



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 12:16 PM UTC

PDB ID : 1KOO / pdb\_00001koo  
Title : THE CRYSTAL STRUCTURE AND MUTATIONAL ANALYSIS OF A NOVEL RNA-BINDING DOMAIN FOUND IN THE HUMAN TAP NUCLEAR MRNA EXPORT FACTOR  
Authors : Ho, D.N.; Coburn, G.A.; Kang, Y.; Cullen, B.R.; Georgiadis, M.M.  
Deposited on : 2001-12-21  
Resolution : 3.80 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                                                             |

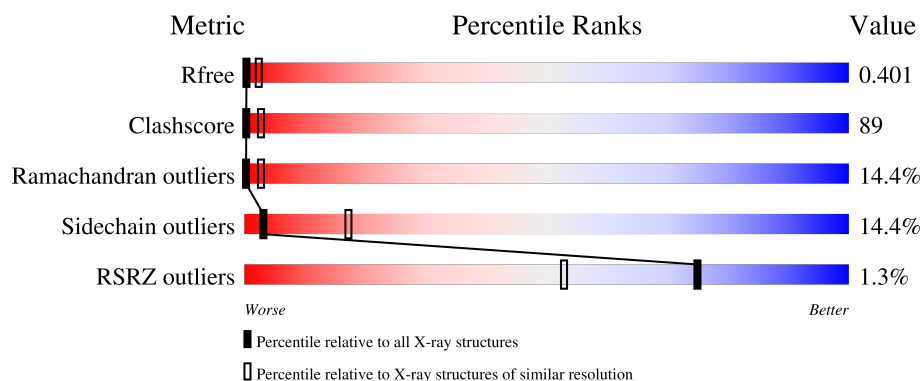
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.80 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                      | 1065 (3.96-3.64)                                      |
| Clashscore            | 190562                      | 1012 (3.94-3.66)                                      |
| Ramachandran outliers | 187476                      | 1048 (3.96-3.64)                                      |
| Sidechain outliers    | 187428                      | 1043 (3.96-3.64)                                      |
| RSRZ outliers         | 180081                      | 1064 (3.96-3.64)                                      |

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     | 277    | <div> <div>12%</div> <div>56%</div> <div>23%</div> <div>7%</div> </div>  |
| 1   | B     | 277    | <div> <div>14%</div> <div>32%</div> <div>11%</div> <div>40%</div> </div> |
| 1   | C     | 277    | <div> <div>13%</div> <div>53%</div> <div>25%</div> <div>5%</div> </div>  |
| 1   | D     | 277    | <div> <div>6%</div> <div>36%</div> <div>15%</div> <div>39%</div> </div>  |

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 6832 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 TIP ASSOCIATING PROTEIN.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 1   | A     | 258      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2067  | 1305 | 365 | 391 | 6 |         |         |       |
| 1   | B     | 165      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1321  | 829  | 232 | 256 | 4 |         |         |       |
| 1   | C     | 262      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2095  | 1323 | 369 | 397 | 6 |         |         |       |
| 1   | D     | 169      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1349  | 848  | 236 | 261 | 4 |         |         |       |

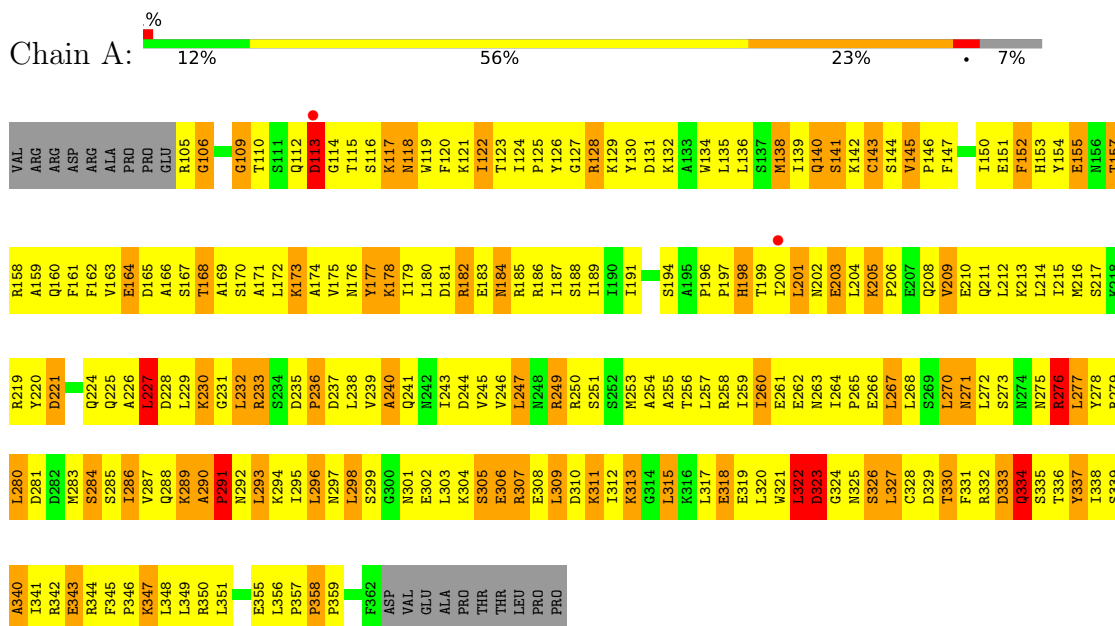
There are 4 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment             | Reference  |
|-------|---------|----------|--------|---------------------|------------|
| A     | 252     | SER      | CYS    | engineered mutation | UNP Q9UBU9 |
| B     | 252     | SER      | CYS    | engineered mutation | UNP Q9UBU9 |
| C     | 252     | SER      | CYS    | engineered mutation | UNP Q9UBU9 |
| D     | 252     | SER      | CYS    | engineered mutation | UNP Q9UBU9 |

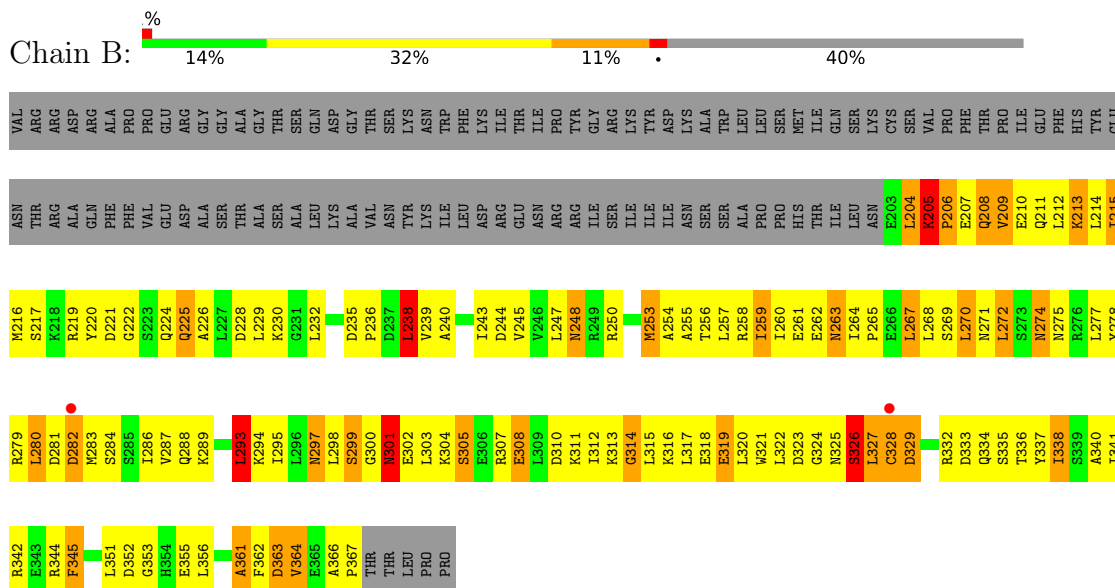
### 3 Residue-property plots

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

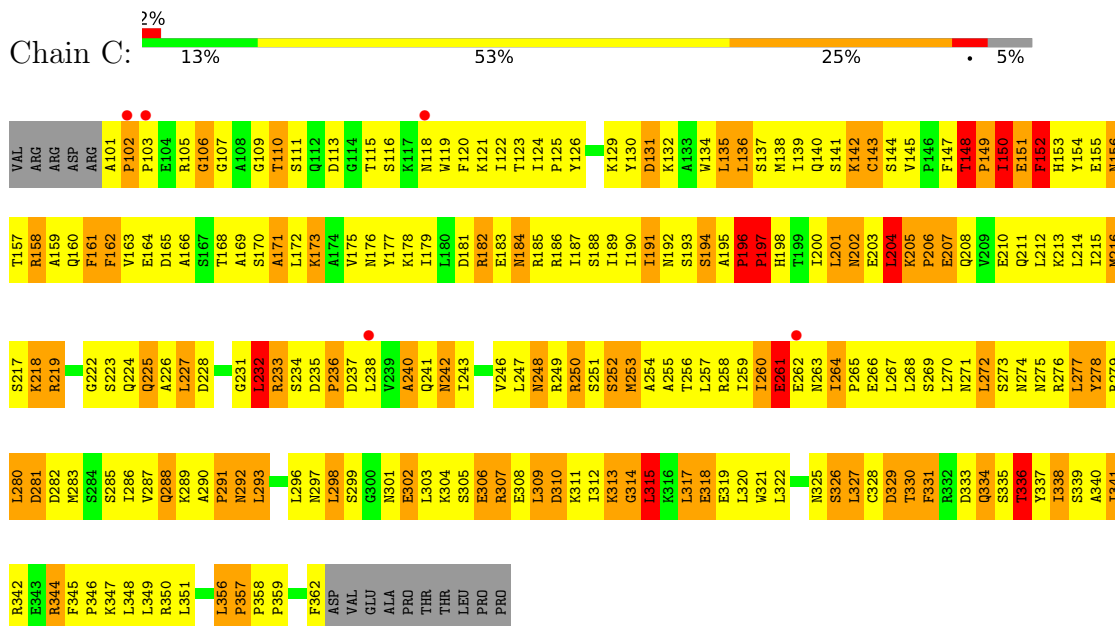
- Molecule 1: TIP ASSOCIATING PROTEIN



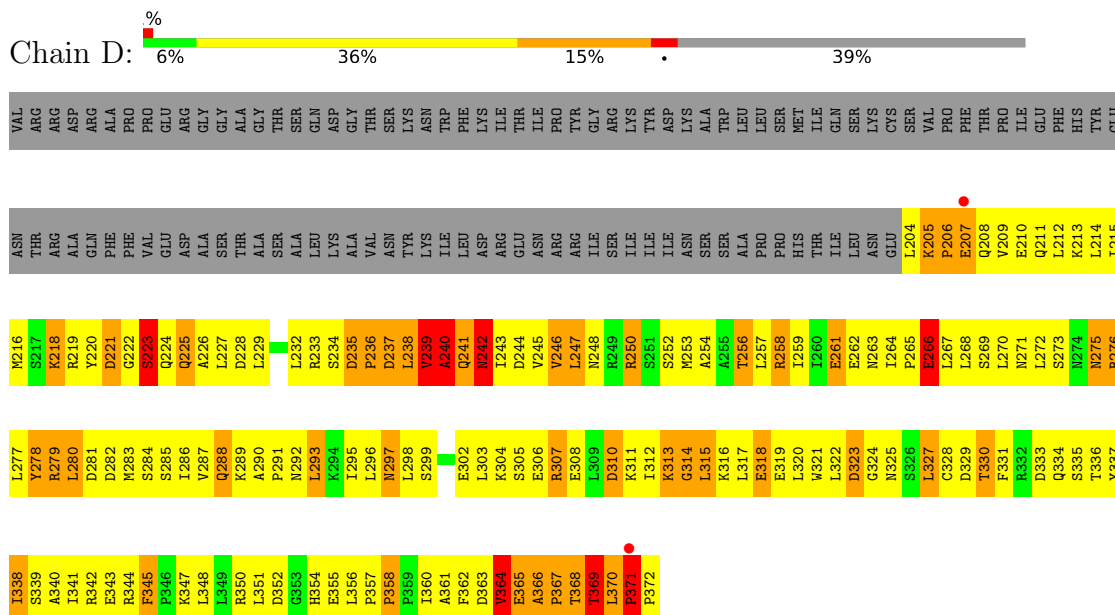
- Molecule 1: TIP ASSOCIATING PROTEIN



• Molecule 1: TIP ASSOCIATING PROTEIN



- Molecule 1: TIP ASSOCIATING PROTEIN



## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 41 21 2                                                   | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 138.25Å 138.25Å 205.00Å<br>90.00° 90.00° 90.00°             | Depositor        |
| Resolution (Å)                                                          | 8.00 – 3.80<br>8.00 – 3.82                                  | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 84.9 (8.00-3.80)<br>78.7 (8.00-3.82)                        | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.13                                                        | Depositor        |
| $R_{sym}$                                                               | 0.13                                                        | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.44 (at 3.77Å)                                             | Xtriage          |
| Refinement program                                                      | CNS 1.0                                                     | Depositor        |
| R, $R_{free}$                                                           | 0.317 , 0.395<br>0.313 , 0.401                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 981 reflections (2.90%)                                     | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 99.2                                                        | Xtriage          |
| Anisotropy                                                              | 0.040                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.44 , 117.0                                                | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$ | Xtriage          |
| Estimated twinning fraction                                             | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.79                                                        | EDS              |
| Total number of atoms                                                   | 6832                                                        | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 63.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.83% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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         | 0/2103        | 1.28        | 25/2840 (0.9%) |
| 1   | B     | 0.66         | 0/1338        | 1.24        | 15/1805 (0.8%) |
| 1   | C     | 0.64         | 0/2133        | 1.19        | 22/2883 (0.8%) |
| 1   | D     | 0.75         | 2/1368 (0.1%) | 1.31        | 20/1848 (1.1%) |
| All | All   | 0.67         | 2/6942 (0.0%) | 1.25        | 82/9376 (0.9%) |

All (2) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 1   | D     | 369 | THR  | CA-CB | 6.28 | 1.60        | 1.54     |
| 1   | D     | 371 | PRO  | CA-C  | 5.43 | 1.57        | 1.52     |

All (82) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|--------|-------------|----------|
| 1   | A     | 168 | THR  | N-CA-C | -11.06 | 98.92       | 110.97   |
| 1   | C     | 196 | PRO  | CA-C-N | 10.81  | 133.35      | 119.84   |
| 1   | C     | 196 | PRO  | C-N-CA | 10.81  | 133.35      | 119.84   |
| 1   | B     | 328 | CYS  | N-CA-C | -10.70 | 101.62      | 112.97   |
| 1   | D     | 369 | THR  | N-CA-C | 10.19  | 120.20      | 108.49   |
| 1   | C     | 253 | MET  | N-CA-C | -9.70  | 101.36      | 113.01   |
| 1   | A     | 334 | GLN  | N-CA-C | -9.69  | 103.58      | 114.62   |
| 1   | A     | 337 | TYR  | N-CA-C | -9.44  | 100.87      | 112.38   |
| 1   | A     | 290 | ALA  | CA-C-N | 9.35   | 131.52      | 119.84   |
| 1   | A     | 290 | ALA  | C-N-CA | 9.35   | 131.52      | 119.84   |
| 1   | A     | 114 | GLY  | N-CA-C | -9.21  | 103.72      | 114.69   |
| 1   | A     | 113 | ASP  | N-CA-C | 9.02   | 121.50      | 110.41   |
| 1   | D     | 306 | GLU  | N-CA-C | -8.97  | 102.32      | 113.18   |
| 1   | A     | 194 | SER  | N-CA-C | 8.86   | 119.61      | 108.45   |
| 1   | B     | 308 | GLU  | N-CA-C | -8.66  | 103.14      | 114.31   |
| 1   | B     | 215 | ILE  | N-CA-C | -8.19  | 103.83      | 111.45   |
| 1   | A     | 173 | LYS  | N-CA-C | -8.19  | 103.29      | 113.20   |
| 1   | D     | 324 | GLY  | N-CA-C | -7.70  | 105.23      | 115.40   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | A     | 306 | GLU  | N-CA-C | -7.64 | 103.93      | 113.18   |
| 1   | D     | 236 | PRO  | N-CA-C | -7.63 | 103.57      | 113.57   |
| 1   | A     | 177 | TYR  | N-CA-C | -7.49 | 103.73      | 112.86   |
| 1   | C     | 336 | THR  | N-CA-C | -7.47 | 103.90      | 113.16   |
| 1   | B     | 238 | LEU  | N-CA-C | -7.26 | 104.02      | 113.17   |
| 1   | C     | 307 | ARG  | N-CA-C | -7.24 | 104.32      | 113.01   |
| 1   | D     | 340 | ALA  | N-CA-C | -7.15 | 104.02      | 112.89   |
| 1   | C     | 281 | ASP  | N-CA-C | -7.12 | 104.41      | 113.23   |
| 1   | B     | 345 | PHE  | CA-C-N | 7.07  | 126.33      | 118.97   |
| 1   | B     | 345 | PHE  | C-N-CA | 7.07  | 126.33      | 118.97   |
| 1   | C     | 311 | LYS  | N-CA-C | -7.04 | 103.69      | 111.36   |
| 1   | D     | 239 | VAL  | N-CA-C | 6.91  | 123.72      | 109.34   |
| 1   | A     | 233 | ARG  | N-CA-C | -6.85 | 103.93      | 112.90   |
| 1   | A     | 280 | LEU  | N-CA-C | 6.70  | 121.47      | 113.16   |
| 1   | D     | 205 | LYS  | CA-C-N | 6.70  | 128.22      | 119.84   |
| 1   | D     | 205 | LYS  | C-N-CA | 6.70  | 128.22      | 119.84   |
| 1   | D     | 318 | GLU  | N-CA-C | -6.61 | 103.27      | 112.45   |
| 1   | D     | 250 | ARG  | N-CA-C | -6.42 | 104.36      | 111.36   |
| 1   | D     | 329 | ASP  | N-CA-C | -6.38 | 105.25      | 113.16   |
| 1   | A     | 117 | LYS  | N-CA-C | -6.33 | 104.72      | 112.88   |
| 1   | C     | 191 | ILE  | N-CA-C | 6.30  | 117.10      | 107.77   |
| 1   | D     | 364 | VAL  | N-CA-C | 6.28  | 122.41      | 109.34   |
| 1   | C     | 205 | LYS  | CA-C-N | 6.26  | 127.67      | 119.84   |
| 1   | C     | 205 | LYS  | C-N-CA | 6.26  | 127.67      | 119.84   |
| 1   | A     | 157 | THR  | N-CA-C | -6.21 | 105.28      | 112.92   |
| 1   | B     | 259 | ILE  | N-CA-C | -6.19 | 106.77      | 112.96   |
| 1   | D     | 262 | GLU  | N-CA-C | 6.13  | 117.83      | 111.03   |
| 1   | C     | 171 | ALA  | N-CA-C | -5.97 | 104.86      | 111.36   |
| 1   | A     | 205 | LYS  | CA-C-N | 5.96  | 125.64      | 119.56   |
| 1   | A     | 205 | LYS  | C-N-CA | 5.96  | 125.64      | 119.56   |
| 1   | D     | 285 | SER  | N-CA-C | -5.91 | 105.89      | 112.57   |
| 1   | A     | 209 | VAL  | N-CA-C | -5.88 | 104.18      | 110.36   |
| 1   | A     | 305 | SER  | N-CA-C | 5.87  | 117.89      | 109.14   |
| 1   | D     | 345 | PHE  | CA-C-N | 5.81  | 126.69      | 120.47   |
| 1   | D     | 345 | PHE  | C-N-CA | 5.81  | 126.69      | 120.47   |
| 1   | D     | 284 | SER  | N-CA-C | -5.72 | 106.26      | 113.18   |
| 1   | D     | 223 | SER  | N-CA-C | 5.72  | 122.98      | 110.80   |
| 1   | B     | 204 | LEU  | N-CA-C | -5.69 | 106.14      | 112.57   |
| 1   | D     | 328 | CYS  | N-CA-C | -5.69 | 106.32      | 113.20   |
| 1   | C     | 131 | ASP  | N-CA-C | 5.60  | 117.22      | 109.15   |
| 1   | C     | 356 | LEU  | CA-C-N | 5.60  | 126.15      | 120.38   |
| 1   | C     | 356 | LEU  | C-N-CA | 5.60  | 126.15      | 120.38   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | A     | 152 | PHE  | N-CA-C  | -5.60 | 103.31      | 110.53   |
| 1   | B     | 205 | LYS  | CA-C-N  | 5.51  | 126.72      | 119.84   |
| 1   | B     | 205 | LYS  | C-N-CA  | 5.51  | 126.72      | 119.84   |
| 1   | B     | 274 | ASN  | N-CA-C  | -5.50 | 104.14      | 111.02   |
| 1   | C     | 240 | ALA  | N-CA-C  | -5.47 | 106.65      | 113.55   |
| 1   | A     | 247 | LEU  | N-CA-C  | 5.46  | 117.94      | 111.33   |
| 1   | D     | 240 | ALA  | N-CA-C  | 5.41  | 122.33      | 110.80   |
| 1   | B     | 225 | GLN  | N-CA-C  | -5.41 | 103.94      | 111.30   |
| 1   | B     | 305 | SER  | N-CA-C  | 5.38  | 118.03      | 109.96   |
| 1   | C     | 173 | LYS  | N-CA-C  | -5.37 | 103.88      | 110.65   |
| 1   | C     | 194 | SER  | N-CA-C  | 5.35  | 118.33      | 109.94   |
| 1   | C     | 357 | PRO  | CA-C-N  | 5.26  | 125.80      | 120.38   |
| 1   | C     | 357 | PRO  | C-N-CA  | 5.26  | 125.80      | 120.38   |
| 1   | B     | 213 | LYS  | N-CA-C  | -5.26 | 106.13      | 112.54   |
| 1   | A     | 203 | GLU  | N-CA-C  | 5.20  | 121.87      | 110.80   |
| 1   | A     | 143 | CYS  | N-CA-C  | 5.15  | 117.18      | 110.53   |
| 1   | C     | 232 | LEU  | CB-CA-C | -5.15 | 110.22      | 117.23   |
| 1   | A     | 260 | ILE  | N-CA-C  | 5.11  | 115.33      | 110.53   |
| 1   | C     | 148 | THR  | N-CA-C  | 5.10  | 114.00      | 108.14   |
| 1   | B     | 361 | ALA  | N-CA-C  | 5.08  | 117.89      | 109.46   |
| 1   | C     | 136 | LEU  | N-CA-C  | -5.06 | 108.13      | 114.56   |
| 1   | A     | 340 | ALA  | N-CA-C  | -5.06 | 104.71      | 111.24   |

There are no chirality outliers.

There are no planarity outliers.

## 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     | 2067  | 0        | 2107     | 395     | 0            |
| 1   | B     | 1321  | 0        | 1359     | 214     | 0            |
| 1   | C     | 2095  | 0        | 2132     | 430     | 0            |
| 1   | D     | 1349  | 0        | 1392     | 217     | 0            |
| All | All   | 6832  | 0        | 6990     | 1228    | 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 89.

All (1228) 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:295:ILE:HG12 | 1:A:319:GLU:HB3  | 1.25                     | 1.16              |
| 1:C:304:LYS:HA   | 1:C:326:SER:HB2  | 1.31                     | 1.13              |
| 1:A:229:LEU:HB3  | 1:A:232:LEU:HD21 | 1.33                     | 1.10              |
| 1:B:338:ILE:HD11 | 1:B:356:LEU:HD22 | 1.30                     | 1.09              |
| 1:A:296:LEU:HD12 | 1:A:297:ASN:H    | 0.98                     | 1.08              |
| 1:C:306:GLU:H    | 1:C:327:LEU:HD13 | 1.14                     | 1.07              |
| 1:C:204:LEU:HA   | 1:C:208:GLN:NE2  | 1.68                     | 1.07              |
| 1:A:306:GLU:HG3  | 1:A:344:ARG:HH21 | 1.19                     | 1.06              |
| 1:C:237:ASP:HA   | 1:C:240:ALA:HB3  | 1.33                     | 1.04              |
| 1:C:257:LEU:HA   | 1:C:260:ILE:HD12 | 1.39                     | 1.04              |
| 1:C:121:LYS:HB2  | 1:C:192:ASN:HB2  | 1.42                     | 1.01              |
| 1:C:120:PHE:H    | 1:C:163:VAL:HB   | 1.22                     | 1.00              |
| 1:A:127:GLY:HA3  | 1:A:159:ALA:HB2  | 1.42                     | 1.00              |
| 1:D:232:LEU:HD23 | 1:D:247:LEU:HG   | 1.43                     | 1.00              |
| 1:A:276:ARG:HH21 | 1:A:276:ARG:HB3  | 1.26                     | 0.98              |
| 1:C:273:SER:HB2  | 1:C:299:SER:HB3  | 1.45                     | 0.98              |
| 1:A:293:LEU:HD23 | 1:A:315:LEU:HD11 | 1.47                     | 0.97              |
| 1:B:216:MET:HE1  | 1:B:256:THR:HA   | 1.47                     | 0.96              |
| 1:C:134:TRP:HA   | 1:C:137:SER:HB2  | 1.47                     | 0.96              |
| 1:A:257:LEU:HD11 | 1:A:283:MET:HA   | 1.45                     | 0.96              |
| 1:C:152:PHE:HD1  | 1:C:161:PHE:HB3  | 1.29                     | 0.96              |
| 1:B:351:LEU:HB3  | 1:B:356:LEU:HD21 | 1.45                     | 0.95              |
| 1:C:201:LEU:HD23 | 1:C:201:LEU:H    | 1.30                     | 0.94              |
| 1:A:296:LEU:HD12 | 1:A:297:ASN:N    | 1.81                     | 0.94              |
| 1:C:121:LYS:HE3  | 1:C:194:SER:HB2  | 1.49                     | 0.94              |
| 1:A:173:LYS:HB2  | 1:A:191:ILE:HG21 | 1.49                     | 0.94              |
| 1:B:269:SER:HB2  | 1:B:295:ILE:HD12 | 1.47                     | 0.94              |
| 1:B:294:LYS:HA   | 1:B:317:LEU:HA   | 1.51                     | 0.92              |
| 1:A:296:LEU:CD1  | 1:A:297:ASN:H    | 1.83                     | 0.92              |
| 1:A:281:ASP:HA   | 1:A:284:SER:HB3  | 1.51                     | 0.92              |
| 1:C:183:GLU:H    | 1:C:185:ARG:NH2  | 1.67                     | 0.91              |
| 1:C:118:ASN:HB2  | 1:C:166:ALA:H    | 1.33                     | 0.91              |
| 1:A:144:SER:O    | 1:A:145:VAL:HG13 | 1.70                     | 0.91              |
| 1:D:347:LYS:H    | 1:D:347:LYS:HD3  | 1.36                     | 0.91              |
| 1:A:214:LEU:HD22 | 1:D:361:ALA:H    | 1.33                     | 0.90              |
| 1:C:257:LEU:HD22 | 1:C:286:ILE:HB   | 1.53                     | 0.89              |
| 1:C:175:VAL:HG13 | 1:C:178:LYS:HB3  | 1.52                     | 0.89              |
| 1:D:241:GLN:HE22 | 1:D:243:ILE:HG13 | 1.34                     | 0.88              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:205:LYS:HG2  | 1:B:208:GLN:HG3  | 1.52                     | 0.88              |
| 1:A:208:GLN:HE21 | 1:A:243:ILE:HG12 | 1.40                     | 0.87              |
| 1:C:241:GLN:HG3  | 1:C:242:ASN:H    | 1.39                     | 0.87              |
| 1:A:140:GLN:HE21 | 1:A:140:GLN:HA   | 1.36                     | 0.87              |
| 1:A:270:LEU:HD22 | 1:A:271:ASN:H    | 1.36                     | 0.87              |
| 1:C:342:ARG:HD3  | 1:C:348:LEU:HB3  | 1.57                     | 0.86              |
| 1:A:124:ILE:HB   | 1:A:159:ALA:HB3  | 1.57                     | 0.86              |
| 1:D:360:ILE:HG12 | 1:D:364:VAL:O    | 1.76                     | 0.86              |
| 1:A:175:VAL:HA   | 1:A:178:LYS:HG3  | 1.58                     | 0.86              |
| 1:C:320:LEU:HD12 | 1:C:321:TRP:H    | 1.41                     | 0.85              |
| 1:D:297:ASN:HD22 | 1:D:298:LEU:N    | 1.73                     | 0.85              |
| 1:B:335:SER:O    | 1:B:338:ILE:HG22 | 1.75                     | 0.85              |
| 1:C:258:ARG:NH1  | 1:C:262:GLU:HB2  | 1.91                     | 0.85              |
| 1:D:254:ALA:O    | 1:D:258:ARG:HB2  | 1.76                     | 0.85              |
| 1:B:338:ILE:CD1  | 1:B:356:LEU:HD22 | 2.07                     | 0.84              |
| 1:C:120:PHE:HB2  | 1:C:163:VAL:HG21 | 1.58                     | 0.84              |
| 1:C:303:LEU:HB2  | 1:C:325:ASN:OD1  | 1.77                     | 0.84              |
| 1:C:344:ARG:HG2  | 1:C:344:ARG:HH11 | 1.41                     | 0.84              |
| 1:B:230:LYS:HB2  | 1:B:271:ASN:HD21 | 1.41                     | 0.84              |
| 1:B:212:LEU:HG   | 1:B:216:MET:HE3  | 1.58                     | 0.84              |
| 1:D:295:ILE:HG13 | 1:D:319:GLU:HB3  | 1.58                     | 0.83              |
| 1:B:257:LEU:HD21 | 1:B:289:LYS:HG3  | 1.60                     | 0.83              |
| 1:B:322:LEU:CD1  | 1:B:341:ILE:HD11 | 2.07                     | 0.83              |
| 1:C:101:ALA:HB3  | 1:C:102:PRO:HD3  | 1.61                     | 0.82              |
| 1:C:152:PHE:CD1  | 1:C:161:PHE:HB3  | 2.14                     | 0.82              |
| 1:D:240:ALA:C    | 1:D:242:ASN:H    | 1.87                     | 0.82              |
| 1:C:207:GLU:HA   | 1:C:210:GLU:HG2  | 1.62                     | 0.82              |
| 1:C:306:GLU:N    | 1:C:327:LEU:HD13 | 1.93                     | 0.82              |
| 1:D:239:VAL:HG23 | 1:D:240:ALA:H    | 1.44                     | 0.82              |
| 1:A:199:THR:HG22 | 1:A:200:ILE:H    | 1.44                     | 0.82              |
| 1:D:297:ASN:HA   | 1:D:321:TRP:HB2  | 1.59                     | 0.82              |
| 1:C:270:LEU:HD21 | 1:C:272:LEU:HD21 | 1.61                     | 0.81              |
| 1:C:342:ARG:HD2  | 1:C:346:PRO:O    | 1.80                     | 0.81              |
| 1:B:225:GLN:O    | 1:B:267:LEU:HD12 | 1.80                     | 0.81              |
| 1:A:276:ARG:HB3  | 1:A:276:ARG:NH2  | 1.95                     | 0.81              |
| 1:A:278:TYR:O    | 1:A:303:LEU:HD23 | 1.80                     | 0.81              |
| 1:B:337:TYR:O    | 1:B:341:ILE:HB   | 1.81                     | 0.81              |
| 1:C:125:PRO:HA   | 1:C:158:ARG:HA   | 1.62                     | 0.81              |
| 1:C:102:PRO:HB2  | 1:C:103:PRO:HD3  | 1.62                     | 0.81              |
| 1:C:271:ASN:HD22 | 1:C:272:LEU:N    | 1.78                     | 0.81              |
| 1:D:369:THR:HG23 | 1:D:370:LEU:N    | 1.95                     | 0.81              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:173:LYS:HD3  | 1:A:191:ILE:HG22 | 1.61                     | 0.81              |
| 1:C:158:ARG:HH11 | 1:C:158:ARG:HB3  | 1.46                     | 0.80              |
| 1:C:232:LEU:O    | 1:C:238:LEU:HG   | 1.82                     | 0.80              |
| 1:D:335:SER:O    | 1:D:338:ILE:HG13 | 1.82                     | 0.80              |
| 1:A:286:ILE:HG13 | 1:A:290:ALA:HB3  | 1.62                     | 0.80              |
| 1:B:351:LEU:HB2  | 1:B:356:LEU:HD11 | 1.63                     | 0.80              |
| 1:A:280:LEU:HD13 | 1:A:312:ILE:HD11 | 1.64                     | 0.79              |
| 1:B:254:ALA:C    | 1:B:258:ARG:HB2  | 2.06                     | 0.79              |
| 1:B:304:LYS:O    | 1:B:327:LEU:HB3  | 1.81                     | 0.79              |
| 1:A:304:LYS:HA   | 1:A:326:SER:HB2  | 1.64                     | 0.79              |
| 1:A:219:ARG:HD3  | 1:A:228:ASP:O    | 1.83                     | 0.78              |
| 1:B:338:ILE:HD11 | 1:B:356:LEU:CD2  | 2.13                     | 0.78              |
| 1:D:263:ASN:C    | 1:D:265:PRO:HD3  | 2.09                     | 0.78              |
| 1:D:297:ASN:HD22 | 1:D:297:ASN:C    | 1.91                     | 0.78              |
| 1:C:271:ASN:HD22 | 1:C:272:LEU:H    | 1.30                     | 0.78              |
| 1:C:286:ILE:HA   | 1:C:289:LYS:HB2  | 1.64                     | 0.78              |
| 1:D:331:PHE:HD2  | 1:D:336:THR:HG22 | 1.48                     | 0.78              |
| 1:B:269:SER:HA   | 1:B:295:ILE:HB   | 1.66                     | 0.78              |
| 1:A:271:ASN:C    | 1:A:271:ASN:HD22 | 1.92                     | 0.78              |
| 1:B:212:LEU:HG   | 1:B:216:MET:CE   | 2.13                     | 0.78              |
| 1:D:269:SER:HA   | 1:D:295:ILE:HG23 | 1.66                     | 0.77              |
| 1:B:213:LYS:HB3  | 1:B:259:ILE:HD13 | 1.64                     | 0.77              |
| 1:B:238:LEU:HG   | 1:B:243:ILE:HB   | 1.66                     | 0.77              |
| 1:C:317:LEU:O    | 1:C:318:GLU:HG3  | 1.84                     | 0.77              |
| 1:A:132:LYS:HG3  | 1:A:152:PHE:CE2  | 2.19                     | 0.77              |
| 1:D:337:TYR:O    | 1:D:341:ILE:HD13 | 1.83                     | 0.77              |
| 1:A:143:CYS:SG   | 1:A:144:SER:N    | 2.57                     | 0.77              |
| 1:A:320:LEU:HD12 | 1:A:321:TRP:H    | 1.50                     | 0.77              |
| 1:A:238:LEU:HD21 | 1:A:243:ILE:HG22 | 1.67                     | 0.76              |
| 1:D:241:GLN:NE2  | 1:D:243:ILE:HG13 | 2.01                     | 0.76              |
| 1:A:278:TYR:CD1  | 1:A:279:ARG:N    | 2.53                     | 0.76              |
| 1:B:323:ASP:HB2  | 1:C:186:ARG:HH11 | 1.50                     | 0.76              |
| 1:C:341:ILE:O    | 1:C:341:ILE:HG22 | 1.84                     | 0.76              |
| 1:A:297:ASN:HD21 | 1:A:299:SER:HB3  | 1.50                     | 0.76              |
| 1:A:309:LEU:HD22 | 1:A:309:LEU:H    | 1.51                     | 0.76              |
| 1:A:249:ARG:HE   | 1:A:249:ARG:HA   | 1.51                     | 0.76              |
| 1:A:280:LEU:HD12 | 1:A:308:GLU:HB3  | 1.68                     | 0.76              |
| 1:C:204:LEU:HA   | 1:C:208:GLN:HE21 | 1.49                     | 0.76              |
| 1:D:259:ILE:HG23 | 1:D:263:ASN:ND2  | 2.01                     | 0.76              |
| 1:D:297:ASN:ND2  | 1:D:299:SER:H    | 1.83                     | 0.75              |
| 1:A:329:ASP:C    | 1:A:331:PHE:H    | 1.95                     | 0.75              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:279:ARG:O    | 1:D:280:LEU:HG   | 1.87                     | 0.75              |
| 1:B:255:ALA:O    | 1:B:259:ILE:HG13 | 1.86                     | 0.75              |
| 1:B:228:ASP:O    | 1:B:229:LEU:HD23 | 1.86                     | 0.75              |
| 1:C:126:TYR:HA   | 1:C:157:THR:HG22 | 1.68                     | 0.75              |
| 1:D:233:ARG:HE   | 1:D:244:ASP:CG   | 1.94                     | 0.75              |
| 1:C:170:SER:HA   | 1:C:173:LYS:HB3  | 1.69                     | 0.74              |
| 1:C:272:LEU:HD12 | 1:C:298:LEU:HG   | 1.68                     | 0.74              |
| 1:A:197:PRO:O    | 1:A:198:HIS:HB2  | 1.88                     | 0.74              |
| 1:B:257:LEU:CD2  | 1:B:289:LYS:HG3  | 2.17                     | 0.74              |
| 1:B:248:ASN:ND2  | 1:B:248:ASN:H    | 1.83                     | 0.74              |
| 1:C:118:ASN:HB2  | 1:C:166:ALA:N    | 2.03                     | 0.74              |
| 1:D:259:ILE:HG23 | 1:D:263:ASN:HD22 | 1.51                     | 0.74              |
| 1:A:303:LEU:HD12 | 1:A:325:ASN:OD1  | 1.88                     | 0.74              |
| 1:A:212:LEU:HD11 | 1:A:216:MET:HE3  | 1.69                     | 0.73              |
| 1:C:241:GLN:HG3  | 1:C:242:ASN:N    | 1.99                     | 0.73              |
| 1:A:125:PRO:HD2  | 1:A:188:SER:HB2  | 1.70                     | 0.73              |
| 1:A:132:LYS:HE3  | 1:A:152:PHE:HD2  | 1.53                     | 0.73              |
| 1:A:267:LEU:HD12 | 1:A:268:LEU:N    | 2.03                     | 0.73              |
| 1:B:338:ILE:O    | 1:B:341:ILE:HG22 | 1.88                     | 0.73              |
| 1:C:181:ASP:OD2  | 1:C:185:ARG:HB2  | 1.88                     | 0.73              |
| 1:B:261:GLU:HB2  | 1:B:289:LYS:CD   | 2.17                     | 0.73              |
| 1:C:246:VAL:HG11 | 1:C:249:ARG:HD3  | 1.70                     | 0.73              |
| 1:B:211:GLN:HA   | 1:B:214:LEU:HB3  | 1.69                     | 0.73              |
| 1:B:287:VAL:HG11 | 1:B:314:GLY:HA3  | 1.70                     | 0.73              |
| 1:C:134:TRP:NE1  | 1:C:138:MET:HG2  | 2.02                     | 0.73              |
| 1:A:175:VAL:HG12 | 1:A:175:VAL:O    | 1.86                     | 0.73              |
| 1:A:342:ARG:HD3  | 1:A:348:LEU:HB3  | 1.69                     | 0.73              |
| 1:C:136:LEU:HA   | 1:C:139:ILE:HD12 | 1.71                     | 0.73              |
| 1:C:305:SER:C    | 1:C:307:ARG:H    | 1.96                     | 0.73              |
| 1:A:276:ARG:HH21 | 1:A:276:ARG:CB   | 1.99                     | 0.73              |
| 1:C:287:VAL:HG13 | 1:C:314:GLY:HA3  | 1.71                     | 0.73              |
| 1:C:120:PHE:HB2  | 1:C:163:VAL:CG2  | 2.19                     | 0.73              |
| 1:A:286:ILE:CG1  | 1:A:290:ALA:HB3  | 2.18                     | 0.72              |
| 1:A:336:THR:HA   | 1:A:339:SER:HB2  | 1.72                     | 0.72              |
| 1:A:214:LEU:HD13 | 1:D:360:ILE:HA   | 1.70                     | 0.72              |
| 1:B:304:LYS:HD3  | 1:B:326:SER:HB2  | 1.70                     | 0.72              |
| 1:C:121:LYS:CE   | 1:C:194:SER:HB2  | 2.18                     | 0.72              |
| 1:C:237:ASP:C    | 1:C:238:LEU:HD22 | 2.15                     | 0.71              |
| 1:D:208:GLN:HA   | 1:D:211:GLN:HE21 | 1.54                     | 0.71              |
| 1:D:369:THR:HG23 | 1:D:370:LEU:H    | 1.55                     | 0.71              |
| 1:B:327:LEU:C    | 1:B:329:ASP:H    | 1.99                     | 0.71              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:250:ARG:HG3  | 1:C:251:SER:N    | 2.04                     | 0.71              |
| 1:A:311:LYS:HA   | 1:A:311:LYS:HZ3  | 1.53                     | 0.71              |
| 1:D:204:LEU:HD23 | 1:D:205:LYS:H    | 1.56                     | 0.71              |
| 1:A:271:ASN:HD21 | 1:A:273:SER:CB   | 2.03                     | 0.71              |
| 1:C:261:GLU:O    | 1:C:265:PRO:HG3  | 1.90                     | 0.71              |
| 1:D:220:TYR:HB2  | 1:D:227:LEU:HD13 | 1.71                     | 0.71              |
| 1:D:316:LYS:HA   | 1:D:347:LYS:HE3  | 1.73                     | 0.70              |
| 1:C:155:GLU:HB3  | 1:C:158:ARG:CG   | 2.21                     | 0.70              |
| 1:C:261:GLU:HB2  | 1:C:289:LYS:O    | 1.92                     | 0.70              |
| 1:C:265:PRO:C    | 1:C:266:GLU:HG3  | 2.17                     | 0.70              |
| 1:B:327:LEU:C    | 1:B:327:LEU:HD12 | 2.16                     | 0.70              |
| 1:A:173:LYS:HB2  | 1:A:191:ILE:CG2  | 2.22                     | 0.70              |
| 1:B:325:ASN:O    | 1:B:327:LEU:N    | 2.23                     | 0.70              |
| 1:C:238:LEU:CA   | 1:C:241:GLN:HG2  | 2.22                     | 0.70              |
| 1:A:120:PHE:CE1  | 1:A:166:ALA:HA   | 2.27                     | 0.70              |
| 1:A:305:SER:OG   | 1:A:307:ARG:HB2  | 1.92                     | 0.70              |
| 1:B:261:GLU:HB2  | 1:B:289:LYS:HD2  | 1.73                     | 0.70              |
| 1:B:279:ARG:C    | 1:B:281:ASP:H    | 2.00                     | 0.70              |
| 1:A:220:TYR:CG   | 1:A:221:ASP:N    | 2.54                     | 0.69              |
| 1:A:309:LEU:H    | 1:A:309:LEU:CD2  | 2.05                     | 0.69              |
| 1:A:317:LEU:O    | 1:A:318:GLU:HG3  | 1.91                     | 0.69              |
| 1:C:196:PRO:O    | 1:C:198:HIS:N    | 2.22                     | 0.69              |
| 1:A:208:GLN:HE21 | 1:A:243:ILE:CG1  | 2.04                     | 0.69              |
| 1:A:270:LEU:HD22 | 1:A:271:ASN:N    | 2.07                     | 0.69              |
| 1:C:131:ASP:O    | 1:C:135:LEU:N    | 2.20                     | 0.69              |
| 1:C:205:LYS:H    | 1:C:208:GLN:CD   | 2.00                     | 0.69              |
| 1:A:206:PRO:HA   | 1:A:209:VAL:HG23 | 1.73                     | 0.69              |
| 1:A:257:LEU:CD1  | 1:A:283:MET:HA   | 2.20                     | 0.69              |
| 1:A:297:ASN:ND2  | 1:A:321:TRP:HB2  | 2.07                     | 0.69              |
| 1:C:258:ARG:HH12 | 1:C:262:GLU:HB2  | 1.57                     | 0.69              |
| 1:D:213:LYS:HG3  | 1:D:259:ILE:HD13 | 1.73                     | 0.69              |
| 1:A:130:TYR:HB2  | 1:A:135:LEU:HD22 | 1.73                     | 0.69              |
| 1:A:229:LEU:HB3  | 1:A:232:LEU:CD2  | 2.18                     | 0.69              |
| 1:A:278:TYR:HD1  | 1:A:279:ARG:N    | 1.90                     | 0.69              |
| 1:C:310:ASP:HB3  | 1:C:344:ARG:NH1  | 2.08                     | 0.69              |
| 1:C:308:GLU:C    | 1:C:310:ASP:H    | 2.00                     | 0.69              |
| 1:A:270:LEU:H    | 1:A:293:LEU:HD11 | 1.56                     | 0.68              |
| 1:C:162:PHE:CE2  | 1:C:197:PRO:HD3  | 2.27                     | 0.68              |
| 1:B:328:CYS:SG   | 1:C:177:TYR:HE1  | 2.16                     | 0.68              |
| 1:C:132:LYS:HA   | 1:C:135:LEU:HD22 | 1.76                     | 0.68              |
| 1:D:204:LEU:HD23 | 1:D:205:LYS:N    | 2.09                     | 0.68              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:225:GLN:HB3  | 1:A:268:LEU:H    | 1.59                     | 0.68              |
| 1:D:313:LYS:HA   | 1:D:344:ARG:HB3  | 1.75                     | 0.68              |
| 1:D:322:LEU:N    | 1:D:352:ASP:OD1  | 2.27                     | 0.68              |
| 1:A:109:GLY:HA2  | 1:A:116:SER:OG   | 1.93                     | 0.68              |
| 1:D:307:ARG:CB   | 1:D:307:ARG:HH21 | 2.07                     | 0.68              |
| 1:C:147:PHE:HB3  | 1:C:168:THR:HG21 | 1.75                     | 0.68              |
| 1:C:120:PHE:HA   | 1:C:193:SER:HA   | 1.75                     | 0.68              |
| 1:C:290:ALA:C    | 1:C:292:ASN:H    | 2.02                     | 0.68              |
| 1:D:323:ASP:C    | 1:D:325:ASN:H    | 2.02                     | 0.68              |
| 1:A:267:LEU:HD12 | 1:A:268:LEU:H    | 1.58                     | 0.68              |
| 1:C:120:PHE:N    | 1:C:163:VAL:HB   | 2.03                     | 0.68              |
| 1:B:205:LYS:O    | 1:B:208:GLN:HB2  | 1.94                     | 0.68              |
| 1:C:151:GLU:HG2  | 1:C:162:PHE:CD1  | 2.29                     | 0.68              |
| 1:A:235:ASP:H    | 1:A:239:VAL:HG23 | 1.59                     | 0.67              |
| 1:B:294:LYS:HD2  | 1:B:316:LYS:O    | 1.94                     | 0.67              |
| 1:C:130:TYR:HB2  | 1:C:135:LEU:HD12 | 1.76                     | 0.67              |
| 1:C:237:ASP:HA   | 1:C:240:ALA:CB   | 2.17                     | 0.67              |
| 1:D:257:LEU:HD11 | 1:D:283:MET:HA   | 1.75                     | 0.67              |
| 1:C:246:VAL:HG21 | 1:C:249:ARG:NH2  | 2.09                     | 0.67              |
| 1:D:305:SER:O    | 1:D:308:GLU:HG2  | 1.94                     | 0.67              |
| 1:D:283:MET:O    | 1:D:286:ILE:HG22 | 1.94                     | 0.67              |
| 1:A:212:LEU:HD13 | 1:A:245:VAL:HG21 | 1.75                     | 0.67              |
| 1:C:342:ARG:NH1  | 1:C:359:PRO:HG3  | 2.10                     | 0.67              |
| 1:D:214:LEU:O    | 1:D:218:LYS:HG2  | 1.93                     | 0.67              |
| 1:C:257:LEU:HD11 | 1:C:283:MET:CB   | 2.25                     | 0.67              |
| 1:A:229:LEU:CB   | 1:A:232:LEU:HD21 | 2.18                     | 0.67              |
| 1:B:207:GLU:C    | 1:B:207:GLU:CD   | 2.62                     | 0.67              |
| 1:A:288:GLN:NE2  | 1:B:288:GLN:HE22 | 1.93                     | 0.67              |
| 1:A:342:ARG:CZ   | 1:A:359:PRO:HG3  | 2.25                     | 0.67              |
| 1:B:326:SER:HA   | 1:B:329:ASP:OD1  | 1.95                     | 0.67              |
| 1:D:212:LEU:O    | 1:D:215:ILE:N    | 2.27                     | 0.67              |
| 1:C:320:LEU:HD12 | 1:C:321:TRP:N    | 2.08                     | 0.66              |
| 1:A:233:ARG:HD2  | 1:A:244:ASP:HB2  | 1.77                     | 0.66              |
| 1:B:253:MET:HE3  | 1:B:283:MET:HB3  | 1.78                     | 0.66              |
| 1:B:280:LEU:CD2  | 1:B:303:LEU:HD22 | 2.26                     | 0.66              |
| 1:B:327:LEU:HD12 | 1:B:328:CYS:N    | 2.10                     | 0.66              |
| 1:C:123:THR:HA   | 1:C:160:GLN:HG2  | 1.77                     | 0.66              |
| 1:D:360:ILE:HD13 | 1:D:365:GLU:HB3  | 1.77                     | 0.66              |
| 1:C:297:ASN:ND2  | 1:C:299:SER:H    | 1.94                     | 0.66              |
| 1:C:333:ASP:C    | 1:C:335:SER:H    | 2.03                     | 0.66              |
| 1:A:127:GLY:HA3  | 1:A:159:ALA:CB   | 2.21                     | 0.66              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:299:SER:HB3  | 1:C:186:ARG:NH1  | 2.11                     | 0.66              |
| 1:C:155:GLU:HB3  | 1:C:158:ARG:HG3  | 1.77                     | 0.66              |
| 1:B:207:GLU:OE2  | 1:B:210:GLU:HB3  | 1.96                     | 0.66              |
| 1:C:255:ALA:O    | 1:C:258:ARG:HB3  | 1.94                     | 0.66              |
| 1:A:309:LEU:HD12 | 1:A:345:PHE:CE1  | 2.31                     | 0.65              |
| 1:A:216:MET:CE   | 1:A:256:THR:HG23 | 2.26                     | 0.65              |
| 1:B:226:ALA:HB2  | 1:B:269:SER:HB3  | 1.78                     | 0.65              |
| 1:C:238:LEU:HA   | 1:C:241:GLN:HG2  | 1.79                     | 0.65              |
| 1:C:342:ARG:CD   | 1:C:348:LEU:HB3  | 2.25                     | 0.65              |
| 1:C:344:ARG:HG2  | 1:C:344:ARG:NH1  | 2.12                     | 0.65              |
| 1:B:305:SER:HB2  | 1:D:330:THR:HG23 | 1.79                     | 0.65              |
| 1:B:333:ASP:OD2  | 1:B:336:THR:HB   | 1.96                     | 0.65              |
| 1:B:248:ASN:HB3  | 1:B:277:LEU:HD23 | 1.78                     | 0.65              |
| 1:B:286:ILE:HG23 | 1:B:315:LEU:HD21 | 1.77                     | 0.65              |
| 1:C:315:LEU:HD23 | 1:C:315:LEU:H    | 1.62                     | 0.65              |
| 1:A:158:ARG:HH21 | 1:A:206:PRO:HD2  | 1.60                     | 0.65              |
| 1:A:238:LEU:HD12 | 1:A:241:GLN:HB2  | 1.79                     | 0.65              |
| 1:A:285:SER:O    | 1:A:287:VAL:N    | 2.30                     | 0.65              |
| 1:A:297:ASN:HD21 | 1:A:299:SER:CB   | 2.10                     | 0.65              |
| 1:B:293:LEU:HD12 | 1:B:295:ILE:H    | 1.62                     | 0.65              |
| 1:C:213:LYS:HA   | 1:C:259:ILE:HD13 | 1.79                     | 0.65              |
| 1:C:277:LEU:O    | 1:C:278:TYR:HB3  | 1.97                     | 0.65              |
| 1:D:269:SER:HA   | 1:D:295:ILE:CG2  | 2.27                     | 0.64              |
| 1:A:105:ARG:HA   | 1:A:110:THR:HA   | 1.79                     | 0.64              |
| 1:A:200:ILE:HG22 | 1:A:202:ASN:ND2  | 2.12                     | 0.64              |
| 1:A:330:THR:O    | 1:A:330:THR:HG22 | 1.95                     | 0.64              |
| 1:C:122:ILE:HD13 | 1:C:191:ILE:HG23 | 1.78                     | 0.64              |
| 1:D:224:GLN:O    | 1:D:268:LEU:HD12 | 1.97                     | 0.64              |
| 1:C:330:THR:HB   | 1:C:331:PHE:HD1  | 1.61                     | 0.64              |
| 1:A:309:LEU:HD22 | 1:A:309:LEU:N    | 2.12                     | 0.64              |
| 1:C:241:GLN:NE2  | 1:C:243:ILE:HG13 | 2.12                     | 0.64              |
| 1:A:132:LYS:HG3  | 1:A:152:PHE:HE2  | 1.59                     | 0.64              |
| 1:C:141:SER:O    | 1:C:142:LYS:HB2  | 1.96                     | 0.64              |
| 1:C:148:THR:O    | 1:C:150:ILE:HG13 | 1.98                     | 0.64              |
| 1:C:312:ILE:HG13 | 1:C:345:PHE:HZ   | 1.62                     | 0.64              |
| 1:A:128:ARG:HG2  | 1:A:154:TYR:CD2  | 2.33                     | 0.64              |
| 1:A:214:LEU:HD22 | 1:D:361:ALA:N    | 2.10                     | 0.64              |
| 1:C:251:SER:HA   | 1:C:254:ALA:HB2  | 1.79                     | 0.64              |
| 1:D:232:LEU:HD23 | 1:D:247:LEU:CG   | 2.24                     | 0.64              |
| 1:A:212:LEU:O    | 1:A:216:MET:HG3  | 1.98                     | 0.64              |
| 1:A:219:ARG:HH12 | 1:A:231:GLY:H    | 1.43                     | 0.64              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:305:SER:O    | 1:C:307:ARG:N    | 2.31                     | 0.64              |
| 1:D:320:LEU:O    | 1:D:351:LEU:HD12 | 1.98                     | 0.64              |
| 1:A:123:THR:O    | 1:A:125:PRO:HD3  | 1.98                     | 0.63              |
| 1:A:297:ASN:ND2  | 1:A:299:SER:HB3  | 2.13                     | 0.63              |
| 1:A:200:ILE:HG22 | 1:A:202:ASN:HD21 | 1.61                     | 0.63              |
| 1:B:216:MET:CE   | 1:B:256:THR:HA   | 2.26                     | 0.63              |
| 1:C:152:PHE:HA   | 1:C:160:GLN:O    | 1.99                     | 0.63              |
| 1:C:296:LEU:HG   | 1:C:298:LEU:HD11 | 1.79                     | 0.63              |
| 1:D:268:LEU:O    | 1:D:295:ILE:HG22 | 1.99                     | 0.63              |
| 1:A:212:LEU:CD1  | 1:A:216:MET:HE3  | 2.28                     | 0.63              |
| 1:C:118:ASN:O    | 1:C:165:ASP:HA   | 1.98                     | 0.63              |
| 1:C:158:ARG:HB3  | 1:C:158:ARG:NH1  | 2.13                     | 0.63              |
| 1:C:264:ILE:N    | 1:C:265:PRO:HD3  | 2.13                     | 0.63              |
| 1:C:290:ALA:O    | 1:C:292:ASN:N    | 2.30                     | 0.63              |
| 1:A:180:LEU:CD2  | 1:A:184:ASN:HA   | 2.29                     | 0.63              |
| 1:B:235:ASP:OD1  | 1:B:238:LEU:N    | 2.31                     | 0.63              |
| 1:C:319:GLU:HB2  | 1:C:350:ARG:HE   | 1.64                     | 0.63              |
| 1:A:271:ASN:ND2  | 1:A:273:SER:H    | 1.97                     | 0.63              |
| 1:A:296:LEU:HD21 | 1:A:298:LEU:HD21 | 1.78                     | 0.63              |
| 1:D:228:ASP:O    | 1:D:229:LEU:HD23 | 1.98                     | 0.63              |
| 1:D:240:ALA:C    | 1:D:242:ASN:N    | 2.57                     | 0.63              |
| 1:A:259:ILE:HG22 | 1:A:263:ASN:HD22 | 1.63                     | 0.63              |
| 1:B:272:LEU:C    | 1:B:275:ASN:HD22 | 2.07                     | 0.63              |
| 1:B:363:ASP:O    | 1:B:367:PRO:HG3  | 1.98                     | 0.63              |
| 1:C:315:LEU:HD12 | 1:C:317:LEU:HD21 | 1.81                     | 0.63              |
| 1:C:137:SER:HA   | 1:C:140:GLN:HG2  | 1.80                     | 0.62              |
| 1:D:313:LYS:HG3  | 1:D:344:ARG:HG3  | 1.81                     | 0.62              |
| 1:D:307:ARG:HH21 | 1:D:307:ARG:HB3  | 1.64                     | 0.62              |
| 1:D:331:PHE:CD2  | 1:D:336:THR:HG22 | 2.33                     | 0.62              |
| 1:A:167:SER:O    | 1:A:170:SER:HB3  | 1.99                     | 0.62              |
| 1:B:272:LEU:HD22 | 1:B:277:LEU:HD11 | 1.81                     | 0.62              |
| 1:C:105:ARG:HH21 | 1:D:238:LEU:HB3  | 1.64                     | 0.62              |
| 1:C:270:LEU:HD12 | 1:C:271:ASN:H    | 1.62                     | 0.62              |
| 1:C:305:SER:CB   | 1:C:307:ARG:HG3  | 2.30                     | 0.62              |
| 1:D:237:ASP:O    | 1:D:238:LEU:HB2  | 1.99                     | 0.62              |
| 1:C:305:SER:HB3  | 1:C:307:ARG:HG3  | 1.81                     | 0.62              |
| 1:D:207:GLU:CD   | 1:D:207:GLU:H    | 2.05                     | 0.62              |
| 1:A:263:ASN:O    | 1:A:265:PRO:HD3  | 1.99                     | 0.62              |
| 1:C:130:TYR:HB2  | 1:C:135:LEU:CD1  | 2.30                     | 0.62              |
| 1:C:134:TRP:HA   | 1:C:137:SER:CB   | 2.28                     | 0.62              |
| 1:D:205:LYS:HB2  | 1:D:208:GLN:OE1  | 1.99                     | 0.62              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:221:ASP:HB3  | 1:D:226:ALA:HB3  | 1.81                     | 0.62              |
| 1:C:172:LEU:N    | 1:C:172:LEU:HD12 | 2.14                     | 0.62              |
| 1:A:155:GLU:O    | 1:A:158:ARG:HB2  | 2.00                     | 0.61              |
| 1:A:216:MET:HE1  | 1:A:256:THR:HG23 | 1.81                     | 0.61              |
| 1:A:271:ASN:HD21 | 1:A:273:SER:HB3  | 1.65                     | 0.61              |
| 1:C:168:THR:HG22 | 1:C:168:THR:O    | 2.00                     | 0.61              |
| 1:C:241:GLN:NE2  | 1:C:243:ILE:O    | 2.33                     | 0.61              |
| 1:A:251:SER:O    | 1:A:254:ALA:HB3  | 2.00                     | 0.61              |
| 1:B:212:LEU:O    | 1:B:216:MET:HG3  | 1.99                     | 0.61              |
| 1:C:130:TYR:O    | 1:C:135:LEU:HD13 | 1.99                     | 0.61              |
| 1:A:253:MET:O    | 1:A:257:LEU:HG   | 2.01                     | 0.61              |
| 1:B:250:ARG:HA   | 1:B:282:ASP:OD2  | 1.99                     | 0.61              |
| 1:C:151:GLU:HB3  | 1:C:161:PHE:HA   | 1.82                     | 0.61              |
| 1:C:184:ASN:O    | 1:C:185:ARG:HG3  | 2.01                     | 0.61              |
| 1:C:279:ARG:O    | 1:C:281:ASP:N    | 2.33                     | 0.61              |
| 1:D:226:ALA:HA   | 1:D:269:SER:HB3  | 1.82                     | 0.61              |
| 1:D:347:LYS:H    | 1:D:347:LYS:CD   | 2.11                     | 0.61              |
| 1:C:140:GLN:HG3  | 1:C:141:SER:N    | 2.15                     | 0.61              |
| 1:D:267:LEU:HD21 | 1:D:270:LEU:HD13 | 1.80                     | 0.61              |
| 1:D:280:LEU:HD12 | 1:D:308:GLU:O    | 2.00                     | 0.61              |
| 1:B:342:ARG:HG3  | 1:B:345:PHE:O    | 2.00                     | 0.61              |
| 1:B:297:ASN:HA   | 1:B:321:TRP:HB2  | 1.83                     | 0.61              |
| 1:B:366:ALA:N    | 1:B:367:PRO:HD2  | 2.14                     | 0.61              |
| 1:A:188:SER:C    | 1:A:189:ILE:HG13 | 2.26                     | 0.61              |
| 1:B:261:GLU:CD   | 1:B:289:LYS:HD3  | 2.26                     | 0.61              |
| 1:C:177:TYR:H    | 1:C:188:SER:HA   | 1.66                     | 0.61              |
| 1:A:175:VAL:O    | 1:A:189:ILE:HD12 | 2.01                     | 0.61              |
| 1:C:171:ALA:HB3  | 1:C:172:LEU:HD12 | 1.82                     | 0.61              |
| 1:C:251:SER:HA   | 1:C:254:ALA:CB   | 2.29                     | 0.61              |
| 1:A:122:ILE:H    | 1:A:122:ILE:HD12 | 1.65                     | 0.61              |
| 1:C:253:MET:HG2  | 1:C:282:ASP:OD2  | 2.01                     | 0.61              |
| 1:D:367:PRO:O    | 1:D:368:THR:O    | 2.19                     | 0.61              |
| 1:A:348:LEU:HD11 | 1:A:350:ARG:O    | 2.00                     | 0.60              |
| 1:C:331:PHE:CD1  | 1:C:331:PHE:N    | 2.69                     | 0.60              |
| 1:B:219:ARG:NH2  | 1:B:228:ASP:OD2  | 2.34                     | 0.60              |
| 1:B:229:LEU:HB3  | 1:B:232:LEU:HD13 | 1.82                     | 0.60              |
| 1:C:297:ASN:HD22 | 1:C:298:LEU:N    | 1.99                     | 0.60              |
| 1:A:188:SER:O    | 1:A:189:ILE:HG13 | 2.00                     | 0.60              |
| 1:D:240:ALA:O    | 1:D:241:GLN:HG3  | 2.01                     | 0.60              |
| 1:A:204:LEU:HD22 | 1:A:208:GLN:HE22 | 1.66                     | 0.60              |
| 1:B:280:LEU:HD11 | 1:B:298:LEU:HD11 | 1.83                     | 0.60              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:150:ILE:O    | 1:C:151:GLU:HB3  | 2.01                     | 0.60              |
| 1:C:232:LEU:O    | 1:C:233:ARG:C    | 2.44                     | 0.60              |
| 1:D:297:ASN:C    | 1:D:297:ASN:ND2  | 2.53                     | 0.60              |
| 1:A:180:LEU:HA   | 1:A:185:ARG:O    | 2.01                     | 0.60              |
| 1:A:342:ARG:NH1  | 1:A:348:LEU:O    | 2.35                     | 0.60              |
| 1:B:313:LYS:HA   | 1:B:344:ARG:HB3  | 1.83                     | 0.60              |
| 1:A:140:GLN:HA   | 1:A:140:GLN:NE2  | 2.14                     | 0.60              |
| 1:A:327:LEU:HD12 | 1:A:328:CYS:N    | 2.16                     | 0.60              |
| 1:C:260:ILE:C    | 1:C:262:GLU:H    | 2.10                     | 0.60              |
| 1:A:122:ILE:HD12 | 1:A:122:ILE:N    | 2.17                     | 0.59              |
| 1:A:122:ILE:HG13 | 1:A:191:ILE:HG13 | 1.84                     | 0.59              |
| 1:A:230:LYS:HA   | 1:A:230:LYS:HE3  | 1.84                     | 0.59              |
| 1:A:342:ARG:NH1  | 1:A:356:LEU:HD13 | 2.17                     | 0.59              |
| 1:B:264:ILE:HG22 | 1:B:267:LEU:HB2  | 1.84                     | 0.59              |
| 1:A:281:ASP:O    | 1:A:284:SER:OG   | 2.20                     | 0.59              |
| 1:A:289:LYS:C    | 1:A:291:PRO:HD3  | 2.27                     | 0.59              |
| 1:B:334:GLN:NE2  | 1:B:351:LEU:HD23 | 2.17                     | 0.59              |
| 1:C:265:PRO:O    | 1:C:266:GLU:HG3  | 2.01                     | 0.59              |
| 1:A:153:HIS:CD2  | 1:A:160:GLN:HG3  | 2.37                     | 0.59              |
| 1:A:340:ALA:O    | 1:A:343:GLU:HB3  | 2.02                     | 0.59              |
| 1:D:297:ASN:HD21 | 1:D:299:SER:H    | 1.48                     | 0.59              |
| 1:A:271:ASN:C    | 1:A:271:ASN:ND2  | 2.58                     | 0.59              |
| 1:C:308:GLU:C    | 1:C:310:ASP:N    | 2.59                     | 0.59              |
| 1:C:310:ASP:O    | 1:C:313:LYS:HB3  | 2.02                     | 0.59              |
| 1:A:311:LYS:HA   | 1:A:311:LYS:NZ   | 2.16                     | 0.59              |
| 1:D:229:LEU:O    | 1:D:232:LEU:HB2  | 2.02                     | 0.59              |
| 1:D:360:ILE:HG21 | 1:D:363:ASP:O    | 2.03                     | 0.59              |
| 1:A:141:SER:C    | 1:A:143:CYS:H    | 2.09                     | 0.59              |
| 1:B:216:MET:HE3  | 1:B:259:ILE:HD12 | 1.83                     | 0.59              |
| 1:C:163:VAL:HG12 | 1:C:164:GLU:N    | 2.17                     | 0.59              |
| 1:C:252:SER:C    | 1:C:254:ALA:N    | 2.58                     | 0.59              |
| 1:A:306:GLU:HG3  | 1:A:344:ARG:NH2  | 2.03                     | 0.59              |
| 1:D:208:GLN:HA   | 1:D:211:GLN:NE2  | 2.17                     | 0.59              |
| 1:C:175:VAL:CG1  | 1:C:178:LYS:HB3  | 2.30                     | 0.59              |
| 1:C:261:GLU:HB3  | 1:C:289:LYS:HB3  | 1.85                     | 0.59              |
| 1:A:158:ARG:HH21 | 1:A:206:PRO:CD   | 2.15                     | 0.59              |
| 1:A:230:LYS:HA   | 1:A:230:LYS:CE   | 2.33                     | 0.59              |
| 1:A:336:THR:C    | 1:A:339:SER:H    | 2.11                     | 0.59              |
| 1:B:278:TYR:HA   | 1:B:303:LEU:HD23 | 1.84                     | 0.58              |
| 1:B:293:LEU:HD12 | 1:B:293:LEU:C    | 2.28                     | 0.58              |
| 1:C:233:ARG:HH12 | 1:C:249:ARG:NH2  | 2.01                     | 0.58              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:281:ASP:HB2  | 1:D:311:LYS:HE3  | 1.85                     | 0.58              |
| 1:D:369:THR:CG2  | 1:D:370:LEU:N    | 2.65                     | 0.58              |
| 1:A:320:LEU:C    | 1:A:321:TRP:CD1  | 2.81                     | 0.58              |
| 1:C:308:GLU:O    | 1:C:310:ASP:N    | 2.36                     | 0.58              |
| 1:D:236:PRO:O    | 1:D:237:ASP:HB2  | 2.03                     | 0.58              |
| 1:D:344:ARG:H    | 1:D:344:ARG:HD2  | 1.68                     | 0.58              |
| 1:A:135:LEU:O    | 1:A:139:ILE:HG13 | 2.03                     | 0.58              |
| 1:D:358:PRO:C    | 1:D:360:ILE:H    | 2.11                     | 0.58              |
| 1:D:367:PRO:O    | 1:D:368:THR:C    | 2.46                     | 0.58              |
| 1:A:199:THR:HG22 | 1:A:200:ILE:N    | 2.17                     | 0.58              |
| 1:A:271:ASN:HD22 | 1:A:273:SER:H    | 1.51                     | 0.58              |
| 1:A:320:LEU:CD1  | 1:A:321:TRP:H    | 2.16                     | 0.58              |
| 1:B:322:LEU:HD13 | 1:B:341:ILE:HD11 | 1.84                     | 0.58              |
| 1:C:121:LYS:HG2  | 1:C:162:PHE:CE2  | 2.38                     | 0.58              |
| 1:D:323:ASP:C    | 1:D:323:ASP:OD1  | 2.46                     | 0.58              |
| 1:A:179:ILE:CG2  | 1:A:187:ILE:HD13 | 2.34                     | 0.58              |
| 1:A:228:ASP:CG   | 1:A:230:LYS:HG2  | 2.27                     | 0.58              |
| 1:A:268:LEU:HD21 | 1:A:292:ASN:HB3  | 1.85                     | 0.58              |
| 1:C:137:SER:HA   | 1:C:140:GLN:HE21 | 1.68                     | 0.58              |
| 1:C:252:SER:C    | 1:C:254:ALA:H    | 2.11                     | 0.58              |
| 1:C:341:ILE:HG22 | 1:C:348:LEU:HD22 | 1.85                     | 0.58              |
| 1:D:264:ILE:N    | 1:D:265:PRO:HD3  | 2.18                     | 0.58              |
| 1:B:275:ASN:HB3  | 1:B:277:LEU:HD21 | 1.86                     | 0.58              |
| 1:C:257:LEU:HD11 | 1:C:283:MET:HB3  | 1.85                     | 0.57              |
| 1:C:337:TYR:CE2  | 1:C:351:LEU:HD21 | 2.39                     | 0.57              |
| 1:B:332:ARG:NH1  | 1:D:304:LYS:HG2  | 2.18                     | 0.57              |
| 1:B:332:ARG:O    | 1:C:190:ILE:HG21 | 2.05                     | 0.57              |
| 1:C:150:ILE:O    | 1:C:151:GLU:CB   | 2.52                     | 0.57              |
| 1:D:250:ARG:O    | 1:D:254:ALA:HB2  | 2.04                     | 0.57              |
| 1:D:278:TYR:CD2  | 1:D:279:ARG:N    | 2.72                     | 0.57              |
| 1:D:281:ASP:HA   | 1:D:311:LYS:HD2  | 1.86                     | 0.57              |
| 1:A:132:LYS:O    | 1:A:136:LEU:HD12 | 2.04                     | 0.57              |
| 1:A:176:ASN:OD1  | 1:A:189:ILE:N    | 2.37                     | 0.57              |
| 1:A:278:TYR:O    | 1:A:303:LEU:CD2  | 2.51                     | 0.57              |
| 1:B:247:LEU:HD11 | 1:B:272:LEU:HD21 | 1.86                     | 0.57              |
| 1:B:264:ILE:CG2  | 1:B:267:LEU:HB2  | 2.35                     | 0.57              |
| 1:A:124:ILE:HD12 | 1:A:159:ALA:HB1  | 1.86                     | 0.57              |
| 1:B:205:LYS:HG2  | 1:B:208:GLN:CG   | 2.29                     | 0.57              |
| 1:B:212:LEU:HD21 | 1:B:256:THR:OG1  | 2.03                     | 0.57              |
| 1:B:332:ARG:HH12 | 1:D:304:LYS:HG2  | 1.69                     | 0.57              |
| 1:B:341:ILE:HG21 | 1:B:351:LEU:HD22 | 1.85                     | 0.57              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:344:ARG:HD2  | 1:B:344:ARG:N    | 2.20                     | 0.57              |
| 1:C:136:LEU:HA   | 1:C:139:ILE:CD1  | 2.33                     | 0.57              |
| 1:C:246:VAL:HG12 | 1:C:248:ASN:HB3  | 1.86                     | 0.57              |
| 1:C:271:ASN:ND2  | 1:C:272:LEU:N    | 2.49                     | 0.57              |
| 1:A:235:ASP:O    | 1:A:236:PRO:O    | 2.23                     | 0.57              |
| 1:C:250:ARG:HG3  | 1:C:251:SER:H    | 1.68                     | 0.57              |
| 1:D:225:GLN:CB   | 1:D:268:LEU:HG   | 2.35                     | 0.57              |
| 1:A:197:PRO:O    | 1:A:198:HIS:CB   | 2.52                     | 0.57              |
| 1:D:342:ARG:HG2  | 1:D:342:ARG:HH11 | 1.69                     | 0.57              |
| 1:A:220:TYR:CD2  | 1:A:221:ASP:N    | 2.72                     | 0.57              |
| 1:B:340:ALA:HB2  | 1:D:307:ARG:HH11 | 1.70                     | 0.57              |
| 1:C:227:LEU:HD12 | 1:C:228:ASP:N    | 2.19                     | 0.57              |
| 1:C:331:PHE:HD1  | 1:C:331:PHE:H    | 1.51                     | 0.57              |
| 1:C:341:ILE:O    | 1:C:348:LEU:HD22 | 2.04                     | 0.57              |
| 1:A:272:LEU:O    | 1:A:273:SER:C    | 2.48                     | 0.57              |
| 1:A:334:GLN:OE1  | 1:A:338:ILE:HG13 | 2.05                     | 0.57              |
| 1:C:132:LYS:HA   | 1:C:135:LEU:CD2  | 2.33                     | 0.57              |
| 1:C:233:ARG:HH11 | 1:C:246:VAL:HG21 | 1.69                     | 0.57              |
| 1:C:256:THR:O    | 1:C:260:ILE:HG13 | 2.05                     | 0.57              |
| 1:A:228:ASP:OD2  | 1:A:230:LYS:HG2  | 2.05                     | 0.57              |
| 1:C:296:LEU:HG   | 1:C:298:LEU:CD1  | 2.34                     | 0.57              |
| 1:C:334:GLN:HA   | 1:C:337:TYR:HB2  | 1.86                     | 0.57              |
| 1:D:273:SER:HA   | 1:D:299:SER:O    | 2.04                     | 0.57              |
| 1:A:325:ASN:O    | 1:A:327:LEU:N    | 2.38                     | 0.56              |
| 1:B:213:LYS:CB   | 1:B:259:ILE:HD13 | 2.33                     | 0.56              |
| 1:C:246:VAL:CG1  | 1:C:248:ASN:HB3  | 2.35                     | 0.56              |
| 1:C:282:ASP:CG   | 1:C:283:MET:N    | 2.63                     | 0.56              |
| 1:C:306:GLU:HA   | 1:C:309:LEU:HG   | 1.85                     | 0.56              |
| 1:C:263:ASN:C    | 1:C:265:PRO:HD3  | 2.30                     | 0.56              |
| 1:A:177:TYR:CD1  | 1:A:186:ARG:HG3  | 2.41                     | 0.56              |
| 1:A:236:PRO:O    | 1:A:237:ASP:HB2  | 2.06                     | 0.56              |
| 1:A:270:LEU:HD11 | 1:A:272:LEU:CD2  | 2.35                     | 0.56              |
| 1:B:301:ASN:O    | 1:B:325:ASN:OD1  | 2.23                     | 0.56              |
| 1:B:328:CYS:HG   | 1:C:177:TYR:HE1  | 1.50                     | 0.56              |
| 1:C:162:PHE:CD2  | 1:C:197:PRO:HD3  | 2.41                     | 0.56              |
| 1:A:112:GLN:O    | 1:A:115:THR:OG1  | 2.24                     | 0.56              |
| 1:A:283:MET:O    | 1:A:285:SER:N    | 2.28                     | 0.56              |
| 1:C:123:THR:HB   | 1:C:190:ILE:HB   | 1.86                     | 0.56              |
| 1:A:235:ASP:H    | 1:A:239:VAL:CG2  | 2.19                     | 0.56              |
| 1:B:294:LYS:HA   | 1:B:317:LEU:CA   | 2.30                     | 0.56              |
| 1:C:270:LEU:H    | 1:C:293:LEU:HD11 | 1.71                     | 0.56              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:227:LEU:HB3  | 1:A:270:LEU:HA   | 1.87                     | 0.56              |
| 1:A:270:LEU:H    | 1:A:293:LEU:CD1  | 2.17                     | 0.56              |
| 1:B:277:LEU:H    | 1:B:301:ASN:HB3  | 1.69                     | 0.56              |
| 1:C:151:GLU:HG3  | 1:C:152:PHE:H    | 1.69                     | 0.56              |
| 1:A:125:PRO:HB3  | 1:D:334:GLN:HG2  | 1.86                     | 0.56              |
| 1:C:310:ASP:N    | 1:C:310:ASP:OD2  | 2.38                     | 0.56              |
| 1:A:268:LEU:CD2  | 1:A:292:ASN:HB3  | 2.36                     | 0.56              |
| 1:C:231:GLY:HA3  | 1:C:235:ASP:OD2  | 2.05                     | 0.56              |
| 1:B:287:VAL:HA   | 1:B:315:LEU:HD23 | 1.88                     | 0.56              |
| 1:C:205:LYS:HB3  | 1:C:208:GLN:HG3  | 1.87                     | 0.56              |
| 1:C:273:SER:O    | 1:C:275:ASN:ND2  | 2.39                     | 0.56              |
| 1:C:315:LEU:HD12 | 1:C:317:LEU:CD2  | 2.36                     | 0.56              |
| 1:A:346:PRO:C    | 1:A:348:LEU:H    | 2.14                     | 0.55              |
| 1:B:338:ILE:C    | 1:B:341:ILE:HG22 | 2.30                     | 0.55              |
| 1:D:204:LEU:HD23 | 1:D:205:LYS:O    | 2.05                     | 0.55              |
| 1:D:322:LEU:O    | 1:D:323:ASP:O    | 2.24                     | 0.55              |
| 1:B:253:MET:C    | 1:B:255:ALA:H    | 2.14                     | 0.55              |
| 1:B:305:SER:CB   | 1:D:330:THR:HG23 | 2.37                     | 0.55              |
| 1:C:296:LEU:HB3  | 1:C:317:LEU:HD11 | 1.88                     | 0.55              |
| 1:C:267:LEU:HD21 | 1:C:270:LEU:HB2  | 1.86                     | 0.55              |
| 1:C:273:SER:OG   | 1:C:274:ASN:ND2  | 2.40                     | 0.55              |
| 1:C:341:ILE:HG21 | 1:C:351:LEU:HD13 | 1.86                     | 0.55              |
| 1:A:206:PRO:HA   | 1:A:209:VAL:CG2  | 2.36                     | 0.55              |
| 1:C:166:ALA:HA   | 1:C:169:ALA:HB3  | 1.89                     | 0.55              |
| 1:C:183:GLU:HB2  | 1:C:185:ARG:CZ   | 2.36                     | 0.55              |
| 1:C:207:GLU:CA   | 1:C:210:GLU:HG2  | 2.33                     | 0.55              |
| 1:C:274:ASN:N    | 1:C:299:SER:O    | 2.36                     | 0.55              |
| 1:D:318:GLU:O    | 1:D:348:LEU:HD12 | 2.05                     | 0.55              |
| 1:D:370:LEU:HD23 | 1:D:370:LEU:C    | 2.31                     | 0.55              |
| 1:A:176:ASN:O    | 1:A:177:TYR:HB3  | 2.06                     | 0.55              |
| 1:A:236:PRO:C    | 1:A:238:LEU:H    | 2.14                     | 0.55              |
| 1:A:268:LEU:HA   | 1:A:293:LEU:HA   | 1.89                     | 0.55              |
| 1:B:271:ASN:HA   | 1:B:297:ASN:HB2  | 1.87                     | 0.55              |
| 1:C:235:ASP:HB3  | 1:C:236:PRO:HD2  | 1.89                     | 0.55              |
| 1:C:260:ILE:C    | 1:C:262:GLU:N    | 2.65                     | 0.55              |
| 1:D:268:LEU:O    | 1:D:293:LEU:HD12 | 2.05                     | 0.55              |
| 1:C:194:SER:O    | 1:C:196:PRO:HD3  | 2.07                     | 0.55              |
| 1:A:329:ASP:C    | 1:A:331:PHE:N    | 2.62                     | 0.55              |
| 1:B:351:LEU:CB   | 1:B:356:LEU:HD11 | 2.34                     | 0.55              |
| 1:A:140:GLN:O    | 1:A:143:CYS:HB3  | 2.06                     | 0.55              |
| 1:C:155:GLU:O    | 1:C:158:ARG:HG2  | 2.07                     | 0.55              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:315:LEU:HB2  | 1:C:317:LEU:CD2  | 2.36                     | 0.55              |
| 1:A:131:ASP:HB3  | 1:A:134:TRP:HB3  | 1.88                     | 0.55              |
| 1:A:343:GLU:HG3  | 1:A:344:ARG:HD2  | 1.89                     | 0.55              |
| 1:A:260:ILE:HG23 | 1:A:264:ILE:O    | 2.07                     | 0.55              |
| 1:D:341:ILE:HG22 | 1:D:348:LEU:HD22 | 1.89                     | 0.55              |
| 1:A:139:ILE:HB   | 1:A:147:PHE:CZ   | 2.41                     | 0.54              |
| 1:C:182:ARG:HB3  | 1:C:185:ARG:NH2  | 2.21                     | 0.54              |
| 1:C:252:SER:H    | 1:C:254:ALA:H    | 1.54                     | 0.54              |
| 1:A:238:LEU:HD11 | 1:A:243:ILE:HG22 | 1.89                     | 0.54              |
| 1:B:258:ARG:NH1  | 1:B:289:LYS:HE3  | 2.22                     | 0.54              |
| 1:A:181:ASP:OD1  | 1:A:185:ARG:N    | 2.39                     | 0.54              |
| 1:A:325:ASN:HD22 | 1:A:325:ASN:N    | 2.03                     | 0.54              |
| 1:C:118:ASN:C    | 1:C:165:ASP:HA   | 2.32                     | 0.54              |
| 1:C:148:THR:OG1  | 1:C:149:PRO:HD2  | 2.07                     | 0.54              |
| 1:C:320:LEU:C    | 1:C:321:TRP:HD1  | 2.15                     | 0.54              |
| 1:D:239:VAL:O    | 1:D:241:GLN:N    | 2.33                     | 0.54              |
| 1:D:258:ARG:HA   | 1:D:258:ARG:HH21 | 1.73                     | 0.54              |
| 1:A:215:ILE:HD11 | 1:A:238:LEU:HB2  | 1.89                     | 0.54              |
| 1:A:286:ILE:HD11 | 1:A:293:LEU:HD22 | 1.89                     | 0.54              |
| 1:B:344:ARG:HD2  | 1:B:344:ARG:H    | 1.72                     | 0.54              |
| 1:A:177:TYR:HA   | 1:A:186:ARG:HB3  | 1.88                     | 0.54              |
| 1:A:308:GLU:O    | 1:A:310:ASP:N    | 2.40                     | 0.54              |
| 1:B:324:GLY:N    | 1:C:177:TYR:CD1  | 2.75                     | 0.54              |
| 1:C:315:LEU:CD1  | 1:C:317:LEU:HD21 | 2.37                     | 0.54              |
| 1:A:301:ASN:O    | 1:A:303:LEU:N    | 2.39                     | 0.54              |
| 1:B:298:LEU:C    | 1:B:301:ASN:HD21 | 2.16                     | 0.54              |
| 1:B:264:ILE:N    | 1:B:265:PRO:HD3  | 2.23                     | 0.54              |
| 1:B:304:LYS:HD3  | 1:B:326:SER:CB   | 2.36                     | 0.54              |
| 1:B:337:TYR:CE1  | 1:B:341:ILE:HD13 | 2.43                     | 0.54              |
| 1:C:137:SER:O    | 1:C:140:GLN:HG2  | 2.08                     | 0.54              |
| 1:D:257:LEU:CD1  | 1:D:283:MET:HA   | 2.37                     | 0.54              |
| 1:C:226:ALA:HB2  | 1:C:269:SER:HB3  | 1.90                     | 0.54              |
| 1:A:277:LEU:HG   | 1:A:301:ASN:CG   | 2.33                     | 0.53              |
| 1:C:122:ILE:HD12 | 1:C:191:ILE:HG12 | 1.90                     | 0.53              |
| 1:C:151:GLU:HG2  | 1:C:162:PHE:HD1  | 1.70                     | 0.53              |
| 1:C:228:ASP:HA   | 1:C:271:ASN:HB3  | 1.91                     | 0.53              |
| 1:C:344:ARG:C    | 1:C:346:PRO:HD3  | 2.34                     | 0.53              |
| 1:A:239:VAL:O    | 1:A:240:ALA:HB3  | 2.08                     | 0.53              |
| 1:C:315:LEU:HB2  | 1:C:317:LEU:HD23 | 1.91                     | 0.53              |
| 1:D:288:GLN:H    | 1:D:288:GLN:NE2  | 2.06                     | 0.53              |
| 1:C:218:LYS:O    | 1:C:219:ARG:CG   | 2.57                     | 0.53              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:308:GLU:C    | 1:A:310:ASP:N    | 2.65                     | 0.53              |
| 1:A:325:ASN:O    | 1:A:327:LEU:HG   | 2.08                     | 0.53              |
| 1:B:262:GLU:HA   | 1:B:262:GLU:OE2  | 2.07                     | 0.53              |
| 1:C:201:LEU:H    | 1:C:201:LEU:CD2  | 2.09                     | 0.53              |
| 1:C:234:SER:O    | 1:C:235:ASP:CG   | 2.52                     | 0.53              |
| 1:B:257:LEU:HD12 | 1:B:286:ILE:HD12 | 1.90                     | 0.53              |
| 1:C:241:GLN:CD   | 1:C:243:ILE:CG1  | 2.82                     | 0.53              |
| 1:C:113:ASP:C    | 1:C:115:THR:H    | 2.17                     | 0.53              |
| 1:C:183:GLU:H    | 1:C:185:ARG:HH21 | 1.52                     | 0.53              |
| 1:C:237:ASP:OD1  | 1:C:241:GLN:HB3  | 2.09                     | 0.53              |
| 1:C:320:LEU:C    | 1:C:321:TRP:CD1  | 2.87                     | 0.53              |
| 1:D:283:MET:HE2  | 1:D:312:ILE:HG21 | 1.90                     | 0.53              |
| 1:A:258:ARG:NH1  | 1:A:262:GLU:OE1  | 2.41                     | 0.53              |
| 1:A:344:ARG:HD2  | 1:A:344:ARG:H    | 1.74                     | 0.53              |
| 1:C:237:ASP:O    | 1:C:238:LEU:HD22 | 2.07                     | 0.53              |
| 1:B:230:LYS:HB2  | 1:B:271:ASN:ND2  | 2.19                     | 0.53              |
| 1:C:224:GLN:O    | 1:C:225:GLN:C    | 2.52                     | 0.53              |
| 1:D:297:ASN:ND2  | 1:D:321:TRP:HB3  | 2.24                     | 0.53              |
| 1:D:333:ASP:OD2  | 1:D:336:THR:HB   | 2.09                     | 0.53              |
| 1:A:280:LEU:CD1  | 1:A:308:GLU:HB3  | 2.38                     | 0.53              |
| 1:D:216:MET:SD   | 1:D:259:ILE:HD12 | 2.49                     | 0.53              |
| 1:A:312:ILE:HG22 | 1:A:315:LEU:HB2  | 1.90                     | 0.53              |
| 1:B:205:LYS:CG   | 1:B:208:GLN:HG3  | 2.34                     | 0.53              |
| 1:C:310:ASP:HB3  | 1:C:344:ARG:HH11 | 1.74                     | 0.53              |
| 1:D:317:LEU:HB2  | 1:D:345:PHE:CD2  | 2.44                     | 0.52              |
| 1:D:365:GLU:O    | 1:D:366:ALA:HB3  | 2.08                     | 0.52              |
| 1:A:155:GLU:HB3  | 1:A:158:ARG:HB2  | 1.90                     | 0.52              |
| 1:A:180:LEU:HD21 | 1:A:184:ASN:HA   | 1.89                     | 0.52              |
| 1:A:182:ARG:H    | 1:A:182:ARG:HE   | 1.56                     | 0.52              |
| 1:A:210:GLU:HG3  | 1:D:361:ALA:HB2  | 1.92                     | 0.52              |
| 1:B:293:LEU:HD12 | 1:B:294:LYS:N    | 2.24                     | 0.52              |
| 1:A:199:THR:H    | 1:A:201:LEU:HD12 | 1.74                     | 0.52              |
| 1:A:208:GLN:O    | 1:A:211:GLN:HB2  | 2.09                     | 0.52              |
| 1:B:211:GLN:HE21 | 1:B:215:ILE:CD1  | 2.21                     | 0.52              |
| 1:B:222:GLY:O    | 1:B:225:GLN:HG3  | 2.08                     | 0.52              |
| 1:D:207:GLU:CD   | 1:D:207:GLU:N    | 2.68                     | 0.52              |
| 1:D:333:ASP:OD1  | 1:D:335:SER:HB2  | 2.10                     | 0.52              |
| 1:A:303:LEU:HB2  | 1:A:325:ASN:HB3  | 1.91                     | 0.52              |
| 1:B:295:ILE:HG23 | 1:B:319:GLU:CD   | 2.34                     | 0.52              |
| 1:C:151:GLU:HG3  | 1:C:152:PHE:N    | 2.23                     | 0.52              |
| 1:A:141:SER:C    | 1:A:143:CYS:N    | 2.65                     | 0.52              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:214:LEU:HD21 | 1:D:360:ILE:HG23 | 1.90                     | 0.52              |
| 1:A:230:LYS:CE   | 1:A:273:SER:HB3  | 2.40                     | 0.52              |
| 1:B:235:ASP:OD1  | 1:B:238:LEU:HB2  | 2.09                     | 0.52              |
| 1:C:267:LEU:HD12 | 1:C:268:LEU:H    | 1.75                     | 0.52              |
| 1:A:208:GLN:HG2  | 1:A:211:GLN:NE2  | 2.25                     | 0.52              |
| 1:B:322:LEU:HD12 | 1:B:341:ILE:HD11 | 1.90                     | 0.52              |
| 1:D:310:ASP:HA   | 1:D:344:ARG:HG2  | 1.91                     | 0.52              |
| 1:A:167:SER:HA   | 1:A:170:SER:HB2  | 1.92                     | 0.52              |
| 1:A:285:SER:C    | 1:A:287:VAL:N    | 2.67                     | 0.52              |
| 1:B:295:ILE:HG23 | 1:B:319:GLU:OE1  | 2.09                     | 0.52              |
| 1:C:121:LYS:HE2  | 1:C:162:PHE:CZ   | 2.45                     | 0.52              |
| 1:C:175:VAL:HG12 | 1:C:175:VAL:O    | 2.10                     | 0.52              |
| 1:D:204:LEU:HG   | 1:D:208:GLN:NE2  | 2.25                     | 0.52              |
| 1:A:200:ILE:O    | 1:A:201:LEU:C    | 2.52                     | 0.52              |
| 1:B:215:ILE:HD11 | 1:B:238:LEU:HD13 | 1.92                     | 0.52              |
| 1:B:236:PRO:O    | 1:B:240:ALA:HB2  | 2.09                     | 0.52              |
| 1:B:261:GLU:O    | 1:B:265:PRO:HG3  | 2.09                     | 0.52              |
| 1:B:334:GLN:HE22 | 1:B:351:LEU:HD23 | 1.73                     | 0.52              |
| 1:C:309:LEU:HD11 | 1:C:322:LEU:HD13 | 1.91                     | 0.52              |
| 1:D:261:GLU:HB2  | 1:D:289:LYS:CG   | 2.40                     | 0.52              |
| 1:A:118:ASN:O    | 1:A:164:GLU:O    | 2.27                     | 0.52              |
| 1:A:323:ASP:OD1  | 1:A:324:GLY:N    | 2.43                     | 0.52              |
| 1:B:207:GLU:O    | 1:B:208:GLN:C    | 2.53                     | 0.52              |
| 1:B:255:ALA:N    | 1:B:258:ARG:HB2  | 2.25                     | 0.52              |
| 1:B:277:LEU:HG   | 1:B:301:ASN:HB3  | 1.92                     | 0.52              |
| 1:B:279:ARG:C    | 1:B:281:ASP:N    | 2.65                     | 0.52              |
| 1:C:341:ILE:O    | 1:C:341:ILE:CG2  | 2.55                     | 0.52              |
| 1:A:182:ARG:C    | 1:A:184:ASN:H    | 2.16                     | 0.51              |
| 1:B:351:LEU:H    | 1:B:356:LEU:HG   | 1.75                     | 0.51              |
| 1:C:102:PRO:CB   | 1:C:103:PRO:HD3  | 2.34                     | 0.51              |
| 1:C:166:ALA:HA   | 1:C:169:ALA:CB   | 2.40                     | 0.51              |
| 1:C:362:PHE:CD1  | 1:C:362:PHE:N    | 2.79                     | 0.51              |
| 1:D:219:ARG:HH12 | 1:D:232:LEU:HA   | 1.75                     | 0.51              |
| 1:D:358:PRO:HG2  | 1:D:360:ILE:O    | 2.09                     | 0.51              |
| 1:A:309:LEU:HD12 | 1:A:345:PHE:CZ   | 2.45                     | 0.51              |
| 1:B:248:ASN:H    | 1:B:248:ASN:HD22 | 1.53                     | 0.51              |
| 1:D:275:ASN:O    | 1:D:276:ARG:C    | 2.53                     | 0.51              |
| 1:A:270:LEU:HD11 | 1:A:272:LEU:HD21 | 1.91                     | 0.51              |
| 1:A:297:ASN:C    | 1:A:297:ASN:HD22 | 2.18                     | 0.51              |
| 1:C:267:LEU:HD12 | 1:C:268:LEU:N    | 2.24                     | 0.51              |
| 1:D:238:LEU:O    | 1:D:242:ASN:ND2  | 2.38                     | 0.51              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:369:THR:CG2  | 1:D:370:LEU:H    | 2.19                     | 0.51              |
| 1:A:181:ASP:OD2  | 1:A:183:GLU:HB2  | 2.11                     | 0.51              |
| 1:B:207:GLU:O    | 1:B:210:GLU:N    | 2.34                     | 0.51              |
| 1:B:280:LEU:HD11 | 1:B:298:LEU:CD1  | 2.41                     | 0.51              |
| 1:B:338:ILE:HA   | 1:B:341:ILE:HG22 | 1.91                     | 0.51              |
| 1:C:175:VAL:CG1  | 1:C:179:ILE:HG12 | 2.40                     | 0.51              |
| 1:C:183:GLU:N    | 1:C:185:ARG:NH2  | 2.48                     | 0.51              |
| 1:C:287:VAL:CG1  | 1:C:314:GLY:HA3  | 2.39                     | 0.51              |
| 1:C:297:ASN:HD22 | 1:C:297:ASN:C    | 2.17                     | 0.51              |
| 1:D:327:LEU:O    | 1:D:330:THR:HB   | 2.10                     | 0.51              |
| 1:A:158:ARG:NH2  | 1:A:206:PRO:CD   | 2.74                     | 0.51              |
| 1:A:230:LYS:HE2  | 1:A:273:SER:HB3  | 1.92                     | 0.51              |
| 1:D:365:GLU:C    | 1:D:365:GLU:OE2  | 2.54                     | 0.51              |
| 1:B:287:VAL:HG22 | 1:B:315:LEU:HG   | 1.92                     | 0.51              |
| 1:C:124:ILE:HG12 | 1:C:189:ILE:HG23 | 1.92                     | 0.51              |
| 1:A:128:ARG:HA   | 1:A:154:TYR:CE2  | 2.46                     | 0.51              |
| 1:A:349:LEU:O    | 1:A:356:LEU:HB2  | 2.11                     | 0.51              |
| 1:B:277:LEU:O    | 1:B:302:GLU:N    | 2.43                     | 0.51              |
| 1:C:261:GLU:C    | 1:C:265:PRO:HG3  | 2.36                     | 0.51              |
| 1:C:301:ASN:O    | 1:C:303:LEU:N    | 2.43                     | 0.51              |
| 1:C:312:ILE:HG13 | 1:C:345:PHE:CZ   | 2.44                     | 0.51              |
| 1:D:225:GLN:HB2  | 1:D:268:LEU:HG   | 1.93                     | 0.51              |
| 1:D:261:GLU:HB2  | 1:D:289:LYS:HB3  | 1.93                     | 0.51              |
| 1:D:204:LEU:C    | 1:D:205:LYS:HD2  | 2.36                     | 0.51              |
| 1:A:153:HIS:HD2  | 1:A:160:GLN:O    | 1.94                     | 0.51              |
| 1:A:165:ASP:HB3  | 1:A:168:THR:OG1  | 2.09                     | 0.51              |
| 1:A:308:GLU:C    | 1:A:310:ASP:H    | 2.18                     | 0.51              |
| 1:B:261:GLU:HB2  | 1:B:289:LYS:HD3  | 1.89                     | 0.51              |
| 1:C:333:ASP:HB2  | 1:C:335:SER:OG   | 2.11                     | 0.51              |
| 1:D:253:MET:O    | 1:D:256:THR:HB   | 2.11                     | 0.51              |
| 1:B:211:GLN:O    | 1:B:215:ILE:N    | 2.44                     | 0.50              |
| 1:B:304:LYS:CD   | 1:B:326:SER:HB2  | 2.40                     | 0.50              |
| 1:B:327:LEU:C    | 1:B:327:LEU:CD1  | 2.84                     | 0.50              |
| 1:C:126:TYR:N    | 1:C:126:TYR:CD2  | 2.77                     | 0.50              |
| 1:A:278:TYR:CE1  | 1:A:279:ARG:HG2  | 2.46                     | 0.50              |
| 1:A:288:GLN:NE2  | 1:B:288:GLN:NE2  | 2.59                     | 0.50              |
| 1:C:243:ILE:HG13 | 1:C:243:ILE:O    | 2.12                     | 0.50              |
| 1:C:280:LEU:HD21 | 1:C:303:LEU:HD21 | 1.94                     | 0.50              |
| 1:D:331:PHE:HD2  | 1:D:336:THR:CG2  | 2.21                     | 0.50              |
| 1:A:268:LEU:CD2  | 1:A:294:LYS:HG2  | 2.41                     | 0.50              |
| 1:C:235:ASP:C    | 1:C:238:LEU:HD23 | 2.37                     | 0.50              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:283:MET:O    | 1:D:286:ILE:CG2  | 2.60                     | 0.50              |
| 1:C:132:LYS:O    | 1:C:135:LEU:HB3  | 2.10                     | 0.50              |
| 1:C:277:LEU:HG   | 1:C:301:ASN:CG   | 2.35                     | 0.50              |
| 1:C:283:MET:HE2  | 1:C:312:ILE:CG2  | 2.42                     | 0.50              |
| 1:C:289:LYS:C    | 1:C:291:PRO:HD3  | 2.37                     | 0.50              |
| 1:C:330:THR:HB   | 1:C:331:PHE:CD1  | 2.45                     | 0.50              |
| 1:A:287:VAL:HG23 | 1:A:315:LEU:HA   | 1.94                     | 0.50              |
| 1:B:320:LEU:HD21 | 1:B:322:LEU:HD11 | 1.94                     | 0.50              |
| 1:A:138:MET:HB3  | 1:A:179:ILE:HD13 | 1.94                     | 0.50              |
| 1:A:297:ASN:ND2  | 1:A:299:SER:CB   | 2.74                     | 0.50              |
| 1:B:264:ILE:HG22 | 1:B:264:ILE:O    | 2.12                     | 0.50              |
| 1:C:267:LEU:HD12 | 1:C:269:SER:H    | 1.76                     | 0.50              |
| 1:C:105:ARG:O    | 1:C:107:GLY:N    | 2.44                     | 0.50              |
| 1:C:118:ASN:ND2  | 1:C:165:ASP:HB2  | 2.27                     | 0.50              |
| 1:C:195:ALA:O    | 1:C:196:PRO:C    | 2.55                     | 0.50              |
| 1:D:212:LEU:O    | 1:D:215:ILE:HB   | 2.12                     | 0.50              |
| 1:D:278:TYR:HD2  | 1:D:279:ARG:H    | 1.59                     | 0.50              |
| 1:D:360:ILE:HD13 | 1:D:365:GLU:CB   | 2.42                     | 0.50              |
| 1:A:167:SER:HA   | 1:A:170:SER:CB   | 2.42                     | 0.50              |
| 1:A:336:THR:O    | 1:A:340:ALA:N    | 2.34                     | 0.50              |
| 1:B:300:GLY:O    | 1:B:301:ASN:C    | 2.55                     | 0.50              |
| 1:C:118:ASN:HD22 | 1:C:165:ASP:HB2  | 1.76                     | 0.50              |
| 1:C:326:SER:C    | 1:C:328:CYS:N    | 2.68                     | 0.50              |
| 1:D:360:ILE:HG12 | 1:D:364:VAL:C    | 2.37                     | 0.50              |
| 1:C:204:LEU:HA   | 1:C:208:GLN:HE22 | 1.65                     | 0.50              |
| 1:B:235:ASP:O    | 1:B:239:VAL:HB   | 2.12                     | 0.49              |
| 1:C:233:ARG:HH11 | 1:C:246:VAL:CG2  | 2.25                     | 0.49              |
| 1:D:212:LEU:O    | 1:D:213:LYS:C    | 2.54                     | 0.49              |
| 1:D:273:SER:HB2  | 1:D:299:SER:HB2  | 1.94                     | 0.49              |
| 1:D:313:LYS:O    | 1:D:314:GLY:O    | 2.29                     | 0.49              |
| 1:B:321:TRP:CH2  | 1:B:353:GLY:HA3  | 2.47                     | 0.49              |
| 1:C:205:LYS:N    | 1:C:208:GLN:CD   | 2.70                     | 0.49              |
| 1:C:241:GLN:O    | 1:C:242:ASN:HB2  | 2.13                     | 0.49              |
| 1:D:365:GLU:OE2  | 1:D:366:ALA:N    | 2.45                     | 0.49              |
| 1:A:119:TRP:C    | 1:A:120:PHE:CD1  | 2.91                     | 0.49              |
| 1:A:204:LEU:HD22 | 1:A:208:GLN:NE2  | 2.26                     | 0.49              |
| 1:A:213:LYS:HG3  | 1:A:259:ILE:HG21 | 1.94                     | 0.49              |
| 1:B:287:VAL:HG12 | 1:B:287:VAL:O    | 2.12                     | 0.49              |
| 1:C:233:ARG:NH1  | 1:C:249:ARG:NH2  | 2.61                     | 0.49              |
| 1:A:140:GLN:HE22 | 1:A:147:PHE:H    | 1.58                     | 0.49              |
| 1:B:216:MET:CE   | 1:B:259:ILE:HD12 | 2.41                     | 0.49              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:267:LEU:HD21 | 1:B:270:LEU:CD1  | 2.42                     | 0.49              |
| 1:C:177:TYR:CD1  | 1:C:188:SER:HB3  | 2.48                     | 0.49              |
| 1:D:270:LEU:O    | 1:D:296:LEU:HA   | 2.11                     | 0.49              |
| 1:B:366:ALA:N    | 1:B:367:PRO:CD   | 2.75                     | 0.49              |
| 1:C:212:LEU:C    | 1:C:214:LEU:N    | 2.69                     | 0.49              |
| 1:D:281:ASP:CA   | 1:D:311:LYS:HD2  | 2.41                     | 0.49              |
| 1:A:169:ALA:O    | 1:A:172:LEU:HB2  | 2.13                     | 0.49              |
| 1:C:110:THR:HG22 | 1:C:110:THR:O    | 2.12                     | 0.49              |
| 1:C:151:GLU:HG2  | 1:C:162:PHE:CE1  | 2.47                     | 0.49              |
| 1:C:273:SER:HA   | 1:C:299:SER:O    | 2.13                     | 0.49              |
| 1:C:313:LYS:HG3  | 1:C:314:GLY:N    | 2.27                     | 0.49              |
| 1:C:344:ARG:NH1  | 1:C:344:ARG:CG   | 2.76                     | 0.49              |
| 1:A:271:ASN:ND2  | 1:A:273:SER:N    | 2.61                     | 0.49              |
| 1:C:163:VAL:CG1  | 1:C:164:GLU:N    | 2.75                     | 0.49              |
| 1:C:168:THR:O    | 1:C:172:LEU:HD13 | 2.13                     | 0.49              |
| 1:C:186:ARG:O    | 1:C:187:ILE:HG13 | 2.13                     | 0.49              |
| 1:C:233:ARG:HH12 | 1:C:249:ARG:HH22 | 1.58                     | 0.49              |
| 1:C:270:LEU:HG   | 1:C:271:ASN:N    | 2.27                     | 0.49              |
| 1:D:241:GLN:HE22 | 1:D:243:ILE:CG1  | 2.16                     | 0.49              |
| 1:A:283:MET:C    | 1:A:285:SER:H    | 2.17                     | 0.49              |
| 1:B:323:ASP:HB3  | 1:C:177:TYR:CD2  | 2.48                     | 0.49              |
| 1:C:143:CYS:SG   | 1:C:172:LEU:HG   | 2.53                     | 0.49              |
| 1:C:155:GLU:OE2  | 1:C:158:ARG:HD2  | 2.12                     | 0.49              |
| 1:C:163:VAL:HG12 | 1:C:165:ASP:N    | 2.28                     | 0.49              |
| 1:C:241:GLN:CD   | 1:C:243:ILE:HG12 | 2.38                     | 0.49              |
| 1:D:358:PRO:C    | 1:D:360:ILE:N    | 2.65                     | 0.49              |
| 1:A:230:LYS:HZ3  | 1:A:271:ASN:CG   | 2.20                     | 0.49              |
| 1:B:220:TYR:CE1  | 1:B:264:ILE:HG21 | 2.48                     | 0.49              |
| 1:C:131:ASP:O    | 1:C:135:LEU:HB2  | 2.13                     | 0.49              |
| 1:C:204:LEU:CA   | 1:C:208:GLN:NE2  | 2.59                     | 0.49              |
| 1:D:279:ARG:O    | 1:D:280:LEU:CG   | 2.60                     | 0.49              |
| 1:A:128:ARG:HA   | 1:A:154:TYR:HE2  | 1.78                     | 0.49              |
| 1:A:139:ILE:HB   | 1:A:147:PHE:HZ   | 1.77                     | 0.49              |
| 1:B:323:ASP:O    | 1:C:186:ARG:NH1  | 2.46                     | 0.49              |
| 1:D:272:LEU:HB2  | 1:D:298:LEU:HD23 | 1.95                     | 0.49              |
| 1:A:150:ILE:C    | 1:A:151:GLU:HG2  | 2.38                     | 0.48              |
| 1:A:321:TRP:O    | 1:A:322:LEU:HG   | 2.13                     | 0.48              |
| 1:A:344:ARG:H    | 1:A:344:ARG:CD   | 2.26                     | 0.48              |
| 1:B:211:GLN:O    | 1:B:214:LEU:HB3  | 2.12                     | 0.48              |
| 1:C:214:LEU:O    | 1:C:217:SER:N    | 2.45                     | 0.48              |
| 1:C:260:ILE:O    | 1:C:262:GLU:N    | 2.46                     | 0.48              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:333:ASP:C    | 1:C:335:SER:N    | 2.71                     | 0.48              |
| 1:A:182:ARG:C    | 1:A:184:ASN:N    | 2.69                     | 0.48              |
| 1:C:138:MET:HE2  | 1:C:138:MET:HA   | 1.94                     | 0.48              |
| 1:C:285:SER:O    | 1:C:289:LYS:HG3  | 2.12                     | 0.48              |
| 1:D:280:LEU:HD12 | 1:D:308:GLU:C    | 2.38                     | 0.48              |
| 1:A:196:PRO:O    | 1:A:198:HIS:N    | 2.46                     | 0.48              |
| 1:C:279:ARG:C    | 1:C:281:ASP:H    | 2.21                     | 0.48              |
| 1:D:281:ASP:O    | 1:D:283:MET:N    | 2.47                     | 0.48              |
| 1:A:257:LEU:HD11 | 1:A:283:MET:CA   | 2.31                     | 0.48              |
| 1:A:271:ASN:HD22 | 1:A:272:LEU:N    | 2.10                     | 0.48              |
| 1:C:124:ILE:HD11 | 1:C:189:ILE:HD13 | 1.95                     | 0.48              |
| 1:C:204:LEU:HD13 | 1:C:255:ALA:HB2  | 1.94                     | 0.48              |
| 1:C:270:LEU:H    | 1:C:293:LEU:CD1  | 2.26                     | 0.48              |
| 1:A:214:LEU:O    | 1:A:217:SER:OG   | 2.28                     | 0.48              |
| 1:A:286:ILE:HG13 | 1:A:290:ALA:CB   | 2.39                     | 0.48              |
| 1:A:285:SER:C    | 1:A:287:VAL:H    | 2.22                     | 0.48              |
| 1:B:220:TYR:OH   | 1:B:225:GLN:HA   | 2.13                     | 0.48              |
| 1:C:122:ILE:CD1  | 1:C:191:ILE:HG23 | 2.42                     | 0.48              |
| 1:C:150:ILE:O    | 1:C:161:PHE:HB2  | 2.13                     | 0.48              |
| 1:C:200:ILE:HG22 | 1:C:202:ASN:OD1  | 2.14                     | 0.48              |
| 1:C:341:ILE:HD12 | 1:C:341:ILE:N    | 2.28                     | 0.48              |
| 1:A:227:LEU:CD1  | 1:A:229:LEU:HD21 | 2.43                     | 0.48              |
| 1:B:262:GLU:O    | 1:B:263:ASN:CG   | 2.57                     | 0.48              |
| 1:B:310:ASP:C    | 1:B:312:ILE:H    | 2.20                     | 0.48              |
| 1:A:236:PRO:HA   | 1:A:239:VAL:HB   | 1.95                     | 0.48              |
| 1:C:241:GLN:NE2  | 1:C:243:ILE:CG1  | 2.77                     | 0.48              |
| 1:C:267:LEU:CD1  | 1:C:269:SER:H    | 2.26                     | 0.48              |
| 1:C:282:ASP:OD1  | 1:C:283:MET:HG2  | 2.14                     | 0.48              |
| 1:B:209:VAL:HG12 | 1:B:259:ILE:HD11 | 1.96                     | 0.48              |
| 1:B:238:LEU:O    | 1:B:243:ILE:N    | 2.41                     | 0.48              |
| 1:B:268:LEU:HA   | 1:B:293:LEU:HA   | 1.96                     | 0.48              |
| 1:C:148:THR:HG23 | 1:C:149:PRO:N    | 2.29                     | 0.48              |
| 1:C:211:GLN:HG2  | 1:C:243:ILE:HD13 | 1.96                     | 0.48              |
| 1:C:222:GLY:O    | 1:C:223:SER:C    | 2.57                     | 0.48              |
| 1:D:257:LEU:HD11 | 1:D:283:MET:HB3  | 1.94                     | 0.48              |
| 1:A:122:ILE:HD13 | 1:A:163:VAL:HG23 | 1.96                     | 0.48              |
| 1:C:159:ALA:C    | 1:C:160:GLN:HG3  | 2.39                     | 0.48              |
| 1:C:246:VAL:HG12 | 1:C:249:ARG:H    | 1.79                     | 0.47              |
| 1:D:293:LEU:HD23 | 1:D:315:LEU:HD13 | 1.96                     | 0.47              |
| 1:A:277:LEU:O    | 1:A:301:ASN:HB3  | 2.13                     | 0.47              |
| 1:A:332:ARG:HE   | 1:A:333:ASP:HB3  | 1.78                     | 0.47              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:257:LEU:HA   | 1:B:260:ILE:HD12 | 1.96                     | 0.47              |
| 1:C:134:TRP:C    | 1:C:136:LEU:H    | 2.22                     | 0.47              |
| 1:A:208:GLN:HA   | 1:A:211:GLN:CG   | 2.44                     | 0.47              |
| 1:A:235:ASP:O    | 1:A:239:VAL:HG23 | 2.14                     | 0.47              |
| 1:A:355:GLU:O    | 1:A:357:PRO:HD3  | 2.14                     | 0.47              |
| 1:C:137:SER:O    | 1:C:141:SER:OG   | 2.31                     | 0.47              |
| 1:C:148:THR:HG23 | 1:C:149:PRO:CD   | 2.44                     | 0.47              |
| 1:C:296:LEU:HB3  | 1:C:317:LEU:CD1  | 2.44                     | 0.47              |
| 1:C:297:ASN:ND2  | 1:C:321:TRP:HB2  | 2.29                     | 0.47              |
| 1:C:342:ARG:HH12 | 1:C:359:PRO:HG3  | 1.78                     | 0.47              |
| 1:C:348:LEU:HG   | 1:C:349:LEU:N    | 2.28                     | 0.47              |
| 1:D:261:GLU:O    | 1:D:265:PRO:HG3  | 2.15                     | 0.47              |
| 1:D:339:SER:O    | 1:D:343:GLU:HG3  | 2.14                     | 0.47              |
| 1:D:371:PRO:CB   | 1:D:372:PRO:CD   | 2.93                     | 0.47              |
| 1:A:122:ILE:CD1  | 1:A:163:VAL:HG23 | 2.44                     | 0.47              |
| 1:A:152:PHE:HA   | 1:A:161:PHE:HB3  | 1.97                     | 0.47              |
| 1:A:216:MET:HE2  | 1:A:256:THR:HG23 | 1.96                     | 0.47              |
| 1:A:271:ASN:HD21 | 1:A:273:SER:HB2  | 1.79                     | 0.47              |
| 1:A:336:THR:HA   | 1:A:339:SER:CB   | 2.44                     | 0.47              |
| 1:C:238:LEU:HA   | 1:C:241:GLN:CG   | 2.44                     | 0.47              |
| 1:C:306:GLU:C    | 1:C:308:GLU:H    | 2.21                     | 0.47              |
| 1:D:288:GLN:NE2  | 1:D:288:GLN:N    | 2.61                     | 0.47              |
| 1:A:238:LEU:O    | 1:A:241:GLN:HB2  | 2.15                     | 0.47              |
| 1:C:235:ASP:HB3  | 1:C:236:PRO:CD   | 2.44                     | 0.47              |
| 1:C:320:LEU:HD11 | 1:C:322:LEU:CD2  | 2.44                     | 0.47              |
| 1:A:304:LYS:HG2  | 1:A:326:SER:CB   | 2.44                     | 0.47              |
| 1:B:298:LEU:CA   | 1:B:301:ASN:HD21 | 2.28                     | 0.47              |
| 1:C:131:ASP:C    | 1:C:135:LEU:HB2  | 2.39                     | 0.47              |
| 1:C:134:TRP:C    | 1:C:136:LEU:N    | 2.72                     | 0.47              |
| 1:A:173:LYS:CD   | 1:A:191:ILE:HG22 | 2.40                     | 0.47              |
| 1:B:248:ASN:ND2  | 1:B:248:ASN:N    | 2.58                     | 0.47              |
| 1:C:205:LYS:H    | 1:C:208:GLN:NE2  | 2.11                     | 0.47              |
| 1:C:250:ARG:CG   | 1:C:251:SER:H    | 2.27                     | 0.47              |
| 1:D:257:LEU:HD11 | 1:D:283:MET:CA   | 2.44                     | 0.47              |
| 1:D:261:GLU:HB2  | 1:D:289:LYS:CB   | 2.45                     | 0.47              |
| 1:D:323:ASP:C    | 1:D:325:ASN:N    | 2.66                     | 0.47              |
| 1:A:125:PRO:O    | 1:A:126:TYR:HB2  | 2.13                     | 0.47              |
| 1:A:179:ILE:HB   | 1:A:187:ILE:HD13 | 1.96                     | 0.47              |
| 1:C:110:THR:O    | 1:C:111:SER:HB2  | 2.14                     | 0.47              |
| 1:C:271:ASN:C    | 1:C:272:LEU:HG   | 2.40                     | 0.47              |
| 1:D:225:GLN:HG2  | 1:D:266:GLU:O    | 2.14                     | 0.47              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:271:ASN:ND2  | 1:D:297:ASN:HB3  | 2.30                     | 0.47              |
| 1:A:168:THR:O    | 1:A:172:LEU:HD13 | 2.14                     | 0.47              |
| 1:C:283:MET:HE2  | 1:C:312:ILE:HG22 | 1.96                     | 0.47              |
| 1:C:336:THR:HA   | 1:C:339:SER:OG   | 2.15                     | 0.47              |
| 1:D:297:ASN:ND2  | 1:D:321:TRP:CB   | 2.78                     | 0.47              |
| 1:A:296:LEU:HG   | 1:A:298:LEU:HG   | 1.97                     | 0.47              |
| 1:A:336:THR:C    | 1:A:338:ILE:N    | 2.66                     | 0.47              |
| 1:A:295:ILE:CG2  | 1:A:296:LEU:N    | 2.77                     | 0.46              |
| 1:B:224:GLN:O    | 1:B:225:GLN:C    | 2.57                     | 0.46              |
| 1:B:262:GLU:O    | 1:B:262:GLU:HG3  | 2.15                     | 0.46              |
| 1:D:287:VAL:HG12 | 1:D:287:VAL:O    | 2.14                     | 0.46              |
| 1:D:347:LYS:HD3  | 1:D:347:LYS:N    | 2.18                     | 0.46              |
| 1:A:125:PRO:HB3  | 1:D:334:GLN:CG   | 2.45                     | 0.46              |
| 1:B:294:LYS:HB3  | 1:B:318:GLU:HG2  | 1.97                     | 0.46              |
| 1:B:362:PHE:O    | 1:B:363:ASP:HB3  | 2.16                     | 0.46              |
| 1:C:173:LYS:HB2  | 1:C:191:ILE:HD12 | 1.96                     | 0.46              |
| 1:C:177:TYR:HA   | 1:C:187:ILE:O    | 2.14                     | 0.46              |
| 1:C:299:SER:O    | 1:C:301:ASN:N    | 2.43                     | 0.46              |
| 1:C:320:LEU:HD11 | 1:C:322:LEU:HD21 | 1.98                     | 0.46              |
| 1:D:229:LEU:HB2  | 1:D:272:LEU:HD23 | 1.98                     | 0.46              |
| 1:D:310:ASP:OD2  | 1:D:344:ARG:NE   | 2.47                     | 0.46              |
| 1:D:335:SER:O    | 1:D:338:ILE:CG1  | 2.57                     | 0.46              |
| 1:A:120:PHE:O    | 1:A:162:PHE:HA   | 2.15                     | 0.46              |
| 1:A:342:ARG:HH22 | 1:A:356:LEU:HB3  | 1.80                     | 0.46              |
| 1:B:243:ILE:HG22 | 1:B:245:VAL:HG23 | 1.97                     | 0.46              |
| 1:C:121:LYS:HE2  | 1:C:162:PHE:CE2  | 2.51                     | 0.46              |
| 1:C:121:LYS:CD   | 1:C:194:SER:HB2  | 2.44                     | 0.46              |
| 1:D:297:ASN:CA   | 1:D:321:TRP:HB2  | 2.37                     | 0.46              |
| 1:A:309:LEU:HB3  | 1:A:345:PHE:CE1  | 2.50                     | 0.46              |
| 1:B:272:LEU:HD23 | 1:B:275:ASN:ND2  | 2.29                     | 0.46              |
| 1:A:235:ASP:C    | 1:A:236:PRO:O    | 2.58                     | 0.46              |
| 1:A:259:ILE:CG2  | 1:A:263:ASN:HD22 | 2.27                     | 0.46              |
| 1:A:342:ARG:NH2  | 1:A:359:PRO:HG3  | 2.29                     | 0.46              |
| 1:B:212:LEU:HG   | 1:B:216:MET:HE2  | 1.97                     | 0.46              |
| 1:B:267:LEU:HD21 | 1:B:270:LEU:HD12 | 1.97                     | 0.46              |
| 1:C:335:SER:HA   | 1:C:338:ILE:HD11 | 1.96                     | 0.46              |
| 1:D:208:GLN:O    | 1:D:211:GLN:HB3  | 2.15                     | 0.46              |
| 1:A:200:ILE:CG2  | 1:A:202:ASN:HD21 | 2.27                     | 0.46              |
| 1:A:216:MET:SD   | 1:A:259:ILE:HD12 | 2.56                     | 0.46              |
| 1:B:214:LEU:HD12 | 1:B:214:LEU:O    | 2.14                     | 0.46              |
| 1:B:338:ILE:O    | 1:B:342:ARG:HB2  | 2.14                     | 0.46              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:306:GLU:C    | 1:C:308:GLU:N    | 2.72                     | 0.46              |
| 1:A:113:ASP:C    | 1:A:115:THR:H    | 2.23                     | 0.46              |
| 1:A:158:ARG:HH22 | 1:A:205:LYS:HE3  | 1.80                     | 0.46              |
| 1:A:263:ASN:C    | 1:A:265:PRO:HD3  | 2.41                     | 0.46              |
| 1:B:328:CYS:HB2  | 1:C:177:TYR:OH   | 2.16                     | 0.46              |
| 1:C:232:LEU:HD22 | 1:C:247:LEU:HG   | 1.98                     | 0.46              |
| 1:C:313:LYS:HD2  | 1:C:313:LYS:C    | 2.41                     | 0.46              |
| 1:A:224:GLN:O    | 1:A:225:GLN:C    | 2.58                     | 0.46              |
| 1:A:264:ILE:N    | 1:A:264:ILE:HD12 | 2.30                     | 0.46              |
| 1:A:275:ASN:HB2  | 1:A:277:LEU:CD2  | 2.46                     | 0.46              |
| 1:C:272:LEU:HD11 | 1:C:296:LEU:HD11 | 1.98                     | 0.46              |
| 1:D:258:ARG:HH21 | 1:D:258:ARG:CA   | 2.29                     | 0.46              |
| 1:A:140:GLN:NE2  | 1:A:147:PHE:CD2  | 2.84                     | 0.46              |
| 1:B:230:LYS:HD2  | 1:B:274:ASN:ND2  | 2.31                     | 0.46              |
| 1:C:315:LEU:HD12 | 1:C:317:LEU:CG   | 2.46                     | 0.46              |
| 1:C:286:ILE:O    | 1:C:289:LYS:N    | 2.42                     | 0.45              |
| 1:A:128:ARG:C    | 1:A:130:TYR:H    | 2.24                     | 0.45              |
| 1:A:173:LYS:HD3  | 1:A:191:ILE:CG2  | 2.38                     | 0.45              |
| 1:B:338:ILE:CA   | 1:B:341:ILE:HG22 | 2.46                     | 0.45              |
| 1:C:184:ASN:C    | 1:C:185:ARG:HG3  | 2.41                     | 0.45              |
| 1:C:200:ILE:O    | 1:C:202:ASN:OD1  | 2.35                     | 0.45              |
| 1:C:248:ASN:ND2  | 1:C:249:ARG:HG3  | 2.31                     | 0.45              |
| 1:C:278:TYR:HB3  | 1:C:302:GLU:O    | 2.17                     | 0.45              |
| 1:D:278:TYR:HD2  | 1:D:279:ARG:N    | 2.14                     | 0.45              |
| 1:A:293:LEU:HB3  | 1:A:315:LEU:HD21 | 1.99                     | 0.45              |
| 1:B:247:LEU:CD1  | 1:B:277:LEU:HD21 | 2.46                     | 0.45              |
| 1:B:338:ILE:HA   | 1:B:341:ILE:CG2  | 2.46                     | 0.45              |
| 1:C:145:VAL:HB   | 1:C:168:THR:OG1  | 2.16                     | 0.45              |
| 1:C:214:LEU:C    | 1:C:216:MET:N    | 2.70                     | 0.45              |
| 1:C:270:LEU:CD1  | 1:C:271:ASN:H    | 2.29                     | 0.45              |
| 1:C:338:ILE:O    | 1:C:342:ARG:HB2  | 2.17                     | 0.45              |
| 1:D:210:GLU:O    | 1:D:214:LEU:HD13 | 2.16                     | 0.45              |
| 1:A:122:ILE:HD11 | 1:A:163:VAL:CG2  | 2.47                     | 0.45              |
| 1:A:320:LEU:CG   | 1:A:321:TRP:N    | 2.80                     | 0.45              |
| 1:B:364:VAL:HG13 | 1:B:364:VAL:O    | 2.16                     | 0.45              |
| 1:C:140:GLN:CG   | 1:C:141:SER:N    | 2.79                     | 0.45              |
| 1:C:150:ILE:HD12 | 1:C:161:PHE:CD1  | 2.52                     | 0.45              |
| 1:C:338:ILE:CG2  | 1:C:356:LEU:HD13 | 2.47                     | 0.45              |
| 1:B:211:GLN:OE1  | 1:B:214:LEU:HD23 | 2.17                     | 0.45              |
| 1:B:301:ASN:HD22 | 1:B:303:LEU:HD11 | 1.81                     | 0.45              |
| 1:C:214:LEU:O    | 1:C:215:ILE:C    | 2.59                     | 0.45              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:288:GLN:O    | 1:D:291:PRO:HD3  | 2.15                     | 0.45              |
| 1:A:247:LEU:O    | 1:A:253:MET:HB2  | 2.16                     | 0.45              |
| 1:A:280:LEU:HD13 | 1:A:312:ILE:CD1  | 2.42                     | 0.45              |
| 1:A:325:ASN:O    | 1:A:326:SER:C    | 2.60                     | 0.45              |
| 1:C:292:ASN:HB2  | 1:C:293:LEU:H    | 1.48                     | 0.45              |
| 1:D:223:SER:HB3  | 1:D:224:GLN:HE21 | 1.81                     | 0.45              |
| 1:A:121:LYS:NZ   | 1:A:160:GLN:NE2  | 2.65                     | 0.45              |
| 1:A:134:TRP:CH2  | 1:A:182:ARG:NH2  | 2.85                     | 0.45              |
| 1:A:334:GLN:O    | 1:A:338:ILE:HG13 | 2.17                     | 0.45              |
| 1:C:130:TYR:CD1  | 1:C:130:TYR:N    | 2.84                     | 0.45              |
| 1:C:327:LEU:HD12 | 1:C:327:LEU:O    | 2.16                     | 0.45              |
| 1:C:357:PRO:HA   | 1:C:358:PRO:HD3  | 1.83                     | 0.45              |
| 1:D:310:ASP:OD1  | 1:D:313:LYS:HD2  | 2.17                     | 0.45              |
| 1:A:268:LEU:HD23 | 1:A:294:LYS:H    | 1.80                     | 0.45              |
| 1:A:296:LEU:HD11 | 1:A:298:LEU:CD2  | 2.47                     | 0.45              |
| 1:C:286:ILE:HA   | 1:C:289:LYS:CB   | 2.43                     | 0.45              |
| 1:A:241:GLN:C    | 1:A:243:ILE:H    | 2.25                     | 0.45              |
| 1:A:245:VAL:HG12 | 1:A:247:LEU:HD23 | 1.98                     | 0.45              |
| 1:C:150:ILE:HD13 | 1:C:162:PHE:C    | 2.41                     | 0.45              |
| 1:A:134:TRP:CZ2  | 1:A:182:ARG:NH2  | 2.85                     | 0.45              |
| 1:A:171:ALA:C    | 1:A:172:LEU:HD12 | 2.42                     | 0.45              |
| 1:A:281:ASP:CA   | 1:A:284:SER:HB3  | 2.34                     | 0.45              |
| 1:A:342:ARG:CZ   | 1:A:356:LEU:HD13 | 2.46                     | 0.45              |
| 1:B:221:ASP:OD2  | 1:B:224:GLN:HG2  | 2.16                     | 0.45              |
| 1:C:286:ILE:O    | 1:C:286:ILE:HG12 | 2.17                     | 0.45              |
| 1:D:250:ARG:O    | 1:D:254:ALA:CB   | 2.65                     | 0.45              |
| 1:A:118:ASN:OD1  | 1:A:164:GLU:O    | 2.35                     | 0.44              |
| 1:A:286:ILE:CD1  | 1:A:293:LEU:HD22 | 2.46                     | 0.44              |
| 1:A:341:ILE:HG22 | 1:A:348:LEU:CD2  | 2.47                     | 0.44              |
| 1:A:119:TRP:CZ3  | 1:A:150:ILE:HD13 | 2.52                     | 0.44              |
| 1:A:182:ARG:HG2  | 1:A:183:GLU:H    | 1.82                     | 0.44              |
| 1:B:208:GLN:HE21 | 1:B:243:ILE:HG23 | 1.81                     | 0.44              |
| 1:D:279:ARG:O    | 1:D:280:LEU:CB   | 2.65                     | 0.44              |
| 1:A:132:LYS:HE3  | 1:A:152:PHE:CD2  | 2.43                     | 0.44              |
| 1:A:165:ASP:HB3  | 1:A:168:THR:CB   | 2.47                     | 0.44              |
| 1:A:191:ILE:CG2  | 1:A:191:ILE:O    | 2.63                     | 0.44              |
| 1:A:246:VAL:CG1  | 1:A:249:ARG:HB2  | 2.47                     | 0.44              |
| 1:A:292:ASN:O    | 1:A:293:LEU:C    | 2.60                     | 0.44              |
| 1:B:220:TYR:CG   | 1:B:221:ASP:N    | 2.85                     | 0.44              |
| 1:C:178:LYS:O    | 1:C:178:LYS:HG2  | 2.17                     | 0.44              |
| 1:C:186:ARG:C    | 1:C:187:ILE:HG13 | 2.42                     | 0.44              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:211:GLN:O    | 1:C:214:LEU:HB3  | 2.17                     | 0.44              |
| 1:C:276:ARG:HG3  | 1:C:276:ARG:HH21 | 1.82                     | 0.44              |
| 1:A:140:GLN:C    | 1:A:143:CYS:HB3  | 2.42                     | 0.44              |
| 1:A:295:ILE:HG22 | 1:A:296:LEU:N    | 2.33                     | 0.44              |
| 1:A:320:LEU:HG   | 1:A:321:TRP:N    | 2.32                     | 0.44              |
| 1:C:120:PHE:HB3  | 1:C:192:ASN:O    | 2.17                     | 0.44              |
| 1:C:315:LEU:HD12 | 1:C:317:LEU:HG   | 1.98                     | 0.44              |
| 1:A:119:TRP:HZ3  | 1:A:150:ILE:CD1  | 2.31                     | 0.44              |
| 1:A:228:ASP:OD1  | 1:A:230:LYS:HG2  | 2.17                     | 0.44              |
| 1:B:315:LEU:CD1  | 1:B:317:LEU:HD23 | 2.47                     | 0.44              |
| 1:C:124:ILE:CG1  | 1:C:189:ILE:HG23 | 2.48                     | 0.44              |
| 1:C:312:ILE:O    | 1:C:313:LYS:C    | 2.60                     | 0.44              |
| 1:A:153:HIS:CD2  | 1:A:160:GLN:O    | 2.71                     | 0.44              |
| 1:B:364:VAL:HA   | 1:B:367:PRO:HG2  | 2.00                     | 0.44              |
| 1:C:280:LEU:CD2  | 1:C:303:LEU:HD21 | 2.47                     | 0.44              |
| 1:D:356:LEU:HA   | 1:D:357:PRO:HD3  | 1.82                     | 0.44              |
| 1:A:172:LEU:C    | 1:A:174:ALA:H    | 2.25                     | 0.44              |
| 1:A:321:TRP:O    | 1:A:322:LEU:CB   | 2.65                     | 0.44              |
| 1:B:308:GLU:OE2  | 1:B:308:GLU:HA   | 2.18                     | 0.44              |
| 1:C:205:LYS:HA   | 1:C:206:PRO:HD3  | 1.83                     | 0.44              |
| 1:C:280:LEU:HG   | 1:C:308:GLU:HB3  | 1.99                     | 0.44              |
| 1:C:282:ASP:CG   | 1:C:283:MET:H    | 2.25                     | 0.44              |
| 1:C:305:SER:OG   | 1:C:307:ARG:HG3  | 2.17                     | 0.44              |
| 1:A:105:ARG:HG3  | 1:A:106:GLY:N    | 2.32                     | 0.44              |
| 1:A:212:LEU:CG   | 1:A:216:MET:HE3  | 2.48                     | 0.44              |
| 1:A:333:ASP:OD1  | 1:A:335:SER:HB2  | 2.17                     | 0.44              |
| 1:A:340:ALA:O    | 1:A:344:ARG:HD3  | 2.17                     | 0.44              |
| 1:A:344:ARG:HB2  | 1:A:345:PHE:CE1  | 2.53                     | 0.44              |
| 1:A:346:PRO:C    | 1:A:348:LEU:N    | 2.72                     | 0.44              |
| 1:B:334:GLN:HA   | 1:B:337:TYR:HB3  | 1.99                     | 0.44              |
| 1:C:340:ALA:C    | 1:C:342:ARG:H    | 2.26                     | 0.44              |
| 1:C:102:PRO:HB2  | 1:C:103:PRO:CD   | 2.43                     | 0.44              |
| 1:C:298:LEU:N    | 1:C:298:LEU:HD12 | 2.33                     | 0.44              |
| 1:C:304:LYS:HD3  | 1:C:326:SER:CB   | 2.48                     | 0.44              |
| 1:D:235:ASP:H    | 1:D:236:PRO:CD   | 2.30                     | 0.44              |
| 1:A:204:LEU:HD22 | 1:A:208:GLN:OE1  | 2.16                     | 0.43              |
| 1:A:249:ARG:HA   | 1:A:249:ARG:NE   | 2.28                     | 0.43              |
| 1:B:238:LEU:HD12 | 1:B:238:LEU:HA   | 1.81                     | 0.43              |
| 1:B:325:ASN:O    | 1:B:327:LEU:HG   | 2.18                     | 0.43              |
| 1:C:346:PRO:C    | 1:C:348:LEU:H    | 2.26                     | 0.43              |
| 1:D:210:GLU:O    | 1:D:214:LEU:CD1  | 2.66                     | 0.43              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:304:LYS:HG2  | 1:A:326:SER:OG   | 2.18                     | 0.43              |
| 1:A:324:GLY:C    | 1:A:325:ASN:HD22 | 2.26                     | 0.43              |
| 1:A:342:ARG:NH1  | 1:A:348:LEU:C    | 2.77                     | 0.43              |
| 1:C:272:LEU:CD1  | 1:C:296:LEU:HD11 | 2.48                     | 0.43              |
| 1:A:140:GLN:N    | 1:A:147:PHE:HE2  | 2.16                     | 0.43              |
| 1:A:176:ASN:C    | 1:A:178:LYS:N    | 2.73                     | 0.43              |
| 1:A:329:ASP:O    | 1:A:331:PHE:N    | 2.51                     | 0.43              |
| 1:C:105:ARG:O    | 1:C:106:GLY:C    | 2.61                     | 0.43              |
| 1:C:192:ASN:N    | 1:C:192:ASN:HD22 | 2.16                     | 0.43              |
| 1:C:203:GLU:O    | 1:C:203:GLU:HG3  | 2.17                     | 0.43              |
| 1:C:257:LEU:CD1  | 1:C:283:MET:HA   | 2.48                     | 0.43              |
| 1:D:287:VAL:HA   | 1:D:315:LEU:HD21 | 2.01                     | 0.43              |
| 1:A:153:HIS:NE2  | 1:A:160:GLN:HG3  | 2.34                     | 0.43              |
| 1:A:251:SER:O    | 1:A:255:ALA:N    | 2.38                     | 0.43              |
| 1:A:312:ILE:O    | 1:A:313:LYS:C    | 2.62                     | 0.43              |
| 1:C:177:TYR:HB3  | 1:C:186:ARG:HD3  | 1.99                     | 0.43              |
| 1:A:263:ASN:HB3  | 1:A:264:ILE:HD12 | 1.99                     | 0.43              |
| 1:A:294:LYS:O    | 1:A:295:ILE:HG13 | 2.19                     | 0.43              |
| 1:A:321:TRP:O    | 1:A:322:LEU:CG   | 2.66                     | 0.43              |
| 1:B:328:CYS:HB2  | 1:C:177:TYR:CE1  | 2.53                     | 0.43              |
| 1:C:148:THR:CB   | 1:C:149:PRO:HD2  | 2.48                     | 0.43              |
| 1:C:296:LEU:CG   | 1:C:298:LEU:HD11 | 2.48                     | 0.43              |
| 1:D:305:SER:O    | 1:D:308:GLU:CG   | 2.62                     | 0.43              |
| 1:A:266:GLU:O    | 1:A:267:LEU:C    | 2.62                     | 0.43              |
| 1:B:361:ALA:HB3  | 1:B:364:VAL:HG23 | 2.01                     | 0.43              |
| 1:C:277:LEU:O    | 1:C:302:GLU:HB2  | 2.19                     | 0.43              |
| 1:C:305:SER:HA   | 1:C:327:LEU:HB2  | 2.00                     | 0.43              |
| 1:A:179:ILE:HG22 | 1:A:187:ILE:HD13 | 2.01                     | 0.43              |
| 1:A:342:ARG:HH11 | 1:A:348:LEU:C    | 2.27                     | 0.43              |
| 1:A:343:GLU:CD   | 1:A:343:GLU:C    | 2.87                     | 0.43              |
| 1:B:211:GLN:CA   | 1:B:214:LEU:HB3  | 2.42                     | 0.43              |
| 1:B:230:LYS:CB   | 1:B:271:ASN:HD21 | 2.22                     | 0.43              |
| 1:B:280:LEU:HD21 | 1:B:303:LEU:HD22 | 1.97                     | 0.43              |
| 1:C:328:CYS:O    | 1:C:330:THR:N    | 2.52                     | 0.43              |
| 1:C:341:ILE:HG22 | 1:C:348:LEU:CD2  | 2.48                     | 0.43              |
| 1:D:240:ALA:O    | 1:D:242:ASN:N    | 2.51                     | 0.43              |
| 1:A:125:PRO:HD2  | 1:A:188:SER:C    | 2.44                     | 0.43              |
| 1:A:168:THR:O    | 1:A:169:ALA:C    | 2.60                     | 0.43              |
| 1:B:247:LEU:HD12 | 1:B:277:LEU:HD21 | 2.00                     | 0.43              |
| 1:C:109:GLY:O    | 1:C:110:THR:CB   | 2.67                     | 0.43              |
| 1:C:309:LEU:HA   | 1:C:312:ILE:HD11 | 2.00                     | 0.43              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:220:TYR:CD1  | 1:D:226:ALA:O    | 2.72                     | 0.43              |
| 1:D:351:LEU:HB2  | 1:D:356:LEU:HD11 | 2.01                     | 0.43              |
| 1:A:221:ASP:HB3  | 1:A:226:ALA:HB3  | 2.01                     | 0.43              |
| 1:A:286:ILE:O    | 1:A:290:ALA:N    | 2.43                     | 0.43              |
| 1:B:213:LYS:HE3  | 1:B:213:LYS:HB2  | 1.73                     | 0.43              |
| 1:C:286:ILE:O    | 1:C:287:VAL:C    | 2.61                     | 0.43              |
| 1:C:334:GLN:HA   | 1:C:337:TYR:CB   | 2.47                     | 0.43              |
| 1:D:335:SER:O    | 1:D:338:ILE:CD1  | 2.67                     | 0.43              |
| 1:D:365:GLU:HB2  | 1:D:366:ALA:H    | 1.56                     | 0.43              |
| 1:B:362:PHE:O    | 1:B:363:ASP:CB   | 2.67                     | 0.42              |
| 1:C:217:SER:O    | 1:C:219:ARG:N    | 2.52                     | 0.42              |
| 1:C:277:LEU:H    | 1:C:301:ASN:HB3  | 1.84                     | 0.42              |
| 1:D:246:VAL:O    | 1:D:252:SER:HB2  | 2.19                     | 0.42              |
| 1:A:158:ARG:NH2  | 1:A:205:LYS:HE3  | 2.34                     | 0.42              |
| 1:A:283:MET:C    | 1:A:285:SER:N    | 2.76                     | 0.42              |
| 1:A:357:PRO:HA   | 1:A:358:PRO:HD3  | 1.93                     | 0.42              |
| 1:B:207:GLU:O    | 1:B:210:GLU:HB2  | 2.19                     | 0.42              |
| 1:B:235:ASP:O    | 1:B:239:VAL:N    | 2.52                     | 0.42              |
| 1:C:134:TRP:O    | 1:C:136:LEU:N    | 2.52                     | 0.42              |
| 1:C:250:ARG:CG   | 1:C:251:SER:N    | 2.73                     | 0.42              |
| 1:C:301:ASN:O    | 1:C:325:ASN:OD1  | 2.36                     | 0.42              |
| 1:D:322:LEU:O    | 1:D:323:ASP:CG   | 2.62                     | 0.42              |
| 1:A:204:LEU:C    | 1:A:205:LYS:HD2  | 2.44                     | 0.42              |
| 1:A:230:LYS:HA   | 1:A:230:LYS:NZ   | 2.34                     | 0.42              |
| 1:A:261:GLU:HB2  | 1:A:289:LYS:HD3  | 2.02                     | 0.42              |
| 1:A:350:ARG:O    | 1:A:351:LEU:HB2  | 2.18                     | 0.42              |
| 1:C:248:ASN:HD22 | 1:C:249:ARG:HG3  | 1.85                     | 0.42              |
| 1:C:267:LEU:HD11 | 1:C:269:SER:C    | 2.43                     | 0.42              |
| 1:A:236:PRO:C    | 1:A:238:LEU:N    | 2.77                     | 0.42              |
| 1:A:328:CYS:O    | 1:A:331:PHE:HB2  | 2.18                     | 0.42              |
| 1:C:134:TRP:CE2  | 1:C:138:MET:HG2  | 2.54                     | 0.42              |
| 1:D:212:LEU:HD12 | 1:D:215:ILE:HB   | 2.00                     | 0.42              |
| 1:A:187:ILE:HD12 | 1:A:187:ILE:H    | 1.85                     | 0.42              |
| 1:A:204:LEU:CD2  | 1:A:208:GLN:HE22 | 2.32                     | 0.42              |
| 1:A:205:LYS:N    | 1:A:208:GLN:OE1  | 2.34                     | 0.42              |
| 1:A:225:GLN:O    | 1:A:267:LEU:CD1  | 2.67                     | 0.42              |
| 1:C:301:ASN:O    | 1:C:325:ASN:CG   | 2.63                     | 0.42              |
| 1:D:207:GLU:N    | 1:D:207:GLU:OE2  | 2.53                     | 0.42              |
| 1:A:119:TRP:HZ3  | 1:A:150:ILE:HD13 | 1.85                     | 0.42              |
| 1:C:196:PRO:HA   | 1:C:197:PRO:HD3  | 1.89                     | 0.42              |
| 1:C:270:LEU:CG   | 1:C:271:ASN:N    | 2.82                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:312:ILE:O    | 1:C:315:LEU:HG   | 2.20                     | 0.42              |
| 1:D:261:GLU:HB2  | 1:D:289:LYS:HD3  | 2.02                     | 0.42              |
| 1:C:119:TRP:CD1  | 1:C:119:TRP:N    | 2.87                     | 0.42              |
| 1:C:130:TYR:C    | 1:C:135:LEU:HD13 | 2.45                     | 0.42              |
| 1:D:286:ILE:O    | 1:D:286:ILE:HG12 | 2.20                     | 0.42              |
| 1:D:347:LYS:CD   | 1:D:347:LYS:N    | 2.81                     | 0.42              |
| 1:A:182:ARG:HG2  | 1:A:183:GLU:N    | 2.35                     | 0.42              |
| 1:A:229:LEU:HB3  | 1:A:232:LEU:HD11 | 2.01                     | 0.42              |
| 1:B:211:GLN:HE21 | 1:B:215:ILE:HD13 | 1.85                     | 0.42              |
| 1:B:277:LEU:CB   | 1:B:301:ASN:HB3  | 2.49                     | 0.42              |
| 1:D:312:ILE:O    | 1:D:314:GLY:N    | 2.53                     | 0.42              |
| 1:A:239:VAL:O    | 1:A:240:ALA:CB   | 2.67                     | 0.42              |
| 1:B:321:TRP:HA   | 1:B:352:ASP:OD1  | 2.20                     | 0.42              |
| 1:C:274:ASN:C    | 1:C:275:ASN:HD22 | 2.28                     | 0.42              |
| 1:D:273:SER:CA   | 1:D:299:SER:O    | 2.68                     | 0.42              |
| 1:D:277:LEU:O    | 1:D:302:GLU:N    | 2.53                     | 0.42              |
| 1:B:310:ASP:C    | 1:B:312:ILE:N    | 2.77                     | 0.42              |
| 1:B:313:LYS:HG2  | 1:B:344:ARG:HB3  | 2.01                     | 0.42              |
| 1:A:312:ILE:HG22 | 1:A:315:LEU:CB   | 2.50                     | 0.41              |
| 1:A:338:ILE:O    | 1:A:342:ARG:CB   | 2.68                     | 0.41              |
| 1:B:305:SER:C    | 1:B:307:ARG:N    | 2.77                     | 0.41              |
| 1:C:109:GLY:O    | 1:C:110:THR:HB   | 2.19                     | 0.41              |
| 1:C:163:VAL:HG12 | 1:C:165:ASP:H    | 1.84                     | 0.41              |
| 1:D:215:ILE:CG2  | 1:D:219:ARG:HD2  | 2.50                     | 0.41              |
| 1:D:220:TYR:HB2  | 1:D:227:LEU:CD1  | 2.46                     | 0.41              |
| 1:D:239:VAL:CG2  | 1:D:240:ALA:H    | 2.21                     | 0.41              |
| 1:D:290:ALA:C    | 1:D:292:ASN:H    | 2.27                     | 0.41              |
| 1:D:303:LEU:O    | 1:D:327:LEU:HD23 | 2.19                     | 0.41              |
| 1:A:268:LEU:O    | 1:A:293:LEU:HD12 | 2.21                     | 0.41              |
| 1:A:309:LEU:CD2  | 1:A:309:LEU:N    | 2.73                     | 0.41              |
| 1:B:344:ARG:C    | 1:B:345:PHE:CD2  | 2.99                     | 0.41              |
| 1:D:363:ASP:HB3  | 1:D:364:VAL:H    | 1.77                     | 0.41              |
| 1:A:181:ASP:OD2  | 1:A:185:ARG:NH2  | 2.53                     | 0.41              |
| 1:A:264:ILE:O    | 1:A:264:ILE:HG22 | 2.19                     | 0.41              |
| 1:A:329:ASP:O    | 1:A:329:ASP:OD2  | 2.38                     | 0.41              |
| 1:A:337:TYR:O    | 1:A:341:ILE:HB   | 2.21                     | 0.41              |
| 1:C:129:LYS:HB3  | 1:C:130:TYR:CE1  | 2.55                     | 0.41              |
| 1:C:313:LYS:O    | 1:C:314:GLY:C    | 2.63                     | 0.41              |
| 1:A:126:TYR:CD1  | 1:D:354:HIS:CE1  | 3.08                     | 0.41              |
| 1:A:196:PRO:HA   | 1:A:197:PRO:HD3  | 1.87                     | 0.41              |
| 1:A:319:GLU:HG3  | 1:A:350:ARG:HB2  | 2.03                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:144:SER:OG   | 1:C:171:ALA:HB1  | 2.20                     | 0.41              |
| 1:C:162:PHE:HB3  | 1:C:163:VAL:H    | 1.52                     | 0.41              |
| 1:C:315:LEU:O    | 1:C:317:LEU:N    | 2.52                     | 0.41              |
| 1:C:358:PRO:HA   | 1:C:359:PRO:HD3  | 1.89                     | 0.41              |
| 1:D:283:MET:CE   | 1:D:312:ILE:HG21 | 2.50                     | 0.41              |
| 1:D:290:ALA:C    | 1:D:292:ASN:N    | 2.78                     | 0.41              |
| 1:B:229:LEU:CB   | 1:B:232:LEU:HD13 | 2.48                     | 0.41              |
| 1:B:272:LEU:C    | 1:B:275:ASN:ND2  | 2.77                     | 0.41              |
| 1:B:313:LYS:HG2  | 1:B:344:ARG:CB   | 2.50                     | 0.41              |
| 1:C:145:VAL:O    | 1:C:168:THR:HG23 | 2.20                     | 0.41              |
| 1:C:175:VAL:HG11 | 1:C:179:ILE:HG12 | 2.02                     | 0.41              |
| 1:C:176:ASN:O    | 1:C:177:TYR:HB2  | 2.20                     | 0.41              |
| 1:C:225:GLN:HB2  | 1:C:268:LEU:HG   | 2.01                     | 0.41              |
| 1:D:246:VAL:HG12 | 1:D:248:ASN:CG   | 2.46                     | 0.41              |
| 1:A:175:VAL:O    | 1:A:175:VAL:CG1  | 2.58                     | 0.41              |
| 1:A:236:PRO:O    | 1:A:238:LEU:N    | 2.47                     | 0.41              |
| 1:A:268:LEU:C    | 1:A:293:LEU:HD12 | 2.46                     | 0.41              |
| 1:A:308:GLU:OE1  | 1:A:308:GLU:HA   | 2.21                     | 0.41              |
| 1:A:315:LEU:HD13 | 1:A:317:LEU:HD21 | 2.03                     | 0.41              |
| 1:C:123:THR:N    | 1:C:190:ILE:O    | 2.48                     | 0.41              |
| 1:C:258:ARG:O    | 1:C:259:ILE:C    | 2.64                     | 0.41              |
| 1:D:205:LYS:HA   | 1:D:206:PRO:HD3  | 1.87                     | 0.41              |
| 1:D:215:ILE:HG22 | 1:D:219:ARG:HD3  | 2.03                     | 0.41              |
| 1:A:246:VAL:HG12 | 1:A:249:ARG:HB2  | 2.02                     | 0.41              |
| 1:B:328:CYS:SG   | 1:C:176:ASN:ND2  | 2.90                     | 0.41              |
| 1:C:233:ARG:NH1  | 1:C:246:VAL:HG21 | 2.35                     | 0.41              |
| 1:C:288:GLN:OE1  | 1:C:289:LYS:HG3  | 2.21                     | 0.41              |
| 1:D:257:LEU:HD11 | 1:D:283:MET:CB   | 2.50                     | 0.41              |
| 1:D:278:TYR:HD2  | 1:D:278:TYR:H    | 1.67                     | 0.41              |
| 1:A:118:ASN:O    | 1:A:118:ASN:OD1  | 2.39                     | 0.41              |
| 1:A:238:LEU:HD11 | 1:A:243:ILE:CG2  | 2.50                     | 0.41              |
| 1:A:283:MET:HE3  | 1:A:283:MET:HB2  | 1.92                     | 0.41              |
| 1:B:264:ILE:N    | 1:B:265:PRO:CD   | 2.84                     | 0.41              |
| 1:B:293:LEU:O    | 1:B:293:LEU:HG   | 2.21                     | 0.41              |
| 1:B:364:VAL:HA   | 1:B:367:PRO:CG   | 2.51                     | 0.41              |
| 1:C:288:GLN:H    | 1:C:288:GLN:HG3  | 1.71                     | 0.41              |
| 1:D:204:LEU:CD2  | 1:D:205:LYS:H    | 2.28                     | 0.41              |
| 1:D:215:ILE:HG23 | 1:D:219:ARG:HD2  | 2.03                     | 0.41              |
| 1:D:270:LEU:O    | 1:D:296:LEU:HD12 | 2.20                     | 0.41              |
| 1:A:122:ILE:HB   | 1:A:161:PHE:CE1  | 2.56                     | 0.41              |
| 1:A:177:TYR:O    | 1:A:177:TYR:CG   | 2.73                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:238:LEU:HD11 | 1:A:243:ILE:CB   | 2.51                     | 0.41              |
| 1:B:268:LEU:O    | 1:B:293:LEU:HA   | 2.21                     | 0.41              |
| 1:B:293:LEU:HD12 | 1:B:295:ILE:N    | 2.32                     | 0.41              |
| 1:C:118:ASN:O    | 1:C:165:ASP:CA   | 2.66                     | 0.41              |
| 1:C:172:LEU:N    | 1:C:172:LEU:CD1  | 2.83                     | 0.41              |
| 1:C:215:ILE:H    | 1:C:215:ILE:HG13 | 1.63                     | 0.41              |
| 1:C:248:ASN:ND2  | 1:C:249:ARG:N    | 2.69                     | 0.41              |
| 1:D:221:ASP:N    | 1:D:226:ALA:O    | 2.53                     | 0.41              |
| 1:D:280:LEU:HD23 | 1:D:280:LEU:HA   | 1.95                     | 0.41              |
| 1:D:290:ALA:N    | 1:D:291:PRO:HD3  | 2.35                     | 0.41              |
| 1:D:369:THR:O    | 1:D:370:LEU:HB2  | 2.21                     | 0.41              |
| 1:A:128:ARG:HH11 | 1:A:128:ARG:HG3  | 1.86                     | 0.41              |
| 1:A:215:ILE:HD11 | 1:A:238:LEU:CB   | 2.50                     | 0.41              |
| 1:A:336:THR:O    | 1:A:339:SER:N    | 2.54                     | 0.41              |
| 1:B:308:GLU:C    | 1:B:310:ASP:N    | 2.79                     | 0.41              |
| 1:C:326:SER:C    | 1:C:328:CYS:H    | 2.28                     | 0.41              |
| 1:D:305:SER:HB3  | 1:D:307:ARG:H    | 1.86                     | 0.41              |
| 1:D:323:ASP:OD1  | 1:D:323:ASP:O    | 2.38                     | 0.41              |
| 1:A:144:SER:O    | 1:A:145:VAL:CG1  | 2.55                     | 0.40              |
| 1:A:152:PHE:O    | 1:A:153:HIS:HB3  | 2.21                     | 0.40              |
| 1:B:328:CYS:CB   | 1:C:177:TYR:HE1  | 2.33                     | 0.40              |
| 1:C:161:PHE:HD2  | 1:C:161:PHE:H    | 1.69                     | 0.40              |
| 1:C:296:LEU:O    | 1:C:320:LEU:HA   | 2.22                     | 0.40              |
| 1:C:303:LEU:HA   | 1:C:303:LEU:HD23 | 1.76                     | 0.40              |
| 1:C:328:CYS:O    | 1:C:329:ASP:C    | 2.64                     | 0.40              |
| 1:C:120:PHE:CD2  | 1:C:193:SER:HB3  | 2.56                     | 0.40              |
| 1:D:258:ARG:HG3  | 1:D:258:ARG:NH2  | 2.36                     | 0.40              |
| 1:D:278:TYR:HA   | 1:D:302:GLU:O    | 2.21                     | 0.40              |
| 1:D:281:ASP:C    | 1:D:283:MET:N    | 2.79                     | 0.40              |
| 1:D:360:ILE:HD13 | 1:D:365:GLU:HA   | 2.02                     | 0.40              |
| 1:A:142:LYS:HD2  | 1:A:178:LYS:CE   | 2.51                     | 0.40              |
| 1:A:325:ASN:N    | 1:A:325:ASN:ND2  | 2.69                     | 0.40              |
| 1:C:271:ASN:ND2  | 1:C:273:SER:H    | 2.19                     | 0.40              |
| 1:C:297:ASN:ND2  | 1:C:297:ASN:C    | 2.79                     | 0.40              |
| 1:B:327:LEU:N    | 1:B:329:ASP:OD2  | 2.55                     | 0.40              |
| 1:B:342:ARG:HA   | 1:B:345:PHE:O    | 2.22                     | 0.40              |
| 1:C:218:LYS:O    | 1:C:219:ARG:CB   | 2.69                     | 0.40              |
| 1:C:348:LEU:HG   | 1:C:349:LEU:H    | 1.87                     | 0.40              |
| 1:A:205:LYS:HE3  | 1:A:205:LYS:HA   | 2.03                     | 0.40              |
| 1:C:156:ASN:ND2  | 1:C:156:ASN:C    | 2.77                     | 0.40              |
| 1:C:248:ASN:HA   | 1:C:277:LEU:HD22 | 2.03                     | 0.40              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1          | Atom-2         | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|----------------|--------------------------|-------------------|
| 1:D:205:LYS:HB2 | 1:D:208:GLN:CD | 2.47                     | 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     | 256/277 (92%)  | 166 (65%) | 57 (22%)  | 33 (13%)  | 0           | 3 |
| 1   | B     | 163/277 (59%)  | 116 (71%) | 33 (20%)  | 14 (9%)   | 0           | 9 |
| 1   | C     | 260/277 (94%)  | 148 (57%) | 66 (25%)  | 46 (18%)  | 0           | 2 |
| 1   | D     | 167/277 (60%)  | 109 (65%) | 29 (17%)  | 29 (17%)  | 0           | 2 |
| All | All   | 846/1108 (76%) | 539 (64%) | 185 (22%) | 122 (14%) | 0           | 3 |

All (122) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 106 | GLY  |
| 1   | A     | 198 | HIS  |
| 1   | A     | 203 | GLU  |
| 1   | A     | 236 | PRO  |
| 1   | A     | 284 | SER  |
| 1   | A     | 286 | ILE  |
| 1   | A     | 302 | GLU  |
| 1   | A     | 313 | LYS  |
| 1   | A     | 322 | LEU  |
| 1   | A     | 326 | SER  |
| 1   | A     | 333 | ASP  |
| 1   | B     | 205 | LYS  |
| 1   | B     | 206 | PRO  |
| 1   | B     | 293 | LEU  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 326 | SER  |
| 1   | B     | 363 | ASP  |
| 1   | C     | 106 | GLY  |
| 1   | C     | 142 | LYS  |
| 1   | C     | 143 | CYS  |
| 1   | C     | 151 | GLU  |
| 1   | C     | 182 | ARG  |
| 1   | C     | 197 | PRO  |
| 1   | C     | 219 | ARG  |
| 1   | C     | 250 | ARG  |
| 1   | C     | 260 | ILE  |
| 1   | C     | 278 | TYR  |
| 1   | C     | 280 | LEU  |
| 1   | C     | 302 | GLU  |
| 1   | C     | 306 | GLU  |
| 1   | D     | 223 | SER  |
| 1   | D     | 237 | ASP  |
| 1   | D     | 239 | VAL  |
| 1   | D     | 240 | ALA  |
| 1   | D     | 242 | ASN  |
| 1   | D     | 280 | LEU  |
| 1   | D     | 315 | LEU  |
| 1   | D     | 323 | ASP  |
| 1   | D     | 367 | PRO  |
| 1   | D     | 368 | THR  |
| 1   | D     | 370 | LEU  |
| 1   | D     | 371 | PRO  |
| 1   | A     | 141 | SER  |
| 1   | A     | 201 | LEU  |
| 1   | A     | 221 | ASP  |
| 1   | A     | 227 | LEU  |
| 1   | A     | 267 | LEU  |
| 1   | A     | 276 | ARG  |
| 1   | A     | 309 | LEU  |
| 1   | A     | 318 | GLU  |
| 1   | A     | 330 | THR  |
| 1   | B     | 208 | GLN  |
| 1   | B     | 263 | ASN  |
| 1   | B     | 301 | ASN  |
| 1   | C     | 116 | SER  |
| 1   | C     | 135 | LEU  |
| 1   | C     | 150 | ILE  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 156 | ASN  |
| 1   | C     | 225 | GLN  |
| 1   | C     | 233 | ARG  |
| 1   | C     | 252 | SER  |
| 1   | C     | 291 | PRO  |
| 1   | C     | 309 | LEU  |
| 1   | C     | 314 | GLY  |
| 1   | D     | 266 | GLU  |
| 1   | D     | 276 | ARG  |
| 1   | D     | 282 | ASP  |
| 1   | D     | 293 | LEU  |
| 1   | D     | 313 | LYS  |
| 1   | D     | 314 | GLY  |
| 1   | A     | 118 | ASN  |
| 1   | A     | 240 | ALA  |
| 1   | A     | 250 | ARG  |
| 1   | A     | 323 | ASP  |
| 1   | A     | 327 | LEU  |
| 1   | A     | 347 | LYS  |
| 1   | B     | 267 | LEU  |
| 1   | B     | 280 | LEU  |
| 1   | B     | 327 | LEU  |
| 1   | C     | 152 | PHE  |
| 1   | C     | 162 | PHE  |
| 1   | C     | 204 | LEU  |
| 1   | C     | 206 | PRO  |
| 1   | C     | 236 | PRO  |
| 1   | C     | 261 | GLU  |
| 1   | C     | 315 | LEU  |
| 1   | C     | 318 | GLU  |
| 1   | C     | 329 | ASP  |
| 1   | C     | 347 | LYS  |
| 1   | D     | 206 | PRO  |
| 1   | D     | 222 | GLY  |
| 1   | D     | 366 | ALA  |
| 1   | A     | 129 | LYS  |
| 1   | A     | 145 | VAL  |
| 1   | B     | 217 | SER  |
| 1   | C     | 110 | THR  |
| 1   | C     | 184 | ASN  |
| 1   | C     | 202 | ASN  |
| 1   | C     | 218 | LYS  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 242 | ASN  |
| 1   | C     | 293 | LEU  |
| 1   | C     | 330 | THR  |
| 1   | C     | 341 | ILE  |
| 1   | D     | 238 | LEU  |
| 1   | D     | 275 | ASN  |
| 1   | A     | 146 | PRO  |
| 1   | A     | 291 | PRO  |
| 1   | A     | 293 | LEU  |
| 1   | A     | 358 | PRO  |
| 1   | B     | 311 | LYS  |
| 1   | C     | 102 | PRO  |
| 1   | C     | 248 | ASN  |
| 1   | D     | 235 | ASP  |
| 1   | D     | 256 | THR  |
| 1   | D     | 327 | LEU  |
| 1   | C     | 334 | GLN  |
| 1   | D     | 364 | VAL  |
| 1   | B     | 314 | GLY  |
| 1   | C     | 149 | PRO  |
| 1   | C     | 196 | PRO  |
| 1   | A     | 109 | GLY  |
| 1   | D     | 358 | PRO  |
| 1   | D     | 209 | VAL  |

### 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     | 232/249 (93%) | 200 (86%) | 32 (14%)  | 3           | 18 |
| 1   | B     | 151/249 (61%) | 130 (86%) | 21 (14%)  | 3           | 18 |
| 1   | C     | 235/249 (94%) | 203 (86%) | 32 (14%)  | 3           | 18 |
| 1   | D     | 155/249 (62%) | 129 (83%) | 26 (17%)  | 2           | 13 |
| All | All   | 773/996 (78%) | 662 (86%) | 111 (14%) | 3           | 17 |

All (111) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 113 | ASP  |
| 1   | A     | 117 | LYS  |
| 1   | A     | 122 | ILE  |
| 1   | A     | 128 | ARG  |
| 1   | A     | 138 | MET  |
| 1   | A     | 140 | GLN  |
| 1   | A     | 155 | GLU  |
| 1   | A     | 157 | THR  |
| 1   | A     | 164 | GLU  |
| 1   | A     | 178 | LYS  |
| 1   | A     | 182 | ARG  |
| 1   | A     | 184 | ASN  |
| 1   | A     | 227 | LEU  |
| 1   | A     | 230 | LYS  |
| 1   | A     | 232 | LEU  |
| 1   | A     | 249 | ARG  |
| 1   | A     | 270 | LEU  |
| 1   | A     | 271 | ASN  |
| 1   | A     | 276 | ARG  |
| 1   | A     | 277 | LEU  |
| 1   | A     | 289 | LYS  |
| 1   | A     | 291 | PRO  |
| 1   | A     | 296 | LEU  |
| 1   | A     | 298 | LEU  |
| 1   | A     | 307 | ARG  |
| 1   | A     | 311 | LYS  |
| 1   | A     | 315 | LEU  |
| 1   | A     | 322 | LEU  |
| 1   | A     | 323 | ASP  |
| 1   | A     | 334 | GLN  |
| 1   | A     | 343 | GLU  |
| 1   | A     | 347 | LYS  |
| 1   | B     | 204 | LEU  |
| 1   | B     | 206 | PRO  |
| 1   | B     | 209 | VAL  |
| 1   | B     | 238 | LEU  |
| 1   | B     | 244 | ASP  |
| 1   | B     | 248 | ASN  |
| 1   | B     | 253 | MET  |
| 1   | B     | 270 | LEU  |
| 1   | B     | 272 | LEU  |
| 1   | B     | 282 | ASP  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 284 | SER  |
| 1   | B     | 293 | LEU  |
| 1   | B     | 297 | ASN  |
| 1   | B     | 299 | SER  |
| 1   | B     | 301 | ASN  |
| 1   | B     | 319 | GLU  |
| 1   | B     | 326 | SER  |
| 1   | B     | 329 | ASP  |
| 1   | B     | 338 | ILE  |
| 1   | B     | 355 | GLU  |
| 1   | B     | 364 | VAL  |
| 1   | C     | 148 | THR  |
| 1   | C     | 150 | ILE  |
| 1   | C     | 152 | PHE  |
| 1   | C     | 153 | HIS  |
| 1   | C     | 154 | TYR  |
| 1   | C     | 158 | ARG  |
| 1   | C     | 161 | PHE  |
| 1   | C     | 196 | PRO  |
| 1   | C     | 197 | PRO  |
| 1   | C     | 201 | LEU  |
| 1   | C     | 204 | LEU  |
| 1   | C     | 207 | GLU  |
| 1   | C     | 216 | MET  |
| 1   | C     | 227 | LEU  |
| 1   | C     | 232 | LEU  |
| 1   | C     | 261 | GLU  |
| 1   | C     | 264 | ILE  |
| 1   | C     | 272 | LEU  |
| 1   | C     | 277 | LEU  |
| 1   | C     | 288 | GLN  |
| 1   | C     | 292 | ASN  |
| 1   | C     | 298 | LEU  |
| 1   | C     | 310 | ASP  |
| 1   | C     | 313 | LYS  |
| 1   | C     | 315 | LEU  |
| 1   | C     | 317 | LEU  |
| 1   | C     | 326 | SER  |
| 1   | C     | 327 | LEU  |
| 1   | C     | 331 | PHE  |
| 1   | C     | 336 | THR  |
| 1   | C     | 338 | ILE  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 344 | ARG  |
| 1   | D     | 207 | GLU  |
| 1   | D     | 218 | LYS  |
| 1   | D     | 221 | ASP  |
| 1   | D     | 225 | GLN  |
| 1   | D     | 234 | SER  |
| 1   | D     | 241 | GLN  |
| 1   | D     | 242 | ASN  |
| 1   | D     | 245 | VAL  |
| 1   | D     | 246 | VAL  |
| 1   | D     | 247 | LEU  |
| 1   | D     | 258 | ARG  |
| 1   | D     | 261 | GLU  |
| 1   | D     | 266 | GLU  |
| 1   | D     | 278 | TYR  |
| 1   | D     | 279 | ARG  |
| 1   | D     | 288 | GLN  |
| 1   | D     | 297 | ASN  |
| 1   | D     | 307 | ARG  |
| 1   | D     | 310 | ASP  |
| 1   | D     | 330 | THR  |
| 1   | D     | 338 | ILE  |
| 1   | D     | 350 | ARG  |
| 1   | D     | 355 | GLU  |
| 1   | D     | 362 | PHE  |
| 1   | D     | 365 | GLU  |
| 1   | D     | 369 | THR  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 112 | GLN  |
| 1   | A     | 140 | GLN  |
| 1   | A     | 153 | HIS  |
| 1   | A     | 160 | GLN  |
| 1   | A     | 202 | ASN  |
| 1   | A     | 242 | ASN  |
| 1   | A     | 263 | ASN  |
| 1   | A     | 271 | ASN  |
| 1   | A     | 274 | ASN  |
| 1   | A     | 275 | ASN  |
| 1   | A     | 288 | GLN  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 292 | ASN  |
| 1   | A     | 297 | ASN  |
| 1   | A     | 325 | ASN  |
| 1   | A     | 354 | HIS  |
| 1   | B     | 241 | GLN  |
| 1   | B     | 248 | ASN  |
| 1   | B     | 271 | ASN  |
| 1   | B     | 274 | ASN  |
| 1   | B     | 275 | ASN  |
| 1   | B     | 297 | ASN  |
| 1   | B     | 301 | ASN  |
| 1   | B     | 334 | GLN  |
| 1   | C     | 118 | ASN  |
| 1   | C     | 140 | GLN  |
| 1   | C     | 153 | HIS  |
| 1   | C     | 156 | ASN  |
| 1   | C     | 160 | GLN  |
| 1   | C     | 192 | ASN  |
| 1   | C     | 198 | HIS  |
| 1   | C     | 208 | GLN  |
| 1   | C     | 241 | GLN  |
| 1   | C     | 248 | ASN  |
| 1   | C     | 263 | ASN  |
| 1   | C     | 271 | ASN  |
| 1   | C     | 274 | ASN  |
| 1   | C     | 275 | ASN  |
| 1   | C     | 297 | ASN  |
| 1   | D     | 208 | GLN  |
| 1   | D     | 211 | GLN  |
| 1   | D     | 224 | GLN  |
| 1   | D     | 241 | GLN  |
| 1   | D     | 242 | ASN  |
| 1   | D     | 263 | ASN  |
| 1   | D     | 271 | ASN  |
| 1   | D     | 288 | GLN  |
| 1   | D     | 297 | ASN  |
| 1   | D     | 334 | GLN  |

### 5.3.3 RNA ⓘ

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](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<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     | 258/277 (93%)  | -0.06  | 2 (0%) 82 62  | 35, 59, 88, 96        | 0     |
| 1   | B     | 165/277 (59%)  | -0.02  | 2 (1%) 76 54  | 36, 55, 78, 84        | 0     |
| 1   | C     | 262/277 (94%)  | 0.09   | 5 (1%) 66 45  | 42, 71, 105, 113      | 0     |
| 1   | D     | 169/277 (61%)  | 0.01   | 2 (1%) 76 54  | 27, 55, 78, 84        | 0     |
| All | All   | 854/1108 (77%) | 0.01   | 11 (1%) 75 53 | 27, 59, 98, 113       | 0     |

All (11) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | A     | 113 | ASP  | 3.9  |
| 1   | B     | 328 | CYS  | 3.3  |
| 1   | C     | 262 | GLU  | 3.1  |
| 1   | D     | 371 | PRO  | 2.8  |
| 1   | C     | 238 | LEU  | 2.8  |
| 1   | B     | 282 | ASP  | 2.5  |
| 1   | C     | 102 | PRO  | 2.5  |
| 1   | C     | 118 | ASN  | 2.3  |
| 1   | C     | 103 | PRO  | 2.2  |
| 1   | D     | 207 | GLU  | 2.1  |
| 1   | A     | 200 | ILE  | 2.1  |

### 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](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.