



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 08:44 AM UTC

PDB ID : 1FPV / pdb\_00001fpv  
Title : STRUCTURE DETERMINATION OF FELINE PANLEUKOPENIA VIRUS  
EMPTY PARTICLES  
Authors : Agbandje, M.; Rossmann, M.G.  
Deposited on : 1993-03-04  
Resolution : 3.30 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)               | : | NOT EXECUTED                                                     |
| EDS                            | : | NOT EXECUTED                                                     |
| Percentile statistics          | : | 20250101.v01 (using entries in the PDB archive January 1st 2025) |
| Ideal geometry (proteins)      | : | Engh & Huber (2001)                                              |
| Ideal geometry (DNA, RNA)      | : | Parkinson et al. (1996)                                          |
| Validation Pipeline (wwPDB-VP) | : | 2.49                                                             |

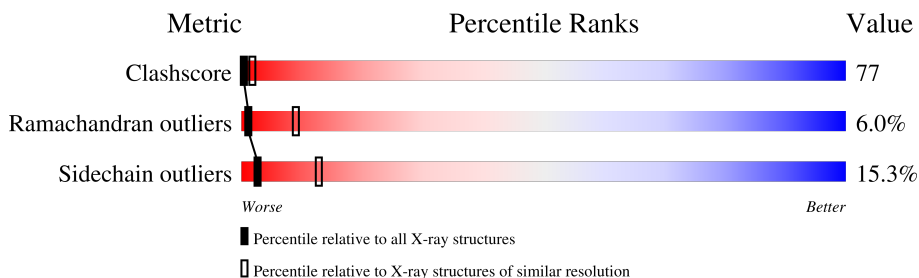
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.30 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)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| Clashscore            | 190562                      | 1209 (3.32-3.28)                                      |
| Ramachandran outliers | 187476                      | 1188 (3.32-3.28)                                      |
| Sidechain outliers    | 187428                      | 1187 (3.32-3.28)                                      |

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  $\leq 5\%$

Note EDS was not executed.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | A     | 584    |                  |

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 4350 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 FELINE PANLEUKOPENIA VIRUS (STRAIN B) VIRAL PROTEIN 2.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | A     | 548      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 4350  | 2766 | 739 | 829 | 16 |         |         |       |

There are 3 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| A     | 104     | GLU      | GLN    | conflict | UNP P24840 |
| A     | 484     | ILE      | VAL    | conflict | UNP P24840 |
| A     | 509     | GLN      | GLU    | conflict | UNP P24840 |



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

| Property                                                 | Value                                           | Source    |
|----------------------------------------------------------|-------------------------------------------------|-----------|
| Space group                                              | P 21 21 21                                      | Depositor |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$ | 380.10Å 379.30Å 350.90Å<br>90.00° 90.00° 90.00° | Depositor |
| Resolution (Å)                                           | (Not available) – 3.30                          | Depositor |
| % Data completeness<br>(in resolution range)             | (Not available) ((Not available)-3.30)          | Depositor |
| $R_{merge}$                                              | (Not available)                                 | Depositor |
| $R_{sym}$                                                | (Not available)                                 | Depositor |
| Refinement program                                       | unknown                                         | Depositor |
| R, $R_{free}$                                            | (Not available) , (Not available)               | Depositor |
| Estimated twinning fraction                              | No twinning to report.                          | Xtriage   |
| Total number of atoms                                    | 4350                                            | wwPDB-VP  |
| Average B, all atoms (Å <sup>2</sup> )                   | 0.0                                             | wwPDB-VP  |

## 5 Model quality

### 5.1 Standard geometry

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

| Mol | Chain | Bond lengths |                | Bond angles |                |
|-----|-------|--------------|----------------|-------------|----------------|
|     |       | RMSZ         | $\# Z  > 5$    | RMSZ        | $\# Z  > 5$    |
| 1   | A     | 1.33         | 33/4479 (0.7%) | 1.63        | 87/6128 (1.4%) |

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   | A     | 0                   | 2                   |

All (33) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 1   | A     | 239 | ASP  | C-N     | -13.06 | 1.15        | 1.33     |
| 1   | A     | 228 | THR  | CA-C    | 12.98  | 1.69        | 1.52     |
| 1   | A     | 263 | THR  | C-O     | 11.90  | 1.39        | 1.23     |
| 1   | A     | 264 | GLY  | N-CA    | 9.86   | 1.59        | 1.45     |
| 1   | A     | 203 | THR  | N-CA    | 8.74   | 1.57        | 1.45     |
| 1   | A     | 47  | ASN  | C-N     | -8.21  | 1.22        | 1.33     |
| 1   | A     | 263 | THR  | CA-C    | -7.19  | 1.43        | 1.52     |
| 1   | A     | 203 | THR  | C-N     | 7.02   | 1.41        | 1.33     |
| 1   | A     | 240 | ASP  | N-CA    | -6.65  | 1.37        | 1.46     |
| 1   | A     | 41  | SER  | N-CA    | 6.33   | 1.53        | 1.45     |
| 1   | A     | 270 | CYS  | N-CA    | 6.19   | 1.53        | 1.46     |
| 1   | A     | 208 | TRP  | NE1-CE2 | -6.06  | 1.30        | 1.37     |
| 1   | A     | 202 | PRO  | CA-C    | 5.74   | 1.59        | 1.52     |
| 1   | A     | 214 | TRP  | NE1-CE2 | -5.72  | 1.31        | 1.37     |
| 1   | A     | 162 | THR  | N-CA    | 5.66   | 1.53        | 1.45     |
| 1   | A     | 202 | PRO  | C-N     | 5.57   | 1.43        | 1.33     |
| 1   | A     | 414 | TRP  | NE1-CE2 | -5.50  | 1.31        | 1.37     |
| 1   | A     | 529 | TRP  | NE1-CE2 | -5.47  | 1.31        | 1.37     |
| 1   | A     | 470 | TRP  | NE1-CE2 | -5.47  | 1.31        | 1.37     |
| 1   | A     | 545 | TRP  | NE1-CE2 | -5.43  | 1.31        | 1.37     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | A     | 269 | ASP  | C-O     | 5.43  | 1.30        | 1.23     |
| 1   | A     | 210 | TYR  | N-CA    | 5.42  | 1.52        | 1.45     |
| 1   | A     | 126 | TRP  | NE1-CE2 | -5.42 | 1.31        | 1.37     |
| 1   | A     | 279 | TRP  | NE1-CE2 | -5.42 | 1.31        | 1.37     |
| 1   | A     | 528 | TRP  | NE1-CE2 | -5.38 | 1.31        | 1.37     |
| 1   | A     | 109 | TRP  | NE1-CE2 | -5.32 | 1.31        | 1.37     |
| 1   | A     | 117 | TRP  | NE1-CE2 | -5.32 | 1.31        | 1.37     |
| 1   | A     | 38  | VAL  | N-CA    | 5.31  | 1.52        | 1.46     |
| 1   | A     | 120 | TRP  | NE1-CE2 | -5.29 | 1.31        | 1.37     |
| 1   | A     | 271 | LYS  | N-CA    | 5.25  | 1.52        | 1.45     |
| 1   | A     | 200 | TRP  | NE1-CE2 | -5.22 | 1.31        | 1.37     |
| 1   | A     | 40  | ILE  | CA-C    | 5.22  | 1.59        | 1.52     |
| 1   | A     | 48  | GLN  | C-N     | -5.06 | 1.25        | 1.33     |

All (87) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|--------|-------------|----------|
| 1   | A     | 342 | TYR  | O-C-N      | 23.35  | 150.59      | 123.27   |
| 1   | A     | 492 | ASN  | CA-CB-CG   | -16.32 | 96.28       | 112.60   |
| 1   | A     | 39  | GLY  | CA-C-N     | -15.91 | 97.03       | 122.64   |
| 1   | A     | 39  | GLY  | C-N-CA     | -15.91 | 97.03       | 122.64   |
| 1   | A     | 228 | THR  | CA-C-O     | -13.05 | 102.28      | 120.16   |
| 1   | A     | 39  | GLY  | O-C-N      | 11.70  | 137.92      | 122.70   |
| 1   | A     | 342 | TYR  | CA-C-N     | 11.22  | 142.98      | 121.54   |
| 1   | A     | 342 | TYR  | C-N-CA     | 11.22  | 142.98      | 121.54   |
| 1   | A     | 263 | THR  | CA-C-O     | -10.54 | 110.07      | 121.56   |
| 1   | A     | 492 | ASN  | CA-C-O     | -10.04 | 109.90      | 120.55   |
| 1   | A     | 263 | THR  | N-CA-CB    | -9.86  | 95.97       | 110.17   |
| 1   | A     | 263 | THR  | O-C-N      | -8.88  | 112.38      | 122.86   |
| 1   | A     | 263 | THR  | CA-C-N     | -8.86  | 111.41      | 122.75   |
| 1   | A     | 263 | THR  | C-N-CA     | -8.86  | 111.41      | 122.75   |
| 1   | A     | 257 | THR  | O-C-N      | 8.03   | 130.64      | 122.12   |
| 1   | A     | 268 | PHE  | CA-CB-CG   | 8.03   | 121.83      | 113.80   |
| 1   | A     | 257 | THR  | CA-CB-OG1  | -7.84  | 97.84       | 109.60   |
| 1   | A     | 130 | VAL  | N-CA-CB    | -7.77  | 99.98       | 110.54   |
| 1   | A     | 265 | THR  | CA-C-O     | -7.50  | 112.06      | 120.54   |
| 1   | A     | 129 | ILE  | CA-C-O     | 7.46   | 129.27      | 121.29   |
| 1   | A     | 263 | THR  | CA-CB-OG1  | -6.97  | 99.15       | 109.60   |
| 1   | A     | 135 | GLU  | CA-C-O     | -6.75  | 113.46      | 120.89   |
| 1   | A     | 253 | HIS  | CA-C-O     | -6.54  | 113.30      | 120.43   |
| 1   | A     | 263 | THR  | OG1-CB-CG2 | 6.50   | 122.29      | 109.30   |
| 1   | A     | 130 | VAL  | CB-CA-C    | 6.40   | 120.78      | 112.14   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | A     | 53  | PHE  | CA-C-N     | 6.36  | 133.69      | 121.54   |
| 1   | A     | 53  | PHE  | C-N-CA     | 6.36  | 133.69      | 121.54   |
| 1   | A     | 255 | LEU  | CA-C-O     | -6.30 | 114.03      | 120.71   |
| 1   | A     | 492 | ASN  | OD1-CG-ND2 | 6.30  | 128.90      | 122.60   |
| 1   | A     | 38  | VAL  | N-CA-C     | 6.23  | 122.31      | 109.34   |
| 1   | A     | 262 | ALA  | CA-C-N     | 6.13  | 130.57      | 120.94   |
| 1   | A     | 262 | ALA  | C-N-CA     | 6.13  | 130.57      | 120.94   |
| 1   | A     | 47  | ASN  | CA-C-N     | 6.08  | 131.75      | 122.93   |
| 1   | A     | 47  | ASN  | C-N-CA     | 6.08  | 131.75      | 122.93   |
| 1   | A     | 132 | THR  | CA-C-O     | -6.03 | 112.42      | 119.05   |
| 1   | A     | 265 | THR  | CA-CB-OG1  | -5.99 | 100.62      | 109.60   |
| 1   | A     | 260 | GLU  | O-C-N      | -5.84 | 116.59      | 123.25   |
| 1   | A     | 520 | ARG  | NE-CZ-NH2  | 5.82  | 124.44      | 119.20   |
| 1   | A     | 194 | THR  | CB-CA-C    | -5.77 | 108.77      | 117.07   |
| 1   | A     | 261 | PHE  | CA-CB-CG   | 5.72  | 119.52      | 113.80   |
| 1   | A     | 286 | GLY  | O-C-N      | 5.66  | 127.77      | 122.90   |
| 1   | A     | 281 | THR  | CB-CA-C    | -5.61 | 108.99      | 117.07   |
| 1   | A     | 486 | ALA  | CB-CA-C    | -5.55 | 101.40      | 109.45   |
| 1   | A     | 493 | ASN  | N-CA-C     | 5.53  | 118.44      | 108.48   |
| 1   | A     | 361 | ARG  | NE-CZ-NH2  | 5.46  | 124.11      | 119.20   |
| 1   | A     | 216 | ARG  | NE-CZ-NH2  | 5.45  | 124.10      | 119.20   |
| 1   | A     | 274 | ARG  | NE-CZ-NH2  | 5.43  | 124.09      | 119.20   |
| 1   | A     | 209 | ARG  | NE-CZ-NH2  | 5.42  | 124.08      | 119.20   |
| 1   | A     | 256 | ARG  | CA-C-O     | -5.42 | 114.83      | 121.88   |
| 1   | A     | 67  | ARG  | NE-CZ-NH2  | 5.39  | 124.05      | 119.20   |
| 1   | A     | 491 | GLN  | CA-C-N     | -5.39 | 113.06      | 120.28   |
| 1   | A     | 491 | GLN  | C-N-CA     | -5.39 | 113.06      | 120.28   |
| 1   | A     | 38  | VAL  | CB-CA-C    | -5.37 | 102.49      | 111.29   |
| 1   | A     | 283 | ARG  | NE-CZ-NH2  | 5.37  | 124.03      | 119.20   |
| 1   | A     | 314 | ARG  | NE-CZ-NH2  | 5.36  | 124.03      | 119.20   |
| 1   | A     | 84  | VAL  | CB-CA-C    | -5.36 | 104.03      | 110.99   |
| 1   | A     | 397 | ARG  | NE-CZ-NH2  | 5.34  | 124.00      | 119.20   |
| 1   | A     | 272 | PRO  | N-CA-CB    | 5.33  | 108.98      | 103.38   |
| 1   | A     | 540 | ARG  | NE-CZ-NH2  | 5.33  | 124.00      | 119.20   |
| 1   | A     | 332 | ARG  | NE-CZ-NH2  | 5.32  | 123.99      | 119.20   |
| 1   | A     | 382 | ARG  | NE-CZ-NH2  | 5.32  | 123.99      | 119.20   |
| 1   | A     | 191 | ARG  | NE-CZ-NH2  | 5.32  | 123.99      | 119.20   |
| 1   | A     | 481 | ARG  | NE-CZ-NH2  | 5.30  | 123.97      | 119.20   |
| 1   | A     | 313 | ARG  | NE-CZ-NH2  | 5.28  | 123.95      | 119.20   |
| 1   | A     | 408 | ARG  | NE-CZ-NH2  | 5.27  | 123.95      | 119.20   |
| 1   | A     | 254 | LEU  | CA-C-N     | -5.26 | 115.31      | 122.93   |
| 1   | A     | 254 | LEU  | C-N-CA     | -5.26 | 115.31      | 122.93   |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | A     | 130 | VAL  | O-C-N     | -5.25 | 116.78      | 121.87   |
| 1   | A     | 580 | PRO  | O-C-N     | 5.25  | 129.26      | 122.91   |
| 1   | A     | 281 | THR  | CA-C-O    | 5.24  | 120.98      | 117.94   |
| 1   | A     | 491 | GLN  | CA-C-O    | 5.22  | 127.98      | 120.51   |
| 1   | A     | 81  | ARG  | NE-CZ-NH2 | 5.22  | 123.90      | 119.20   |
| 1   | A     | 194 | THR  | O-C-N     | 5.22  | 125.38      | 121.47   |
| 1   | A     | 54  | LEU  | O-C-N     | -5.19 | 115.69      | 122.59   |
| 1   | A     | 385 | GLY  | N-CA-C    | -5.16 | 106.35      | 111.56   |
| 1   | A     | 86  | ASN  | O-C-N     | 5.14  | 128.87      | 121.92   |
| 1   | A     | 377 | ARG  | NE-CZ-NH2 | 5.14  | 123.83      | 119.20   |
| 1   | A     | 269 | ASP  | CA-C-N    | -5.14 | 113.53      | 122.37   |
| 1   | A     | 269 | ASP  | C-N-CA    | -5.14 | 113.53      | 122.37   |
| 1   | A     | 560 | ASN  | N-CA-C    | -5.14 | 107.04      | 113.72   |
| 1   | A     | 54  | LEU  | CA-C-O    | 5.09  | 127.79      | 120.51   |
| 1   | A     | 489 | VAL  | CA-C-O    | -5.08 | 115.10      | 120.53   |
| 1   | A     | 581 | ARG  | NE-CZ-NH2 | 5.07  | 123.77      | 119.20   |
| 1   | A     | 444 | TYR  | N-CA-C    | -5.06 | 106.95      | 113.23   |
| 1   | A     | 93  | LYS  | CB-CA-C   | -5.05 | 103.73      | 111.66   |
| 1   | A     | 517 | ASN  | O-C-N     | 5.04  | 129.29      | 122.59   |
| 1   | A     | 269 | ASP  | CA-CB-CG  | 5.01  | 117.61      | 112.60   |

There are no chirality outliers.

All (2) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | A     | 228 | THR  | Mainchain |
| 1   | A     | 39  | GLY  | Mainchain |

## 5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 4350  | 0        | 4153     | 652     | 0            |
| All | All   | 4350  | 0        | 4153     | 652     | 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 77.

All (652) 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:A:96:MET:CE    | 1:A:221:SER:H    | 1.01                     | 1.63              |
| 1:A:424:VAL:HG21 | 1:A:429:VAL:CG2  | 1.37                     | 1.54              |
| 1:A:77:GLU:CG    | 1:A:518:MET:HE3  | 1.30                     | 1.52              |
| 1:A:150:LEU:CD2  | 1:A:525:SER:HB3  | 1.42                     | 1.49              |
| 1:A:361:ARG:NH1  | 1:A:401:ILE:HG22 | 1.10                     | 1.42              |
| 1:A:96:MET:CE    | 1:A:221:SER:N    | 1.83                     | 1.39              |
| 1:A:359:ALA:CB   | 1:A:373:ASP:O    | 1.69                     | 1.39              |
| 1:A:159:GLN:HB2  | 1:A:160:PRO:CD   | 1.54                     | 1.37              |
| 1:A:77:GLU:HG3   | 1:A:518:MET:CE   | 1.52                     | 1.36              |
| 1:A:276:THR:HG21 | 1:A:581:ARG:CB   | 1.51                     | 1.36              |
| 1:A:424:VAL:CG2  | 1:A:429:VAL:CG2  | 2.00                     | 1.35              |
| 1:A:150:LEU:HD23 | 1:A:525:SER:CB   | 1.56                     | 1.33              |
| 1:A:158:THR:O    | 1:A:160:PRO:HD2  | 1.25                     | 1.32              |
| 1:A:361:ARG:O    | 1:A:407:GLY:HA3  | 1.19                     | 1.31              |
| 1:A:276:THR:CG2  | 1:A:581:ARG:HB3  | 1.61                     | 1.28              |
| 1:A:113:ASP:O    | 1:A:195:LEU:HD12 | 1.33                     | 1.26              |
| 1:A:564:ASN:OD1  | 1:A:568:ALA:HB3  | 1.16                     | 1.26              |
| 1:A:113:ASP:O    | 1:A:195:LEU:CD1  | 1.84                     | 1.25              |
| 1:A:516:ALA:C    | 1:A:517:ASN:ND2  | 1.94                     | 1.25              |
| 1:A:424:VAL:CG2  | 1:A:429:VAL:HG23 | 1.63                     | 1.24              |
| 1:A:516:ALA:O    | 1:A:517:ASN:ND2  | 1.66                     | 1.24              |
| 1:A:111:LEU:HD23 | 1:A:112:VAL:N    | 1.52                     | 1.23              |
| 1:A:160:PRO:CB   | 1:A:161:PRO:O    | 1.87                     | 1.22              |
| 1:A:361:ARG:NH1  | 1:A:401:ILE:CG2  | 2.02                     | 1.22              |
| 1:A:77:GLU:CB    | 1:A:518:MET:CE   | 2.20                     | 1.20              |
| 1:A:359:ALA:HB1  | 1:A:373:ASP:CB   | 1.72                     | 1.20              |
| 1:A:359:ALA:CB   | 1:A:373:ASP:HB2  | 1.72                     | 1.18              |
| 1:A:505:ASN:OD1  | 1:A:521:ILE:HD12 | 1.37                     | 1.18              |
| 1:A:564:ASN:OD1  | 1:A:568:ALA:CB   | 1.92                     | 1.17              |
| 1:A:96:MET:HE2   | 1:A:221:SER:N    | 1.46                     | 1.16              |
| 1:A:369:ASN:O    | 1:A:371:ALA:N    | 1.78                     | 1.14              |
| 1:A:193:GLU:HB3  | 1:A:206:THR:HG21 | 1.21                     | 1.14              |
| 1:A:424:VAL:HG22 | 1:A:429:VAL:HG23 | 1.25                     | 1.14              |
| 1:A:77:GLU:CG    | 1:A:518:MET:CE   | 2.12                     | 1.13              |
| 1:A:276:THR:CG2  | 1:A:581:ARG:CB   | 2.20                     | 1.13              |
| 1:A:70:HIS:HD2   | 1:A:526:ASP:OD1  | 1.30                     | 1.12              |
| 1:A:160:PRO:HB2  | 1:A:161:PRO:O    | 0.95                     | 1.12              |
| 1:A:109:TRP:NE1  | 1:A:247:GLU:OE2  | 1.82                     | 1.12              |
| 1:A:359:ALA:HB3  | 1:A:373:ASP:C    | 1.77                     | 1.10              |
| 1:A:276:THR:HG22 | 1:A:581:ARG:HB3  | 1.27                     | 1.10              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:99:ASP:OD1   | 1:A:216:ARG:NH1  | 1.83                     | 1.10              |
| 1:A:194:THR:HG22 | 1:A:195:LEU:H    | 1.12                     | 1.09              |
| 1:A:96:MET:HE3   | 1:A:221:SER:H    | 1.12                     | 1.08              |
| 1:A:157:ALA:HA   | 1:A:161:PRO:HB3  | 1.34                     | 1.08              |
| 1:A:424:VAL:HG21 | 1:A:429:VAL:HG21 | 1.34                     | 1.08              |
| 1:A:99:ASP:CG    | 1:A:216:ARG:NH1  | 2.12                     | 1.07              |
| 1:A:361:ARG:CZ   | 1:A:401:ILE:HG22 | 1.83                     | 1.07              |
| 1:A:174:MET:HE3  | 1:A:503:ALA:HA   | 1.33                     | 1.07              |
| 1:A:465:PRO:HG3  | 1:A:571:ILE:CG2  | 1.85                     | 1.07              |
| 1:A:361:ARG:O    | 1:A:407:GLY:CA   | 2.03                     | 1.06              |
| 1:A:365:GLN:HA   | 1:A:365:GLN:OE1  | 1.53                     | 1.05              |
| 1:A:381:GLY:HA2  | 1:A:386:GLN:HE21 | 1.23                     | 1.04              |
| 1:A:193:GLU:HB3  | 1:A:206:THR:CG2  | 1.87                     | 1.04              |
| 1:A:276:THR:HG21 | 1:A:581:ARG:HB2  | 1.07                     | 1.04              |
| 1:A:74:PRO:O     | 1:A:520:ARG:NH2  | 1.92                     | 1.03              |
| 1:A:424:VAL:HG21 | 1:A:429:VAL:HG22 | 1.36                     | 1.03              |
| 1:A:382:ARG:HH11 | 1:A:382:ARG:HG2  | 1.17                     | 1.03              |
| 1:A:118:GLY:HA3  | 1:A:197:PHE:CE2  | 1.94                     | 1.02              |
| 1:A:159:GLN:CB   | 1:A:160:PRO:HD3  | 1.88                     | 1.02              |
| 1:A:309:GLN:O    | 1:A:313:ARG:HG3  | 1.58                     | 1.00              |
| 1:A:516:ALA:O    | 1:A:517:ASN:CG   | 2.04                     | 1.00              |
| 1:A:93:LYS:NZ    | 1:A:227:GLY:O    | 1.94                     | 1.00              |
| 1:A:516:ALA:C    | 1:A:517:ASN:HD22 | 1.59                     | 0.99              |
| 1:A:576:SER:O    | 1:A:578:LEU:CD2  | 2.11                     | 0.98              |
| 1:A:465:PRO:HG3  | 1:A:571:ILE:HG21 | 1.43                     | 0.97              |
| 1:A:96:MET:HE2   | 1:A:220:PRO:C    | 1.89                     | 0.97              |
| 1:A:213:GLN:OE1  | 1:A:237:ASP:HB3  | 1.63                     | 0.97              |
| 1:A:96:MET:HE2   | 1:A:220:PRO:CA   | 1.94                     | 0.97              |
| 1:A:159:GLN:CB   | 1:A:160:PRO:CD   | 2.42                     | 0.97              |
| 1:A:359:ALA:CB   | 1:A:373:ASP:C    | 2.35                     | 0.97              |
| 1:A:77:GLU:CB    | 1:A:518:MET:HE3  | 1.90                     | 0.97              |
| 1:A:96:MET:HE1   | 1:A:221:SER:H    | 1.28                     | 0.96              |
| 1:A:359:ALA:HB3  | 1:A:373:ASP:O    | 0.79                     | 0.96              |
| 1:A:381:GLY:HA2  | 1:A:386:GLN:NE2  | 1.78                     | 0.96              |
| 1:A:70:HIS:CD2   | 1:A:526:ASP:OD1  | 2.19                     | 0.95              |
| 1:A:429:VAL:HG12 | 1:A:431:LEU:CD1  | 1.97                     | 0.94              |
| 1:A:77:GLU:HB2   | 1:A:518:MET:HE2  | 1.46                     | 0.94              |
| 1:A:158:THR:O    | 1:A:160:PRO:CD   | 2.15                     | 0.94              |
| 1:A:443:ASN:HB2  | 1:A:446:ASN:OD1  | 1.68                     | 0.93              |
| 1:A:99:ASP:CG    | 1:A:216:ARG:HH12 | 1.74                     | 0.93              |
| 1:A:96:MET:HE2   | 1:A:221:SER:H    | 1.03                     | 0.93              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:322:THR:CG2  | 1:A:420:PHE:CD2  | 2.52                     | 0.92              |
| 1:A:159:GLN:HB2  | 1:A:160:PRO:HD3  | 0.92                     | 0.92              |
| 1:A:197:PHE:HE2  | 1:A:465:PRO:HB2  | 1.33                     | 0.91              |
| 1:A:38:VAL:CG2   | 1:A:38:VAL:O     | 2.18                     | 0.91              |
| 1:A:424:VAL:CG2  | 1:A:429:VAL:HG21 | 1.90                     | 0.90              |
| 1:A:466:ASN:O    | 1:A:467:GLY:O    | 1.88                     | 0.90              |
| 1:A:193:GLU:CB   | 1:A:206:THR:HG21 | 2.01                     | 0.90              |
| 1:A:96:MET:HE2   | 1:A:220:PRO:HA   | 1.55                     | 0.89              |
| 1:A:219:ILE:HG13 | 1:A:230:THR:HB   | 1.54                     | 0.89              |
| 1:A:370:GLN:NE2  | 1:A:399:THR:HG21 | 1.87                     | 0.89              |
| 1:A:378:TYR:O    | 1:A:397:ARG:CB   | 2.21                     | 0.88              |
| 1:A:361:ARG:NH1  | 1:A:402:ALA:O    | 2.05                     | 0.88              |
| 1:A:160:PRO:HB2  | 1:A:161:PRO:C    | 1.98                     | 0.88              |
| 1:A:431:LEU:HB3  | 1:A:432:PRO:HD2  | 1.53                     | 0.88              |
| 1:A:469:ILE:CG2  | 1:A:470:TRP:HE3  | 1.86                     | 0.88              |
| 1:A:322:THR:HG21 | 1:A:420:PHE:CE2  | 2.08                     | 0.88              |
| 1:A:73:MET:HE3   | 1:A:520:ARG:NE   | 1.87                     | 0.88              |
| 1:A:150:LEU:CD2  | 1:A:525:SER:CB   | 2.29                     | 0.87              |
| 1:A:99:ASP:OD2   | 1:A:216:ARG:NH1  | 2.08                     | 0.87              |
| 1:A:416:GLN:HB3  | 1:A:429:VAL:HG22 | 1.55                     | 0.87              |
| 1:A:565:ASN:ND2  | 1:A:566:ILE:HG13 | 1.88                     | 0.87              |
| 1:A:279:TRP:HE3  | 1:A:279:TRP:O    | 1.58                     | 0.87              |
| 1:A:415:ILE:HD11 | 1:A:444:TYR:CE2  | 2.10                     | 0.86              |
| 1:A:157:ALA:HA   | 1:A:161:PRO:CB   | 2.05                     | 0.86              |
| 1:A:266:PHE:HZ   | 1:A:493:ASN:O    | 1.58                     | 0.86              |
| 1:A:359:ALA:CB   | 1:A:373:ASP:CA   | 2.53                     | 0.86              |
| 1:A:77:GLU:HG2   | 1:A:520:ARG:NH1  | 1.90                     | 0.86              |
| 1:A:469:ILE:CG2  | 1:A:470:TRP:CE3  | 2.59                     | 0.86              |
| 1:A:111:LEU:CD2  | 1:A:112:VAL:N    | 2.37                     | 0.86              |
| 1:A:38:VAL:O     | 1:A:38:VAL:HG22  | 1.76                     | 0.85              |
| 1:A:364:ALA:O    | 1:A:367:ASP:HB3  | 1.76                     | 0.85              |
| 1:A:382:ARG:HG2  | 1:A:382:ARG:NH1  | 1.89                     | 0.85              |
| 1:A:517:ASN:O    | 1:A:519:SER:N    | 2.10                     | 0.85              |
| 1:A:378:TYR:O    | 1:A:397:ARG:HB3  | 1.76                     | 0.85              |
| 1:A:361:ARG:HH11 | 1:A:401:ILE:HG22 | 1.04                     | 0.85              |
| 1:A:77:GLU:HB2   | 1:A:518:MET:CE   | 1.97                     | 0.84              |
| 1:A:193:GLU:CD   | 1:A:209:ARG:HH22 | 1.85                     | 0.84              |
| 1:A:194:THR:HG22 | 1:A:195:LEU:N    | 1.89                     | 0.84              |
| 1:A:53:PHE:CD1   | 1:A:59:VAL:CG1   | 2.61                     | 0.83              |
| 1:A:233:TYR:O    | 1:A:233:TYR:HD1  | 1.60                     | 0.83              |
| 1:A:313:ARG:O    | 1:A:325:ILE:HD12 | 1.79                     | 0.83              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:343:TYR:OH   | 1:A:371:ALA:HB2  | 1.79                     | 0.83              |
| 1:A:365:GLN:OE1  | 1:A:365:GLN:CA   | 2.26                     | 0.82              |
| 1:A:197:PHE:CE2  | 1:A:465:PRO:HB2  | 2.13                     | 0.82              |
| 1:A:111:LEU:HD23 | 1:A:112:VAL:CA   | 2.09                     | 0.82              |
| 1:A:578:LEU:HD23 | 1:A:578:LEU:H    | 1.45                     | 0.82              |
| 1:A:429:VAL:HG12 | 1:A:431:LEU:HD11 | 1.60                     | 0.82              |
| 1:A:93:LYS:CE    | 1:A:227:GLY:O    | 2.26                     | 0.81              |
| 1:A:340:ALA:HB1  | 1:A:341:PRO:HD2  | 1.62                     | 0.81              |
| 1:A:465:PRO:HG3  | 1:A:571:ILE:HG22 | 1.60                     | 0.81              |
| 1:A:505:ASN:OD1  | 1:A:521:ILE:CD1  | 2.23                     | 0.81              |
| 1:A:53:PHE:CD1   | 1:A:59:VAL:HG12  | 2.15                     | 0.81              |
| 1:A:118:GLY:HA3  | 1:A:197:PHE:CD2  | 2.16                     | 0.81              |
| 1:A:340:ALA:HB3  | 1:A:357:ILE:HD11 | 1.63                     | 0.81              |
| 1:A:359:ALA:HB1  | 1:A:373:ASP:HB2  | 0.85                     | 0.81              |
| 1:A:233:TYR:O    | 1:A:233:TYR:CD1  | 2.32                     | 0.80              |
| 1:A:121:PHE:CE2  | 1:A:129:ILE:HD11 | 2.17                     | 0.80              |
| 1:A:158:THR:O    | 1:A:158:THR:CG2  | 2.30                     | 0.80              |
| 1:A:89:LYS:O     | 1:A:95:ASN:HB2   | 1.82                     | 0.80              |
| 1:A:415:ILE:CD1  | 1:A:444:TYR:CE2  | 2.65                     | 0.80              |
| 1:A:576:SER:O    | 1:A:578:LEU:HD22 | 1.81                     | 0.80              |
| 1:A:415:ILE:HD11 | 1:A:444:TYR:CD2  | 2.16                     | 0.80              |
| 1:A:380:PHE:CD1  | 1:A:466:ASN:OD1  | 2.35                     | 0.79              |
| 1:A:464:TYR:HA   | 1:A:465:PRO:O    | 1.82                     | 0.79              |
| 1:A:359:ALA:CB   | 1:A:373:ASP:CB   | 2.44                     | 0.79              |
| 1:A:432:PRO:O    | 1:A:443:ASN:ND2  | 2.16                     | 0.78              |
| 1:A:99:ASP:OD1   | 1:A:101:ILE:HG22 | 1.82                     | 0.78              |
| 1:A:184:PRO:HD3  | 1:A:244:TYR:CE2  | 2.18                     | 0.78              |
| 1:A:370:GLN:HE22 | 1:A:399:THR:HG21 | 1.44                     | 0.78              |
| 1:A:511:ASP:OD2  | 1:A:513:ASP:C    | 2.27                     | 0.78              |
| 1:A:278:THR:HG21 | 1:A:583:LEU:HD12 | 1.65                     | 0.78              |
| 1:A:341:PRO:HB2  | 1:A:344:SER:OG   | 1.84                     | 0.77              |
| 1:A:193:GLU:OE1  | 1:A:209:ARG:NH2  | 2.16                     | 0.77              |
| 1:A:174:MET:HE3  | 1:A:504:PRO:CD   | 2.14                     | 0.77              |
| 1:A:86:ASN:ND2   | 1:A:100:ASP:HB2  | 1.99                     | 0.77              |
| 1:A:146:PHE:HD2  | 1:A:147:ASN:HD22 | 1.32                     | 0.77              |
| 1:A:73:MET:CE    | 1:A:520:ARG:HG3  | 2.15                     | 0.77              |
| 1:A:174:MET:CE   | 1:A:504:PRO:HD2  | 2.15                     | 0.77              |
| 1:A:361:ARG:NH1  | 1:A:401:ILE:O    | 2.18                     | 0.77              |
| 1:A:471:ASP:O    | 1:A:472:LYS:O    | 2.01                     | 0.77              |
| 1:A:515:SER:O    | 1:A:516:ALA:C    | 2.28                     | 0.77              |
| 1:A:122:ASN:ND2  | 1:A:125:ASP:OD2  | 2.19                     | 0.76              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:564:ASN:O    | 1:A:567:GLY:N    | 2.18                     | 0.76              |
| 1:A:322:THR:HG21 | 1:A:420:PHE:CD2  | 2.19                     | 0.76              |
| 1:A:469:ILE:HG21 | 1:A:470:TRP:CE3  | 2.18                     | 0.76              |
| 1:A:77:GLU:CG    | 1:A:520:ARG:NH1  | 2.48                     | 0.76              |
| 1:A:464:TYR:CD1  | 1:A:464:TYR:C    | 2.64                     | 0.76              |
| 1:A:276:THR:O    | 1:A:577:GLN:NE2  | 2.19                     | 0.75              |
| 1:A:113:ASP:O    | 1:A:195:LEU:HD13 | 1.86                     | 0.75              |
| 1:A:279:TRP:O    | 1:A:279:TRP:CE3  | 2.38                     | 0.75              |
| 1:A:413:ASP:O    | 1:A:414:TRP:HB3  | 1.87                     | 0.75              |
| 1:A:130:VAL:HG13 | 1:A:578:LEU:HD21 | 1.67                     | 0.75              |
| 1:A:469:ILE:HG22 | 1:A:470:TRP:HE3  | 1.50                     | 0.75              |
| 1:A:152:THR:HG23 | 1:A:521:ILE:HG22 | 1.69                     | 0.75              |
| 1:A:429:VAL:HG12 | 1:A:431:LEU:HD12 | 1.68                     | 0.75              |
| 1:A:361:ARG:HH21 | 1:A:365:GLN:HE21 | 1.34                     | 0.74              |
| 1:A:111:LEU:HD23 | 1:A:112:VAL:C    | 2.12                     | 0.74              |
| 1:A:361:ARG:NH1  | 1:A:401:ILE:C    | 2.46                     | 0.74              |
| 1:A:448:PHE:CE2  | 1:A:450:THR:CG2  | 2.70                     | 0.74              |
| 1:A:68:LEU:HB2   | 1:A:528:TRP:CE3  | 2.22                     | 0.74              |
| 1:A:422:LEU:HA   | 1:A:423:PRO:C    | 2.11                     | 0.74              |
| 1:A:66:SER:HA    | 1:A:530:LYS:HA   | 1.67                     | 0.74              |
| 1:A:69:VAL:HG13  | 1:A:205:PRO:HD3  | 1.68                     | 0.74              |
| 1:A:96:MET:CE    | 1:A:220:PRO:CA   | 2.65                     | 0.74              |
| 1:A:138:LEU:HD13 | 1:A:535:PHE:CE1  | 2.22                     | 0.74              |
| 1:A:111:LEU:HD23 | 1:A:112:VAL:H    | 1.52                     | 0.73              |
| 1:A:139:VAL:HG12 | 1:A:140:SER:N    | 2.02                     | 0.73              |
| 1:A:415:ILE:CD1  | 1:A:444:TYR:CD2  | 2.70                     | 0.73              |
| 1:A:533:LEU:HD21 | 1:A:535:PHE:HZ   | 1.53                     | 0.73              |
| 1:A:533:LEU:CD2  | 1:A:535:PHE:CZ   | 2.71                     | 0.73              |
| 1:A:576:SER:O    | 1:A:578:LEU:HD23 | 1.86                     | 0.73              |
| 1:A:266:PHE:HZ   | 1:A:493:ASN:C    | 1.96                     | 0.73              |
| 1:A:465:PRO:CG   | 1:A:571:ILE:HG22 | 2.19                     | 0.73              |
| 1:A:429:VAL:CG1  | 1:A:431:LEU:HD11 | 2.18                     | 0.73              |
| 1:A:444:TYR:O    | 1:A:448:PHE:HB2  | 1.89                     | 0.73              |
| 1:A:424:VAL:HG22 | 1:A:429:VAL:CG2  | 1.93                     | 0.72              |
| 1:A:47:ASN:ND2   | 1:A:65:SER:HA    | 2.05                     | 0.72              |
| 1:A:414:TRP:NE1  | 1:A:416:GLN:HE21 | 1.86                     | 0.72              |
| 1:A:116:ALA:O    | 1:A:120:TRP:HD1  | 1.73                     | 0.72              |
| 1:A:68:LEU:HD23  | 1:A:202:PRO:HB3  | 1.70                     | 0.72              |
| 1:A:99:ASP:CG    | 1:A:216:ARG:HH11 | 1.97                     | 0.72              |
| 1:A:217:THR:O    | 1:A:231:ASN:HA   | 1.90                     | 0.71              |
| 1:A:533:LEU:HD21 | 1:A:535:PHE:CZ   | 2.25                     | 0.71              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:390:THR:HG22 | 1:A:391:THR:N    | 2.04                     | 0.71              |
| 1:A:424:VAL:CG1  | 1:A:429:VAL:HG21 | 2.21                     | 0.71              |
| 1:A:343:TYR:CE1  | 1:A:371:ALA:HB1  | 2.24                     | 0.71              |
| 1:A:343:TYR:OH   | 1:A:371:ALA:CB   | 2.38                     | 0.71              |
| 1:A:417:ASN:OD1  | 1:A:419:ASN:ND2  | 2.20                     | 0.71              |
| 1:A:157:ALA:CA   | 1:A:161:PRO:HB3  | 2.18                     | 0.70              |
| 1:A:409:TYR:C    | 1:A:411:GLU:H    | 1.99                     | 0.70              |
| 1:A:283:ARG:HE   | 1:A:327:GLU:HB3  | 1.57                     | 0.70              |
| 1:A:103:VAL:HG12 | 1:A:212:PHE:HB3  | 1.73                     | 0.70              |
| 1:A:121:PHE:CE2  | 1:A:129:ILE:CD1  | 2.73                     | 0.70              |
| 1:A:152:THR:HG23 | 1:A:521:ILE:CG2  | 2.22                     | 0.70              |
| 1:A:339:SER:HB2  | 1:A:450:THR:OG1  | 1.91                     | 0.70              |
| 1:A:84:VAL:HG21  | 1:A:102:HIS:CE1  | 2.26                     | 0.70              |
| 1:A:424:VAL:HG11 | 1:A:429:VAL:HG21 | 1.73                     | 0.69              |
| 1:A:77:GLU:HG2   | 1:A:520:ARG:HH12 | 1.55                     | 0.69              |
| 1:A:422:LEU:HA   | 1:A:424:VAL:N    | 2.06                     | 0.69              |
| 1:A:465:PRO:CG   | 1:A:571:ILE:CG2  | 2.68                     | 0.69              |
| 1:A:77:GLU:HB3   | 1:A:518:MET:CE   | 2.22                     | 0.69              |
| 1:A:84:VAL:O     | 1:A:101:ILE:HA   | 1.92                     | 0.69              |
| 1:A:139:VAL:O    | 1:A:268:PHE:HD1  | 1.73                     | 0.69              |
| 1:A:482:LEU:N    | 1:A:482:LEU:HD23 | 2.08                     | 0.69              |
| 1:A:578:LEU:HD23 | 1:A:578:LEU:N    | 2.05                     | 0.69              |
| 1:A:409:TYR:CE1  | 1:A:411:GLU:HB2  | 2.27                     | 0.69              |
| 1:A:158:THR:O    | 1:A:158:THR:HG22 | 1.92                     | 0.69              |
| 1:A:322:THR:CG2  | 1:A:420:PHE:HD2  | 2.06                     | 0.69              |
| 1:A:49:THR:HG22  | 1:A:51:PHE:CE1   | 2.27                     | 0.68              |
| 1:A:518:MET:O    | 1:A:518:MET:HG3  | 1.92                     | 0.68              |
| 1:A:378:TYR:CE2  | 1:A:463:VAL:HG11 | 2.27                     | 0.68              |
| 1:A:116:ALA:O    | 1:A:120:TRP:CD1  | 2.47                     | 0.68              |
| 1:A:448:PHE:CE2  | 1:A:450:THR:HG23 | 2.28                     | 0.68              |
| 1:A:452:GLY:C    | 1:A:454:LEU:H    | 2.00                     | 0.68              |
| 1:A:501:LYS:HG2  | 1:A:502:VAL:N    | 2.09                     | 0.68              |
| 1:A:93:LYS:O     | 1:A:221:SER:O    | 2.10                     | 0.68              |
| 1:A:562:VAL:HG13 | 1:A:563:PRO:HD2  | 1.76                     | 0.68              |
| 1:A:101:ILE:HG21 | 1:A:216:ARG:HD2  | 1.76                     | 0.68              |
| 1:A:180:ASN:O    | 1:A:181:ASN:C    | 2.37                     | 0.67              |
| 1:A:109:TRP:CE3  | 1:A:501:LYS:HB2  | 2.29                     | 0.67              |
| 1:A:469:ILE:HG22 | 1:A:470:TRP:CE3  | 2.27                     | 0.67              |
| 1:A:121:PHE:HE2  | 1:A:129:ILE:HD11 | 1.58                     | 0.67              |
| 1:A:103:VAL:CG2  | 1:A:214:TRP:HB3  | 2.25                     | 0.67              |
| 1:A:361:ARG:HH21 | 1:A:365:GLN:NE2  | 1.91                     | 0.67              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:150:LEU:HD23 | 1:A:525:SER:HB3  | 0.70                     | 0.67              |
| 1:A:64:ASN:HA    | 1:A:531:GLY:O    | 1.93                     | 0.67              |
| 1:A:158:THR:C    | 1:A:159:GLN:HG2  | 2.18                     | 0.67              |
| 1:A:174:MET:HE3  | 1:A:504:PRO:HD2  | 1.76                     | 0.67              |
| 1:A:431:LEU:HB3  | 1:A:432:PRO:CD   | 2.24                     | 0.67              |
| 1:A:313:ARG:O    | 1:A:325:ILE:CD1  | 2.43                     | 0.66              |
| 1:A:80:LYS:O     | 1:A:105:ILE:HG23 | 1.95                     | 0.66              |
| 1:A:309:GLN:O    | 1:A:313:ARG:CG   | 2.38                     | 0.66              |
| 1:A:414:TRP:CD1  | 1:A:416:GLN:HE21 | 2.13                     | 0.66              |
| 1:A:158:THR:C    | 1:A:160:PRO:HD2  | 2.16                     | 0.65              |
| 1:A:361:ARG:HA   | 1:A:368:GLU:OE2  | 1.96                     | 0.65              |
| 1:A:150:LEU:HD21 | 1:A:525:SER:HB3  | 1.67                     | 0.65              |
| 1:A:109:TRP:CZ3  | 1:A:501:LYS:HB3  | 2.32                     | 0.65              |
| 1:A:96:MET:HE1   | 1:A:221:SER:N    | 1.93                     | 0.65              |
| 1:A:115:ASN:OD1  | 1:A:469:ILE:HB   | 1.97                     | 0.65              |
| 1:A:174:MET:CE   | 1:A:504:PRO:CD   | 2.72                     | 0.65              |
| 1:A:77:GLU:CB    | 1:A:518:MET:HE2  | 2.06                     | 0.64              |
| 1:A:73:MET:CE    | 1:A:520:ARG:CG   | 2.75                     | 0.64              |
| 1:A:160:PRO:CB   | 1:A:161:PRO:C    | 2.65                     | 0.64              |
| 1:A:364:ALA:O    | 1:A:367:ASP:CB   | 2.45                     | 0.64              |
| 1:A:414:TRP:HE1  | 1:A:416:GLN:NE2  | 1.95                     | 0.64              |
| 1:A:279:TRP:CE3  | 1:A:279:TRP:C    | 2.76                     | 0.64              |
| 1:A:430:LEU:HD11 | 1:A:436:ILE:HD11 | 1.79                     | 0.64              |
| 1:A:361:ARG:HH11 | 1:A:401:ILE:CG2  | 1.91                     | 0.63              |
| 1:A:431:LEU:HD12 | 1:A:431:LEU:N    | 2.13                     | 0.63              |
| 1:A:403:HIS:CE1  | 1:A:575:LYS:HD2  | 2.32                     | 0.63              |
| 1:A:533:LEU:HG   | 1:A:535:PHE:CE2  | 2.33                     | 0.63              |
| 1:A:548:ILE:HG23 | 1:A:580:PRO:HD2  | 1.81                     | 0.63              |
| 1:A:564:ASN:O    | 1:A:566:ILE:N    | 2.32                     | 0.63              |
| 1:A:299:GLY:C    | 1:A:301:THR:H    | 2.06                     | 0.63              |
| 1:A:53:PHE:CE1   | 1:A:59:VAL:HG11  | 2.33                     | 0.63              |
| 1:A:49:THR:HG22  | 1:A:51:PHE:HE1   | 1.64                     | 0.63              |
| 1:A:174:MET:HE3  | 1:A:503:ALA:CA   | 2.19                     | 0.63              |
| 1:A:564:ASN:ND2  | 1:A:566:ILE:H    | 1.97                     | 0.63              |
| 1:A:369:ASN:C    | 1:A:371:ALA:H    | 1.97                     | 0.63              |
| 1:A:107:THR:OG1  | 1:A:208:TRP:HB3  | 1.99                     | 0.62              |
| 1:A:155:GLU:OE2  | 1:A:163:LYS:HE2  | 1.97                     | 0.62              |
| 1:A:385:GLY:O    | 1:A:386:GLN:O    | 2.17                     | 0.62              |
| 1:A:557:ASN:HB3  | 1:A:561:TYR:HE2  | 1.64                     | 0.62              |
| 1:A:203:THR:OG1  | 1:A:204:ILE:N    | 2.32                     | 0.62              |
| 1:A:42:THR:CG2   | 1:A:260:GLU:HB2  | 2.29                     | 0.62              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:245:THR:O    | 1:A:249:SER:OG   | 2.16                     | 0.62              |
| 1:A:471:ASP:C    | 1:A:472:LYS:O    | 2.42                     | 0.62              |
| 1:A:266:PHE:CZ   | 1:A:493:ASN:O    | 2.48                     | 0.62              |
| 1:A:396:GLU:HG3  | 1:A:397:ARG:N    | 2.14                     | 0.62              |
| 1:A:390:THR:CG2  | 1:A:391:THR:N    | 2.62                     | 0.62              |
| 1:A:65:SER:OG    | 1:A:67:ARG:NH2   | 2.23                     | 0.62              |
| 1:A:93:LYS:O     | 1:A:222:HIS:O    | 2.18                     | 0.62              |
| 1:A:508:ASN:ND2  | 1:A:509:GLN:HG3  | 2.15                     | 0.62              |
| 1:A:500:VAL:HG11 | 1:A:527:PHE:CZ   | 2.35                     | 0.61              |
| 1:A:103:VAL:HG23 | 1:A:214:TRP:CB   | 2.29                     | 0.61              |
| 1:A:292:ASN:HB2  | 1:A:306:ILE:O    | 2.00                     | 0.61              |
| 1:A:359:ALA:HB2  | 1:A:373:ASP:CA   | 2.31                     | 0.61              |
| 1:A:326:THR:H    | 1:A:329:THR:HB   | 1.65                     | 0.61              |
| 1:A:219:ILE:HG13 | 1:A:230:THR:CB   | 2.28                     | 0.61              |
| 1:A:414:TRP:HE1  | 1:A:416:GLN:HE21 | 1.46                     | 0.61              |
| 1:A:443:ASN:HB3  | 1:A:445:THR:H    | 1.65                     | 0.61              |
| 1:A:138:LEU:CD1  | 1:A:535:PHE:CE1  | 2.83                     | 0.61              |
| 1:A:174:MET:HE3  | 1:A:504:PRO:HD3  | 1.81                     | 0.61              |
| 1:A:361:ARG:CZ   | 1:A:401:ILE:CG2  | 2.64                     | 0.60              |
| 1:A:426:ASN:C    | 1:A:428:ASN:H    | 2.09                     | 0.60              |
| 1:A:482:LEU:HD23 | 1:A:482:LEU:H    | 1.66                     | 0.60              |
| 1:A:317:THR:HG23 | 1:A:329:THR:HG22 | 1.83                     | 0.60              |
| 1:A:219:ILE:CG1  | 1:A:230:THR:HB   | 2.29                     | 0.60              |
| 1:A:505:ASN:O    | 1:A:520:ARG:HB2  | 2.01                     | 0.60              |
| 1:A:533:LEU:CD2  | 1:A:535:PHE:HZ   | 2.11                     | 0.60              |
| 1:A:551:MET:HE3  | 1:A:574:GLU:CD   | 2.26                     | 0.60              |
| 1:A:390:THR:CG2  | 1:A:391:THR:H    | 2.14                     | 0.60              |
| 1:A:511:ASP:C    | 1:A:513:ASP:H    | 2.06                     | 0.60              |
| 1:A:115:ASN:ND2  | 1:A:470:TRP:O    | 2.30                     | 0.60              |
| 1:A:322:THR:HG22 | 1:A:420:PHE:HD2  | 1.67                     | 0.60              |
| 1:A:84:VAL:O     | 1:A:101:ILE:HG13 | 2.01                     | 0.59              |
| 1:A:38:VAL:O     | 1:A:38:VAL:HG23  | 2.02                     | 0.59              |
| 1:A:111:LEU:CD2  | 1:A:112:VAL:C    | 2.75                     | 0.59              |
| 1:A:369:ASN:HB3  | 1:A:372:ALA:HB3  | 1.84                     | 0.59              |
| 1:A:470:TRP:HA   | 1:A:488:PHE:O    | 2.02                     | 0.59              |
| 1:A:368:GLU:HG2  | 1:A:369:ASN:H    | 1.67                     | 0.59              |
| 1:A:578:LEU:O    | 1:A:578:LEU:HG   | 2.01                     | 0.59              |
| 1:A:409:TYR:O    | 1:A:411:GLU:N    | 2.35                     | 0.59              |
| 1:A:54:LEU:CD1   | 1:A:54:LEU:N     | 2.66                     | 0.59              |
| 1:A:103:VAL:HG23 | 1:A:214:TRP:HB3  | 1.84                     | 0.59              |
| 1:A:343:TYR:CZ   | 1:A:371:ALA:HB1  | 2.37                     | 0.59              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:377:ARG:CZ   | 1:A:397:ARG:HG3  | 2.33                     | 0.59              |
| 1:A:459:ASN:HA   | 1:A:482:LEU:HD12 | 1.83                     | 0.59              |
| 1:A:73:MET:HE3   | 1:A:520:ARG:HE   | 1.68                     | 0.59              |
| 1:A:194:THR:CG2  | 1:A:195:LEU:H    | 1.83                     | 0.59              |
| 1:A:369:ASN:OD1  | 1:A:410:PRO:HG2  | 2.03                     | 0.58              |
| 1:A:417:ASN:HB2  | 1:A:428:ASN:HD22 | 1.68                     | 0.58              |
| 1:A:222:HIS:CE1  | 1:A:225:THR:N    | 2.71                     | 0.58              |
| 1:A:111:LEU:O    | 1:A:205:PRO:CB   | 2.52                     | 0.58              |
| 1:A:250:VAL:HG13 | 1:A:251:PRO:HD2  | 1.85                     | 0.58              |
| 1:A:152:THR:CG2  | 1:A:521:ILE:CG2  | 2.81                     | 0.58              |
| 1:A:111:LEU:O    | 1:A:205:PRO:HB3  | 2.04                     | 0.57              |
| 1:A:183:MET:HG2  | 1:A:208:TRP:HH2  | 1.68                     | 0.57              |
| 1:A:560:ASN:OD1  | 1:A:572:VAL:HG21 | 2.03                     | 0.57              |
| 1:A:77:GLU:HG3   | 1:A:518:MET:HE3  | 0.59                     | 0.57              |
| 1:A:295:PRO:HB3  | 1:A:302:ASN:HB3  | 1.87                     | 0.57              |
| 1:A:324:TYR:O    | 1:A:329:THR:HG21 | 2.04                     | 0.57              |
| 1:A:110:SER:HB2  | 1:A:500:VAL:O    | 2.05                     | 0.57              |
| 1:A:150:LEU:HD21 | 1:A:525:SER:CB   | 2.29                     | 0.57              |
| 1:A:160:PRO:HG2  | 1:A:162:THR:OG1  | 2.03                     | 0.57              |
| 1:A:184:PRO:HD3  | 1:A:244:TYR:CD2  | 2.38                     | 0.57              |
| 1:A:197:PHE:HE2  | 1:A:465:PRO:CB   | 2.11                     | 0.57              |
| 1:A:448:PHE:CE2  | 1:A:450:THR:HG21 | 2.37                     | 0.57              |
| 1:A:247:GLU:CD   | 1:A:247:GLU:H    | 2.13                     | 0.57              |
| 1:A:77:GLU:CG    | 1:A:520:ARG:HH11 | 2.17                     | 0.57              |
| 1:A:213:GLN:OE1  | 1:A:237:ASP:CB   | 2.46                     | 0.57              |
| 1:A:213:GLN:O    | 1:A:236:THR:HG23 | 2.05                     | 0.57              |
| 1:A:361:ARG:HG3  | 1:A:368:GLU:OE2  | 2.04                     | 0.57              |
| 1:A:77:GLU:CB    | 1:A:518:MET:HE1  | 2.30                     | 0.57              |
| 1:A:447:ILE:HG22 | 1:A:447:ILE:O    | 2.05                     | 0.57              |
| 1:A:111:LEU:HD23 | 1:A:111:LEU:C    | 2.27                     | 0.56              |
| 1:A:47:ASN:HD22  | 1:A:66:SER:H     | 1.53                     | 0.56              |
| 1:A:54:LEU:N     | 1:A:54:LEU:HD13  | 2.20                     | 0.56              |
| 1:A:140:SER:H    | 1:A:534:VAL:HB   | 1.70                     | 0.56              |
| 1:A:75:GLU:O     | 1:A:520:ARG:NH2  | 2.39                     | 0.56              |
| 1:A:73:MET:HE1   | 1:A:520:ARG:HG3  | 1.86                     | 0.56              |
| 1:A:93:LYS:O     | 1:A:222:HIS:C    | 2.49                     | 0.56              |
| 1:A:390:THR:HG22 | 1:A:391:THR:H    | 1.70                     | 0.56              |
| 1:A:461:PRO:HB3  | 1:A:577:GLN:OE1  | 2.06                     | 0.56              |
| 1:A:188:ALA:HB1  | 1:A:193:GLU:O    | 2.05                     | 0.56              |
| 1:A:354:LYS:HD2  | 1:A:355:THR:N    | 2.21                     | 0.56              |
| 1:A:118:GLY:CA   | 1:A:465:PRO:HB3  | 2.36                     | 0.56              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:198:TYR:OH   | 1:A:570:LYS:HA   | 2.06                     | 0.56              |
| 1:A:42:THR:HG22  | 1:A:260:GLU:HB2  | 1.88                     | 0.55              |
| 1:A:109:TRP:CE3  | 1:A:501:LYS:CB   | 2.89                     | 0.55              |
| 1:A:193:GLU:HB3  | 1:A:206:THR:HG22 | 1.86                     | 0.55              |
| 1:A:381:GLY:CA   | 1:A:386:GLN:NE2  | 2.64                     | 0.55              |
| 1:A:278:THR:CG2  | 1:A:583:LEU:HD12 | 2.35                     | 0.55              |
| 1:A:538:LYS:HG3  | 1:A:539:LEU:N    | 2.20                     | 0.55              |
| 1:A:68:LEU:HB2   | 1:A:528:TRP:CZ3  | 2.41                     | 0.55              |
| 1:A:86:ASN:ND2   | 1:A:100:ASP:H    | 2.04                     | 0.55              |
| 1:A:53:PHE:CE1   | 1:A:59:VAL:CG1   | 2.89                     | 0.55              |
| 1:A:232:VAL:HG23 | 1:A:233:TYR:N    | 2.21                     | 0.55              |
| 1:A:548:ILE:HG23 | 1:A:580:PRO:CD   | 2.37                     | 0.55              |
| 1:A:62:THR:HG21  | 1:A:532:LYS:HE3  | 1.88                     | 0.55              |
| 1:A:86:ASN:HD21  | 1:A:100:ASP:H    | 1.54                     | 0.55              |
| 1:A:340:ALA:HB1  | 1:A:341:PRO:CD   | 2.35                     | 0.55              |
| 1:A:515:SER:O    | 1:A:516:ALA:O    | 2.23                     | 0.55              |
| 1:A:47:ASN:HA    | 1:A:64:ASN:O     | 2.07                     | 0.55              |
| 1:A:133:MET:SD   | 1:A:539:LEU:HD23 | 2.47                     | 0.55              |
| 1:A:361:ARG:NH1  | 1:A:401:ILE:CB   | 2.68                     | 0.55              |
| 1:A:511:ASP:C    | 1:A:513:ASP:N    | 2.64                     | 0.55              |
| 1:A:103:VAL:CG2  | 1:A:214:TRP:CB   | 2.85                     | 0.55              |
| 1:A:194:THR:HB   | 1:A:384:HIS:CE1  | 2.42                     | 0.55              |
| 1:A:511:ASP:OD2  | 1:A:513:ASP:HB2  | 2.07                     | 0.54              |
| 1:A:415:ILE:HD12 | 1:A:444:TYR:CD2  | 2.41                     | 0.54              |
| 1:A:511:ASP:OD2  | 1:A:513:ASP:CA   | 2.55                     | 0.54              |
| 1:A:52:LYS:O     | 1:A:54:LEU:HD13  | 2.08                     | 0.54              |
| 1:A:73:MET:HE1   | 1:A:520:ARG:CG   | 2.37                     | 0.54              |
| 1:A:366:THR:O    | 1:A:366:THR:HG22 | 2.07                     | 0.54              |
| 1:A:96:MET:CE    | 1:A:220:PRO:CB   | 2.85                     | 0.54              |
| 1:A:409:TYR:CE1  | 1:A:411:GLU:CB   | 2.90                     | 0.54              |
| 1:A:96:MET:CE    | 1:A:220:PRO:C    | 2.62                     | 0.54              |
| 1:A:111:LEU:CD2  | 1:A:112:VAL:H    | 2.14                     | 0.54              |
| 1:A:313:ARG:C    | 1:A:325:ILE:HD12 | 2.32                     | 0.54              |
| 1:A:469:ILE:HG21 | 1:A:470:TRP:HE3  | 1.56                     | 0.54              |
| 1:A:266:PHE:CZ   | 1:A:493:ASN:C    | 2.84                     | 0.54              |
| 1:A:301:THR:O    | 1:A:301:THR:HG22 | 2.06                     | 0.54              |
| 1:A:578:LEU:CD2  | 1:A:578:LEU:N    | 2.71                     | 0.54              |
| 1:A:52:LYS:O     | 1:A:52:LYS:HG2   | 2.08                     | 0.54              |
| 1:A:422:LEU:CA   | 1:A:423:PRO:C    | 2.81                     | 0.54              |
| 1:A:341:PRO:HB2  | 1:A:344:SER:CB   | 2.38                     | 0.53              |
| 1:A:339:SER:O    | 1:A:449:ASN:HA   | 2.09                     | 0.53              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:452:GLY:C    | 1:A:454:LEU:N    | 2.65                     | 0.53              |
| 1:A:103:VAL:CG1  | 1:A:212:PHE:HB3  | 2.38                     | 0.53              |
| 1:A:224:GLY:O    | 1:A:225:THR:C    | 2.49                     | 0.53              |
| 1:A:472:LYS:HG2  | 1:A:473:GLU:H    | 1.72                     | 0.53              |
| 1:A:482:LEU:N    | 1:A:482:LEU:CD2  | 2.71                     | 0.53              |
| 1:A:216:ARG:HG2  | 1:A:232:VAL:O    | 2.08                     | 0.53              |
| 1:A:119:VAL:HG12 | 1:A:119:VAL:O    | 2.08                     | 0.53              |
| 1:A:400:TYR:OH   | 1:A:575:LYS:HA   | 2.09                     | 0.53              |
| 1:A:416:GLN:CB   | 1:A:429:VAL:HG22 | 2.35                     | 0.53              |
| 1:A:432:PRO:HA   | 1:A:443:ASN:ND2  | 2.24                     | 0.53              |
| 1:A:89:LYS:O     | 1:A:95:ASN:CB    | 2.55                     | 0.52              |
| 1:A:422:LEU:HB2  | 1:A:423:PRO:HA   | 1.91                     | 0.52              |
| 1:A:96:MET:CE    | 1:A:220:PRO:HA   | 2.31                     | 0.52              |
| 1:A:77:GLU:OE2   | 1:A:520:ARG:NH1  | 2.42                     | 0.52              |
| 1:A:96:MET:HE1   | 1:A:220:PRO:CB   | 2.39                     | 0.52              |
| 1:A:243:PHE:CD1  | 1:A:243:PHE:C    | 2.87                     | 0.52              |
| 1:A:359:ALA:HB2  | 1:A:373:ASP:HA   | 1.91                     | 0.52              |
| 1:A:343:TYR:CZ   | 1:A:371:ALA:CB   | 2.92                     | 0.52              |
| 1:A:565:ASN:HD21 | 1:A:566:ILE:HG13 | 1.70                     | 0.52              |
| 1:A:110:SER:O    | 1:A:500:VAL:O    | 2.27                     | 0.52              |
| 1:A:501:LYS:CG   | 1:A:502:VAL:N    | 2.71                     | 0.52              |
| 1:A:364:ALA:C    | 1:A:367:ASP:HB3  | 2.34                     | 0.52              |
| 1:A:118:GLY:HA3  | 1:A:465:PRO:HB3  | 1.90                     | 0.52              |
| 1:A:101:ILE:HG23 | 1:A:101:ILE:O    | 2.10                     | 0.52              |
| 1:A:122:ASN:HB2  | 1:A:123:PRO:HD2  | 1.92                     | 0.51              |
| 1:A:276:THR:HG23 | 1:A:579:ALA:O    | 2.09                     | 0.51              |
| 1:A:443:ASN:CB   | 1:A:445:THR:OG1  | 2.58                     | 0.51              |
| 1:A:557:ASN:O    | 1:A:560:ASN:HB2  | 2.11                     | 0.51              |
| 1:A:67:ARG:N     | 1:A:529:TRP:O    | 2.44                     | 0.51              |
| 1:A:233:TYR:CD1  | 1:A:233:TYR:C    | 2.88                     | 0.51              |
| 1:A:426:ASN:O    | 1:A:428:ASN:N    | 2.43                     | 0.51              |
| 1:A:468:GLN:OE1  | 1:A:471:ASP:HB2  | 2.10                     | 0.51              |
| 1:A:308:VAL:HG12 | 1:A:309:GLN:N    | 2.26                     | 0.51              |
| 1:A:198:TYR:CE1  | 1:A:571:ILE:HG13 | 2.46                     | 0.51              |
| 1:A:466:ASN:O    | 1:A:467:GLY:C    | 2.53                     | 0.51              |
| 1:A:96:MET:HE3   | 1:A:221:SER:C    | 2.36                     | 0.51              |
| 1:A:459:ASN:HD22 | 1:A:482:LEU:HB2  | 1.74                     | 0.51              |
| 1:A:197:PHE:CE2  | 1:A:465:PRO:CB   | 2.89                     | 0.51              |
| 1:A:420:PHE:O    | 1:A:421:ASN:C    | 2.53                     | 0.51              |
| 1:A:326:THR:HG22 | 1:A:327:GLU:N    | 2.25                     | 0.51              |
| 1:A:77:GLU:HB3   | 1:A:518:MET:HE1  | 1.93                     | 0.51              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:222:HIS:CD2  | 1:A:225:THR:OG1  | 2.64                     | 0.51              |
| 1:A:409:TYR:C    | 1:A:411:GLU:N    | 2.67                     | 0.51              |
| 1:A:93:LYS:HE2   | 1:A:227:GLY:O    | 2.10                     | 0.50              |
| 1:A:518:MET:O    | 1:A:519:SER:C    | 2.54                     | 0.50              |
| 1:A:73:MET:HE3   | 1:A:520:ARG:CG   | 2.41                     | 0.50              |
| 1:A:75:GLU:C     | 1:A:520:ARG:HH22 | 2.19                     | 0.50              |
| 1:A:511:ASP:OD2  | 1:A:513:ASP:CB   | 2.59                     | 0.50              |
| 1:A:266:PHE:CE1  | 1:A:495:PRO:HD3  | 2.47                     | 0.50              |
| 1:A:360:GLY:O    | 1:A:373:ASP:OD2  | 2.30                     | 0.50              |
| 1:A:45:PHE:HE1   | 1:A:47:ASN:HB2   | 1.76                     | 0.50              |
| 1:A:158:THR:H    | 1:A:161:PRO:HB3  | 1.76                     | 0.50              |
| 1:A:213:GLN:HG3  | 1:A:240:ASP:HB2  | 1.94                     | 0.50              |
| 1:A:361:ARG:HH11 | 1:A:401:ILE:C    | 2.16                     | 0.50              |
| 1:A:564:ASN:HD22 | 1:A:566:ILE:H    | 1.60                     | 0.50              |
| 1:A:233:TYR:CE1  | 1:A:235:GLY:HA2  | 2.47                     | 0.50              |
| 1:A:46:ASN:C     | 1:A:66:SER:HG    | 2.20                     | 0.49              |
| 1:A:282:ASN:O    | 1:A:332:ARG:NE   | 2.45                     | 0.49              |
| 1:A:562:VAL:CG1  | 1:A:563:PRO:HD2  | 2.41                     | 0.49              |
| 1:A:160:PRO:HG2  | 1:A:161:PRO:C    | 2.37                     | 0.49              |
| 1:A:484:ILE:O    | 1:A:484:ILE:CG2  | 2.56                     | 0.49              |
| 1:A:93:LYS:C     | 1:A:221:SER:O    | 2.55                     | 0.49              |
| 1:A:216:ARG:HG2  | 1:A:217:THR:H    | 1.77                     | 0.49              |
| 1:A:231:ASN:O    | 1:A:231:ASN:CG   | 2.55                     | 0.49              |
| 1:A:383:GLN:HB3  | 1:A:384:HIS:CD2  | 2.47                     | 0.49              |
| 1:A:73:MET:HB2   | 1:A:523:THR:O    | 2.12                     | 0.49              |
| 1:A:113:ASP:OD2  | 1:A:188:ALA:N    | 2.43                     | 0.49              |
| 1:A:139:VAL:O    | 1:A:268:PHE:CD1  | 2.59                     | 0.49              |
| 1:A:341:PRO:CB   | 1:A:344:SER:OG   | 2.57                     | 0.49              |
| 1:A:459:ASN:CG   | 1:A:460:VAL:N    | 2.70                     | 0.49              |
| 1:A:435:PRO:HB3  | 1:A:439:LYS:O    | 2.12                     | 0.49              |
| 1:A:361:ARG:NH2  | 1:A:365:GLN:NE2  | 2.59                     | 0.49              |
| 1:A:77:GLU:CD    | 1:A:520:ARG:NH1  | 2.71                     | 0.48              |
| 1:A:126:TRP:O    | 1:A:130:VAL:HB   | 2.13                     | 0.48              |
| 1:A:364:ALA:HB3  | 1:A:367:ASP:CB   | 2.42                     | 0.48              |
| 1:A:554:ASN:HB2  | 1:A:557:ASN:HD22 | 1.77                     | 0.48              |
| 1:A:109:TRP:CG   | 1:A:246:ILE:HD12 | 2.48                     | 0.48              |
| 1:A:160:PRO:CG   | 1:A:161:PRO:C    | 2.86                     | 0.48              |
| 1:A:471:ASP:O    | 1:A:472:LYS:C    | 2.55                     | 0.48              |
| 1:A:136:LEU:HD12 | 1:A:537:ALA:HB2  | 1.94                     | 0.48              |
| 1:A:361:ARG:HH12 | 1:A:401:ILE:C    | 2.16                     | 0.48              |
| 1:A:517:ASN:O    | 1:A:518:MET:C    | 2.56                     | 0.48              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:183:MET:HG2  | 1:A:208:TRP:CH2  | 2.48                     | 0.48              |
| 1:A:326:THR:O    | 1:A:330:ILE:HG13 | 2.13                     | 0.48              |
| 1:A:378:TYR:O    | 1:A:397:ARG:HB2  | 2.11                     | 0.48              |
| 1:A:216:ARG:CG   | 1:A:232:VAL:O    | 2.62                     | 0.48              |
| 1:A:432:PRO:HA   | 1:A:443:ASN:HD22 | 1.79                     | 0.48              |
| 1:A:65:SER:O     | 1:A:529:TRP:CZ3  | 2.67                     | 0.48              |
| 1:A:381:GLY:O    | 1:A:383:GLN:N    | 2.37                     | 0.48              |
| 1:A:219:ILE:HG22 | 1:A:220:PRO:HD2  | 1.95                     | 0.48              |
| 1:A:361:ARG:HE   | 1:A:365:GLN:HE22 | 1.61                     | 0.48              |
| 1:A:463:VAL:O    | 1:A:465:PRO:O    | 2.31                     | 0.48              |
| 1:A:377:ARG:NE   | 1:A:397:ARG:HG3  | 2.29                     | 0.47              |
| 1:A:469:ILE:HG22 | 1:A:470:TRP:N    | 2.29                     | 0.47              |
| 1:A:45:PHE:C     | 1:A:45:PHE:CD1   | 2.92                     | 0.47              |
| 1:A:42:THR:HG21  | 1:A:260:GLU:HB2  | 1.95                     | 0.47              |
| 1:A:109:TRP:HZ3  | 1:A:174:MET:O    | 1.98                     | 0.47              |
| 1:A:158:THR:O    | 1:A:158:THR:HG23 | 2.10                     | 0.47              |
| 1:A:442:ILE:HG22 | 1:A:443:ASN:N    | 2.29                     | 0.47              |
| 1:A:472:LYS:HG2  | 1:A:473:GLU:N    | 2.29                     | 0.47              |
| 1:A:430:LEU:HD21 | 1:A:436:ILE:HD11 | 1.96                     | 0.47              |
| 1:A:484:ILE:O    | 1:A:484:ILE:HG23 | 2.13                     | 0.47              |
| 1:A:540:ARG:O    | 1:A:540:ARG:HG3  | 2.15                     | 0.47              |
| 1:A:557:ASN:O    | 1:A:558:GLN:C    | 2.57                     | 0.47              |
| 1:A:86:ASN:C     | 1:A:88:ASP:H     | 2.23                     | 0.47              |
| 1:A:283:ARG:HD2  | 1:A:327:GLU:O    | 2.15                     | 0.47              |
| 1:A:410:PRO:HA   | 1:A:413:ASP:OD1  | 2.14                     | 0.47              |
| 1:A:545:TRP:CD1  | 1:A:545:TRP:C    | 2.92                     | 0.47              |
| 1:A:572:VAL:HG12 | 1:A:573:TYR:O    | 2.15                     | 0.47              |
| 1:A:368:GLU:HG2  | 1:A:369:ASN:N    | 2.29                     | 0.46              |
| 1:A:73:MET:HE3   | 1:A:520:ARG:CD   | 2.45                     | 0.46              |
| 1:A:380:PHE:CE1  | 1:A:398:PHE:CE1  | 3.04                     | 0.46              |
| 1:A:408:ARG:O    | 1:A:410:PRO:HD3  | 2.16                     | 0.46              |
| 1:A:464:TYR:HA   | 1:A:465:PRO:C    | 2.40                     | 0.46              |
| 1:A:111:LEU:CG   | 1:A:112:VAL:N    | 2.77                     | 0.46              |
| 1:A:109:TRP:CD1  | 1:A:246:ILE:HD12 | 2.51                     | 0.46              |
| 1:A:138:LEU:HD11 | 1:A:533:LEU:HD11 | 1.98                     | 0.46              |
| 1:A:494:CYS:HB3  | 1:A:495:PRO:HD2  | 1.98                     | 0.46              |
| 1:A:533:LEU:CD2  | 1:A:535:PHE:CE2  | 2.99                     | 0.46              |
| 1:A:564:ASN:C    | 1:A:566:ILE:N    | 2.74                     | 0.46              |
| 1:A:138:LEU:HD13 | 1:A:535:PHE:HE1  | 1.77                     | 0.46              |
| 1:A:151:LYS:HE2  | 1:A:167:ASN:OD1  | 2.16                     | 0.46              |
| 1:A:342:TYR:CE1  | 1:A:446:ASN:HA   | 2.50                     | 0.46              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:347:ALA:HB2  | 1:A:352:PRO:HA   | 1.98                     | 0.46              |
| 1:A:551:MET:HE3  | 1:A:574:GLU:OE1  | 2.15                     | 0.46              |
| 1:A:221:SER:CB   | 1:A:229:PRO:HG3  | 2.45                     | 0.46              |
| 1:A:426:ASN:C    | 1:A:428:ASN:N    | 2.69                     | 0.45              |
| 1:A:299:GLY:C    | 1:A:301:THR:N    | 2.73                     | 0.45              |
| 1:A:408:ARG:C    | 1:A:410:PRO:HD3  | 2.42                     | 0.45              |
| 1:A:538:LYS:HG3  | 1:A:539:LEU:H    | 1.81                     | 0.45              |
| 1:A:174:MET:CE   | 1:A:504:PRO:HD3  | 2.43                     | 0.45              |
| 1:A:216:ARG:HG2  | 1:A:217:THR:N    | 2.32                     | 0.45              |
| 1:A:67:ARG:NH1   | 1:A:196:GLY:O    | 2.50                     | 0.45              |
| 1:A:103:VAL:HG23 | 1:A:214:TRP:HB2  | 1.98                     | 0.45              |
| 1:A:552:SER:OG   | 1:A:553:ILE:N    | 2.49                     | 0.45              |
| 1:A:283:ARG:NE   | 1:A:327:GLU:HB3  | 2.28                     | 0.45              |
| 1:A:400:TYR:CE1  | 1:A:575:LYS:HA   | 2.52                     | 0.45              |
| 1:A:286:GLY:O    | 1:A:288:PRO:HD3  | 2.17                     | 0.45              |
| 1:A:177:LEU:CD1  | 1:A:179:SER:OG   | 2.64                     | 0.45              |
| 1:A:199:PRO:C    | 1:A:201:LYS:H    | 2.25                     | 0.45              |
| 1:A:158:THR:O    | 1:A:159:GLN:CB   | 2.65                     | 0.45              |
| 1:A:158:THR:N    | 1:A:161:PRO:HB3  | 2.31                     | 0.45              |
| 1:A:75:GLU:C     | 1:A:520:ARG:NH2  | 2.75                     | 0.45              |
| 1:A:383:GLN:C    | 1:A:384:HIS:CD2  | 2.95                     | 0.45              |
| 1:A:474:PHE:CD1  | 1:A:474:PHE:N    | 2.85                     | 0.45              |
| 1:A:222:HIS:CE1  | 1:A:225:THR:H    | 2.34                     | 0.44              |
| 1:A:322:THR:HG22 | 1:A:420:PHE:CD2  | 2.42                     | 0.44              |
| 1:A:369:ASN:HB3  | 1:A:372:ALA:CB   | 2.48                     | 0.44              |
| 1:A:382:ARG:NH1  | 1:A:382:ARG:CG   | 2.67                     | 0.44              |
| 1:A:414:TRP:NE1  | 1:A:416:GLN:NE2  | 2.56                     | 0.44              |
| 1:A:431:LEU:CD1  | 1:A:431:LEU:N    | 2.79                     | 0.44              |
| 1:A:53:PHE:HD1   | 1:A:59:VAL:CG1   | 2.26                     | 0.44              |
| 1:A:221:SER:HB3  | 1:A:229:PRO:HG3  | 1.99                     | 0.44              |
| 1:A:105:ILE:HD11 | 1:A:212:PHE:CD2  | 2.53                     | 0.44              |
| 1:A:443:ASN:HB3  | 1:A:445:THR:OG1  | 2.17                     | 0.44              |
| 1:A:516:ALA:CA   | 1:A:517:ASN:HD22 | 2.23                     | 0.44              |
| 1:A:45:PHE:CD1   | 1:A:46:ASN:N     | 2.86                     | 0.44              |
| 1:A:120:TRP:CD1  | 1:A:469:ILE:HD11 | 2.52                     | 0.44              |
| 1:A:338:TYR:CE1  | 1:A:357:ILE:HD13 | 2.53                     | 0.44              |
| 1:A:342:TYR:CD1  | 1:A:342:TYR:N    | 2.85                     | 0.44              |
| 1:A:191:ARG:O    | 1:A:193:GLU:HG3  | 2.17                     | 0.44              |
| 1:A:551:MET:CE   | 1:A:574:GLU:OE1  | 2.66                     | 0.44              |
| 1:A:140:SER:HB2  | 1:A:534:VAL:CG2  | 2.47                     | 0.44              |
| 1:A:361:ARG:NE   | 1:A:365:GLN:HE22 | 2.16                     | 0.43              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:383:GLN:O    | 1:A:383:GLN:HG2  | 2.18                     | 0.43              |
| 1:A:62:THR:CG2   | 1:A:532:LYS:HE3  | 2.48                     | 0.43              |
| 1:A:266:PHE:CZ   | 1:A:494:CYS:HA   | 2.53                     | 0.43              |
| 1:A:77:GLU:CG    | 1:A:518:MET:HE1  | 2.33                     | 0.43              |
| 1:A:232:VAL:CG2  | 1:A:233:TYR:N    | 2.82                     | 0.43              |
| 1:A:409:TYR:CD1  | 1:A:411:GLU:HB2  | 2.53                     | 0.43              |
| 1:A:510:TYR:HE1  | 1:A:518:MET:HB3  | 1.84                     | 0.43              |
| 1:A:61:ILE:N     | 1:A:535:PHE:O    | 2.52                     | 0.43              |
| 1:A:378:TYR:O    | 1:A:397:ARG:CA   | 2.66                     | 0.43              |
| 1:A:517:ASN:C    | 1:A:519:SER:N    | 2.76                     | 0.43              |
| 1:A:533:LEU:CG   | 1:A:535:PHE:CE2  | 3.02                     | 0.43              |
| 1:A:266:PHE:CZ   | 1:A:494:CYS:CA   | 3.01                     | 0.43              |
| 1:A:572:VAL:HG12 | 1:A:573:TYR:N    | 2.33                     | 0.43              |
| 1:A:45:PHE:HD1   | 1:A:46:ASN:N     | 2.17                     | 0.43              |
| 1:A:68:LEU:HB2   | 1:A:528:TRP:CD2  | 2.54                     | 0.43              |
| 1:A:160:PRO:CG   | 1:A:161:PRO:O    | 2.62                     | 0.43              |
| 1:A:255:LEU:HB3  | 1:A:259:ASP:HB2  | 2.01                     | 0.43              |
| 1:A:361:ARG:CZ   | 1:A:402:ALA:O    | 2.65                     | 0.43              |
| 1:A:71:LEU:HD21  | 1:A:502:VAL:HG23 | 2.01                     | 0.42              |
| 1:A:91:ALA:C     | 1:A:93:LYS:H     | 2.26                     | 0.42              |
| 1:A:317:THR:HG22 | 1:A:318:GLN:N    | 2.34                     | 0.42              |
| 1:A:448:PHE:CZ   | 1:A:450:THR:CG2  | 3.01                     | 0.42              |
| 1:A:111:LEU:CG   | 1:A:112:VAL:H    | 2.32                     | 0.42              |
| 1:A:139:VAL:CG1  | 1:A:140:SER:N    | 2.69                     | 0.42              |
| 1:A:551:MET:HE3  | 1:A:574:GLU:OE2  | 2.19                     | 0.42              |
| 1:A:71:LEU:HD12  | 1:A:72:ASN:N     | 2.35                     | 0.42              |
| 1:A:196:GLY:HA2  | 1:A:383:GLN:HG2  | 2.01                     | 0.42              |
| 1:A:342:TYR:HE1  | 1:A:445:THR:C    | 2.27                     | 0.42              |
| 1:A:368:GLU:CG   | 1:A:369:ASN:H    | 2.30                     | 0.42              |
| 1:A:368:GLU:OE1  | 1:A:375:ASP:OD2  | 2.37                     | 0.42              |
| 1:A:197:PHE:HB3  | 1:A:571:ILE:HD12 | 2.02                     | 0.42              |
| 1:A:425:THR:O    | 1:A:426:ASN:C    | 2.63                     | 0.42              |
| 1:A:431:LEU:CB   | 1:A:432:PRO:CD   | 2.93                     | 0.42              |
| 1:A:45:PHE:C     | 1:A:45:PHE:HD1   | 2.27                     | 0.42              |
| 1:A:219:ILE:CD1  | 1:A:230:THR:HB   | 2.50                     | 0.42              |
| 1:A:325:ILE:HG23 | 1:A:330:ILE:HG12 | 2.00                     | 0.42              |
| 1:A:380:PHE:HE1  | 1:A:398:PHE:CE1  | 2.38                     | 0.42              |
| 1:A:184:PRO:O    | 1:A:497:GLN:NE2  | 2.53                     | 0.42              |
| 1:A:564:ASN:OD1  | 1:A:568:ALA:HB2  | 2.08                     | 0.42              |
| 1:A:162:THR:HG22 | 1:A:163:LYS:N    | 2.35                     | 0.42              |
| 1:A:177:LEU:HD22 | 1:A:178:ASP:N    | 2.33                     | 0.42              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:279:TRP:C    | 1:A:279:TRP:CD2  | 2.97                     | 0.42              |
| 1:A:562:VAL:HG12 | 1:A:563:PRO:O    | 2.20                     | 0.42              |
| 1:A:382:ARG:HA   | 1:A:382:ARG:HD3  | 1.88                     | 0.41              |
| 1:A:96:MET:HE3   | 1:A:221:SER:N    | 1.90                     | 0.41              |
| 1:A:99:ASP:OD1   | 1:A:101:ILE:CG2  | 2.62                     | 0.41              |
| 1:A:158:THR:HG23 | 1:A:159:GLN:HG2  | 2.01                     | 0.41              |
| 1:A:339:SER:O    | 1:A:450:THR:N    | 2.46                     | 0.41              |
| 1:A:452:GLY:O    | 1:A:454:LEU:N    | 2.54                     | 0.41              |
| 1:A:212:PHE:HE1  | 1:A:236:THR:HG21 | 1.85                     | 0.41              |
| 1:A:308:VAL:CG1  | 1:A:309:GLN:N    | 2.84                     | 0.41              |
| 1:A:101:ILE:HD11 | 1:A:233:TYR:HB2  | 2.01                     | 0.41              |
| 1:A:237:ASP:HB3  | 1:A:240:ASP:OD1  | 2.21                     | 0.41              |
| 1:A:265:THR:HG21 | 1:A:267:PHE:CZ   | 2.54                     | 0.41              |
| 1:A:440:THR:O    | 1:A:442:ILE:N    | 2.53                     | 0.41              |
| 1:A:443:ASN:HB3  | 1:A:445:THR:N    | 2.34                     | 0.41              |
| 1:A:44:THR:HG22  | 1:A:45:PHE:N     | 2.35                     | 0.41              |
| 1:A:126:TRP:NE1  | 1:A:130:VAL:HG21 | 2.36                     | 0.41              |
| 1:A:55:GLU:O     | 1:A:56:ASN:HB2   | 2.21                     | 0.41              |
| 1:A:68:LEU:HD13  | 1:A:528:TRP:CE2  | 2.56                     | 0.41              |
| 1:A:73:MET:SD    | 1:A:520:ARG:HG3  | 2.60                     | 0.41              |
| 1:A:84:VAL:CG1   | 1:A:100:ASP:O    | 2.68                     | 0.41              |
| 1:A:143:GLN:O    | 1:A:263:THR:HB   | 2.21                     | 0.41              |
| 1:A:187:PRO:HB2  | 1:A:468:GLN:NE2  | 2.36                     | 0.41              |
| 1:A:425:THR:O    | 1:A:428:ASN:HB2  | 2.20                     | 0.41              |
| 1:A:555:VAL:HG12 | 1:A:555:VAL:O    | 2.21                     | 0.41              |
| 1:A:359:ALA:HB2  | 1:A:373:ASP:C    | 2.34                     | 0.40              |
| 1:A:419:ASN:O    | 1:A:421:ASN:N    | 2.50                     | 0.40              |
| 1:A:466:ASN:C    | 1:A:467:GLY:O    | 2.62                     | 0.40              |
| 1:A:470:TRP:CD1  | 1:A:470:TRP:C    | 2.99                     | 0.40              |
| 1:A:54:LEU:HB2   | 1:A:58:TRP:O     | 2.21                     | 0.40              |
| 1:A:105:ILE:CD1  | 1:A:212:PHE:CD2  | 3.05                     | 0.40              |
| 1:A:173:LEU:HD23 | 1:A:175:VAL:HG23 | 2.02                     | 0.40              |
| 1:A:342:TYR:N    | 1:A:342:TYR:HD1  | 2.19                     | 0.40              |
| 1:A:247:GLU:CD   | 1:A:247:GLU:N    | 2.76                     | 0.40              |
| 1:A:346:GLU:O    | 1:A:352:PRO:HA   | 2.21                     | 0.40              |
| 1:A:481:ARG:HB2  | 1:A:482:LEU:CD2  | 2.52                     | 0.40              |
| 1:A:110:SER:O    | 1:A:500:VAL:N    | 2.50                     | 0.40              |
| 1:A:474:PHE:N    | 1:A:474:PHE:HD1  | 2.19                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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     | 546/584 (94%) | 448 (82%) | 65 (12%) | 33 (6%)  | <b>1</b> <b>9</b> |

All (33) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 159 | GLN  |
| 1   | A     | 370 | GLN  |
| 1   | A     | 386 | GLN  |
| 1   | A     | 402 | ALA  |
| 1   | A     | 465 | PRO  |
| 1   | A     | 466 | ASN  |
| 1   | A     | 467 | GLY  |
| 1   | A     | 472 | LYS  |
| 1   | A     | 516 | ALA  |
| 1   | A     | 518 | MET  |
| 1   | A     | 558 | GLN  |
| 1   | A     | 565 | ASN  |
| 1   | A     | 38  | VAL  |
| 1   | A     | 157 | ALA  |
| 1   | A     | 181 | ASN  |
| 1   | A     | 229 | PRO  |
| 1   | A     | 343 | TYR  |
| 1   | A     | 374 | GLY  |
| 1   | A     | 382 | ARG  |
| 1   | A     | 421 | ASN  |
| 1   | A     | 427 | ASP  |
| 1   | A     | 522 | VAL  |
| 1   | A     | 221 | SER  |
| 1   | A     | 414 | TRP  |
| 1   | A     | 441 | GLY  |
| 1   | A     | 426 | ASN  |
| 1   | A     | 230 | THR  |
| 1   | A     | 300 | ALA  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 362 | GLY  |
| 1   | A     | 410 | PRO  |
| 1   | A     | 517 | ASN  |
| 1   | A     | 453 | PRO  |
| 1   | A     | 94  | 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     | 477/496 (96%) | 404 (85%) | 73 (15%) | 3 13        |

All (73) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 38  | VAL  |
| 1   | A     | 40  | ILE  |
| 1   | A     | 41  | SER  |
| 1   | A     | 42  | THR  |
| 1   | A     | 47  | ASN  |
| 1   | A     | 48  | GLN  |
| 1   | A     | 54  | LEU  |
| 1   | A     | 65  | SER  |
| 1   | A     | 66  | SER  |
| 1   | A     | 67  | ARG  |
| 1   | A     | 68  | LEU  |
| 1   | A     | 71  | LEU  |
| 1   | A     | 78  | ASN  |
| 1   | A     | 80  | LYS  |
| 1   | A     | 85  | ASN  |
| 1   | A     | 87  | MET  |
| 1   | A     | 96  | MET  |
| 1   | A     | 130 | VAL  |
| 1   | A     | 158 | THR  |
| 1   | A     | 170 | THR  |
| 1   | A     | 173 | LEU  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 177 | LEU  |
| 1   | A     | 179 | SER  |
| 1   | A     | 180 | ASN  |
| 1   | A     | 182 | THR  |
| 1   | A     | 183 | MET  |
| 1   | A     | 191 | ARG  |
| 1   | A     | 203 | THR  |
| 1   | A     | 208 | TRP  |
| 1   | A     | 213 | GLN  |
| 1   | A     | 215 | ASP  |
| 1   | A     | 219 | ILE  |
| 1   | A     | 228 | THR  |
| 1   | A     | 230 | THR  |
| 1   | A     | 231 | ASN  |
| 1   | A     | 232 | VAL  |
| 1   | A     | 233 | TYR  |
| 1   | A     | 240 | ASP  |
| 1   | A     | 249 | SER  |
| 1   | A     | 255 | LEU  |
| 1   | A     | 263 | THR  |
| 1   | A     | 271 | LYS  |
| 1   | A     | 342 | TYR  |
| 1   | A     | 344 | SER  |
| 1   | A     | 349 | THR  |
| 1   | A     | 354 | LYS  |
| 1   | A     | 355 | THR  |
| 1   | A     | 357 | ILE  |
| 1   | A     | 361 | ARG  |
| 1   | A     | 365 | GLN  |
| 1   | A     | 369 | ASN  |
| 1   | A     | 382 | ARG  |
| 1   | A     | 387 | LYS  |
| 1   | A     | 396 | GLU  |
| 1   | A     | 404 | GLN  |
| 1   | A     | 411 | GLU  |
| 1   | A     | 417 | ASN  |
| 1   | A     | 420 | PHE  |
| 1   | A     | 421 | ASN  |
| 1   | A     | 422 | LEU  |
| 1   | A     | 464 | TYR  |
| 1   | A     | 482 | LEU  |
| 1   | A     | 484 | ILE  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 491 | GLN  |
| 1   | A     | 493 | ASN  |
| 1   | A     | 517 | ASN  |
| 1   | A     | 520 | ARG  |
| 1   | A     | 560 | ASN  |
| 1   | A     | 564 | ASN  |
| 1   | A     | 575 | LYS  |
| 1   | A     | 578 | LEU  |
| 1   | A     | 581 | ARG  |
| 1   | A     | 582 | LYS  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 47  | ASN  |
| 1   | A     | 48  | GLN  |
| 1   | A     | 64  | ASN  |
| 1   | A     | 70  | HIS  |
| 1   | A     | 86  | ASN  |
| 1   | A     | 95  | ASN  |
| 1   | A     | 102 | HIS  |
| 1   | A     | 122 | ASN  |
| 1   | A     | 147 | ASN  |
| 1   | A     | 180 | ASN  |
| 1   | A     | 282 | ASN  |
| 1   | A     | 292 | ASN  |
| 1   | A     | 370 | GLN  |
| 1   | A     | 384 | HIS  |
| 1   | A     | 386 | GLN  |
| 1   | A     | 403 | HIS  |
| 1   | A     | 416 | GLN  |
| 1   | A     | 428 | ASN  |
| 1   | A     | 443 | ASN  |
| 1   | A     | 459 | ASN  |
| 1   | A     | 491 | GLN  |
| 1   | A     | 493 | ASN  |
| 1   | A     | 508 | ASN  |
| 1   | A     | 517 | ASN  |
| 1   | A     | 549 | GLN  |
| 1   | A     | 557 | ASN  |
| 1   | A     | 565 | ASN  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|-----|-------|------------------|
| 1   | A     | 1                |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1     | A     | 239:ASP   | C      | 240:ASP   | N      | 1.15         |

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.