



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 03:45 AM UTC

PDB ID : 4LLF / pdb\_00004llf  
Title : Crystal structure of Cucumber Necrosis Virus  
Authors : Smith, T.  
Deposited on : 2013-07-09  
Resolution : 2.89 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

---

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

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

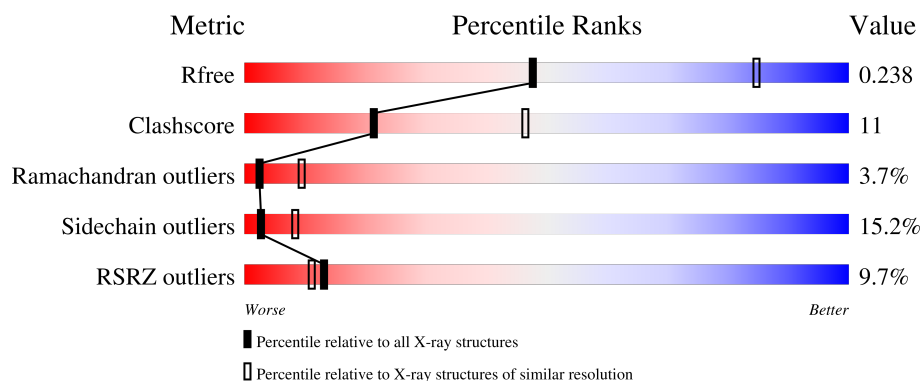
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.89 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                      | 3557 (2.90-2.86)                                      |
| Clashscore            | 190562                      | 3801 (2.90-2.86)                                      |
| Ramachandran outliers | 187476                      | 3699 (2.90-2.86)                                      |
| Sidechain outliers    | 187428                      | 3702 (2.90-2.86)                                      |
| RSRZ outliers         | 180081                      | 3558 (2.90-2.86)                                      |

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     | 380    | <div> <div>6%</div> <div> <div>51%</div> <div>21%</div> <div>•</div> <div>24%</div> </div> </div>                |
| 1   | B     | 380    | <div> <div>12%</div> <div> <div>48%</div> <div>22%</div> <div>6%</div> <div>•</div> <div>23%</div> </div> </div> |
| 1   | D     | 380    | <div> <div>5%</div> <div> <div>54%</div> <div>27%</div> <div>••</div> <div>16%</div> </div> </div>               |
| 1   | E     | 380    | <div> <div>6%</div> <div> <div>51%</div> <div>22%</div> <div>••</div> <div>24%</div> </div> </div>               |
| 1   | F     | 380    | <div> <div>13%</div> <div> <div>47%</div> <div>22%</div> <div>6%</div> <div>•</div> <div>23%</div> </div> </div> |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | G     | 380    |                  |
| 1   | H     | 380    |                  |
| 1   | I     | 380    |                  |
| 1   | J     | 380    |                  |
| 1   | K     | 380    |                  |
| 1   | L     | 380    |                  |
| 1   | M     | 380    |                  |
| 1   | N     | 380    |                  |
| 1   | O     | 380    |                  |
| 1   | P     | 380    |                  |

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 34586 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 Capsid protein.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 1   | A     | 289      | Total | C    | N   | O   | S | 0       | 1       | 0     |
|     |       |          | 2212  | 1408 | 370 | 433 | 1 |         |         |       |
| 1   | B     | 291      | Total | C    | N   | O   | S | 0       | 1       | 0     |
|     |       |          | 2226  | 1417 | 373 | 435 | 1 |         |         |       |
| 1   | D     | 321      | Total | C    | N   | O   | S | 0       | 2       | 0     |
|     |       |          | 2462  | 1573 | 417 | 471 | 1 |         |         |       |
| 1   | E     | 289      | Total | C    | N   | O   | S | 0       | 1       | 0     |
|     |       |          | 2212  | 1408 | 370 | 433 | 1 |         |         |       |
| 1   | F     | 291      | Total | C    | N   | O   | S | 0       | 1       | 0     |
|     |       |          | 2226  | 1417 | 373 | 435 | 1 |         |         |       |
| 1   | G     | 321      | Total | C    | N   | O   | S | 0       | 2       | 0     |
|     |       |          | 2462  | 1573 | 417 | 471 | 1 |         |         |       |
| 1   | H     | 289      | Total | C    | N   | O   | S | 0       | 1       | 0     |
|     |       |          | 2212  | 1408 | 370 | 433 | 1 |         |         |       |
| 1   | I     | 291      | Total | C    | N   | O   | S | 0       | 1       | 0     |
|     |       |          | 2226  | 1417 | 373 | 435 | 1 |         |         |       |
| 1   | J     | 321      | Total | C    | N   | O   | S | 0       | 2       | 0     |
|     |       |          | 2462  | 1573 | 417 | 471 | 1 |         |         |       |
| 1   | K     | 289      | Total | C    | N   | O   | S | 0       | 1       | 0     |
|     |       |          | 2212  | 1408 | 370 | 433 | 1 |         |         |       |
| 1   | L     | 291      | Total | C    | N   | O   | S | 0       | 1       | 0     |
|     |       |          | 2226  | 1417 | 373 | 435 | 1 |         |         |       |
| 1   | M     | 321      | Total | C    | N   | O   | S | 0       | 2       | 0     |
|     |       |          | 2462  | 1573 | 417 | 471 | 1 |         |         |       |
| 1   | N     | 289      | Total | C    | N   | O   | S | 0       | 1       | 0     |
|     |       |          | 2212  | 1408 | 370 | 433 | 1 |         |         |       |
| 1   | O     | 291      | Total | C    | N   | O   | S | 0       | 1       | 0     |
|     |       |          | 2226  | 1417 | 373 | 435 | 1 |         |         |       |
| 1   | P     | 321      | Total | C    | N   | O   | S | 0       | 2       | 0     |
|     |       |          | 2462  | 1573 | 417 | 471 | 1 |         |         |       |

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

| Mol | Chain | Residues | Atoms           | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 2   | B     | 2        | Total Ca<br>2 2 | 0       | 0       |
| 2   | D     | 1        | Total Ca<br>1 1 | 0       | 0       |
| 2   | E     | 2        | Total Ca<br>2 2 | 0       | 0       |
| 2   | F     | 1        | Total Ca<br>1 1 | 0       | 0       |
| 2   | H     | 1        | Total Ca<br>1 1 | 0       | 0       |
| 2   | I     | 2        | Total Ca<br>2 2 | 0       | 0       |
| 2   | K     | 2        | Total Ca<br>2 2 | 0       | 0       |
| 2   | M     | 1        | Total Ca<br>1 1 | 0       | 0       |
| 2   | N     | 1        | Total Ca<br>1 1 | 0       | 0       |
| 2   | O     | 2        | Total Ca<br>2 2 | 0       | 0       |

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms           | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 3   | D     | 1        | Total Zn<br>2 2 | 0       | 1       |
| 3   | G     | 1        | Total Zn<br>2 2 | 0       | 1       |
| 3   | J     | 1        | Total Zn<br>2 2 | 0       | 1       |
| 3   | M     | 1        | Total Zn<br>2 2 | 0       | 1       |
| 3   | P     | 1        | Total Zn<br>2 2 | 0       | 1       |

- Molecule 4 is water.

| Mol | Chain | Residues | Atoms          | ZeroOcc | AltConf |
|-----|-------|----------|----------------|---------|---------|
| 4   | A     | 5        | Total O<br>5 5 | 0       | 0       |
| 4   | B     | 5        | Total O<br>5 5 | 0       | 0       |
| 4   | D     | 4        | Total O<br>4 4 | 0       | 0       |

*Continued on next page...*

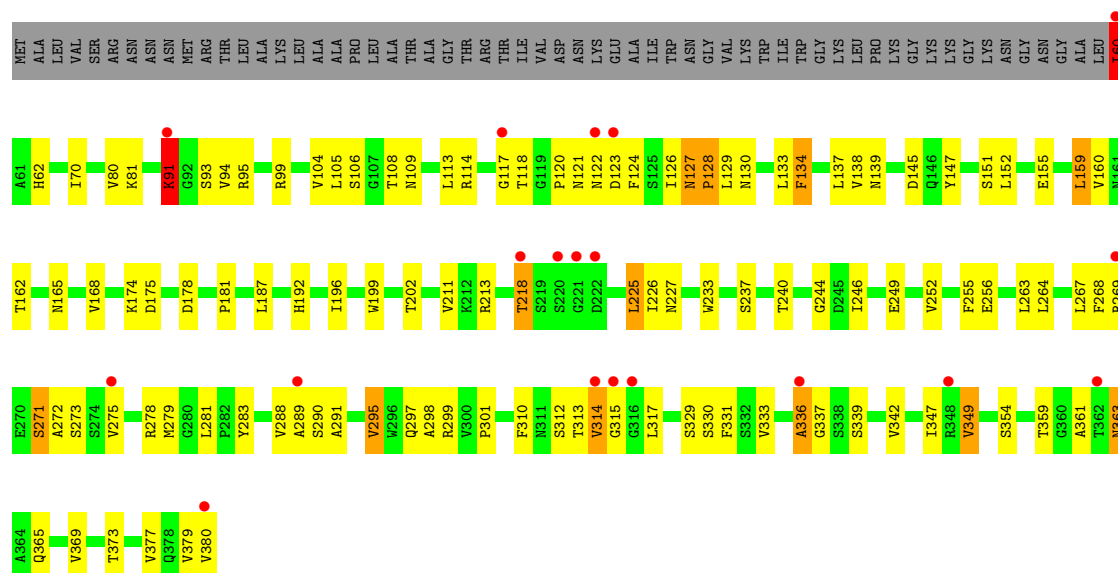
*Continued from previous page...*

| Mol | Chain | Residues | Atoms      |        | ZeroOcc | AltConf |
|-----|-------|----------|------------|--------|---------|---------|
| 4   | E     | 3        | Total<br>3 | O<br>3 | 0       | 0       |
| 4   | F     | 1        | Total<br>1 | O<br>1 | 0       | 0       |
| 4   | G     | 5        | Total<br>5 | O<br>5 | 0       | 0       |
| 4   | H     | 4        | Total<br>4 | O<br>4 | 0       | 0       |
| 4   | I     | 3        | Total<br>3 | O<br>3 | 0       | 0       |
| 4   | J     | 3        | Total<br>3 | O<br>3 | 0       | 0       |
| 4   | K     | 3        | Total<br>3 | O<br>3 | 0       | 0       |
| 4   | L     | 5        | Total<br>5 | O<br>5 | 0       | 0       |
| 4   | M     | 4        | Total<br>4 | O<br>4 | 0       | 0       |
| 4   | N     | 5        | Total<br>5 | O<br>5 | 0       | 0       |
| 4   | O     | 4        | Total<br>4 | O<br>4 | 0       | 0       |
| 4   | P     | 7        | Total<br>7 | O<br>7 | 0       | 0       |

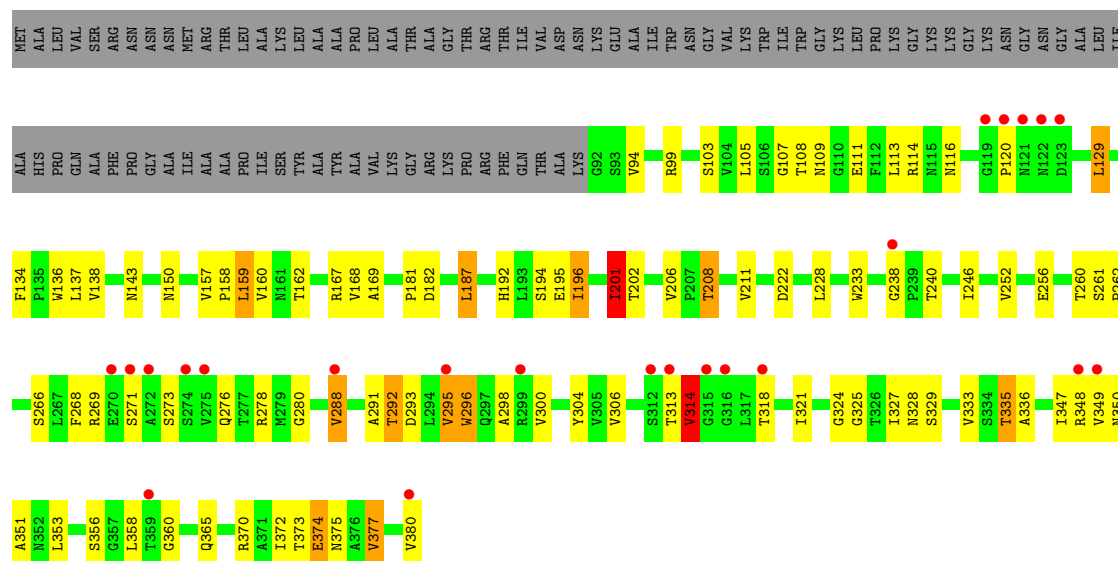




• Molecule 1: Capsid protein

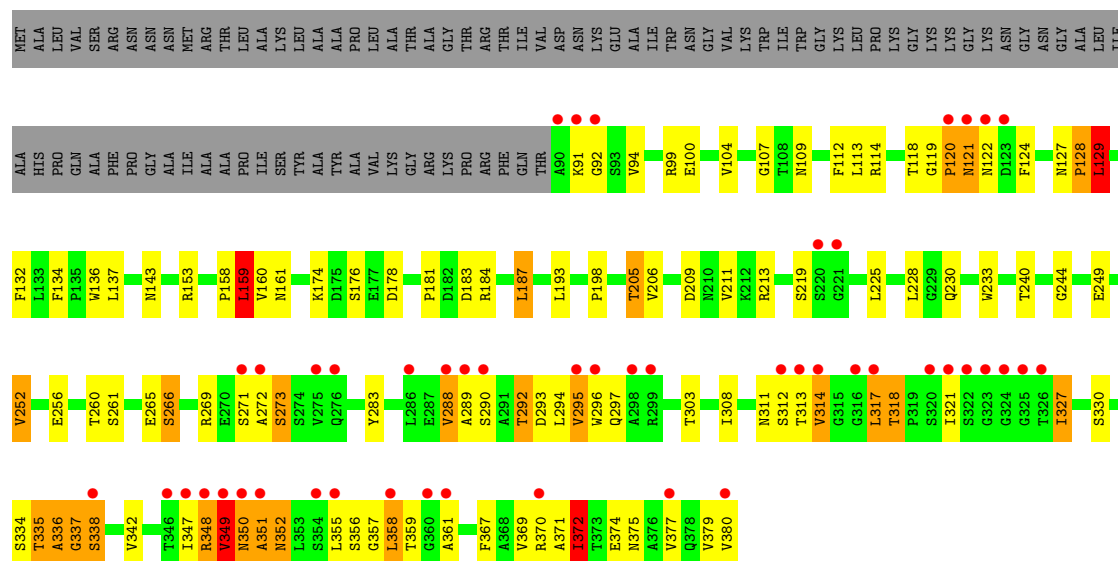


• Molecule 1: Capsid protein

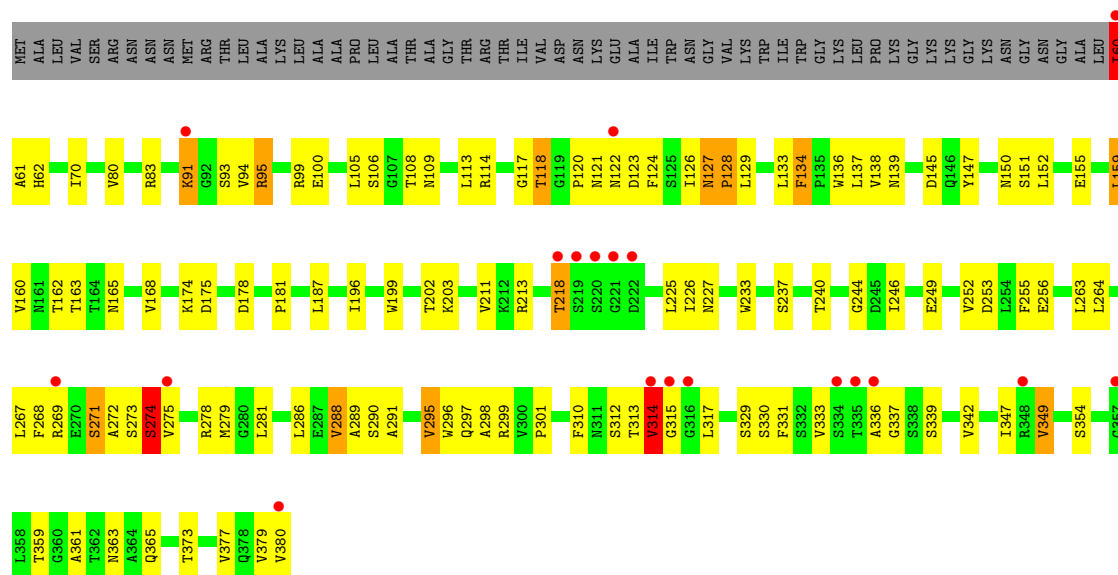


• Molecule 1: Capsid protein

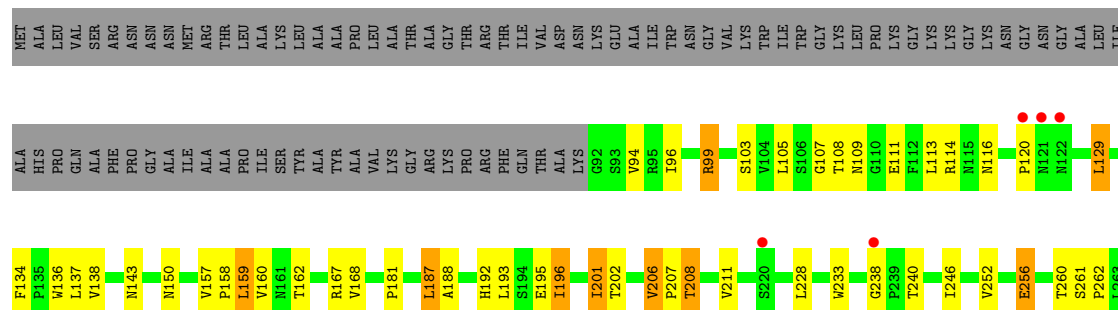




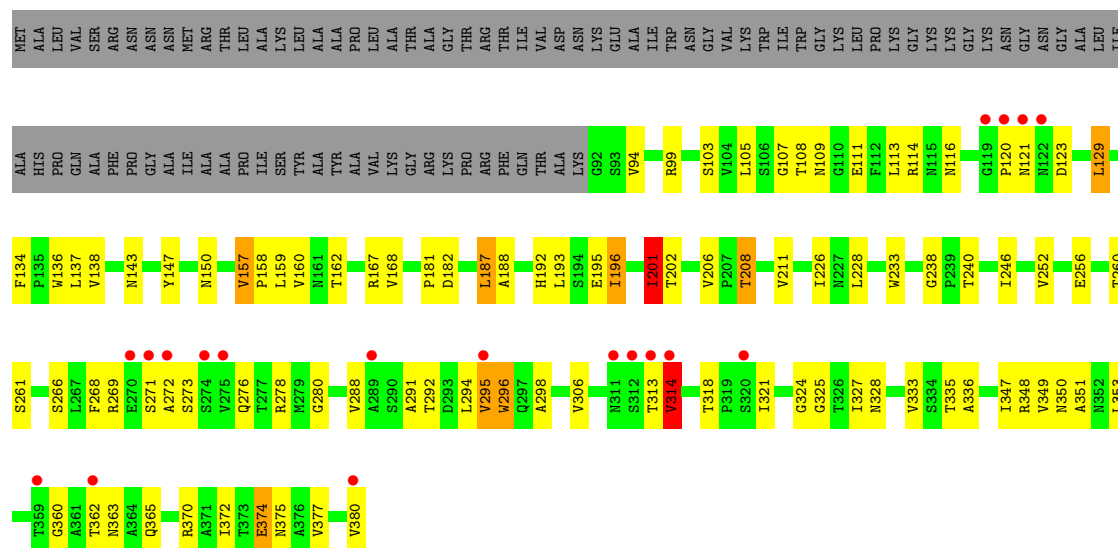
• Molecule 1: Capsid protein



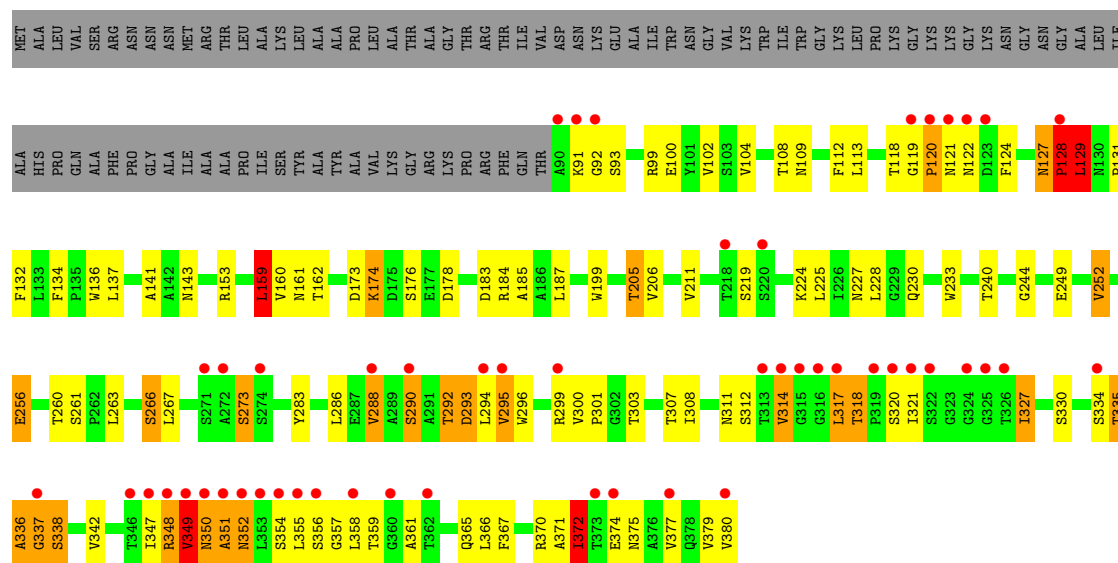
• Molecule 1: Capsid protein



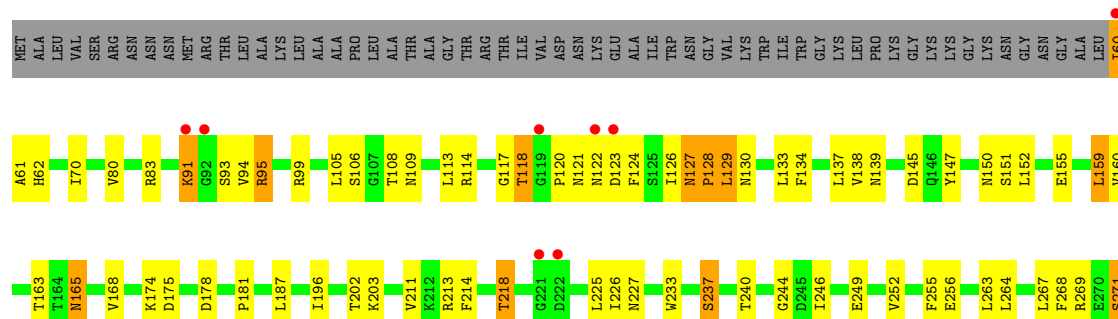


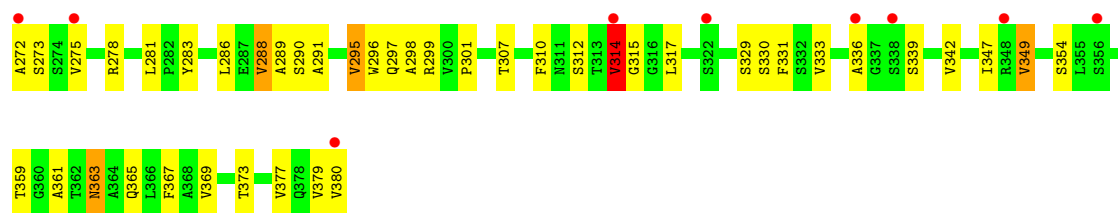


• Molecule 1: Capsid protein

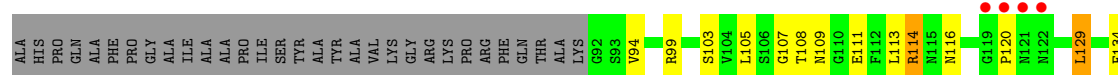
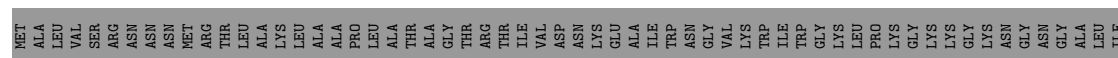


• Molecule 1: Capsid protein

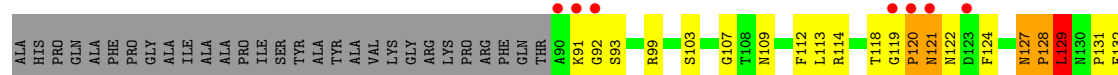




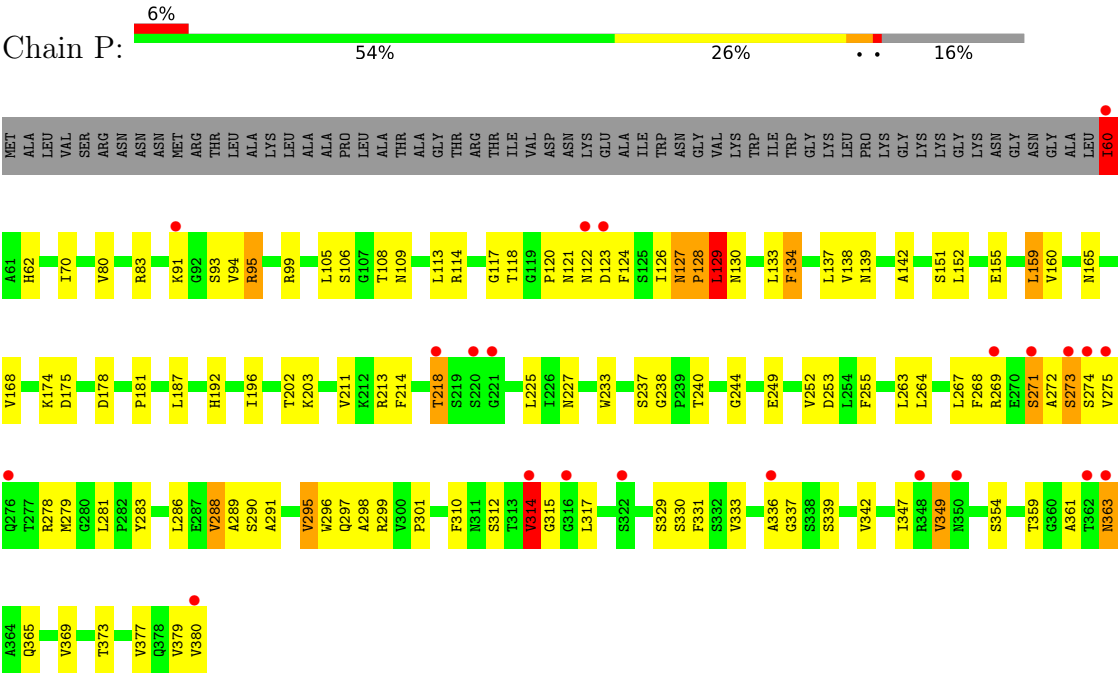
• Molecule 1: Capsid protein



• Molecule 1: Capsid protein



• Molecule 1: Capsid protein



## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | I 2 3                                                       | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 384.00Å 384.00Å 384.00Å<br>90.00° 90.00° 90.00°             | Depositor        |
| Resolution (Å)                                                          | 75.31 – 2.89<br>75.31 – 2.89                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 64.4 (75.31-2.89)<br>63.6 (75.31-2.89)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | (Not available)                                             | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 0.52 (at 2.91Å)                                             | Xtriage          |
| Refinement program                                                      | PHENIX (phenix.refine: 1.8.2_1309)                          | Depositor        |
| R, $R_{free}$                                                           | 0.213 , 0.242<br>0.212 , 0.238                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 9645 reflections (4.63%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 32.6                                                        | Xtriage          |
| Anisotropy                                                              | 0.000                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.35 , 64.2                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$ | Xtriage          |
| Estimated twinning fraction                                             | 0.013 for -l,-k,-h                                          | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.90                                                        | EDS              |
| Total number of atoms                                                   | 34586                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 53.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.01% 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: ZN, CA

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     | 0.64         | 0/2267          | 0.97        | 5/3102 (0.2%)    |
| 1   | B     | 0.69         | 0/2281          | 1.11        | 11/3120 (0.4%)   |
| 1   | D     | 0.65         | 0/2530          | 1.16        | 16/3461 (0.5%)   |
| 1   | E     | 0.66         | 0/2267          | 0.95        | 3/3102 (0.1%)    |
| 1   | F     | 0.68         | 3/2281 (0.1%)   | 1.10        | 11/3120 (0.4%)   |
| 1   | G     | 0.66         | 0/2530          | 1.16        | 20/3461 (0.6%)   |
| 1   | H     | 0.77         | 3/2267 (0.1%)   | 1.04        | 7/3102 (0.2%)    |
| 1   | I     | 0.67         | 1/2281 (0.0%)   | 1.17        | 18/3120 (0.6%)   |
| 1   | J     | 0.70         | 1/2530 (0.0%)   | 1.19        | 22/3461 (0.6%)   |
| 1   | K     | 0.66         | 1/2267 (0.0%)   | 0.95        | 1/3102 (0.0%)    |
| 1   | L     | 0.66         | 2/2281 (0.1%)   | 1.02        | 8/3120 (0.3%)    |
| 1   | M     | 0.67         | 1/2530 (0.0%)   | 1.16        | 19/3461 (0.5%)   |
| 1   | N     | 0.63         | 0/2267          | 0.96        | 2/3102 (0.1%)    |
| 1   | O     | 0.66         | 3/2281 (0.1%)   | 1.10        | 11/3120 (0.4%)   |
| 1   | P     | 0.65         | 0/2530          | 1.17        | 18/3461 (0.5%)   |
| All | All   | 0.67         | 15/35390 (0.0%) | 1.09        | 172/48415 (0.4%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | L     | 0                   | 1                   |

All (15) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 1   | H     | 296 | TRP  | CG-CD1  | -10.51 | 1.10        | 1.36     |
| 1   | H     | 296 | TRP  | NE1-CE2 | -7.80  | 1.28        | 1.37     |
| 1   | F     | 297 | GLN  | CD-NE2  | -6.98  | 1.18        | 1.33     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | O     | 297 | GLN  | CD-NE2  | -6.81 | 1.19        | 1.33     |
| 1   | H     | 296 | TRP  | CD2-CE3 | -6.70 | 1.29        | 1.40     |
| 1   | M     | 314 | VAL  | CA-CB   | 6.39  | 1.63        | 1.54     |
| 1   | L     | 127 | ASN  | C-O     | 6.00  | 1.29        | 1.24     |
| 1   | F     | 297 | GLN  | CD-OE1  | -5.92 | 1.12        | 1.23     |
| 1   | J     | 123 | ASP  | N-CA    | -5.82 | 1.42        | 1.47     |
| 1   | O     | 297 | GLN  | CD-OE1  | -5.75 | 1.12        | 1.23     |
| 1   | F     | 349 | VAL  | CA-CB   | 5.72  | 1.62        | 1.54     |
| 1   | K     | 157 | VAL  | CA-CB   | -5.54 | 1.49        | 1.54     |
| 1   | L     | 349 | VAL  | CA-CB   | 5.21  | 1.61        | 1.54     |
| 1   | I     | 349 | VAL  | CA-CB   | 5.13  | 1.61        | 1.54     |
| 1   | O     | 349 | VAL  | CA-CB   | 5.05  | 1.61        | 1.54     |

All (172) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|--------|-------------|----------|
| 1   | D     | 127 | ASN  | CA-C-N     | -20.14 | 94.66       | 119.84   |
| 1   | D     | 127 | ASN  | C-N-CA     | -20.14 | 94.66       | 119.84   |
| 1   | P     | 127 | ASN  | CA-C-N     | -19.86 | 95.02       | 119.84   |
| 1   | P     | 127 | ASN  | C-N-CA     | -19.86 | 95.02       | 119.84   |
| 1   | M     | 127 | ASN  | CA-C-N     | -19.36 | 95.64       | 119.84   |
| 1   | M     | 127 | ASN  | C-N-CA     | -19.36 | 95.64       | 119.84   |
| 1   | J     | 127 | ASN  | CA-C-N     | -18.90 | 96.22       | 119.84   |
| 1   | J     | 127 | ASN  | C-N-CA     | -18.90 | 96.22       | 119.84   |
| 1   | G     | 127 | ASN  | CA-C-N     | -18.59 | 96.60       | 119.84   |
| 1   | G     | 127 | ASN  | C-N-CA     | -18.59 | 96.60       | 119.84   |
| 1   | F     | 127 | ASN  | CA-C-N     | -17.92 | 97.44       | 119.84   |
| 1   | F     | 127 | ASN  | C-N-CA     | -17.92 | 97.44       | 119.84   |
| 1   | I     | 127 | ASN  | CA-C-N     | -17.88 | 97.49       | 119.84   |
| 1   | I     | 127 | ASN  | C-N-CA     | -17.88 | 97.49       | 119.84   |
| 1   | O     | 127 | ASN  | CA-C-N     | -17.66 | 97.76       | 119.84   |
| 1   | O     | 127 | ASN  | C-N-CA     | -17.66 | 97.76       | 119.84   |
| 1   | B     | 127 | ASN  | CA-C-N     | -17.14 | 98.42       | 119.84   |
| 1   | B     | 127 | ASN  | C-N-CA     | -17.14 | 98.42       | 119.84   |
| 1   | H     | 296 | TRP  | CB-CG-CD2  | 10.42  | 141.39      | 126.80   |
| 1   | H     | 296 | TRP  | CG-CD1-NE1 | 9.91   | 123.08      | 110.20   |
| 1   | I     | 348 | ARG  | NE-CZ-NH2  | 9.04   | 127.33      | 119.20   |
| 1   | I     | 348 | ARG  | NE-CZ-NH1  | -8.60  | 112.90      | 121.50   |
| 1   | H     | 296 | TRP  | CB-CG-CD1  | -8.36  | 114.36      | 126.90   |
| 1   | L     | 159 | LEU  | N-CA-C     | -8.26  | 102.98      | 113.72   |
| 1   | I     | 330 | SER  | CA-CB-OG   | 7.96   | 127.02      | 111.10   |
| 1   | L     | 129 | LEU  | N-CA-C     | 7.70   | 127.19      | 110.80   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res   | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-------|------|------------|-------|-------------|----------|
| 1   | I     | 92    | GLY  | N-CA-C     | -7.62 | 102.54      | 115.80   |
| 1   | L     | 127   | ASN  | CA-C-O     | -7.46 | 113.64      | 120.50   |
| 1   | M     | 60    | ILE  | CG1-CB-CG2 | -7.31 | 88.78       | 110.70   |
| 1   | I     | 128   | PRO  | CA-C-N     | 7.22  | 134.70      | 121.70   |
| 1   | I     | 128   | PRO  | C-N-CA     | 7.22  | 134.70      | 121.70   |
| 1   | F     | 128   | PRO  | CA-C-N     | 7.21  | 134.67      | 121.70   |
| 1   | F     | 128   | PRO  | C-N-CA     | 7.21  | 134.67      | 121.70   |
| 1   | O     | 159   | LEU  | N-CA-C     | -7.18 | 104.38      | 113.72   |
| 1   | L     | 92    | GLY  | N-CA-C     | -7.09 | 103.46      | 115.80   |
| 1   | B     | 128   | PRO  | CA-C-N     | 6.99  | 134.28      | 121.70   |
| 1   | B     | 128   | PRO  | C-N-CA     | 6.99  | 134.28      | 121.70   |
| 1   | B     | 92    | GLY  | N-CA-C     | -6.98 | 103.66      | 115.80   |
| 1   | O     | 128   | PRO  | CA-C-N     | 6.92  | 134.16      | 121.70   |
| 1   | O     | 128   | PRO  | C-N-CA     | 6.92  | 134.16      | 121.70   |
| 1   | O     | 92    | GLY  | N-CA-C     | -6.89 | 103.80      | 115.80   |
| 1   | I     | 159   | LEU  | N-CA-C     | -6.84 | 104.83      | 113.72   |
| 1   | P     | 62[A] | HIS  | CA-C-N     | 6.82  | 126.78      | 119.76   |
| 1   | P     | 62[A] | HIS  | C-N-CA     | 6.82  | 126.78      | 119.76   |
| 1   | P     | 62[B] | HIS  | CA-C-N     | 6.82  | 126.78      | 119.76   |
| 1   | P     | 62[B] | HIS  | C-N-CA     | 6.82  | 126.78      | 119.76   |
| 1   | F     | 92    | GLY  | N-CA-C     | -6.74 | 104.07      | 115.80   |
| 1   | J     | 60    | ILE  | CG1-CB-CG2 | -6.72 | 90.55       | 110.70   |
| 1   | D     | 62[A] | HIS  | CA-C-N     | 6.71  | 126.67      | 119.76   |
| 1   | D     | 62[A] | HIS  | C-N-CA     | 6.71  | 126.67      | 119.76   |
| 1   | D     | 62[B] | HIS  | CA-C-N     | 6.71  | 126.67      | 119.76   |
| 1   | D     | 62[B] | HIS  | C-N-CA     | 6.71  | 126.67      | 119.76   |
| 1   | J     | 128   | PRO  | CA-C-N     | 6.62  | 133.61      | 121.70   |
| 1   | J     | 128   | PRO  | C-N-CA     | 6.62  | 133.61      | 121.70   |
| 1   | F     | 159   | LEU  | N-CA-C     | -6.56 | 105.19      | 113.72   |
| 1   | J     | 62[A] | HIS  | CA-C-N     | 6.55  | 126.50      | 119.76   |
| 1   | J     | 62[A] | HIS  | C-N-CA     | 6.55  | 126.50      | 119.76   |
| 1   | J     | 62[B] | HIS  | CA-C-N     | 6.55  | 126.50      | 119.76   |
| 1   | J     | 62[B] | HIS  | C-N-CA     | 6.55  | 126.50      | 119.76   |
| 1   | M     | 128   | PRO  | CA-C-N     | 6.54  | 133.47      | 121.70   |
| 1   | M     | 128   | PRO  | C-N-CA     | 6.54  | 133.47      | 121.70   |
| 1   | J     | 122   | ASN  | CB-CA-C    | -6.46 | 102.50      | 112.07   |
| 1   | P     | 128   | PRO  | CA-C-N     | 6.33  | 133.09      | 121.70   |
| 1   | P     | 128   | PRO  | C-N-CA     | 6.33  | 133.09      | 121.70   |
| 1   | G     | 128   | PRO  | CA-C-N     | 6.30  | 133.04      | 121.70   |
| 1   | G     | 128   | PRO  | C-N-CA     | 6.30  | 133.04      | 121.70   |
| 1   | D     | 128   | PRO  | CA-C-N     | 6.24  | 132.94      | 121.70   |
| 1   | D     | 128   | PRO  | C-N-CA     | 6.24  | 132.94      | 121.70   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res   | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-------|------|------------|-------|-------------|----------|
| 1   | J     | 314   | VAL  | CB-CA-C    | 6.16  | 121.39      | 111.29   |
| 1   | P     | 314   | VAL  | CB-CA-C    | 6.16  | 121.39      | 111.29   |
| 1   | M     | 163   | THR  | N-CA-C     | -6.11 | 105.41      | 112.92   |
| 1   | B     | 159   | LEU  | N-CA-C     | -6.09 | 105.80      | 113.72   |
| 1   | K     | 201   | ILE  | CB-CA-C    | -6.08 | 104.90      | 111.59   |
| 1   | J     | 130   | ASN  | CA-C-N     | 6.08  | 126.52      | 119.47   |
| 1   | J     | 130   | ASN  | C-N-CA     | 6.08  | 126.52      | 119.47   |
| 1   | J     | 123   | ASP  | N-CA-C     | -6.05 | 104.75      | 113.21   |
| 1   | M     | 314   | VAL  | CB-CA-C    | 6.03  | 121.18      | 111.29   |
| 1   | D     | 130   | ASN  | CA-C-N     | 6.02  | 126.19      | 119.32   |
| 1   | D     | 130   | ASN  | C-N-CA     | 6.02  | 126.19      | 119.32   |
| 1   | G     | 127   | ASN  | N-CA-C     | -5.99 | 102.74      | 108.13   |
| 1   | G     | 128   | PRO  | CA-C-O     | -5.97 | 109.73      | 120.60   |
| 1   | P     | 124   | PHE  | N-CA-C     | -5.94 | 105.34      | 112.59   |
| 1   | M     | 130   | ASN  | CA-C-N     | 5.92  | 126.33      | 119.47   |
| 1   | M     | 130   | ASN  | C-N-CA     | 5.92  | 126.33      | 119.47   |
| 1   | M     | 124   | PHE  | N-CA-C     | -5.90 | 105.39      | 112.59   |
| 1   | P     | 130   | ASN  | CA-C-N     | 5.88  | 126.03      | 119.32   |
| 1   | P     | 130   | ASN  | C-N-CA     | 5.88  | 126.03      | 119.32   |
| 1   | I     | 330   | SER  | N-CA-C     | 5.87  | 118.20      | 108.99   |
| 1   | H     | 295   | VAL  | N-CA-C     | 5.84  | 116.89      | 108.48   |
| 1   | D     | 124   | PHE  | N-CA-C     | -5.84 | 105.46      | 112.59   |
| 1   | I     | 252   | VAL  | CB-CA-C    | -5.81 | 101.59      | 110.95   |
| 1   | J     | 127   | ASN  | N-CA-C     | -5.78 | 102.93      | 108.13   |
| 1   | O     | 119   | GLY  | CA-C-N     | 5.78  | 127.06      | 119.84   |
| 1   | O     | 119   | GLY  | C-N-CA     | 5.78  | 127.06      | 119.84   |
| 1   | G     | 124   | PHE  | N-CA-C     | -5.76 | 105.45      | 112.88   |
| 1   | I     | 330   | SER  | CB-CA-C    | 5.73  | 122.15      | 109.94   |
| 1   | D     | 128   | PRO  | CA-C-O     | -5.71 | 110.20      | 120.60   |
| 1   | G     | 60    | ILE  | CG1-CB-CG2 | -5.71 | 93.57       | 110.70   |
| 1   | I     | 128   | PRO  | CA-C-O     | -5.66 | 110.30      | 120.60   |
| 1   | P     | 60    | ILE  | CG1-CB-CG2 | -5.63 | 93.81       | 110.70   |
| 1   | F     | 119   | GLY  | CA-C-N     | 5.63  | 126.87      | 119.84   |
| 1   | F     | 119   | GLY  | C-N-CA     | 5.63  | 126.87      | 119.84   |
| 1   | F     | 128   | PRO  | CA-C-O     | -5.62 | 110.38      | 120.60   |
| 1   | P     | 123   | ASP  | N-CA-C     | -5.61 | 105.36      | 113.21   |
| 1   | A     | 201   | ILE  | CB-CA-C    | -5.59 | 105.44      | 111.59   |
| 1   | G     | 62[A] | HIS  | CA-C-N     | 5.58  | 125.51      | 119.76   |
| 1   | G     | 62[A] | HIS  | C-N-CA     | 5.58  | 125.51      | 119.76   |
| 1   | G     | 62[B] | HIS  | CA-C-N     | 5.58  | 125.51      | 119.76   |
| 1   | G     | 62[B] | HIS  | C-N-CA     | 5.58  | 125.51      | 119.76   |
| 1   | O     | 128   | PRO  | CA-C-O     | -5.58 | 110.45      | 120.60   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res   | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-------|------|------------|-------|-------------|----------|
| 1   | B     | 128   | PRO  | CA-C-O     | -5.56 | 110.48      | 120.60   |
| 1   | J     | 122   | ASN  | N-CA-C     | 5.55  | 117.54      | 109.71   |
| 1   | M     | 128   | PRO  | CA-C-O     | -5.53 | 110.54      | 120.60   |
| 1   | D     | 134   | PHE  | CA-C-N     | 5.52  | 124.98      | 119.24   |
| 1   | D     | 134   | PHE  | C-N-CA     | 5.52  | 124.98      | 119.24   |
| 1   | G     | 314   | VAL  | CB-CA-C    | 5.51  | 120.32      | 111.29   |
| 1   | G     | 274   | SER  | CA-CB-OG   | 5.50  | 122.11      | 111.10   |
| 1   | I     | 119   | GLY  | CA-C-N     | 5.50  | 126.71      | 119.84   |
| 1   | I     | 119   | GLY  | C-N-CA     | 5.50  | 126.71      | 119.84   |
| 1   | D     | 60    | ILE  | CG1-CB-CG2 | -5.50 | 94.21       | 110.70   |
| 1   | M     | 62[A] | HIS  | CA-C-N     | 5.49  | 125.42      | 119.76   |
| 1   | M     | 62[A] | HIS  | C-N-CA     | 5.49  | 125.42      | 119.76   |
| 1   | M     | 62[B] | HIS  | CA-C-N     | 5.49  | 125.42      | 119.76   |
| 1   | M     | 62[B] | HIS  | C-N-CA     | 5.49  | 125.42      | 119.76   |
| 1   | J     | 134   | PHE  | CA-C-N     | 5.46  | 124.92      | 119.24   |
| 1   | J     | 134   | PHE  | C-N-CA     | 5.46  | 124.92      | 119.24   |
| 1   | P     | 128   | PRO  | CA-C-O     | -5.46 | 110.67      | 120.60   |
| 1   | J     | 124   | PHE  | N-CA-C     | -5.42 | 106.25      | 112.92   |
| 1   | A     | 356   | SER  | N-CA-CB    | -5.41 | 101.34      | 110.49   |
| 1   | M     | 237   | SER  | CB-CA-C    | -5.41 | 109.35      | 115.79   |
| 1   | L     | 127   | ASN  | C-N-CD     | -5.39 | 102.91      | 125.00   |
| 1   | J     | 210   | ASN  | CB-CA-C    | 5.39  | 124.05      | 111.77   |
| 1   | J     | 237   | SER  | CB-CA-C    | -5.38 | 109.38      | 115.79   |
| 1   | M     | 123   | ASP  | N-CA-C     | -5.38 | 105.68      | 113.21   |
| 1   | P     | 134   | PHE  | CA-C-N     | 5.29  | 124.74      | 119.24   |
| 1   | P     | 134   | PHE  | C-N-CA     | 5.29  | 124.74      | 119.24   |
| 1   | B     | 129   | LEU  | N-CA-C     | 5.26  | 125.72      | 111.00   |
| 1   | H     | 316   | GLY  | N-CA-C     | -5.23 | 106.15      | 112.48   |
| 1   | I     | 288   | VAL  | N-CA-C     | 5.21  | 115.23      | 108.35   |
| 1   | G     | 134   | PHE  | CA-C-N     | 5.21  | 124.66      | 119.24   |
| 1   | G     | 134   | PHE  | C-N-CA     | 5.21  | 124.66      | 119.24   |
| 1   | J     | 128   | PRO  | CA-C-O     | -5.21 | 111.12      | 120.60   |
| 1   | L     | 119   | GLY  | CA-C-N     | 5.20  | 126.34      | 119.84   |
| 1   | L     | 119   | GLY  | C-N-CA     | 5.20  | 126.34      | 119.84   |
| 1   | G     | 128   | PRO  | N-CA-C     | 5.20  | 123.18      | 112.47   |
| 1   | I     | 348   | ARG  | CD-NE-CZ   | 5.18  | 131.65      | 124.40   |
| 1   | I     | 129   | LEU  | N-CA-C     | 5.17  | 125.49      | 111.00   |
| 1   | B     | 119   | GLY  | CA-C-N     | 5.17  | 126.31      | 119.84   |
| 1   | B     | 119   | GLY  | C-N-CA     | 5.17  | 126.31      | 119.84   |
| 1   | E     | 201   | ILE  | CB-CA-C    | -5.17 | 105.90      | 111.59   |
| 1   | G     | 123   | ASP  | N-CA-C     | -5.17 | 105.97      | 113.21   |
| 1   | D     | 123   | ASP  | N-CA-C     | -5.16 | 105.98      | 113.21   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | F     | 129 | LEU  | N-CA-C    | 5.16  | 125.45      | 111.00   |
| 1   | G     | 163 | THR  | N-CA-C    | -5.14 | 106.85      | 113.02   |
| 1   | H     | 201 | ILE  | CB-CA-C   | -5.13 | 105.94      | 111.59   |
| 1   | H     | 349 | VAL  | N-CA-C    | -5.13 | 102.27      | 108.53   |
| 1   | M     | 60  | ILE  | CA-CB-CG1 | 5.12  | 119.11      | 110.40   |
| 1   | F     | 252 | VAL  | CB-CA-C   | -5.12 | 102.71      | 110.95   |
| 1   | B     | 252 | VAL  | CB-CA-C   | -5.12 | 102.71      | 110.95   |
| 1   | M     | 288 | VAL  | N-CA-C    | 5.11  | 115.27      | 108.11   |
| 1   | L     | 252 | VAL  | CB-CA-C   | -5.11 | 102.73      | 110.95   |
| 1   | N     | 201 | ILE  | CB-CA-C   | -5.06 | 106.02      | 111.59   |
| 1   | G     | 274 | SER  | N-CA-C    | 5.03  | 121.52      | 110.80   |
| 1   | N     | 349 | VAL  | N-CA-C    | -5.03 | 102.39      | 108.53   |
| 1   | A     | 252 | VAL  | CB-CA-C   | -5.02 | 103.09      | 110.82   |
| 1   | E     | 222 | ASP  | CA-C-N    | 5.02  | 124.80      | 119.28   |
| 1   | E     | 222 | ASP  | C-N-CA    | 5.02  | 124.80      | 119.28   |
| 1   | O     | 252 | VAL  | CB-CA-C   | -5.02 | 102.87      | 110.95   |
| 1   | P     | 129 | LEU  | N-CA-C    | 5.01  | 125.04      | 111.00   |
| 1   | O     | 129 | LEU  | N-CA-C    | 5.01  | 125.04      | 111.00   |
| 1   | A     | 222 | ASP  | CA-C-N    | 5.01  | 124.79      | 119.28   |
| 1   | A     | 222 | ASP  | C-N-CA    | 5.01  | 124.79      | 119.28   |

There are no chirality outliers.

All (1) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 1   | L     | 128 | PRO  | Peptide |

## 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     | 2212  | 0        | 2159     | 45      | 0            |
| 1   | B     | 2226  | 0        | 2177     | 57      | 0            |
| 1   | D     | 2462  | 0        | 2418     | 51      | 0            |
| 1   | E     | 2212  | 0        | 2159     | 47      | 0            |
| 1   | F     | 2226  | 0        | 2177     | 59      | 0            |
| 1   | G     | 2462  | 0        | 2418     | 51      | 0            |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | H     | 2212  | 0        | 2159     | 57      | 0            |
| 1   | I     | 2226  | 0        | 2177     | 59      | 0            |
| 1   | J     | 2462  | 0        | 2418     | 52      | 0            |
| 1   | K     | 2212  | 0        | 2159     | 44      | 0            |
| 1   | L     | 2226  | 0        | 2177     | 65      | 0            |
| 1   | M     | 2462  | 0        | 2418     | 50      | 0            |
| 1   | N     | 2212  | 0        | 2159     | 49      | 0            |
| 1   | O     | 2226  | 0        | 2177     | 60      | 0            |
| 1   | P     | 2462  | 0        | 2418     | 50      | 0            |
| 2   | B     | 2     | 0        | 0        | 0       | 0            |
| 2   | D     | 1     | 0        | 0        | 0       | 0            |
| 2   | E     | 2     | 0        | 0        | 0       | 0            |
| 2   | F     | 1     | 0        | 0        | 0       | 0            |
| 2   | H     | 1     | 0        | 0        | 0       | 0            |
| 2   | I     | 2     | 0        | 0        | 0       | 0            |
| 2   | K     | 2     | 0        | 0        | 0       | 0            |
| 2   | M     | 1     | 0        | 0        | 0       | 0            |
| 2   | N     | 1     | 0        | 0        | 0       | 0            |
| 2   | O     | 2     | 0        | 0        | 0       | 0            |
| 3   | D     | 2     | 0        | 0        | 0       | 0            |
| 3   | G     | 2     | 0        | 0        | 0       | 0            |
| 3   | J     | 2     | 0        | 0        | 0       | 0            |
| 3   | M     | 2     | 0        | 0        | 0       | 0            |
| 3   | P     | 2     | 0        | 0        | 0       | 0            |
| 4   | A     | 5     | 0        | 0        | 0       | 0            |
| 4   | B     | 5     | 0        | 0        | 0       | 0            |
| 4   | D     | 4     | 0        | 0        | 0       | 0            |
| 4   | E     | 3     | 0        | 0        | 0       | 0            |
| 4   | F     | 1     | 0        | 0        | 0       | 0            |
| 4   | G     | 5     | 0        | 0        | 0       | 0            |
| 4   | H     | 4     | 0        | 0        | 1       | 0            |
| 4   | I     | 3     | 0        | 0        | 1       | 0            |
| 4   | J     | 3     | 0        | 0        | 0       | 0            |
| 4   | K     | 3     | 0        | 0        | 0       | 0            |
| 4   | L     | 5     | 0        | 0        | 2       | 0            |
| 4   | M     | 4     | 0        | 0        | 0       | 0            |
| 4   | N     | 5     | 0        | 0        | 1       | 0            |
| 4   | O     | 4     | 0        | 0        | 0       | 0            |
| 4   | P     | 7     | 0        | 0        | 0       | 0            |
| All | All   | 34586 | 0        | 33770    | 744     | 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 11.

All (744) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:296:TRP:CZ3  | 1:H:366:LEU:HB2  | 1.73                     | 1.24              |
| 1:H:296:TRP:HE3  | 1:H:366:LEU:HD22 | 1.19                     | 1.07              |
| 1:H:296:TRP:HZ3  | 1:H:366:LEU:HB2  | 1.20                     | 1.01              |
| 1:H:296:TRP:HD1  | 1:H:296:TRP:N    | 1.56                     | 0.98              |
| 1:H:295:VAL:C    | 1:H:296:TRP:HD1  | 1.78                     | 0.91              |
| 1:J:122:ASN:HB3  | 1:J:218:THR:HG21 | 1.56                     | 0.87              |
| 1:H:296:TRP:CE3  | 1:H:366:LEU:HD22 | 2.10                     | 0.86              |
| 1:H:296:TRP:CE3  | 1:H:366:LEU:HB2  | 2.10                     | 0.86              |
| 1:L:348:ARG:HG2  | 1:L:349:VAL:HG12 | 1.64                     | 0.79              |
| 1:J:109:ASN:H    | 1:J:240:THR:HB   | 1.48                     | 0.79              |
| 1:H:296:TRP:N    | 1:H:296:TRP:CD1  | 2.41                     | 0.78              |
| 1:H:295:VAL:C    | 1:H:296:TRP:CD1  | 2.61                     | 0.77              |
| 1:L:335:THR:OG1  | 1:L:336:ALA:N    | 2.18                     | 0.77              |
| 1:O:335:THR:OG1  | 1:O:336:ALA:N    | 2.18                     | 0.76              |
| 1:F:348:ARG:HG2  | 1:F:349:VAL:HG12 | 1.67                     | 0.74              |
| 1:I:335:THR:OG1  | 1:I:336:ALA:N    | 2.19                     | 0.74              |
| 1:F:109:ASN:H    | 1:F:240:THR:HB   | 1.54                     | 0.73              |
| 1:L:128:PRO:O    | 1:L:141:ALA:CB   | 2.37                     | 0.73              |
| 1:B:335:THR:OG1  | 1:B:336:ALA:N    | 2.20                     | 0.73              |
| 1:G:109:ASN:H    | 1:G:240:THR:HB   | 1.53                     | 0.73              |
| 1:M:109:ASN:H    | 1:M:240:THR:HB   | 1.54                     | 0.73              |
| 1:M:268:PHE:HB2  | 1:M:365:GLN:HG3  | 1.71                     | 0.73              |
| 1:A:298:ALA:HB3  | 1:A:347:ILE:HG21 | 1.71                     | 0.73              |
| 1:D:122:ASN:HB3  | 1:D:218:THR:HG21 | 1.70                     | 0.72              |
| 1:E:298:ALA:HB3  | 1:E:347:ILE:HG21 | 1.71                     | 0.72              |
| 1:G:108:THR:HG23 | 1:G:113:LEU:HD22 | 1.70                     | 0.72              |
| 1:P:109:ASN:H    | 1:P:240:THR:HB   | 1.56                     | 0.71              |
| 1:D:268:PHE:HB2  | 1:D:365:GLN:HG3  | 1.72                     | 0.71              |
| 1:G:268:PHE:HB2  | 1:G:365:GLN:HG3  | 1.72                     | 0.71              |
| 1:N:298:ALA:HB3  | 1:N:347:ILE:HG21 | 1.71                     | 0.71              |
| 1:B:348:ARG:HG2  | 1:B:349:VAL:HG12 | 1.71                     | 0.71              |
| 1:I:348:ARG:O    | 1:I:350:ASN:N    | 2.24                     | 0.71              |
| 1:H:296:TRP:HZ3  | 1:H:366:LEU:CB   | 2.01                     | 0.70              |
| 1:B:348:ARG:O    | 1:B:350:ASN:N    | 2.25                     | 0.70              |
| 1:H:298:ALA:HB3  | 1:H:347:ILE:HG21 | 1.73                     | 0.70              |
| 1:O:109:ASN:H    | 1:O:240:THR:HB   | 1.57                     | 0.69              |
| 1:J:210:ASN:OD1  | 1:J:210:ASN:O    | 2.09                     | 0.69              |
| 1:K:298:ALA:HB3  | 1:K:347:ILE:HG21 | 1.73                     | 0.69              |
| 1:F:121:ASN:HB3  | 1:F:230:GLN:OE1  | 1.92                     | 0.69              |
| 1:P:268:PHE:HB2  | 1:P:365:GLN:HG3  | 1.73                     | 0.69              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:I:159:LEU:HB2   | 1:I:244:GLY:HA2  | 1.74                     | 0.69              |
| 1:A:269:ARG:NH2   | 1:A:271:SER:OG   | 2.26                     | 0.69              |
| 1:I:348:ARG:HG3   | 1:I:349:VAL:HG12 | 1.74                     | 0.69              |
| 1:O:348:ARG:HG2   | 1:O:349:VAL:HG12 | 1.72                     | 0.69              |
| 1:A:268:PHE:HB2   | 1:A:365:GLN:HG3  | 1.73                     | 0.69              |
| 1:F:335:THR:OG1   | 1:F:336:ALA:N    | 2.18                     | 0.68              |
| 1:D:297:GLN:OE1   | 1:D:299:ARG:NH1  | 2.24                     | 0.68              |
| 1:F:348:ARG:O     | 1:F:350:ASN:N    | 2.26                     | 0.68              |
| 1:H:99[B]:ARG:NH2 | 4:H:502:HOH:O    | 2.25                     | 0.68              |
| 1:B:109:ASN:H     | 1:B:240:THR:HB   | 1.57                     | 0.68              |
| 1:E:269:ARG:NH2   | 1:E:271:SER:OG   | 2.26                     | 0.68              |
| 1:M:297:GLN:OE1   | 1:M:299:ARG:NH1  | 2.26                     | 0.68              |
| 1:O:348:ARG:O     | 1:O:350:ASN:N    | 2.26                     | 0.68              |
| 1:E:268:PHE:HB2   | 1:E:365:GLN:HG3  | 1.74                     | 0.68              |
| 1:N:268:PHE:HB2   | 1:N:365:GLN:HG3  | 1.76                     | 0.67              |
| 1:D:165:ASN:HB3   | 1:O:161:ASN:HB3  | 1.76                     | 0.67              |
| 1:D:108:THR:HG23  | 1:D:113:LEU:HD22 | 1.75                     | 0.67              |
| 1:J:268:PHE:HB2   | 1:J:365:GLN:HG3  | 1.75                     | 0.67              |
| 1:F:161:ASN:HB3   | 1:J:165:ASN:HB3  | 1.75                     | 0.67              |
| 1:J:108:THR:HG23  | 1:J:113:LEU:HD22 | 1.76                     | 0.67              |
| 1:B:159:LEU:HB2   | 1:B:244:GLY:HA2  | 1.77                     | 0.67              |
| 1:L:348:ARG:O     | 1:L:350:ASN:N    | 2.28                     | 0.67              |
| 1:P:297:GLN:OE1   | 1:P:299:ARG:NH1  | 2.26                     | 0.67              |
| 1:K:268:PHE:HB2   | 1:K:365:GLN:HG3  | 1.75                     | 0.67              |
| 1:H:192:HIS:NE2   | 1:I:256:GLU:OE2  | 2.25                     | 0.66              |
| 1:D:109:ASN:H     | 1:D:240:THR:HB   | 1.61                     | 0.66              |
| 1:A:296:TRP:N     | 1:A:296:TRP:CD1  | 2.63                     | 0.66              |
| 1:E:196:ILE:HG12  | 1:E:202:THR:HB   | 1.78                     | 0.66              |
| 1:E:296:TRP:CD1   | 1:E:296:TRP:N    | 2.62                     | 0.66              |
| 1:H:268:PHE:HB2   | 1:H:365:GLN:HG3  | 1.77                     | 0.66              |
| 1:M:108:THR:HG23  | 1:M:113:LEU:HD22 | 1.77                     | 0.66              |
| 1:N:296:TRP:CD1   | 1:N:296:TRP:N    | 2.64                     | 0.65              |
| 1:H:278:ARG:NH1   | 1:H:280:GLY:O    | 2.30                     | 0.65              |
| 1:K:296:TRP:N     | 1:K:296:TRP:CD1  | 2.61                     | 0.65              |
| 1:H:196:ILE:HG12  | 1:H:202:THR:HB   | 1.78                     | 0.65              |
| 1:J:297:GLN:OE1   | 1:J:299:ARG:NH1  | 2.29                     | 0.64              |
| 1:O:159:LEU:HB2   | 1:O:244:GLY:HA2  | 1.80                     | 0.64              |
| 1:P:108:THR:HG23  | 1:P:113:LEU:HD22 | 1.78                     | 0.64              |
| 1:L:109:ASN:H     | 1:L:240:THR:HB   | 1.63                     | 0.64              |
| 1:A:196:ILE:HG12  | 1:A:202:THR:HB   | 1.78                     | 0.64              |
| 1:B:318:THR:OG1   | 1:B:357:GLY:N    | 2.22                     | 0.64              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:318:THR:OG1  | 1:F:357:GLY:N    | 2.21                     | 0.64              |
| 1:N:269:ARG:NH2  | 1:N:271:SER:OG   | 2.31                     | 0.64              |
| 1:A:278:ARG:NH1  | 1:A:280:GLY:O    | 2.31                     | 0.64              |
| 1:H:296:TRP:HB2  | 1:H:353:LEU:CD2  | 2.27                     | 0.64              |
| 1:K:109:ASN:H    | 1:K:240:THR:HB   | 1.63                     | 0.64              |
| 1:K:196:ILE:HG12 | 1:K:202:THR:HB   | 1.80                     | 0.64              |
| 1:B:318:THR:HB   | 1:B:356:SER:HB2  | 1.78                     | 0.63              |
| 1:K:192:HIS:NE2  | 1:L:256:GLU:OE2  | 2.28                     | 0.63              |
| 1:K:269:ARG:NH2  | 1:K:271:SER:OG   | 2.31                     | 0.63              |
| 1:F:318:THR:HB   | 1:F:356:SER:HB2  | 1.79                     | 0.63              |
| 1:L:318:THR:OG1  | 1:L:357:GLY:N    | 2.23                     | 0.63              |
| 1:N:192:HIS:NE2  | 1:O:256:GLU:OE2  | 2.28                     | 0.63              |
| 1:O:318:THR:HB   | 1:O:356:SER:HB2  | 1.80                     | 0.63              |
| 1:E:278:ARG:NH1  | 1:E:280:GLY:O    | 2.30                     | 0.63              |
| 1:I:318:THR:OG1  | 1:I:357:GLY:N    | 2.22                     | 0.63              |
| 1:K:278:ARG:NH1  | 1:K:280:GLY:O    | 2.32                     | 0.63              |
| 1:N:196:ILE:HG12 | 1:N:202:THR:HB   | 1.80                     | 0.63              |
| 1:O:288:VAL:H    | 1:O:295:VAL:HG23 | 1.62                     | 0.63              |
| 1:I:161:ASN:HB3  | 1:M:165:ASN:HB3  | 1.81                     | 0.62              |
| 1:L:161:ASN:HB3  | 1:P:165:ASN:HB3  | 1.81                     | 0.62              |
| 1:G:297:GLN:OE1  | 1:G:299:ARG:NH1  | 2.30                     | 0.62              |
| 1:I:318:THR:HB   | 1:I:356:SER:HB2  | 1.81                     | 0.62              |
| 1:D:314:VAL:HG22 | 1:D:315:GLY:H    | 1.64                     | 0.62              |
| 1:B:288:VAL:H    | 1:B:295:VAL:HG23 | 1.65                     | 0.62              |
| 1:H:269:ARG:NH2  | 1:H:271:SER:OG   | 2.33                     | 0.62              |
| 1:L:288:VAL:H    | 1:L:295:VAL:HG23 | 1.64                     | 0.62              |
| 1:L:159:LEU:HB2  | 1:L:244:GLY:HA2  | 1.81                     | 0.62              |
| 1:O:358:LEU:HD23 | 1:O:361:ALA:HB2  | 1.82                     | 0.61              |
| 1:A:192:HIS:NE2  | 1:B:256:GLU:OE2  | 2.30                     | 0.61              |
| 1:I:348:ARG:NH2  | 4:I:501:HOH:O    | 2.33                     | 0.61              |
| 1:G:122:ASN:HB3  | 1:G:218:THR:HG21 | 1.84                     | 0.60              |
| 1:F:118:THR:O    | 1:F:120:PRO:HD2  | 2.01                     | 0.60              |
| 1:F:288:VAL:H    | 1:F:295:VAL:HG23 | 1.65                     | 0.60              |
| 1:I:118:THR:O    | 1:I:120:PRO:HD2  | 2.02                     | 0.60              |
| 1:D:288:VAL:HG22 | 1:D:295:VAL:HG22 | 1.83                     | 0.60              |
| 1:I:109:ASN:H    | 1:I:240:THR:HB   | 1.66                     | 0.60              |
| 1:F:159:LEU:HB2  | 1:F:244:GLY:HA2  | 1.83                     | 0.60              |
| 1:K:362:THR:OG1  | 1:K:363:ASN:N    | 2.34                     | 0.60              |
| 1:P:122:ASN:HB3  | 1:P:218:THR:HG21 | 1.84                     | 0.60              |
| 1:I:348:ARG:HG3  | 1:I:349:VAL:N    | 2.15                     | 0.60              |
| 1:J:288:VAL:HG22 | 1:J:295:VAL:HG22 | 1.83                     | 0.60              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:K:129:LEU:HD22   | 1:K:138:VAL:HG23   | 1.82                     | 0.60              |
| 1:L:358:LEU:HD23   | 1:L:361:ALA:HB2    | 1.82                     | 0.60              |
| 1:P:288:VAL:HG22   | 1:P:295:VAL:HG22   | 1.82                     | 0.60              |
| 1:B:161:ASN:HB3    | 1:G:165:ASN:HB3    | 1.83                     | 0.60              |
| 1:E:134:PHE:HB3    | 1:E:137:LEU:HB3    | 1.84                     | 0.60              |
| 1:M:288:VAL:HG22   | 1:M:295:VAL:HG22   | 1.84                     | 0.60              |
| 1:N:134:PHE:HB3    | 1:N:137:LEU:HB3    | 1.84                     | 0.60              |
| 1:B:118:THR:O      | 1:B:120:PRO:HD2    | 2.01                     | 0.60              |
| 1:H:296:TRP:CZ3    | 1:H:366:LEU:CB     | 2.67                     | 0.60              |
| 1:O:371:ALA:HB1    | 1:O:375:ASN:OD1    | 2.02                     | 0.60              |
| 1:O:318:THR:OG1    | 1:O:357:GLY:N      | 2.21                     | 0.59              |
| 1:H:321:ILE:HG21   | 1:H:325:GLY:HA3    | 1.84                     | 0.59              |
| 1:I:176:SER:HA     | 1:I:230:GLN:HB2    | 1.83                     | 0.59              |
| 1:G:99[A]:ARG:HH11 | 1:G:99[A]:ARG:HG2  | 1.67                     | 0.59              |
| 1:B:153:ARG:HD3    | 1:B:205:THR:HG23   | 1.84                     | 0.59              |
| 1:N:278:ARG:NH1    | 1:N:280:GLY:O      | 2.36                     | 0.59              |
| 1:K:134:PHE:HB3    | 1:K:137:LEU:HB3    | 1.83                     | 0.59              |
| 1:O:118:THR:O      | 1:O:120:PRO:HD2    | 2.02                     | 0.59              |
| 1:L:118:THR:O      | 1:L:120:PRO:HD2    | 2.02                     | 0.58              |
| 1:A:134:PHE:HB3    | 1:A:137:LEU:HB3    | 1.83                     | 0.58              |
| 1:B:176:SER:HA     | 1:B:230:GLN:HB2    | 1.84                     | 0.58              |
| 1:E:182:ASP:OD1    | 1:H:373:THR:OG1    | 2.18                     | 0.58              |
| 1:E:113:LEU:HD21   | 1:E:116:ASN:HA     | 1.84                     | 0.58              |
| 1:H:134:PHE:HB3    | 1:H:137:LEU:HB3    | 1.85                     | 0.58              |
| 1:H:296:TRP:HE3    | 1:H:366:LEU:CD2    | 2.04                     | 0.58              |
| 1:M:99[A]:ARG:HG2  | 1:M:99[A]:ARG:HH11 | 1.69                     | 0.58              |
| 1:P:93:SER:HB3     | 1:P:255:PHE:CE1    | 2.38                     | 0.58              |
| 1:E:192:HIS:NE2    | 1:F:256:GLU:OE2    | 2.30                     | 0.58              |
| 1:O:176:SER:HA     | 1:O:230:GLN:HB2    | 1.86                     | 0.58              |
| 1:D:147:TYR:OH     | 1:D:226:ILE:O      | 2.22                     | 0.57              |
| 1:P:314:VAL:HG22   | 1:P:315:GLY:H      | 1.68                     | 0.57              |
| 1:G:288:VAL:HG22   | 1:G:295:VAL:HG22   | 1.87                     | 0.57              |
| 1:H:109:ASN:H      | 1:H:240:THR:HB     | 1.69                     | 0.57              |
| 1:L:176:SER:HA     | 1:L:230:GLN:HB2    | 1.85                     | 0.57              |
| 1:M:122:ASN:HB3    | 1:M:218:THR:HG21   | 1.86                     | 0.57              |
| 1:J:99[A]:ARG:HG2  | 1:J:99[A]:ARG:HH11 | 1.70                     | 0.57              |
| 1:M:312:SER:HA     | 1:M:361:ALA:HA     | 1.86                     | 0.57              |
| 1:M:314:VAL:HG22   | 1:M:315:GLY:H      | 1.70                     | 0.57              |
| 1:O:347:ILE:HG13   | 1:O:351:ALA:HB3    | 1.87                     | 0.57              |
| 1:H:296:TRP:HB2    | 1:H:353:LEU:HD23   | 1.86                     | 0.56              |
| 1:L:128:PRO:O      | 1:L:141:ALA:HB1    | 2.05                     | 0.56              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:F:371:ALA:HB1   | 1:F:375:ASN:OD1    | 2.06                     | 0.56              |
| 1:A:109:ASN:H     | 1:A:240:THR:HB     | 1.70                     | 0.56              |
| 1:A:113:LEU:HD21  | 1:A:116:ASN:HA     | 1.87                     | 0.56              |
| 1:M:93:SER:HB3    | 1:M:255:PHE:CE1    | 2.40                     | 0.56              |
| 1:A:372:ILE:HD12  | 1:A:374:GLU:HG2    | 1.87                     | 0.56              |
| 1:B:371:ALA:HB1   | 1:B:375:ASN:OD1    | 2.05                     | 0.56              |
| 1:N:109:ASN:H     | 1:N:240:THR:HB     | 1.69                     | 0.56              |
| 1:P:99[A]:ARG:HG2 | 1:P:99[A]:ARG:HH11 | 1.70                     | 0.56              |
| 1:B:336:ALA:O     | 1:B:338:SER:N      | 2.37                     | 0.56              |
| 1:G:312:SER:HA    | 1:G:361:ALA:HA     | 1.87                     | 0.56              |
| 1:I:371:ALA:HB1   | 1:I:375:ASN:OD1    | 2.06                     | 0.56              |
| 1:F:176:SER:HA    | 1:F:230:GLN:HB2    | 1.87                     | 0.55              |
| 1:G:314:VAL:HG22  | 1:G:315:GLY:H      | 1.70                     | 0.55              |
| 1:I:336:ALA:O     | 1:I:338:SER:N      | 2.39                     | 0.55              |
| 1:M:147:TYR:OH    | 1:M:226:ILE:O      | 2.20                     | 0.55              |
| 1:K:113:LEU:HD21  | 1:K:116:ASN:HA     | 1.88                     | 0.55              |
| 1:M:127:ASN:HB2   | 1:M:227:ASN:OD1    | 2.06                     | 0.55              |
| 1:N:129:LEU:HD22  | 1:N:138:VAL:HG23   | 1.88                     | 0.55              |
| 1:A:321:ILE:HG21  | 1:A:325:GLY:HA3    | 1.89                     | 0.55              |
| 1:L:371:ALA:HB1   | 1:L:375:ASN:OD1    | 2.05                     | 0.55              |
| 1:N:321:ILE:HG21  | 1:N:325:GLY:HA3    | 1.87                     | 0.55              |
| 1:E:321:ILE:HG21  | 1:E:325:GLY:HA3    | 1.89                     | 0.55              |
| 1:I:120:PRO:O     | 1:I:122:ASN:N      | 2.37                     | 0.55              |
| 1:N:372:ILE:HD12  | 1:N:374:GLU:HG2    | 1.88                     | 0.55              |
| 1:G:114:ARG:HE    | 1:G:120:PRO:HD3    | 1.72                     | 0.55              |
| 1:A:105:LEU:HG    | 1:A:233:TRP:CD1    | 2.42                     | 0.55              |
| 1:I:288:VAL:H     | 1:I:295:VAL:HG23   | 1.72                     | 0.55              |
| 1:K:321:ILE:HG21  | 1:K:325:GLY:HA3    | 1.88                     | 0.55              |
| 1:P:105:LEU:HG    | 1:P:233:TRP:CD1    | 2.42                     | 0.55              |
| 1:J:93:SER:HB3    | 1:J:255:PHE:CE1    | 2.42                     | 0.54              |
| 1:E:109:ASN:H     | 1:E:240:THR:HB     | 1.72                     | 0.54              |
| 1:J:127:ASN:HB2   | 1:J:227:ASN:OD1    | 2.07                     | 0.54              |
| 1:A:129:LEU:HD22  | 1:A:138:VAL:HG23   | 1.88                     | 0.54              |
| 1:F:336:ALA:O     | 1:F:338:SER:N      | 2.38                     | 0.54              |
| 1:O:336:ALA:O     | 1:O:338:SER:N      | 2.39                     | 0.54              |
| 1:K:288:VAL:HG22  | 1:K:295:VAL:HG22   | 1.90                     | 0.54              |
| 1:N:113:LEU:HD21  | 1:N:116:ASN:HA     | 1.90                     | 0.54              |
| 1:A:150:ASN:O     | 1:A:208:THR:HG21   | 2.08                     | 0.54              |
| 1:A:347:ILE:HG23  | 1:A:351:ALA:HB3    | 1.88                     | 0.54              |
| 1:A:373:THR:OG1   | 1:N:182:ASP:OD1    | 2.25                     | 0.54              |
| 1:H:113:LEU:HD21  | 1:H:116:ASN:HA     | 1.88                     | 0.54              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:K:105:LEU:HD12  | 1:K:246:ILE:HD11   | 1.89                     | 0.54              |
| 1:K:182:ASP:OD1   | 1:N:373:THR:OG1    | 2.23                     | 0.54              |
| 1:E:181:PRO:HG3   | 1:E:187:LEU:HD23   | 1.90                     | 0.54              |
| 1:H:105:LEU:HG    | 1:H:233:TRP:CD1    | 2.42                     | 0.54              |
| 1:J:312:SER:HA    | 1:J:361:ALA:HA     | 1.90                     | 0.54              |
| 1:D:99[A]:ARG:HG2 | 1:D:99[A]:ARG:HH11 | 1.73                     | 0.54              |
| 1:D:312:SER:HA    | 1:D:361:ALA:HA     | 1.89                     | 0.54              |
| 1:K:150:ASN:O     | 1:K:208:THR:HG21   | 2.08                     | 0.54              |
| 1:P:312:SER:HA    | 1:P:361:ALA:HA     | 1.89                     | 0.54              |
| 1:L:358:LEU:HD23  | 1:L:361:ALA:CB     | 2.38                     | 0.53              |
| 1:O:358:LEU:HD23  | 1:O:361:ALA:CB     | 2.38                     | 0.53              |
| 1:E:129:LEU:HD22  | 1:E:138:VAL:HG23   | 1.90                     | 0.53              |
| 1:G:93:SER:HB3    | 1:G:255:PHE:CE1    | 2.42                     | 0.53              |
| 1:N:362:THR:OG1   | 1:N:363:ASN:N      | 2.38                     | 0.53              |
| 1:G:147:TYR:OH    | 1:G:226:ILE:O      | 2.25                     | 0.53              |
| 1:N:108:THR:HG23  | 1:N:113:LEU:HD13   | 1.89                     | 0.53              |
| 1:B:134:PHE:HB3   | 1:B:137:LEU:HB3    | 1.90                     | 0.53              |
| 1:E:150:ASN:O     | 1:E:208:THR:HG21   | 2.09                     | 0.53              |
| 1:O:120:PRO:O     | 1:O:122:ASN:N      | 2.39                     | 0.53              |
| 1:D:93:SER:HB3    | 1:D:255:PHE:CE1    | 2.44                     | 0.53              |
| 1:G:159:LEU:HB2   | 1:G:244:GLY:HA2    | 1.91                     | 0.53              |
| 1:B:120:PRO:O     | 1:B:122:ASN:N      | 2.40                     | 0.53              |
| 1:D:127:ASN:HB2   | 1:D:227:ASN:OD1    | 2.08                     | 0.53              |
| 1:P:159:LEU:HB2   | 1:P:244:GLY:HA2    | 1.91                     | 0.53              |
| 1:H:260:THR:HG22  | 1:H:261:SER:O      | 2.09                     | 0.52              |
| 1:G:105:LEU:HG    | 1:G:233:TRP:CD1    | 2.44                     | 0.52              |
| 1:J:114:ARG:HE    | 1:J:120:PRO:HD3    | 1.73                     | 0.52              |
| 1:L:120:PRO:O     | 1:L:122:ASN:N      | 2.38                     | 0.52              |
| 1:L:336:ALA:O     | 1:L:338:SER:N      | 2.40                     | 0.52              |
| 1:M:105:LEU:HG    | 1:M:233:TRP:CD1    | 2.45                     | 0.52              |
| 1:N:347:ILE:HG23  | 1:N:351:ALA:HB3    | 1.92                     | 0.52              |
| 1:H:129:LEU:HD22  | 1:H:138:VAL:HG23   | 1.92                     | 0.52              |
| 1:L:320:SER:HG    | 1:L:354:SER:HG     | 1.57                     | 0.52              |
| 1:D:105:LEU:HG    | 1:D:233:TRP:CD1    | 2.45                     | 0.52              |
| 1:E:107:GLY:HA2   | 1:E:113:LEU:HD22   | 1.92                     | 0.52              |
| 1:J:267:LEU:HD13  | 1:J:278:ARG:HB2    | 1.92                     | 0.52              |
| 1:N:107:GLY:HA2   | 1:N:113:LEU:HD22   | 1.91                     | 0.52              |
| 1:P:126:ILE:HD13  | 1:P:152:LEU:HD21   | 1.91                     | 0.52              |
| 1:D:99[B]:ARG:NH2 | 1:D:155:GLU:OE1    | 2.43                     | 0.52              |
| 1:K:107:GLY:HA2   | 1:K:113:LEU:HD22   | 1.92                     | 0.52              |
| 1:L:372:ILE:HD11  | 1:N:262:PRO:HG3    | 1.92                     | 0.52              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:M:114:ARG:HE    | 1:M:120:PRO:HD3  | 1.73                     | 0.52              |
| 1:P:127:ASN:HB2   | 1:P:227:ASN:OD1  | 2.09                     | 0.52              |
| 1:A:260:THR:HG22  | 1:A:261:SER:O    | 2.10                     | 0.52              |
| 1:G:127:ASN:HB2   | 1:G:227:ASN:OD1  | 2.09                     | 0.52              |
| 1:I:372:ILE:HD12  | 1:I:374:GLU:HG2  | 1.92                     | 0.52              |
| 1:J:105:LEU:HG    | 1:J:233:TRP:CD1  | 2.45                     | 0.52              |
| 1:D:126:ILE:HD13  | 1:D:152:LEU:HD21 | 1.92                     | 0.52              |
| 1:F:134:PHE:HB3   | 1:F:137:LEU:HB3  | 1.92                     | 0.52              |
| 1:D:159:LEU:HB2   | 1:D:244:GLY:HA2  | 1.92                     | 0.52              |
| 1:F:120:PRO:O     | 1:F:122:ASN:N    | 2.38                     | 0.52              |
| 1:O:209:ASP:OD2   | 1:O:213:ARG:NH2  | 2.37                     | 0.52              |
| 1:P:267:LEU:HD13  | 1:P:278:ARG:HB2  | 1.92                     | 0.52              |
| 1:A:105:LEU:HD12  | 1:A:246:ILE:HD11 | 1.92                     | 0.51              |
| 1:I:134:PHE:HB3   | 1:I:137:LEU:HB3  | 1.91                     | 0.51              |
| 1:A:269:ARG:HG3   | 1:A:276:GLN:HB3  | 1.92                     | 0.51              |
| 1:E:105:LEU:HG    | 1:E:233:TRP:CD1  | 2.45                     | 0.51              |
| 1:J:109:ASN:N     | 1:J:240:THR:HB   | 2.21                     | 0.51              |
| 1:N:105:LEU:HG    | 1:N:233:TRP:CD1  | 2.45                     | 0.51              |
| 1:O:134:PHE:HB3   | 1:O:137:LEU:HB3  | 1.91                     | 0.51              |
| 1:P:331:PHE:CD2   | 1:P:379:VAL:HG23 | 2.44                     | 0.51              |
| 1:D:114:ARG:HE    | 1:D:120:PRO:HD3  | 1.76                     | 0.51              |
| 1:B:358:LEU:HD23  | 1:B:361:ALA:HB2  | 1.93                     | 0.51              |
| 1:H:347:ILE:HG23  | 1:H:351:ALA:HB3  | 1.91                     | 0.51              |
| 1:L:134:PHE:HB3   | 1:L:137:LEU:HB3  | 1.91                     | 0.51              |
| 1:M:126:ILE:HD13  | 1:M:152:LEU:HD21 | 1.92                     | 0.51              |
| 1:D:175:ASP:HB3   | 1:D:178:ASP:HB2  | 1.93                     | 0.51              |
| 1:I:143:ASN:HB3   | 1:K:136:TRP:CZ2  | 2.46                     | 0.51              |
| 1:B:124:PHE:CE1   | 1:B:132:PHE:HE2  | 2.29                     | 0.51              |
| 1:F:109:ASN:N     | 1:F:240:THR:HB   | 2.25                     | 0.51              |
| 1:M:99[B]:ARG:NH2 | 1:M:155:GLU:OE1  | 2.44                     | 0.51              |
| 1:H:108:THR:HG23  | 1:H:113:LEU:HD13 | 1.92                     | 0.51              |
| 1:F:153:ARG:HD3   | 1:F:205:THR:HG23 | 1.92                     | 0.50              |
| 1:G:126:ILE:HD13  | 1:G:152:LEU:HD21 | 1.93                     | 0.50              |
| 1:H:181:PRO:HG3   | 1:H:187:LEU:HD23 | 1.93                     | 0.50              |
| 1:M:301:PRO:HD3   | 1:M:349:VAL:HG22 | 1.93                     | 0.50              |
| 1:E:105:LEU:HD12  | 1:E:246:ILE:HD11 | 1.93                     | 0.50              |
| 1:L:260:THR:HG22  | 1:L:261:SER:O    | 2.10                     | 0.50              |
| 1:B:358:LEU:HD23  | 1:B:361:ALA:CB   | 2.41                     | 0.50              |
| 1:I:320:SER:HG    | 1:I:354:SER:HG   | 1.58                     | 0.50              |
| 1:F:303:THR:HB    | 1:F:371:ALA:O    | 2.12                     | 0.50              |
| 1:G:331:PHE:CD2   | 1:G:379:VAL:HG23 | 2.47                     | 0.50              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:K:105:LEU:HG    | 1:K:233:TRP:CD1  | 2.46                     | 0.50              |
| 1:I:124:PHE:CE1   | 1:I:132:PHE:HE2  | 2.30                     | 0.50              |
| 1:J:99[B]:ARG:NH2 | 1:J:155:GLU:OE1  | 2.45                     | 0.50              |
| 1:K:269:ARG:HG3   | 1:K:276:GLN:HB3  | 1.93                     | 0.50              |
| 1:E:372:ILE:HD12  | 1:E:374:GLU:HG2  | 1.93                     | 0.50              |
| 1:B:266:SER:HB3   | 1:E:375:ASN:HD22 | 1.77                     | 0.50              |
| 1:D:331:PHE:CD1   | 1:D:379:VAL:HG23 | 2.46                     | 0.50              |
| 1:M:331:PHE:CD2   | 1:M:379:VAL:HG23 | 2.47                     | 0.50              |
| 1:F:107:GLY:HA2   | 1:F:113:LEU:HD23 | 1.93                     | 0.50              |
| 1:O:124:PHE:CE1   | 1:O:132:PHE:HE2  | 2.29                     | 0.50              |
| 1:G:109:ASN:N     | 1:G:240:THR:HB   | 2.25                     | 0.49              |
| 1:K:313:THR:O     | 1:K:314:VAL:HG12 | 2.11                     | 0.49              |
| 1:F:99[A]:ARG:HD2 | 1:F:249:GLU:OE1  | 2.12                     | 0.49              |
| 1:F:292:THR:O     | 1:F:358:LEU:HB2  | 2.11                     | 0.49              |
| 1:J:175:ASP:HB3   | 1:J:178:ASP:HB2  | 1.93                     | 0.49              |
| 1:K:108:THR:HG23  | 1:K:113:LEU:HD13 | 1.94                     | 0.49              |
| 1:N:150:ASN:O     | 1:N:208:THR:HG21 | 2.11                     | 0.49              |
| 1:N:269:ARG:HG3   | 1:N:276:GLN:HB3  | 1.93                     | 0.49              |
| 1:A:182:ASP:OD1   | 1:E:373:THR:OG1  | 2.23                     | 0.49              |
| 1:F:124:PHE:CE1   | 1:F:132:PHE:HE2  | 2.30                     | 0.49              |
| 1:L:318:THR:HB    | 1:L:356:SER:HB2  | 1.94                     | 0.49              |
| 1:L:321:ILE:HA    | 1:L:352:ASN:O    | 2.12                     | 0.49              |
| 1:K:347:ILE:HG23  | 1:K:351:ALA:HB3  | 1.94                     | 0.49              |
| 1:N:105:LEU:HD12  | 1:N:246:ILE:HD11 | 1.94                     | 0.49              |
| 1:I:136:TRP:CZ2   | 1:K:143:ASN:HB3  | 2.48                     | 0.49              |
| 1:J:331:PHE:CD1   | 1:J:379:VAL:HG23 | 2.47                     | 0.49              |
| 1:K:181:PRO:HG3   | 1:K:187:LEU:HD23 | 1.95                     | 0.49              |
| 1:N:299:ARG:NH2   | 4:N:503:HOH:O    | 2.45                     | 0.49              |
| 1:E:108:THR:HG23  | 1:E:113:LEU:HD13 | 1.94                     | 0.49              |
| 1:H:107:GLY:HA2   | 1:H:113:LEU:HD22 | 1.94                     | 0.49              |
| 1:I:292:THR:O     | 1:I:358:LEU:HB2  | 2.13                     | 0.49              |
| 1:E:167:ARG:NH2   | 1:H:159:LEU:HD13 | 2.28                     | 0.49              |
| 1:O:99[A]:ARG:HD2 | 1:O:249:GLU:OE1  | 2.13                     | 0.49              |
| 1:A:107:GLY:HA2   | 1:A:113:LEU:HD22 | 1.94                     | 0.49              |
| 1:I:372:ILE:HG13  | 1:I:375:ASN:OD1  | 2.13                     | 0.49              |
| 1:A:136:TRP:CZ2   | 1:O:143:ASN:HB3  | 2.47                     | 0.48              |
| 1:F:372:ILE:HD11  | 1:H:262:PRO:HG3  | 1.94                     | 0.48              |
| 1:N:167:ARG:HD2   | 1:N:195:GLU:HB3  | 1.94                     | 0.48              |
| 1:E:298:ALA:CB    | 1:E:347:ILE:HG21 | 2.41                     | 0.48              |
| 1:E:347:ILE:HG23  | 1:E:351:ALA:HB3  | 1.94                     | 0.48              |
| 1:A:262:PRO:HG3   | 1:O:372:ILE:HD11 | 1.95                     | 0.48              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:J:295:VAL:HG12  | 1:J:354:SER:HB2   | 1.96                     | 0.48              |
| 1:L:294:LEU:HB2   | 1:L:355:LEU:HB2   | 1.96                     | 0.48              |
| 1:B:260:THR:HG22  | 1:B:261:SER:O     | 2.14                     | 0.48              |
| 1:F:143:ASN:HB3   | 1:H:136:TRP:CZ2   | 2.48                     | 0.48              |
| 1:N:181:PRO:HG3   | 1:N:187:LEU:HD23  | 1.95                     | 0.48              |
| 1:P:114:ARG:HE    | 1:P:120:PRO:HD3   | 1.78                     | 0.48              |
| 1:H:105:LEU:HD12  | 1:H:246:ILE:HD11  | 1.95                     | 0.48              |
| 1:I:153:ARG:HD3   | 1:I:205:THR:HG23  | 1.96                     | 0.48              |
| 1:O:121:ASN:HB3   | 1:O:230:GLN:OE1   | 2.13                     | 0.48              |
| 1:B:311:ASN:O     | 1:B:361:ALA:HA    | 2.13                     | 0.48              |
| 1:G:99[B]:ARG:NH2 | 1:G:155:GLU:OE1   | 2.45                     | 0.48              |
| 1:L:124:PHE:CE1   | 1:L:132:PHE:HE2   | 2.31                     | 0.48              |
| 1:L:303:THR:HB    | 1:L:371:ALA:O     | 2.13                     | 0.48              |
| 1:K:372:ILE:HD12  | 1:K:374:GLU:HG2   | 1.95                     | 0.48              |
| 1:D:271:SER:HA    | 1:D:272:ALA:HA    | 1.62                     | 0.48              |
| 1:P:134:PHE:HB3   | 1:P:137:LEU:HB3   | 1.95                     | 0.48              |
| 1:K:298:ALA:CB    | 1:K:347:ILE:HG21  | 2.42                     | 0.48              |
| 1:H:372:ILE:HD12  | 1:H:374:GLU:HG2   | 1.96                     | 0.47              |
| 1:A:108:THR:HG23  | 1:A:113:LEU:HD13  | 1.95                     | 0.47              |
| 1:L:153:ARG:HD3   | 1:L:205:THR:HG23  | 1.95                     | 0.47              |
| 1:A:181:PRO:HG3   | 1:A:187:LEU:HD23  | 1.95                     | 0.47              |
| 1:B:99[A]:ARG:HD2 | 1:B:249:GLU:OE1   | 2.14                     | 0.47              |
| 1:B:114:ARG:HD2   | 1:B:181:PRO:HD2   | 1.96                     | 0.47              |
| 1:D:301:PRO:HD3   | 1:D:349:VAL:HG22  | 1.95                     | 0.47              |
| 1:H:269:ARG:HG3   | 1:H:276:GLN:HB3   | 1.97                     | 0.47              |
| 1:I:266:SER:HB3   | 1:K:375:ASN:HD22  | 1.77                     | 0.47              |
| 1:M:121:ASN:HD21  | 1:M:299:ARG:HE    | 1.62                     | 0.47              |
| 1:M:159:LEU:HB2   | 1:M:244:GLY:HA2   | 1.96                     | 0.47              |
| 1:P:121:ASN:HD21  | 1:P:299:ARG:HE    | 1.61                     | 0.47              |
| 1:L:266:SER:HB3   | 1:N:375:ASN:HD22  | 1.79                     | 0.47              |
| 1:A:294:LEU:HD12  | 1:A:294:LEU:HA    | 1.78                     | 0.47              |
| 1:J:159:LEU:HB2   | 1:J:244:GLY:HA2   | 1.97                     | 0.47              |
| 1:D:81:LYS:O      | 1:D:99[A]:ARG:NH2 | 2.47                     | 0.47              |
| 1:D:91:LYS:HA     | 1:D:91:LYS:HD2    | 1.67                     | 0.47              |
| 1:L:292:THR:O     | 1:L:358:LEU:HB2   | 2.15                     | 0.47              |
| 1:L:299:ARG:NH2   | 4:L:404:HOH:O     | 2.39                     | 0.47              |
| 1:M:175:ASP:HB3   | 1:M:178:ASP:HB2   | 1.97                     | 0.47              |
| 1:E:260:THR:HG22  | 1:E:261:SER:O     | 2.14                     | 0.47              |
| 1:G:134:PHE:HB3   | 1:G:137:LEU:HB3   | 1.96                     | 0.47              |
| 1:I:161:ASN:O     | 1:I:199:TRP:HB3   | 2.15                     | 0.47              |
| 1:L:143:ASN:HB3   | 1:N:136:TRP:CZ2   | 2.50                     | 0.47              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:H:150:ASN:O     | 1:H:208:THR:HG21  | 2.15                     | 0.47              |
| 1:N:260:THR:HG22  | 1:N:261:SER:O     | 2.15                     | 0.47              |
| 1:O:292:THR:O     | 1:O:358:LEU:HB2   | 2.15                     | 0.47              |
| 1:B:113:LEU:HD12  | 1:B:113:LEU:HA    | 1.75                     | 0.47              |
| 1:B:136:TRP:CZ2   | 1:E:143:ASN:HB3   | 2.50                     | 0.47              |
| 1:B:303:THR:HB    | 1:B:371:ALA:O     | 2.15                     | 0.47              |
| 1:G:295:VAL:HG12  | 1:G:354:SER:HB2   | 1.97                     | 0.47              |
| 1:I:311:ASN:O     | 1:I:361:ALA:HA    | 2.15                     | 0.47              |
| 1:P:129:LEU:HA    | 1:P:129:LEU:HD22  | 1.70                     | 0.47              |
| 1:B:109:ASN:N     | 1:B:240:THR:HB    | 2.27                     | 0.46              |
| 1:D:109:ASN:N     | 1:D:240:THR:HB    | 2.28                     | 0.46              |
| 1:G:134:PHE:O     | 1:G:138:VAL:HG23  | 2.15                     | 0.46              |
| 1:G:267:LEU:HD13  | 1:G:278:ARG:HB2   | 1.97                     | 0.46              |
| 1:P:99[B]:ARG:NH2 | 1:P:155:GLU:OE1   | 2.47                     | 0.46              |
| 1:G:91:LYS:HD2    | 1:G:91:LYS:HA     | 1.63                     | 0.46              |
| 1:G:114:ARG:HD2   | 1:G:181:PRO:HD2   | 1.97                     | 0.46              |
| 1:J:95:ARG:NH2    | 1:J:150:ASN:HD21  | 2.13                     | 0.46              |
| 1:O:303:THR:HB    | 1:O:371:ALA:O     | 2.15                     | 0.46              |
| 1:B:143:ASN:HB3   | 1:E:136:TRP:CZ2   | 2.51                     | 0.46              |
| 1:D:290:SER:OG    | 1:D:291:ALA:N     | 2.48                     | 0.46              |
| 1:J:134:PHE:HB3   | 1:J:137:LEU:HB3   | 1.98                     | 0.46              |
| 1:P:312:SER:O     | 1:P:337:GLY:HA2   | 2.16                     | 0.46              |
| 1:A:313:THR:O     | 1:A:314:VAL:HG12  | 2.15                     | 0.46              |
| 1:B:372:ILE:HG13  | 1:B:375:ASN:OD1   | 2.15                     | 0.46              |
| 1:L:286:LEU:HD13  | 1:L:296:TRP:CZ3   | 2.51                     | 0.46              |
| 1:O:114:ARG:HD2   | 1:O:181:PRO:HD2   | 1.97                     | 0.46              |
| 1:E:370:ARG:HA    | 1:E:370:ARG:HD3   | 1.61                     | 0.46              |
| 1:F:161:ASN:N     | 1:J:165:ASN:HB3   | 2.30                     | 0.46              |
| 1:G:175:ASP:HB3   | 1:G:178:ASP:HB2   | 1.97                     | 0.46              |
| 1:J:312:SER:O     | 1:J:337:GLY:HA2   | 2.14                     | 0.46              |
| 1:M:109:ASN:N     | 1:M:240:THR:HB    | 2.25                     | 0.46              |
| 1:M:263:LEU:HD22  | 1:M:281:LEU:HD11  | 1.97                     | 0.46              |
| 1:P:175:ASP:HB3   | 1:P:178:ASP:HB2   | 1.98                     | 0.46              |
| 1:D:165:ASN:HD22  | 1:O:161:ASN:HD22  | 1.64                     | 0.46              |
| 1:D:196:ILE:HD13  | 1:D:202:THR:HB    | 1.98                     | 0.46              |
| 1:I:108:THR:HG23  | 1:I:113:LEU:HD22  | 1.97                     | 0.46              |
| 1:E:300:VAL:O     | 1:E:304:TYR:OH    | 2.30                     | 0.46              |
| 1:G:95:ARG:HG3    | 1:G:253:ASP:OD1   | 2.16                     | 0.46              |
| 1:H:313:THR:O     | 1:H:314:VAL:HG12  | 2.16                     | 0.46              |
| 1:J:81:LYS:O      | 1:J:99[A]:ARG:NH2 | 2.49                     | 0.46              |
| 1:B:372:ILE:HD11  | 1:E:262:PRO:HG3   | 1.97                     | 0.46              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:E:269:ARG:HG3   | 1:E:276:GLN:HB3  | 1.98                     | 0.46              |
| 1:J:301:PRO:HD3   | 1:J:349:VAL:HG22 | 1.98                     | 0.46              |
| 1:M:134:PHE:HB3   | 1:M:137:LEU:HB3  | 1.98                     | 0.46              |
| 1:D:134:PHE:HB3   | 1:D:137:LEU:HB3  | 1.98                     | 0.46              |
| 1:G:301:PRO:HD3   | 1:G:349:VAL:HG22 | 1.98                     | 0.46              |
| 1:J:126:ILE:HD13  | 1:J:152:LEU:HD21 | 1.98                     | 0.46              |
| 1:L:120:PRO:HG2   | 4:L:404:HOH:O    | 2.15                     | 0.46              |
| 1:B:318:THR:HG1   | 1:B:357:GLY:H    | 1.56                     | 0.45              |
| 1:G:105:LEU:HD12  | 1:G:246:ILE:HD11 | 1.97                     | 0.45              |
| 1:I:123:ASP:OD1   | 1:I:123:ASP:N    | 2.47                     | 0.45              |
| 1:J:121:ASN:HD21  | 1:J:299:ARG:HE   | 1.64                     | 0.45              |
| 1:J:196:ILE:HG21  | 1:J:202:THR:HB   | 1.98                     | 0.45              |
| 1:L:108:THR:HG23  | 1:L:113:LEU:HD22 | 1.98                     | 0.45              |
| 1:L:161:ASN:N     | 1:P:165:ASN:HB3  | 2.31                     | 0.45              |
| 1:N:298:ALA:CB    | 1:N:347:ILE:HG21 | 2.42                     | 0.45              |
| 1:N:313:THR:O     | 1:N:314:VAL:HG12 | 2.16                     | 0.45              |
| 1:O:260:THR:HG22  | 1:O:261:SER:O    | 2.16                     | 0.45              |
| 1:P:109:ASN:N     | 1:P:240:THR:HB   | 2.26                     | 0.45              |
| 1:D:312:SER:O     | 1:D:337:GLY:HA2  | 2.15                     | 0.45              |
| 1:I:303:THR:HB    | 1:I:371:ALA:O    | 2.17                     | 0.45              |
| 1:B:271:SER:HA    | 1:B:272:ALA:HA   | 1.79                     | 0.45              |
| 1:D:165:ASN:HB3   | 1:O:161:ASN:N    | 2.32                     | 0.45              |
| 1:J:60:ILE:HG21   | 1:J:60:ILE:HD13  | 1.35                     | 0.45              |
| 1:K:157:VAL:HA    | 1:K:158:PRO:HD3  | 1.77                     | 0.45              |
| 1:K:370:ARG:HD3   | 1:K:370:ARG:HA   | 1.63                     | 0.45              |
| 1:D:267:LEU:HD13  | 1:D:278:ARG:HB2  | 1.98                     | 0.45              |
| 1:G:60:ILE:HG22   | 1:G:61:ALA:N     | 2.32                     | 0.45              |
| 1:M:298:ALA:HB2   | 1:M:347:ILE:HD13 | 1.98                     | 0.45              |
| 1:E:157:VAL:HA    | 1:E:158:PRO:HD3  | 1.80                     | 0.45              |
| 1:A:375:ASN:HD22  | 1:O:266:SER:HB3  | 1.82                     | 0.45              |
| 1:N:157:VAL:HA    | 1:N:158:PRO:HD3  | 1.77                     | 0.45              |
| 1:O:107:GLY:HA2   | 1:O:113:LEU:HD23 | 1.99                     | 0.45              |
| 1:E:288:VAL:HG22  | 1:E:295:VAL:HG13 | 1.99                     | 0.45              |
| 1:E:313:THR:O     | 1:E:314:VAL:HG12 | 2.16                     | 0.45              |
| 1:F:283:TYR:OH    | 1:F:370:ARG:NH2  | 2.49                     | 0.45              |
| 1:L:99[A]:ARG:HD2 | 1:L:249:GLU:OE1  | 2.16                     | 0.45              |
| 1:M:60:ILE:HD13   | 1:M:60:ILE:HG21  | 1.28                     | 0.45              |
| 1:N:291:ALA:HB1   | 1:N:360:GLY:HA2  | 1.99                     | 0.45              |
| 1:B:347:ILE:HG13  | 1:B:351:ALA:HB3  | 1.99                     | 0.45              |
| 1:G:121:ASN:HD21  | 1:G:299:ARG:HE   | 1.64                     | 0.45              |
| 1:H:298:ALA:CB    | 1:H:347:ILE:HG21 | 2.45                     | 0.45              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:G:271:SER:HA    | 1:G:272:ALA:HA   | 1.59                     | 0.45              |
| 1:I:347:ILE:HG13  | 1:I:351:ALA:HB3  | 1.99                     | 0.45              |
| 1:M:307:THR:HB    | 1:M:367:PHE:HB2  | 1.99                     | 0.45              |
| 1:H:256:GLU:OE1   | 1:J:192:HIS:NE2  | 2.49                     | 0.44              |
| 1:K:260:THR:HG22  | 1:K:261:SER:O    | 2.17                     | 0.44              |
| 1:M:264:LEU:HD23  | 1:M:264:LEU:H    | 1.81                     | 0.44              |
| 1:P:142:ALA:HB2   | 1:P:263:LEU:HD21 | 1.98                     | 0.44              |
| 1:A:167:ARG:HD2   | 1:A:195:GLU:HB3  | 1.98                     | 0.44              |
| 1:E:109:ASN:N     | 1:E:240:THR:HB   | 2.32                     | 0.44              |
| 1:F:313:THR:O     | 1:F:313:THR:OG1  | 2.34                     | 0.44              |
| 1:I:296:TRP:NE1   | 1:I:308:ILE:HD13 | 2.32                     | 0.44              |
| 1:L:296:TRP:NE1   | 1:L:308:ILE:HD13 | 2.32                     | 0.44              |
| 1:G:263:LEU:HD22  | 1:G:281:LEU:HD11 | 1.99                     | 0.44              |
| 1:I:318:THR:HG1   | 1:I:357:GLY:H    | 1.57                     | 0.44              |
| 1:K:109:ASN:N     | 1:K:240:THR:HB   | 2.30                     | 0.44              |
| 1:N:271:SER:HA    | 1:N:272:ALA:HA   | 1.71                     | 0.44              |
| 1:O:294:LEU:HB2   | 1:O:355:LEU:HB2  | 2.00                     | 0.44              |
| 1:O:318:THR:CB    | 1:O:356:SER:HB2  | 2.47                     | 0.44              |
| 1:D:279:MET:HE3   | 1:D:279:MET:HB2  | 1.89                     | 0.44              |
| 1:J:196:ILE:HD13  | 1:J:202:THR:HB   | 2.00                     | 0.44              |
| 1:J:271:SER:HA    | 1:J:272:ALA:HA   | 1.61                     | 0.44              |
| 1:K:167:ARG:HD2   | 1:K:195:GLU:HB3  | 1.99                     | 0.44              |
| 1:O:284:PHE:CE1   | 1:O:298:ALA:HB2  | 2.53                     | 0.44              |
| 1:O:311:ASN:O     | 1:O:361:ALA:HA   | 2.18                     | 0.44              |
| 1:B:124:PHE:HE1   | 1:B:233:TRP:CH2  | 2.34                     | 0.44              |
| 1:E:292:THR:O     | 1:E:358:LEU:HB2  | 2.18                     | 0.44              |
| 1:F:209:ASP:OD2   | 1:F:213:ARG:NH2  | 2.37                     | 0.44              |
| 1:I:99[A]:ARG:HD2 | 1:I:249:GLU:OE1  | 2.18                     | 0.44              |
| 1:M:129:LEU:HD22  | 1:M:129:LEU:HA   | 1.68                     | 0.44              |
| 1:M:281:LEU:HD12  | 1:M:283:TYR:OH   | 2.18                     | 0.44              |
| 1:F:114:ARG:HD2   | 1:F:181:PRO:HD2  | 1.99                     | 0.44              |
| 1:F:269:ARG:HE    | 1:F:289:ALA:HB3  | 1.83                     | 0.44              |
| 1:K:314:VAL:H     | 1:K:336:ALA:HA   | 1.83                     | 0.44              |
| 1:O:271:SER:HA    | 1:O:272:ALA:HA   | 1.73                     | 0.44              |
| 1:O:312:SER:HB2   | 1:O:313:THR:H    | 1.65                     | 0.44              |
| 1:P:264:LEU:HB2   | 1:P:369:VAL:HG12 | 1.99                     | 0.44              |
| 1:I:100:GLU:OE2   | 1:I:250:TYR:OH   | 2.26                     | 0.44              |
| 1:J:225:LEU:HD23  | 1:J:225:LEU:HA   | 1.84                     | 0.44              |
| 1:M:114:ARG:HD2   | 1:M:181:PRO:HD2  | 1.99                     | 0.44              |
| 1:A:109:ASN:N     | 1:A:240:THR:HB   | 2.33                     | 0.44              |
| 1:B:347:ILE:HD12  | 1:B:347:ILE:HA   | 1.89                     | 0.44              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:N:370:ARG:HD3  | 1:N:370:ARG:HA   | 1.62                     | 0.44              |
| 1:O:224:LYS:HB3  | 1:P:214:PHE:CE2  | 2.53                     | 0.44              |
| 1:P:264:LEU:HD23 | 1:P:264:LEU:H    | 1.83                     | 0.44              |
| 1:F:311:ASN:O    | 1:F:361:ALA:HA   | 2.17                     | 0.44              |
| 1:F:372:ILE:HG13 | 1:F:375:ASN:OD1  | 2.18                     | 0.44              |
| 1:G:196:ILE:HD13 | 1:G:202:THR:HB   | 2.00                     | 0.44              |
| 1:I:270:GLU:HA   | 1:I:271:SER:HB2  | 2.00                     | 0.44              |
| 1:M:290:SER:OG   | 1:M:291:ALA:N    | 2.51                     | 0.44              |
| 1:A:143:ASN:HB3  | 1:O:136:TRP:CZ2  | 2.53                     | 0.43              |
| 1:B:158:PRO:HB3  | 1:B:198:PRO:O    | 2.18                     | 0.43              |
| 1:I:260:THR:HG22 | 1:I:261:SER:O    | 2.18                     | 0.43              |
| 1:L:113:LEU:HD12 | 1:L:113:LEU:HA   | 1.75                     | 0.43              |
| 1:L:129:LEU:O    | 1:L:131:PRO:HD3  | 2.18                     | 0.43              |
| 1:L:300:VAL:HA   | 1:L:301:PRO:HD2  | 1.79                     | 0.43              |
| 1:M:203:LYS:HE2  | 1:M:203:LYS:HB3  | 1.81                     | 0.43              |
| 1:G:60:ILE:HD13  | 1:G:60:ILE:HG21  | 1.51                     | 0.43              |
| 1:G:100:GLU:OE2  | 1:G:136:TRP:HB3  | 2.18                     | 0.43              |
| 1:I:113:LEU:HD12 | 1:I:113:LEU:HA   | 1.81                     | 0.43              |
| 1:B:284:PHE:CE2  | 1:B:298:ALA:HB2  | 2.53                     | 0.43              |
| 1:G:286:LEU:HD13 | 1:G:296:TRP:CE3  | 2.53                     | 0.43              |
| 1:H:167:ARG:HD2  | 1:H:195:GLU:HB3  | 2.00                     | 0.43              |
| 1:I:129:LEU:HD22 | 1:I:129:LEU:HA   | 1.81                     | 0.43              |
| 1:L:100:GLU:CD   | 1:L:136:TRP:HB3  | 2.43                     | 0.43              |
| 1:J:290:SER:OG   | 1:J:291:ALA:N    | 2.51                     | 0.43              |
| 1:J:314:VAL:HG13 | 1:J:315:GLY:N    | 2.33                     | 0.43              |
| 1:L:290:SER:HG   | 1:L:293:ASP:H    | 1.63                     | 0.43              |
| 1:D:313:THR:O    | 1:D:314:VAL:HG12 | 2.19                     | 0.43              |
| 1:I:224:LYS:HB3  | 1:J:214:PHE:CE2  | 2.53                     | 0.43              |
| 1:O:307:THR:HB   | 1:O:367:PHE:HB2  | 1.99                     | 0.43              |
| 1:J:281:LEU:HD12 | 1:J:283:TYR:OH   | 2.18                     | 0.43              |
| 1:M:134:PHE:O    | 1:M:138:VAL:HG23 | 2.19                     | 0.43              |
| 1:M:295:VAL:HG12 | 1:M:354:SER:HB2  | 2.01                     | 0.43              |
| 1:N:109:ASN:N    | 1:N:240:THR:HB   | 2.32                     | 0.43              |
| 1:O:127:ASN:HB2  | 1:O:227:ASN:OD1  | 2.18                     | 0.43              |
| 1:P:295:VAL:HG12 | 1:P:354:SER:HB2  | 1.99                     | 0.43              |
| 1:B:296:TRP:NE1  | 1:B:308:ILE:HD13 | 2.34                     | 0.43              |
| 1:D:134:PHE:O    | 1:D:138:VAL:HG23 | 2.17                     | 0.43              |
| 1:D:295:VAL:HG12 | 1:D:354:SER:HB2  | 2.00                     | 0.43              |
| 1:D:298:ALA:HB2  | 1:D:347:ILE:HD13 | 2.01                     | 0.43              |
| 1:F:129:LEU:HD22 | 1:F:129:LEU:HA   | 1.78                     | 0.43              |
| 1:F:187:LEU:HD22 | 1:F:193:LEU:HD13 | 2.01                     | 0.43              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:312:SER:O    | 1:G:337:GLY:HA2  | 2.17                     | 0.43              |
| 1:G:313:THR:O    | 1:G:314:VAL:HG12 | 2.18                     | 0.43              |
| 1:M:267:LEU:HD13 | 1:M:278:ARG:HB2  | 2.00                     | 0.43              |
| 1:N:256:GLU:OE1  | 1:P:192:HIS:NE2  | 2.50                     | 0.43              |
| 1:D:114:ARG:HD2  | 1:D:181:PRO:HD2  | 2.00                     | 0.43              |
| 1:G:310:PHE:CE1  | 1:G:339:SER:HB2  | 2.54                     | 0.43              |
| 1:M:271:SER:HA   | 1:M:272:ALA:HA   | 1.63                     | 0.43              |
| 1:O:372:ILE:HG13 | 1:O:375:ASN:OD1  | 2.19                     | 0.43              |
| 1:B:294:LEU:HB2  | 1:B:355:LEU:HB2  | 2.00                     | 0.43              |
| 1:F:124:PHE:HE1  | 1:F:233:TRP:CH2  | 2.37                     | 0.43              |
| 1:F:260:THR:HG22 | 1:F:261:SER:O    | 2.19                     | 0.43              |
| 1:G:290:SER:OG   | 1:G:291:ALA:N    | 2.52                     | 0.43              |
| 1:M:91:LYS:HD2   | 1:M:91:LYS:HA    | 1.67                     | 0.43              |
| 1:N:159:LEU:HD12 | 1:N:159:LEU:HA   | 1.83                     | 0.43              |
| 1:B:129:LEU:HD22 | 1:B:129:LEU:HA   | 1.85                     | 0.43              |
| 1:B:307:THR:HB   | 1:B:367:PHE:HB2  | 2.01                     | 0.43              |
| 1:D:281:LEU:HD12 | 1:D:283:TYR:OH   | 2.19                     | 0.43              |
| 1:J:314:VAL:HG13 | 1:J:315:GLY:H    | 1.84                     | 0.43              |
| 1:K:147:TYR:OH   | 1:K:226:ILE:O    | 2.25                     | 0.43              |
| 1:L:311:ASN:O    | 1:L:361:ALA:HA   | 2.19                     | 0.43              |
| 1:M:95:ARG:NH2   | 1:M:150:ASN:HD21 | 2.17                     | 0.43              |
| 1:M:310:PHE:CE1  | 1:M:339:SER:HB2  | 2.54                     | 0.43              |
| 1:O:270:GLU:HB2  | 1:O:271:SER:C    | 2.44                     | 0.43              |
| 1:A:329:SER:HB2  | 1:A:377:VAL:HG13 | 2.01                     | 0.42              |
| 1:I:173:ASP:OD1  | 1:I:174:LYS:N    | 2.52                     | 0.42              |
| 1:I:294:LEU:HB2  | 1:I:355:LEU:HB2  | 2.01                     | 0.42              |
| 1:J:60:ILE:HG22  | 1:J:61:ALA:N     | 2.33                     | 0.42              |
| 1:L:159:LEU:HD12 | 1:L:159:LEU:HA   | 1.83                     | 0.42              |
| 1:N:292:THR:O    | 1:N:358:LEU:HB2  | 2.19                     | 0.42              |
| 1:B:348:ARG:CG   | 1:B:349:VAL:N    | 2.82                     | 0.42              |
| 1:H:206:VAL:HG23 | 1:H:207:PRO:HD2  | 2.02                     | 0.42              |
| 1:I:114:ARG:HD2  | 1:I:181:PRO:HD2  | 2.01                     | 0.42              |
| 1:I:209:ASP:OD2  | 1:I:213:ARG:NH2  | 2.41                     | 0.42              |
| 1:L:136:TRP:CZ2  | 1:N:143:ASN:HB3  | 2.54                     | 0.42              |
| 1:L:348:ARG:CG   | 1:L:349:VAL:N    | 2.83                     | 0.42              |
| 1:J:271:SER:HB3  | 1:J:363:ASN:H    | 1.84                     | 0.42              |
| 1:D:162:THR:HA   | 1:D:199:TRP:CG   | 2.53                     | 0.42              |
| 1:E:187:LEU:O    | 1:E:187:LEU:HD22 | 2.19                     | 0.42              |
| 1:G:298:ALA:HB2  | 1:G:347:ILE:HD13 | 2.02                     | 0.42              |
| 1:M:196:ILE:HG21 | 1:M:202:THR:HB   | 2.01                     | 0.42              |
| 1:B:107:GLY:HA2  | 1:B:113:LEU:HD23 | 2.00                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:91:LYS:HA    | 1:J:91:LYS:HD2   | 1.65                     | 0.42              |
| 1:K:188:ALA:HA   | 1:K:193:LEU:HD22 | 2.01                     | 0.42              |
| 1:K:294:LEU:HA   | 1:K:294:LEU:HD12 | 1.80                     | 0.42              |
| 1:L:372:ILE:HG13 | 1:L:375:ASN:OD1  | 2.19                     | 0.42              |
| 1:O:321:ILE:HA   | 1:O:352:ASN:O    | 2.20                     | 0.42              |
| 1:P:196:ILE:HG21 | 1:P:202:THR:HB   | 2.01                     | 0.42              |
| 1:B:292:THR:O    | 1:B:358:LEU:HB2  | 2.19                     | 0.42              |
| 1:D:60:ILE:HG21  | 1:D:60:ILE:HD13  | 1.44                     | 0.42              |
| 1:D:121:ASN:HD21 | 1:D:299:ARG:HE   | 1.68                     | 0.42              |
| 1:D:271:SER:HB3  | 1:D:363:ASN:H    | 1.84                     | 0.42              |
| 1:E:335:THR:OG1  | 1:E:336:ALA:N    | 2.52                     | 0.42              |
| 1:F:112:PHE:HE1  | 1:F:184:ARG:HG2  | 1.85                     | 0.42              |
| 1:G:114:ARG:NE   | 1:G:120:PRO:HD3  | 2.34                     | 0.42              |
| 1:K:201:ILE:HG22 | 1:K:202:THR:N    | 2.34                     | 0.42              |
| 1:M:196:ILE:HD13 | 1:M:202:THR:HB   | 2.00                     | 0.42              |
| 1:A:298:ALA:CB   | 1:A:347:ILE:HG21 | 2.43                     | 0.42              |
| 1:B:127:ASN:HB2  | 1:B:227:ASN:OD1  | 2.19                     | 0.42              |
| 1:L:318:THR:HG1  | 1:L:357:GLY:H    | 1.59                     | 0.42              |
| 1:F:321:ILE:HA   | 1:F:352:ASN:O    | 2.19                     | 0.42              |
| 1:I:172:PHE:CE2  | 1:I:207:PRO:HD2  | 2.55                     | 0.42              |
| 1:L:263:LEU:HD23 | 1:L:263:LEU:HA   | 1.88                     | 0.42              |
| 1:L:307:THR:HB   | 1:L:367:PHE:HB2  | 2.01                     | 0.42              |
| 1:M:114:ARG:NE   | 1:M:120:PRO:HD3  | 2.35                     | 0.42              |
| 1:M:218:THR:HB   | 1:M:278:ARG:HH22 | 1.85                     | 0.42              |
| 1:O:313:THR:O    | 1:O:313:THR:OG1  | 2.36                     | 0.42              |
| 1:O:348:ARG:CG   | 1:O:349:VAL:N    | 2.83                     | 0.42              |
| 1:B:276:GLN:OE1  | 1:B:286:LEU:HB3  | 2.20                     | 0.42              |
| 1:D:196:ILE:HG21 | 1:D:202:THR:HB   | 2.01                     | 0.42              |
| 1:D:263:LEU:HD22 | 1:D:281:LEU:HD11 | 2.00                     | 0.42              |
| 1:F:348:ARG:CG   | 1:F:349:VAL:N    | 2.82                     | 0.42              |
| 1:H:370:ARG:HD3  | 1:H:370:ARG:HA   | 1.74                     | 0.42              |
| 1:L:283:TYR:OH   | 1:L:370:ARG:NH2  | 2.53                     | 0.42              |
| 1:N:187:LEU:HD22 | 1:N:187:LEU:O    | 2.20                     | 0.42              |
| 1:O:158:PRO:HB3  | 1:O:198:PRO:O    | 2.19                     | 0.42              |
| 1:P:95:ARG:HG3   | 1:P:253:ASP:OD1  | 2.20                     | 0.42              |
| 1:P:134:PHE:O    | 1:P:138:VAL:HG23 | 2.19                     | 0.42              |
| 1:P:218:THR:HB   | 1:P:278:ARG:HH22 | 1.85                     | 0.42              |
| 1:P:271:SER:HA   | 1:P:272:ALA:HA   | 1.61                     | 0.42              |
| 1:F:94:VAL:HG21  | 1:H:96:ILE:HD13  | 2.02                     | 0.42              |
| 1:F:335:THR:HG1  | 1:F:336:ALA:H    | 1.58                     | 0.42              |
| 1:L:183:ASP:OD2  | 1:L:185:ALA:HB3  | 2.20                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:347:ILE:HG13 | 1:L:351:ALA:HB3  | 2.01                     | 0.42              |
| 1:M:286:LEU:HD13 | 1:M:296:TRP:CE3  | 2.54                     | 0.42              |
| 1:P:273:SER:O    | 1:P:274:SER:HB2  | 2.20                     | 0.42              |
| 1:A:206:VAL:HG23 | 1:A:207:PRO:HD2  | 2.01                     | 0.41              |
| 1:A:271:SER:HA   | 1:A:272:ALA:HA   | 1.70                     | 0.41              |
| 1:B:321:ILE:HA   | 1:B:352:ASN:O    | 2.20                     | 0.41              |
| 1:F:294:LEU:HB2  | 1:F:355:LEU:HB2  | 2.02                     | 0.41              |
| 1:G:95:ARG:NH2   | 1:G:150:ASN:HD21 | 2.18                     | 0.41              |
| 1:G:203:LYS:HB3  | 1:G:203:LYS:HE2  | 1.79                     | 0.41              |
| 1:H:157:VAL:HA   | 1:H:158:PRO:HD3  | 1.79                     | 0.41              |
| 1:L:127:ASN:HB2  | 1:L:227:ASN:OD1  | 2.20                     | 0.41              |
| 1:L:312:SER:O    | 1:L:337:GLY:HA2  | 2.20                     | 0.41              |
| 1:O:300:VAL:O    | 1:O:304:TYR:OH   | 2.30                     | 0.41              |
| 1:P:271:SER:HB3  | 1:P:363:ASN:H    | 1.84                     | 0.41              |
| 1:P:298:ALA:HB2  | 1:P:347:ILE:HD13 | 2.02                     | 0.41              |
| 1:F:266:SER:HB3  | 1:H:375:ASN:HD22 | 1.85                     | 0.41              |
| 1:I:127:ASN:HB2  | 1:I:227:ASN:OD1  | 2.20                     | 0.41              |
| 1:L:129:LEU:O    | 1:L:129:LEU:HD13 | 2.20                     | 0.41              |
| 1:O:312:SER:O    | 1:O:337:GLY:HA2  | 2.21                     | 0.41              |
| 1:P:290:SER:OG   | 1:P:291:ALA:N    | 2.53                     | 0.41              |
| 1:B:269:ARG:HE   | 1:B:289:ALA:HB3  | 1.85                     | 0.41              |
| 1:F:129:LEU:HD13 | 1:F:129:LEU:O    | 2.20                     | 0.41              |
| 1:F:347:ILE:HG13 | 1:F:351:ALA:HB3  | 2.02                     | 0.41              |
| 1:J:210:ASN:OD1  | 1:J:210:ASN:C    | 2.63                     | 0.41              |
| 1:K:271:SER:HA   | 1:K:272:ALA:HA   | 1.73                     | 0.41              |
| 1:O:296:TRP:NE1  | 1:O:308:ILE:HD13 | 2.36                     | 0.41              |
| 1:G:264:LEU:H    | 1:G:264:LEU:HD23 | 1.84                     | 0.41              |
| 1:H:109:ASN:N    | 1:H:240:THR:HB   | 2.32                     | 0.41              |
| 1:I:269:ARG:HE   | 1:I:289:ALA:HB3  | 1.84                     | 0.41              |
| 1:I:299:ARG:HA   | 1:I:299:ARG:HD2  | 1.95                     | 0.41              |
| 1:J:114:ARG:NE   | 1:J:120:PRO:HD3  | 2.36                     | 0.41              |
| 1:N:114:ARG:H    | 1:N:114:ARG:HG2  | 1.76                     | 0.41              |
| 1:O:153:ARG:HD3  | 1:O:205:THR:HG23 | 2.02                     | 0.41              |
| 1:P:286:LEU:HD13 | 1:P:296:TRP:CE3  | 2.56                     | 0.41              |
| 1:A:162:THR:HG23 | 1:E:162:THR:HG21 | 2.01                     | 0.41              |
| 1:A:178:ASP:HA   | 1:A:179:PRO:HD3  | 1.94                     | 0.41              |
| 1:E:329:SER:HB2  | 1:E:377:VAL:HG13 | 2.02                     | 0.41              |
| 1:F:158:PRO:HB3  | 1:F:198:PRO:O    | 2.20                     | 0.41              |
| 1:J:134:PHE:O    | 1:J:138:VAL:HG23 | 2.20                     | 0.41              |
| 1:N:294:LEU:HD12 | 1:N:294:LEU:HA   | 1.80                     | 0.41              |
| 1:P:196:ILE:HD13 | 1:P:202:THR:HB   | 2.01                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:P:301:PRO:HD3  | 1:P:349:VAL:HG22 | 2.02                     | 0.41              |
| 1:A:159:LEU:HD13 | 1:N:167:ARG:NH2  | 2.35                     | 0.41              |
| 1:D:105:LEU:HD12 | 1:D:246:ILE:HD11 | 2.02                     | 0.41              |
| 1:D:225:LEU:HD23 | 1:D:225:LEU:HA   | 1.82                     | 0.41              |
| 1:D:310:PHE:CE1  | 1:D:339:SER:HB2  | 2.56                     | 0.41              |
| 1:F:136:TRP:CZ2  | 1:H:143:ASN:HB3  | 2.55                     | 0.41              |
| 1:F:296:TRP:NE1  | 1:F:308:ILE:HD13 | 2.35                     | 0.41              |
| 1:F:318:THR:HG1  | 1:F:357:GLY:H    | 1.54                     | 0.41              |
| 1:M:271:SER:HB3  | 1:M:363:ASN:H    | 1.86                     | 0.41              |
| 1:P:60:ILE:HD13  | 1:P:60:ILE:HG21  | 1.49                     | 0.41              |
| 1:P:114:ARG:HD2  | 1:P:181:PRO:HD2  | 2.02                     | 0.41              |
| 1:P:203:LYS:HB3  | 1:P:203:LYS:HE2  | 1.81                     | 0.41              |
| 1:P:310:PHE:CE1  | 1:P:339:SER:HB2  | 2.55                     | 0.41              |
| 1:A:292:THR:O    | 1:A:358:LEU:HB2  | 2.20                     | 0.41              |
| 1:B:312:SER:HB2  | 1:B:313:THR:H    | 1.67                     | 0.41              |
| 1:D:264:LEU:HB2  | 1:D:369:VAL:HG12 | 2.02                     | 0.41              |
| 1:H:187:LEU:HD22 | 1:H:187:LEU:O    | 2.21                     | 0.41              |
| 1:H:188:ALA:HA   | 1:H:193:LEU:HD22 | 2.02                     | 0.41              |
| 1:I:263:LEU:HD23 | 1:I:263:LEU:HA   | 1.93                     | 0.41              |
| 1:I:267:LEU:O    | 1:I:365:GLN:HA   | 2.21                     | 0.41              |
| 1:I:284:PHE:CE1  | 1:I:298:ALA:HB2  | 2.55                     | 0.41              |
| 1:J:142:ALA:HB2  | 1:J:263:LEU:HD21 | 2.02                     | 0.41              |
| 1:K:121:ASN:HB3  | 1:K:123:ASP:H    | 1.86                     | 0.41              |
| 1:L:173:ASP:OD1  | 1:L:174:LYS:N    | 2.54                     | 0.41              |
| 1:O:269:ARG:HE   | 1:O:289:ALA:HB3  | 1.86                     | 0.41              |
| 1:P:279:MET:HE3  | 1:P:279:MET:HB2  | 1.90                     | 0.41              |
| 1:B:296:TRP:CD2  | 1:B:366:LEU:HD12 | 2.55                     | 0.41              |
| 1:B:300:VAL:O    | 1:B:304:TYR:OH   | 2.28                     | 0.41              |
| 1:B:312:SER:O    | 1:B:337:GLY:HA2  | 2.21                     | 0.41              |
| 1:B:335:THR:HG1  | 1:B:336:ALA:H    | 1.60                     | 0.41              |
| 1:E:293:ASP:OD2  | 1:E:356:SER:HB2  | 2.21                     | 0.41              |
| 1:F:100:GLU:CD   | 1:F:136:TRP:HB3  | 2.46                     | 0.41              |
| 1:G:196:ILE:HG21 | 1:G:202:THR:HB   | 2.03                     | 0.41              |
| 1:I:169:ALA:CB   | 1:I:195:GLU:HG2  | 2.51                     | 0.41              |
| 1:J:95:ARG:HG3   | 1:J:253:ASP:OD1  | 2.21                     | 0.41              |
| 1:N:349:VAL:O    | 1:N:351:ALA:N    | 2.54                     | 0.41              |
| 1:F:209:ASP:CG   | 1:F:213:ARG:HH22 | 2.27                     | 0.41              |
| 1:F:271:SER:HA   | 1:F:272:ALA:HA   | 1.80                     | 0.41              |
| 1:F:369:VAL:HG11 | 1:H:264:LEU:HD13 | 2.01                     | 0.41              |
| 1:G:279:MET:HE3  | 1:G:279:MET:HB2  | 1.99                     | 0.41              |
| 1:I:288:VAL:HG12 | 1:I:295:VAL:CG2  | 2.51                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:312:SER:O    | 1:I:337:GLY:HA2  | 2.20                     | 0.41              |
| 1:I:321:ILE:HA   | 1:I:352:ASN:O    | 2.21                     | 0.41              |
| 1:L:161:ASN:O    | 1:L:199:TRP:HB3  | 2.21                     | 0.41              |
| 1:L:224:LYS:HB3  | 1:M:214:PHE:CE2  | 2.55                     | 0.41              |
| 1:O:103:SER:HB2  | 1:O:132:PHE:CZ   | 2.56                     | 0.41              |
| 1:O:124:PHE:HE1  | 1:O:233:TRP:CH2  | 2.38                     | 0.41              |
| 1:A:169:ALA:HA   | 1:A:194:SER:O    | 2.21                     | 0.41              |
| 1:A:256:GLU:OE1  | 1:D:192:HIS:NE2  | 2.52                     | 0.41              |
| 1:F:312:SER:O    | 1:F:337:GLY:HA2  | 2.20                     | 0.41              |
| 1:K:167:ARG:NH2  | 1:N:159:LEU:HD13 | 2.36                     | 0.41              |
| 1:L:112:PHE:HE1  | 1:L:184:ARG:HG2  | 1.86                     | 0.41              |
| 1:A:159:LEU:HD12 | 1:A:159:LEU:HA   | 1.83                     | 0.40              |
| 1:E:291:ALA:HB1  | 1:E:360:GLY:HA2  | 2.04                     | 0.40              |
| 1:H:291:ALA:HB1  | 1:H:360:GLY:HA2  | 2.03                     | 0.40              |
| 1:H:294:LEU:HD12 | 1:H:294:LEU:HA   | 1.74                     | 0.40              |
| 1:L:124:PHE:HE1  | 1:L:233:TRP:CH2  | 2.39                     | 0.40              |
| 1:A:167:ARG:NH2  | 1:E:159:LEU:HD13 | 2.37                     | 0.40              |
| 1:H:162:THR:HG23 | 1:K:162:THR:HG21 | 2.04                     | 0.40              |
| 1:I:158:PRO:HB3  | 1:I:198:PRO:O    | 2.20                     | 0.40              |
| 1:K:291:ALA:HB1  | 1:K:360:GLY:HA2  | 2.02                     | 0.40              |
| 1:L:296:TRP:CD2  | 1:L:366:LEU:HD12 | 2.56                     | 0.40              |
| 1:O:109:ASN:N    | 1:O:240:THR:HB   | 2.30                     | 0.40              |
| 1:O:129:LEU:O    | 1:O:131:PRO:HD3  | 2.22                     | 0.40              |
| 1:P:281:LEU:HD12 | 1:P:283:TYR:OH   | 2.22                     | 0.40              |
| 1:D:314:VAL:N    | 1:D:336:ALA:O    | 2.44                     | 0.40              |
| 1:E:167:ARG:HD2  | 1:E:195:GLU:HB3  | 2.02                     | 0.40              |
| 1:E:201:ILE:H    | 1:E:201:ILE:HG12 | 1.72                     | 0.40              |
| 1:F:265:GLU:O    | 1:F:367:PHE:HA   | 2.21                     | 0.40              |
| 1:J:95:ARG:NH2   | 1:J:150:ASN:ND2  | 2.69                     | 0.40              |
| 1:J:279:MET:HE3  | 1:J:279:MET:HB2  | 1.85                     | 0.40              |
| 1:L:267:LEU:O    | 1:L:365:GLN:HA   | 2.21                     | 0.40              |
| 1:M:264:LEU:HB2  | 1:M:369:VAL:HG12 | 2.03                     | 0.40              |
| 1:N:335:THR:OG1  | 1:N:336:ALA:N    | 2.53                     | 0.40              |
| 1:B:276:GLN:CD   | 1:B:286:LEU:HD23 | 2.47                     | 0.40              |
| 1:E:169:ALA:HA   | 1:E:194:SER:O    | 2.20                     | 0.40              |
| 1:F:113:LEU:HD12 | 1:F:113:LEU:HA   | 1.77                     | 0.40              |
| 1:F:161:ASN:CB   | 1:J:165:ASN:HB3  | 2.48                     | 0.40              |
| 1:J:263:LEU:HD22 | 1:J:281:LEU:HD11 | 2.04                     | 0.40              |
| 1:M:105:LEU:HD12 | 1:M:246:ILE:HD11 | 2.02                     | 0.40              |
| 1:O:112:PHE:HE1  | 1:O:184:ARG:HG2  | 1.87                     | 0.40              |
| 1:A:370:ARG:HD3  | 1:A:370:ARG:HA   | 1.63                     | 0.40              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:318:THR:CB   | 1:B:356:SER:HB2  | 2.48                     | 0.40              |
| 1:G:162:THR:HA   | 1:G:199:TRP:CG   | 2.56                     | 0.40              |
| 1:G:272:ALA:O    | 1:G:274:SER:N    | 2.55                     | 0.40              |
| 1:I:129:LEU:HD13 | 1:I:129:LEU:O    | 2.22                     | 0.40              |
| 1:L:109:ASN:N    | 1:L:240:THR:HB   | 2.32                     | 0.40              |
| 1:N:310:PHE:CE1  | 1:N:339:SER:HB2  | 2.57                     | 0.40              |
| 1:O:149:PHE:CD1  | 1:O:252:VAL:HG13 | 2.57                     | 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     | 288/380 (76%) | 264 (92%) | 17 (6%) | 7 (2%)   | 4           | 16 |
| 1   | B     | 290/380 (76%) | 250 (86%) | 24 (8%) | 16 (6%)  | 1           | 4  |
| 1   | D     | 321/380 (84%) | 286 (89%) | 25 (8%) | 10 (3%)  | 3           | 12 |
| 1   | E     | 288/380 (76%) | 268 (93%) | 13 (4%) | 7 (2%)   | 4           | 16 |
| 1   | F     | 290/380 (76%) | 249 (86%) | 25 (9%) | 16 (6%)  | 1           | 4  |
| 1   | G     | 321/380 (84%) | 286 (89%) | 25 (8%) | 10 (3%)  | 3           | 12 |
| 1   | H     | 288/380 (76%) | 264 (92%) | 17 (6%) | 7 (2%)   | 4           | 16 |
| 1   | I     | 290/380 (76%) | 248 (86%) | 26 (9%) | 16 (6%)  | 1           | 4  |
| 1   | J     | 321/380 (84%) | 287 (89%) | 24 (8%) | 10 (3%)  | 3           | 12 |
| 1   | K     | 288/380 (76%) | 265 (92%) | 16 (6%) | 7 (2%)   | 4           | 16 |
| 1   | L     | 290/380 (76%) | 249 (86%) | 23 (8%) | 18 (6%)  | 1           | 3  |
| 1   | M     | 321/380 (84%) | 286 (89%) | 24 (8%) | 11 (3%)  | 3           | 11 |
| 1   | N     | 288/380 (76%) | 264 (92%) | 17 (6%) | 7 (2%)   | 4           | 16 |
| 1   | O     | 290/380 (76%) | 249 (86%) | 25 (9%) | 16 (6%)  | 1           | 4  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|----------|----------|-------------|----|
| 1   | P     | 321/380 (84%)   | 284 (88%)  | 28 (9%)  | 9 (3%)   | 4           | 14 |
| All | All   | 4495/5700 (79%) | 3999 (89%) | 329 (7%) | 167 (4%) | 2           | 9  |

All (167) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 128 | PRO  |
| 1   | B     | 273 | SER  |
| 1   | B     | 314 | VAL  |
| 1   | B     | 317 | LEU  |
| 1   | B     | 350 | ASN  |
| 1   | D     | 118 | THR  |
| 1   | D     | 128 | PRO  |
| 1   | D     | 314 | VAL  |
| 1   | F     | 128 | PRO  |
| 1   | F     | 273 | SER  |
| 1   | F     | 314 | VAL  |
| 1   | F     | 317 | LEU  |
| 1   | F     | 350 | ASN  |
| 1   | G     | 118 | THR  |
| 1   | G     | 128 | PRO  |
| 1   | G     | 314 | VAL  |
| 1   | I     | 128 | PRO  |
| 1   | I     | 273 | SER  |
| 1   | I     | 314 | VAL  |
| 1   | I     | 317 | LEU  |
| 1   | I     | 350 | ASN  |
| 1   | J     | 118 | THR  |
| 1   | J     | 128 | PRO  |
| 1   | J     | 314 | VAL  |
| 1   | L     | 128 | PRO  |
| 1   | L     | 273 | SER  |
| 1   | L     | 314 | VAL  |
| 1   | L     | 317 | LEU  |
| 1   | L     | 350 | ASN  |
| 1   | M     | 118 | THR  |
| 1   | M     | 128 | PRO  |
| 1   | M     | 314 | VAL  |
| 1   | O     | 128 | PRO  |
| 1   | O     | 273 | SER  |
| 1   | O     | 314 | VAL  |
| 1   | O     | 317 | LEU  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | O     | 350 | ASN  |
| 1   | P     | 118 | THR  |
| 1   | P     | 128 | PRO  |
| 1   | P     | 314 | VAL  |
| 1   | A     | 273 | SER  |
| 1   | A     | 350 | ASN  |
| 1   | B     | 121 | ASN  |
| 1   | B     | 219 | SER  |
| 1   | B     | 336 | ALA  |
| 1   | B     | 337 | GLY  |
| 1   | B     | 349 | VAL  |
| 1   | D     | 117 | GLY  |
| 1   | E     | 273 | SER  |
| 1   | E     | 350 | ASN  |
| 1   | F     | 121 | ASN  |
| 1   | F     | 219 | SER  |
| 1   | F     | 327 | ILE  |
| 1   | F     | 336 | ALA  |
| 1   | F     | 337 | GLY  |
| 1   | F     | 349 | VAL  |
| 1   | G     | 117 | GLY  |
| 1   | G     | 273 | SER  |
| 1   | H     | 273 | SER  |
| 1   | H     | 350 | ASN  |
| 1   | I     | 121 | ASN  |
| 1   | I     | 219 | SER  |
| 1   | I     | 336 | ALA  |
| 1   | I     | 337 | GLY  |
| 1   | I     | 349 | VAL  |
| 1   | J     | 117 | GLY  |
| 1   | K     | 273 | SER  |
| 1   | K     | 350 | ASN  |
| 1   | L     | 121 | ASN  |
| 1   | L     | 129 | LEU  |
| 1   | L     | 219 | SER  |
| 1   | L     | 327 | ILE  |
| 1   | L     | 336 | ALA  |
| 1   | L     | 337 | GLY  |
| 1   | L     | 349 | VAL  |
| 1   | N     | 273 | SER  |
| 1   | N     | 350 | ASN  |
| 1   | O     | 121 | ASN  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | O     | 219 | SER  |
| 1   | O     | 336 | ALA  |
| 1   | O     | 337 | GLY  |
| 1   | O     | 349 | VAL  |
| 1   | B     | 120 | PRO  |
| 1   | B     | 338 | SER  |
| 1   | D     | 336 | ALA  |
| 1   | D     | 363 | ASN  |
| 1   | F     | 120 | PRO  |
| 1   | F     | 338 | SER  |
| 1   | G     | 274 | SER  |
| 1   | G     | 289 | ALA  |
| 1   | G     | 336 | ALA  |
| 1   | I     | 120 | PRO  |
| 1   | I     | 338 | SER  |
| 1   | J     | 336 | ALA  |
| 1   | J     | 363 | ASN  |
| 1   | L     | 120 | PRO  |
| 1   | L     | 338 | SER  |
| 1   | M     | 117 | GLY  |
| 1   | M     | 336 | ALA  |
| 1   | O     | 120 | PRO  |
| 1   | O     | 327 | ILE  |
| 1   | O     | 338 | SER  |
| 1   | P     | 117 | GLY  |
| 1   | P     | 273 | SER  |
| 1   | P     | 336 | ALA  |
| 1   | P     | 363 | ASN  |
| 1   | B     | 327 | ILE  |
| 1   | D     | 273 | SER  |
| 1   | G     | 363 | ASN  |
| 1   | I     | 327 | ILE  |
| 1   | J     | 273 | SER  |
| 1   | M     | 61  | ALA  |
| 1   | M     | 273 | SER  |
| 1   | M     | 289 | ALA  |
| 1   | M     | 363 | ASN  |
| 1   | N     | 256 | GLU  |
| 1   | A     | 120 | PRO  |
| 1   | A     | 256 | GLU  |
| 1   | A     | 314 | VAL  |
| 1   | B     | 351 | ALA  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | E     | 120 | PRO  |
| 1   | E     | 256 | GLU  |
| 1   | H     | 120 | PRO  |
| 1   | H     | 256 | GLU  |
| 1   | H     | 314 | VAL  |
| 1   | I     | 290 | SER  |
| 1   | I     | 351 | ALA  |
| 1   | J     | 61  | ALA  |
| 1   | J     | 91  | LYS  |
| 1   | K     | 120 | PRO  |
| 1   | K     | 256 | GLU  |
| 1   | L     | 290 | SER  |
| 1   | L     | 351 | ALA  |
| 1   | M     | 165 | ASN  |
| 1   | M     | 256 | GLU  |
| 1   | N     | 120 | PRO  |
| 1   | O     | 290 | SER  |
| 1   | O     | 351 | ALA  |
| 1   | P     | 289 | ALA  |
| 1   | B     | 290 | SER  |
| 1   | D     | 91  | LYS  |
| 1   | D     | 256 | GLU  |
| 1   | D     | 289 | ALA  |
| 1   | F     | 290 | SER  |
| 1   | F     | 351 | ALA  |
| 1   | G     | 256 | GLU  |
| 1   | H     | 324 | GLY  |
| 1   | I     | 372 | ILE  |
| 1   | J     | 289 | ALA  |
| 1   | L     | 372 | ILE  |
| 1   | N     | 314 | VAL  |
| 1   | N     | 324 | GLY  |
| 1   | O     | 372 | ILE  |
| 1   | B     | 372 | ILE  |
| 1   | E     | 238 | GLY  |
| 1   | F     | 372 | ILE  |
| 1   | K     | 314 | VAL  |
| 1   | A     | 324 | GLY  |
| 1   | E     | 314 | VAL  |
| 1   | E     | 324 | GLY  |
| 1   | K     | 324 | GLY  |
| 1   | N     | 238 | GLY  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 238 | GLY  |
| 1   | H     | 238 | GLY  |
| 1   | L     | 102 | VAL  |
| 1   | P     | 238 | GLY  |
| 1   | K     | 238 | GLY  |

### 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     | 244/309 (79%)   | 206 (84%)  | 38 (16%)  | 2           | 8 |
| 1   | B     | 245/309 (79%)   | 206 (84%)  | 39 (16%)  | 2           | 7 |
| 1   | D     | 267/309 (86%)   | 228 (85%)  | 39 (15%)  | 3           | 9 |
| 1   | E     | 244/309 (79%)   | 208 (85%)  | 36 (15%)  | 3           | 9 |
| 1   | F     | 245/309 (79%)   | 206 (84%)  | 39 (16%)  | 2           | 7 |
| 1   | G     | 267/309 (86%)   | 225 (84%)  | 42 (16%)  | 2           | 7 |
| 1   | H     | 244/309 (79%)   | 209 (86%)  | 35 (14%)  | 3           | 9 |
| 1   | I     | 245/309 (79%)   | 205 (84%)  | 40 (16%)  | 2           | 7 |
| 1   | J     | 267/309 (86%)   | 226 (85%)  | 41 (15%)  | 2           | 8 |
| 1   | K     | 244/309 (79%)   | 209 (86%)  | 35 (14%)  | 3           | 9 |
| 1   | L     | 245/309 (79%)   | 205 (84%)  | 40 (16%)  | 2           | 7 |
| 1   | M     | 267/309 (86%)   | 228 (85%)  | 39 (15%)  | 3           | 9 |
| 1   | N     | 244/309 (79%)   | 208 (85%)  | 36 (15%)  | 3           | 9 |
| 1   | O     | 245/309 (79%)   | 205 (84%)  | 40 (16%)  | 2           | 7 |
| 1   | P     | 267/309 (86%)   | 228 (85%)  | 39 (15%)  | 3           | 9 |
| All | All   | 3780/4635 (82%) | 3202 (85%) | 578 (15%) | 3           | 8 |

All (578) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 94  | VAL  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res   | Type |
|-----|-------|-------|------|
| 1   | A     | 99[A] | ARG  |
| 1   | A     | 99[B] | ARG  |
| 1   | A     | 103   | SER  |
| 1   | A     | 111   | GLU  |
| 1   | A     | 114   | ARG  |
| 1   | A     | 129   | LEU  |
| 1   | A     | 159   | LEU  |
| 1   | A     | 160   | VAL  |
| 1   | A     | 168   | VAL  |
| 1   | A     | 187   | LEU  |
| 1   | A     | 196   | ILE  |
| 1   | A     | 201   | ILE  |
| 1   | A     | 206   | VAL  |
| 1   | A     | 208   | THR  |
| 1   | A     | 211   | VAL  |
| 1   | A     | 228   | LEU  |
| 1   | A     | 252   | VAL  |
| 1   | A     | 266   | SER  |
| 1   | A     | 288   | VAL  |
| 1   | A     | 292   | THR  |
| 1   | A     | 295   | VAL  |
| 1   | A     | 296   | TRP  |
| 1   | A     | 306   | VAL  |
| 1   | A     | 314   | VAL  |
| 1   | A     | 318   | THR  |
| 1   | A     | 327   | ILE  |
| 1   | A     | 328   | ASN  |
| 1   | A     | 333   | VAL  |
| 1   | A     | 335   | THR  |
| 1   | A     | 348   | ARG  |
| 1   | A     | 349   | VAL  |
| 1   | A     | 353   | LEU  |
| 1   | A     | 356   | SER  |
| 1   | A     | 362   | THR  |
| 1   | A     | 374   | GLU  |
| 1   | A     | 377   | VAL  |
| 1   | A     | 380   | VAL  |
| 1   | B     | 91    | LYS  |
| 1   | B     | 129   | LEU  |
| 1   | B     | 159   | LEU  |
| 1   | B     | 160   | VAL  |
| 1   | B     | 162   | THR  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 174 | LYS  |
| 1   | B     | 178 | ASP  |
| 1   | B     | 183 | ASP  |
| 1   | B     | 187 | LEU  |
| 1   | B     | 205 | THR  |
| 1   | B     | 206 | VAL  |
| 1   | B     | 211 | VAL  |
| 1   | B     | 225 | LEU  |
| 1   | B     | 228 | LEU  |
| 1   | B     | 252 | VAL  |
| 1   | B     | 266 | SER  |
| 1   | B     | 273 | SER  |
| 1   | B     | 288 | VAL  |
| 1   | B     | 292 | THR  |
| 1   | B     | 293 | ASP  |
| 1   | B     | 295 | VAL  |
| 1   | B     | 314 | VAL  |
| 1   | B     | 317 | LEU  |
| 1   | B     | 318 | THR  |
| 1   | B     | 327 | ILE  |
| 1   | B     | 330 | SER  |
| 1   | B     | 334 | SER  |
| 1   | B     | 335 | THR  |
| 1   | B     | 342 | VAL  |
| 1   | B     | 348 | ARG  |
| 1   | B     | 349 | VAL  |
| 1   | B     | 352 | ASN  |
| 1   | B     | 359 | THR  |
| 1   | B     | 372 | ILE  |
| 1   | B     | 373 | THR  |
| 1   | B     | 374 | GLU  |
| 1   | B     | 377 | VAL  |
| 1   | B     | 379 | VAL  |
| 1   | B     | 380 | VAL  |
| 1   | D     | 60  | ILE  |
| 1   | D     | 70  | ILE  |
| 1   | D     | 80  | VAL  |
| 1   | D     | 91  | LYS  |
| 1   | D     | 94  | VAL  |
| 1   | D     | 95  | ARG  |
| 1   | D     | 104 | VAL  |
| 1   | D     | 106 | SER  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res   | Type |
|-----|-------|-------|------|
| 1   | D     | 129   | LEU  |
| 1   | D     | 133   | LEU  |
| 1   | D     | 139   | ASN  |
| 1   | D     | 145   | ASP  |
| 1   | D     | 151   | SER  |
| 1   | D     | 159   | LEU  |
| 1   | D     | 160   | VAL  |
| 1   | D     | 168   | VAL  |
| 1   | D     | 174   | LYS  |
| 1   | D     | 187   | LEU  |
| 1   | D     | 211   | VAL  |
| 1   | D     | 213   | ARG  |
| 1   | D     | 218   | THR  |
| 1   | D     | 225   | LEU  |
| 1   | D     | 237   | SER  |
| 1   | D     | 249   | GLU  |
| 1   | D     | 252   | VAL  |
| 1   | D     | 269   | ARG  |
| 1   | D     | 271   | SER  |
| 1   | D     | 275   | VAL  |
| 1   | D     | 295   | VAL  |
| 1   | D     | 317   | LEU  |
| 1   | D     | 329   | SER  |
| 1   | D     | 330   | SER  |
| 1   | D     | 333   | VAL  |
| 1   | D     | 342   | VAL  |
| 1   | D     | 349   | VAL  |
| 1   | D     | 359   | THR  |
| 1   | D     | 373   | THR  |
| 1   | D     | 377   | VAL  |
| 1   | D     | 380   | VAL  |
| 1   | E     | 94    | VAL  |
| 1   | E     | 99[A] | ARG  |
| 1   | E     | 99[B] | ARG  |
| 1   | E     | 103   | SER  |
| 1   | E     | 111   | GLU  |
| 1   | E     | 114   | ARG  |
| 1   | E     | 129   | LEU  |
| 1   | E     | 159   | LEU  |
| 1   | E     | 160   | VAL  |
| 1   | E     | 168   | VAL  |
| 1   | E     | 187   | LEU  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | E     | 196 | ILE  |
| 1   | E     | 201 | ILE  |
| 1   | E     | 206 | VAL  |
| 1   | E     | 208 | THR  |
| 1   | E     | 211 | VAL  |
| 1   | E     | 228 | LEU  |
| 1   | E     | 252 | VAL  |
| 1   | E     | 266 | SER  |
| 1   | E     | 288 | VAL  |
| 1   | E     | 292 | THR  |
| 1   | E     | 295 | VAL  |
| 1   | E     | 296 | TRP  |
| 1   | E     | 306 | VAL  |
| 1   | E     | 314 | VAL  |
| 1   | E     | 318 | THR  |
| 1   | E     | 327 | ILE  |
| 1   | E     | 328 | ASN  |
| 1   | E     | 333 | VAL  |
| 1   | E     | 335 | THR  |
| 1   | E     | 348 | ARG  |
| 1   | E     | 349 | VAL  |
| 1   | E     | 353 | LEU  |
| 1   | E     | 374 | GLU  |
| 1   | E     | 377 | VAL  |
| 1   | E     | 380 | VAL  |
| 1   | F     | 91  | LYS  |
| 1   | F     | 104 | VAL  |
| 1   | F     | 129 | LEU  |
| 1   | F     | 159 | LEU  |
| 1   | F     | 160 | VAL  |
| 1   | F     | 174 | LYS  |
| 1   | F     | 178 | ASP  |
| 1   | F     | 183 | ASP  |
| 1   | F     | 187 | LEU  |
| 1   | F     | 205 | THR  |
| 1   | F     | 206 | VAL  |
| 1   | F     | 211 | VAL  |
| 1   | F     | 225 | LEU  |
| 1   | F     | 228 | LEU  |
| 1   | F     | 252 | VAL  |
| 1   | F     | 266 | SER  |
| 1   | F     | 273 | SER  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | F     | 288 | VAL  |
| 1   | F     | 292 | THR  |
| 1   | F     | 293 | ASP  |
| 1   | F     | 295 | VAL  |
| 1   | F     | 314 | VAL  |
| 1   | F     | 317 | LEU  |
| 1   | F     | 318 | THR  |
| 1   | F     | 327 | ILE  |
| 1   | F     | 330 | SER  |
| 1   | F     | 334 | SER  |
| 1   | F     | 335 | THR  |
| 1   | F     | 342 | VAL  |
| 1   | F     | 348 | ARG  |
| 1   | F     | 349 | VAL  |
| 1   | F     | 352 | ASN  |
| 1   | F     | 358 | LEU  |
| 1   | F     | 359 | THR  |
| 1   | F     | 372 | ILE  |
| 1   | F     | 374 | GLU  |
| 1   | F     | 377 | VAL  |
| 1   | F     | 379 | VAL  |
| 1   | F     | 380 | VAL  |
| 1   | G     | 60  | ILE  |
| 1   | G     | 70  | ILE  |
| 1   | G     | 80  | VAL  |
| 1   | G     | 83  | ARG  |
| 1   | G     | 91  | LYS  |
| 1   | G     | 94  | VAL  |
| 1   | G     | 95  | ARG  |
| 1   | G     | 106 | SER  |
| 1   | G     | 118 | THR  |
| 1   | G     | 129 | LEU  |
| 1   | G     | 133 | LEU  |
| 1   | G     | 139 | ASN  |
| 1   | G     | 145 | ASP  |
| 1   | G     | 151 | SER  |
| 1   | G     | 159 | LEU  |
| 1   | G     | 160 | VAL  |
| 1   | G     | 168 | VAL  |
| 1   | G     | 174 | LYS  |
| 1   | G     | 187 | LEU  |
| 1   | G     | 211 | VAL  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res   | Type |
|-----|-------|-------|------|
| 1   | G     | 213   | ARG  |
| 1   | G     | 218   | THR  |
| 1   | G     | 225   | LEU  |
| 1   | G     | 237   | SER  |
| 1   | G     | 249   | GLU  |
| 1   | G     | 252   | VAL  |
| 1   | G     | 269   | ARG  |
| 1   | G     | 271   | SER  |
| 1   | G     | 274   | SER  |
| 1   | G     | 275   | VAL  |
| 1   | G     | 288   | VAL  |
| 1   | G     | 295   | VAL  |
| 1   | G     | 317   | LEU  |
| 1   | G     | 329   | SER  |
| 1   | G     | 330   | SER  |
| 1   | G     | 333   | VAL  |
| 1   | G     | 342   | VAL  |
| 1   | G     | 349   | VAL  |
| 1   | G     | 359   | THR  |
| 1   | G     | 373   | THR  |
| 1   | G     | 377   | VAL  |
| 1   | G     | 380   | VAL  |
| 1   | H     | 94    | VAL  |
| 1   | H     | 99[A] | ARG  |
| 1   | H     | 99[B] | ARG  |
| 1   | H     | 103   | SER  |
| 1   | H     | 111   | GLU  |
| 1   | H     | 114   | ARG  |
| 1   | H     | 129   | LEU  |
| 1   | H     | 159   | LEU  |
| 1   | H     | 160   | VAL  |
| 1   | H     | 168   | VAL  |
| 1   | H     | 187   | LEU  |
| 1   | H     | 196   | ILE  |
| 1   | H     | 201   | ILE  |
| 1   | H     | 206   | VAL  |
| 1   | H     | 208   | THR  |
| 1   | H     | 211   | VAL  |
| 1   | H     | 228   | LEU  |
| 1   | H     | 252   | VAL  |
| 1   | H     | 266   | SER  |
| 1   | H     | 288   | VAL  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | H     | 292 | THR  |
| 1   | H     | 295 | VAL  |
| 1   | H     | 306 | VAL  |
| 1   | H     | 314 | VAL  |
| 1   | H     | 318 | THR  |
| 1   | H     | 327 | ILE  |
| 1   | H     | 328 | ASN  |
| 1   | H     | 333 | VAL  |
| 1   | H     | 335 | THR  |
| 1   | H     | 348 | ARG  |
| 1   | H     | 349 | VAL  |
| 1   | H     | 353 | LEU  |
| 1   | H     | 374 | GLU  |
| 1   | H     | 377 | VAL  |
| 1   | H     | 380 | VAL  |
| 1   | I     | 91  | LYS  |
| 1   | I     | 93  | SER  |
| 1   | I     | 104 | VAL  |
| 1   | I     | 129 | LEU  |
| 1   | I     | 159 | LEU  |
| 1   | I     | 160 | VAL  |
| 1   | I     | 174 | LYS  |
| 1   | I     | 178 | ASP  |
| 1   | I     | 183 | ASP  |
| 1   | I     | 187 | LEU  |
| 1   | I     | 205 | THR  |
| 1   | I     | 206 | VAL  |
| 1   | I     | 211 | VAL  |
| 1   | I     | 225 | LEU  |
| 1   | I     | 228 | LEU  |
| 1   | I     | 252 | VAL  |
| 1   | I     | 266 | SER  |
| 1   | I     | 273 | SER  |
| 1   | I     | 288 | VAL  |
| 1   | I     | 292 | THR  |
| 1   | I     | 293 | ASP  |
| 1   | I     | 295 | VAL  |
| 1   | I     | 314 | VAL  |
| 1   | I     | 317 | LEU  |
| 1   | I     | 318 | THR  |
| 1   | I     | 327 | ILE  |
| 1   | I     | 330 | SER  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | I     | 334 | SER  |
| 1   | I     | 335 | THR  |
| 1   | I     | 342 | VAL  |
| 1   | I     | 348 | ARG  |
| 1   | I     | 349 | VAL  |
| 1   | I     | 352 | ASN  |
| 1   | I     | 358 | LEU  |
| 1   | I     | 359 | THR  |
| 1   | I     | 372 | ILE  |
| 1   | I     | 374 | GLU  |
| 1   | I     | 377 | VAL  |
| 1   | I     | 379 | VAL  |
| 1   | I     | 380 | VAL  |
| 1   | J     | 70  | ILE  |
| 1   | J     | 80  | VAL  |
| 1   | J     | 83  | ARG  |
| 1   | J     | 91  | LYS  |
| 1   | J     | 94  | VAL  |
| 1   | J     | 95  | ARG  |
| 1   | J     | 106 | SER  |
| 1   | J     | 122 | ASN  |
| 1   | J     | 129 | LEU  |
| 1   | J     | 133 | LEU  |
| 1   | J     | 139 | ASN  |
| 1   | J     | 145 | ASP  |
| 1   | J     | 151 | SER  |
| 1   | J     | 159 | LEU  |
| 1   | J     | 160 | VAL  |
| 1   | J     | 168 | VAL  |
| 1   | J     | 174 | LYS  |
| 1   | J     | 187 | LEU  |
| 1   | J     | 210 | ASN  |
| 1   | J     | 211 | VAL  |
| 1   | J     | 213 | ARG  |
| 1   | J     | 218 | THR  |
| 1   | J     | 225 | LEU  |
| 1   | J     | 237 | SER  |
| 1   | J     | 252 | VAL  |
| 1   | J     | 269 | ARG  |
| 1   | J     | 271 | SER  |
| 1   | J     | 275 | VAL  |
| 1   | J     | 288 | VAL  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res   | Type |
|-----|-------|-------|------|
| 1   | J     | 295   | VAL  |
| 1   | J     | 314   | VAL  |
| 1   | J     | 317   | LEU  |
| 1   | J     | 329   | SER  |
| 1   | J     | 330   | SER  |
| 1   | J     | 333   | VAL  |
| 1   | J     | 342   | VAL  |
| 1   | J     | 349   | VAL  |
| 1   | J     | 359   | THR  |
| 1   | J     | 373   | THR  |
| 1   | J     | 377   | VAL  |
| 1   | J     | 380   | VAL  |
| 1   | K     | 94    | VAL  |
| 1   | K     | 99[A] | ARG  |
| 1   | K     | 99[B] | ARG  |
| 1   | K     | 103   | SER  |
| 1   | K     | 111   | GLU  |
| 1   | K     | 114   | ARG  |
| 1   | K     | 129   | LEU  |
| 1   | K     | 159   | LEU  |
| 1   | K     | 160   | VAL  |
| 1   | K     | 168   | VAL  |
| 1   | K     | 187   | LEU  |
| 1   | K     | 196   | ILE  |
| 1   | K     | 201   | ILE  |
| 1   | K     | 206   | VAL  |
| 1   | K     | 208   | THR  |
| 1   | K     | 211   | VAL  |
| 1   | K     | 228   | LEU  |
| 1   | K     | 252   | VAL  |
| 1   | K     | 266   | SER  |
| 1   | K     | 292   | THR  |
| 1   | K     | 295   | VAL  |
| 1   | K     | 296   | TRP  |
| 1   | K     | 306   | VAL  |
| 1   | K     | 314   | VAL  |
| 1   | K     | 318   | THR  |
| 1   | K     | 327   | ILE  |
| 1   | K     | 328   | ASN  |
| 1   | K     | 333   | VAL  |
| 1   | K     | 335   | THR  |
| 1   | K     | 348   | ARG  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | K     | 349 | VAL  |
| 1   | K     | 353 | LEU  |
| 1   | K     | 374 | GLU  |
| 1   | K     | 377 | VAL  |
| 1   | K     | 380 | VAL  |
| 1   | L     | 91  | LYS  |
| 1   | L     | 93  | SER  |
| 1   | L     | 104 | VAL  |
| 1   | L     | 129 | LEU  |
| 1   | L     | 159 | LEU  |
| 1   | L     | 160 | VAL  |
| 1   | L     | 162 | THR  |
| 1   | L     | 174 | LYS  |
| 1   | L     | 178 | ASP  |
| 1   | L     | 187 | LEU  |
| 1   | L     | 205 | THR  |
| 1   | L     | 206 | VAL  |
| 1   | L     | 211 | VAL  |
| 1   | L     | 225 | LEU  |
| 1   | L     | 228 | LEU  |
| 1   | L     | 252 | VAL  |
| 1   | L     | 256 | GLU  |
| 1   | L     | 266 | SER  |
| 1   | L     | 273 | SER  |
| 1   | L     | 288 | VAL  |
| 1   | L     | 292 | THR  |
| 1   | L     | 293 | ASP  |
| 1   | L     | 295 | VAL  |
| 1   | L     | 314 | VAL  |
| 1   | L     | 317 | LEU  |
| 1   | L     | 318 | THR  |
| 1   | L     | 327 | ILE  |
| 1   | L     | 330 | SER  |
| 1   | L     | 334 | SER  |
| 1   | L     | 335 | THR  |
| 1   | L     | 342 | VAL  |
| 1   | L     | 348 | ARG  |
| 1   | L     | 349 | VAL  |
| 1   | L     | 352 | ASN  |
| 1   | L     | 359 | THR  |
| 1   | L     | 372 | ILE  |
| 1   | L     | 374 | GLU  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | L     | 377 | VAL  |
| 1   | L     | 379 | VAL  |
| 1   | L     | 380 | VAL  |
| 1   | M     | 70  | ILE  |
| 1   | M     | 80  | VAL  |
| 1   | M     | 83  | ARG  |
| 1   | M     | 91  | LYS  |
| 1   | M     | 94  | VAL  |
| 1   | M     | 95  | ARG  |
| 1   | M     | 106 | SER  |
| 1   | M     | 118 | THR  |
| 1   | M     | 129 | LEU  |
| 1   | M     | 133 | LEU  |
| 1   | M     | 139 | ASN  |
| 1   | M     | 145 | ASP  |
| 1   | M     | 151 | SER  |
| 1   | M     | 159 | LEU  |
| 1   | M     | 160 | VAL  |
| 1   | M     | 168 | VAL  |
| 1   | M     | 174 | LYS  |
| 1   | M     | 187 | LEU  |
| 1   | M     | 211 | VAL  |
| 1   | M     | 213 | ARG  |
| 1   | M     | 218 | THR  |
| 1   | M     | 225 | LEU  |
| 1   | M     | 237 | SER  |
| 1   | M     | 249 | GLU  |
| 1   | M     | 252 | VAL  |
| 1   | M     | 269 | ARG  |
| 1   | M     | 271 | SER  |
| 1   | M     | 275 | VAL  |
| 1   | M     | 295 | VAL  |
| 1   | M     | 317 | LEU  |
| 1   | M     | 329 | SER  |
| 1   | M     | 330 | SER  |
| 1   | M     | 333 | VAL  |
| 1   | M     | 342 | VAL  |
| 1   | M     | 349 | VAL  |
| 1   | M     | 359 | THR  |
| 1   | M     | 373 | THR  |
| 1   | M     | 377 | VAL  |
| 1   | M     | 380 | VAL  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res   | Type |
|-----|-------|-------|------|
| 1   | N     | 94    | VAL  |
| 1   | N     | 99[A] | ARG  |
| 1   | N     | 99[B] | ARG  |
| 1   | N     | 103   | SER  |
| 1   | N     | 111   | GLU  |
| 1   | N     | 114   | ARG  |
| 1   | N     | 129   | LEU  |
| 1   | N     | 159   | LEU  |
| 1   | N     | 160   | VAL  |
| 1   | N     | 168   | VAL  |
| 1   | N     | 187   | LEU  |
| 1   | N     | 196   | ILE  |
| 1   | N     | 201   | ILE  |
| 1   | N     | 206   | VAL  |
| 1   | N     | 208   | THR  |
| 1   | N     | 211   | VAL  |
| 1   | N     | 228   | LEU  |
| 1   | N     | 252   | VAL  |
| 1   | N     | 266   | SER  |
| 1   | N     | 288   | VAL  |
| 1   | N     | 292   | THR  |
| 1   | N     | 295   | VAL  |
| 1   | N     | 296   | TRP  |
| 1   | N     | 306   | VAL  |
| 1   | N     | 314   | VAL  |
| 1   | N     | 318   | THR  |
| 1   | N     | 327   | ILE  |
| 1   | N     | 333   | VAL  |
| 1   | N     | 335   | THR  |
| 1   | N     | 348   | ARG  |
| 1   | N     | 349   | VAL  |
| 1   | N     | 353   | LEU  |
| 1   | N     | 374   | GLU  |
| 1   | N     | 377   | VAL  |
| 1   | N     | 378   | GLN  |
| 1   | N     | 380   | VAL  |
| 1   | O     | 91    | LYS  |
| 1   | O     | 93    | SER  |
| 1   | O     | 129   | LEU  |
| 1   | O     | 159   | LEU  |
| 1   | O     | 160   | VAL  |
| 1   | O     | 162   | THR  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | O     | 174 | LYS  |
| 1   | O     | 178 | ASP  |
| 1   | O     | 183 | ASP  |
| 1   | O     | 187 | LEU  |
| 1   | O     | 205 | THR  |
| 1   | O     | 206 | VAL  |
| 1   | O     | 211 | VAL  |
| 1   | O     | 225 | LEU  |
| 1   | O     | 228 | LEU  |
| 1   | O     | 252 | VAL  |
| 1   | O     | 256 | GLU  |
| 1   | O     | 266 | SER  |
| 1   | O     | 273 | SER  |
| 1   | O     | 288 | VAL  |
| 1   | O     | 292 | THR  |
| 1   | O     | 293 | ASP  |
| 1   | O     | 295 | VAL  |
| 1   | O     | 314 | VAL  |
| 1   | O     | 317 | LEU  |
| 1   | O     | 318 | THR  |
| 1   | O     | 327 | ILE  |
| 1   | O     | 330 | SER  |
| 1   | O     | 334 | SER  |
| 1   | O     | 335 | THR  |
| 1   | O     | 342 | VAL  |
| 1   | O     | 348 | ARG  |
| 1   | O     | 349 | VAL  |
| 1   | O     | 352 | ASN  |
| 1   | O     | 359 | THR  |
| 1   | O     | 372 | ILE  |
| 1   | O     | 374 | GLU  |
| 1   | O     | 377 | VAL  |
| 1   | O     | 379 | VAL  |
| 1   | O     | 380 | VAL  |
| 1   | P     | 60  | ILE  |
| 1   | P     | 70  | ILE  |
| 1   | P     | 80  | VAL  |
| 1   | P     | 83  | ARG  |
| 1   | P     | 91  | LYS  |
| 1   | P     | 94  | VAL  |
| 1   | P     | 95  | ARG  |
| 1   | P     | 106 | SER  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | P     | 129 | LEU  |
| 1   | P     | 133 | LEU  |
| 1   | P     | 139 | ASN  |
| 1   | P     | 151 | SER  |
| 1   | P     | 159 | LEU  |
| 1   | P     | 160 | VAL  |
| 1   | P     | 168 | VAL  |
| 1   | P     | 174 | LYS  |
| 1   | P     | 187 | LEU  |
| 1   | P     | 211 | VAL  |
| 1   | P     | 213 | ARG  |
| 1   | P     | 218 | THR  |
| 1   | P     | 225 | LEU  |
| 1   | P     | 237 | SER  |
| 1   | P     | 249 | GLU  |
| 1   | P     | 252 | VAL  |
| 1   | P     | 269 | ARG  |
| 1   | P     | 271 | SER  |
| 1   | P     | 275 | VAL  |
| 1   | P     | 288 | VAL  |
| 1   | P     | 295 | VAL  |
| 1   | P     | 317 | LEU  |
| 1   | P     | 329 | SER  |
| 1   | P     | 330 | SER  |
| 1   | P     | 333 | VAL  |
| 1   | P     | 342 | VAL  |
| 1   | P     | 349 | VAL  |
| 1   | P     | 359 | THR  |
| 1   | P     | 373 | THR  |
| 1   | P     | 377 | VAL  |
| 1   | P     | 380 | VAL  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 297 | GLN  |
| 1   | A     | 344 | ASN  |
| 1   | A     | 378 | GLN  |
| 1   | B     | 139 | ASN  |
| 1   | B     | 146 | GLN  |
| 1   | B     | 297 | GLN  |
| 1   | B     | 378 | GLN  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 165 | ASN  |
| 1   | D     | 328 | ASN  |
| 1   | E     | 146 | GLN  |
| 1   | E     | 210 | ASN  |
| 1   | E     | 378 | GLN  |
| 1   | F     | 139 | ASN  |
| 1   | F     | 146 | GLN  |
| 1   | F     | 276 | GLN  |
| 1   | G     | 328 | ASN  |
| 1   | H     | 146 | GLN  |
| 1   | H     | 210 | ASN  |
| 1   | H     | 378 | GLN  |
| 1   | I     | 146 | GLN  |
| 1   | I     | 276 | GLN  |
| 1   | I     | 297 | GLN  |
| 1   | J     | 150 | ASN  |
| 1   | J     | 328 | ASN  |
| 1   | K     | 210 | ASN  |
| 1   | K     | 311 | ASN  |
| 1   | K     | 344 | ASN  |
| 1   | K     | 363 | ASN  |
| 1   | K     | 378 | GLN  |
| 1   | L     | 139 | ASN  |
| 1   | L     | 276 | GLN  |
| 1   | L     | 297 | GLN  |
| 1   | M     | 150 | ASN  |
| 1   | M     | 328 | ASN  |
| 1   | N     | 210 | ASN  |
| 1   | N     | 344 | ASN  |
| 1   | N     | 363 | ASN  |
| 1   | N     | 378 | GLN  |
| 1   | O     | 297 | GLN  |
| 1   | P     | 328 | ASN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 25 ligands modelled in this entry, 25 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 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     | 289/380 (76%)   | 0.34   | 21 (7%) 21 17  | 22, 46, 93, 118       | 1 (0%)  |
| 1   | B     | 291/380 (76%)   | 0.65   | 46 (15%) 5 4   | 20, 51, 102, 117      | 1 (0%)  |
| 1   | D     | 321/380 (84%)   | 0.31   | 19 (5%) 28 22  | 21, 46, 91, 107       | 2 (0%)  |
| 1   | E     | 289/380 (76%)   | 0.36   | 23 (7%) 18 15  | 21, 46, 87, 110       | 1 (0%)  |
| 1   | F     | 291/380 (76%)   | 0.72   | 48 (16%) 4 4   | 22, 51, 107, 124      | 1 (0%)  |
| 1   | G     | 321/380 (84%)   | 0.28   | 19 (5%) 28 22  | 23, 45, 87, 105       | 2 (0%)  |
| 1   | H     | 289/380 (76%)   | 0.36   | 21 (7%) 21 17  | 23, 46, 92, 103       | 1 (0%)  |
| 1   | I     | 291/380 (76%)   | 0.63   | 41 (14%) 6 5   | 20, 51, 104, 120      | 1 (0%)  |
| 1   | J     | 321/380 (84%)   | 0.29   | 19 (5%) 28 22  | 21, 46, 87, 111       | 2 (0%)  |
| 1   | K     | 289/380 (76%)   | 0.32   | 19 (6%) 24 19  | 22, 47, 85, 111       | 1 (0%)  |
| 1   | L     | 291/380 (76%)   | 0.73   | 51 (17%) 4 3   | 20, 51, 105, 124      | 1 (0%)  |
| 1   | M     | 321/380 (84%)   | 0.29   | 17 (5%) 32 25  | 20, 46, 85, 102       | 2 (0%)  |
| 1   | N     | 289/380 (76%)   | 0.36   | 21 (7%) 21 17  | 21, 48, 89, 117       | 1 (0%)  |
| 1   | O     | 291/380 (76%)   | 0.73   | 49 (16%) 4 3   | 20, 52, 107, 125      | 1 (0%)  |
| 1   | P     | 321/380 (84%)   | 0.32   | 22 (6%) 23 18  | 24, 47, 93, 111       | 2 (0%)  |
| All | All   | 4505/5700 (79%) | 0.44   | 436 (9%) 13 11 | 20, 47, 99, 125       | 20 (0%) |

All (436) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | I     | 317 | LEU  | 6.8  |
| 1   | B     | 317 | LEU  | 6.2  |
| 1   | L     | 90  | ALA  | 5.9  |
| 1   | B     | 349 | VAL  | 5.8  |
| 1   | D     | 221 | GLY  | 5.7  |
| 1   | L     | 349 | VAL  | 5.6  |
| 1   | F     | 349 | VAL  | 5.5  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | O     | 317 | LEU  | 5.4  |
| 1   | F     | 317 | LEU  | 5.3  |
| 1   | F     | 272 | ALA  | 5.2  |
| 1   | I     | 272 | ALA  | 5.2  |
| 1   | F     | 90  | ALA  | 5.2  |
| 1   | G     | 221 | GLY  | 5.1  |
| 1   | F     | 121 | ASN  | 5.0  |
| 1   | B     | 121 | ASN  | 4.9  |
| 1   | L     | 317 | LEU  | 4.8  |
| 1   | L     | 325 | GLY  | 4.8  |
| 1   | O     | 90  | ALA  | 4.7  |
| 1   | O     | 322 | SER  | 4.7  |
| 1   | G     | 122 | ASN  | 4.7  |
| 1   | I     | 90  | ALA  | 4.6  |
| 1   | L     | 122 | ASN  | 4.6  |
| 1   | L     | 121 | ASN  | 4.5  |
| 1   | P     | 221 | GLY  | 4.5  |
| 1   | G     | 314 | VAL  | 4.5  |
| 1   | O     | 121 | ASN  | 4.5  |
| 1   | J     | 221 | GLY  | 4.4  |
| 1   | O     | 348 | ARG  | 4.4  |
| 1   | I     | 288 | VAL  | 4.4  |
| 1   | L     | 91  | LYS  | 4.3  |
| 1   | B     | 324 | GLY  | 4.3  |
| 1   | G     | 91  | LYS  | 4.3  |
| 1   | N     | 120 | PRO  | 4.3  |
| 1   | A     | 314 | VAL  | 4.2  |
| 1   | D     | 314 | VAL  | 4.2  |
| 1   | J     | 314 | VAL  | 4.2  |
| 1   | I     | 314 | VAL  | 4.2  |
| 1   | O     | 272 | ALA  | 4.2  |
| 1   | B     | 90  | ALA  | 4.1  |
| 1   | B     | 348 | ARG  | 4.1  |
| 1   | N     | 119 | GLY  | 4.1  |
| 1   | O     | 351 | ALA  | 4.0  |
| 1   | M     | 122 | ASN  | 4.0  |
| 1   | F     | 348 | ARG  | 4.0  |
| 1   | B     | 288 | VAL  | 4.0  |
| 1   | I     | 349 | VAL  | 4.0  |
| 1   | E     | 120 | PRO  | 4.0  |
| 1   | B     | 272 | ALA  | 4.0  |
| 1   | D     | 122 | ASN  | 3.9  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | J     | 91  | LYS  | 3.9  |
| 1   | I     | 120 | PRO  | 3.9  |
| 1   | L     | 348 | ARG  | 3.9  |
| 1   | D     | 91  | LYS  | 3.9  |
| 1   | I     | 121 | ASN  | 3.9  |
| 1   | P     | 350 | ASN  | 3.9  |
| 1   | A     | 380 | VAL  | 3.9  |
| 1   | F     | 288 | VAL  | 3.9  |
| 1   | O     | 288 | VAL  | 3.9  |
| 1   | O     | 324 | GLY  | 3.8  |
| 1   | P     | 91  | LYS  | 3.8  |
| 1   | B     | 119 | GLY  | 3.8  |
| 1   | P     | 275 | VAL  | 3.8  |
| 1   | L     | 351 | ALA  | 3.8  |
| 1   | P     | 314 | VAL  | 3.8  |
| 1   | M     | 221 | GLY  | 3.8  |
| 1   | L     | 320 | SER  | 3.7  |
| 1   | B     | 299 | ARG  | 3.7  |
| 1   | I     | 348 | ARG  | 3.7  |
| 1   | O     | 120 | PRO  | 3.7  |
| 1   | J     | 336 | ALA  | 3.7  |
| 1   | F     | 320 | SER  | 3.7  |
| 1   | J     | 122 | ASN  | 3.7  |
| 1   | O     | 299 | ARG  | 3.6  |
| 1   | E     | 119 | GLY  | 3.6  |
| 1   | L     | 272 | ALA  | 3.6  |
| 1   | I     | 290 | SER  | 3.6  |
| 1   | F     | 91  | LYS  | 3.6  |
| 1   | L     | 92  | GLY  | 3.6  |
| 1   | L     | 324 | GLY  | 3.5  |
| 1   | E     | 121 | ASN  | 3.5  |
| 1   | M     | 91  | LYS  | 3.5  |
| 1   | O     | 334 | SER  | 3.5  |
| 1   | K     | 119 | GLY  | 3.5  |
| 1   | M     | 275 | VAL  | 3.5  |
| 1   | O     | 349 | VAL  | 3.5  |
| 1   | F     | 220 | SER  | 3.5  |
| 1   | B     | 91  | LYS  | 3.5  |
| 1   | L     | 314 | VAL  | 3.5  |
| 1   | O     | 271 | SER  | 3.5  |
| 1   | H     | 362 | THR  | 3.4  |
| 1   | B     | 92  | GLY  | 3.4  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | B     | 316 | GLY  | 3.4  |
| 1   | L     | 347 | ILE  | 3.4  |
| 1   | M     | 60  | ILE  | 3.4  |
| 1   | K     | 271 | SER  | 3.4  |
| 1   | J     | 218 | THR  | 3.4  |
| 1   | L     | 352 | ASN  | 3.3  |
| 1   | M     | 119 | GLY  | 3.3  |
| 1   | G     | 275 | VAL  | 3.3  |
| 1   | F     | 377 | VAL  | 3.3  |
| 1   | N     | 275 | VAL  | 3.3  |
| 1   | E     | 270 | GLU  | 3.3  |
| 1   | K     | 362 | THR  | 3.3  |
| 1   | F     | 92  | GLY  | 3.3  |
| 1   | J     | 275 | VAL  | 3.3  |
| 1   | O     | 320 | SER  | 3.3  |
| 1   | B     | 120 | PRO  | 3.2  |
| 1   | L     | 316 | GLY  | 3.2  |
| 1   | M     | 314 | VAL  | 3.2  |
| 1   | B     | 313 | THR  | 3.2  |
| 1   | I     | 313 | THR  | 3.2  |
| 1   | H     | 296 | TRP  | 3.2  |
| 1   | F     | 354 | SER  | 3.2  |
| 1   | H     | 312 | SER  | 3.2  |
| 1   | A     | 275 | VAL  | 3.2  |
| 1   | A     | 119 | GLY  | 3.2  |
| 1   | F     | 360 | GLY  | 3.2  |
| 1   | L     | 120 | PRO  | 3.2  |
| 1   | B     | 352 | ASN  | 3.2  |
| 1   | F     | 324 | GLY  | 3.2  |
| 1   | B     | 290 | SER  | 3.1  |
| 1   | F     | 326 | THR  | 3.1  |
| 1   | O     | 380 | VAL  | 3.1  |
| 1   | K     | 359 | THR  | 3.1  |
| 1   | I     | 91  | LYS  | 3.1  |
| 1   | A     | 312 | SER  | 3.1  |
| 1   | L     | 322 | SER  | 3.1  |
| 1   | F     | 295 | VAL  | 3.0  |
| 1   | I     | 295 | VAL  | 3.0  |
| 1   | F     | 325 | GLY  | 3.0  |
| 1   | I     | 316 | GLY  | 3.0  |
| 1   | I     | 299 | ARG  | 3.0  |
| 1   | L     | 380 | VAL  | 3.0  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | E     | 238 | GLY  | 3.0  |
| 1   | E     | 316 | GLY  | 3.0  |
| 1   | L     | 294 | LEU  | 3.0  |
| 1   | O     | 298 | ALA  | 3.0  |
| 1   | P     | 380 | VAL  | 3.0  |
| 1   | J     | 60  | ILE  | 3.0  |
| 1   | B     | 123 | ASP  | 3.0  |
| 1   | B     | 322 | SER  | 3.0  |
| 1   | F     | 380 | VAL  | 3.0  |
| 1   | G     | 60  | ILE  | 3.0  |
| 1   | E     | 380 | VAL  | 3.0  |
| 1   | G     | 315 | GLY  | 2.9  |
| 1   | G     | 220 | SER  | 2.9  |
| 1   | I     | 334 | SER  | 2.9  |
| 1   | G     | 348 | ARG  | 2.9  |
| 1   | P     | 60  | ILE  | 2.9  |
| 1   | F     | 298 | ALA  | 2.9  |
| 1   | O     | 220 | SER  | 2.9  |
| 1   | A     | 348 | ARG  | 2.9  |
| 1   | N     | 362 | THR  | 2.9  |
| 1   | O     | 313 | THR  | 2.9  |
| 1   | F     | 316 | GLY  | 2.9  |
| 1   | B     | 276 | GLN  | 2.9  |
| 1   | M     | 222 | ASP  | 2.9  |
| 1   | O     | 336 | ALA  | 2.9  |
| 1   | E     | 348 | ARG  | 2.9  |
| 1   | F     | 322 | SER  | 2.9  |
| 1   | P     | 220 | SER  | 2.9  |
| 1   | D     | 336 | ALA  | 2.8  |
| 1   | A     | 120 | PRO  | 2.8  |
| 1   | H     | 314 | VAL  | 2.8  |
| 1   | I     | 380 | VAL  | 2.8  |
| 1   | K     | 312 | SER  | 2.8  |
| 1   | N     | 359 | THR  | 2.8  |
| 1   | A     | 238 | GLY  | 2.8  |
| 1   | I     | 360 | GLY  | 2.8  |
| 1   | F     | 299 | ARG  | 2.8  |
| 1   | I     | 351 | ALA  | 2.8  |
| 1   | L     | 321 | ILE  | 2.8  |
| 1   | L     | 334 | SER  | 2.8  |
| 1   | N     | 322 | SER  | 2.8  |
| 1   | B     | 295 | VAL  | 2.8  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | B     | 380 | VAL  | 2.8  |
| 1   | K     | 380 | VAL  | 2.8  |
| 1   | L     | 288 | VAL  | 2.8  |
| 1   | D     | 60  | ILE  | 2.8  |
| 1   | P     | 122 | ASN  | 2.8  |
| 1   | D     | 218 | THR  | 2.8  |
| 1   | F     | 313 | THR  | 2.8  |
| 1   | H     | 316 | GLY  | 2.8  |
| 1   | L     | 128 | PRO  | 2.8  |
| 1   | H     | 122 | ASN  | 2.7  |
| 1   | H     | 220 | SER  | 2.7  |
| 1   | L     | 220 | SER  | 2.7  |
| 1   | O     | 119 | GLY  | 2.7  |
| 1   | H     | 380 | VAL  | 2.7  |
| 1   | N     | 380 | VAL  | 2.7  |
| 1   | L     | 362 | THR  | 2.7  |
| 1   | B     | 320 | SER  | 2.7  |
| 1   | B     | 354 | SER  | 2.7  |
| 1   | I     | 322 | SER  | 2.7  |
| 1   | J     | 348 | ARG  | 2.7  |
| 1   | F     | 351 | ALA  | 2.7  |
| 1   | I     | 119 | GLY  | 2.7  |
| 1   | I     | 337 | GLY  | 2.7  |
| 1   | L     | 326 | THR  | 2.7  |
| 1   | D     | 117 | GLY  | 2.7  |
| 1   | I     | 359 | THR  | 2.7  |
| 1   | N     | 121 | ASN  | 2.7  |
| 1   | B     | 314 | VAL  | 2.7  |
| 1   | D     | 275 | VAL  | 2.7  |
| 1   | F     | 314 | VAL  | 2.7  |
| 1   | L     | 355 | LEU  | 2.7  |
| 1   | B     | 315 | GLY  | 2.6  |
| 1   | I     | 92  | GLY  | 2.6  |
| 1   | M     | 380 | VAL  | 2.6  |
| 1   | O     | 91  | LYS  | 2.6  |
| 1   | I     | 320 | SER  | 2.6  |
| 1   | F     | 221 | GLY  | 2.6  |
| 1   | H     | 120 | PRO  | 2.6  |
| 1   | K     | 120 | PRO  | 2.6  |
| 1   | L     | 337 | GLY  | 2.6  |
| 1   | E     | 122 | ASN  | 2.6  |
| 1   | K     | 314 | VAL  | 2.6  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | D     | 289 | ALA  | 2.6  |
| 1   | O     | 295 | VAL  | 2.6  |
| 1   | O     | 321 | ILE  | 2.6  |
| 1   | O     | 347 | ILE  | 2.6  |
| 1   | F     | 276 | GLN  | 2.6  |
| 1   | H     | 121 | ASN  | 2.6  |
| 1   | A     | 272 | ALA  | 2.6  |
| 1   | J     | 272 | ALA  | 2.6  |
| 1   | P     | 336 | ALA  | 2.6  |
| 1   | I     | 271 | SER  | 2.6  |
| 1   | E     | 315 | GLY  | 2.6  |
| 1   | F     | 286 | LEU  | 2.6  |
| 1   | O     | 362 | THR  | 2.6  |
| 1   | M     | 348 | ARG  | 2.5  |
| 1   | B     | 319 | PRO  | 2.5  |
| 1   | O     | 316 | GLY  | 2.5  |
| 1   | L     | 295 | VAL  | 2.5  |
| 1   | B     | 351 | ALA  | 2.5  |
| 1   | H     | 273 | SER  | 2.5  |
| 1   | L     | 290 | SER  | 2.5  |
| 1   | D     | 315 | GLY  | 2.5  |
| 1   | I     | 324 | GLY  | 2.5  |
| 1   | O     | 92  | GLY  | 2.5  |
| 1   | E     | 288 | VAL  | 2.5  |
| 1   | G     | 218 | THR  | 2.5  |
| 1   | P     | 218 | THR  | 2.5  |
| 1   | N     | 272 | ALA  | 2.5  |
| 1   | G     | 222 | ASP  | 2.5  |
| 1   | N     | 312 | SER  | 2.5  |
| 1   | I     | 319 | PRO  | 2.5  |
| 1   | H     | 288 | VAL  | 2.5  |
| 1   | A     | 270 | GLU  | 2.5  |
| 1   | B     | 291 | ALA  | 2.5  |
| 1   | A     | 123 | ASP  | 2.5  |
| 1   | F     | 347 | ILE  | 2.5  |
| 1   | O     | 314 | VAL  | 2.5  |
| 1   | L     | 374 | GLU  | 2.5  |
| 1   | L     | 299 | ARG  | 2.5  |
| 1   | M     | 123 | ASP  | 2.4  |
| 1   | L     | 119 | GLY  | 2.4  |
| 1   | L     | 315 | GLY  | 2.4  |
| 1   | K     | 320 | SER  | 2.4  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | M     | 356 | SER  | 2.4  |
| 1   | O     | 291 | ALA  | 2.4  |
| 1   | D     | 362 | THR  | 2.4  |
| 1   | B     | 122 | ASN  | 2.4  |
| 1   | J     | 210 | ASN  | 2.4  |
| 1   | K     | 122 | ASN  | 2.4  |
| 1   | H     | 317 | LEU  | 2.4  |
| 1   | I     | 347 | ILE  | 2.4  |
| 1   | B     | 360 | GLY  | 2.4  |
| 1   | E     | 275 | VAL  | 2.4  |
| 1   | D     | 348 | ARG  | 2.4  |
| 1   | M     | 322 | SER  | 2.4  |
| 1   | O     | 312 | SER  | 2.4  |
| 1   | O     | 339 | SER  | 2.4  |
| 1   | G     | 336 | ALA  | 2.4  |
| 1   | M     | 272 | ALA  | 2.4  |
| 1   | E     | 313 | THR  | 2.4  |
| 1   | F     | 120 | PRO  | 2.4  |
| 1   | L     | 123 | ASP  | 2.4  |
| 1   | L     | 377 | VAL  | 2.4  |
| 1   | N     | 238 | GLY  | 2.4  |
| 1   | O     | 315 | GLY  | 2.4  |
| 1   | O     | 377 | VAL  | 2.4  |
| 1   | E     | 312 | SER  | 2.4  |
| 1   | F     | 271 | SER  | 2.4  |
| 1   | E     | 318 | THR  | 2.4  |
| 1   | I     | 122 | ASN  | 2.4  |
| 1   | N     | 122 | ASN  | 2.4  |
| 1   | P     | 316 | GLY  | 2.4  |
| 1   | F     | 123 | ASP  | 2.4  |
| 1   | E     | 272 | ALA  | 2.4  |
| 1   | I     | 277 | THR  | 2.4  |
| 1   | A     | 121 | ASN  | 2.3  |
| 1   | A     | 299 | ARG  | 2.3  |
| 1   | H     | 275 | VAL  | 2.3  |
| 1   | J     | 117 | GLY  | 2.3  |
| 1   | K     | 274 | SER  | 2.3  |
| 1   | I     | 294 | LEU  | 2.3  |
| 1   | G     | 269 | ARG  | 2.3  |
| 1   | N     | 314 | VAL  | 2.3  |
| 1   | G     | 316 | GLY  | 2.3  |
| 1   | O     | 357 | GLY  | 2.3  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | I     | 276 | GLN  | 2.3  |
| 1   | B     | 294 | LEU  | 2.3  |
| 1   | H     | 274 | SER  | 2.3  |
| 1   | I     | 220 | SER  | 2.3  |
| 1   | J     | 219 | SER  | 2.3  |
| 1   | B     | 362 | THR  | 2.3  |
| 1   | H     | 313 | THR  | 2.3  |
| 1   | L     | 218 | THR  | 2.3  |
| 1   | L     | 313 | THR  | 2.3  |
| 1   | O     | 301 | PRO  | 2.3  |
| 1   | P     | 269 | ARG  | 2.3  |
| 1   | K     | 295 | VAL  | 2.3  |
| 1   | F     | 323 | GLY  | 2.3  |
| 1   | L     | 350 | ASN  | 2.3  |
| 1   | O     | 123 | ASP  | 2.3  |
| 1   | F     | 321 | ILE  | 2.3  |
| 1   | P     | 271 | SER  | 2.3  |
| 1   | B     | 269 | ARG  | 2.3  |
| 1   | J     | 269 | ARG  | 2.3  |
| 1   | H     | 295 | VAL  | 2.3  |
| 1   | K     | 272 | ALA  | 2.3  |
| 1   | M     | 336 | ALA  | 2.3  |
| 1   | A     | 362 | THR  | 2.3  |
| 1   | B     | 271 | SER  | 2.3  |
| 1   | B     | 326 | THR  | 2.3  |
| 1   | D     | 220 | SER  | 2.3  |
| 1   | E     | 359 | THR  | 2.3  |
| 1   | J     | 220 | SER  | 2.3  |
| 1   | L     | 354 | SER  | 2.3  |
| 1   | N     | 295 | VAL  | 2.3  |
| 1   | L     | 360 | GLY  | 2.3  |
| 1   | F     | 361 | ALA  | 2.2  |
| 1   | K     | 121 | ASN  | 2.2  |
| 1   | N     | 270 | GLU  | 2.2  |
| 1   | P     | 363 | ASN  | 2.2  |
| 1   | F     | 358 | LEU  | 2.2  |
| 1   | L     | 353 | LEU  | 2.2  |
| 1   | D     | 222 | ASP  | 2.2  |
| 1   | E     | 299 | ARG  | 2.2  |
| 1   | F     | 296 | TRP  | 2.2  |
| 1   | P     | 362 | THR  | 2.2  |
| 1   | K     | 275 | VAL  | 2.2  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | L     | 319 | PRO  | 2.2  |
| 1   | O     | 373 | THR  | 2.2  |
| 1   | A     | 322 | SER  | 2.2  |
| 1   | B     | 312 | SER  | 2.2  |
| 1   | F     | 350 | ASN  | 2.2  |
| 1   | G     | 380 | VAL  | 2.2  |
| 1   | K     | 313 | THR  | 2.2  |
| 1   | E     | 274 | SER  | 2.2  |
| 1   | F     | 290 | SER  | 2.2  |
| 1   | F     | 312 | SER  | 2.2  |
| 1   | F     | 338 | SER  | 2.2  |
| 1   | I     | 312 | SER  | 2.2  |
| 1   | M     | 92  | GLY  | 2.2  |
| 1   | O     | 325 | GLY  | 2.2  |
| 1   | O     | 354 | SER  | 2.2  |
| 1   | I     | 350 | ASN  | 2.2  |
| 1   | N     | 350 | ASN  | 2.2  |
| 1   | P     | 276 | GLN  | 2.2  |
| 1   | E     | 349 | VAL  | 2.2  |
| 1   | F     | 275 | VAL  | 2.2  |
| 1   | I     | 275 | VAL  | 2.2  |
| 1   | G     | 335 | THR  | 2.2  |
| 1   | L     | 373 | THR  | 2.2  |
| 1   | J     | 119 | GLY  | 2.2  |
| 1   | B     | 355 | LEU  | 2.2  |
| 1   | G     | 334 | SER  | 2.2  |
| 1   | N     | 273 | SER  | 2.2  |
| 1   | O     | 358 | LEU  | 2.2  |
| 1   | P     | 273 | SER  | 2.2  |
| 1   | H     | 348 | ARG  | 2.1  |
| 1   | B     | 377 | VAL  | 2.1  |
| 1   | O     | 360 | GLY  | 2.1  |
| 1   | L     | 358 | LEU  | 2.1  |
| 1   | A     | 273 | SER  | 2.1  |
| 1   | B     | 361 | ALA  | 2.1  |
| 1   | J     | 271 | SER  | 2.1  |
| 1   | N     | 274 | SER  | 2.1  |
| 1   | P     | 274 | SER  | 2.1  |
| 1   | I     | 321 | ILE  | 2.1  |
| 1   | F     | 122 | ASN  | 2.1  |
| 1   | J     | 350 | ASN  | 2.1  |
| 1   | J     | 380 | VAL  | 2.1  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | D     | 123 | ASP  | 2.1  |
| 1   | A     | 316 | GLY  | 2.1  |
| 1   | A     | 274 | SER  | 2.1  |
| 1   | L     | 271 | SER  | 2.1  |
| 1   | M     | 338 | SER  | 2.1  |
| 1   | N     | 349 | VAL  | 2.1  |
| 1   | B     | 217 | ASP  | 2.1  |
| 1   | B     | 325 | GLY  | 2.1  |
| 1   | B     | 337 | GLY  | 2.1  |
| 1   | E     | 123 | ASP  | 2.1  |
| 1   | F     | 355 | LEU  | 2.1  |
| 1   | H     | 324 | GLY  | 2.1  |
| 1   | O     | 353 | LEU  | 2.1  |
| 1   | I     | 289 | ALA  | 2.1  |
| 1   | K     | 270 | GLU  | 2.1  |
| 1   | L     | 274 | SER  | 2.1  |
| 1   | N     | 271 | SER  | 2.1  |
| 1   | P     | 322 | SER  | 2.1  |
| 1   | B     | 275 | VAL  | 2.1  |
| 1   | K     | 311 | ASN  | 2.1  |
| 1   | O     | 352 | ASN  | 2.1  |
| 1   | O     | 355 | LEU  | 2.1  |
| 1   | H     | 238 | GLY  | 2.1  |
| 1   | O     | 337 | GLY  | 2.1  |
| 1   | B     | 370 | ARG  | 2.1  |
| 1   | D     | 269 | ARG  | 2.1  |
| 1   | F     | 346 | THR  | 2.1  |
| 1   | F     | 289 | ALA  | 2.1  |
| 1   | I     | 343 | ALA  | 2.1  |
| 1   | E     | 271 | SER  | 2.0  |
| 1   | G     | 219 | SER  | 2.0  |
| 1   | H     | 320 | SER  | 2.0  |
| 1   | L     | 356 | SER  | 2.0  |
| 1   | O     | 319 | PRO  | 2.0  |
| 1   | A     | 315 | GLY  | 2.0  |
| 1   | D     | 316 | GLY  | 2.0  |
| 1   | F     | 370 | ARG  | 2.0  |
| 1   | L     | 346 | THR  | 2.0  |
| 1   | K     | 289 | ALA  | 2.0  |
| 1   | N     | 291 | ALA  | 2.0  |
| 1   | A     | 271 | SER  | 2.0  |
| 1   | E     | 295 | VAL  | 2.0  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | I     | 370 | ARG  | 2.0  |
| 1   | P     | 348 | ARG  | 2.0  |
| 1   | G     | 357 | GLY  | 2.0  |
| 1   | O     | 221 | GLY  | 2.0  |
| 1   | A     | 359 | THR  | 2.0  |
| 1   | B     | 359 | THR  | 2.0  |
| 1   | O     | 277 | THR  | 2.0  |
| 1   | P     | 123 | ASP  | 2.0  |
| 1   | D     | 380 | VAL  | 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(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|--------|-------|------|------|----------------------------|-------|
| 2   | CA   | B     | 402    | 1/1   | 0.78 | 0.14 | 84,84,84,84                | 0     |
| 2   | CA   | I     | 402    | 1/1   | 0.78 | 0.12 | 91,91,91,91                | 0     |
| 2   | CA   | O     | 402    | 1/1   | 0.78 | 0.16 | 87,87,87,87                | 0     |
| 2   | CA   | I     | 401    | 1/1   | 0.79 | 0.20 | 99,99,99,99                | 0     |
| 2   | CA   | K     | 402    | 1/1   | 0.86 | 0.18 | 83,83,83,83                | 0     |
| 2   | CA   | F     | 401    | 1/1   | 0.86 | 0.11 | 82,82,82,82                | 0     |
| 2   | CA   | E     | 402    | 1/1   | 0.88 | 0.14 | 93,93,93,93                | 0     |
| 2   | CA   | B     | 401    | 1/1   | 0.88 | 0.15 | 89,89,89,89                | 0     |
| 2   | CA   | M     | 402    | 1/1   | 0.89 | 0.11 | 74,74,74,74                | 0     |
| 2   | CA   | E     | 401    | 1/1   | 0.89 | 0.13 | 82,82,82,82                | 0     |
| 2   | CA   | O     | 401    | 1/1   | 0.90 | 0.13 | 76,76,76,76                | 0     |
| 3   | ZN   | P     | 401[A] | 1/1   | 0.91 | 0.34 | 120,120,120,120            | 1     |
| 3   | ZN   | P     | 401[B] | 1/1   | 0.91 | 0.34 | 102,102,102,102            | 0     |
| 3   | ZN   | G     | 401[A] | 1/1   | 0.93 | 0.13 | 99,99,99,99                | 1     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res    | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|--------|-------|------|------|-----------------------------|-------|
| 3   | ZN   | G     | 401[B] | 1/1   | 0.93 | 0.13 | 124,124,124,124             | 1     |
| 3   | ZN   | D     | 401[A] | 1/1   | 0.93 | 0.30 | 97,97,97,97                 | 1     |
| 3   | ZN   | D     | 401[B] | 1/1   | 0.93 | 0.30 | 121,121,121,121             | 1     |
| 2   | CA   | H     | 401    | 1/1   | 0.94 | 0.10 | 77,77,77,77                 | 0     |
| 3   | ZN   | J     | 401[A] | 1/1   | 0.94 | 0.31 | 97,97,97,97                 | 1     |
| 3   | ZN   | J     | 401[B] | 1/1   | 0.94 | 0.31 | 121,121,121,121             | 1     |
| 2   | CA   | K     | 401    | 1/1   | 0.94 | 0.11 | 77,77,77,77                 | 0     |
| 2   | CA   | D     | 402    | 1/1   | 0.94 | 0.10 | 77,77,77,77                 | 0     |
| 2   | CA   | N     | 401    | 1/1   | 0.95 | 0.14 | 88,88,88,88                 | 0     |
| 3   | ZN   | M     | 401[A] | 1/1   | 0.98 | 0.10 | 107,107,107,107             | 1     |
| 3   | ZN   | M     | 401[B] | 1/1   | 0.98 | 0.10 | 118,118,118,118             | 1     |

## 6.5 Other polymers [i](#)

There are no such residues in this entry.