



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 27, 2026 – 04:47 PM UTC

PDB ID : 4PUO / pdb\_00004puo  
Title : Crystal structure of HIV-1 reverse transcriptase in complex with RNA/DNA and Nevirapine  
Authors : Das, K.; Martinez, S.E.; Arnold, E.  
Deposited on : 2014-03-13  
Resolution : 2.90 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

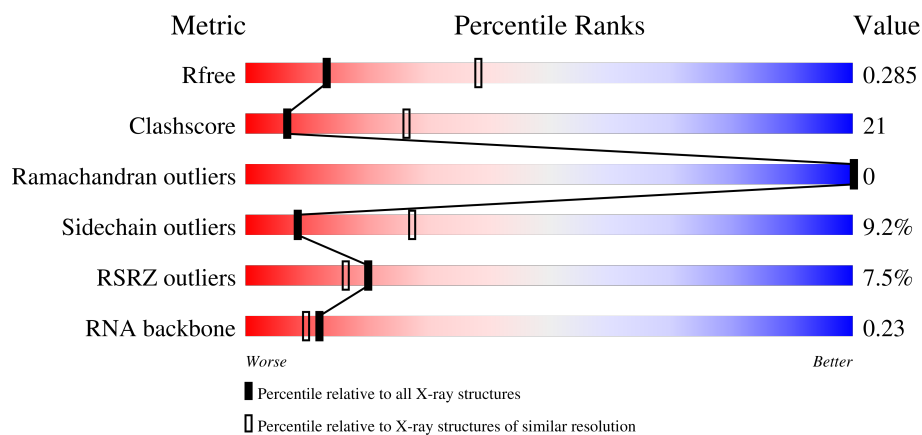
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 Å.

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



| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| $R_{free}$            | 180053                      | 2481 (2.90-2.90)                                      |
| Clashscore            | 190562                      | 2690 (2.90-2.90)                                      |
| Ramachandran outliers | 187476                      | 2623 (2.90-2.90)                                      |
| Sidechain outliers    | 187428                      | 2625 (2.90-2.90)                                      |
| RSRZ outliers         | 180081                      | 2481 (2.90-2.90)                                      |
| RNA backbone          | 3983                        | 1120 (3.10-2.70)                                      |

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

| Mol | Chain | Length | Quality of chain                                                        |
|-----|-------|--------|-------------------------------------------------------------------------|
| 1   | A     | 556    | <div> <div>8%</div> <div>48%</div> <div>44%</div> <div>8%</div> </div>  |
| 1   | C     | 556    | <div> <div>10%</div> <div>57%</div> <div>35%</div> <div>7%</div> </div> |
| 2   | B     | 428    | <div> <div>4%</div> <div>52%</div> <div>35%</div> <div>8%</div> </div>  |
| 2   | D     | 428    | <div> <div>6%</div> <div>51%</div> <div>37%</div> <div>8%</div> </div>  |

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| Mol | Chain | Length | Quality of chain                                                                             |
|-----|-------|--------|----------------------------------------------------------------------------------------------|
| 3   | E     | 27     | <div><div></div><div>4%</div><div>15%</div><div>33%</div><div>22%</div><div>30%</div></div>  |
| 3   | T     | 27     | <div><div></div><div>7%</div><div>19%</div><div>26%</div><div>30%</div><div>26%</div></div>  |
| 4   | F     | 21     | <div><div></div><div>14%</div><div>43%</div><div>33%</div><div>14%</div><div>10%</div></div> |
| 4   | P     | 21     | <div><div></div><div>10%</div><div>14%</div><div>52%</div><div>24%</div><div>10%</div></div> |

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 17462 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called HIV-1 Reverse Transcriptase, p66 subunit.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 1   | A     | 555      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 4512  | 2920 | 751 | 833 | 8 |         |         |       |
| 1   | C     | 555      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 4506  | 2917 | 748 | 833 | 8 |         |         |       |

There are 10 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment             | Reference  |
|-------|---------|----------|--------|---------------------|------------|
| A     | -1      | MET      | -      | expression tag      | UNP P03366 |
| A     | 0       | VAL      | -      | expression tag      | UNP P03366 |
| A     | 258     | CYS      | GLN    | engineered mutation | UNP P03366 |
| A     | 280     | SER      | CYS    | engineered mutation | UNP P03366 |
| A     | 498     | ASN      | ASP    | engineered mutation | UNP P03366 |
| C     | -1      | MET      | -      | expression tag      | UNP P03366 |
| C     | 0       | VAL      | -      | expression tag      | UNP P03366 |
| C     | 258     | CYS      | GLN    | engineered mutation | UNP P03366 |
| C     | 280     | SER      | CYS    | engineered mutation | UNP P03366 |
| C     | 498     | ASN      | ASP    | engineered mutation | UNP P03366 |

- Molecule 2 is a protein called HIV-1 Reverse Transcriptase, p51 subunit.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 2   | B     | 412      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 3400  | 2212 | 563 | 619 | 6 |         |         |       |
| 2   | D     | 412      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 3400  | 2212 | 563 | 619 | 6 |         |         |       |

There are 2 discrepancies between the modelled and reference sequences:

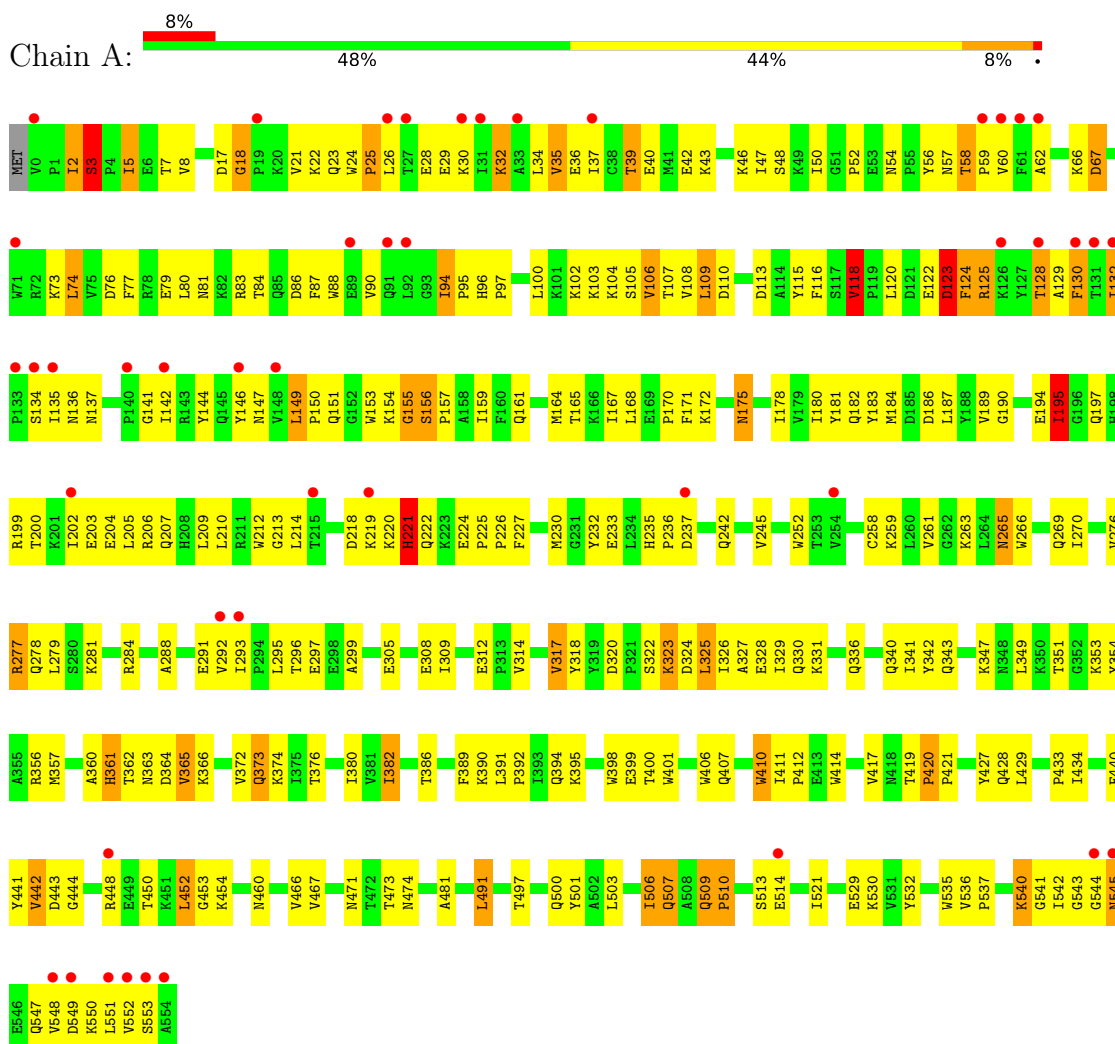
| Chain | Residue | Modelled | Actual | Comment             | Reference  |
|-------|---------|----------|--------|---------------------|------------|
| B     | 280     | SER      | CYS    | engineered mutation | UNP P03366 |
| D     | 280     | SER      | CYS    | engineered mutation | UNP P03366 |



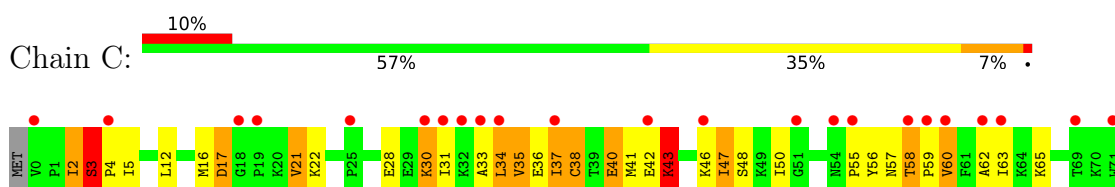
### 3 Residue-property plots

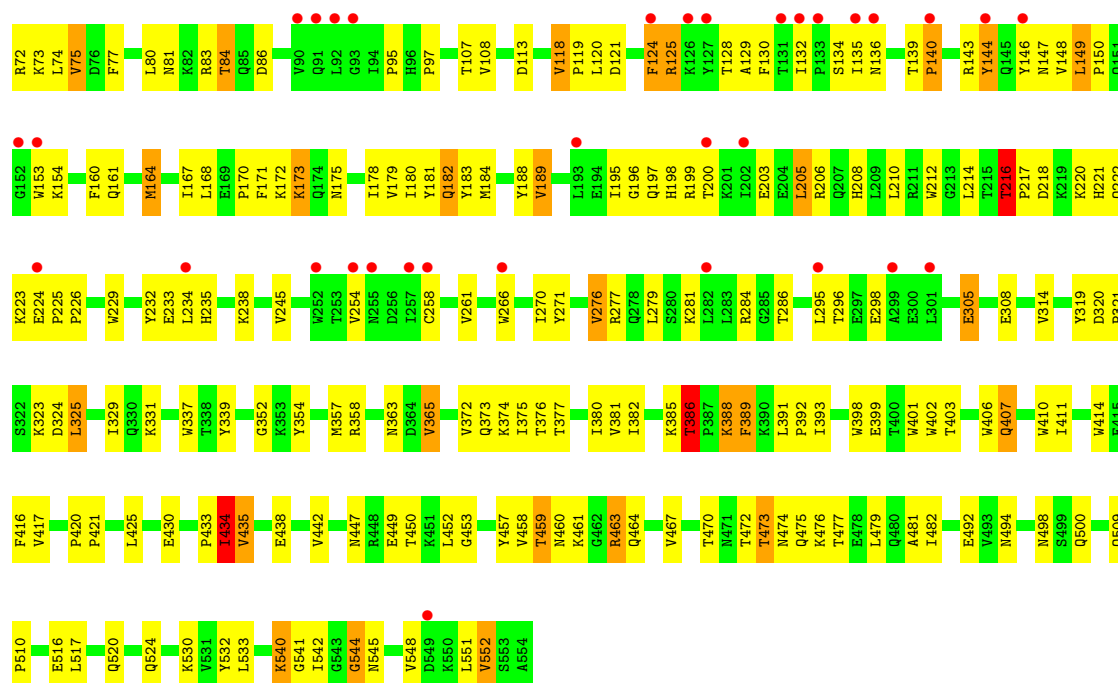
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: HIV-1 Reverse Transcriptase, p66 subunit

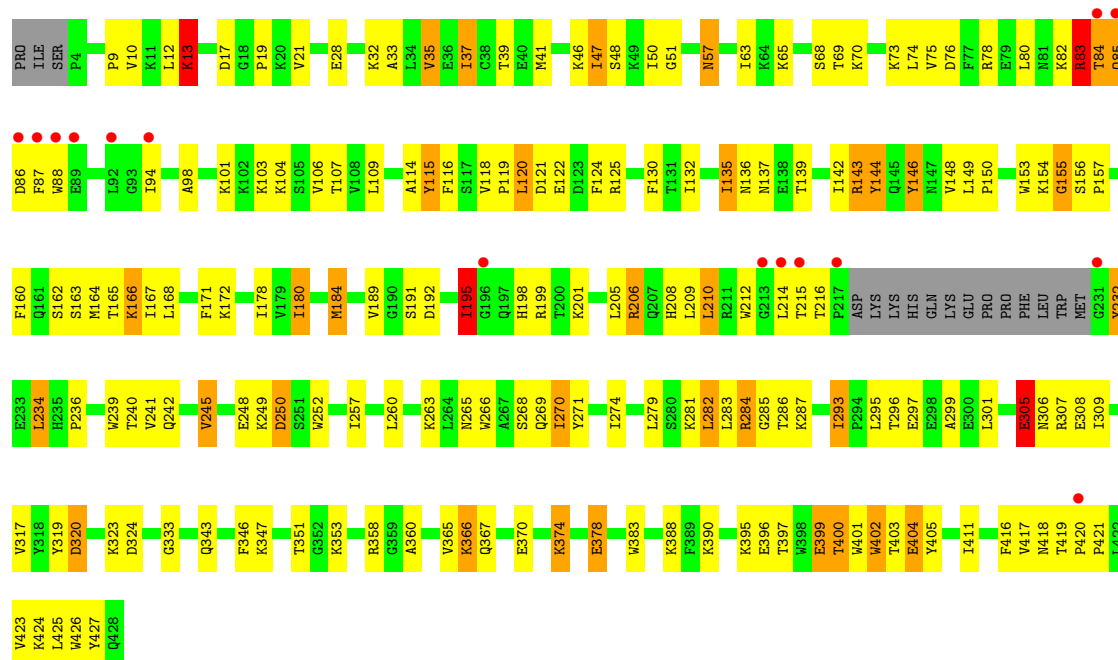


- Molecule 1: HIV-1 Reverse Transcriptase, p66 subunit

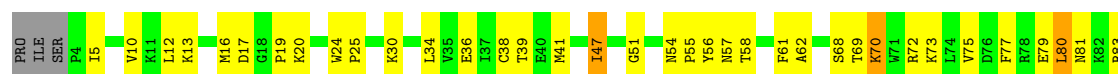


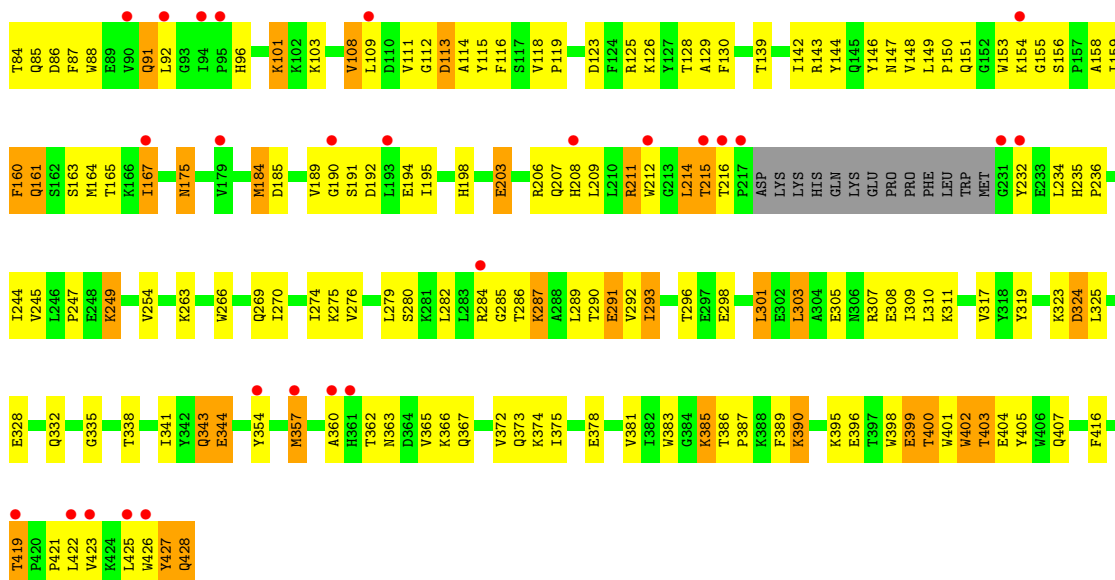


• Molecule 2: HIV-1 Reverse Transcriptase, p51 subunit



• Molecule 2: HIV-1 Reverse Transcriptase, p51 subunit

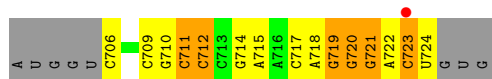




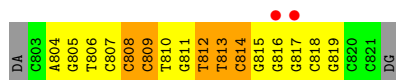
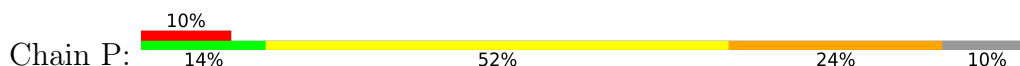
• Molecule 3: 5'-R(P\*AP\*UP\*GP\*GP\*UP\*CP\*GP\*GP\*CP\*GP\*CP\*CP\*CP\*GP\*AP\*AP\*CP\*AP\*GP\*GP\*GP\*AP\*CP\*UP\*GP\*UP\*G)-3'



• Molecule 3: 5'-R(P\*AP\*UP\*GP\*GP\*UP\*CP\*GP\*GP\*CP\*GP\*CP\*CP\*CP\*GP\*AP\*AP\*CP\*AP\*GP\*GP\*GP\*AP\*CP\*UP\*GP\*UP\*G)-3'



• Molecule 4: 5'-D(\*A\*CP\*AP\*GP\*TP\*CP\*CP\*CP\*TP\*GP\*TP\*TP\*CP\*GP\*GP\*GP\*CP\*GP\*CP\*CP\*G)-3'



• Molecule 4: 5'-D(\*A\*CP\*AP\*GP\*TP\*CP\*CP\*CP\*TP\*GP\*TP\*TP\*CP\*GP\*GP\*GP\*CP\*GP\*CP\*CP\*G)-3'





## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 1 21 1                                                    | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 89.74Å 132.13Å 141.96Å<br>90.00° 100.63° 90.00°             | Depositor        |
| Resolution (Å)                                                          | 46.51 – 2.90<br>46.51 – 2.90                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 98.5 (46.51-2.90)<br>98.4 (46.51-2.90)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.09                                                        | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.68 (at 2.91Å)                                             | Xtriage          |
| Refinement program                                                      | PHENIX (phenix.refine: 1.8.4_1496)                          | Depositor        |
| R, $R_{free}$                                                           | 0.228 , 0.285<br>0.232 , 0.285                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 2136 reflections (2.96%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 61.8                                                        | Xtriage          |
| Anisotropy                                                              | 0.021                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.32 , 81.0                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$ | Xtriage          |
| Estimated twinning fraction                                             | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.91                                                        | EDS              |
| Total number of atoms                                                   | 17462                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 85.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.83% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

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

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

| Mol | Chain | Bond lengths |                 | Bond angles |                  |
|-----|-------|--------------|-----------------|-------------|------------------|
|     |       | RMSZ         | $\# Z  > 5$     | RMSZ        | $\# Z  > 5$      |
| 1   | A     | 0.93         | 7/4630 (0.2%)   | 1.34        | 63/6290 (1.0%)   |
| 1   | C     | 0.92         | 5/4624 (0.1%)   | 1.30        | 56/6283 (0.9%)   |
| 2   | B     | 1.01         | 7/3497 (0.2%)   | 1.40        | 41/4751 (0.9%)   |
| 2   | D     | 0.93         | 4/3497 (0.1%)   | 1.36        | 48/4751 (1.0%)   |
| 3   | E     | 0.61         | 1/456 (0.2%)    | 0.75        | 1/709 (0.1%)     |
| 3   | T     | 0.70         | 1/483 (0.2%)    | 0.79        | 0/752            |
| 4   | F     | 0.78         | 3/426 (0.7%)    | 0.84        | 4/655 (0.6%)     |
| 4   | P     | 0.79         | 3/426 (0.7%)    | 0.97        | 6/655 (0.9%)     |
| All | All   | 0.93         | 31/18039 (0.2%) | 1.30        | 219/24846 (0.9%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | A     | 0                   | 2                   |
| 1   | C     | 0                   | 1                   |
| 2   | B     | 0                   | 2                   |
| All | All   | 0                   | 5                   |

All (31) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 1   | C     | 389 | PHE  | CA-C    | -11.51 | 1.39        | 1.52     |
| 4   | P     | 809 | DC   | O3'-P   | -9.54  | 1.46        | 1.61     |
| 2   | B     | 400 | THR  | C-O     | 8.72   | 1.34        | 1.24     |
| 2   | D     | 400 | THR  | C-O     | 8.62   | 1.34        | 1.24     |
| 4   | F     | 816 | DG   | C3'-C2' | -8.27  | 1.36        | 1.52     |
| 2   | B     | 399 | GLU  | C-O     | 8.07   | 1.33        | 1.24     |
| 1   | A     | 365 | VAL  | CA-CB   | -7.79  | 1.45        | 1.54     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 3   | T     | 706 | C    | C1'-N1  | 7.37  | 1.59        | 1.48     |
| 4   | F     | 811 | DG   | C3'-C2' | -7.30 | 1.38        | 1.52     |
| 1   | C     | 467 | VAL  | CA-CB   | -7.18 | 1.45        | 1.54     |
| 3   | E     | 706 | C    | C1'-N1  | 6.60  | 1.58        | 1.48     |
| 1   | A     | 467 | VAL  | CA-C    | -6.50 | 1.48        | 1.52     |
| 1   | A     | 3   | SER  | CA-C    | 6.45  | 1.59        | 1.52     |
| 2   | B     | 83  | ARG  | C-O     | 6.05  | 1.32        | 1.24     |
| 2   | D     | 270 | ILE  | CA-CB   | -6.00 | 1.49        | 1.55     |
| 4   | P     | 814 | DC   | C3'-C2' | -5.81 | 1.41        | 1.52     |
| 4   | P     | 809 | DC   | C3'-C2' | -5.79 | 1.41        | 1.52     |
| 2   | D     | 159 | ILE  | C-O     | 5.64  | 1.30        | 1.24     |
| 1   | C     | 365 | VAL  | CA-CB   | -5.60 | 1.47        | 1.54     |
| 1   | A     | 265 | ASN  | C-O     | 5.56  | 1.30        | 1.24     |
| 2   | D     | 399 | GLU  | C-O     | 5.51  | 1.30        | 1.24     |
| 2   | B     | 397 | THR  | CA-CB   | -5.49 | 1.44        | 1.53     |
| 1   | A     | 466 | VAL  | CA-CB   | -5.42 | 1.47        | 1.54     |
| 1   | A     | 536 | VAL  | C-O     | -5.42 | 1.20        | 1.24     |
| 2   | B     | 84  | THR  | N-CA    | -5.39 | 1.38        | 1.46     |
| 2   | B     | 135 | ILE  | CA-CB   | -5.39 | 1.48        | 1.54     |
| 1   | C     | 434 | ILE  | CA-CB   | -5.36 | 1.47        | 1.53     |
| 4   | F     | 815 | DG   | C3'-C2' | 5.19  | 1.63        | 1.52     |
| 1   | C     | 389 | PHE  | N-CA    | -5.16 | 1.39        | 1.46     |
| 1   | A     | 521 | ILE  | CA-CB   | -5.14 | 1.48        | 1.54     |
| 2   | B     | 419 | THR  | C-N     | 5.14  | 1.39        | 1.33     |

All (219) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|--------|-------------|----------|
| 2   | B     | 139 | THR  | CA-C-N | -15.30 | 104.61      | 120.98   |
| 2   | B     | 139 | THR  | C-N-CA | -15.30 | 104.61      | 120.98   |
| 1   | A     | 149 | LEU  | CA-C-N | 12.62  | 132.38      | 119.76   |
| 1   | A     | 149 | LEU  | C-N-CA | 12.62  | 132.38      | 119.76   |
| 2   | D     | 402 | TRP  | N-CA-C | -12.47 | 97.69       | 111.28   |
| 2   | B     | 402 | TRP  | N-CA-C | -12.16 | 98.10       | 111.36   |
| 2   | D     | 139 | THR  | CA-C-N | -11.71 | 105.20      | 119.84   |
| 2   | D     | 139 | THR  | C-N-CA | -11.71 | 105.20      | 119.84   |
| 2   | B     | 84  | THR  | N-CA-C | -11.29 | 99.49       | 113.38   |
| 1   | A     | 545 | ASN  | N-CA-C | -11.29 | 99.00       | 113.12   |
| 1   | C     | 4   | PRO  | N-CA-C | 11.01  | 129.21      | 113.47   |
| 1   | C     | 118 | VAL  | CA-C-N | 10.95  | 131.65      | 119.83   |
| 1   | C     | 118 | VAL  | C-N-CA | 10.95  | 131.65      | 119.83   |
| 2   | B     | 85  | GLN  | N-CA-C | -10.24 | 100.11      | 111.07   |

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| Mol | Chain | Res | Type | Atoms       | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|--------|-------------|----------|
| 1   | A     | 156 | SER  | N-CA-C      | -10.18 | 98.32       | 112.17   |
| 2   | D     | 54  | ASN  | CA-C-N      | 10.13  | 130.40      | 119.87   |
| 2   | D     | 54  | ASN  | C-N-CA      | 10.13  | 130.40      | 119.87   |
| 2   | B     | 400 | THR  | CA-C-N      | -10.09 | 104.81      | 122.26   |
| 2   | B     | 400 | THR  | C-N-CA      | -10.09 | 104.81      | 122.26   |
| 1   | C     | 40  | GLU  | N-CA-C      | -9.88  | 99.34       | 111.40   |
| 1   | A     | 28  | GLU  | N-CA-C      | 9.78   | 123.17      | 111.82   |
| 1   | C     | 382 | ILE  | N-CA-C      | 9.66   | 120.19      | 110.82   |
| 2   | B     | 284 | ARG  | N-CA-C      | 9.50   | 122.51      | 111.11   |
| 2   | D     | 161 | GLN  | N-CA-C      | -9.34  | 101.18      | 111.36   |
| 1   | A     | 540 | LYS  | N-CA-C      | -9.34  | 101.40      | 113.17   |
| 2   | B     | 51  | GLY  | CA-C-N      | 9.10   | 129.34      | 119.87   |
| 2   | B     | 51  | GLY  | C-N-CA      | 9.10   | 129.34      | 119.87   |
| 1   | C     | 386 | THR  | CA-C-N      | 9.09   | 129.03      | 120.03   |
| 1   | C     | 386 | THR  | C-N-CA      | 9.09   | 129.03      | 120.03   |
| 4   | P     | 809 | DC   | C2'-C3'-O3' | -8.90  | 98.15       | 111.50   |
| 2   | D     | 235 | HIS  | CA-C-N      | 8.56   | 130.54      | 119.84   |
| 2   | D     | 235 | HIS  | C-N-CA      | 8.56   | 130.54      | 119.84   |
| 4   | P     | 814 | DC   | C2'-C3'-O3' | -8.53  | 98.71       | 111.50   |
| 1   | A     | 320 | ASP  | CA-C-N      | 8.45   | 130.40      | 119.84   |
| 1   | A     | 320 | ASP  | C-N-CA      | 8.45   | 130.40      | 119.84   |
| 1   | C     | 544 | GLY  | N-CA-C      | -8.41  | 102.01      | 112.77   |
| 4   | P     | 812 | DT   | P-O3'-C3'   | 8.24   | 132.56      | 120.20   |
| 2   | B     | 21  | VAL  | N-CA-C      | 8.19   | 120.15      | 109.58   |
| 1   | C     | 224 | GLU  | CA-C-N      | 8.15   | 128.77      | 120.38   |
| 1   | C     | 224 | GLU  | C-N-CA      | 8.15   | 128.77      | 120.38   |
| 1   | A     | 221 | HIS  | N-CA-C      | 8.14   | 121.70      | 108.34   |
| 1   | A     | 382 | ILE  | N-CA-C      | 7.98   | 118.00      | 110.74   |
| 3   | E     | 719 | G    | C3'-C2'-O2' | -7.93  | 98.80       | 110.70   |
| 2   | B     | 426 | TRP  | N-CA-C      | -7.90  | 103.21      | 113.17   |
| 2   | D     | 160 | PHE  | N-CA-C      | -7.90  | 103.36      | 113.16   |
| 2   | D     | 175 | ASN  | CA-C-N      | 7.83   | 127.46      | 119.56   |
| 2   | D     | 175 | ASN  | C-N-CA      | 7.83   | 127.46      | 119.56   |
| 1   | C     | 388 | LYS  | CA-C-N      | -7.74  | 111.71      | 122.93   |
| 1   | C     | 388 | LYS  | C-N-CA      | -7.74  | 111.71      | 122.93   |
| 1   | C     | 509 | GLN  | CB-CA-C     | -7.71  | 105.72      | 111.20   |
| 1   | A     | 293 | ILE  | CA-C-N      | 7.70   | 128.31      | 120.14   |
| 1   | A     | 293 | ILE  | C-N-CA      | 7.70   | 128.31      | 120.14   |
| 4   | F     | 816 | DG   | C2'-C3'-O3' | 7.70   | 123.05      | 111.50   |
| 2   | B     | 400 | THR  | O-C-N       | -7.62  | 114.22      | 122.07   |
| 2   | D     | 324 | ASP  | N-CA-C      | 7.59   | 121.20      | 110.50   |
| 2   | D     | 400 | THR  | CA-C-N      | -7.58  | 108.31      | 121.66   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2   | D     | 400 | THR  | C-N-CA  | -7.58 | 108.31      | 121.66   |
| 2   | B     | 83  | ARG  | CA-C-N  | -7.55 | 109.19      | 122.26   |
| 2   | B     | 83  | ARG  | C-N-CA  | -7.55 | 109.19      | 122.26   |
| 2   | D     | 386 | THR  | CA-C-N  | 7.40  | 127.56      | 120.31   |
| 2   | D     | 386 | THR  | C-N-CA  | 7.40  | 127.56      | 120.31   |
| 1   | A     | 509 | GLN  | CA-C-N  | 7.38  | 127.36      | 119.76   |
| 1   | A     | 509 | GLN  | C-N-CA  | 7.38  | 127.36      | 119.76   |
| 1   | A     | 29  | GLU  | N-CA-C  | 7.32  | 119.15      | 111.03   |
| 1   | C     | 43  | LYS  | N-CA-C  | 7.30  | 118.93      | 110.97   |
| 1   | C     | 30  | LYS  | N-CA-C  | 7.27  | 122.33      | 113.17   |
| 1   | C     | 41  | MET  | N-CA-C  | -7.27 | 103.35      | 111.71   |
| 1   | A     | 125 | ARG  | N-CA-C  | -7.25 | 102.56      | 111.33   |
| 1   | A     | 8   | VAL  | CA-C-N  | 7.17  | 128.80      | 119.84   |
| 1   | A     | 8   | VAL  | C-N-CA  | 7.17  | 128.80      | 119.84   |
| 2   | B     | 195 | ILE  | N-CA-C  | 7.04  | 118.65      | 110.62   |
| 2   | B     | 206 | ARG  | N-CA-C  | -6.98 | 103.67      | 111.28   |
| 2   | D     | 51  | GLY  | CA-C-N  | 6.96  | 126.64      | 119.82   |
| 2   | D     | 51  | GLY  | C-N-CA  | 6.96  | 126.64      | 119.82   |
| 2   | B     | 146 | TYR  | N-CA-C  | 6.95  | 119.88      | 109.25   |
| 1   | A     | 58  | THR  | CA-C-N  | 6.95  | 128.52      | 119.84   |
| 1   | A     | 58  | THR  | C-N-CA  | 6.95  | 128.52      | 119.84   |
| 1   | A     | 67  | ASP  | N-CA-C  | 6.91  | 121.45      | 111.56   |
| 2   | B     | 271 | TYR  | CA-C-N  | 6.89  | 126.58      | 119.82   |
| 2   | B     | 271 | TYR  | C-N-CA  | 6.89  | 126.58      | 119.82   |
| 1   | C     | 38  | CYS  | CA-C-N  | -6.89 | 109.91      | 122.38   |
| 1   | C     | 38  | CYS  | C-N-CA  | -6.89 | 109.91      | 122.38   |
| 1   | C     | 125 | ARG  | N-CA-C  | -6.74 | 103.17      | 111.33   |
| 2   | D     | 195 | ILE  | N-CA-C  | 6.73  | 117.42      | 110.36   |
| 1   | C     | 320 | ASP  | CA-C-N  | 6.69  | 128.21      | 119.84   |
| 1   | C     | 320 | ASP  | C-N-CA  | 6.69  | 128.21      | 119.84   |
| 2   | D     | 184 | MET  | CB-CA-C | -6.67 | 108.86      | 116.54   |
| 2   | D     | 276 | VAL  | N-CA-C  | 6.67  | 119.31      | 112.90   |
| 2   | D     | 159 | ILE  | CA-C-N  | -6.62 | 110.39      | 122.38   |
| 2   | D     | 159 | ILE  | C-N-CA  | -6.62 | 110.39      | 122.38   |
| 1   | C     | 35  | VAL  | N-CA-C  | 6.59  | 117.28      | 110.36   |
| 1   | C     | 277 | ARG  | N-CA-C  | 6.58  | 118.11      | 111.07   |
| 1   | A     | 453 | GLY  | N-CA-C  | 6.54  | 121.28      | 110.55   |
| 1   | A     | 74  | LEU  | N-CA-C  | 6.54  | 119.25      | 108.99   |
| 2   | B     | 305 | GLU  | N-CA-C  | -6.50 | 104.29      | 111.82   |
| 1   | A     | 30  | LYS  | N-CA-C  | 6.45  | 119.30      | 111.82   |
| 2   | B     | 234 | LEU  | CA-C-N  | -6.44 | 115.67      | 122.89   |
| 2   | B     | 234 | LEU  | C-N-CA  | -6.44 | 115.67      | 122.89   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 1   | A     | 124 | PHE  | N-CA-C      | -6.38 | 105.50      | 113.28   |
| 2   | B     | 83  | ARG  | CA-C-O      | 6.33  | 126.37      | 119.15   |
| 1   | C     | 62  | ALA  | N-CA-C      | 6.33  | 118.57      | 109.14   |
| 2   | D     | 190 | GLY  | N-CA-C      | 6.33  | 121.62      | 110.80   |
| 1   | A     | 141 | GLY  | N-CA-C      | 6.32  | 119.35      | 110.38   |
| 4   | P     | 813 | DT   | P-O3'-C3'   | 6.29  | 129.64      | 120.20   |
| 1   | C     | 453 | GLY  | N-CA-C      | 6.24  | 119.92      | 110.18   |
| 1   | A     | 219 | LYS  | N-CA-C      | -6.15 | 105.50      | 112.87   |
| 2   | D     | 96  | HIS  | N-CA-C      | 6.14  | 118.52      | 109.50   |
| 2   | B     | 245 | VAL  | N-CA-C      | 6.13  | 117.13      | 108.17   |
| 1   | A     | 491 | LEU  | N-CA-C      | 6.13  | 118.76      | 111.71   |
| 2   | D     | 249 | LYS  | N-CA-C      | 6.11  | 119.09      | 108.76   |
| 2   | B     | 419 | THR  | CA-C-N      | -6.11 | 114.08      | 120.38   |
| 2   | B     | 419 | THR  | C-N-CA      | -6.11 | 114.08      | 120.38   |
| 1   | A     | 312 | GLU  | CA-C-N      | -6.10 | 114.45      | 120.98   |
| 1   | A     | 312 | GLU  | C-N-CA      | -6.10 | 114.45      | 120.98   |
| 2   | D     | 400 | THR  | CA-C-O      | 6.06  | 127.18      | 120.82   |
| 4   | F     | 811 | DG   | C2'-C3'-O3' | -6.02 | 102.47      | 111.50   |
| 2   | D     | 284 | ARG  | N-CA-C      | 6.01  | 118.63      | 111.71   |
| 1   | A     | 277 | ARG  | N-CA-C      | 6.00  | 118.31      | 111.11   |
| 1   | C     | 435 | VAL  | CA-C-N      | -5.98 | 113.72      | 122.46   |
| 1   | C     | 435 | VAL  | C-N-CA      | -5.98 | 113.72      | 122.46   |
| 2   | B     | 404 | GLU  | N-CA-C      | 5.98  | 119.76      | 112.23   |
| 1   | A     | 541 | GLY  | CA-C-N      | -5.95 | 115.43      | 122.93   |
| 1   | A     | 541 | GLY  | C-N-CA      | -5.95 | 115.43      | 122.93   |
| 1   | A     | 118 | VAL  | N-CA-C      | 5.95  | 114.51      | 107.73   |
| 2   | B     | 13  | LYS  | CA-C-N      | 5.92  | 126.26      | 119.93   |
| 2   | B     | 13  | LYS  | C-N-CA      | 5.92  | 126.26      | 119.93   |
| 1   | C     | 118 | VAL  | N-CA-C      | 5.88  | 117.00      | 107.71   |
| 1   | A     | 62  | ALA  | N-CA-C      | 5.87  | 118.33      | 109.41   |
| 2   | D     | 419 | THR  | CA-C-N      | -5.86 | 114.34      | 120.38   |
| 2   | D     | 419 | THR  | C-N-CA      | -5.86 | 114.34      | 120.38   |
| 1   | C     | 234 | LEU  | N-CA-C      | 5.85  | 117.94      | 108.41   |
| 4   | P     | 808 | DC   | O3'-P-O5'   | 5.85  | 112.77      | 104.00   |
| 1   | A     | 128 | THR  | N-CA-C      | 5.82  | 120.10      | 112.89   |
| 1   | A     | 410 | TRP  | N-CA-C      | 5.81  | 117.94      | 108.76   |
| 2   | B     | 420 | PRO  | CA-C-N      | -5.79 | 113.27      | 120.79   |
| 2   | B     | 420 | PRO  | C-N-CA      | -5.79 | 113.27      | 120.79   |
| 1   | C     | 467 | VAL  | N-CA-C      | 5.77  | 114.31      | 107.73   |
| 1   | C     | 221 | HIS  | N-CA-C      | -5.77 | 99.12       | 108.41   |
| 1   | C     | 216 | THR  | CA-C-N      | 5.76  | 125.73      | 120.03   |
| 1   | C     | 216 | THR  | C-N-CA      | 5.76  | 125.73      | 120.03   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 1   | A     | 106 | VAL  | N-CA-C      | 5.74  | 116.33      | 107.78   |
| 1   | C     | 276 | VAL  | N-CA-C      | 5.73  | 118.50      | 112.83   |
| 1   | A     | 452 | LEU  | N-CA-C      | 5.70  | 118.85      | 109.72   |
| 1   | C     | 266 | TRP  | N-CA-C      | -5.69 | 105.07      | 111.28   |
| 4   | F     | 804 | DA   | C2'-C3'-O3' | 5.68  | 120.02      | 111.50   |
| 1   | C     | 46  | LYS  | N-CA-C      | -5.67 | 106.32      | 113.18   |
| 1   | C     | 389 | PHE  | CA-C-O      | -5.66 | 114.71      | 120.71   |
| 2   | B     | 400 | THR  | N-CA-C      | 5.66  | 117.13      | 111.07   |
| 1   | A     | 510 | PRO  | CA-C-O      | -5.66 | 114.89      | 121.34   |
| 2   | D     | 407 | GLN  | N-CA-C      | 5.65  | 120.29      | 113.17   |
| 1   | A     | 509 | GLN  | CB-CA-C     | -5.64 | 106.09      | 111.00   |
| 1   | C     | 541 | GLY  | N-CA-C      | -5.58 | 105.27      | 114.76   |
| 1   | A     | 155 | GLY  | N-CA-C      | -5.58 | 106.08      | 115.62   |
| 1   | C     | 34  | LEU  | N-CA-C      | 5.56  | 118.53      | 111.69   |
| 2   | D     | 195 | ILE  | CB-CA-C     | -5.55 | 104.78      | 111.88   |
| 2   | B     | 400 | THR  | CA-C-O      | 5.54  | 126.64      | 120.82   |
| 4   | F     | 815 | DG   | C2'-C3'-O3' | 5.54  | 119.81      | 111.50   |
| 1   | C     | 31  | ILE  | N-CA-C      | 5.52  | 120.63      | 113.07   |
| 2   | B     | 320 | ASP  | CA-C-N      | 5.49  | 125.84      | 119.47   |
| 2   | B     | 320 | ASP  | C-N-CA      | 5.49  | 125.84      | 119.47   |
| 1   | A     | 279 | LEU  | N-CA-C      | -5.49 | 105.38      | 111.36   |
| 1   | A     | 3   | SER  | N-CA-C      | 5.48  | 121.38      | 108.40   |
| 1   | A     | 184 | MET  | CB-CA-C     | -5.46 | 110.29      | 116.63   |
| 1   | C     | 386 | THR  | CB-CA-C     | -5.46 | 102.60      | 109.31   |
| 2   | D     | 285 | GLY  | N-CA-C      | 5.45  | 122.41      | 112.27   |
| 2   | D     | 291 | GLU  | CA-C-N      | -5.45 | 115.34      | 122.37   |
| 2   | D     | 291 | GLU  | C-N-CA      | -5.45 | 115.34      | 122.37   |
| 1   | A     | 32  | LYS  | N-CA-C      | -5.43 | 106.16      | 112.89   |
| 1   | A     | 129 | ALA  | N-CA-C      | 5.43  | 117.89      | 110.24   |
| 2   | D     | 301 | LEU  | CA-CB-CG    | -5.42 | 97.31       | 116.30   |
| 1   | C     | 540 | LYS  | N-CA-C      | -5.42 | 106.34      | 113.17   |
| 1   | C     | 60  | VAL  | N-CA-C      | 5.40  | 115.76      | 107.77   |
| 1   | A     | 501 | TYR  | N-CA-C      | 5.39  | 117.58      | 111.11   |
| 1   | C     | 28  | GLU  | N-CA-C      | 5.39  | 119.48      | 113.01   |
| 1   | C     | 58  | THR  | CA-C-N      | 5.38  | 126.57      | 119.84   |
| 1   | C     | 58  | THR  | C-N-CA      | 5.38  | 126.57      | 119.84   |
| 1   | A     | 8   | VAL  | CB-CA-C     | 5.38  | 116.12      | 110.37   |
| 1   | A     | 108 | VAL  | N-CA-C      | 5.37  | 115.72      | 107.77   |
| 2   | B     | 57  | ASN  | N-CA-C      | 5.35  | 117.90      | 108.75   |
| 2   | B     | 333 | GLY  | N-CA-C      | 5.35  | 119.60      | 112.65   |
| 2   | B     | 143 | ARG  | N-CA-C      | 5.35  | 117.95      | 109.24   |
| 2   | B     | 155 | GLY  | N-CA-C      | -5.34 | 106.21      | 113.37   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | C     | 33  | ALA  | N-CA-C    | 5.34  | 118.96      | 112.23   |
| 2   | D     | 91  | GLN  | N-CA-C    | 5.32  | 116.93      | 111.03   |
| 1   | A     | 356 | ARG  | N-CA-C    | 5.31  | 117.40      | 109.59   |
| 2   | D     | 25  | PRO  | CA-C-O    | -5.31 | 115.36      | 121.36   |
| 2   | B     | 270 | ILE  | N-CA-C    | 5.30  | 115.96      | 110.82   |
| 2   | D     | 198 | HIS  | N-CA-C    | -5.30 | 105.41      | 111.14   |
| 1   | C     | 3   | SER  | N-CA-C    | 5.30  | 119.41      | 108.71   |
| 1   | A     | 54  | ASN  | CA-C-N    | -5.29 | 116.31      | 121.65   |
| 1   | A     | 54  | ASN  | C-N-CA    | -5.29 | 116.31      | 121.65   |
| 1   | C     | 4   | PRO  | CB-CA-C   | -5.27 | 104.68      | 113.06   |
| 2   | D     | 344 | GLU  | CA-C-N    | 5.27  | 125.57      | 119.93   |
| 2   | D     | 344 | GLU  | C-N-CA    | 5.27  | 125.57      | 119.93   |
| 1   | A     | 151 | GLN  | N-CA-C    | 5.27  | 117.34      | 109.59   |
| 1   | C     | 389 | PHE  | N-CA-C    | -5.26 | 101.12      | 109.59   |
| 2   | D     | 381 | VAL  | CA-C-N    | -5.25 | 117.83      | 122.97   |
| 2   | D     | 381 | VAL  | C-N-CA    | -5.25 | 117.83      | 122.97   |
| 2   | D     | 385 | LYS  | N-CA-C    | -5.24 | 101.11      | 109.07   |
| 1   | C     | 124 | PHE  | N-CA-C    | -5.22 | 106.76      | 113.23   |
| 1   | C     | 37  | ILE  | N-CA-C    | -5.21 | 106.22      | 113.00   |
| 1   | A     | 18  | GLY  | CA-C-N    | 5.20  | 125.41      | 120.31   |
| 1   | A     | 18  | GLY  | C-N-CA    | 5.20  | 125.41      | 120.31   |
| 1   | A     | 25  | PRO  | N-CA-C    | 5.19  | 119.34      | 111.15   |
| 2   | D     | 165 | THR  | N-CA-C    | -5.19 | 105.62      | 111.28   |
| 2   | D     | 69  | THR  | N-CA-C    | -5.17 | 106.75      | 113.16   |
| 2   | D     | 58  | THR  | CA-C-N    | -5.14 | 114.69      | 120.14   |
| 2   | D     | 58  | THR  | C-N-CA    | -5.14 | 114.69      | 120.14   |
| 4   | P     | 813 | DT   | O3'-P-O5' | -5.14 | 96.29       | 104.00   |
| 1   | A     | 195 | ILE  | N-CA-C    | 5.07  | 116.39      | 110.62   |
| 1   | A     | 386 | THR  | CA-C-N    | -5.06 | 115.03      | 120.03   |
| 1   | A     | 386 | THR  | C-N-CA    | -5.06 | 115.03      | 120.03   |
| 1   | C     | 75  | VAL  | N-CA-C    | 5.04  | 115.23      | 107.77   |
| 1   | C     | 510 | PRO  | CA-C-O    | -5.03 | 115.27      | 121.31   |
| 1   | A     | 175 | ASN  | N-CA-C    | 5.03  | 116.79      | 109.30   |
| 1   | A     | 132 | ILE  | CA-C-N    | 5.02  | 125.30      | 119.93   |
| 1   | A     | 132 | ILE  | C-N-CA    | 5.02  | 125.30      | 119.93   |
| 1   | C     | 149 | LEU  | CA-C-N    | 5.01  | 126.10      | 119.84   |
| 1   | C     | 149 | LEU  | C-N-CA    | 5.01  | 126.10      | 119.84   |

There are no chirality outliers.

All (5) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | A     | 123 | ASP  | Mainchain |
| 1   | A     | 35  | VAL  | Mainchain |
| 2   | B     | 400 | THR  | Mainchain |
| 2   | B     | 83  | ARG  | Mainchain |
| 1   | C     | 389 | PHE  | Mainchain |

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 4512  | 0        | 4571     | 202     | 0            |
| 1   | C     | 4506  | 0        | 4560     | 171     | 0            |
| 2   | B     | 3400  | 0        | 3433     | 167     | 0            |
| 2   | D     | 3400  | 0        | 3433     | 145     | 0            |
| 3   | E     | 408   | 0        | 207      | 10      | 0            |
| 3   | T     | 432   | 0        | 218      | 11      | 0            |
| 4   | F     | 382   | 0        | 215      | 21      | 0            |
| 4   | P     | 382   | 0        | 215      | 30      | 0            |
| 5   | A     | 20    | 0        | 14       | 0       | 0            |
| 5   | C     | 20    | 0        | 14       | 1       | 0            |
| All | All   | 17462 | 0        | 16880    | 726     | 0            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 21.

All (726) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:423:VAL:HG13 | 2:D:426:TRP:HD1  | 1.11                     | 1.13              |
| 2:B:421:PRO:HB3  | 2:B:424:LYS:HB2  | 1.32                     | 1.11              |
| 1:A:545:ASN:HA   | 1:A:548:VAL:HG12 | 1.31                     | 1.05              |
| 4:P:812:DT:H2'   | 4:P:813:DT:H71   | 1.39                     | 1.02              |
| 1:A:128:THR:HG21 | 1:A:146:TYR:HB2  | 1.41                     | 1.01              |
| 1:C:498:ASN:HD22 | 1:C:545:ASN:HD21 | 1.13                     | 0.96              |
| 2:B:115:TYR:HD2  | 2:B:156:SER:HB3  | 1.30                     | 0.96              |
| 1:C:21:VAL:H     | 1:C:57:ASN:HB2   | 1.28                     | 0.96              |
| 1:A:545:ASN:CA   | 1:A:548:VAL:HG12 | 1.97                     | 0.93              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:423:VAL:HG13 | 2:D:426:TRP:CD1  | 2.04                     | 0.92              |
| 2:B:191:SER:HG   | 2:B:198:HIS:HD1  | 1.08                     | 0.91              |
| 1:A:434:ILE:HD13 | 1:A:530:LYS:HB3  | 1.52                     | 0.91              |
| 1:C:474:ASN:HD21 | 3:E:723:C:H4'    | 1.37                     | 0.90              |
| 1:A:545:ASN:HA   | 1:A:548:VAL:CG1  | 2.02                     | 0.88              |
| 2:B:282:LEU:HD22 | 2:B:293:ILE:HD11 | 1.55                     | 0.88              |
| 4:F:815:DG:N3    | 4:F:816:DG:N7    | 2.21                     | 0.88              |
| 2:B:28:GLU:HB2   | 2:B:135:ILE:HD11 | 1.54                     | 0.87              |
| 2:B:13:LYS:HD3   | 2:B:83:ARG:HA    | 1.54                     | 0.87              |
| 1:C:107:THR:HG1  | 1:C:198:HIS:HE2  | 1.15                     | 0.87              |
| 1:A:547:GLN:O    | 1:A:550:LYS:HG2  | 1.75                     | 0.87              |
| 1:A:434:ILE:CD1  | 1:A:530:LYS:HB3  | 2.05                     | 0.87              |
| 1:A:544:GLY:O    | 1:A:548:VAL:HB   | 1.75                     | 0.86              |
| 2:B:122:GLU:HA   | 2:B:125:ARG:HD2  | 1.57                     | 0.86              |
| 1:C:500:GLN:HE22 | 2:D:422:LEU:HD23 | 1.40                     | 0.86              |
| 2:D:209:LEU:HB3  | 2:D:214:LEU:HD23 | 1.59                     | 0.85              |
| 1:C:452:LEU:HD11 | 1:C:470:THR:HG22 | 1.58                     | 0.84              |
| 1:C:56:TYR:HB2   | 1:C:129:ALA:HB3  | 1.59                     | 0.83              |
| 1:A:395:LYS:HD3  | 1:A:414:TRP:CZ2  | 2.15                     | 0.81              |
| 2:D:125:ARG:HE   | 2:D:147:ASN:HA   | 1.44                     | 0.81              |
| 1:A:90:VAL:HG11  | 1:A:161:GLN:HB3  | 1.63                     | 0.80              |
| 1:A:94:ILE:HD13  | 1:A:230:MET:HE1  | 1.63                     | 0.80              |
| 2:B:85:GLN:HA    | 2:B:88:TRP:CE2   | 2.16                     | 0.80              |
| 4:F:815:DG:C2    | 4:F:816:DG:C5    | 2.70                     | 0.80              |
| 1:C:180:ILE:HG13 | 1:C:189:VAL:HG13 | 1.65                     | 0.79              |
| 1:A:125:ARG:HD3  | 1:A:147:ASN:HA   | 1.64                     | 0.79              |
| 1:A:545:ASN:O    | 1:A:549:ASP:HB2  | 1.83                     | 0.78              |
| 1:C:372:VAL:HG11 | 1:C:411:ILE:HG23 | 1.66                     | 0.78              |
| 1:C:435:VAL:HG13 | 2:D:290:THR:HG21 | 1.66                     | 0.77              |
| 2:B:421:PRO:CB   | 2:B:424:LYS:HB2  | 2.12                     | 0.77              |
| 1:A:5:ILE:HG22   | 1:A:212:TRP:HD1  | 1.51                     | 0.76              |
| 2:B:263:LYS:NZ   | 2:B:425:LEU:HB3  | 2.00                     | 0.76              |
| 4:P:807:DC:H2'   | 4:P:808:DC:C6    | 2.20                     | 0.76              |
| 1:A:406:TRP:CZ3  | 1:A:407:GLN:HG3  | 2.22                     | 0.75              |
| 2:B:115:TYR:CD2  | 2:B:156:SER:HB3  | 2.18                     | 0.75              |
| 1:C:5:ILE:HG22   | 1:C:212:TRP:HD1  | 1.52                     | 0.75              |
| 1:C:498:ASN:ND2  | 1:C:545:ASN:HD21 | 1.84                     | 0.75              |
| 2:D:423:VAL:CG1  | 2:D:426:TRP:HD1  | 1.96                     | 0.75              |
| 1:C:57:ASN:HA    | 1:C:130:PHE:HA   | 1.68                     | 0.74              |
| 2:D:421:PRO:HB2  | 2:D:423:VAL:H    | 1.50                     | 0.73              |
| 2:B:206:ARG:NH2  | 2:B:216:THR:O    | 2.22                     | 0.73              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:458:VAL:HG23 | 1:C:548:VAL:HB   | 1.69                     | 0.73              |
| 4:P:812:DT:C6    | 4:P:813:DT:C7    | 2.71                     | 0.72              |
| 2:D:422:LEU:HD12 | 2:D:422:LEU:C    | 2.15                     | 0.72              |
| 2:B:425:LEU:N    | 2:B:425:LEU:HD12 | 2.04                     | 0.72              |
| 1:C:261:VAL:HG13 | 1:C:276:VAL:HG21 | 1.71                     | 0.71              |
| 2:D:86:ASP:OD1   | 2:D:87:PHE:N     | 2.24                     | 0.71              |
| 1:A:32:LYS:NZ    | 1:A:134:SER:OG   | 2.20                     | 0.71              |
| 4:F:807:DC:H2'   | 4:F:808:DC:C6    | 2.26                     | 0.70              |
| 1:A:450:THR:O    | 1:A:452:LEU:HG   | 1.92                     | 0.70              |
| 1:A:245:VAL:O    | 1:A:263:LYS:NZ   | 2.20                     | 0.70              |
| 1:A:79:GLU:OE1   | 1:A:83:ARG:NH1   | 2.25                     | 0.69              |
| 3:T:711:C:H2'    | 3:T:712:C:C6     | 2.26                     | 0.69              |
| 2:B:195:ILE:HD11 | 2:B:199:ARG:HH21 | 1.58                     | 0.69              |
| 2:B:250:ASP:OD1  | 2:B:250:ASP:N    | 2.14                     | 0.69              |
| 1:A:175:ASN:HB3  | 1:A:178:ILE:HG12 | 1.75                     | 0.68              |
| 2:D:317:VAL:HG23 | 2:D:317:VAL:O    | 1.92                     | 0.68              |
| 1:A:324:ASP:O    | 1:A:343:GLN:HG2  | 1.93                     | 0.68              |
| 4:P:808:DC:H2''  | 4:P:809:DC:C5'   | 2.23                     | 0.68              |
| 1:C:65:LYS:HG2   | 1:C:72:ARG:HH22  | 1.59                     | 0.68              |
| 2:B:47:ILE:HD12  | 2:B:144:TYR:CD2  | 2.29                     | 0.68              |
| 3:E:711:C:H2'    | 3:E:712:C:C6     | 2.29                     | 0.68              |
| 2:B:142:ILE:HG22 | 2:B:144:TYR:HE1  | 1.58                     | 0.67              |
| 1:C:58:THR:HB    | 1:C:77:PHE:HB3   | 1.76                     | 0.67              |
| 1:A:60:VAL:HG21  | 1:A:132:ILE:HD12 | 1.75                     | 0.67              |
| 1:A:261:VAL:HG13 | 1:A:276:VAL:HG21 | 1.77                     | 0.67              |
| 2:B:164:MET:HE3  | 2:B:168:LEU:HG   | 1.76                     | 0.67              |
| 4:P:812:DT:C6    | 4:P:813:DT:H71   | 2.30                     | 0.66              |
| 1:A:544:GLY:O    | 1:A:548:VAL:CB   | 2.43                     | 0.66              |
| 2:B:164:MET:HE1  | 2:B:209:LEU:HD21 | 1.78                     | 0.66              |
| 1:A:218:ASP:HA   | 1:A:220:LYS:HG2  | 1.77                     | 0.66              |
| 2:D:332:GLN:NE2  | 2:D:427:TYR:HB3  | 2.10                     | 0.66              |
| 1:A:305:GLU:O    | 1:A:309:ILE:HG13 | 1.95                     | 0.66              |
| 1:C:434:ILE:CD1  | 1:C:530:LYS:HB3  | 2.26                     | 0.66              |
| 1:C:305:GLU:HA   | 1:C:308:GLU:HB3  | 1.79                     | 0.65              |
| 1:A:24:TRP:CD2   | 1:A:25:PRO:HD2   | 2.32                     | 0.65              |
| 1:A:221:HIS:HB2  | 1:A:224:GLU:HB2  | 1.78                     | 0.65              |
| 1:C:354:TYR:HD1  | 1:C:374:LYS:HD2  | 1.61                     | 0.65              |
| 3:E:721:G:H2'    | 3:E:722:A:C8     | 2.31                     | 0.65              |
| 1:A:167:ILE:O    | 1:A:170:PRO:HD2  | 1.97                     | 0.65              |
| 4:F:809:DC:C5    | 4:F:810:DT:H73   | 2.31                     | 0.65              |
| 2:D:80:LEU:HD23  | 2:D:153:TRP:CD1  | 2.32                     | 0.65              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:372:VAL:HG11 | 1:A:411:ILE:HG23 | 1.78                     | 0.65              |
| 1:A:123:ASP:N    | 1:A:123:ASP:OD1  | 2.29                     | 0.64              |
| 1:A:26:LEU:HD22  | 1:A:60:VAL:HG11  | 1.79                     | 0.64              |
| 2:B:28:GLU:HB2   | 2:B:135:ILE:CD1  | 2.27                     | 0.64              |
| 2:D:101:LYS:O    | 2:D:236:PRO:HB2  | 1.97                     | 0.64              |
| 2:D:423:VAL:O    | 2:D:426:TRP:HB2  | 1.96                     | 0.64              |
| 1:A:118:VAL:HB   | 1:A:149:LEU:HG   | 1.78                     | 0.64              |
| 1:A:427:TYR:OH   | 1:A:510:PRO:HD2  | 1.98                     | 0.64              |
| 3:E:709:C:H2'    | 3:E:710:G:H8     | 1.61                     | 0.64              |
| 3:T:710:G:C6     | 3:T:711:C:C4     | 2.85                     | 0.64              |
| 2:B:107:THR:HG23 | 2:B:232:TYR:HB2  | 1.79                     | 0.63              |
| 1:A:5:ILE:HG22   | 1:A:212:TRP:CD1  | 2.32                     | 0.63              |
| 2:D:365:VAL:HG11 | 2:D:401:TRP:HB2  | 1.78                     | 0.63              |
| 1:A:395:LYS:HD3  | 1:A:414:TRP:CH2  | 2.32                     | 0.63              |
| 2:B:84:THR:HG21  | 2:B:153:TRP:CZ2  | 2.33                     | 0.63              |
| 4:F:815:DG:C2    | 4:F:816:DG:N7    | 2.65                     | 0.63              |
| 1:A:225:PRO:HA   | 1:A:226:PRO:C    | 2.24                     | 0.63              |
| 1:C:75:VAL:HG12  | 1:C:77:PHE:HD1   | 1.64                     | 0.63              |
| 4:P:810:DT:C2    | 4:P:811:DG:C8    | 2.87                     | 0.63              |
| 4:P:812:DT:C2'   | 4:P:813:DT:H71   | 2.22                     | 0.63              |
| 2:B:180:ILE:HD13 | 2:B:189:VAL:HG22 | 1.81                     | 0.62              |
| 1:A:135:ILE:HG23 | 1:A:136:ASN:H    | 1.63                     | 0.62              |
| 2:D:279:LEU:O    | 2:D:282:LEU:HB2  | 1.98                     | 0.62              |
| 1:A:365:VAL:HG11 | 1:A:401:TRP:CD1  | 2.35                     | 0.62              |
| 1:C:35:VAL:HG23  | 1:C:134:SER:OG   | 1.99                     | 0.62              |
| 2:D:422:LEU:HD12 | 2:D:422:LEU:O    | 1.99                     | 0.62              |
| 2:B:249:LYS:HB2  | 2:B:252:TRP:CE2  | 2.35                     | 0.62              |
| 1:C:60:VAL:HG23  | 1:C:132:ILE:HG21 | 1.80                     | 0.62              |
| 2:B:142:ILE:CG2  | 2:B:144:TYR:HE1  | 2.13                     | 0.61              |
| 1:C:48:SER:O     | 1:C:144:TYR:HB2  | 2.00                     | 0.61              |
| 1:C:164:MET:HA   | 1:C:167:ILE:HD12 | 1.82                     | 0.61              |
| 1:A:406:TRP:CH2  | 2:B:418:ASN:HA   | 2.35                     | 0.61              |
| 1:C:21:VAL:HG12  | 1:C:22:LYS:H     | 1.64                     | 0.61              |
| 2:B:323:LYS:HB2  | 2:B:343:GLN:NE2  | 2.15                     | 0.61              |
| 2:B:88:TRP:NE1   | 2:B:154:LYS:HB2  | 2.16                     | 0.61              |
| 2:B:263:LYS:HZ2  | 2:B:425:LEU:HB3  | 1.64                     | 0.61              |
| 1:C:40:GLU:O     | 1:C:43:LYS:HB2   | 2.01                     | 0.61              |
| 1:A:175:ASN:HB3  | 1:A:178:ILE:CG1  | 2.31                     | 0.61              |
| 2:B:317:VAL:HG12 | 2:B:347:LYS:HG2  | 1.82                     | 0.61              |
| 2:D:41:MET:HE2   | 2:D:47:ILE:HD13  | 1.83                     | 0.61              |
| 2:D:254:VAL:HG22 | 2:D:293:ILE:HD11 | 1.82                     | 0.61              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:161:GLN:OE1  | 1:C:182:GLN:NE2  | 2.33                     | 0.60              |
| 2:D:303:LEU:O    | 2:D:307:ARG:HG3  | 2.01                     | 0.60              |
| 1:A:21:VAL:O     | 1:A:57:ASN:ND2   | 2.34                     | 0.60              |
| 1:C:325:LEU:HB2  | 1:C:385:LYS:HE2  | 1.83                     | 0.60              |
| 4:P:812:DT:C5    | 4:P:813:DT:H73   | 2.37                     | 0.60              |
| 1:C:434:ILE:HD13 | 1:C:530:LYS:HB3  | 1.83                     | 0.60              |
| 1:C:492:GLU:HG2  | 1:C:530:LYS:HB2  | 1.83                     | 0.60              |
| 4:P:807:DC:H2'   | 4:P:808:DC:H6    | 1.64                     | 0.60              |
| 1:A:109:LEU:HD11 | 1:A:205:LEU:HD23 | 1.84                     | 0.60              |
| 1:A:120:LEU:HD23 | 1:A:125:ARG:HA   | 1.84                     | 0.60              |
| 1:A:296:THR:HG23 | 1:A:299:ALA:H    | 1.67                     | 0.60              |
| 2:B:214:LEU:HD12 | 2:B:215:THR:H    | 1.65                     | 0.60              |
| 1:C:329:ILE:O    | 1:C:392:PRO:HD3  | 2.01                     | 0.60              |
| 1:C:498:ASN:HD22 | 1:C:545:ASN:ND2  | 1.93                     | 0.60              |
| 1:A:128:THR:HG22 | 1:A:128:THR:O    | 2.02                     | 0.60              |
| 1:C:125:ARG:HE   | 1:C:147:ASN:HA   | 1.67                     | 0.60              |
| 2:D:357:MET:O    | 2:D:360:ALA:HB2  | 2.01                     | 0.60              |
| 2:B:118:VAL:HG12 | 2:B:119:PRO:O    | 2.01                     | 0.59              |
| 2:B:403:THR:HG22 | 2:B:403:THR:O    | 2.02                     | 0.59              |
| 1:A:81:ASN:HD21  | 1:A:153:TRP:HA   | 1.67                     | 0.59              |
| 1:A:199:ARG:NE   | 1:A:222:GLN:OE1  | 2.24                     | 0.59              |
| 2:B:252:TRP:NE1  | 2:B:295:LEU:HD11 | 2.17                     | 0.59              |
| 2:B:353:LYS:HE3  | 2:B:427:TYR:CE1  | 2.37                     | 0.59              |
| 1:A:543:GLY:HA2  | 2:B:283:LEU:O    | 2.02                     | 0.59              |
| 2:B:84:THR:HG21  | 2:B:153:TRP:HZ2  | 1.68                     | 0.59              |
| 2:B:120:LEU:HD23 | 2:B:125:ARG:HG3  | 1.84                     | 0.58              |
| 1:C:235:HIS:CD2  | 1:C:238:LYS:HE3  | 2.38                     | 0.58              |
| 1:C:457:TYR:HE1  | 1:C:463:ARG:HG2  | 1.67                     | 0.58              |
| 2:D:399:GLU:HA   | 2:D:402:TRP:HD1  | 1.67                     | 0.58              |
| 4:P:808:DC:H2''  | 4:P:809:DC:H5''  | 1.84                     | 0.58              |
| 2:B:209:LEU:HD22 | 2:B:214:LEU:HD23 | 1.85                     | 0.58              |
| 1:C:58:THR:H     | 1:C:130:PHE:HB2  | 1.68                     | 0.58              |
| 1:A:362:THR:OG1  | 1:A:363:ASN:N    | 2.36                     | 0.58              |
| 2:D:142:ILE:HG22 | 2:D:144:TYR:HE1  | 1.68                     | 0.58              |
| 4:F:807:DC:H2''  | 4:F:808:DC:C5'   | 2.33                     | 0.58              |
| 2:B:195:ILE:CG1  | 2:B:199:ARG:HE   | 2.16                     | 0.58              |
| 1:C:206:ARG:HG2  | 1:C:216:THR:OG1  | 2.03                     | 0.58              |
| 2:D:24:TRP:HZ2   | 2:D:61:PHE:CE2   | 2.22                     | 0.58              |
| 2:D:84:THR:HG21  | 2:D:153:TRP:HZ2  | 1.67                     | 0.58              |
| 3:E:721:G:H2'    | 3:E:722:A:H8     | 1.68                     | 0.58              |
| 1:C:80:LEU:O     | 1:C:84:THR:OG1   | 2.20                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:111:VAL:HG23 | 2:D:115:TYR:HE2  | 1.66                     | 0.58              |
| 2:D:354:TYR:CZ   | 2:D:374:LYS:HG2  | 2.39                     | 0.58              |
| 1:C:223:LYS:O    | 1:C:225:PRO:HD3  | 2.03                     | 0.58              |
| 1:A:46:LYS:HE3   | 1:A:116:PHE:HB3  | 1.85                     | 0.58              |
| 1:A:161:GLN:O    | 1:A:165:THR:OG1  | 2.21                     | 0.58              |
| 1:A:544:GLY:O    | 1:A:548:VAL:N    | 2.35                     | 0.58              |
| 2:D:115:TYR:HE1  | 2:D:156:SER:C    | 2.12                     | 0.58              |
| 4:P:809:DC:H1'   | 4:P:810:DT:H5'   | 1.85                     | 0.58              |
| 1:A:34:LEU:HD22  | 1:A:73:LYS:HZ3   | 1.67                     | 0.58              |
| 2:D:398:TRP:O    | 2:D:402:TRP:HB3  | 2.04                     | 0.58              |
| 4:P:812:DT:C2    | 4:P:813:DT:C6    | 2.91                     | 0.58              |
| 2:B:88:TRP:CD1   | 2:B:154:LYS:HB2  | 2.38                     | 0.57              |
| 1:A:103:LYS:O    | 1:A:236:PRO:HB3  | 2.04                     | 0.57              |
| 1:C:494:ASN:HB3  | 2:D:289:LEU:HD12 | 1.86                     | 0.57              |
| 2:D:125:ARG:NE   | 2:D:147:ASN:HA   | 2.15                     | 0.57              |
| 2:D:274:ILE:O    | 2:D:275:LYS:HD3  | 2.04                     | 0.57              |
| 2:B:13:LYS:HD2   | 2:B:86:ASP:HB3   | 1.87                     | 0.57              |
| 1:A:204:GLU:O    | 1:A:207:GLN:HB2  | 2.05                     | 0.57              |
| 1:A:210:LEU:O    | 1:A:213:GLY:N    | 2.29                     | 0.57              |
| 2:B:366:LYS:HG3  | 2:B:405:TYR:CD1  | 2.40                     | 0.57              |
| 1:A:330:GLN:NE2  | 1:A:340:GLN:OE1  | 2.28                     | 0.57              |
| 1:C:181:TYR:CE2  | 1:C:183:TYR:HB2  | 2.40                     | 0.56              |
| 1:A:149:LEU:HD13 | 1:A:156:SER:HA   | 1.87                     | 0.56              |
| 1:C:376:THR:HG23 | 1:C:386:THR:HG23 | 1.87                     | 0.56              |
| 2:D:387:PRO:HG2  | 2:D:389:PHE:CE1  | 2.41                     | 0.56              |
| 2:B:205:LEU:O    | 2:B:209:LEU:HD12 | 2.04                     | 0.56              |
| 2:B:142:ILE:HG22 | 2:B:144:TYR:CE1  | 2.39                     | 0.56              |
| 4:F:815:DG:C4    | 4:F:816:DG:N7    | 2.74                     | 0.56              |
| 2:D:73:LYS:NZ    | 2:D:146:TYR:OH   | 2.29                     | 0.56              |
| 1:C:295:LEU:HG   | 1:C:296:THR:H    | 1.71                     | 0.56              |
| 1:C:457:TYR:HA   | 1:C:548:VAL:HG21 | 1.86                     | 0.56              |
| 2:D:85:GLN:HA    | 2:D:88:TRP:NE1   | 2.21                     | 0.56              |
| 1:A:58:THR:OG1   | 1:A:130:PHE:HB2  | 2.05                     | 0.56              |
| 4:F:815:DG:C2    | 4:F:816:DG:C6    | 2.94                     | 0.56              |
| 2:D:401:TRP:O    | 2:D:404:GLU:N    | 2.38                     | 0.55              |
| 4:F:807:DC:H2'   | 4:F:808:DC:H6    | 1.69                     | 0.55              |
| 1:A:354:TYR:HD1  | 1:A:374:LYS:HD2  | 1.70                     | 0.55              |
| 2:B:403:THR:O    | 2:B:403:THR:CG2  | 2.55                     | 0.55              |
| 1:C:35:VAL:HB    | 1:C:134:SER:HB3  | 1.88                     | 0.55              |
| 4:P:807:DC:H2''  | 4:P:808:DC:H5'   | 1.88                     | 0.55              |
| 1:A:195:ILE:HG22 | 1:A:199:ARG:NH1  | 2.22                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:77:PHE:O     | 1:A:80:LEU:N     | 2.40                     | 0.55              |
| 1:C:77:PHE:CD2   | 1:C:80:LEU:HB3   | 2.40                     | 0.55              |
| 2:D:17:ASP:O     | 2:D:83:ARG:NH1   | 2.40                     | 0.55              |
| 1:A:221:HIS:CG   | 1:A:224:GLU:HB2  | 2.41                     | 0.55              |
| 1:A:503:LEU:O    | 1:A:507:GLN:HB2  | 2.07                     | 0.55              |
| 2:B:120:LEU:HD12 | 2:B:149:LEU:HD23 | 1.87                     | 0.55              |
| 1:A:86:ASP:OD1   | 1:A:154:LYS:NZ   | 2.39                     | 0.55              |
| 1:A:373:GLN:HG3  | 2:B:401:TRP:CH2  | 2.42                     | 0.55              |
| 2:D:263:LYS:HA   | 2:D:425:LEU:HD13 | 1.88                     | 0.55              |
| 2:B:114:ALA:HB2  | 2:B:214:LEU:HD22 | 1.88                     | 0.55              |
| 2:B:242:GLN:O    | 2:B:351:THR:OG1  | 2.25                     | 0.55              |
| 1:C:95:PRO:HG2   | 1:C:229:TRP:HH2  | 1.71                     | 0.55              |
| 4:F:807:DC:H2''  | 4:F:808:DC:H5'   | 1.89                     | 0.55              |
| 1:A:328:GLU:HB2  | 1:A:390:LYS:HB2  | 1.88                     | 0.54              |
| 1:C:35:VAL:HG13  | 1:C:36:GLU:HG3   | 1.89                     | 0.54              |
| 2:D:282:LEU:HD21 | 2:D:296:THR:HG23 | 1.89                     | 0.54              |
| 1:A:105:SER:O    | 1:A:190:GLY:HA2  | 2.07                     | 0.54              |
| 2:D:114:ALA:H    | 2:D:214:LEU:HD13 | 1.73                     | 0.54              |
| 1:C:38:CYS:O     | 1:C:42:GLU:OE1   | 2.25                     | 0.54              |
| 3:T:711:C:O2'    | 3:T:712:C:OP1    | 2.25                     | 0.54              |
| 1:A:322:SER:OG   | 1:A:323:LYS:HG2  | 2.07                     | 0.54              |
| 1:A:59:PRO:O     | 1:A:76:ASP:HB3   | 2.07                     | 0.54              |
| 2:B:69:THR:HG23  | 2:B:70:LYS:HE2   | 1.90                     | 0.54              |
| 2:D:395:LYS:HG3  | 2:D:416:PHE:CE2  | 2.41                     | 0.54              |
| 1:A:168:LEU:HD21 | 1:A:187:LEU:HD13 | 1.89                     | 0.54              |
| 1:C:540:LYS:HB2  | 1:C:542:ILE:HG13 | 1.89                     | 0.54              |
| 2:D:72:ARG:HD3   | 2:D:73:LYS:O     | 2.07                     | 0.54              |
| 2:D:423:VAL:O    | 2:D:423:VAL:HG12 | 2.08                     | 0.54              |
| 1:A:317:VAL:HG23 | 1:A:318:TYR:N    | 2.23                     | 0.54              |
| 2:D:421:PRO:HB2  | 2:D:423:VAL:HB   | 1.90                     | 0.54              |
| 3:T:714:G:C2     | 3:T:715:A:C4     | 2.96                     | 0.54              |
| 1:C:452:LEU:CD1  | 1:C:470:THR:HG22 | 2.36                     | 0.54              |
| 1:C:474:ASN:ND2  | 3:E:723:C:H4'    | 2.16                     | 0.54              |
| 3:T:720:G:H2'    | 3:T:721:G:O4'    | 2.08                     | 0.54              |
| 1:C:452:LEU:HD12 | 1:C:470:THR:HA   | 1.89                     | 0.53              |
| 1:C:120:LEU:HD13 | 1:C:148:VAL:O    | 2.08                     | 0.53              |
| 2:D:19:PRO:HD3   | 2:D:80:LEU:HD12  | 1.90                     | 0.53              |
| 2:D:427:TYR:C    | 2:D:427:TYR:CD1  | 2.86                     | 0.53              |
| 4:P:812:DT:C6    | 4:P:813:DT:H73   | 2.42                     | 0.53              |
| 2:B:423:VAL:HG12 | 2:B:423:VAL:O    | 2.08                     | 0.53              |
| 1:A:94:ILE:HD13  | 1:A:230:MET:CE   | 2.38                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:59:PRO:O     | 1:C:75:VAL:HG13  | 2.08                     | 0.53              |
| 1:C:121:ASP:O    | 1:C:125:ARG:HG3  | 2.08                     | 0.53              |
| 1:C:339:TYR:CZ   | 1:C:352:GLY:HA3  | 2.44                     | 0.53              |
| 2:D:401:TRP:HB3  | 2:D:405:TYR:HE2  | 1.74                     | 0.53              |
| 1:C:417:VAL:O    | 1:C:417:VAL:HG13 | 2.09                     | 0.53              |
| 1:A:547:GLN:N    | 1:A:547:GLN:OE1  | 2.41                     | 0.53              |
| 2:B:116:PHE:O    | 2:B:148:VAL:HG11 | 2.09                     | 0.53              |
| 1:C:125:ARG:O    | 1:C:128:THR:OG1  | 2.25                     | 0.53              |
| 1:C:354:TYR:CD1  | 1:C:374:LYS:HD2  | 2.43                     | 0.53              |
| 1:C:442:VAL:HB   | 1:C:481:ALA:HB1  | 1.91                     | 0.53              |
| 2:B:82:LYS:O     | 2:B:85:GLN:HB3   | 2.09                     | 0.52              |
| 2:B:76:ASP:OD1   | 2:B:78:ARG:NE    | 2.38                     | 0.52              |
| 1:C:438:GLU:HG3  | 1:C:461:LYS:HD3  | 1.92                     | 0.52              |
| 2:D:287:LYS:HG2  | 2:D:291:GLU:OE2  | 2.09                     | 0.52              |
| 3:T:714:G:H2'    | 3:T:715:A:C8     | 2.45                     | 0.52              |
| 2:D:85:GLN:HA    | 2:D:88:TRP:CE2   | 2.45                     | 0.52              |
| 1:A:18:GLY:HA3   | 1:A:56:TYR:CD1   | 2.43                     | 0.52              |
| 2:B:162:SER:O    | 2:B:165:THR:HG22 | 2.10                     | 0.52              |
| 2:D:24:TRP:HZ2   | 2:D:61:PHE:HE2   | 1.57                     | 0.52              |
| 1:C:406:TRP:CH2  | 1:C:407:GLN:HG3  | 2.44                     | 0.52              |
| 4:P:809:DC:C5    | 4:P:810:DT:H73   | 2.44                     | 0.52              |
| 2:B:115:TYR:O    | 2:B:149:LEU:HB2  | 2.09                     | 0.52              |
| 1:C:97:PRO:HG2   | 1:C:232:TYR:CE1  | 2.44                     | 0.52              |
| 1:C:197:GLN:O    | 1:C:200:THR:HB   | 2.10                     | 0.52              |
| 1:A:37:ILE:HA    | 1:A:40:GLU:CD    | 2.34                     | 0.52              |
| 1:C:271:TYR:CZ   | 1:C:314:VAL:HG12 | 2.45                     | 0.52              |
| 1:A:96:HIS:N     | 2:B:136:ASN:HD21 | 2.08                     | 0.51              |
| 1:A:373:GLN:HG3  | 2:B:401:TRP:HH2  | 1.75                     | 0.51              |
| 1:A:452:LEU:HD23 | 1:A:471:ASN:H    | 1.73                     | 0.51              |
| 1:C:167:ILE:O    | 1:C:170:PRO:HD2  | 2.11                     | 0.51              |
| 4:P:807:DC:H2''  | 4:P:808:DC:C5'   | 2.40                     | 0.51              |
| 2:B:401:TRP:O    | 2:B:404:GLU:N    | 2.42                     | 0.51              |
| 1:C:544:GLY:O    | 1:C:548:VAL:HG12 | 2.09                     | 0.51              |
| 2:D:88:TRP:CD1   | 2:D:154:LYS:HB3  | 2.45                     | 0.51              |
| 3:T:714:G:H2'    | 3:T:715:A:H8     | 1.74                     | 0.51              |
| 4:P:804:DA:H2''  | 4:P:805:DG:H8    | 1.75                     | 0.51              |
| 2:B:425:LEU:N    | 2:B:425:LEU:CD1  | 2.73                     | 0.51              |
| 2:D:154:LYS:HD2  | 2:D:184:MET:HE1  | 1.93                     | 0.51              |
| 2:D:305:GLU:O    | 2:D:309:ILE:HG13 | 2.11                     | 0.51              |
| 1:A:48:SER:O     | 1:A:144:TYR:HB2  | 2.11                     | 0.51              |
| 1:A:233:GLU:HG3  | 1:A:242:GLN:HG2  | 1.92                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:17:ASP:O     | 2:B:83:ARG:NH1   | 2.38                     | 0.51              |
| 2:B:390:LYS:HB3  | 2:B:417:VAL:HG21 | 1.91                     | 0.51              |
| 2:D:84:THR:HG21  | 2:D:153:TRP:CZ2  | 2.45                     | 0.51              |
| 2:D:92:LEU:HD21  | 2:D:161:GLN:OE1  | 2.11                     | 0.51              |
| 1:A:155:GLY:O    | 1:A:159:ILE:HB   | 2.11                     | 0.51              |
| 1:C:220:LYS:HE2  | 1:C:222:GLN:HA   | 1.92                     | 0.51              |
| 1:A:441:TYR:CD1  | 2:B:286:THR:HG23 | 2.46                     | 0.51              |
| 1:C:139:THR:HB   | 1:C:140:PRO:HD2  | 1.93                     | 0.51              |
| 2:D:109:LEU:HD22 | 2:D:216:THR:HG21 | 1.93                     | 0.51              |
| 1:A:317:VAL:HG23 | 1:A:318:TYR:O    | 2.11                     | 0.51              |
| 1:C:199:ARG:NH2  | 1:C:223:LYS:HD3  | 2.26                     | 0.51              |
| 2:B:130:PHE:CE2  | 2:B:144:TYR:HB2  | 2.46                     | 0.51              |
| 1:C:2:ILE:HG22   | 1:C:3:SER:H      | 1.77                     | 0.51              |
| 2:D:118:VAL:HG12 | 2:D:119:PRO:O    | 2.11                     | 0.51              |
| 4:P:808:DC:H2''  | 4:P:809:DC:H5'   | 1.92                     | 0.51              |
| 1:A:226:PRO:HB3  | 1:A:235:HIS:NE2  | 2.25                     | 0.50              |
| 1:A:382:ILE:HA   | 2:B:136:ASN:OD1  | 2.11                     | 0.50              |
| 1:A:500:GLN:HG3  | 1:A:535:TRP:NE1  | 2.26                     | 0.50              |
| 1:C:35:VAL:HG13  | 1:C:36:GLU:N     | 2.27                     | 0.50              |
| 2:D:68:SER:HB3   | 2:D:70:LYS:HE2   | 1.93                     | 0.50              |
| 1:A:32:LYS:HZ2   | 1:A:35:VAL:HG21  | 1.76                     | 0.50              |
| 1:A:34:LEU:HD21  | 1:A:132:ILE:HG21 | 1.92                     | 0.50              |
| 1:C:34:LEU:HD13  | 1:C:73:LYS:HE3   | 1.92                     | 0.50              |
| 3:E:720:G:H2'    | 3:E:721:G:C8     | 2.47                     | 0.50              |
| 1:A:225:PRO:HD3  | 1:A:227:PHE:CE1  | 2.47                     | 0.50              |
| 1:C:430:GLU:HG3  | 1:C:434:ILE:HD11 | 1.94                     | 0.50              |
| 2:D:142:ILE:HG22 | 2:D:144:TYR:CE1  | 2.46                     | 0.50              |
| 1:A:197:GLN:O    | 1:A:200:THR:HB   | 2.11                     | 0.50              |
| 4:P:812:DT:C2    | 4:P:813:DT:C5    | 2.99                     | 0.50              |
| 2:B:85:GLN:HG3   | 2:B:88:TRP:CH2   | 2.47                     | 0.50              |
| 1:C:5:ILE:HG22   | 1:C:212:TRP:CD1  | 2.40                     | 0.50              |
| 1:C:218:ASP:OD1  | 1:C:222:GLN:NE2  | 2.45                     | 0.50              |
| 2:B:249:LYS:HG3  | 2:B:252:TRP:CH2  | 2.46                     | 0.50              |
| 2:B:270:ILE:HG13 | 2:B:346:PHE:HD1  | 1.76                     | 0.50              |
| 2:D:87:PHE:CE2   | 2:D:155:GLY:HA2  | 2.46                     | 0.50              |
| 2:D:292:VAL:C    | 2:D:293:ILE:HD13 | 2.36                     | 0.50              |
| 1:C:420:PRO:HA   | 1:C:421:PRO:C    | 2.36                     | 0.50              |
| 1:A:106:VAL:HG12 | 1:A:227:PHE:HE2  | 1.77                     | 0.49              |
| 1:A:410:TRP:CZ2  | 1:A:412:PRO:HA   | 2.47                     | 0.49              |
| 2:B:13:LYS:HD2   | 2:B:86:ASP:CB    | 2.42                     | 0.49              |
| 2:B:252:TRP:CB   | 2:B:257:ILE:HD11 | 2.41                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:401:TRP:O    | 2:B:402:TRP:C    | 2.55                     | 0.49              |
| 1:C:391:LEU:HD12 | 1:C:414:TRP:CE3  | 2.47                     | 0.49              |
| 2:B:47:ILE:HG22  | 2:B:146:TYR:HA   | 1.94                     | 0.49              |
| 2:B:195:ILE:HG12 | 2:B:199:ARG:HE   | 1.77                     | 0.49              |
| 2:B:252:TRP:HB3  | 2:B:257:ILE:HD11 | 1.93                     | 0.49              |
| 2:B:374:LYS:O    | 2:B:378:GLU:HG3  | 2.12                     | 0.49              |
| 2:D:354:TYR:HE2  | 2:D:375:ILE:HG13 | 1.77                     | 0.49              |
| 1:A:410:TRP:CH2  | 1:A:412:PRO:HA   | 2.47                     | 0.49              |
| 4:F:815:DG:N3    | 4:F:816:DG:C8    | 2.79                     | 0.49              |
| 2:B:74:LEU:HD12  | 2:B:75:VAL:N     | 2.27                     | 0.49              |
| 2:D:56:TYR:O     | 2:D:143:ARG:NH2  | 2.45                     | 0.49              |
| 2:D:57:ASN:OD1   | 2:D:130:PHE:HA   | 2.13                     | 0.49              |
| 1:A:5:ILE:CG2    | 1:A:212:TRP:HD1  | 2.23                     | 0.49              |
| 1:A:327:ALA:O    | 1:A:389:PHE:HA   | 2.12                     | 0.49              |
| 1:A:360:ALA:HA   | 1:A:514:GLU:OE2  | 2.12                     | 0.49              |
| 2:D:47:ILE:HB    | 2:D:144:TYR:HD2  | 1.77                     | 0.49              |
| 2:D:244:ILE:HB   | 2:D:310:LEU:HD22 | 1.94                     | 0.49              |
| 2:D:400:THR:HB   | 2:D:401:TRP:CD1  | 2.47                     | 0.49              |
| 1:A:21:VAL:HB    | 1:A:59:PRO:HD3   | 1.95                     | 0.49              |
| 1:A:186:ASP:C    | 1:A:187:LEU:HD23 | 2.38                     | 0.49              |
| 2:B:154:LYS:C    | 2:B:157:PRO:HD2  | 2.37                     | 0.49              |
| 2:B:206:ARG:HE   | 2:B:216:THR:HB   | 1.77                     | 0.49              |
| 1:C:524:GLN:HA   | 1:C:524:GLN:NE2  | 2.27                     | 0.49              |
| 1:A:164:MET:O    | 1:A:168:LEU:HD13 | 2.12                     | 0.49              |
| 1:A:442:VAL:HB   | 1:A:481:ALA:HB1  | 1.94                     | 0.49              |
| 2:D:116:PHE:O    | 2:D:148:VAL:HG11 | 2.13                     | 0.49              |
| 2:D:155:GLY:O    | 2:D:158:ALA:N    | 2.46                     | 0.49              |
| 1:A:97:PRO:HG2   | 1:A:232:TYR:CD1  | 2.48                     | 0.49              |
| 2:B:191:SER:OG   | 2:B:198:HIS:ND1  | 2.21                     | 0.49              |
| 1:C:97:PRO:HG2   | 1:C:232:TYR:CD1  | 2.48                     | 0.49              |
| 1:A:549:ASP:O    | 1:A:553:SER:HB2  | 2.13                     | 0.49              |
| 2:B:136:ASN:O    | 2:B:137:ASN:HB2  | 2.12                     | 0.49              |
| 2:B:266:TRP:O    | 2:B:269:GLN:N    | 2.41                     | 0.49              |
| 2:B:285:GLY:H    | 2:B:287:LYS:HE2  | 1.78                     | 0.49              |
| 2:D:13:LYS:HD3   | 2:D:86:ASP:H     | 1.78                     | 0.49              |
| 2:D:164:MET:HE1  | 2:D:209:LEU:HD21 | 1.95                     | 0.49              |
| 2:B:41:MET:HE2   | 2:B:47:ILE:CD1   | 2.43                     | 0.48              |
| 1:C:35:VAL:O     | 1:C:38:CYS:HB3   | 2.12                     | 0.48              |
| 1:C:172:LYS:HG2  | 1:C:180:ILE:HD13 | 1.94                     | 0.48              |
| 4:F:815:DG:N2    | 4:F:816:DG:C5    | 2.81                     | 0.48              |
| 1:C:391:LEU:O    | 1:C:393:ILE:N    | 2.39                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:214:LEU:HD12 | 2:D:215:THR:H    | 1.77                     | 0.48              |
| 2:D:338:THR:HG21 | 2:D:427:TYR:HB2  | 1.95                     | 0.48              |
| 2:D:366:LYS:HG3  | 2:D:405:TYR:CD1  | 2.48                     | 0.48              |
| 2:D:401:TRP:O    | 2:D:402:TRP:C    | 2.53                     | 0.48              |
| 2:B:395:LYS:HG3  | 2:B:416:PHE:CE2  | 2.47                     | 0.48              |
| 1:C:500:GLN:NE2  | 2:D:422:LEU:HD23 | 2.18                     | 0.48              |
| 1:A:209:LEU:HD22 | 1:A:214:LEU:HD13 | 1.94                     | 0.48              |
| 1:C:516:GLU:O    | 1:C:520:GLN:HG3  | 2.14                     | 0.48              |
| 2:D:354:TYR:OH   | 2:D:374:LYS:HG2  | 2.14                     | 0.48              |
| 1:A:24:TRP:CE3   | 1:A:25:PRO:HD2   | 2.49                     | 0.48              |
| 1:A:128:THR:O    | 1:A:128:THR:CG2  | 2.61                     | 0.48              |
| 3:T:711:C:HO2'   | 3:T:712:C:P      | 2.35                     | 0.48              |
| 1:A:545:ASN:C    | 1:A:548:VAL:HG12 | 2.36                     | 0.48              |
| 1:A:281:LYS:HG2  | 1:A:284:ARG:NH2  | 2.29                     | 0.48              |
| 1:C:358:ARG:NH2  | 2:D:396:GLU:OE1  | 2.46                     | 0.48              |
| 1:C:447:ASN:OD1  | 1:C:450:THR:HG23 | 2.13                     | 0.48              |
| 1:A:32:LYS:HD2   | 1:A:32:LYS:HA    | 1.62                     | 0.48              |
| 1:A:171:PHE:CZ   | 1:A:205:LEU:HB2  | 2.49                     | 0.48              |
| 1:C:160:PHE:C    | 1:C:160:PHE:CD1  | 2.91                     | 0.48              |
| 1:C:457:TYR:C    | 1:C:457:TYR:CD1  | 2.91                     | 0.48              |
| 2:D:247:PRO:O    | 2:D:307:ARG:NH2  | 2.46                     | 0.48              |
| 2:D:374:LYS:O    | 2:D:378:GLU:HG3  | 2.14                     | 0.48              |
| 3:E:709:C:H2'    | 3:E:710:G:C8     | 2.45                     | 0.48              |
| 1:A:77:PHE:CE1   | 1:A:128:THR:HG23 | 2.48                     | 0.48              |
| 2:B:263:LYS:HZ3  | 2:B:425:LEU:HB3  | 1.78                     | 0.48              |
| 1:C:473:THR:O    | 1:C:477:THR:HG23 | 2.13                     | 0.48              |
| 1:C:548:VAL:O    | 1:C:552:VAL:HG13 | 2.14                     | 0.48              |
| 1:A:365:VAL:HG11 | 1:A:401:TRP:CG   | 2.48                     | 0.47              |
| 1:C:65:LYS:HB3   | 1:C:72:ARG:HH12  | 1.79                     | 0.47              |
| 1:A:448:ARG:NH1  | 4:P:806:DT:O2    | 2.47                     | 0.47              |
| 2:B:106:VAL:O    | 2:B:234:LEU:N    | 2.45                     | 0.47              |
| 1:C:130:PHE:O    | 1:C:143:ARG:HB2  | 2.14                     | 0.47              |
| 2:D:111:VAL:HG23 | 2:D:115:TYR:CE2  | 2.49                     | 0.47              |
| 1:A:252:TRP:CD1  | 1:A:295:LEU:HG   | 2.50                     | 0.47              |
| 1:C:398:TRP:CZ2  | 1:C:411:ILE:HG13 | 2.50                     | 0.47              |
| 1:A:50:ILE:HG22  | 1:A:52:PRO:HD2   | 1.95                     | 0.47              |
| 1:A:94:ILE:CD1   | 1:A:230:MET:HE1  | 2.41                     | 0.47              |
| 2:B:65:LYS:O     | 2:B:68:SER:HB3   | 2.15                     | 0.47              |
| 1:C:365:VAL:HG11 | 1:C:401:TRP:CD1  | 2.50                     | 0.47              |
| 2:D:30:LYS:HD3   | 2:D:62:ALA:O     | 2.15                     | 0.47              |
| 2:D:291:GLU:HG2  | 2:D:293:ILE:CD1  | 2.44                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:218:ASP:C    | 1:A:220:LYS:N    | 2.72                     | 0.47              |
| 1:A:331:LYS:NZ   | 1:A:364:ASP:OD2  | 2.47                     | 0.47              |
| 1:C:37:ILE:HA    | 1:C:40:GLU:HB2   | 1.97                     | 0.47              |
| 3:T:714:G:N2     | 3:T:715:A:C4     | 2.83                     | 0.47              |
| 1:C:435:VAL:HG22 | 2:D:290:THR:HG21 | 1.97                     | 0.47              |
| 1:C:135:ILE:HG12 | 1:C:136:ASN:OD1  | 2.15                     | 0.47              |
| 1:C:161:GLN:NE2  | 1:C:184:MET:O    | 2.48                     | 0.47              |
| 1:A:32:LYS:NZ    | 1:A:35:VAL:HG21  | 2.29                     | 0.46              |
| 2:B:154:LYS:O    | 2:B:157:PRO:HD2  | 2.15                     | 0.46              |
| 2:B:401:TRP:HB3  | 2:B:405:TYR:HE2  | 1.79                     | 0.46              |
| 1:C:65:LYS:HG2   | 1:C:72:ARG:NH2   | 2.27                     | 0.46              |
| 1:A:376:THR:O    | 1:A:380:ILE:HG12 | 2.15                     | 0.46              |
| 2:B:73:LYS:NZ    | 2:B:130:PHE:CZ   | 2.83                     | 0.46              |
| 2:B:425:LEU:HD12 | 2:B:425:LEU:H    | 1.79                     | 0.46              |
| 1:C:473:THR:OG1  | 1:C:476:LYS:HG3  | 2.15                     | 0.46              |
| 1:A:149:LEU:HA   | 1:A:150:PRO:HD3  | 1.48                     | 0.46              |
| 1:A:194:GLU:CD   | 1:A:197:GLN:H    | 2.24                     | 0.46              |
| 2:B:284:ARG:HH11 | 2:B:284:ARG:HG3  | 1.81                     | 0.46              |
| 2:D:208:HIS:O    | 2:D:211:ARG:HG2  | 2.15                     | 0.46              |
| 4:F:809:DC:C5    | 4:F:810:DT:C7    | 2.97                     | 0.46              |
| 1:A:2:ILE:HG22   | 1:A:3:SER:H      | 1.80                     | 0.46              |
| 2:D:206:ARG:NH2  | 2:D:216:THR:O    | 2.49                     | 0.46              |
| 2:D:319:TYR:HD1  | 2:D:343:GLN:HE22 | 1.58                     | 0.46              |
| 1:A:342:TYR:HA   | 1:A:349:LEU:HD12 | 1.98                     | 0.46              |
| 1:A:545:ASN:O    | 1:A:549:ASP:N    | 2.41                     | 0.46              |
| 2:B:101:LYS:O    | 2:B:236:PRO:HB2  | 2.15                     | 0.46              |
| 1:C:179:VAL:HG12 | 5:C:901:NVP:HCC2 | 1.97                     | 0.46              |
| 4:F:809:DC:C4    | 4:F:810:DT:H73   | 2.50                     | 0.46              |
| 1:A:406:TRP:HH2  | 2:B:418:ASN:HA   | 1.79                     | 0.46              |
| 2:B:297:GLU:O    | 2:B:301:LEU:HG   | 2.16                     | 0.46              |
| 1:C:120:LEU:HG   | 1:C:121:ASP:H    | 1.81                     | 0.46              |
| 1:C:206:ARG:HH21 | 1:C:217:PRO:C    | 2.23                     | 0.46              |
| 3:T:717:C:H2'    | 3:T:718:A:C8     | 2.51                     | 0.46              |
| 1:C:2:ILE:HD12   | 1:C:2:ILE:H      | 1.80                     | 0.46              |
| 1:C:17:ASP:O     | 1:C:83:ARG:HD3   | 2.15                     | 0.46              |
| 1:C:281:LYS:O    | 1:C:284:ARG:HG3  | 2.15                     | 0.46              |
| 1:C:463:ARG:HE   | 1:C:463:ARG:HB2  | 1.23                     | 0.46              |
| 2:D:280:SER:C    | 2:D:282:LEU:N    | 2.72                     | 0.46              |
| 4:F:809:DC:C6    | 4:F:810:DT:H71   | 2.51                     | 0.46              |
| 1:A:88:TRP:CD1   | 2:B:143:ARG:CZ   | 2.99                     | 0.46              |
| 1:A:326:ILE:O    | 1:A:341:ILE:HA   | 2.16                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:360:ALA:HA   | 2:B:367:GLN:OE1  | 2.15                     | 0.46              |
| 1:A:77:PHE:HB3   | 1:A:80:LEU:HB3   | 1.98                     | 0.46              |
| 1:A:202:ILE:HG21 | 1:A:220:LYS:NZ   | 2.30                     | 0.46              |
| 2:B:279:LEU:HD23 | 2:B:299:ALA:HB1  | 1.98                     | 0.46              |
| 1:C:58:THR:N     | 1:C:130:PHE:HB2  | 2.31                     | 0.46              |
| 1:A:156:SER:HB2  | 1:A:157:PRO:HD3  | 1.98                     | 0.46              |
| 2:B:85:GLN:HA    | 2:B:88:TRP:CZ2   | 2.49                     | 0.46              |
| 2:D:19:PRO:CD    | 2:D:80:LEU:HD12  | 2.46                     | 0.46              |
| 2:D:108:VAL:HG12 | 2:D:232:TYR:O    | 2.15                     | 0.46              |
| 2:B:85:GLN:HA    | 2:B:88:TRP:NE1   | 2.30                     | 0.45              |
| 1:C:173:LYS:HD2  | 1:C:173:LYS:HA   | 1.71                     | 0.45              |
| 2:D:103:LYS:HD2  | 2:D:191:SER:HA   | 1.98                     | 0.45              |
| 1:C:331:LYS:HB2  | 1:C:337:TRP:CZ3  | 2.51                     | 0.45              |
| 3:E:710:G:C6     | 3:E:711:C:C4     | 3.05                     | 0.45              |
| 1:A:34:LEU:HA    | 1:A:37:ILE:HB    | 1.97                     | 0.45              |
| 1:A:391:LEU:HD12 | 1:A:414:TRP:CE3  | 2.51                     | 0.45              |
| 1:C:406:TRP:CZ3  | 1:C:407:GLN:HG3  | 2.52                     | 0.45              |
| 2:D:282:LEU:HD21 | 2:D:296:THR:CG2  | 2.46                     | 0.45              |
| 1:A:102:LYS:HE2  | 1:A:237:ASP:HA   | 1.98                     | 0.45              |
| 1:A:428:GLN:HA   | 1:A:509:GLN:OE1  | 2.17                     | 0.45              |
| 2:B:9:PRO:HA     | 2:B:121:ASP:CG   | 2.41                     | 0.45              |
| 2:D:160:PHE:O    | 2:D:160:PHE:CD1  | 2.69                     | 0.45              |
| 1:A:347:LYS:HB2  | 1:A:347:LYS:HE3  | 1.77                     | 0.45              |
| 2:B:10:VAL:HG13  | 2:B:87:PHE:CD1   | 2.50                     | 0.45              |
| 2:B:50:ILE:HG12  | 2:B:143:ARG:HB2  | 1.98                     | 0.45              |
| 2:B:84:THR:O     | 2:B:85:GLN:C     | 2.58                     | 0.45              |
| 2:D:341:ILE:HD11 | 2:D:375:ILE:HG23 | 1.98                     | 0.45              |
| 1:A:22:LYS:HE3   | 1:A:23:GLN:O     | 2.17                     | 0.45              |
| 1:A:221:HIS:CB   | 1:A:224:GLU:HB2  | 2.44                     | 0.45              |
| 2:B:78:ARG:O     | 2:B:82:LYS:HG3   | 2.15                     | 0.45              |
| 1:A:270:ILE:HD12 | 1:A:270:ILE:HA   | 1.80                     | 0.45              |
| 1:A:340:GLN:HG3  | 1:A:351:THR:HG22 | 1.98                     | 0.45              |
| 1:A:398:TRP:CE2  | 1:A:411:ILE:HD12 | 2.52                     | 0.45              |
| 1:A:420:PRO:HA   | 1:A:421:PRO:C    | 2.41                     | 0.45              |
| 2:B:124:PHE:CE2  | 2:B:153:TRP:CZ2  | 3.04                     | 0.45              |
| 1:C:77:PHE:HD2   | 1:C:80:LEU:HB3   | 1.79                     | 0.45              |
| 1:C:195:ILE:HG12 | 1:C:199:ARG:HE   | 1.82                     | 0.45              |
| 1:C:226:PRO:HB3  | 1:C:235:HIS:CE1  | 2.52                     | 0.45              |
| 1:C:254:VAL:HG21 | 1:C:286:THR:HG21 | 1.97                     | 0.45              |
| 1:C:270:ILE:HG23 | 1:C:271:TYR:N    | 2.31                     | 0.45              |
| 2:D:115:TYR:O    | 2:D:149:LEU:HB2  | 2.17                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:172:LYS:HE3  | 1:A:180:ILE:HD12 | 1.98                     | 0.45              |
| 2:B:35:VAL:O     | 2:B:39:THR:HG23  | 2.16                     | 0.45              |
| 2:B:274:ILE:HA   | 2:B:306:ASN:OD1  | 2.16                     | 0.45              |
| 2:B:358:ARG:NH2  | 2:B:405:TYR:O    | 2.50                     | 0.45              |
| 1:C:203:GLU:OE1  | 1:C:206:ARG:HD2  | 2.15                     | 0.45              |
| 2:D:79:GLU:O     | 2:D:83:ARG:HD2   | 2.17                     | 0.45              |
| 2:D:142:ILE:CG2  | 2:D:144:TYR:HE1  | 2.30                     | 0.45              |
| 2:D:373:GLN:HE21 | 2:D:373:GLN:HB3  | 1.59                     | 0.45              |
| 2:B:320:ASP:OD1  | 2:B:320:ASP:C    | 2.60                     | 0.45              |
| 1:C:149:LEU:HA   | 1:C:150:PRO:HD3  | 1.78                     | 0.45              |
| 2:B:84:THR:O     | 2:B:87:PHE:N     | 2.49                     | 0.45              |
| 2:B:98:ALA:O     | 2:B:101:LYS:HE2  | 2.16                     | 0.45              |
| 1:A:39:THR:HA    | 1:A:42:GLU:CD    | 2.42                     | 0.44              |
| 1:A:115:TYR:CE2  | 1:A:156:SER:HB3  | 2.52                     | 0.44              |
| 1:A:443:ASP:OD1  | 1:A:444:GLY:N    | 2.50                     | 0.44              |
| 1:C:107:THR:OG1  | 1:C:198:HIS:NE2  | 2.27                     | 0.44              |
| 1:C:199:ARG:HH22 | 1:C:223:LYS:HD3  | 1.82                     | 0.44              |
| 2:D:17:ASP:OD1   | 2:D:56:TYR:OH    | 2.31                     | 0.44              |
| 4:F:803:DC:H2'   | 4:F:804:DA:C8    | 2.52                     | 0.44              |
| 2:B:115:TYR:N    | 2:B:115:TYR:CD1  | 2.85                     | 0.44              |
| 2:B:279:LEU:HD23 | 2:B:279:LEU:HA   | 1.71                     | 0.44              |
| 1:C:63:ILE:H     | 1:C:74:LEU:HD12  | 1.82                     | 0.44              |
| 1:C:128:THR:CB   | 1:C:146:TYR:HB2  | 2.47                     | 0.44              |
| 2:D:427:TYR:CD1  | 2:D:428:GLN:O    | 2.70                     | 0.44              |
| 3:E:718:A:C6     | 3:E:719:G:C5     | 3.05                     | 0.44              |
| 1:A:366:LYS:HE3  | 1:A:401:TRP:HH2  | 1.82                     | 0.44              |
| 1:C:30:LYS:HD2   | 1:C:30:LYS:N     | 2.31                     | 0.44              |
| 1:C:135:ILE:HG12 | 1:C:136:ASN:CG   | 2.43                     | 0.44              |
| 1:A:265:ASN:OD1  | 1:A:353:LYS:HD3  | 2.18                     | 0.44              |
| 2:B:166:LYS:HB2  | 2:B:166:LYS:HE3  | 1.66                     | 0.44              |
| 1:C:164:MET:HE2  | 1:C:168:LEU:CD1  | 2.47                     | 0.44              |
| 2:D:167:ILE:O    | 2:D:167:ILE:HG12 | 2.17                     | 0.44              |
| 1:A:142:ILE:HD12 | 1:A:142:ILE:HA   | 1.88                     | 0.44              |
| 1:A:329:ILE:O    | 1:A:392:PRO:HD3  | 2.18                     | 0.44              |
| 1:C:388:LYS:H    | 1:C:388:LYS:HG3  | 1.65                     | 0.44              |
| 2:D:12:LEU:HD23  | 2:D:16:MET:O     | 2.18                     | 0.44              |
| 4:P:809:DC:C5    | 4:P:810:DT:C7    | 3.00                     | 0.44              |
| 1:A:440:PHE:N    | 1:A:440:PHE:CD1  | 2.86                     | 0.44              |
| 1:C:410:TRP:CE2  | 2:D:363:ASN:ND2  | 2.86                     | 0.44              |
| 1:C:430:GLU:HB2  | 1:C:532:TYR:HB2  | 1.98                     | 0.44              |
| 1:A:125:ARG:HD3  | 1:A:147:ASN:HD22 | 1.83                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:78:ARG:HD3   | 2:B:411:ILE:O    | 2.18                     | 0.44              |
| 2:D:396:GLU:OE2  | 2:D:396:GLU:N    | 2.46                     | 0.44              |
| 1:A:128:THR:HG21 | 1:A:146:TYR:CD2  | 2.52                     | 0.44              |
| 2:D:112:GLY:HA3  | 2:D:151:GLN:OE1  | 2.18                     | 0.44              |
| 2:D:149:LEU:HD13 | 2:D:156:SER:HA   | 2.00                     | 0.44              |
| 1:A:203:GLU:HA   | 1:A:206:ARG:HD3  | 2.00                     | 0.44              |
| 2:B:206:ARG:NE   | 2:B:216:THR:HB   | 2.32                     | 0.44              |
| 1:C:473:THR:HG21 | 4:F:809:DC:P     | 2.57                     | 0.44              |
| 1:A:342:TYR:CD1  | 1:A:342:TYR:C    | 2.95                     | 0.43              |
| 2:D:323:LYS:O    | 2:D:385:LYS:NZ   | 2.51                     | 0.43              |
| 1:A:325:LEU:HA   | 1:A:325:LEU:HD23 | 1.66                     | 0.43              |
| 2:B:210:LEU:HA   | 2:B:214:LEU:O    | 2.18                     | 0.43              |
| 1:C:416:PHE:CD1  | 1:C:417:VAL:N    | 2.86                     | 0.43              |
| 2:D:266:TRP:CD1  | 2:D:269:GLN:HE21 | 2.36                     | 0.43              |
| 2:D:301:LEU:HA   | 2:D:301:LEU:HD23 | 1.45                     | 0.43              |
| 2:B:28:GLU:HG3   | 2:B:32:LYS:HD3   | 1.99                     | 0.43              |
| 2:B:214:LEU:HD12 | 2:B:215:THR:N    | 2.33                     | 0.43              |
| 2:B:281:LYS:O    | 2:B:284:ARG:HG2  | 2.18                     | 0.43              |
| 2:B:305:GLU:O    | 2:B:309:ILE:HG13 | 2.18                     | 0.43              |
| 1:C:206:ARG:HH22 | 1:C:218:ASP:HB2  | 1.83                     | 0.43              |
| 2:D:20:LYS:HD3   | 2:D:55:PRO:O     | 2.18                     | 0.43              |
| 2:D:372:VAL:HG13 | 2:D:389:PHE:CE2  | 2.53                     | 0.43              |
| 1:A:278:GLN:HB2  | 1:A:299:ALA:HA   | 2.01                     | 0.43              |
| 1:A:361:HIS:ND1  | 1:A:513:SER:OG   | 2.38                     | 0.43              |
| 1:C:226:PRO:HB2  | 1:C:233:GLU:HG2  | 2.00                     | 0.43              |
| 2:B:82:LYS:HA    | 2:B:85:GLN:HB2   | 2.01                     | 0.43              |
| 1:C:21:VAL:HG23  | 1:C:57:ASN:O     | 2.19                     | 0.43              |
| 2:D:47:ILE:HD12  | 2:D:144:TYR:CD2  | 2.53                     | 0.43              |
| 2:D:113:ASP:HB2  | 2:D:214:LEU:HD12 | 2.00                     | 0.43              |
| 4:P:817:DG:C6    | 4:P:818:DC:C4    | 3.07                     | 0.43              |
| 1:A:181:TYR:CE2  | 1:A:183:TYR:HB2  | 2.54                     | 0.43              |
| 2:B:82:LYS:C     | 2:B:85:GLN:H     | 2.27                     | 0.43              |
| 2:D:81:ASN:HB3   | 2:D:154:LYS:HD3  | 2.00                     | 0.43              |
| 2:D:114:ALA:N    | 2:D:214:LEU:HD13 | 2.33                     | 0.43              |
| 2:D:422:LEU:C    | 2:D:422:LEU:CD1  | 2.85                     | 0.43              |
| 4:P:806:DT:H2'   | 4:P:807:DC:C6    | 2.53                     | 0.43              |
| 1:A:544:GLY:HA2  | 1:A:547:GLN:HB2  | 2.01                     | 0.43              |
| 2:B:115:TYR:HD1  | 2:B:115:TYR:H    | 1.65                     | 0.43              |
| 2:D:75:VAL:HB    | 2:D:77:PHE:CE2   | 2.54                     | 0.43              |
| 2:D:335:GLY:HA2  | 2:D:367:GLN:HE22 | 1.84                     | 0.43              |
| 1:A:542:ILE:HG12 | 2:B:283:LEU:CD1  | 2.49                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:171:PHE:CZ   | 1:C:205:LEU:HB2  | 2.54                     | 0.43              |
| 2:D:68:SER:HA    | 2:D:70:LYS:HZ1   | 1.84                     | 0.43              |
| 1:A:22:LYS:HG2   | 1:A:23:GLN:N     | 2.34                     | 0.43              |
| 1:A:104:LYS:HE2  | 1:A:104:LYS:HB2  | 1.79                     | 0.43              |
| 1:A:497:THR:O    | 1:A:535:TRP:HA   | 2.19                     | 0.43              |
| 2:B:365:VAL:HG11 | 2:B:401:TRP:HB2  | 2.01                     | 0.43              |
| 1:C:205:LEU:O    | 1:C:205:LEU:HG   | 2.17                     | 0.43              |
| 1:C:463:ARG:C    | 1:C:464:GLN:HG2  | 2.43                     | 0.43              |
| 1:A:224:GLU:N    | 1:A:225:PRO:HD2  | 2.34                     | 0.42              |
| 1:A:259:LYS:HG3  | 4:P:819:DG:OP1   | 2.18                     | 0.42              |
| 2:B:120:LEU:HD13 | 2:B:150:PRO:HD3  | 2.01                     | 0.42              |
| 1:C:524:GLN:HA   | 1:C:524:GLN:HE21 | 1.84                     | 0.42              |
| 1:A:128:THR:HG21 | 1:A:146:TYR:HD2  | 1.83                     | 0.42              |
| 2:B:41:MET:HG2   | 2:B:46:LYS:HD3   | 2.01                     | 0.42              |
| 4:P:815:DG:N3    | 4:P:816:DG:C8    | 2.87                     | 0.42              |
| 1:A:34:LEU:HD22  | 1:A:73:LYS:NZ    | 2.33                     | 0.42              |
| 1:A:88:TRP:CZ2   | 2:B:57:ASN:HB2   | 2.54                     | 0.42              |
| 2:B:239:TRP:CZ3  | 2:B:378:GLU:HB3  | 2.54                     | 0.42              |
| 2:D:111:VAL:HG22 | 2:D:185:ASP:O    | 2.19                     | 0.42              |
| 2:B:172:LYS:HE2  | 2:B:180:ILE:HB   | 2.01                     | 0.42              |
| 1:C:35:VAL:HG23  | 1:C:134:SER:CB   | 2.49                     | 0.42              |
| 1:C:124:PHE:O    | 1:C:125:ARG:C    | 2.62                     | 0.42              |
| 1:A:87:PHE:HE2   | 1:A:154:LYS:HB2  | 1.85                     | 0.42              |
| 1:A:94:ILE:CD1   | 1:A:230:MET:CE   | 2.97                     | 0.42              |
| 1:A:95:PRO:HA    | 2:B:136:ASN:O    | 2.20                     | 0.42              |
| 1:C:175:ASN:HB3  | 1:C:178:ILE:HD13 | 2.00                     | 0.42              |
| 2:D:325:LEU:HB2  | 2:D:387:PRO:HA   | 2.01                     | 0.42              |
| 1:A:43:LYS:HD3   | 1:A:43:LYS:HA    | 1.63                     | 0.42              |
| 1:A:433:PRO:HD3  | 1:A:532:TYR:CZ   | 2.55                     | 0.42              |
| 1:C:324:ASP:OD2  | 1:C:388:LYS:NZ   | 2.47                     | 0.42              |
| 1:C:479:LEU:HB2  | 1:C:517:LEU:HD21 | 2.00                     | 0.42              |
| 2:D:34:LEU:HD23  | 2:D:34:LEU:HA    | 1.78                     | 0.42              |
| 2:D:149:LEU:HA   | 2:D:150:PRO:HD3  | 1.80                     | 0.42              |
| 1:A:406:TRP:HH2  | 2:B:418:ASN:CB   | 2.33                     | 0.42              |
| 2:B:319:TYR:CD2  | 2:B:383:TRP:HD1  | 2.38                     | 0.42              |
| 1:C:279:LEU:HD23 | 1:C:279:LEU:HA   | 1.72                     | 0.42              |
| 1:C:323:LYS:HE2  | 1:C:323:LYS:HB3  | 1.51                     | 0.42              |
| 1:A:550:LYS:CG   | 1:A:551:LEU:N    | 2.82                     | 0.42              |
| 2:B:160:PHE:O    | 2:B:160:PHE:CD1  | 2.73                     | 0.42              |
| 2:D:328:GLU:HG3  | 2:D:390:LYS:HG3  | 2.02                     | 0.42              |
| 1:A:429:LEU:HD11 | 1:A:506:ILE:HG22 | 2.02                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:370:GLU:HG3  | 2:B:374:LYS:HD2  | 2.02                     | 0.42              |
| 1:A:276:VAL:HG12 | 1:A:353:LYS:NZ   | 2.35                     | 0.42              |
| 1:A:454:LYS:HG3  | 1:A:552:VAL:HG13 | 2.02                     | 0.42              |
| 2:B:19:PRO:HG3   | 2:B:80:LEU:HB2   | 2.02                     | 0.42              |
| 2:B:33:ALA:O     | 2:B:37:ILE:HD12  | 2.20                     | 0.42              |
| 2:B:248:GLU:HG2  | 2:B:307:ARG:HH12 | 1.85                     | 0.42              |
| 2:B:257:ILE:H    | 2:B:257:ILE:HG12 | 1.66                     | 0.42              |
| 1:C:363:ASN:OD1  | 1:C:363:ASN:C    | 2.63                     | 0.42              |
| 1:C:475:GLN:CD   | 4:F:809:DC:H5'   | 2.45                     | 0.42              |
| 2:B:132:ILE:HB   | 2:B:142:ILE:HB   | 2.02                     | 0.41              |
| 1:C:63:ILE:H     | 1:C:74:LEU:CD1   | 2.33                     | 0.41              |
| 1:C:153:TRP:CD1  | 1:C:154:LYS:H    | 2.38                     | 0.41              |
| 1:C:399:GLU:O    | 1:C:403:THR:HG23 | 2.20                     | 0.41              |
| 1:C:433:PRO:HD3  | 1:C:532:TYR:CZ   | 2.55                     | 0.41              |
| 1:C:551:LEU:HD23 | 1:C:551:LEU:HA   | 1.70                     | 0.41              |
| 2:D:128:THR:OG1  | 2:D:146:TYR:HB2  | 2.20                     | 0.41              |
| 2:D:303:LEU:HG   | 2:D:307:ARG:NH1  | 2.35                     | 0.41              |
| 2:D:395:LYS:NZ   | 4:F:813:DT:OP1   | 2.32                     | 0.41              |
| 4:F:807:DC:H2''  | 4:F:808:DC:O5'   | 2.19                     | 0.41              |
| 1:A:288:ALA:HB3  | 1:A:291:GLU:HG3  | 2.02                     | 0.41              |
| 1:A:448:ARG:HE   | 1:A:448:ARG:HB2  | 1.52                     | 0.41              |
| 2:B:153:TRP:CZ2  | 2:B:155:GLY:HA3  | 2.55                     | 0.41              |
| 2:D:10:VAL:HG13  | 2:D:87:PHE:CD1   | 2.56                     | 0.41              |
| 2:D:203:GLU:O    | 2:D:207:GLN:HG2  | 2.20                     | 0.41              |
| 3:T:720:G:C4     | 3:T:721:G:C8     | 3.08                     | 0.41              |
| 1:A:60:VAL:HA    | 1:A:76:ASP:HB3   | 2.01                     | 0.41              |
| 2:B:154:LYS:HG2  | 2:B:184:MET:SD   | 2.61                     | 0.41              |
| 2:B:171:PHE:CE2  | 2:B:205:LEU:HB2  | 2.55                     | 0.41              |
| 2:B:206:ARG:NH1  | 2:B:232:TYR:OH   | 2.53                     | 0.41              |
| 2:B:252:TRP:CZ3  | 2:B:260:LEU:HD22 | 2.54                     | 0.41              |
| 2:B:265:ASN:O    | 2:B:268:SER:OG   | 2.31                     | 0.41              |
| 1:C:399:GLU:HA   | 1:C:402:TRP:CD1  | 2.56                     | 0.41              |
| 1:C:434:ILE:HG13 | 1:C:494:ASN:OD1  | 2.20                     | 0.41              |
| 2:B:12:LEU:HD12  | 2:B:124:PHE:HE1  | 1.84                     | 0.41              |
| 2:B:167:ILE:HG23 | 2:B:212:TRP:CG   | 2.56                     | 0.41              |
| 2:B:209:LEU:O    | 2:B:214:LEU:N    | 2.53                     | 0.41              |
| 1:C:167:ILE:HG22 | 1:C:208:HIS:HE1  | 1.85                     | 0.41              |
| 4:P:809:DC:C6    | 4:P:810:DT:C7    | 3.04                     | 0.41              |
| 4:P:810:DT:C2    | 4:P:811:DG:N7    | 2.89                     | 0.41              |
| 4:P:814:DC:H2''  | 4:P:815:DG:H8    | 1.85                     | 0.41              |
| 1:A:84:THR:HG23  | 1:A:124:PHE:CZ   | 2.55                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:128:THR:HG21 | 1:A:146:TYR:CB   | 2.29                     | 0.41              |
| 1:A:277:ARG:HB2  | 1:A:336:GLN:CD   | 2.45                     | 0.41              |
| 2:B:396:GLU:OE2  | 2:B:396:GLU:N    | 2.50                     | 0.41              |
| 2:D:209:LEU:HB3  | 2:D:214:LEU:CD2  | 2.39                     | 0.41              |
| 2:D:308:GLU:O    | 2:D:311:LYS:HB2  | 2.19                     | 0.41              |
| 4:P:809:DC:C6    | 4:P:810:DT:H71   | 2.55                     | 0.41              |
| 1:C:319:TYR:CZ   | 1:C:321:PRO:HA   | 2.56                     | 0.41              |
| 2:D:402:TRP:CG   | 2:D:403:THR:N    | 2.88                     | 0.41              |
| 1:A:540:LYS:HA   | 1:A:540:LYS:HD3  | 1.70                     | 0.41              |
| 2:B:249:LYS:HB2  | 2:B:252:TRP:CZ2  | 2.54                     | 0.41              |
| 2:B:421:PRO:HB3  | 2:B:424:LYS:CB   | 2.24                     | 0.41              |
| 1:C:12:LEU:HG    | 1:C:124:PHE:HE2  | 1.85                     | 0.41              |
| 1:C:108:VAL:HG22 | 1:C:188:TYR:CD2  | 2.56                     | 0.41              |
| 1:C:118:VAL:HA   | 1:C:119:PRO:HD2  | 1.63                     | 0.41              |
| 2:D:112:GLY:O    | 2:D:115:TYR:HB2  | 2.21                     | 0.41              |
| 2:D:319:TYR:CD2  | 2:D:383:TRP:HD1  | 2.38                     | 0.41              |
| 2:B:252:TRP:HB3  | 2:B:257:ILE:CD1  | 2.50                     | 0.41              |
| 1:C:460:ASN:HA   | 2:D:286:THR:HG22 | 2.01                     | 0.41              |
| 2:D:317:VAL:O    | 2:D:317:VAL:CG2  | 2.63                     | 0.41              |
| 1:A:434:ILE:HD11 | 1:A:530:LYS:HB3  | 1.97                     | 0.41              |
| 1:A:460:ASN:HA   | 2:B:286:THR:O    | 2.21                     | 0.41              |
| 1:C:417:VAL:O    | 1:C:417:VAL:CG1  | 2.69                     | 0.41              |
| 2:D:56:TYR:HD2   | 2:D:126:LYS:O    | 2.04                     | 0.41              |
| 2:D:324:ASP:O    | 2:D:343:GLN:HG3  | 2.20                     | 0.41              |
| 1:A:194:GLU:OE2  | 1:A:197:GLN:HB2  | 2.21                     | 0.41              |
| 1:A:419:THR:O    | 1:A:420:PRO:C    | 2.63                     | 0.41              |
| 2:B:104:LYS:HB2  | 2:B:192:ASP:HA   | 2.03                     | 0.41              |
| 2:B:189:VAL:HG21 | 2:B:205:LEU:HD23 | 2.03                     | 0.41              |
| 1:C:139:THR:HB   | 1:C:140:PRO:CD   | 2.50                     | 0.41              |
| 2:D:163:SER:O    | 2:D:167:ILE:HG22 | 2.21                     | 0.41              |
| 1:A:96:HIS:H     | 2:B:136:ASN:HD21 | 1.68                     | 0.40              |
| 1:A:100:LEU:O    | 1:A:318:TYR:HB3  | 2.22                     | 0.40              |
| 1:A:326:ILE:HB   | 1:A:342:TYR:CE1  | 2.55                     | 0.40              |
| 1:A:491:LEU:HD23 | 1:A:491:LEU:HA   | 1.87                     | 0.40              |
| 2:B:109:LEU:HD22 | 2:B:206:ARG:NH1  | 2.36                     | 0.40              |
| 1:C:196:GLY:HA2  | 1:C:199:ARG:HD2  | 2.02                     | 0.40              |
| 2:D:103:LYS:HD3  | 2:D:192:ASP:OD1  | 2.21                     | 0.40              |
| 2:D:357:MET:HE2  | 2:D:357:MET:HB3  | 1.99                     | 0.40              |
| 4:F:809:DC:C6    | 4:F:810:DT:C7    | 3.04                     | 0.40              |
| 1:A:266:TRP:O    | 1:A:269:GLN:HG2  | 2.22                     | 0.40              |
| 1:A:537:PRO:O    | 1:A:542:ILE:HD12 | 2.21                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:270:ILE:HG13 | 2:B:346:PHE:CD1  | 2.56                     | 0.40              |
| 2:B:423:VAL:O    | 2:B:423:VAL:CG1  | 2.69                     | 0.40              |
| 1:A:218:ASP:C    | 1:A:220:LYS:H    | 2.29                     | 0.40              |
| 2:B:130:PHE:CZ   | 2:B:144:TYR:HB2  | 2.56                     | 0.40              |
| 1:A:46:LYS:O     | 1:A:47:ILE:HG13  | 2.22                     | 0.40              |
| 1:A:545:ASN:O    | 1:A:548:VAL:HG12 | 2.21                     | 0.40              |
| 2:B:282:LEU:HD23 | 2:B:282:LEU:HA   | 1.74                     | 0.40              |
| 2:B:421:PRO:CB   | 2:B:424:LYS:CB   | 2.92                     | 0.40              |
| 1:C:47:ILE:HG21  | 1:C:144:TYR:CE2  | 2.56                     | 0.40              |
| 1:C:81:ASN:HB3   | 1:C:154:LYS:HG3  | 2.02                     | 0.40              |
| 1:C:214:LEU:HA   | 1:C:214:LEU:HD23 | 1.51                     | 0.40              |
| 1:C:459:THR:CG2  | 1:C:461:LYS:H    | 2.34                     | 0.40              |
| 4:P:814:DC:H2''  | 4:P:815:DG:C8    | 2.57                     | 0.40              |
| 1:A:325:LEU:HD21 | 1:A:349:LEU:HD13 | 2.03                     | 0.40              |
| 1:A:543:GLY:HA2  | 2:B:285:GLY:O    | 2.21                     | 0.40              |
| 1:C:55:PRO:HA    | 1:C:143:ARG:NH2  | 2.36                     | 0.40              |
| 1:C:380:ILE:O    | 1:C:381:VAL:C    | 2.63                     | 0.40              |
| 2:D:57:ASN:HA    | 2:D:129:ALA:O    | 2.21                     | 0.40              |
| 2:D:87:PHE:O     | 2:D:91:GLN:HB3   | 2.21                     | 0.40              |
| 2:D:423:VAL:CG1  | 2:D:423:VAL:O    | 2.70                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

| Mol | Chain | Analysed        | Favoured   | Allowed | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|---------|----------|-------------|-----|
| 1   | A     | 553/556 (100%)  | 523 (95%)  | 30 (5%) | 0        | 100         | 100 |
| 1   | C     | 553/556 (100%)  | 522 (94%)  | 31 (6%) | 0        | 100         | 100 |
| 2   | B     | 408/428 (95%)   | 396 (97%)  | 12 (3%) | 0        | 100         | 100 |
| 2   | D     | 408/428 (95%)   | 398 (98%)  | 10 (2%) | 0        | 100         | 100 |
| All | All   | 1922/1968 (98%) | 1839 (96%) | 83 (4%) | 0        | 100         | 100 |

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|----------|-------------|----|
| 1   | A     | 495/497 (100%)  | 449 (91%)  | 46 (9%)  | 8           | 27 |
| 1   | C     | 494/497 (99%)   | 453 (92%)  | 41 (8%)  | 10          | 32 |
| 2   | B     | 374/390 (96%)   | 338 (90%)  | 36 (10%) | 8           | 26 |
| 2   | D     | 374/390 (96%)   | 338 (90%)  | 36 (10%) | 8           | 26 |
| All | All   | 1737/1774 (98%) | 1578 (91%) | 159 (9%) | 8           | 27 |

All (159) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 2   | ILE  |
| 1   | A     | 3   | SER  |
| 1   | A     | 5   | ILE  |
| 1   | A     | 7   | THR  |
| 1   | A     | 17  | ASP  |
| 1   | A     | 36  | GLU  |
| 1   | A     | 39  | THR  |
| 1   | A     | 66  | LYS  |
| 1   | A     | 67  | ASP  |
| 1   | A     | 74  | LEU  |
| 1   | A     | 94  | ILE  |
| 1   | A     | 107 | THR  |
| 1   | A     | 109 | LEU  |
| 1   | A     | 110 | ASP  |
| 1   | A     | 113 | ASP  |
| 1   | A     | 118 | VAL  |
| 1   | A     | 122 | GLU  |
| 1   | A     | 123 | ASP  |
| 1   | A     | 130 | PHE  |
| 1   | A     | 137 | ASN  |
| 1   | A     | 182 | GLN  |
| 1   | A     | 189 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 195 | ILE  |
| 1   | A     | 221 | HIS  |
| 1   | A     | 258 | CYS  |
| 1   | A     | 292 | VAL  |
| 1   | A     | 297 | GLU  |
| 1   | A     | 308 | GLU  |
| 1   | A     | 314 | VAL  |
| 1   | A     | 317 | VAL  |
| 1   | A     | 323 | LYS  |
| 1   | A     | 325 | LEU  |
| 1   | A     | 357 | MET  |
| 1   | A     | 361 | HIS  |
| 1   | A     | 373 | GLN  |
| 1   | A     | 394 | GLN  |
| 1   | A     | 399 | GLU  |
| 1   | A     | 400 | THR  |
| 1   | A     | 417 | VAL  |
| 1   | A     | 420 | PRO  |
| 1   | A     | 442 | VAL  |
| 1   | A     | 473 | THR  |
| 1   | A     | 474 | ASN  |
| 1   | A     | 506 | ILE  |
| 1   | A     | 507 | GLN  |
| 1   | A     | 529 | GLU  |
| 2   | B     | 13  | LYS  |
| 2   | B     | 35  | VAL  |
| 2   | B     | 37  | ILE  |
| 2   | B     | 47  | ILE  |
| 2   | B     | 48  | SER  |
| 2   | B     | 63  | ILE  |
| 2   | B     | 94  | ILE  |
| 2   | B     | 103 | LYS  |
| 2   | B     | 115 | TYR  |
| 2   | B     | 120 | LEU  |
| 2   | B     | 144 | TYR  |
| 2   | B     | 163 | SER  |
| 2   | B     | 166 | LYS  |
| 2   | B     | 178 | ILE  |
| 2   | B     | 180 | ILE  |
| 2   | B     | 184 | MET  |
| 2   | B     | 195 | ILE  |
| 2   | B     | 201 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 208 | HIS  |
| 2   | B     | 210 | LEU  |
| 2   | B     | 232 | TYR  |
| 2   | B     | 240 | THR  |
| 2   | B     | 241 | VAL  |
| 2   | B     | 245 | VAL  |
| 2   | B     | 250 | ASP  |
| 2   | B     | 282 | LEU  |
| 2   | B     | 293 | ILE  |
| 2   | B     | 296 | THR  |
| 2   | B     | 305 | GLU  |
| 2   | B     | 308 | GLU  |
| 2   | B     | 324 | ASP  |
| 2   | B     | 366 | LYS  |
| 2   | B     | 374 | LYS  |
| 2   | B     | 378 | GLU  |
| 2   | B     | 388 | LYS  |
| 2   | B     | 399 | GLU  |
| 1   | C     | 2   | ILE  |
| 1   | C     | 3   | SER  |
| 1   | C     | 16  | MET  |
| 1   | C     | 17  | ASP  |
| 1   | C     | 21  | VAL  |
| 1   | C     | 43  | LYS  |
| 1   | C     | 47  | ILE  |
| 1   | C     | 50  | ILE  |
| 1   | C     | 84  | THR  |
| 1   | C     | 86  | ASP  |
| 1   | C     | 113 | ASP  |
| 1   | C     | 140 | PRO  |
| 1   | C     | 144 | TYR  |
| 1   | C     | 164 | MET  |
| 1   | C     | 173 | LYS  |
| 1   | C     | 182 | GLN  |
| 1   | C     | 189 | VAL  |
| 1   | C     | 205 | LEU  |
| 1   | C     | 210 | LEU  |
| 1   | C     | 216 | THR  |
| 1   | C     | 245 | VAL  |
| 1   | C     | 258 | CYS  |
| 1   | C     | 298 | GLU  |
| 1   | C     | 305 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 325 | LEU  |
| 1   | C     | 357 | MET  |
| 1   | C     | 373 | GLN  |
| 1   | C     | 375 | ILE  |
| 1   | C     | 377 | THR  |
| 1   | C     | 386 | THR  |
| 1   | C     | 407 | GLN  |
| 1   | C     | 425 | LEU  |
| 1   | C     | 434 | ILE  |
| 1   | C     | 449 | GLU  |
| 1   | C     | 459 | THR  |
| 1   | C     | 463 | ARG  |
| 1   | C     | 472 | THR  |
| 1   | C     | 473 | THR  |
| 1   | C     | 482 | ILE  |
| 1   | C     | 533 | LEU  |
| 1   | C     | 552 | VAL  |
| 2   | D     | 5   | ILE  |
| 2   | D     | 36  | GLU  |
| 2   | D     | 38  | CYS  |
| 2   | D     | 39  | THR  |
| 2   | D     | 47  | ILE  |
| 2   | D     | 70  | LYS  |
| 2   | D     | 80  | LEU  |
| 2   | D     | 101 | LYS  |
| 2   | D     | 108 | VAL  |
| 2   | D     | 113 | ASP  |
| 2   | D     | 123 | ASP  |
| 2   | D     | 167 | ILE  |
| 2   | D     | 175 | ASN  |
| 2   | D     | 189 | VAL  |
| 2   | D     | 194 | GLU  |
| 2   | D     | 203 | GLU  |
| 2   | D     | 211 | ARG  |
| 2   | D     | 212 | TRP  |
| 2   | D     | 214 | LEU  |
| 2   | D     | 215 | THR  |
| 2   | D     | 234 | LEU  |
| 2   | D     | 245 | VAL  |
| 2   | D     | 249 | LYS  |
| 2   | D     | 287 | LYS  |
| 2   | D     | 293 | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | D     | 298 | GLU  |
| 2   | D     | 303 | LEU  |
| 2   | D     | 343 | GLN  |
| 2   | D     | 344 | GLU  |
| 2   | D     | 357 | MET  |
| 2   | D     | 362 | THR  |
| 2   | D     | 390 | LYS  |
| 2   | D     | 403 | THR  |
| 2   | D     | 419 | THR  |
| 2   | D     | 427 | TYR  |
| 2   | D     | 428 | GLN  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 147 | ASN  |
| 1   | A     | 373 | GLN  |
| 1   | A     | 394 | GLN  |
| 1   | A     | 407 | GLN  |
| 1   | A     | 524 | GLN  |
| 2   | B     | 161 | GLN  |
| 2   | B     | 258 | GLN  |
| 2   | B     | 361 | HIS  |
| 1   | C     | 222 | GLN  |
| 1   | C     | 474 | ASN  |
| 1   | C     | 500 | GLN  |
| 1   | C     | 520 | GLN  |
| 1   | C     | 545 | ASN  |
| 1   | C     | 547 | GLN  |
| 2   | D     | 54  | ASN  |
| 2   | D     | 145 | GLN  |
| 2   | D     | 242 | GLN  |
| 2   | D     | 269 | GLN  |
| 2   | D     | 428 | GLN  |

### 5.3.3 RNA ⓘ

| Mol | Chain | Analysed    | Backbone Outliers | Pucker Outliers |
|-----|-------|-------------|-------------------|-----------------|
| 3   | E     | 18/27 (66%) | 8 (44%)           | 3 (16%)         |
| 3   | T     | 19/27 (70%) | 10 (52%)          | 4 (21%)         |

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| Mol | Chain | Analysed    | Backbone Outliers | Pucker Outliers |
|-----|-------|-------------|-------------------|-----------------|
| All | All   | 37/54 (68%) | 18 (48%)          | 7 (18%)         |

All (18) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | T     | 708 | G    |
| 3   | T     | 712 | C    |
| 3   | T     | 715 | A    |
| 3   | T     | 716 | A    |
| 3   | T     | 717 | C    |
| 3   | T     | 718 | A    |
| 3   | T     | 720 | G    |
| 3   | T     | 721 | G    |
| 3   | T     | 724 | U    |
| 3   | T     | 725 | G    |
| 3   | E     | 712 | C    |
| 3   | E     | 714 | G    |
| 3   | E     | 715 | A    |
| 3   | E     | 717 | C    |
| 3   | E     | 720 | G    |
| 3   | E     | 721 | G    |
| 3   | E     | 723 | C    |
| 3   | E     | 724 | U    |

All (7) RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | T     | 711 | C    |
| 3   | T     | 714 | G    |
| 3   | T     | 719 | G    |
| 3   | T     | 720 | G    |
| 3   | E     | 711 | C    |
| 3   | E     | 714 | G    |
| 3   | E     | 720 | G    |

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

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

| Mol | Type | Chain | Res | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |     |      | Counts       | RMSZ | # $ Z  > 2$ | Counts      | RMSZ | # $ Z  > 2$ |
| 5   | NVP  | A     | 901 | -    | 23,23,23     | 1.57 | 6 (26%)     | 34,34,34    | 4.50 | 18 (52%)    |
| 5   | NVP  | C     | 901 | -    | 23,23,23     | 1.55 | 5 (21%)     | 34,34,34    | 4.50 | 20 (58%)    |

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   |
|-----|------|-------|-----|------|---------|----------|---------|
| 5   | NVP  | A     | 901 | -    | -       | 2/4/6/6  | 0/4/4/4 |
| 5   | NVP  | C     | 901 | -    | -       | 0/4/6/6  | 0/4/4/4 |

All (11) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 5   | A     | 901 | NVP  | C2-N3   | 3.31  | 1.40        | 1.34     |
| 5   | C     | 901 | NVP  | C15-N14 | 3.27  | 1.40        | 1.34     |
| 5   | C     | 901 | NVP  | C2-N3   | 2.87  | 1.39        | 1.34     |
| 5   | C     | 901 | NVP  | C13-N14 | 2.69  | 1.40        | 1.34     |
| 5   | A     | 901 | NVP  | C15-N14 | 2.67  | 1.39        | 1.34     |
| 5   | C     | 901 | NVP  | C4-N3   | 2.59  | 1.40        | 1.34     |
| 5   | A     | 901 | NVP  | C13-N14 | 2.53  | 1.39        | 1.34     |
| 5   | A     | 901 | NVP  | C4-N3   | 2.47  | 1.39        | 1.34     |
| 5   | A     | 901 | NVP  | C10-C15 | -2.21 | 1.37        | 1.40     |
| 5   | C     | 901 | NVP  | C10-C9  | 2.14  | 1.52        | 1.49     |
| 5   | A     | 901 | NVP  | C7-C6   | 2.06  | 1.43        | 1.40     |

All (38) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 5   | C     | 901 | NVP  | C7-C2-N1    | 18.19 | 127.13      | 120.14   |
| 5   | A     | 901 | NVP  | C7-C2-N1    | 18.05 | 127.07      | 120.14   |
| 5   | A     | 901 | NVP  | C7-N8-C9    | -8.81 | 121.02      | 128.29   |
| 5   | C     | 901 | NVP  | N3-C2-N1    | -7.38 | 111.09      | 116.67   |
| 5   | C     | 901 | NVP  | C6-C7-N8    | -6.30 | 113.60      | 119.18   |
| 5   | A     | 901 | NVP  | CB-CA-N1    | 5.88  | 119.57      | 116.09   |
| 5   | C     | 901 | NVP  | C7-N8-C9    | -5.77 | 123.53      | 128.29   |
| 5   | C     | 901 | NVP  | OE-C9-N8    | -5.32 | 115.19      | 120.38   |
| 5   | A     | 901 | NVP  | C11-C10-C15 | 5.14  | 122.28      | 117.23   |
| 5   | C     | 901 | NVP  | N14-C15-N1  | -4.90 | 112.96      | 116.67   |
| 5   | A     | 901 | NVP  | C10-C9-N8   | 4.78  | 124.88      | 120.22   |
| 5   | A     | 901 | NVP  | N3-C2-N1    | -4.63 | 113.17      | 116.67   |
| 5   | C     | 901 | NVP  | C2-C7-N8    | 4.57  | 125.77      | 121.46   |
| 5   | C     | 901 | NVP  | CB-CA-N1    | 4.52  | 118.77      | 116.09   |
| 5   | A     | 901 | NVP  | C6-C7-C2    | 4.28  | 122.37      | 119.03   |
| 5   | C     | 901 | NVP  | C10-C9-N8   | 4.22  | 124.34      | 120.22   |
| 5   | C     | 901 | NVP  | C10-C15-N1  | 4.18  | 126.16      | 120.95   |
| 5   | A     | 901 | NVP  | OE-C9-N8    | -4.16 | 116.33      | 120.38   |
| 5   | A     | 901 | NVP  | CC-CA-N1    | -4.12 | 113.65      | 116.09   |
| 5   | C     | 901 | NVP  | C15-N1-CA   | 4.04  | 119.53      | 116.34   |
| 5   | A     | 901 | NVP  | C10-C15-N1  | 3.96  | 125.88      | 120.95   |
| 5   | C     | 901 | NVP  | C15-N1-C2   | 3.95  | 119.64      | 115.29   |
| 5   | C     | 901 | NVP  | C15-C10-C9  | 3.91  | 127.83      | 124.01   |
| 5   | A     | 901 | NVP  | CD-C6-C7    | 3.88  | 126.14      | 121.42   |
| 5   | A     | 901 | NVP  | C11-C10-C9  | -3.83 | 110.35      | 116.76   |
| 5   | A     | 901 | NVP  | N14-C15-N1  | -3.80 | 113.79      | 116.67   |
| 5   | A     | 901 | NVP  | C15-N1-CA   | 3.72  | 119.28      | 116.34   |
| 5   | A     | 901 | NVP  | C15-C10-C9  | 3.43  | 127.36      | 124.01   |
| 5   | A     | 901 | NVP  | C6-C7-N8    | -3.36 | 116.21      | 119.18   |
| 5   | C     | 901 | NVP  | C11-C10-C15 | 2.92  | 120.11      | 117.23   |
| 5   | C     | 901 | NVP  | C11-C10-C9  | -2.81 | 112.06      | 116.76   |
| 5   | C     | 901 | NVP  | CC-CA-N1    | -2.65 | 114.52      | 116.09   |
| 5   | C     | 901 | NVP  | C5-C4-N3    | -2.63 | 120.75      | 123.97   |
| 5   | C     | 901 | NVP  | C12-C13-N14 | -2.34 | 119.71      | 123.42   |
| 5   | C     | 901 | NVP  | C2-N1-CA    | -2.18 | 114.62      | 116.34   |
| 5   | A     | 901 | NVP  | C12-C13-N14 | -2.14 | 120.04      | 123.42   |
| 5   | A     | 901 | NVP  | CD-C6-C5    | -2.08 | 116.27      | 120.28   |
| 5   | C     | 901 | NVP  | C6-C7-C2    | 2.05  | 120.62      | 119.03   |

There are no chirality outliers.

All (2) torsion outliers are listed below:

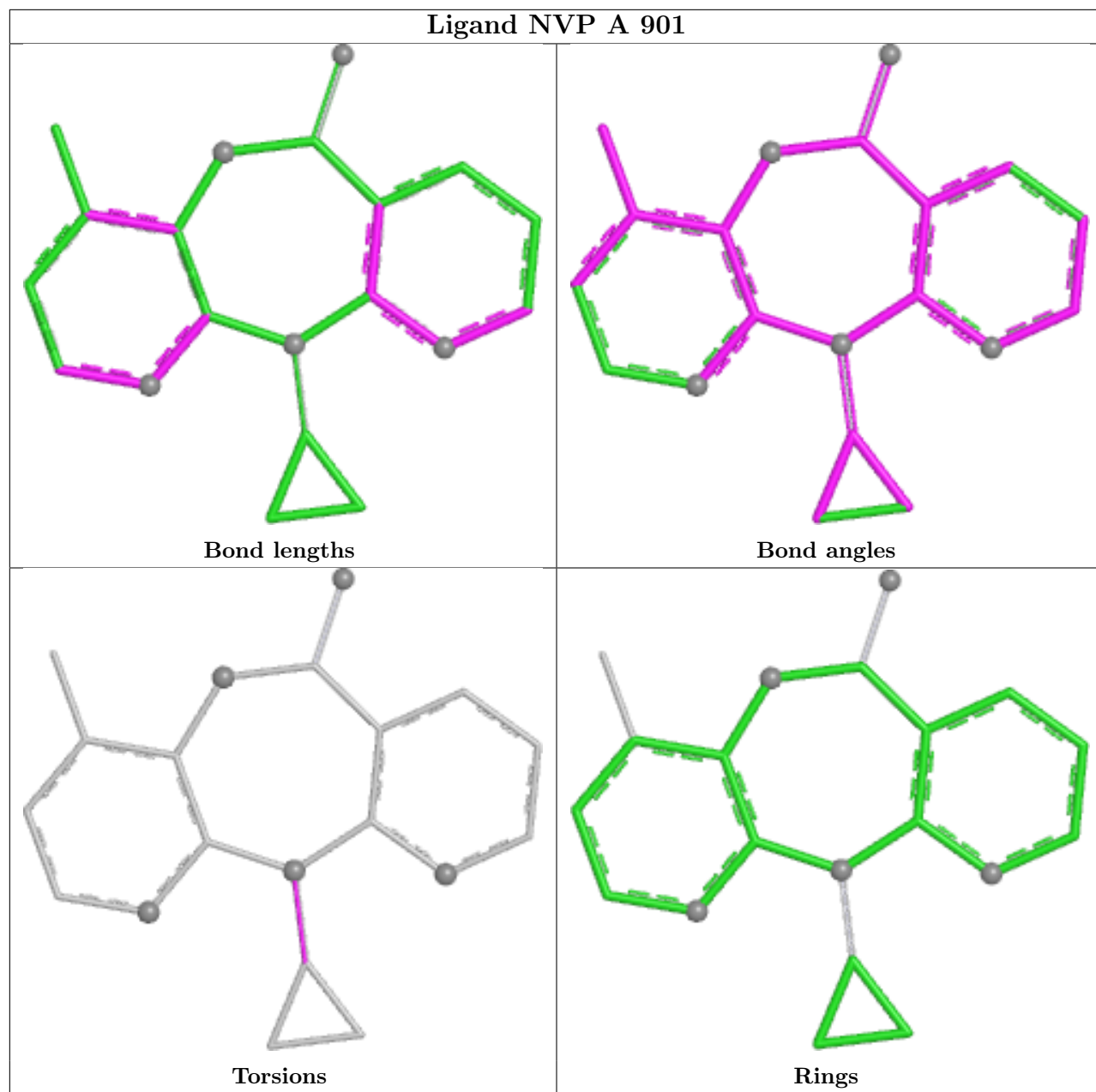
| Mol | Chain | Res | Type | Atoms        |
|-----|-------|-----|------|--------------|
| 5   | A     | 901 | NVP  | CC-CA-N1-C15 |
| 5   | A     | 901 | NVP  | CB-CA-N1-C15 |

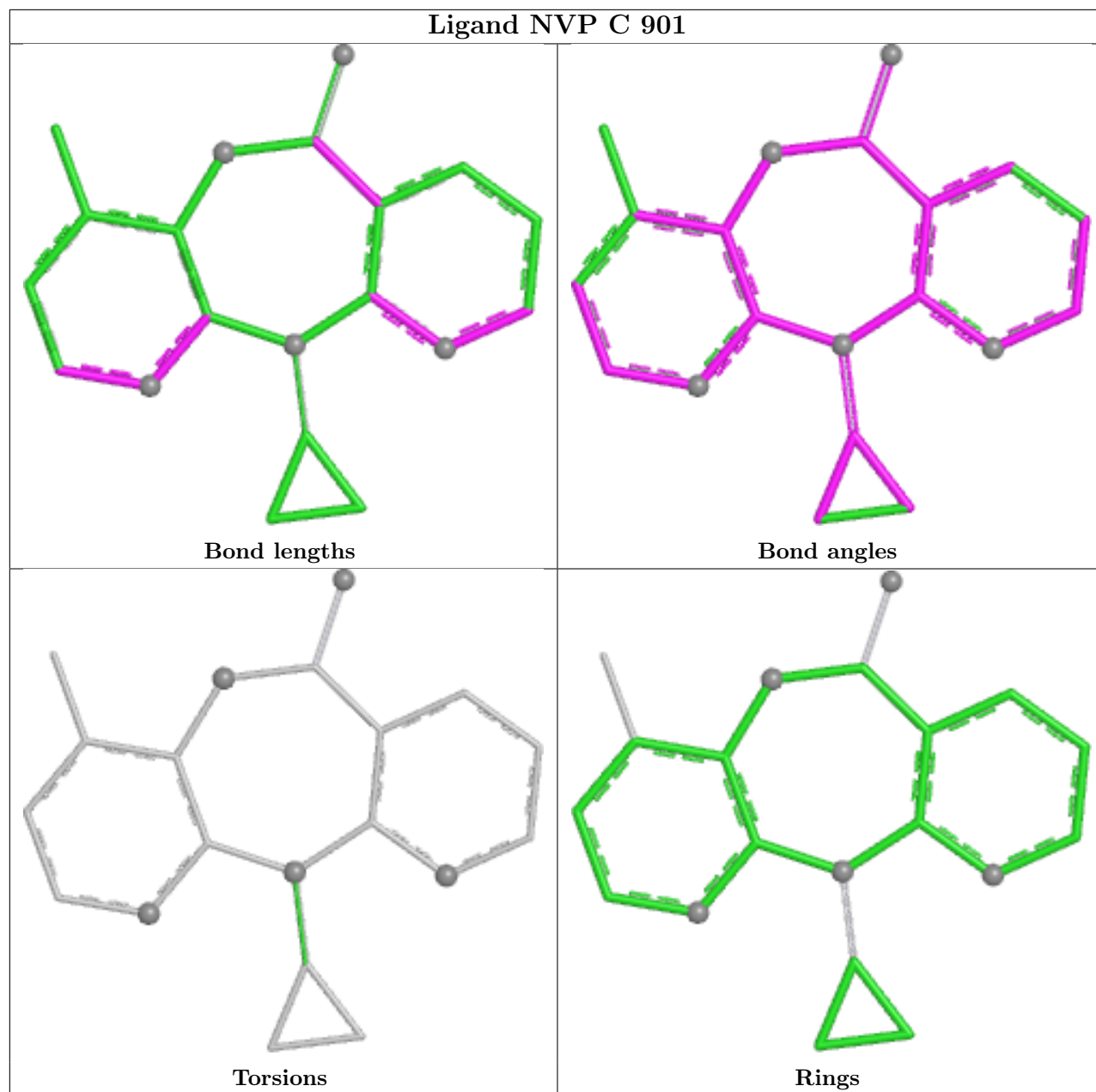
There are no ring outliers.

1 monomer is involved in 1 short contact:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 5   | C     | 901 | NVP  | 1       | 0            |

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





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2        | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|----------------|-----------------------|-------|
| 1   | A     | 555/556 (99%)   | 0.48   | 45 (8%) 18 15  | 17, 82, 185, 221      | 0     |
| 1   | C     | 555/556 (99%)   | 0.49   | 56 (10%) 12 10 | 13, 89, 191, 219      | 0     |
| 2   | B     | 412/428 (96%)   | 0.02   | 15 (3%) 46 38  | 18, 58, 108, 135      | 0     |
| 2   | D     | 412/428 (96%)   | 0.28   | 27 (6%) 24 19  | 20, 67, 119, 144      | 0     |
| 3   | E     | 19/27 (70%)     | 1.08   | 1 (5%) 32 25   | 130, 171, 195, 201    | 0     |
| 3   | T     | 20/27 (74%)     | 1.29   | 2 (10%) 12 10  | 123, 141, 184, 191    | 0     |
| 4   | F     | 19/21 (90%)     | 0.87   | 3 (15%) 5 4    | 91, 157, 195, 202     | 0     |
| 4   | P     | 19/21 (90%)     | 0.98   | 2 (10%) 11 10  | 85, 134, 175, 177     | 0     |
| All | All   | 2011/2064 (97%) | 0.37   | 151 (7%) 20 16 | 13, 73, 179, 221      | 0     |

All (151) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | A     | 132 | ILE  | 10.5 |
| 1   | A     | 133 | PRO  | 9.6  |
| 1   | A     | 60  | VAL  | 5.9  |
| 1   | C     | 30  | LYS  | 5.5  |
| 1   | C     | 33  | ALA  | 5.5  |
| 2   | D     | 360 | ALA  | 4.6  |
| 2   | B     | 214 | LEU  | 4.5  |
| 1   | A     | 26  | LEU  | 4.4  |
| 2   | B     | 88  | TRP  | 4.3  |
| 1   | A     | 33  | ALA  | 4.2  |
| 1   | A     | 544 | GLY  | 4.2  |
| 1   | C     | 63  | ILE  | 4.0  |
| 1   | C     | 31  | ILE  | 4.0  |
| 1   | A     | 27  | THR  | 3.9  |
| 1   | A     | 71  | TRP  | 3.9  |
| 2   | D     | 354 | TYR  | 3.7  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | C     | 90  | VAL  | 3.6  |
| 1   | A     | 131 | THR  | 3.5  |
| 2   | B     | 217 | PRO  | 3.5  |
| 2   | B     | 215 | THR  | 3.5  |
| 2   | D     | 90  | VAL  | 3.4  |
| 2   | D     | 232 | TYR  | 3.4  |
| 1   | A     | 62  | ALA  | 3.3  |
| 1   | C     | 91  | GLN  | 3.3  |
| 2   | B     | 231 | GLY  | 3.3  |
| 1   | C     | 92  | LEU  | 3.3  |
| 1   | A     | 551 | LEU  | 3.3  |
| 1   | C     | 257 | ILE  | 3.2  |
| 1   | A     | 135 | ILE  | 3.2  |
| 1   | C     | 60  | VAL  | 3.2  |
| 2   | D     | 231 | GLY  | 3.2  |
| 2   | D     | 215 | THR  | 3.1  |
| 1   | A     | 31  | ILE  | 3.1  |
| 1   | A     | 219 | LYS  | 3.1  |
| 1   | C     | 301 | LEU  | 3.1  |
| 2   | D     | 94  | ILE  | 3.1  |
| 1   | C     | 254 | VAL  | 3.0  |
| 1   | C     | 32  | LYS  | 3.0  |
| 2   | B     | 84  | THR  | 3.0  |
| 1   | A     | 61  | PHE  | 3.0  |
| 1   | A     | 92  | LEU  | 3.0  |
| 2   | B     | 87  | PHE  | 3.0  |
| 2   | D     | 179 | VAL  | 3.0  |
| 1   | C     | 255 | ASN  | 3.0  |
| 1   | C     | 59  | PRO  | 3.0  |
| 2   | D     | 212 | TRP  | 2.9  |
| 1   | A     | 142 | ILE  | 2.9  |
| 2   | D     | 422 | LEU  | 2.9  |
| 2   | B     | 85  | GLN  | 2.9  |
| 2   | B     | 86  | ASP  | 2.9  |
| 2   | D     | 208 | HIS  | 2.9  |
| 2   | D     | 419 | THR  | 2.9  |
| 1   | A     | 37  | ILE  | 2.9  |
| 2   | D     | 190 | GLY  | 2.9  |
| 1   | A     | 89  | GLU  | 2.9  |
| 1   | A     | 514 | GLU  | 2.9  |
| 1   | A     | 148 | VAL  | 2.8  |
| 1   | C     | 93  | GLY  | 2.8  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2   | D     | 217 | PRO  | 2.8  |
| 1   | C     | 234 | LEU  | 2.8  |
| 1   | A     | 553 | SER  | 2.8  |
| 1   | A     | 549 | ASP  | 2.8  |
| 1   | C     | 58  | THR  | 2.8  |
| 1   | C     | 71  | TRP  | 2.7  |
| 1   | C     | 135 | ILE  | 2.7  |
| 1   | C     | 299 | ALA  | 2.7  |
| 1   | A     | 128 | THR  | 2.7  |
| 2   | D     | 95  | PRO  | 2.7  |
| 1   | C     | 37  | ILE  | 2.7  |
| 1   | A     | 126 | LYS  | 2.7  |
| 1   | A     | 146 | TYR  | 2.7  |
| 3   | E     | 723 | C    | 2.6  |
| 1   | A     | 448 | ARG  | 2.6  |
| 3   | T     | 725 | G    | 2.6  |
| 1   | A     | 19  | PRO  | 2.6  |
| 1   | C     | 55  | PRO  | 2.6  |
| 1   | C     | 54  | ASN  | 2.6  |
| 1   | C     | 252 | TRP  | 2.5  |
| 1   | C     | 18  | GLY  | 2.5  |
| 1   | C     | 295 | LEU  | 2.5  |
| 1   | C     | 282 | LEU  | 2.5  |
| 1   | C     | 200 | THR  | 2.5  |
| 1   | C     | 133 | PRO  | 2.5  |
| 2   | B     | 89  | GLU  | 2.5  |
| 1   | A     | 554 | ALA  | 2.5  |
| 4   | F     | 816 | DG   | 2.5  |
| 2   | B     | 94  | ILE  | 2.5  |
| 1   | C     | 153 | TRP  | 2.5  |
| 1   | C     | 69  | THR  | 2.5  |
| 4   | P     | 817 | DG   | 2.5  |
| 1   | C     | 19  | PRO  | 2.4  |
| 2   | B     | 213 | GLY  | 2.4  |
| 1   | C     | 62  | ALA  | 2.4  |
| 1   | A     | 293 | ILE  | 2.4  |
| 1   | C     | 224 | GLU  | 2.4  |
| 1   | A     | 91  | GLN  | 2.4  |
| 1   | A     | 292 | VAL  | 2.4  |
| 1   | C     | 152 | GLY  | 2.4  |
| 1   | C     | 34  | LEU  | 2.4  |
| 2   | B     | 92  | LEU  | 2.4  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | A     | 202 | ILE  | 2.4  |
| 1   | A     | 545 | ASN  | 2.4  |
| 1   | A     | 130 | PHE  | 2.4  |
| 2   | D     | 109 | LEU  | 2.4  |
| 2   | D     | 361 | HIS  | 2.4  |
| 1   | C     | 131 | THR  | 2.3  |
| 4   | F     | 815 | DG   | 2.3  |
| 1   | A     | 140 | PRO  | 2.3  |
| 1   | C     | 202 | ILE  | 2.3  |
| 1   | C     | 0   | VAL  | 2.3  |
| 1   | C     | 124 | PHE  | 2.3  |
| 4   | F     | 817 | DG   | 2.3  |
| 2   | D     | 154 | LYS  | 2.3  |
| 2   | D     | 357 | MET  | 2.2  |
| 2   | D     | 426 | TRP  | 2.2  |
| 1   | A     | 254 | VAL  | 2.2  |
| 1   | C     | 4   | PRO  | 2.2  |
| 2   | B     | 420 | PRO  | 2.2  |
| 2   | D     | 92  | LEU  | 2.2  |
| 1   | C     | 132 | ILE  | 2.2  |
| 1   | A     | 0   | VAL  | 2.2  |
| 1   | A     | 548 | VAL  | 2.2  |
| 3   | T     | 707 | G    | 2.2  |
| 1   | C     | 136 | ASN  | 2.2  |
| 2   | D     | 284 | ARG  | 2.2  |
| 1   | A     | 134 | SER  | 2.2  |
| 1   | C     | 127 | TYR  | 2.2  |
| 1   | A     | 59  | PRO  | 2.2  |
| 1   | A     | 215 | THR  | 2.2  |
| 1   | C     | 126 | LYS  | 2.2  |
| 1   | C     | 144 | TYR  | 2.2  |
| 4   | P     | 816 | DG   | 2.2  |
| 1   | C     | 258 | CYS  | 2.1  |
| 2   | D     | 216 | THR  | 2.1  |
| 2   | D     | 167 | ILE  | 2.1  |
| 1   | A     | 552 | VAL  | 2.1  |
| 1   | C     | 193 | LEU  | 2.1  |
| 2   | D     | 425 | LEU  | 2.1  |
| 1   | C     | 46  | LYS  | 2.1  |
| 1   | C     | 25  | PRO  | 2.1  |
| 2   | B     | 196 | GLY  | 2.1  |
| 2   | D     | 193 | LEU  | 2.0  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | C     | 549 | ASP  | 2.0  |
| 1   | C     | 266 | TRP  | 2.0  |
| 2   | D     | 423 | VAL  | 2.0  |
| 1   | C     | 140 | PRO  | 2.0  |
| 1   | C     | 51  | GLY  | 2.0  |
| 1   | A     | 237 | ASP  | 2.0  |
| 1   | A     | 30  | LYS  | 2.0  |
| 1   | C     | 42  | GLU  | 2.0  |
| 1   | C     | 146 | TYR  | 2.0  |

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

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

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

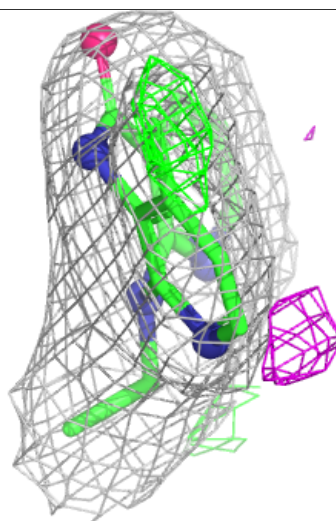
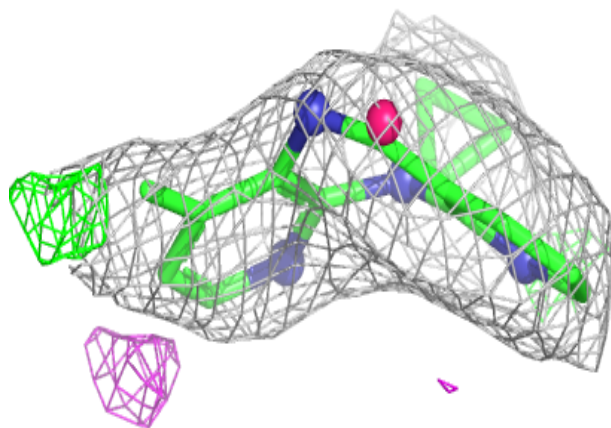
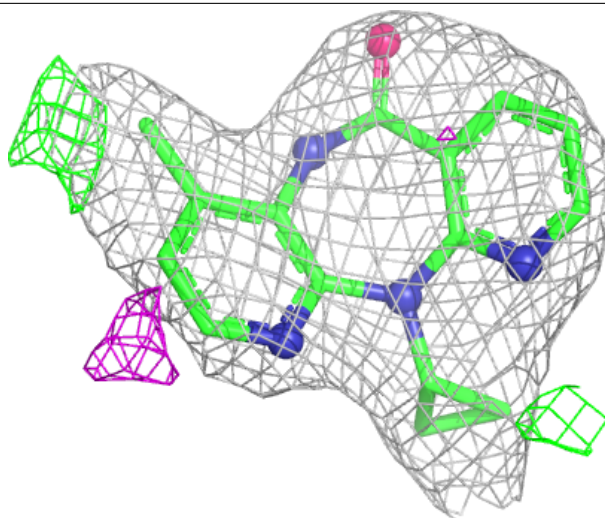
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 5   | NVP  | A     | 901 | 20/20 | 0.90 | 0.13 | 49,56,65,67                 | 0     |
| 5   | NVP  | C     | 901 | 20/20 | 0.96 | 0.10 | 58,68,80,81                 | 0     |

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

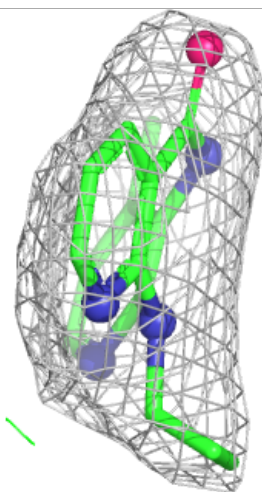
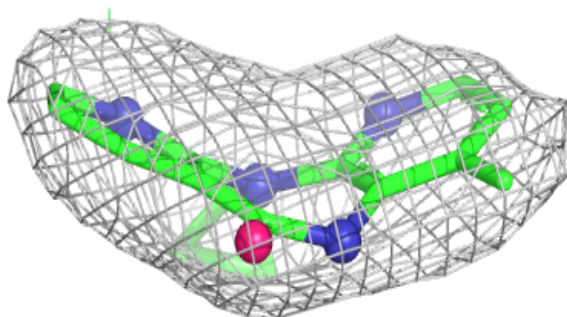
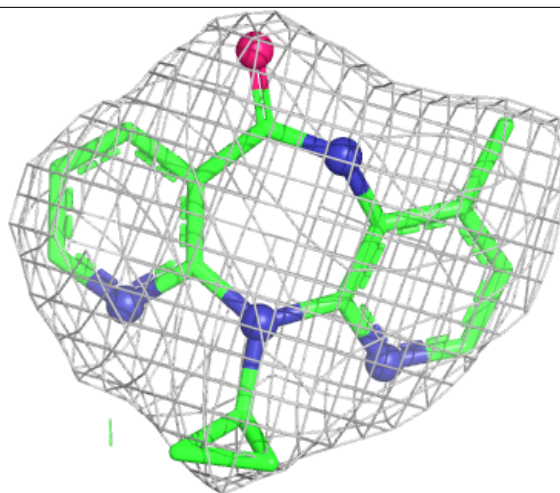
**Electron density around NVP A 901:**

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



**Electron density around NVP C 901:**

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



## 6.5 Other polymers [i](#)

There are no such residues in this entry.