



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 11:16 PM UTC

PDB ID : 4F35 / pdb\_00004f35  
Title : Crystal Structure of a bacterial dicarboxylate/sodium symporter  
Authors : Mancusso, R.L.; Gregorio, G.G.; Liu, Q.; Wang, D.N.  
Deposited on : 2012-05-08  
Resolution : 3.20 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  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

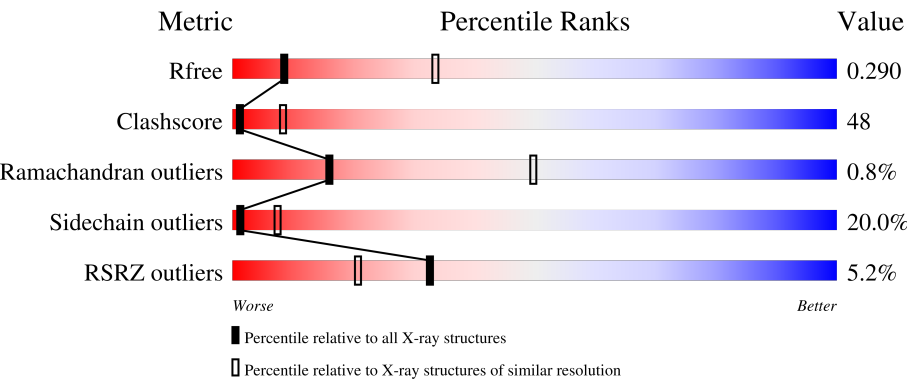
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 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                      | 1466 (3.20-3.20)                                      |
| Clashscore            | 190562                      | 1573 (3.20-3.20)                                      |
| Ramachandran outliers | 187476                      | 1548 (3.20-3.20)                                      |
| Sidechain outliers    | 187428                      | 1547 (3.20-3.20)                                      |
| RSRZ outliers         | 180081                      | 1466 (3.20-3.20)                                      |

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     | 449    | <div><div>6%</div><div><div></div><div></div><div></div><div></div></div><div>40%43%13% . .</div></div> |
| 1   | B     | 449    | <div><div>7%</div><div><div></div><div></div><div></div><div></div></div><div>36%44%12%8%</div></div>   |
| 1   | C     | 449    | <div><div>3%</div><div><div></div><div></div><div></div><div></div></div><div>33%50%12% . .</div></div> |
| 1   | D     | 449    | <div><div>3%</div><div><div></div><div></div><div></div><div></div></div><div>37%48%10% . .</div></div> |

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 4   | CIT  | B     | 501 | -         | -        | X       | -                |

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12390 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.

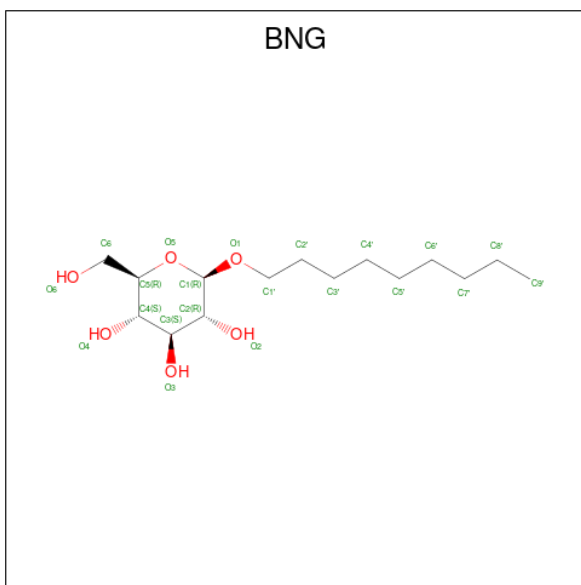
- Molecule 1 is a protein called Transporter, NadC family.

| Mol | Chain | Residues | Atoms |      |     |     |   |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|----|---------|---------|-------|
| 1   | D     | 430      | Total | C    | N   | O   | S | Se | 3       | 0       | 0     |
|     |       |          | 3076  | 2046 | 479 | 526 | 3 | 22 |         |         |       |
| 1   | B     | 414      | Total | C    | N   | O   | S | Se | 0       | 0       | 0     |
|     |       |          | 2980  | 1991 | 457 | 508 | 3 | 21 |         |         |       |
| 1   | A     | 434      | Total | C    | N   | O   | S | Se | 0       | 0       | 0     |
|     |       |          | 3110  | 2068 | 481 | 536 | 3 | 22 |         |         |       |
| 1   | C     | 430      | Total | C    | N   | O   | S | Se | 0       | 0       | 0     |
|     |       |          | 3113  | 2077 | 482 | 529 | 3 | 22 |         |         |       |

- Molecule 2 is SODIUM ION (CCD ID: NA) (formula: Na).

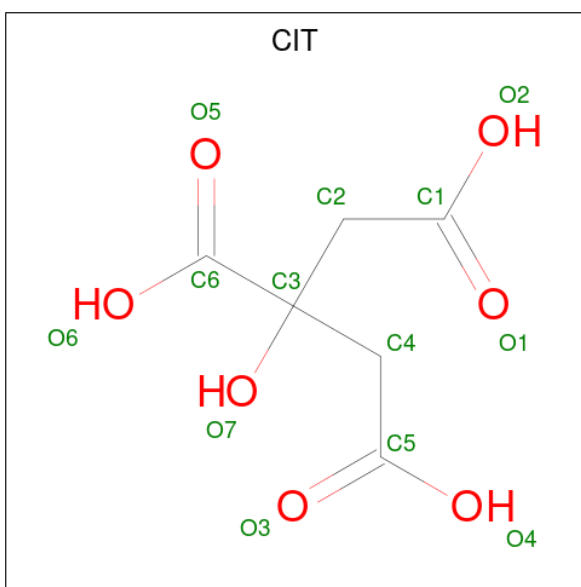
| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 2   | D     | 1        | Total | Na | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 2   | B     | 1        | Total | Na | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 2   | A     | 1        | Total | Na | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 2   | C     | 1        | Total | Na | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

- Molecule 3 is nonyl beta-D-glucopyranoside (CCD ID: BNG) (formula: C<sub>15</sub>H<sub>30</sub>O<sub>6</sub>).



| Mol | Chain | Residues | Atoms       |         |        | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|--------|---------|---------|
| 3   | D     | 1        | Total<br>21 | C<br>15 | O<br>6 | 0       | 0       |
| 3   | B     | 1        | Total<br>21 | C<br>15 | O<br>6 | 0       | 0       |
| 3   | C     | 1        | Total<br>21 | C<br>15 | O<br>6 | 0       | 0       |

- Molecule 4 is CITRIC ACID (CCD ID: CIT) (formula:  $\text{C}_6\text{H}_8\text{O}_7$ ).



| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 4   | B     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 13    | 6 | 7 |         |         |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 4   | A     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 13    | 6 | 7 |         |         |
| 4   | C     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 13    | 6 | 7 |         |         |

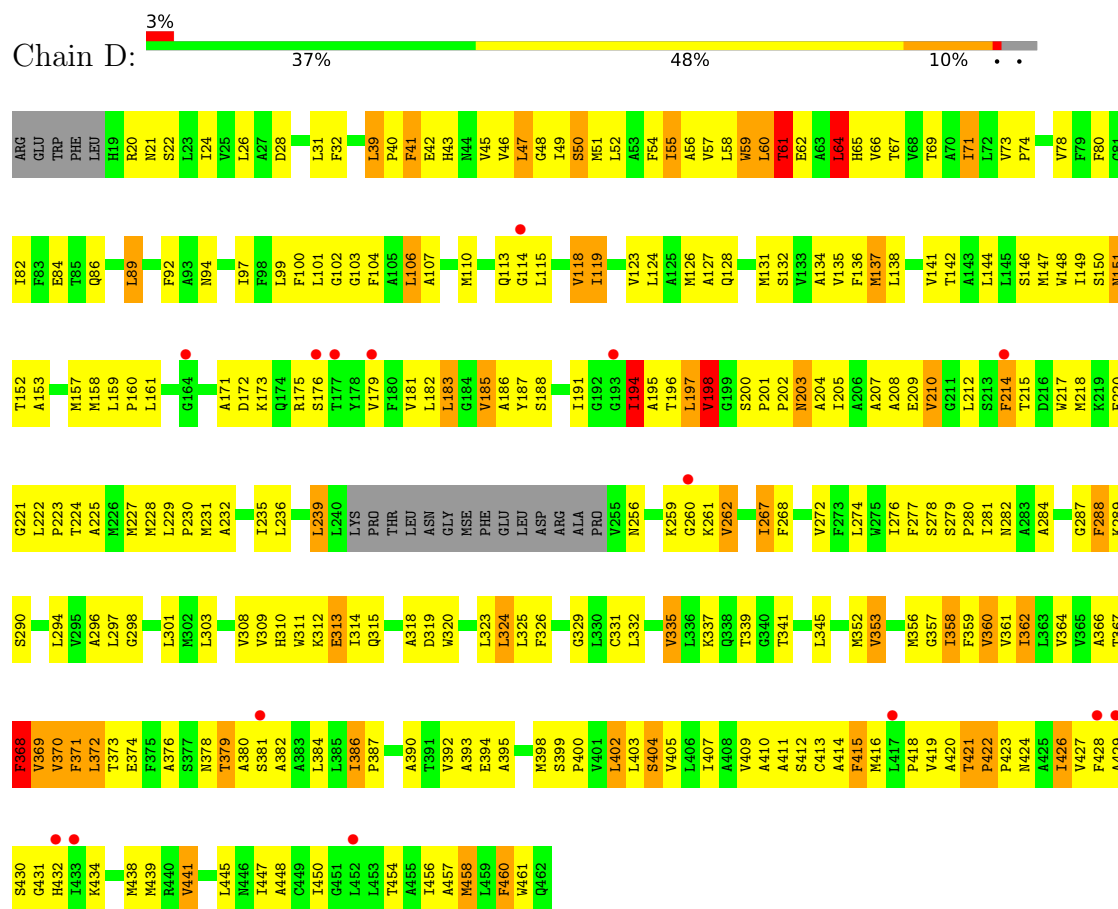
- Molecule 5 is water.

| Mol | Chain | Residues | Atoms |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---------|---------|
| 5   | D     | 3        | Total | O | 0       | 0       |
|     |       |          | 3     | 3 |         |         |
| 5   | B     | 1        | Total | O | 0       | 0       |
|     |       |          | 1     | 1 |         |         |
| 5   | C     | 1        | Total | O | 0       | 0       |
|     |       |          | 1     | 1 |         |         |

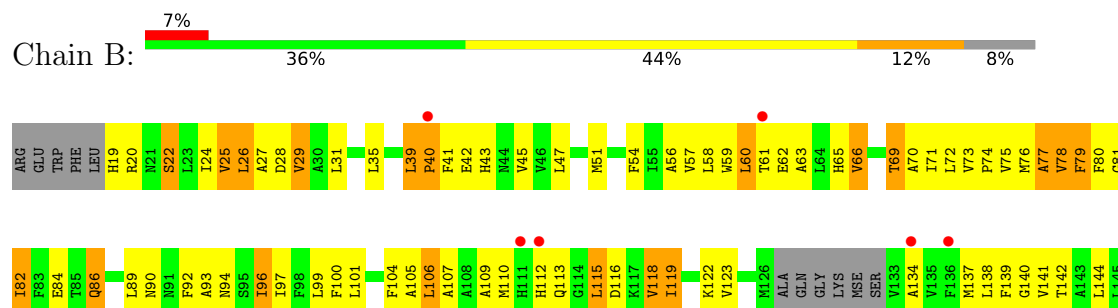
### 3 Residue-property plots

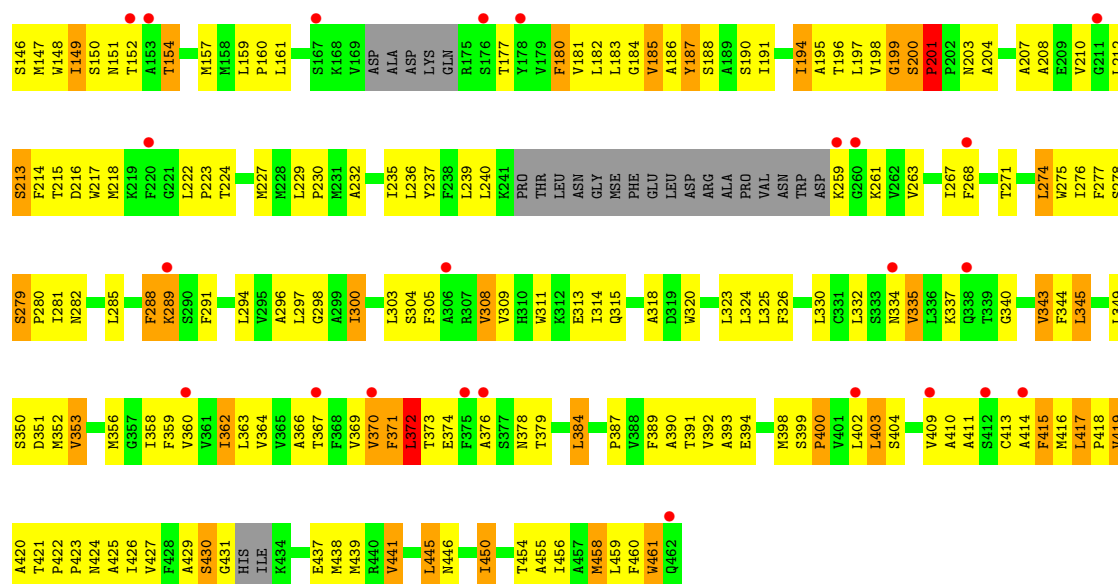
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Transporter, NadC family

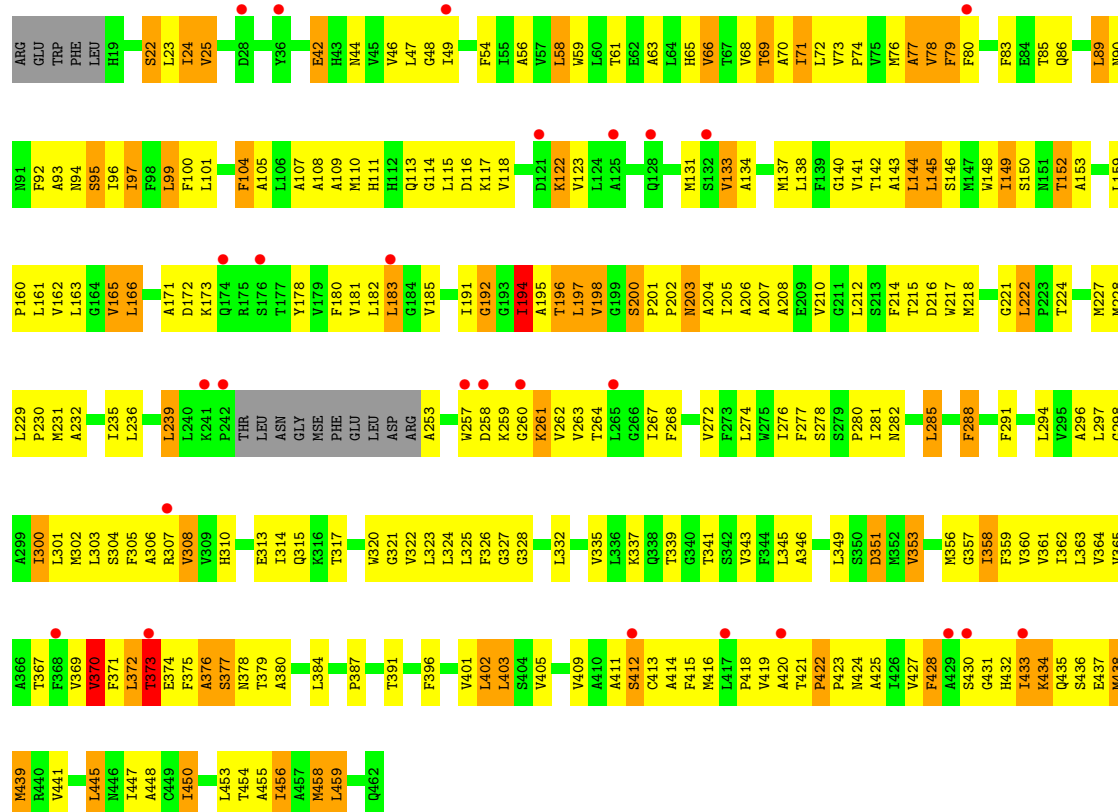


#### • Molecule 1: Transporter, NadC family





• Molecule 1: Transporter, NadC family



• Molecule 1: Transporter, NadC family





## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 1 21 1                                                    | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 101.33Å 100.87Å 164.57Å<br>90.00° 101.74° 90.00°            | Depositor        |
| Resolution (Å)                                                          | 44.38 – 3.20<br>44.38 – 3.20                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 96.5 (44.38-3.20)<br>96.5 (44.38-3.20)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | (Not available)                                             | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.53 (at 3.19Å)                                             | Xtriage          |
| Refinement program                                                      | PHENIX (phenix.refine: 1.7.1_743)                           | Depositor        |
| R, $R_{free}$                                                           | 0.228 , 0.291<br>0.226 , 0.290                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 2026 reflections (3.88%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 93.9                                                        | Xtriage          |
| Anisotropy                                                              | 0.263                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.29 , 123.5                                                | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$ | Xtriage          |
| Estimated twinning fraction                                             | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.93                                                        | EDS              |
| Total number of atoms                                                   | 12390                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 98.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.48% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NA, CIT, BNG

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     | 0.66         | 1/3153 (0.0%)  | 1.09        | 11/4278 (0.3%)  |
| 1   | B     | 0.58         | 0/3024         | 1.06        | 15/4106 (0.4%)  |
| 1   | C     | 0.67         | 1/3163 (0.0%)  | 1.15        | 26/4292 (0.6%)  |
| 1   | D     | 0.68         | 0/3119         | 1.16        | 17/4231 (0.4%)  |
| All | All   | 0.65         | 2/12459 (0.0%) | 1.12        | 69/16907 (0.4%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | A     | 0                   | 1                   |
| 1   | C     | 0                   | 2                   |
| 1   | D     | 0                   | 3                   |
| All | All   | 0                   | 6                   |

All (2) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 1   | A     | 370 | VAL  | CA-CB | 8.16 | 1.62        | 1.54     |
| 1   | C     | 370 | VAL  | CA-CB | 6.14 | 1.62        | 1.54     |

All (69) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|--------|-------------|----------|
| 1   | D     | 256 | ASN  | N-CA-C | 10.51  | 124.62      | 111.69   |
| 1   | A     | 373 | THR  | N-CA-C | -10.44 | 100.55      | 113.18   |
| 1   | B     | 372 | LEU  | N-CA-C | -8.79  | 102.56      | 113.28   |
| 1   | D     | 415 | PHE  | N-CA-C | -8.57  | 97.65       | 108.45   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | B     | 201 | PRO  | N-CA-C | 8.35  | 120.89      | 110.70   |
| 1   | C     | 422 | PRO  | CA-C-N | -7.87 | 110.34      | 119.32   |
| 1   | C     | 422 | PRO  | C-N-CA | -7.87 | 110.34      | 119.32   |
| 1   | A     | 79  | PHE  | N-CA-C | -7.76 | 100.16      | 110.24   |
| 1   | C     | 430 | SER  | N-CA-C | 7.62  | 119.27      | 108.00   |
| 1   | B     | 200 | SER  | CA-C-N | 7.40  | 128.00      | 120.38   |
| 1   | B     | 200 | SER  | C-N-CA | 7.40  | 128.00      | 120.38   |
| 1   | C     | 401 | VAL  | N-CA-C | 7.37  | 117.50      | 110.42   |
| 1   | A     | 370 | VAL  | N-CA-C | -7.28 | 98.28       | 109.78   |
| 1   | C     | 417 | LEU  | CA-C-N | -7.20 | 112.22      | 119.99   |
| 1   | C     | 417 | LEU  | C-N-CA | -7.20 | 112.22      | 119.99   |
| 1   | A     | 253 | ALA  | CA-C-N | 7.02  | 128.61      | 119.84   |
| 1   | A     | 253 | ALA  | C-N-CA | 7.02  | 128.61      | 119.84   |
| 1   | A     | 192 | GLY  | N-CA-C | -7.00 | 105.03      | 113.99   |
| 1   | D     | 370 | VAL  | N-CA-C | -6.99 | 102.35      | 111.09   |
| 1   | D     | 60  | LEU  | N-CA-C | -6.94 | 101.37      | 110.53   |
| 1   | C     | 201 | PRO  | CA-C-N | -6.85 | 111.85      | 118.97   |
| 1   | C     | 201 | PRO  | C-N-CA | -6.85 | 111.85      | 118.97   |
| 1   | C     | 103 | GLY  | N-CA-C | -6.56 | 104.56      | 112.49   |
| 1   | D     | 39  | LEU  | CA-C-N | 6.52  | 128.23      | 121.65   |
| 1   | D     | 39  | LEU  | C-N-CA | 6.52  | 128.23      | 121.65   |
| 1   | D     | 368 | PHE  | N-CA-C | -6.46 | 105.27      | 113.02   |
| 1   | A     | 422 | PRO  | N-CA-C | 6.29  | 118.37      | 110.70   |
| 1   | B     | 415 | PHE  | N-CA-C | -6.23 | 97.53       | 110.80   |
| 1   | C     | 371 | PHE  | N-CA-C | 6.22  | 120.61      | 112.89   |
| 1   | C     | 77  | ALA  | N-CA-C | -6.17 | 100.16      | 109.60   |
| 1   | D     | 429 | ALA  | N-CA-C | -6.10 | 99.12       | 108.76   |
| 1   | D     | 421 | THR  | CA-C-N | -6.06 | 114.14      | 120.38   |
| 1   | D     | 421 | THR  | C-N-CA | -6.06 | 114.14      | 120.38   |
| 1   | C     | 422 | PRO  | N-CA-C | 6.05  | 118.08      | 110.70   |
| 1   | C     | 129 | GLY  | N-CA-C | 6.00  | 120.32      | 110.97   |
| 1   | A     | 172 | ASP  | N-CA-C | -5.97 | 105.98      | 113.20   |
| 1   | D     | 284 | ALA  | N-CA-C | -5.96 | 105.98      | 113.20   |
| 1   | B     | 77  | ALA  | N-CA-C | -5.93 | 100.53      | 109.60   |
| 1   | B     | 20  | ARG  | N-CA-C | -5.73 | 104.23      | 111.11   |
| 1   | D     | 172 | ASP  | N-CA-C | -5.72 | 106.15      | 113.01   |
| 1   | A     | 77  | ALA  | N-CA-C | -5.70 | 100.89      | 109.60   |
| 1   | C     | 206 | ALA  | N-CA-C | -5.65 | 104.81      | 110.97   |
| 1   | C     | 95  | SER  | N-CA-C | 5.61  | 118.16      | 111.71   |
| 1   | C     | 168 | LYS  | N-CA-C | -5.60 | 106.53      | 113.19   |
| 1   | B     | 429 | ALA  | N-CA-C | -5.58 | 99.95       | 108.76   |
| 1   | C     | 69  | THR  | N-CA-C | -5.56 | 105.22      | 111.28   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | B     | 60  | LEU  | N-CA-C  | -5.56 | 102.25      | 110.48   |
| 1   | C     | 300 | ILE  | N-CA-C  | -5.53 | 104.98      | 110.62   |
| 1   | D     | 20  | ARG  | CB-CA-C | -5.40 | 109.89      | 117.23   |
| 1   | C     | 300 | ILE  | N-CA-CB | 5.39  | 117.88      | 110.54   |
| 1   | B     | 79  | PHE  | N-CA-C  | -5.36 | 102.68      | 110.24   |
| 1   | B     | 430 | SER  | CB-CA-C | -5.36 | 110.38      | 116.54   |
| 1   | C     | 374 | GLU  | N-CA-C  | -5.29 | 101.50      | 109.60   |
| 1   | D     | 198 | VAL  | N-CA-C  | 5.28  | 115.19      | 107.37   |
| 1   | A     | 431 | GLY  | N-CA-C  | -5.28 | 103.62      | 110.38   |
| 1   | B     | 370 | VAL  | N-CA-C  | -5.26 | 104.26      | 110.21   |
| 1   | B     | 199 | GLY  | N-CA-C  | -5.25 | 98.08       | 113.30   |
| 1   | A     | 46  | VAL  | CB-CA-C | -5.22 | 105.19      | 111.88   |
| 1   | C     | 235 | ILE  | CB-CA-C | -5.19 | 105.24      | 111.88   |
| 1   | C     | 430 | SER  | CB-CA-C | -5.18 | 109.09      | 116.34   |
| 1   | D     | 422 | PRO  | N-CA-C  | 5.18  | 117.01      | 110.70   |
| 1   | D     | 426 | ILE  | CB-CA-C | -5.11 | 105.42      | 111.81   |
| 1   | C     | 318 | ALA  | CA-C-N  | -5.11 | 114.89      | 122.41   |
| 1   | C     | 318 | ALA  | C-N-CA  | -5.11 | 114.89      | 122.41   |
| 1   | B     | 400 | PRO  | N-CA-C  | -5.07 | 107.25      | 113.84   |
| 1   | D     | 294 | LEU  | N-CA-C  | -5.06 | 105.45      | 110.97   |
| 1   | C     | 461 | TRP  | N-CA-C  | -5.04 | 107.15      | 113.15   |
| 1   | C     | 415 | PHE  | N-CA-C  | -5.04 | 101.75      | 108.86   |
| 1   | B     | 437 | GLU  | N-CA-C  | -5.01 | 106.95      | 113.16   |

There are no chirality outliers.

All (6) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 1   | A     | 433 | ILE  | Peptide |
| 1   | C     | 430 | SER  | Peptide |
| 1   | C     | 61  | THR  | Peptide |
| 1   | D     | 371 | PHE  | Peptide |
| 1   | D     | 61  | THR  | Peptide |
| 1   | D     | 64  | LEU  | Peptide |

## 5.2 Too-close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 3110  | 0        | 3137     | 291     | 0            |
| 1   | B     | 2980  | 0        | 3005     | 312     | 0            |
| 1   | C     | 3113  | 0        | 3139     | 300     | 0            |
| 1   | D     | 3076  | 0        | 3109     | 301     | 0            |
| 2   | A     | 1     | 0        | 0        | 0       | 0            |
| 2   | B     | 1     | 0        | 0        | 0       | 0            |
| 2   | C     | 1     | 0        | 0        | 0       | 0            |
| 2   | D     | 1     | 0        | 0        | 0       | 0            |
| 3   | B     | 21    | 0        | 30       | 5       | 0            |
| 3   | C     | 21    | 0        | 30       | 1       | 0            |
| 3   | D     | 21    | 0        | 30       | 3       | 0            |
| 4   | A     | 13    | 0        | 5        | 3       | 0            |
| 4   | B     | 13    | 0        | 5        | 6       | 0            |
| 4   | C     | 13    | 0        | 5        | 5       | 0            |
| 5   | B     | 1     | 0        | 0        | 0       | 0            |
| 5   | C     | 1     | 0        | 0        | 0       | 0            |
| 5   | D     | 3     | 0        | 0        | 1       | 0            |
| All | All   | 12390 | 0        | 12495    | 1184    | 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 48.

All (1184) 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:419:VAL:HG11 | 1:A:425:ALA:HB2  | 1.25                     | 1.13              |
| 1:C:420:ALA:HB1  | 1:C:421:THR:HA   | 1.36                     | 1.07              |
| 1:B:420:ALA:HB1  | 1:B:421:THR:HA   | 1.38                     | 1.06              |
| 1:C:200:SER:HB2  | 1:C:201:PRO:HD2  | 1.37                     | 1.04              |
| 1:A:377:SER:HB3  | 1:A:380:ALA:HB3  | 1.40                     | 1.03              |
| 1:B:373:THR:HG21 | 1:B:416:MSE:HE2  | 1.41                     | 1.02              |
| 1:B:372:LEU:HD13 | 1:B:414:ALA:HB2  | 1.38                     | 1.01              |
| 1:A:372:LEU:HA   | 1:A:376:ALA:HA   | 1.39                     | 1.01              |
| 1:C:372:LEU:O    | 1:C:376:ALA:HB2  | 1.59                     | 1.01              |
| 1:A:61:THR:HG23  | 1:A:63:ALA:H     | 1.23                     | 1.00              |
| 1:D:259:LYS:HG2  | 1:D:261:LYS:HE3  | 1.42                     | 1.00              |
| 1:C:191:ILE:HG12 | 1:C:228:MSE:HE3  | 1.44                     | 0.98              |
| 1:D:71:ILE:HD13  | 1:C:300:ILE:HD11 | 1.41                     | 0.98              |
| 1:A:196:THR:HG22 | 1:A:198:VAL:H    | 1.27                     | 0.98              |
| 1:D:42:GLU:HG2   | 1:D:43:HIS:H     | 1.26                     | 0.98              |
| 1:A:108:ALA:HB2  | 1:A:317:THR:HG21 | 1.44                     | 0.97              |
| 1:D:372:LEU:HD21 | 1:D:378:ASN:HA   | 1.47                     | 0.97              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:196:THR:HG22 | 1:C:198:VAL:H    | 1.28                     | 0.97              |
| 1:A:372:LEU:O    | 1:A:372:LEU:HD22 | 1.64                     | 0.96              |
| 1:C:151:ASN:HD21 | 1:C:200:SER:HB3  | 1.28                     | 0.96              |
| 1:C:362:ILE:HD11 | 1:C:454:THR:HA   | 1.47                     | 0.96              |
| 1:B:318:ALA:HB3  | 1:B:320:TRP:CZ3  | 2.01                     | 0.95              |
| 1:B:90:ASN:HD22  | 1:A:90:ASN:HD22  | 1.14                     | 0.95              |
| 1:D:58:LEU:HD11  | 1:D:64:LEU:HD23  | 1.48                     | 0.94              |
| 1:A:235:ILE:O    | 1:A:239:LEU:HB2  | 1.67                     | 0.93              |
| 1:B:282:ASN:OD1  | 1:B:288:PHE:HB2  | 1.68                     | 0.93              |
| 1:B:282:ASN:HD21 | 1:B:288:PHE:H    | 1.13                     | 0.92              |
| 1:C:419:VAL:HG21 | 1:C:425:ALA:HB2  | 1.52                     | 0.90              |
| 1:D:368:PHE:O    | 1:D:371:PHE:HB3  | 1.71                     | 0.90              |
| 1:A:71:ILE:O     | 1:A:74:PRO:HD2   | 1.71                     | 0.90              |
| 1:A:371:PHE:O    | 1:A:372:LEU:HB3  | 1.71                     | 0.89              |
| 1:C:434:LYS:CB   | 1:C:437:GLU:HB2  | 2.03                     | 0.88              |
| 1:C:418:PRO:HD3  | 1:C:438:MSE:SE   | 2.23                     | 0.88              |
| 1:D:103:GLY:HA3  | 1:D:198:VAL:HG11 | 1.57                     | 0.87              |
| 1:D:203:ASN:HB3  | 1:D:217:TRP:CZ2  | 2.10                     | 0.87              |
| 1:B:372:LEU:O    | 1:B:376:ALA:HB2  | 1.74                     | 0.86              |
| 1:C:229:LEU:HB3  | 1:C:230:PRO:HD3  | 1.57                     | 0.85              |
| 1:D:51:MSE:CE    | 1:D:335:VAL:HG11 | 2.07                     | 0.85              |
| 1:A:419:VAL:HB   | 1:A:420:ALA:HA   | 1.57                     | 0.85              |
| 1:C:356:MSE:HE3  | 1:C:360:VAL:HG12 | 1.59                     | 0.85              |
| 1:D:367:THR:HG23 | 1:D:450:ILE:HD13 | 1.58                     | 0.85              |
| 1:A:97:ILE:HD12  | 1:A:97:ILE:H     | 1.42                     | 0.84              |
| 1:C:191:ILE:HD13 | 1:C:229:LEU:HA   | 1.59                     | 0.84              |
| 1:B:80:PHE:CE2   | 3:B:503:BNG:H3'1 | 2.11                     | 0.84              |
| 1:D:191:ILE:HG12 | 1:D:228:MSE:HE2  | 1.59                     | 0.84              |
| 1:A:419:VAL:HG11 | 1:A:425:ALA:CB   | 2.07                     | 0.83              |
| 1:A:357:GLY:HA3  | 1:A:361:VAL:HG23 | 1.60                     | 0.83              |
| 1:A:73:VAL:HB    | 1:A:74:PRO:HD3   | 1.61                     | 0.83              |
| 1:B:196:THR:OG1  | 1:B:198:VAL:O    | 1.96                     | 0.83              |
| 1:B:200:SER:HB2  | 1:B:201:PRO:HD2  | 1.59                     | 0.82              |
| 1:B:236:LEU:HD23 | 1:B:441:VAL:HG11 | 1.61                     | 0.82              |
| 1:B:315:GLN:HA   | 1:B:320:TRP:CH2  | 2.15                     | 0.81              |
| 1:B:282:ASN:ND2  | 1:B:288:PHE:H    | 1.78                     | 0.81              |
| 1:D:159:LEU:HB3  | 1:D:160:PRO:HD3  | 1.63                     | 0.81              |
| 1:D:376:ALA:HB3  | 1:D:420:ALA:H    | 1.46                     | 0.81              |
| 1:A:59:TRP:NE1   | 1:A:69:THR:OG1   | 2.13                     | 0.81              |
| 1:D:372:LEU:CD2  | 1:D:378:ASN:HA   | 2.11                     | 0.81              |
| 1:A:282:ASN:OD1  | 1:A:288:PHE:HB2  | 1.81                     | 0.81              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:80:PHE:CE2   | 3:C:503:BNG:H4'2 | 2.15                     | 0.80              |
| 1:B:152:THR:HG22 | 1:B:423:PRO:HD3  | 1.62                     | 0.80              |
| 1:B:229:LEU:HB3  | 1:B:230:PRO:HD3  | 1.63                     | 0.80              |
| 1:C:418:PRO:HA   | 1:C:419:VAL:HG23 | 1.63                     | 0.80              |
| 1:B:123:VAL:HG13 | 1:B:137:MSE:HE2  | 1.64                     | 0.80              |
| 1:C:367:THR:OG1  | 1:C:450:ILE:HD11 | 1.82                     | 0.80              |
| 1:B:367:THR:HA   | 1:B:450:ILE:HD13 | 1.63                     | 0.80              |
| 1:A:207:ALA:HA   | 1:A:212:LEU:HB2  | 1.62                     | 0.80              |
| 1:B:79:PHE:O     | 1:B:80:PHE:HB2   | 1.80                     | 0.79              |
| 1:A:346:ALA:HA   | 1:A:396:PHE:HE2  | 1.47                     | 0.79              |
| 1:C:151:ASN:ND2  | 1:C:200:SER:HB3  | 1.97                     | 0.79              |
| 1:D:357:GLY:HA3  | 1:D:361:VAL:HG23 | 1.62                     | 0.79              |
| 1:A:420:ALA:HB1  | 1:A:421:THR:HA   | 1.64                     | 0.79              |
| 1:A:418:PRO:HD3  | 1:A:438:MSE:SE   | 2.32                     | 0.79              |
| 1:C:419:VAL:HG13 | 1:C:420:ALA:HA   | 1.63                     | 0.79              |
| 1:B:99:LEU:HD12  | 1:B:197:LEU:HD22 | 1.63                     | 0.78              |
| 1:A:315:GLN:HA   | 1:A:320:TRP:CH2  | 2.17                     | 0.78              |
| 1:C:127:ALA:HB1  | 1:C:133:VAL:HG23 | 1.64                     | 0.78              |
| 1:C:130:LYS:HE3  | 1:C:130:LYS:HA   | 1.65                     | 0.78              |
| 1:B:300:ILE:HD11 | 1:A:71:ILE:HD13  | 1.64                     | 0.78              |
| 1:A:267:ILE:HD12 | 1:A:303:LEU:HD23 | 1.65                     | 0.78              |
| 1:B:372:LEU:HD22 | 1:B:376:ALA:HB1  | 1.65                     | 0.78              |
| 1:D:46:VAL:O     | 1:D:50:SER:HB2   | 1.84                     | 0.77              |
| 1:C:78:VAL:O     | 1:C:81:GLY:N     | 2.16                     | 0.77              |
| 1:A:258:ASP:HA   | 1:A:261:LYS:HD3  | 1.67                     | 0.77              |
| 1:A:337:LYS:HE2  | 1:A:391:THR:HG22 | 1.64                     | 0.77              |
| 1:B:358:ILE:O    | 1:B:362:ILE:HG23 | 1.85                     | 0.77              |
| 1:B:210:VAL:HG12 | 1:B:400:PRO:HB2  | 1.65                     | 0.77              |
| 1:C:57:VAL:O     | 1:C:60:LEU:O     | 2.02                     | 0.77              |
| 1:B:159:LEU:HB3  | 1:B:160:PRO:HD3  | 1.66                     | 0.77              |
| 1:B:232:ALA:HA   | 1:B:445:LEU:HD11 | 1.67                     | 0.76              |
| 1:A:349:LEU:O    | 1:A:353:VAL:HG13 | 1.85                     | 0.76              |
| 1:B:418:PRO:HB3  | 1:B:419:VAL:HG13 | 1.67                     | 0.76              |
| 1:A:92:PHE:HD2   | 1:A:327:GLY:HA3  | 1.49                     | 0.76              |
| 1:D:220:PHE:HD1  | 1:D:460:PHE:CE2  | 2.04                     | 0.76              |
| 1:A:210:VAL:HG11 | 1:A:401:VAL:HA   | 1.66                     | 0.76              |
| 1:C:119:ILE:O    | 1:C:123:VAL:HG12 | 1.85                     | 0.76              |
| 1:A:150:SER:HB3  | 1:A:153:ALA:HB3  | 1.68                     | 0.75              |
| 1:A:413:CYS:HB3  | 1:A:415:PHE:CE2  | 2.20                     | 0.75              |
| 1:B:394:GLU:HG2  | 1:B:400:PRO:HG3  | 1.67                     | 0.75              |
| 1:A:47:LEU:HD11  | 1:A:80:PHE:HD1   | 1.50                     | 0.75              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:373:THR:HG22 | 1:D:374:GLU:H    | 1.50                     | 0.75              |
| 1:A:196:THR:N    | 1:A:217:TRP:HZ3  | 1.85                     | 0.75              |
| 1:A:419:VAL:CG1  | 1:A:425:ALA:HB2  | 2.13                     | 0.75              |
| 1:A:434:LYS:HB3  | 1:A:434:LYS:NZ   | 2.02                     | 0.74              |
| 1:B:349:LEU:O    | 1:B:353:VAL:HG13 | 1.86                     | 0.74              |
| 1:B:352:MSE:O    | 1:B:356:MSE:HG3  | 1.86                     | 0.74              |
| 1:B:414:ALA:HB3  | 1:B:421:THR:HG23 | 1.69                     | 0.74              |
| 1:A:48:GLY:HA3   | 1:A:341:THR:OG1  | 1.88                     | 0.74              |
| 1:B:208:ALA:HB1  | 1:B:330:LEU:HD11 | 1.70                     | 0.74              |
| 1:C:144:LEU:HA   | 1:C:147:MSE:HE3  | 1.68                     | 0.74              |
| 1:B:72:LEU:HD13  | 1:A:301:LEU:HD22 | 1.69                     | 0.74              |
| 1:D:67:THR:O     | 1:D:71:ILE:HD12  | 1.88                     | 0.74              |
| 1:D:200:SER:HB2  | 1:D:201:PRO:CD   | 2.17                     | 0.74              |
| 1:A:315:GLN:HG3  | 1:A:320:TRP:CZ3  | 2.23                     | 0.74              |
| 1:D:373:THR:HG22 | 1:D:374:GLU:N    | 2.03                     | 0.74              |
| 1:C:110:MSE:HG2  | 1:C:115:LEU:HD23 | 1.69                     | 0.73              |
| 1:A:196:THR:HG23 | 1:A:214:PHE:HE1  | 1.53                     | 0.73              |
| 1:A:356:MSE:HE3  | 1:A:360:VAL:HG12 | 1.68                     | 0.73              |
| 1:A:162:VAL:O    | 1:A:166:LEU:HD22 | 1.87                     | 0.73              |
| 1:C:362:ILE:CD1  | 1:C:454:THR:HA   | 2.16                     | 0.73              |
| 1:D:200:SER:HB2  | 1:D:201:PRO:HD3  | 1.69                     | 0.73              |
| 1:A:159:LEU:HB3  | 1:A:160:PRO:HD3  | 1.71                     | 0.73              |
| 1:A:108:ALA:HB2  | 1:A:317:THR:CG2  | 2.18                     | 0.73              |
| 1:D:123:VAL:O    | 1:D:126:MSE:HB3  | 1.88                     | 0.73              |
| 1:D:392:VAL:O    | 1:D:395:ALA:N    | 2.22                     | 0.73              |
| 1:A:59:TRP:NE1   | 1:A:69:THR:HG1   | 1.85                     | 0.72              |
| 1:A:24:ILE:HD11  | 1:A:61:THR:HG21  | 1.69                     | 0.72              |
| 1:D:370:VAL:O    | 1:D:373:THR:HB   | 1.89                     | 0.72              |
| 1:D:430:SER:C    | 1:D:432:HIS:H    | 1.94                     | 0.72              |
| 1:C:200:SER:HB2  | 1:C:201:PRO:CD   | 2.17                     | 0.72              |
| 1:A:285:LEU:HD23 | 1:A:285:LEU:O    | 1.90                     | 0.72              |
| 1:D:127:ALA:C    | 1:D:128:GLN:HG2  | 2.15                     | 0.72              |
| 1:A:99:LEU:HD22  | 1:A:296:ALA:HB2  | 1.72                     | 0.72              |
| 1:C:213:SER:H    | 1:C:216:ASP:HB2  | 1.54                     | 0.72              |
| 1:D:114:GLY:O    | 1:D:118:VAL:HG12 | 1.90                     | 0.72              |
| 1:C:373:THR:HG22 | 1:C:417:LEU:HG   | 1.71                     | 0.72              |
| 1:A:339:THR:OG1  | 1:A:341:THR:OG1  | 2.04                     | 0.72              |
| 1:C:282:ASN:OD1  | 1:C:288:PHE:HB2  | 1.90                     | 0.72              |
| 1:D:236:LEU:HD12 | 1:D:441:VAL:HG21 | 1.71                     | 0.71              |
| 1:A:141:VAL:O    | 1:A:145:LEU:HB2  | 1.91                     | 0.71              |
| 1:C:194:ILE:O    | 1:C:195:ALA:HB3  | 1.91                     | 0.71              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:372:LEU:HD21 | 1:D:378:ASN:CA   | 2.20                     | 0.71              |
| 1:B:109:ALA:HA   | 1:B:309:VAL:HG22 | 1.72                     | 0.71              |
| 1:A:134:ALA:O    | 1:A:138:LEU:HB2  | 1.90                     | 0.71              |
| 1:B:106:LEU:HD12 | 1:B:268:PHE:HD1  | 1.55                     | 0.71              |
| 1:C:390:ALA:HB2  | 1:C:404:SER:OG   | 1.90                     | 0.71              |
| 1:D:86:GLN:HE22  | 1:C:94:ASN:HA    | 1.56                     | 0.71              |
| 1:B:139:PHE:O    | 1:B:142:THR:HG22 | 1.91                     | 0.70              |
| 1:D:131:MSE:O    | 1:D:134:ALA:N    | 2.24                     | 0.70              |
| 1:B:337:LYS:HE2  | 1:B:391:THR:HG22 | 1.73                     | 0.70              |
| 1:A:372:LEU:HD21 | 1:A:411:ALA:O    | 1.90                     | 0.70              |
| 1:D:259:LYS:HG3  | 1:D:261:LYS:H    | 1.56                     | 0.70              |
| 1:A:107:ALA:HA   | 1:A:110:MSE:HE2  | 1.73                     | 0.70              |
| 1:D:71:ILE:HD13  | 1:C:300:ILE:CD1  | 2.19                     | 0.70              |
| 1:D:402:LEU:HD23 | 1:D:403:LEU:N    | 2.07                     | 0.70              |
| 1:B:182:LEU:HD22 | 1:B:427:VAL:HB   | 1.73                     | 0.70              |
| 1:B:340:GLY:O    | 1:B:343:VAL:N    | 2.25                     | 0.70              |
| 1:A:92:PHE:HE2   | 1:A:328:GLY:N    | 1.89                     | 0.70              |
| 1:A:346:ALA:HA   | 1:A:396:PHE:CE2  | 2.27                     | 0.70              |
| 1:B:332:LEU:HA   | 1:B:335:VAL:HG12 | 1.73                     | 0.69              |
| 1:C:151:ASN:O    | 1:C:154:THR:HG22 | 1.92                     | 0.69              |
| 1:D:259:LYS:CG   | 1:D:261:LYS:HE3  | 2.22                     | 0.69              |
| 1:A:66:VAL:HG13  | 1:A:325:LEU:HD13 | 1.73                     | 0.69              |
| 1:B:106:LEU:O    | 1:B:110:MSE:HE2  | 1.92                     | 0.69              |
| 1:B:372:LEU:HG   | 1:B:411:ALA:HA   | 1.74                     | 0.69              |
| 1:D:73:VAL:HB    | 1:D:74:PRO:HD3   | 1.75                     | 0.68              |
| 1:A:59:TRP:CD1   | 1:A:69:THR:HG1   | 2.11                     | 0.68              |
| 1:C:115:LEU:O    | 1:C:118:VAL:HG13 | 1.93                     | 0.68              |
| 1:A:267:ILE:CD1  | 1:A:303:LEU:HD23 | 2.23                     | 0.68              |
| 1:D:42:GLU:HG2   | 1:D:43:HIS:N     | 2.03                     | 0.68              |
| 1:B:315:GLN:HA   | 1:B:320:TRP:HH2  | 1.58                     | 0.68              |
| 1:C:198:VAL:O    | 1:C:198:VAL:HG23 | 1.92                     | 0.68              |
| 1:B:152:THR:HG23 | 4:B:501:CIT:H41  | 1.76                     | 0.68              |
| 1:A:58:LEU:HA    | 1:A:61:THR:HG22  | 1.76                     | 0.68              |
| 1:A:357:GLY:CA   | 1:A:358:ILE:C    | 2.66                     | 0.68              |
| 1:A:166:LEU:HD23 | 1:A:166:LEU:O    | 1.94                     | 0.67              |
| 1:D:323:LEU:HA   | 1:D:326:PHE:HD2  | 1.59                     | 0.67              |
| 1:D:362:ILE:HG21 | 1:D:458:MSE:HE1  | 1.76                     | 0.67              |
| 1:C:212:LEU:HD22 | 1:C:216:ASP:HB3  | 1.76                     | 0.67              |
| 1:B:311:TRP:HB3  | 1:A:65:HIS:CD2   | 2.30                     | 0.67              |
| 1:C:145:LEU:HD22 | 1:C:149:ILE:HD11 | 1.77                     | 0.67              |
| 1:C:447:ILE:HA   | 1:C:450:ILE:HG22 | 1.77                     | 0.67              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:47:LEU:HD21  | 1:D:80:PHE:HB3   | 1.74                     | 0.67              |
| 1:B:45:VAL:HG11  | 1:B:344:PHE:CD1  | 2.30                     | 0.67              |
| 1:B:455:ALA:O    | 1:B:459:LEU:HB2  | 1.95                     | 0.67              |
| 1:B:194:ILE:HA   | 1:B:203:ASN:HD21 | 1.60                     | 0.67              |
| 1:A:384:LEU:O    | 1:A:387:PRO:HD2  | 1.95                     | 0.67              |
| 1:A:430:SER:O    | 1:A:430:SER:OG   | 2.08                     | 0.67              |
| 1:C:25:VAL:O     | 1:C:29:VAL:HG23  | 1.95                     | 0.67              |
| 1:B:115:LEU:O    | 1:B:119:ILE:HG12 | 1.95                     | 0.66              |
| 1:A:373:THR:HG23 | 1:A:415:PHE:O    | 1.95                     | 0.66              |
| 1:B:360:VAL:O    | 1:B:364:VAL:HG23 | 1.95                     | 0.66              |
| 1:D:420:ALA:HB1  | 1:D:421:THR:HA   | 1.75                     | 0.66              |
| 1:B:372:LEU:O    | 1:B:372:LEU:HD22 | 1.96                     | 0.66              |
| 1:D:21:ASN:HA    | 1:D:24:ILE:HD12  | 1.78                     | 0.66              |
| 1:A:97:ILE:H     | 1:A:97:ILE:CD1   | 2.09                     | 0.66              |
| 1:C:196:THR:HG22 | 1:C:198:VAL:N    | 2.07                     | 0.66              |
| 1:A:403:LEU:N    | 1:A:403:LEU:HD23 | 2.11                     | 0.66              |
| 1:A:418:PRO:HG3  | 1:A:428:PHE:CE1  | 2.30                     | 0.66              |
| 1:D:201:PRO:HD2  | 1:D:202:PRO:HD2  | 1.76                     | 0.66              |
| 1:C:146:SER:HB2  | 1:C:154:THR:HG21 | 1.78                     | 0.66              |
| 1:D:152:THR:HG23 | 1:D:422:PRO:HB2  | 1.78                     | 0.65              |
| 1:B:24:ILE:O     | 1:B:27:ALA:HB3   | 1.96                     | 0.65              |
| 1:B:73:VAL:HB    | 1:B:74:PRO:HD3   | 1.78                     | 0.65              |
| 1:A:97:ILE:HD12  | 1:A:97:ILE:N     | 2.12                     | 0.65              |
| 1:A:332:LEU:HA   | 1:A:335:VAL:HG22 | 1.77                     | 0.65              |
| 1:B:372:LEU:HD11 | 1:B:411:ALA:O    | 1.97                     | 0.65              |
| 1:C:418:PRO:HG3  | 1:C:428:PHE:CD2  | 2.32                     | 0.65              |
| 1:D:51:MSE:HE3   | 1:D:335:VAL:HG11 | 1.79                     | 0.65              |
| 1:C:141:VAL:O    | 1:C:145:LEU:HB2  | 1.97                     | 0.65              |
| 1:C:358:ILE:O    | 1:C:362:ILE:HG23 | 1.95                     | 0.65              |
| 1:B:376:ALA:HB3  | 1:B:420:ALA:HB3  | 1.79                     | 0.65              |
| 1:D:320:TRP:CE3  | 1:D:323:LEU:HD12 | 2.32                     | 0.64              |
| 1:D:360:VAL:O    | 1:D:364:VAL:HG23 | 1.95                     | 0.64              |
| 1:D:101:LEU:HD13 | 1:D:323:LEU:HD11 | 1.78                     | 0.64              |
| 1:B:384:LEU:O    | 1:B:387:PRO:HD2  | 1.98                     | 0.64              |
| 1:A:100:PHE:CE1  | 1:A:198:VAL:HG13 | 2.31                     | 0.64              |
| 1:A:277:PHE:HB3  | 1:A:281:ILE:HD13 | 1.79                     | 0.64              |
| 1:C:379:THR:OG1  | 4:C:501:CIT:H22  | 1.98                     | 0.64              |
| 1:D:432:HIS:C    | 1:D:434:LYS:H    | 2.04                     | 0.64              |
| 1:C:69:THR:O     | 1:C:72:LEU:HB3   | 1.98                     | 0.64              |
| 1:C:331:CYS:O    | 1:C:335:VAL:HG23 | 1.98                     | 0.64              |
| 1:C:394:GLU:HG3  | 1:C:400:PRO:HG3  | 1.78                     | 0.64              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:92:PHE:CD2   | 1:A:327:GLY:HA3  | 2.32                     | 0.64              |
| 1:B:372:LEU:CD1  | 1:B:414:ALA:HB2  | 2.20                     | 0.64              |
| 1:D:267:ILE:HD13 | 1:D:303:LEU:HD23 | 1.78                     | 0.63              |
| 1:B:372:LEU:O    | 1:B:376:ALA:CB   | 2.44                     | 0.63              |
| 1:C:259:LYS:CB   | 1:C:261:LYS:HE3  | 2.27                     | 0.63              |
| 1:D:194:ILE:CG1  | 1:D:195:ALA:N    | 2.62                     | 0.63              |
| 1:A:357:GLY:HA3  | 1:A:358:ILE:C    | 2.22                     | 0.63              |
| 1:A:320:TRP:CD1  | 1:A:323:LEU:HD12 | 2.33                     | 0.63              |
| 1:C:123:VAL:HG22 | 1:C:137:MSE:HG3  | 1.79                     | 0.63              |
| 1:D:372:LEU:HG   | 1:D:414:ALA:HB2  | 1.81                     | 0.63              |
| 1:C:48:GLY:HA3   | 1:C:341:THR:OG1  | 1.98                     | 0.63              |
| 1:B:461:TRP:HA   | 1:B:461:TRP:CE3  | 2.34                     | 0.63              |
| 1:A:163:LEU:O    | 1:A:166:LEU:O    | 2.17                     | 0.63              |
| 1:D:182:LEU:HB3  | 1:D:427:VAL:HB   | 1.81                     | 0.63              |
| 1:C:261:LYS:H    | 1:C:261:LYS:HD2  | 1.62                     | 0.63              |
| 1:C:310:HIS:O    | 1:C:313:GLU:HG2  | 1.99                     | 0.63              |
| 1:B:82:ILE:HD13  | 1:B:335:VAL:HG23 | 1.81                     | 0.62              |
| 1:C:79:PHE:O     | 1:C:80:PHE:HB2   | 1.98                     | 0.62              |
| 1:B:418:PRO:HD3  | 1:B:438:MSE:SE   | 2.49                     | 0.62              |
| 1:C:115:LEU:O    | 1:C:119:ILE:HG13 | 1.99                     | 0.62              |
| 1:B:362:ILE:HG21 | 1:B:458:MSE:HE1  | 1.81                     | 0.62              |
| 1:A:315:GLN:HG3  | 1:A:320:TRP:HZ3  | 1.62                     | 0.62              |
| 1:A:335:VAL:O    | 1:A:339:THR:HG23 | 1.98                     | 0.62              |
| 1:C:105:ALA:HA   | 1:C:314:ILE:HD12 | 1.80                     | 0.62              |
| 1:A:232:ALA:HB1  | 1:A:445:LEU:HD21 | 1.81                     | 0.62              |
| 1:C:145:LEU:HD22 | 1:C:149:ILE:CD1  | 2.29                     | 0.62              |
| 1:C:222:LEU:O    | 1:C:222:LEU:HD22 | 1.99                     | 0.62              |
| 1:B:109:ALA:HA   | 1:B:309:VAL:CG2  | 2.30                     | 0.62              |
| 1:A:458:MSE:HE3  | 1:A:458:MSE:HA   | 1.80                     | 0.62              |
| 1:C:263:VAL:O    | 1:C:267:ILE:HG13 | 1.99                     | 0.62              |
| 1:B:105:ALA:HA   | 1:B:314:ILE:HD12 | 1.81                     | 0.62              |
| 1:C:213:SER:N    | 1:C:216:ASP:HB2  | 2.13                     | 0.62              |
| 1:C:201:PRO:O    | 1:C:205:ILE:CG1  | 2.47                     | 0.62              |
| 1:D:422:PRO:O    | 1:D:426:ILE:HG12 | 2.00                     | 0.62              |
| 1:C:212:LEU:CD2  | 1:C:216:ASP:HB3  | 2.29                     | 0.62              |
| 1:D:403:LEU:O    | 1:D:407:ILE:HG13 | 2.00                     | 0.62              |
| 1:B:151:ASN:O    | 1:B:154:THR:HG22 | 1.99                     | 0.62              |
| 1:A:201:PRO:HB2  | 1:A:379:THR:HG23 | 1.81                     | 0.62              |
| 1:D:309:VAL:CG2  | 1:D:313:GLU:HG3  | 2.30                     | 0.62              |
| 1:D:366:ALA:O    | 1:D:369:VAL:N    | 2.31                     | 0.62              |
| 1:C:203:ASN:OD1  | 1:C:203:ASN:N    | 2.33                     | 0.62              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:201:PRO:CD   | 1:D:202:PRO:HD2  | 2.29                     | 0.61              |
| 1:D:42:GLU:CG    | 1:D:43:HIS:H     | 2.04                     | 0.61              |
| 1:B:28:ASP:HB2   | 1:B:57:VAL:HG11  | 1.81                     | 0.61              |
| 1:B:194:ILE:O    | 1:B:195:ALA:HB3  | 1.99                     | 0.61              |
| 1:A:447:ILE:HA   | 1:A:450:ILE:HG23 | 1.80                     | 0.61              |
| 1:C:191:ILE:CG1  | 1:C:228:MSE:HE3  | 2.26                     | 0.61              |
| 1:D:267:ILE:HG21 | 1:D:303:LEU:CD2  | 2.30                     | 0.61              |
| 1:D:73:VAL:HG12  | 1:D:331:CYS:SG   | 2.40                     | 0.61              |
| 1:D:259:LYS:O    | 1:D:262:VAL:HG12 | 2.00                     | 0.61              |
| 1:D:207:ALA:CB   | 1:D:212:LEU:HB2  | 2.30                     | 0.61              |
| 1:D:362:ILE:HG12 | 1:D:454:THR:HG23 | 1.82                     | 0.61              |
| 1:D:432:HIS:C    | 1:D:434:LYS:N    | 2.56                     | 0.61              |
| 1:A:22:SER:O     | 1:A:25:VAL:N     | 2.33                     | 0.61              |
| 1:A:196:THR:HG22 | 1:A:198:VAL:N    | 2.09                     | 0.61              |
| 1:D:115:LEU:HA   | 1:D:118:VAL:CG1  | 2.31                     | 0.61              |
| 1:B:101:LEU:O    | 1:B:101:LEU:HD23 | 1.99                     | 0.61              |
| 1:C:362:ILE:HG12 | 1:C:458:MSE:CE   | 2.31                     | 0.61              |
| 1:B:267:ILE:HG21 | 1:B:303:LEU:HG   | 1.81                     | 0.61              |
| 1:B:308:VAL:HG12 | 1:B:309:VAL:HG23 | 1.83                     | 0.61              |
| 1:C:111:HIS:O    | 1:C:114:GLY:N    | 2.29                     | 0.61              |
| 1:D:194:ILE:HG13 | 1:D:195:ALA:N    | 2.16                     | 0.61              |
| 1:D:185:VAL:HG12 | 1:D:186:ALA:N    | 2.16                     | 0.60              |
| 1:A:203:ASN:HB3  | 1:A:217:TRP:CZ2  | 2.35                     | 0.60              |
| 1:C:418:PRO:CD   | 1:C:438:MSE:SE   | 2.99                     | 0.60              |
| 1:A:203:ASN:N    | 1:A:203:ASN:OD1  | 2.32                     | 0.60              |
| 1:B:374:GLU:O    | 1:B:374:GLU:HG3  | 2.01                     | 0.60              |
| 1:C:194:ILE:HG13 | 1:C:195:ALA:N    | 2.15                     | 0.60              |
| 1:D:376:ALA:HB1  | 1:D:420:ALA:HB3  | 1.83                     | 0.60              |
| 1:A:24:ILE:HG12  | 1:A:63:ALA:HB2   | 1.83                     | 0.60              |
| 1:A:206:ALA:O    | 1:A:210:VAL:HG22 | 2.00                     | 0.60              |
| 1:D:74:PRO:HG2   | 1:D:92:PHE:CE1   | 2.37                     | 0.60              |
| 1:D:374:GLU:C    | 1:D:376:ALA:H    | 2.09                     | 0.60              |
| 1:D:430:SER:O    | 1:D:432:HIS:N    | 2.34                     | 0.60              |
| 1:B:144:LEU:O    | 1:B:147:MSE:HE2  | 2.01                     | 0.60              |
| 1:C:152:THR:HG23 | 4:C:501:CIT:O4   | 2.02                     | 0.60              |
| 1:C:423:PRO:O    | 1:C:427:VAL:HG22 | 2.02                     | 0.60              |
| 1:D:277:PHE:O    | 1:D:280:PRO:HD2  | 2.00                     | 0.60              |
| 1:B:267:ILE:HD12 | 1:B:303:LEU:HD23 | 1.84                     | 0.60              |
| 1:A:47:LEU:HD11  | 1:A:80:PHE:CD1   | 2.33                     | 0.60              |
| 1:C:214:PHE:CD2  | 1:C:214:PHE:C    | 2.80                     | 0.60              |
| 1:A:133:VAL:O    | 1:A:137:MSE:HB2  | 2.02                     | 0.60              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:419:VAL:HG21 | 1:C:425:ALA:CB   | 2.28                     | 0.60              |
| 1:C:442:GLY:O    | 1:C:446:ASN:HB2  | 2.01                     | 0.60              |
| 1:D:201:PRO:N    | 1:D:202:PRO:HD2  | 2.16                     | 0.60              |
| 1:B:378:ASN:HD21 | 1:B:421:THR:HG21 | 1.66                     | 0.60              |
| 1:A:180:PHE:CD2  | 1:A:180:PHE:O    | 2.55                     | 0.60              |
| 1:C:455:ALA:O    | 1:C:459:LEU:HD12 | 2.02                     | 0.60              |
| 1:C:325:LEU:CD2  | 1:C:379:THR:HG22 | 2.31                     | 0.60              |
| 1:A:196:THR:HG23 | 1:A:214:PHE:CE1  | 2.35                     | 0.59              |
| 1:C:197:LEU:HD12 | 1:C:214:PHE:HA   | 1.82                     | 0.59              |
| 1:A:201:PRO:HG2  | 1:A:379:THR:OG1  | 2.02                     | 0.59              |
| 1:A:285:LEU:HD23 | 1:A:285:LEU:C    | 2.27                     | 0.59              |
| 1:C:419:VAL:HG13 | 1:C:420:ALA:CA   | 2.32                     | 0.59              |
| 1:D:80:PHE:CZ    | 3:D:502:BNG:H3'1 | 2.37                     | 0.59              |
| 1:B:152:THR:HG23 | 4:B:501:CIT:C4   | 2.31                     | 0.59              |
| 1:D:282:ASN:OD1  | 1:D:288:PHE:HB2  | 2.02                     | 0.59              |
| 1:B:93:ALA:HB2   | 1:A:93:ALA:HB2   | 1.84                     | 0.59              |
| 1:B:118:VAL:O    | 1:B:122:LYS:N    | 2.30                     | 0.59              |
| 1:C:367:THR:O    | 1:C:370:VAL:HG23 | 2.03                     | 0.59              |
| 1:D:67:THR:HG21  | 1:C:311:TRP:CZ2  | 2.38                     | 0.59              |
| 1:B:70:ALA:HB2   | 1:B:325:LEU:HD12 | 1.83                     | 0.59              |
| 1:B:239:LEU:HD13 | 1:B:441:VAL:HA   | 1.84                     | 0.59              |
| 1:A:282:ASN:HD21 | 1:A:288:PHE:H    | 1.49                     | 0.59              |
| 1:D:183:LEU:HG   | 1:D:187:TYR:CZ   | 2.38                     | 0.59              |
| 1:B:31:LEU:HG    | 1:B:35:LEU:HD11  | 1.85                     | 0.59              |
| 1:C:38:PHE:O     | 1:C:39:LEU:C     | 2.46                     | 0.59              |
| 1:D:135:VAL:O    | 1:D:138:LEU:HB2  | 2.02                     | 0.59              |
| 1:B:410:ALA:O    | 1:B:413:CYS:HB2  | 2.03                     | 0.59              |
| 1:A:152:THR:HB   | 1:A:422:PRO:HG2  | 1.84                     | 0.59              |
| 1:A:231:MSE:HE3  | 1:A:448:ALA:HB1  | 1.84                     | 0.59              |
| 1:A:372:LEU:HD22 | 1:A:376:ALA:HB1  | 1.84                     | 0.59              |
| 1:C:232:ALA:HA   | 1:C:445:LEU:CD1  | 2.32                     | 0.59              |
| 1:D:335:VAL:O    | 1:D:339:THR:HG23 | 2.02                     | 0.59              |
| 1:B:149:ILE:HD13 | 1:B:154:THR:HB   | 1.85                     | 0.59              |
| 1:C:222:LEU:O    | 1:C:226:MSE:HG2  | 2.02                     | 0.59              |
| 1:C:282:ASN:HD21 | 1:C:288:PHE:H    | 1.49                     | 0.59              |
| 1:D:366:ALA:O    | 1:D:369:VAL:HB   | 2.02                     | 0.59              |
| 1:D:430:SER:C    | 1:D:432:HIS:N    | 2.60                     | 0.59              |
| 1:A:370:VAL:O    | 1:A:371:PHE:HB3  | 2.02                     | 0.59              |
| 1:A:372:LEU:HD23 | 1:A:378:ASN:HA   | 1.85                     | 0.59              |
| 1:B:372:LEU:HD21 | 1:B:378:ASN:HA   | 1.85                     | 0.59              |
| 1:A:420:ALA:HB1  | 1:A:421:THR:CA   | 2.32                     | 0.59              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:434:LYS:HB3  | 1:A:434:LYS:HZ3  | 1.68                     | 0.58              |
| 1:C:175:ARG:O    | 1:C:179:VAL:O    | 2.21                     | 0.58              |
| 1:D:203:ASN:HB3  | 1:D:217:TRP:CE2  | 2.38                     | 0.58              |
| 1:C:215:THR:HA   | 1:C:218:MSE:HB3  | 1.84                     | 0.58              |
| 1:D:289:LYS:O    | 1:C:85:THR:OG1   | 2.17                     | 0.58              |
| 1:B:214:PHE:HE2  | 1:B:218:MSE:SE   | 2.36                     | 0.58              |
| 1:B:373:THR:CG2  | 1:B:416:MSE:HE2  | 2.26                     | 0.58              |
| 1:B:424:ASN:CG   | 1:B:438:MSE:HE1  | 2.28                     | 0.58              |
| 1:C:123:VAL:HG11 | 1:C:141:VAL:CG2  | 2.32                     | 0.58              |
| 1:C:144:LEU:O    | 1:C:147:MSE:HB2  | 2.02                     | 0.58              |
| 1:B:101:LEU:HD23 | 1:B:101:LEU:C    | 2.28                     | 0.58              |
| 1:A:372:LEU:C    | 1:A:372:LEU:HD13 | 2.28                     | 0.58              |
| 1:C:73:VAL:HB    | 1:C:74:PRO:HD3   | 1.84                     | 0.58              |
| 1:C:447:ILE:O    | 1:C:450:ILE:HG22 | 2.03                     | 0.58              |
| 1:C:210:VAL:HG12 | 1:C:400:PRO:HB2  | 1.86                     | 0.58              |
| 1:D:65:HIS:CG    | 1:D:66:VAL:H     | 2.21                     | 0.58              |
| 1:A:294:LEU:O    | 1:A:298:GLY:N    | 2.28                     | 0.58              |
| 1:C:183:LEU:HD11 | 1:C:438:MSE:HG2  | 1.85                     | 0.58              |
| 1:D:200:SER:O    | 1:D:203:ASN:OD1  | 2.22                     | 0.58              |
| 1:B:43:HIS:HE1   | 3:B:503:BNG:H4   | 1.69                     | 0.58              |
| 1:C:336:LEU:HB3  | 1:C:342:SER:OG   | 2.04                     | 0.58              |
| 1:A:282:ASN:HB2  | 1:A:291:PHE:CD2  | 2.39                     | 0.57              |
| 1:A:297:LEU:O    | 1:A:300:ILE:HG23 | 2.04                     | 0.57              |
| 1:B:123:VAL:HG13 | 1:B:137:MSE:CE   | 2.35                     | 0.57              |
| 1:B:123:VAL:HG11 | 1:B:141:VAL:HG23 | 1.84                     | 0.57              |
| 1:D:80:PHE:CE1   | 3:D:502:BNG:H5'1 | 2.39                     | 0.57              |
| 1:B:378:ASN:OD1  | 1:B:421:THR:HG22 | 2.04                     | 0.57              |
| 1:C:135:VAL:HG23 | 1:C:136:PHE:N    | 2.20                     | 0.57              |
| 1:C:180:PHE:O    | 1:C:184:GLY:N    | 2.20                     | 0.57              |
| 1:D:59:TRP:CD1   | 1:D:69:THR:HG21  | 2.39                     | 0.57              |
| 1:B:461:TRP:HA   | 1:B:461:TRP:HE3  | 1.69                     | 0.57              |
| 1:A:267:ILE:HG21 | 1:A:303:LEU:CD2  | 2.35                     | 0.57              |
| 1:A:424:ASN:O    | 1:A:427:VAL:HG22 | 2.05                     | 0.57              |
| 1:D:115:LEU:O    | 1:D:119:ILE:HG13 | 2.04                     | 0.57              |
| 1:C:54:PHE:C     | 1:C:54:PHE:CD2   | 2.81                     | 0.57              |
| 1:C:362:ILE:HD11 | 1:C:454:THR:CA   | 2.30                     | 0.57              |
| 1:D:372:LEU:CD1  | 1:D:376:ALA:HB1  | 2.34                     | 0.57              |
| 1:B:350:SER:O    | 1:B:353:VAL:HG22 | 2.04                     | 0.57              |
| 1:A:372:LEU:O    | 1:A:376:ALA:HB2  | 2.05                     | 0.57              |
| 1:D:203:ASN:ND2  | 1:D:217:TRP:CH2  | 2.71                     | 0.57              |
| 1:B:419:VAL:HG12 | 1:B:421:THR:O    | 2.04                     | 0.57              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:279:SER:HB3  | 1:B:280:PRO:HD3  | 1.87                     | 0.57              |
| 1:A:78:VAL:HA    | 1:A:83:PHE:O     | 2.05                     | 0.57              |
| 1:A:372:LEU:O    | 1:A:372:LEU:CD2  | 2.47                     | 0.57              |
| 1:D:372:LEU:HD21 | 1:D:378:ASN:CB   | 2.35                     | 0.56              |
| 1:C:282:ASN:ND2  | 1:C:288:PHE:H    | 2.03                     | 0.56              |
| 1:D:61:THR:OG1   | 1:D:62:GLU:N     | 2.37                     | 0.56              |
| 1:B:318:ALA:HB3  | 1:B:320:TRP:CH2  | 2.38                     | 0.56              |
| 1:A:200:SER:HB2  | 1:A:201:PRO:HD2  | 1.86                     | 0.56              |
| 1:C:40:PRO:HG2   | 1:C:41:PHE:H     | 1.70                     | 0.56              |
| 1:C:110:MSE:CG   | 1:C:115:LEU:HD23 | 2.34                     | 0.56              |
| 1:C:201:PRO:O    | 1:C:205:ILE:HG13 | 2.04                     | 0.56              |
| 1:D:56:ALA:HB2   | 1:D:384:LEU:HD11 | 1.87                     | 0.56              |
| 1:B:418:PRO:CB   | 1:B:419:VAL:HG13 | 2.36                     | 0.56              |
| 1:A:351:ASP:OD1  | 1:A:351:ASP:N    | 2.39                     | 0.56              |
| 1:D:183:LEU:HB3  | 1:D:236:LEU:HD21 | 1.85                     | 0.56              |
| 1:D:207:ALA:HA   | 1:D:212:LEU:HB2  | 1.87                     | 0.56              |
| 1:D:267:ILE:HG21 | 1:D:303:LEU:HD21 | 1.87                     | 0.56              |
| 1:D:279:SER:HB3  | 1:D:280:PRO:HD3  | 1.87                     | 0.56              |
| 1:B:86:GLN:OE1   | 1:A:95:SER:N     | 2.39                     | 0.56              |
| 1:D:210:VAL:HG11 | 1:D:404:SER:OG   | 2.06                     | 0.56              |
| 1:B:320:TRP:O    | 1:B:324:LEU:HD13 | 2.05                     | 0.56              |
| 1:C:114:GLY:O    | 1:C:118:VAL:HG12 | 2.06                     | 0.56              |
| 1:B:194:ILE:HB   | 1:B:217:TRP:HH2  | 1.70                     | 0.56              |
| 1:B:282:ASN:HD21 | 1:B:288:PHE:N    | 1.95                     | 0.56              |
| 1:C:373:THR:HG21 | 1:C:416:MSE:HE2  | 1.87                     | 0.56              |
| 1:D:214:PHE:HD2  | 1:D:214:PHE:O    | 1.89                     | 0.56              |
| 1:A:86:GLN:O     | 1:A:89:LEU:N     | 2.39                     | 0.56              |
| 1:D:99:LEU:O     | 1:D:99:LEU:HD12  | 2.06                     | 0.56              |
| 1:D:194:ILE:HG12 | 1:D:225:ALA:HB2  | 1.88                     | 0.56              |
| 1:B:146:SER:HA   | 1:B:149:ILE:CD1  | 2.35                     | 0.56              |
| 4:B:501:CIT:H42  | 4:B:501:CIT:O2   | 2.06                     | 0.56              |
| 1:B:39:LEU:HD13  | 1:B:40:PRO:HD2   | 1.87                     | 0.55              |
| 1:B:100:PHE:CD1  | 1:B:198:VAL:HG12 | 2.41                     | 0.55              |
| 1:A:92:PHE:CE2   | 1:A:328:GLY:N    | 2.74                     | 0.55              |
| 1:A:195:ALA:O    | 1:A:218:MSE:HG3  | 2.06                     | 0.55              |
| 1:D:150:SER:HB3  | 1:D:153:ALA:HB3  | 1.88                     | 0.55              |
| 1:A:77:ALA:O     | 1:A:78:VAL:HB    | 2.05                     | 0.55              |
| 1:D:372:LEU:O    | 1:D:373:THR:C    | 2.49                     | 0.55              |
| 1:D:203:ASN:OD1  | 1:D:203:ASN:N    | 2.37                     | 0.55              |
| 1:B:325:LEU:HD23 | 1:B:379:THR:HG22 | 1.88                     | 0.55              |
| 1:A:24:ILE:O     | 1:A:24:ILE:HD12  | 2.07                     | 0.55              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:422:PRO:O    | 1:C:423:PRO:C    | 2.47                     | 0.55              |
| 1:B:66:VAL:CG1   | 1:B:325:LEU:HD13 | 2.36                     | 0.55              |
| 1:B:372:LEU:HD22 | 1:B:376:ALA:CB   | 2.34                     | 0.55              |
| 1:D:60:LEU:C     | 1:D:61:THR:O     | 2.48                     | 0.55              |
| 1:A:145:LEU:HD13 | 1:A:149:ILE:HG13 | 1.89                     | 0.55              |
| 1:B:31:LEU:O     | 1:B:35:LEU:HD12  | 2.07                     | 0.55              |
| 1:B:213:SER:H    | 1:B:216:ASP:HB2  | 1.72                     | 0.55              |
| 1:B:413:CYS:O    | 1:B:415:PHE:CD2  | 2.60                     | 0.55              |
| 1:B:414:ALA:HB3  | 1:B:421:THR:CG2  | 2.35                     | 0.55              |
| 1:B:418:PRO:HG3  | 1:B:438:MSE:SE   | 2.57                     | 0.55              |
| 1:A:227:MSE:O    | 1:A:230:PRO:HD2  | 2.06                     | 0.55              |
| 1:C:152:THR:HG22 | 1:C:423:PRO:HD3  | 1.89                     | 0.55              |
| 1:D:341:THR:O    | 1:D:345:LEU:HG   | 2.07                     | 0.55              |
| 1:C:159:LEU:HB3  | 1:C:160:PRO:HD3  | 1.88                     | 0.55              |
| 1:D:418:PRO:HB3  | 1:D:424:ASN:HB3  | 1.88                     | 0.55              |
| 1:B:373:THR:HG23 | 1:B:415:PHE:O    | 2.07                     | 0.55              |
| 1:D:103:GLY:HA3  | 1:D:198:VAL:CG1  | 2.35                     | 0.54              |
| 1:D:268:PHE:O    | 1:D:272:VAL:HG23 | 2.06                     | 0.54              |
| 1:D:372:LEU:CD2  | 1:D:411:ALA:O    | 2.55                     | 0.54              |
| 1:A:111:HIS:O    | 1:A:114:GLY:N    | 2.40                     | 0.54              |
| 1:A:268:PHE:O    | 1:A:272:VAL:HG23 | 2.07                     | 0.54              |
| 1:A:373:THR:HG21 | 1:A:416:MSE:HB2  | 1.88                     | 0.54              |
| 1:C:132:SER:O    | 1:C:135:VAL:HG22 | 2.07                     | 0.54              |
| 1:D:372:LEU:HA   | 1:D:376:ALA:HA   | 1.88                     | 0.54              |
| 1:B:183:LEU:HD11 | 1:B:438:MSE:HE3  | 1.90                     | 0.54              |
| 1:A:362:ILE:HG13 | 1:A:454:THR:HG23 | 1.87                     | 0.54              |
| 1:B:227:MSE:O    | 1:B:230:PRO:HD2  | 2.06                     | 0.54              |
| 1:A:78:VAL:HG12  | 1:A:79:PHE:N     | 2.21                     | 0.54              |
| 1:C:362:ILE:HG12 | 1:C:458:MSE:HE1  | 1.87                     | 0.54              |
| 1:C:435:GLN:O    | 1:C:439:MSE:HG3  | 2.07                     | 0.54              |
| 1:A:70:ALA:HB2   | 1:A:325:LEU:HD12 | 1.89                     | 0.54              |
| 1:D:357:GLY:HA3  | 1:D:361:VAL:CG2  | 2.34                     | 0.54              |
| 1:B:152:THR:CG2  | 4:B:501:CIT:H41  | 2.38                     | 0.54              |
| 1:B:194:ILE:HG21 | 1:B:409:VAL:HG23 | 1.89                     | 0.54              |
| 1:C:127:ALA:HA   | 1:C:137:MSE:HE2  | 1.89                     | 0.54              |
| 1:C:325:LEU:HD21 | 1:C:379:THR:HG22 | 1.89                     | 0.54              |
| 1:B:107:ALA:HA   | 1:B:110:MSE:CE   | 2.36                     | 0.54              |
| 1:A:94:ASN:O     | 1:A:97:ILE:HD13  | 2.07                     | 0.54              |
| 1:A:194:ILE:HG22 | 1:A:195:ALA:H    | 1.73                     | 0.54              |
| 1:A:282:ASN:ND2  | 1:A:288:PHE:H    | 2.06                     | 0.54              |
| 1:A:358:ILE:O    | 1:A:361:VAL:N    | 2.39                     | 0.54              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:436:SER:HA   | 1:C:439:MSE:HG3  | 1.88                     | 0.54              |
| 1:D:214:PHE:C    | 1:D:214:PHE:CD2  | 2.86                     | 0.54              |
| 1:D:227:MSE:O    | 1:D:230:PRO:HD2  | 2.07                     | 0.54              |
| 1:B:90:ASN:HD22  | 1:A:90:ASN:ND2   | 1.96                     | 0.54              |
| 1:B:107:ALA:HA   | 1:B:110:MSE:HE3  | 1.88                     | 0.54              |
| 1:D:229:LEU:HB3  | 1:D:230:PRO:HD3  | 1.90                     | 0.54              |
| 1:A:258:ASP:N    | 1:A:259:LYS:CB   | 2.71                     | 0.54              |
| 1:A:298:GLY:O    | 1:A:301:LEU:HB2  | 2.08                     | 0.54              |
| 1:D:194:ILE:HG13 | 1:D:195:ALA:H    | 1.73                     | 0.53              |
| 1:D:239:LEU:HD13 | 1:D:441:VAL:HG23 | 1.90                     | 0.53              |
| 1:D:309:VAL:HG23 | 1:D:313:GLU:HG3  | 1.89                     | 0.53              |
| 1:A:276:ILE:HG22 | 1:A:277:PHE:CD2  | 2.44                     | 0.53              |
| 1:C:220:PHE:CD2  | 1:C:405:VAL:HG21 | 2.43                     | 0.53              |
| 1:C:418:PRO:HA   | 1:C:419:VAL:CG2  | 2.37                     | 0.53              |
| 1:A:86:GLN:HG3   | 1:A:90:ASN:OD1   | 2.08                     | 0.53              |
| 1:A:196:THR:HG22 | 1:A:198:VAL:O    | 2.09                     | 0.53              |
| 1:D:104:PHE:CD1  | 1:D:318:ALA:HA   | 2.44                     | 0.53              |
| 1:A:54:PHE:HE2   | 1:A:72:LEU:HD21  | 1.73                     | 0.53              |
| 1:A:146:SER:C    | 1:A:148:TRP:H    | 2.15                     | 0.53              |
| 1:A:307:ARG:HG2  | 1:A:307:ARG:O    | 2.08                     | 0.53              |
| 1:D:58:LEU:HD11  | 1:D:64:LEU:CD2   | 2.31                     | 0.53              |
| 1:B:134:ALA:O    | 1:B:138:LEU:HG   | 2.09                     | 0.53              |
| 1:B:370:VAL:O    | 1:B:371:PHE:HB3  | 2.07                     | 0.53              |
| 1:C:150:SER:O    | 1:C:154:THR:HB   | 2.09                     | 0.53              |
| 1:C:182:LEU:O    | 1:C:427:VAL:HG11 | 2.08                     | 0.53              |
| 1:C:235:ILE:HD12 | 1:C:445:LEU:HD12 | 1.90                     | 0.53              |
| 1:D:61:THR:O     | 1:D:62:GLU:HG3   | 2.08                     | 0.53              |
| 1:D:418:PRO:HD3  | 1:D:438:MSE:SE   | 2.59                     | 0.53              |
| 1:B:78:VAL:HG12  | 1:B:79:PHE:N     | 2.24                     | 0.53              |
| 1:A:178:TYR:CB   | 1:A:432:HIS:H    | 2.22                     | 0.53              |
| 1:A:325:LEU:CD2  | 1:A:379:THR:HG22 | 2.38                     | 0.53              |
| 1:A:377:SER:HB3  | 1:A:380:ALA:CB   | 2.25                     | 0.53              |
| 1:C:198:VAL:O    | 1:C:198:VAL:CG2  | 2.57                     | 0.53              |
| 1:B:106:LEU:O    | 1:B:109:ALA:HB3  | 2.08                     | 0.53              |
| 1:B:372:LEU:HD13 | 1:B:414:ALA:CB   | 2.27                     | 0.53              |
| 1:C:123:VAL:CG1  | 1:C:141:VAL:HG21 | 2.39                     | 0.53              |
| 1:C:127:ALA:HB1  | 1:C:133:VAL:CG2  | 2.38                     | 0.53              |
| 1:C:227:MSE:O    | 1:C:230:PRO:HD2  | 2.08                     | 0.53              |
| 1:C:232:ALA:HA   | 1:C:445:LEU:HD11 | 1.91                     | 0.53              |
| 1:C:359:PHE:C    | 1:C:359:PHE:CD2  | 2.87                     | 0.53              |
| 1:B:188:SER:HB2  | 1:B:229:LEU:HD11 | 1.91                     | 0.53              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:200:SER:HB2  | 1:B:201:PRO:CD   | 2.32                     | 0.53              |
| 1:B:204:ALA:CB   | 1:B:326:PHE:CZ   | 2.92                     | 0.53              |
| 1:B:389:PHE:HD1  | 1:B:403:LEU:HD13 | 1.74                     | 0.53              |
| 1:A:96:ILE:O     | 1:A:97:ILE:C     | 2.52                     | 0.53              |
| 1:C:116:ASP:OD1  | 1:C:117:LYS:N    | 2.42                     | 0.53              |
| 1:C:171:ALA:C    | 1:C:173:LYS:N    | 2.67                     | 0.53              |
| 1:D:272:VAL:O    | 1:D:276:ILE:HG13 | 2.09                     | 0.53              |
| 1:A:359:PHE:HD1  | 1:A:458:MSE:SE   | 2.42                     | 0.53              |
| 1:C:86:GLN:O     | 1:C:86:GLN:HG3   | 2.09                     | 0.53              |
| 1:D:97:ILE:HD12  | 1:D:97:ILE:N     | 2.24                     | 0.52              |
| 1:A:42:GLU:OE1   | 1:A:44:ASN:HB2   | 2.09                     | 0.52              |
| 1:A:212:LEU:HD22 | 1:A:216:ASP:HB3  | 1.89                     | 0.52              |
| 1:D:195:ALA:N    | 1:D:217:TRP:HZ3  | 2.08                     | 0.52              |
| 1:B:390:ALA:O    | 1:B:394:GLU:HG3  | 2.09                     | 0.52              |
| 1:A:456:ILE:HA   | 1:A:459:LEU:HD22 | 1.92                     | 0.52              |
| 1:D:220:PHE:CD1  | 1:D:460:PHE:CE2  | 2.93                     | 0.52              |
| 1:D:382:ALA:O    | 1:D:386:ILE:HG12 | 2.10                     | 0.52              |
| 1:D:394:GLU:HG3  | 1:D:400:PRO:HG3  | 1.91                     | 0.52              |
| 1:B:378:ASN:HD21 | 1:B:421:THR:CG2  | 2.22                     | 0.52              |
| 1:A:195:ALA:C    | 1:A:217:TRP:HZ3  | 2.17                     | 0.52              |
| 1:A:376:ALA:HB3  | 1:A:420:ALA:HB3  | 1.91                     | 0.52              |
| 1:C:31:LEU:HD12  | 1:C:31:LEU:O     | 2.09                     | 0.52              |
| 1:D:214:PHE:HD2  | 1:D:214:PHE:C    | 2.17                     | 0.52              |
| 1:D:379:THR:HG22 | 1:D:380:ALA:N    | 2.23                     | 0.52              |
| 1:B:77:ALA:O     | 1:B:78:VAL:HB    | 2.09                     | 0.52              |
| 1:B:279:SER:HB3  | 1:B:280:PRO:CD   | 2.40                     | 0.52              |
| 1:A:108:ALA:CB   | 1:A:317:THR:HG21 | 2.28                     | 0.52              |
| 1:C:210:VAL:HG21 | 1:C:401:VAL:HG22 | 1.91                     | 0.52              |
| 1:C:265:LEU:O    | 1:C:268:PHE:HB3  | 2.10                     | 0.52              |
| 1:C:386:ILE:HD11 | 1:C:408:ALA:HB2  | 1.91                     | 0.52              |
| 1:C:428:PHE:HZ   | 1:C:435:GLN:HB3  | 1.72                     | 0.52              |
| 1:D:52:LEU:HD12  | 1:D:52:LEU:O     | 2.10                     | 0.52              |
| 1:D:373:THR:O    | 1:D:376:ALA:HB2  | 2.10                     | 0.52              |
| 1:D:74:PRO:HG2   | 1:D:92:PHE:HE1   | 1.74                     | 0.52              |
| 1:D:142:THR:HG23 | 1:D:158:MSE:HG3  | 1.92                     | 0.52              |
| 1:D:422:PRO:N    | 1:D:423:PRO:HD2  | 2.25                     | 0.52              |
| 1:B:71:ILE:O     | 1:B:75:VAL:HG23  | 2.09                     | 0.52              |
| 1:B:187:TYR:CZ   | 1:B:415:PHE:HB3  | 2.45                     | 0.52              |
| 1:B:197:LEU:HD12 | 1:B:214:PHE:HA   | 1.91                     | 0.52              |
| 1:C:377:SER:HB3  | 1:C:380:ALA:HB3  | 1.90                     | 0.52              |
| 1:D:201:PRO:O    | 1:D:202:PRO:C    | 2.52                     | 0.52              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:72:LEU:O     | 1:B:76:MSE:HG3   | 2.10                     | 0.52              |
| 1:B:94:ASN:O     | 1:B:97:ILE:HB    | 2.10                     | 0.52              |
| 1:B:180:PHE:C    | 1:B:180:PHE:CD2  | 2.87                     | 0.52              |
| 1:A:274:LEU:O    | 1:A:278:SER:N    | 2.43                     | 0.52              |
| 1:C:35:LEU:HD22  | 1:C:39:LEU:HD22  | 1.91                     | 0.52              |
| 1:D:151:ASN:OD1  | 1:D:151:ASN:N    | 2.42                     | 0.52              |
| 1:D:405:VAL:O    | 1:D:409:VAL:HG23 | 2.10                     | 0.52              |
| 1:B:54:PHE:C     | 1:B:54:PHE:CD2   | 2.87                     | 0.52              |
| 1:A:315:GLN:HA   | 1:A:320:TRP:CZ3  | 2.45                     | 0.52              |
| 1:D:57:VAL:O     | 1:D:61:THR:HG23  | 2.10                     | 0.52              |
| 1:B:24:ILE:HG21  | 1:B:63:ALA:HB2   | 1.92                     | 0.52              |
| 1:B:149:ILE:C    | 1:B:149:ILE:HD12 | 2.35                     | 0.52              |
| 1:B:151:ASN:HB2  | 4:B:501:CIT:C5   | 2.40                     | 0.52              |
| 1:C:123:VAL:HG11 | 1:C:141:VAL:HG21 | 1.92                     | 0.52              |
| 1:D:107:ALA:HA   | 1:D:110:MSE:HG2  | 1.92                     | 0.51              |
| 1:A:96:ILE:HG13  | 1:A:208:ALA:HA   | 1.92                     | 0.51              |
| 1:A:196:THR:N    | 1:A:217:TRP:CZ3  | 2.72                     | 0.51              |
| 1:C:18:LEU:CB    | 1:C:19:HIS:HA    | 2.40                     | 0.51              |
| 1:C:100:PHE:CD1  | 1:C:198:VAL:HG12 | 2.44                     | 0.51              |
| 1:C:374:GLU:O    | 1:C:375:PHE:C    | 2.50                     | 0.51              |
| 1:D:201:PRO:HD2  | 1:D:202:PRO:CD   | 2.38                     | 0.51              |
| 1:C:23:LEU:O     | 1:C:26:LEU:N     | 2.43                     | 0.51              |
| 1:C:371:PHE:O    | 1:C:371:PHE:CG   | 2.61                     | 0.51              |
| 1:B:235:ILE:HD12 | 1:B:445:LEU:HD12 | 1.91                     | 0.51              |
| 1:D:311:TRP:NE1  | 1:D:315:GLN:OE1  | 2.44                     | 0.51              |
| 1:B:139:PHE:HA   | 1:B:142:THR:HG22 | 1.92                     | 0.51              |
| 1:B:359:PHE:O    | 1:B:363:LEU:HB2  | 2.11                     | 0.51              |
| 1:B:389:PHE:HD1  | 1:B:403:LEU:CD1  | 2.23                     | 0.51              |
| 1:A:298:GLY:HA2  | 1:A:301:LEU:HD12 | 1.92                     | 0.51              |
| 1:D:298:GLY:HA2  | 1:D:301:LEU:HD12 | 1.92                     | 0.51              |
| 1:A:197:LEU:HD12 | 1:A:214:PHE:HA   | 1.92                     | 0.51              |
| 1:A:277:PHE:O    | 1:A:280:PRO:HD2  | 2.11                     | 0.51              |
| 1:A:325:LEU:O    | 1:A:326:PHE:C    | 2.54                     | 0.51              |
| 1:C:202:PRO:HA   | 1:C:205:ILE:HG13 | 1.92                     | 0.51              |
| 1:B:180:PHE:CD2  | 1:B:181:VAL:N    | 2.78                     | 0.51              |
| 1:A:138:LEU:HD22 | 1:A:165:VAL:HG11 | 1.93                     | 0.51              |
| 1:A:376:ALA:O    | 1:A:377:SER:C    | 2.51                     | 0.51              |
| 1:C:178:TYR:HA   | 1:C:182:LEU:CB   | 2.41                     | 0.51              |
| 1:C:390:ALA:HB1  | 1:C:400:PRO:HB3  | 1.92                     | 0.51              |
| 1:D:56:ALA:HB1   | 1:D:384:LEU:HD21 | 1.92                     | 0.51              |
| 1:C:388:VAL:HG12 | 1:C:389:PHE:CD2  | 2.46                     | 0.51              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:205:ILE:O    | 1:D:208:ALA:HB3  | 2.11                     | 0.51              |
| 1:B:123:VAL:HG11 | 1:B:141:VAL:CG2  | 2.41                     | 0.51              |
| 1:B:147:MSE:O    | 1:B:198:VAL:O    | 2.28                     | 0.51              |
| 1:B:152:THR:CG2  | 1:B:422:PRO:HB2  | 2.40                     | 0.51              |
| 1:C:282:ASN:OD1  | 1:C:288:PHE:N    | 2.44                     | 0.51              |
| 1:D:147:MSE:O    | 1:D:196:THR:OG1  | 2.22                     | 0.51              |
| 1:D:372:LEU:HD13 | 1:D:376:ALA:HB1  | 1.90                     | 0.51              |
| 1:B:418:PRO:CG   | 1:B:438:MSE:SE   | 3.09                     | 0.51              |
| 1:C:131:MSE:O    | 1:C:132:SER:C    | 2.54                     | 0.51              |
| 1:C:369:VAL:HG11 | 1:C:450:ILE:HB   | 1.93                     | 0.51              |
| 1:D:236:LEU:HD12 | 1:D:441:VAL:CG2  | 2.39                     | 0.50              |
| 1:D:386:ILE:O    | 1:D:387:PRO:C    | 2.55                     | 0.50              |
| 1:C:394:GLU:CG   | 1:C:400:PRO:HG3  | 2.41                     | 0.50              |
| 1:C:428:PHE:HZ   | 1:C:435:GLN:CB   | 2.24                     | 0.50              |
| 1:C:58:LEU:HD23  | 1:C:64:LEU:HD12  | 1.93                     | 0.50              |
| 1:C:362:ILE:HD12 | 1:C:362:ILE:O    | 2.12                     | 0.50              |
| 1:B:106:LEU:HD21 | 1:B:271:THR:HG21 | 1.93                     | 0.50              |
| 1:C:235:ILE:HD12 | 1:C:445:LEU:CD1  | 2.40                     | 0.50              |
| 1:C:373:THR:CG2  | 1:C:417:LEU:HG   | 2.41                     | 0.50              |
| 1:D:288:PHE:O    | 1:D:289:LYS:HB2  | 2.10                     | 0.50              |
| 1:D:337:LYS:HD3  | 5:D:601:HOH:O    | 2.09                     | 0.50              |
| 1:D:372:LEU:CA   | 1:D:376:ALA:HA   | 2.42                     | 0.50              |
| 1:B:31:LEU:HG    | 1:B:35:LEU:CD1   | 2.42                     | 0.50              |
| 1:A:372:LEU:N    | 1:A:374:GLU:H    | 2.10                     | 0.50              |
| 1:D:47:LEU:HD21  | 1:D:80:PHE:CB    | 2.40                     | 0.50              |
| 1:D:127:ALA:O    | 1:D:128:GLN:HG2  | 2.12                     | 0.50              |
| 1:D:309:VAL:HG22 | 1:D:313:GLU:HG3  | 1.94                     | 0.50              |
| 1:A:152:THR:HG22 | 4:A:501:CIT:H41  | 1.93                     | 0.50              |
| 1:C:40:PRO:O     | 1:C:41:PHE:C     | 2.53                     | 0.50              |
| 1:B:332:LEU:HA   | 1:B:335:VAL:CG1  | 2.41                     | 0.50              |
| 1:D:195:ALA:N    | 1:D:217:TRP:CZ3  | 2.79                     | 0.50              |
| 1:D:386:ILE:HB   | 1:D:387:PRO:HD3  | 1.94                     | 0.50              |
| 1:B:369:VAL:HG11 | 1:B:450:ILE:HG12 | 1.94                     | 0.50              |
| 1:A:371:PHE:O    | 1:A:371:PHE:CD2  | 2.64                     | 0.50              |
| 1:D:220:PHE:HD1  | 1:D:460:PHE:CZ   | 2.29                     | 0.50              |
| 1:B:110:MSE:HG2  | 1:B:115:LEU:HD23 | 1.94                     | 0.50              |
| 1:A:325:LEU:HD23 | 1:A:379:THR:HG22 | 1.93                     | 0.50              |
| 1:C:195:ALA:N    | 1:C:217:TRP:CZ3  | 2.80                     | 0.50              |
| 1:D:201:PRO:HG2  | 1:D:379:THR:OG1  | 2.12                     | 0.49              |
| 1:B:227:MSE:SE   | 1:B:456:ILE:HD11 | 2.61                     | 0.49              |
| 1:A:405:VAL:O    | 1:A:409:VAL:HG23 | 2.12                     | 0.49              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:185:VAL:CG1  | 1:B:186:ALA:N    | 2.75                     | 0.49              |
| 1:B:324:LEU:N    | 1:B:324:LEU:HD12 | 2.26                     | 0.49              |
| 1:B:372:LEU:HG   | 1:B:411:ALA:CA   | 2.40                     | 0.49              |
| 1:A:162:VAL:HA   | 1:A:165:VAL:HG12 | 1.93                     | 0.49              |
| 1:A:195:ALA:N    | 1:A:217:TRP:CH2  | 2.80                     | 0.49              |
| 1:A:372:LEU:H    | 1:A:374:GLU:H    | 1.60                     | 0.49              |
| 1:D:106:LEU:HD12 | 1:D:303:LEU:HD11 | 1.93                     | 0.49              |
| 1:B:356:MSE:HE3  | 1:B:360:VAL:HG12 | 1.93                     | 0.49              |
| 1:B:372:LEU:HD21 | 1:B:378:ASN:CG   | 2.37                     | 0.49              |
| 1:A:191:ILE:HG12 | 1:A:228:MSE:HE2  | 1.94                     | 0.49              |
| 1:A:358:ILE:N    | 1:A:358:ILE:HD12 | 2.26                     | 0.49              |
| 1:B:372:LEU:CD2  | 1:B:378:ASN:HA   | 2.43                     | 0.49              |
| 1:A:413:CYS:HB3  | 1:A:415:PHE:HE2  | 1.75                     | 0.49              |
| 1:A:421:THR:HG23 | 1:A:423:PRO:HD2  | 1.94                     | 0.49              |
| 1:C:152:THR:HG23 | 4:C:501:CIT:C5   | 2.42                     | 0.49              |
| 1:D:86:GLN:NE2   | 1:C:94:ASN:HA    | 2.25                     | 0.49              |
| 1:C:127:ALA:CA   | 1:C:137:MSE:HE2  | 2.43                     | 0.49              |
| 1:D:135:VAL:HG23 | 1:D:136:PHE:N    | 2.28                     | 0.49              |
| 1:B:25:VAL:O     | 1:B:28:ASP:N     | 2.46                     | 0.49              |
| 1:A:306:ALA:C    | 1:A:308:VAL:H    | 2.20                     | 0.49              |
| 1:A:357:GLY:CA   | 1:A:361:VAL:HG23 | 2.37                     | 0.49              |
| 1:C:31:LEU:HD11  | 1:C:35:LEU:HD11  | 1.94                     | 0.49              |
| 1:D:104:PHE:CE1  | 1:D:319:ASP:N    | 2.67                     | 0.49              |
| 1:D:182:LEU:O    | 1:D:427:VAL:HG11 | 2.13                     | 0.49              |
| 1:D:416:MSE:HE3  | 1:D:439:MSE:HG3  | 1.95                     | 0.49              |
| 1:B:19:HIS:HA    | 1:B:22:SER:HB2   | 1.93                     | 0.49              |
| 1:A:231:MSE:HE3  | 1:A:448:ALA:CB   | 2.43                     | 0.49              |
| 1:A:377:SER:O    | 1:A:378:ASN:C    | 2.55                     | 0.49              |
| 1:C:196:THR:CG2  | 1:C:198:VAL:O    | 2.60                     | 0.49              |
| 1:D:362:ILE:HD12 | 1:D:457:ALA:HB3  | 1.95                     | 0.49              |
| 1:A:191:ILE:O    | 1:A:194:ILE:HG12 | 2.13                     | 0.49              |
| 1:A:263:VAL:HG13 | 1:A:308:VAL:HG21 | 1.94                     | 0.49              |
| 1:B:57:VAL:O     | 1:B:60:LEU:O     | 2.31                     | 0.49              |
| 1:B:214:PHE:C    | 1:B:214:PHE:CD2  | 2.91                     | 0.49              |
| 1:A:260:GLY:O    | 1:A:263:VAL:HG12 | 2.13                     | 0.49              |
| 1:C:221:GLY:O    | 1:C:222:LEU:C    | 2.55                     | 0.49              |
| 1:C:325:LEU:CD2  | 1:C:379:THR:CG2  | 2.91                     | 0.49              |
| 1:D:175:ARG:HB2  | 1:D:179:VAL:CB   | 2.43                     | 0.48              |
| 1:B:180:PHE:HD2  | 1:B:181:VAL:N    | 2.10                     | 0.48              |
| 1:C:264:THR:OG1  | 1:C:308:VAL:HG21 | 2.13                     | 0.48              |
| 1:B:288:PHE:O    | 1:B:289:LYS:HB3  | 2.13                     | 0.48              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:455:ALA:O    | 1:A:459:LEU:HD13 | 2.13                     | 0.48              |
| 1:C:67:THR:O     | 1:C:71:ILE:HG13  | 2.12                     | 0.48              |
| 1:C:156:ALA:O    | 1:C:160:PRO:HD3  | 2.13                     | 0.48              |
| 1:C:161:LEU:O    | 1:C:165:VAL:HG22 | 2.13                     | 0.48              |
| 1:D:65:HIS:CG    | 1:D:66:VAL:N     | 2.81                     | 0.48              |
| 1:D:80:PHE:CE2   | 3:D:502:BNG:H3'1 | 2.49                     | 0.48              |
| 1:D:323:LEU:O    | 1:D:326:PHE:HB2  | 2.12                     | 0.48              |
| 1:B:43:HIS:CE1   | 3:B:503:BNG:H62  | 2.48                     | 0.48              |
| 1:B:151:ASN:HB2  | 4:B:501:CIT:O3   | 2.13                     | 0.48              |
| 1:B:371:PHE:CD2  | 1:B:371:PHE:C    | 2.87                     | 0.48              |
| 1:A:146:SER:O    | 1:A:148:TRP:N    | 2.47                     | 0.48              |
| 1:A:239:LEU:HD13 | 1:A:441:VAL:HA   | 1.94                     | 0.48              |
| 1:B:150:SER:O    | 1:B:154:THR:HB   | 2.13                     | 0.48              |
| 1:A:65:HIS:HB3   | 1:A:68:VAL:HG23  | 1.94                     | 0.48              |
| 1:A:229:LEU:HB3  | 1:A:230:PRO:HD3  | 1.94                     | 0.48              |
| 1:A:263:VAL:HG13 | 1:A:264:THR:N    | 2.29                     | 0.48              |
| 1:A:282:ASN:HB2  | 1:A:291:PHE:CG   | 2.49                     | 0.48              |
| 1:A:377:SER:O    | 1:A:380:ALA:N    | 2.46                     | 0.48              |
| 1:C:112:HIS:ND1  | 1:C:112:HIS:C    | 2.71                     | 0.48              |
| 1:D:141:VAL:CG1  | 1:D:158:MSE:HE1  | 2.44                     | 0.48              |
| 1:D:195:ALA:HA   | 1:D:221:GLY:C    | 2.38                     | 0.48              |
| 1:B:115:LEU:O    | 1:B:118:VAL:HG13 | 2.14                     | 0.48              |
| 1:B:197:LEU:O    | 1:B:197:LEU:HD23 | 2.13                     | 0.48              |
| 1:B:389:PHE:CD1  | 1:B:403:LEU:HD13 | 2.48                     | 0.48              |
| 1:A:369:VAL:HG12 | 1:A:370:VAL:N    | 2.26                     | 0.48              |
| 1:D:110:MSE:HE1  | 1:D:148:TRP:HB3  | 1.95                     | 0.48              |
| 1:B:195:ALA:N    | 1:B:217:TRP:CZ3  | 2.81                     | 0.48              |
| 1:B:362:ILE:O    | 1:B:366:ALA:HB2  | 2.14                     | 0.48              |
| 1:B:420:ALA:CB   | 1:B:421:THR:HA   | 2.20                     | 0.48              |
| 1:B:430:SER:O    | 1:B:431:GLY:C    | 2.57                     | 0.48              |
| 1:A:203:ASN:CB   | 1:A:217:TRP:CZ2  | 2.97                     | 0.48              |
| 1:D:61:THR:O     | 1:D:62:GLU:CG    | 2.62                     | 0.48              |
| 1:D:369:VAL:HG23 | 1:D:410:ALA:HB1  | 1.94                     | 0.48              |
| 1:B:149:ILE:CD1  | 1:B:149:ILE:C    | 2.87                     | 0.48              |
| 1:D:113:GLN:O    | 1:D:261:LYS:HE2  | 2.14                     | 0.48              |
| 1:D:186:ALA:HB2  | 1:D:427:VAL:HG11 | 1.95                     | 0.48              |
| 1:D:372:LEU:C    | 1:D:376:ALA:HA   | 2.39                     | 0.48              |
| 1:D:402:LEU:HD23 | 1:D:402:LEU:C    | 2.38                     | 0.48              |
| 1:B:107:ALA:HB1  | 1:B:149:ILE:HG22 | 1.96                     | 0.48              |
| 1:B:362:ILE:HD11 | 1:B:454:THR:HG23 | 1.96                     | 0.48              |
| 1:A:181:VAL:HG12 | 1:A:182:LEU:HD23 | 1.96                     | 0.48              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:51:MSE:HE2   | 1:C:51:MSE:HB3   | 1.71                     | 0.48              |
| 1:C:191:ILE:C    | 1:C:193:GLY:H    | 2.21                     | 0.48              |
| 1:C:367:THR:O    | 1:C:367:THR:HG22 | 2.13                     | 0.48              |
| 1:D:228:MSE:CE   | 1:D:415:PHE:HZ   | 2.27                     | 0.48              |
| 1:A:403:LEU:N    | 1:A:403:LEU:CD2  | 2.77                     | 0.48              |
| 1:B:288:PHE:CZ   | 1:A:79:PHE:HA    | 2.49                     | 0.48              |
| 1:B:313:GLU:HA   | 1:B:313:GLU:OE2  | 2.14                     | 0.48              |
| 1:B:374:GLU:O    | 1:B:374:GLU:CG   | 2.61                     | 0.48              |
| 1:A:204:ALA:HB3  | 1:A:326:PHE:CE1  | 2.48                     | 0.48              |
| 1:C:139:PHE:CE1  | 1:C:184:GLY:HA3  | 2.49                     | 0.48              |
| 1:D:73:VAL:HB    | 1:D:74:PRO:CD    | 2.44                     | 0.47              |
| 1:D:185:VAL:CG1  | 1:D:186:ALA:N    | 2.77                     | 0.47              |
| 1:D:259:LYS:HG2  | 1:D:261:LYS:CE   | 2.30                     | 0.47              |
| 1:B:99:LEU:CD1   | 1:B:197:LEU:HD22 | 2.37                     | 0.47              |
| 1:A:113:GLN:HG3  | 1:A:264:THR:OG1  | 2.14                     | 0.47              |
| 1:A:166:LEU:CD1  | 1:A:181:VAL:HG21 | 2.44                     | 0.47              |
| 1:C:229:LEU:HB3  | 1:C:230:PRO:CD   | 2.35                     | 0.47              |
| 1:C:356:MSE:HE3  | 1:C:360:VAL:CG1  | 2.39                     | 0.47              |
| 1:D:134:ALA:HA   | 1:D:137:MSE:HB2  | 1.96                     | 0.47              |
| 1:A:66:VAL:CG1   | 1:A:325:LEU:HD13 | 2.43                     | 0.47              |
| 1:A:108:ALA:HB2  | 1:A:317:THR:CB   | 2.43                     | 0.47              |
| 1:A:374:GLU:O    | 1:A:375:PHE:C    | 2.55                     | 0.47              |
| 1:C:77:ALA:O     | 1:C:78:VAL:HB    | 2.14                     | 0.47              |
| 1:C:393:ALA:HB1  | 1:C:398:MSE:HG2  | 1.96                     | 0.47              |
| 1:B:140:GLY:O    | 1:B:144:LEU:HB2  | 2.14                     | 0.47              |
| 1:B:212:LEU:HD13 | 1:B:217:TRP:HD1  | 1.78                     | 0.47              |
| 1:A:71:ILE:C     | 1:A:74:PRO:HD2   | 2.38                     | 0.47              |
| 1:A:372:LEU:CD2  | 1:A:376:ALA:HB1  | 2.43                     | 0.47              |
| 1:C:325:LEU:HD23 | 1:C:379:THR:CG2  | 2.44                     | 0.47              |
| 1:D:41:PHE:CD2   | 1:D:41:PHE:N     | 2.82                     | 0.47              |
| 1:D:159:LEU:CB   | 1:D:160:PRO:HD3  | 2.38                     | 0.47              |
| 1:D:222:LEU:HB3  | 1:D:223:PRO:HD3  | 1.96                     | 0.47              |
| 1:D:353:VAL:HA   | 1:D:356:MSE:HB3  | 1.96                     | 0.47              |
| 1:B:80:PHE:CZ    | 3:B:503:BNG:H5'2 | 2.49                     | 0.47              |
| 1:B:106:LEU:HD11 | 1:B:268:PHE:HA   | 1.97                     | 0.47              |
| 1:B:148:TRP:CD1  | 1:B:268:PHE:HZ   | 2.33                     | 0.47              |
| 1:A:262:VAL:HG13 | 1:A:263:VAL:N    | 2.28                     | 0.47              |
| 1:A:297:LEU:HA   | 1:A:300:ILE:CG2  | 2.43                     | 0.47              |
| 1:A:414:ALA:CB   | 1:A:421:THR:H    | 2.27                     | 0.47              |
| 1:C:23:LEU:O     | 1:C:26:LEU:HB2   | 2.14                     | 0.47              |
| 1:C:194:ILE:CA   | 1:C:217:TRP:HH2  | 2.28                     | 0.47              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:124:LEU:CD2  | 1:D:161:LEU:HD11 | 2.45                     | 0.47              |
| 1:D:369:VAL:CG2  | 1:D:413:CYS:HB2  | 2.45                     | 0.47              |
| 1:B:56:ALA:CB    | 1:B:384:LEU:HD21 | 2.44                     | 0.47              |
| 1:B:274:LEU:O    | 1:B:278:SER:N    | 2.47                     | 0.47              |
| 1:B:334:ASN:O    | 1:B:335:VAL:C    | 2.56                     | 0.47              |
| 1:A:79:PHE:O     | 1:A:80:PHE:HB2   | 2.14                     | 0.47              |
| 1:A:379:THR:OG1  | 4:A:501:CIT:H22  | 2.14                     | 0.47              |
| 1:A:416:MSE:HG2  | 1:A:439:MSE:HA   | 1.95                     | 0.47              |
| 1:C:113:GLN:HG3  | 1:C:308:VAL:HG22 | 1.95                     | 0.47              |
| 1:C:191:ILE:HG12 | 1:C:228:MSE:CE   | 2.30                     | 0.47              |
| 1:B:35:LEU:O     | 1:B:39:LEU:HB2   | 2.15                     | 0.47              |
| 1:B:66:VAL:HG13  | 1:B:325:LEU:HD13 | 1.96                     | 0.47              |
| 1:A:146:SER:C    | 1:A:148:TRP:N    | 2.72                     | 0.47              |
| 1:C:359:PHE:CD2  | 1:C:359:PHE:O    | 2.67                     | 0.47              |
| 1:D:31:LEU:HD12  | 1:D:31:LEU:O     | 2.14                     | 0.47              |
| 1:D:32:PHE:CE1   | 1:D:50:SER:HB3   | 2.49                     | 0.47              |
| 1:D:48:GLY:HA3   | 1:D:341:THR:OG1  | 2.14                     | 0.47              |
| 1:D:358:ILE:O    | 1:D:359:PHE:C    | 2.57                     | 0.47              |
| 1:D:430:SER:OG   | 1:D:431:GLY:N    | 2.48                     | 0.47              |
| 1:B:275:TRP:HZ2  | 1:B:296:ALA:HB2  | 1.80                     | 0.47              |
| 1:B:289:LYS:HB2  | 1:B:289:LYS:HE3  | 1.66                     | 0.47              |
| 1:B:320:TRP:CD1  | 1:A:320:TRP:CD2  | 3.03                     | 0.47              |
| 1:A:78:VAL:C     | 1:A:79:PHE:O     | 2.50                     | 0.47              |
| 1:A:85:THR:O     | 1:A:86:GLN:C     | 2.57                     | 0.47              |
| 1:A:257:TRP:O    | 1:A:258:ASP:HB3  | 2.15                     | 0.47              |
| 1:C:194:ILE:HA   | 1:C:217:TRP:HH2  | 1.78                     | 0.47              |
| 1:C:356:MSE:HE2  | 1:C:361:VAL:HG22 | 1.95                     | 0.47              |
| 1:D:207:ALA:CA   | 1:D:212:LEU:HB2  | 2.45                     | 0.47              |
| 1:D:260:GLY:C    | 1:D:262:VAL:H    | 2.23                     | 0.47              |
| 1:B:139:PHE:HE2  | 1:B:185:VAL:N    | 2.13                     | 0.47              |
| 1:C:89:LEU:C     | 1:C:91:ASN:N     | 2.72                     | 0.47              |
| 1:C:410:ALA:O    | 1:C:413:CYS:HB2  | 2.15                     | 0.47              |
| 1:A:195:ALA:HB1  | 1:A:222:LEU:HD23 | 1.96                     | 0.47              |
| 1:A:210:VAL:HG23 | 1:A:212:LEU:HG   | 1.95                     | 0.47              |
| 1:C:194:ILE:O    | 1:C:195:ALA:CB   | 2.56                     | 0.47              |
| 1:C:195:ALA:N    | 1:C:217:TRP:HZ3  | 2.12                     | 0.47              |
| 1:C:222:LEU:HD22 | 1:C:222:LEU:C    | 2.39                     | 0.47              |
| 1:D:41:PHE:O     | 1:D:42:GLU:C     | 2.58                     | 0.47              |
| 1:D:110:MSE:HB2  | 1:D:115:LEU:HB3  | 1.97                     | 0.47              |
| 1:D:362:ILE:HD11 | 1:D:454:THR:HA   | 1.97                     | 0.47              |
| 1:D:419:VAL:CB   | 1:D:420:ALA:HA   | 2.45                     | 0.47              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:191:ILE:HD11 | 1:B:232:ALA:HB2  | 1.97                     | 0.47              |
| 1:B:419:VAL:HG11 | 1:B:425:ALA:HB2  | 1.97                     | 0.47              |
| 1:C:377:SER:O    | 1:C:378:ASN:C    | 2.57                     | 0.47              |
| 1:D:191:ILE:HD13 | 1:D:228:MSE:HG2  | 1.97                     | 0.46              |
| 1:B:421:THR:OG1  | 1:B:423:PRO:HD2  | 2.15                     | 0.46              |
| 1:A:140:GLY:O    | 1:A:144:LEU:HB2  | 2.16                     | 0.46              |
| 1:C:18:LEU:C     | 1:C:20:ARG:N     | 2.72                     | 0.46              |
| 1:C:76:MSE:C     | 1:C:77:ALA:O     | 2.55                     | 0.46              |
| 1:C:281:ILE:O    | 1:C:285:LEU:HG   | 2.14                     | 0.46              |
| 1:D:124:LEU:HD22 | 1:D:161:LEU:HD11 | 1.96                     | 0.46              |
| 1:B:305:PHE:CD1  | 1:B:305:PHE:C    | 2.92                     | 0.46              |
| 1:A:315:GLN:HA   | 1:A:320:TRP:HH2  | 1.74                     | 0.46              |
| 1:A:371:PHE:O    | 1:A:371:PHE:CG   | 2.67                     | 0.46              |
| 1:D:28:ASP:OD2   | 1:D:54:PHE:HA    | 2.15                     | 0.46              |
| 1:D:51:MSE:O     | 1:D:55:ILE:HB    | 2.16                     | 0.46              |
| 1:B:372:LEU:CD2  | 1:B:376:ALA:HB1  | 2.40                     | 0.46              |
| 1:A:200:SER:CB   | 1:A:201:PRO:HD2  | 2.45                     | 0.46              |
| 1:C:392:VAL:C    | 1:C:394:GLU:N    | 2.74                     | 0.46              |
| 1:D:194:ILE:O    | 1:D:195:ALA:HB3  | 2.16                     | 0.46              |
| 1:D:282:ASN:HD21 | 1:D:288:PHE:H    | 1.63                     | 0.46              |
| 1:C:213:SER:H    | 1:C:216:ASP:CB   | 2.24                     | 0.46              |
| 1:D:323:LEU:HA   | 1:D:326:PHE:CD2  | 2.45                     | 0.46              |
| 1:B:66:VAL:HG13  | 1:B:325:LEU:CD1  | 2.45                     | 0.46              |
| 1:B:149:ILE:HD12 | 1:B:149:ILE:O    | 2.16                     | 0.46              |
| 1:C:96:ILE:HG13  | 1:C:208:ALA:HA   | 1.96                     | 0.46              |
| 1:C:369:VAL:HG13 | 1:C:446:ASN:OD1  | 2.16                     | 0.46              |
| 1:A:422:PRO:HG2  | 1:A:423:PRO:HD3  | 1.98                     | 0.46              |
| 1:C:135:VAL:O    | 1:C:138:LEU:HB2  | 2.16                     | 0.46              |
| 1:C:421:THR:OG1  | 1:C:423:PRO:HD2  | 2.16                     | 0.46              |
| 4:C:501:CIT:O3   | 4:C:501:CIT:H21  | 2.16                     | 0.46              |
| 1:D:58:LEU:CD1   | 1:D:64:LEU:HD23  | 2.33                     | 0.46              |
| 1:D:171:ALA:HB1  | 1:D:173:LYS:H    | 1.81                     | 0.46              |
| 1:B:194:ILE:O    | 1:B:195:ALA:CB   | 2.63                     | 0.46              |
| 1:B:362:ILE:O    | 1:B:366:ALA:CB   | 2.63                     | 0.46              |
| 1:C:282:ASN:CG   | 1:C:288:PHE:H    | 2.23                     | 0.46              |
| 1:D:102:GLY:HA3  | 1:D:296:ALA:HB1  | 1.98                     | 0.46              |
| 1:D:210:VAL:HG23 | 1:D:210:VAL:O    | 2.15                     | 0.46              |
| 1:A:70:ALA:O     | 1:A:74:PRO:HD3   | 2.16                     | 0.46              |
| 1:C:130:LYS:HB3  | 1:C:131:MSE:H    | 1.59                     | 0.46              |
| 1:C:161:LEU:HD12 | 1:C:161:LEU:HA   | 1.82                     | 0.46              |
| 1:C:452:LEU:O    | 1:C:456:ILE:HG13 | 2.15                     | 0.46              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:64:LEU:HD13  | 1:D:64:LEU:HA    | 1.44                     | 0.46              |
| 1:B:180:PHE:HB2  | 1:B:240:LEU:CD1  | 2.46                     | 0.46              |
| 1:C:150:SER:HB3  | 1:C:153:ALA:HB3  | 1.97                     | 0.46              |
| 1:D:141:VAL:HG12 | 1:D:158:MSE:CE   | 2.45                     | 0.46              |
| 1:B:152:THR:HG22 | 1:B:423:PRO:CD   | 2.40                     | 0.46              |
| 1:A:94:ASN:HB3   | 1:A:97:ILE:CD1   | 2.45                     | 0.46              |
| 1:C:223:PRO:HA   | 1:C:226:MSE:CG   | 2.46                     | 0.46              |
| 1:D:183:LEU:HD11 | 1:D:438:MSE:HG3  | 1.97                     | 0.45              |
| 1:A:107:ALA:HA   | 1:A:110:MSE:CE   | 2.42                     | 0.45              |
| 1:C:53:ALA:O     | 1:C:54:PHE:C     | 2.58                     | 0.45              |
| 1:C:232:ALA:HA   | 1:C:445:LEU:HD13 | 1.96                     | 0.45              |
| 1:C:420:ALA:HB1  | 1:C:421:THR:CA   | 2.26                     | 0.45              |
| 1:B:187:TYR:CD1  | 1:B:415:PHE:HD1  | 2.34                     | 0.45              |
| 1:B:210:VAL:CG1  | 1:B:400:PRO:HB2  | 2.43                     | 0.45              |
| 1:B:214:PHE:CE2  | 1:B:218:MSE:SE   | 3.17                     | 0.45              |
| 1:A:161:LEU:O    | 1:A:165:VAL:HG12 | 2.15                     | 0.45              |
| 1:C:32:PHE:O     | 1:C:33:LEU:C     | 2.58                     | 0.45              |
| 1:D:146:SER:O    | 1:D:147:MSE:C    | 2.59                     | 0.45              |
| 1:B:146:SER:HA   | 1:B:149:ILE:HD12 | 1.98                     | 0.45              |
| 1:A:231:MSE:CE   | 1:A:448:ALA:HB1  | 2.46                     | 0.45              |
| 1:C:356:MSE:HE2  | 1:C:361:VAL:HA   | 1.99                     | 0.45              |
| 1:B:106:LEU:C    | 1:B:110:MSE:HE2  | 2.40                     | 0.45              |
| 1:B:213:SER:N    | 1:B:216:ASP:HB2  | 2.32                     | 0.45              |
| 1:B:400:PRO:O    | 1:B:404:SER:OG   | 2.34                     | 0.45              |
| 1:A:310:HIS:HB2  | 1:A:313:GLU:HG2  | 1.99                     | 0.45              |
| 1:D:393:ALA:O    | 1:D:398:MSE:HB3  | 2.17                     | 0.45              |
| 1:B:372:LEU:CD1  | 1:B:411:ALA:O    | 2.63                     | 0.45              |
| 1:A:182:LEU:O    | 1:A:427:VAL:HG11 | 2.16                     | 0.45              |
| 1:A:239:LEU:HD13 | 1:A:441:VAL:HG22 | 1.99                     | 0.45              |
| 1:A:414:ALA:HB1  | 1:A:421:THR:H    | 1.82                     | 0.45              |
| 1:D:39:LEU:HD22  | 1:D:41:PHE:HE2   | 1.81                     | 0.45              |
| 1:A:58:LEU:HA    | 1:A:58:LEU:HD12  | 1.71                     | 0.45              |
| 1:C:294:LEU:O    | 1:C:298:GLY:N    | 2.43                     | 0.45              |
| 1:D:274:LEU:O    | 1:D:278:SER:N    | 2.50                     | 0.45              |
| 1:D:288:PHE:CZ   | 1:C:79:PHE:HD1   | 2.35                     | 0.45              |
| 1:A:137:MSE:O    | 1:A:141:VAL:HG23 | 2.16                     | 0.45              |
| 1:C:261:LYS:O    | 1:C:264:THR:N    | 2.50                     | 0.45              |
| 1:D:100:PHE:CE1  | 1:D:198:VAL:HA   | 2.51                     | 0.45              |
| 1:D:141:VAL:HG12 | 1:D:158:MSE:HE2  | 1.99                     | 0.45              |
| 1:D:188:SER:OG   | 1:D:229:LEU:HD11 | 2.16                     | 0.45              |
| 1:D:376:ALA:CB   | 1:D:420:ALA:H    | 2.21                     | 0.45              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:207:ALA:HA   | 1:B:212:LEU:HB2  | 1.98                     | 0.45              |
| 1:A:131:MSE:O    | 1:A:134:ALA:N    | 2.50                     | 0.45              |
| 1:D:386:ILE:HG23 | 1:D:404:SER:HB3  | 1.99                     | 0.45              |
| 1:D:392:VAL:O    | 1:D:393:ALA:C    | 2.58                     | 0.45              |
| 1:A:78:VAL:HG12  | 1:A:79:PHE:H     | 1.82                     | 0.45              |
| 1:A:267:ILE:HG21 | 1:A:303:LEU:HD23 | 1.98                     | 0.45              |
| 1:C:418:PRO:CA   | 1:C:419:VAL:HG23 | 2.40                     | 0.45              |
| 1:B:187:TYR:HD2  | 1:B:236:LEU:HD11 | 1.82                     | 0.44              |
| 1:C:52:LEU:HD22  | 1:C:336:LEU:HD21 | 1.99                     | 0.44              |
| 1:C:208:ALA:HB1  | 1:C:330:LEU:HD21 | 1.98                     | 0.44              |
| 1:D:447:ILE:O    | 1:D:448:ALA:C    | 2.59                     | 0.44              |
| 1:B:320:TRP:O    | 1:B:324:LEU:CD1  | 2.65                     | 0.44              |
| 1:A:66:VAL:HG13  | 1:A:325:LEU:CD1  | 2.43                     | 0.44              |
| 1:A:171:ALA:HB1  | 1:A:173:LYS:O    | 2.17                     | 0.44              |
| 1:C:83:PHE:HZ    | 1:C:334:ASN:HB3  | 1.82                     | 0.44              |
| 1:C:157:MSE:O    | 1:C:160:PRO:HD2  | 2.17                     | 0.44              |
| 1:D:66:VAL:CG1   | 1:D:325:LEU:HD23 | 2.47                     | 0.44              |
| 1:D:97:ILE:H     | 1:D:97:ILE:CD1   | 2.30                     | 0.44              |
| 1:D:235:ILE:O    | 1:D:239:LEU:HB2  | 2.17                     | 0.44              |
| 1:B:139:PHE:C    | 1:B:142:THR:HG22 | 2.43                     | 0.44              |
| 1:B:180:PHE:HE1  | 1:B:237:TYR:HB2  | 1.83                     | 0.44              |
| 1:A:197:LEU:CD1  | 1:A:214:PHE:HA   | 2.47                     | 0.44              |
| 1:A:372:LEU:HA   | 1:A:376:ALA:CA   | 2.29                     | 0.44              |
| 1:C:372:LEU:O    | 1:C:376:ALA:CB   | 2.48                     | 0.44              |
| 1:D:222:LEU:HB3  | 1:D:223:PRO:CD   | 2.47                     | 0.44              |
| 1:D:279:SER:HB3  | 1:D:280:PRO:CD   | 2.47                     | 0.44              |
| 1:D:372:LEU:HD21 | 1:D:411:ALA:O    | 2.16                     | 0.44              |
| 1:B:86:GLN:OE1   | 1:A:94:ASN:HA    | 2.18                     | 0.44              |
| 1:B:186:ALA:HB2  | 1:B:427:VAL:CG1  | 2.47                     | 0.44              |
| 1:B:277:PHE:O    | 1:B:281:ILE:HG13 | 2.17                     | 0.44              |
| 1:A:101:LEU:O    | 1:A:104:PHE:HB2  | 2.18                     | 0.44              |
| 1:A:445:LEU:O    | 1:A:448:ALA:HB3  | 2.17                     | 0.44              |
| 1:C:79:PHE:O     | 1:C:80:PHE:CB    | 2.65                     | 0.44              |
| 1:C:261:LYS:HD2  | 1:C:261:LYS:N    | 2.32                     | 0.44              |
| 1:A:159:LEU:CB   | 1:A:160:PRO:HD3  | 2.45                     | 0.44              |
| 1:C:147:MSE:HA   | 1:C:192:GLY:O    | 2.17                     | 0.44              |
| 1:C:318:ALA:HB3  | 1:C:320:TRP:NE1  | 2.33                     | 0.44              |
| 1:C:388:VAL:HG12 | 1:C:389:PHE:HD2  | 1.82                     | 0.44              |
| 1:D:26:LEU:HD23  | 1:D:26:LEU:HA    | 1.78                     | 0.44              |
| 1:D:110:MSE:HE3  | 1:D:149:ILE:HG13 | 1.99                     | 0.44              |
| 1:B:82:ILE:CD1   | 1:B:335:VAL:HG23 | 2.46                     | 0.44              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:201:PRO:O    | 1:B:204:ALA:HB3  | 2.18                     | 0.44              |
| 1:B:367:THR:CA   | 1:B:450:ILE:HD13 | 2.40                     | 0.44              |
| 1:B:418:PRO:CA   | 1:B:419:VAL:HG13 | 2.47                     | 0.44              |
| 1:C:52:LEU:HD12  | 1:C:52:LEU:HA    | 1.72                     | 0.44              |
| 1:C:61:THR:OG1   | 1:C:62:GLU:N     | 2.49                     | 0.44              |
| 1:C:286:GLY:O    | 1:C:287:GLY:C    | 2.60                     | 0.44              |
| 1:C:293:THR:O    | 1:C:297:LEU:N    | 2.43                     | 0.44              |
| 1:D:311:TRP:O    | 1:D:312:LYS:C    | 2.59                     | 0.44              |
| 1:B:51:MSE:HG2   | 1:B:76:MSE:CE    | 2.48                     | 0.44              |
| 1:A:24:ILE:CG1   | 1:A:63:ALA:HB2   | 2.46                     | 0.44              |
| 1:C:201:PRO:O    | 1:C:205:ILE:HG12 | 2.16                     | 0.44              |
| 1:D:426:ILE:O    | 1:D:428:PHE:N    | 2.51                     | 0.44              |
| 1:B:152:THR:HG22 | 1:B:422:PRO:HB2  | 2.00                     | 0.44              |
| 1:B:180:PHE:HB2  | 1:B:240:LEU:HD11 | 1.99                     | 0.44              |
| 1:A:268:PHE:C    | 1:A:268:PHE:CD2  | 2.95                     | 0.44              |
| 1:A:320:TRP:O    | 1:A:321:GLY:C    | 2.60                     | 0.44              |
| 1:A:401:VAL:O    | 1:A:405:VAL:HG23 | 2.18                     | 0.44              |
| 1:A:453:LEU:HA   | 1:A:456:ILE:HD11 | 2.00                     | 0.44              |
| 1:C:178:TYR:O    | 1:C:179:VAL:C    | 2.61                     | 0.44              |
| 1:C:369:VAL:HG23 | 1:C:413:CYS:HB2  | 2.00                     | 0.44              |
| 1:C:419:VAL:CG1  | 1:C:420:ALA:HA   | 2.43                     | 0.44              |
| 1:D:67:THR:HG21  | 1:C:311:TRP:CE2  | 2.53                     | 0.44              |
| 1:D:161:LEU:O    | 1:D:161:LEU:HD12 | 2.18                     | 0.44              |
| 1:D:303:LEU:HD23 | 1:D:303:LEU:HA   | 1.87                     | 0.44              |
| 1:B:56:ALA:HB1   | 1:B:384:LEU:HD21 | 1.99                     | 0.44              |
| 1:B:320:TRP:CD1  | 1:A:320:TRP:CG   | 3.06                     | 0.44              |
| 1:C:346:ALA:HB1  | 1:C:396:PHE:CE1  | 2.53                     | 0.44              |
| 1:D:86:GLN:O     | 1:D:89:LEU:N     | 2.51                     | 0.43              |
| 1:D:94:ASN:HA    | 1:C:86:GLN:HE22  | 1.83                     | 0.43              |
| 1:B:80:PHE:CD2   | 3:B:503:BNG:H3'1 | 2.51                     | 0.43              |
| 1:A:109:ALA:HB2  | 1:A:303:LEU:HD13 | 2.01                     | 0.43              |
| 1:C:137:MSE:O    | 1:C:141:VAL:HG23 | 2.18                     | 0.43              |
| 1:C:273:PHE:CD2  | 1:C:273:PHE:C    | 2.96                     | 0.43              |
| 1:C:358:ILE:HD13 | 1:C:458:MSE:SE   | 2.68                     | 0.43              |
| 1:B:232:ALA:HB1  | 1:B:445:LEU:HD21 | 2.00                     | 0.43              |
| 1:B:402:LEU:HD12 | 1:B:402:LEU:HA   | 1.57                     | 0.43              |
| 1:A:433:ILE:HG13 | 1:A:437:GLU:OE1  | 2.18                     | 0.43              |
| 1:A:458:MSE:HA   | 1:A:458:MSE:CE   | 2.46                     | 0.43              |
| 1:B:418:PRO:CD   | 1:B:438:MSE:SE   | 3.17                     | 0.43              |
| 1:A:297:LEU:HA   | 1:A:300:ILE:HG23 | 2.00                     | 0.43              |
| 1:D:418:PRO:HB3  | 1:D:424:ASN:CB   | 2.49                     | 0.43              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:313:GLU:OE2  | 1:B:313:GLU:CA   | 2.66                     | 0.43              |
| 1:B:345:LEU:HD12 | 1:B:345:LEU:HA   | 1.77                     | 0.43              |
| 1:C:356:MSE:HE2  | 1:C:361:VAL:CG2  | 2.48                     | 0.43              |
| 1:B:198:VAL:HA   | 1:B:199:GLY:HA2  | 1.84                     | 0.43              |
| 1:B:323:LEU:HD23 | 1:B:323:LEU:HA   | 1.84                     | 0.43              |
| 1:D:55:ILE:HG22  | 1:D:56:ALA:N     | 2.34                     | 0.43              |
| 1:D:207:ALA:HB1  | 1:D:212:LEU:HB2  | 1.99                     | 0.43              |
| 1:B:69:THR:O     | 1:B:72:LEU:HB3   | 2.19                     | 0.43              |
| 1:B:110:MSE:HE3  | 1:B:110:MSE:HB2  | 1.95                     | 0.43              |
| 1:B:416:MSE:HG2  | 1:B:439:MSE:HA   | 1.99                     | 0.43              |
| 1:B:418:PRO:HA   | 1:B:419:VAL:HG13 | 2.00                     | 0.43              |
| 1:A:346:ALA:CA   | 1:A:396:PHE:CE2  | 3.00                     | 0.43              |
| 1:A:372:LEU:CD2  | 1:A:378:ASN:OD1  | 2.67                     | 0.43              |
| 1:D:374:GLU:C    | 1:D:376:ALA:N    | 2.75                     | 0.43              |
| 1:A:162:VAL:HA   | 1:A:165:VAL:CG1  | 2.49                     | 0.43              |
| 1:C:323:LEU:HD23 | 1:C:326:PHE:CE2  | 2.54                     | 0.43              |
| 1:B:40:PRO:C     | 1:B:41:PHE:CD1   | 2.97                     | 0.43              |
| 1:B:78:VAL:O     | 1:B:79:PHE:C     | 2.61                     | 0.43              |
| 1:A:306:ALA:C    | 1:A:308:VAL:N    | 2.75                     | 0.43              |
| 1:A:378:ASN:ND2  | 1:A:412:SER:HA   | 2.33                     | 0.43              |
| 1:C:265:LEU:HD13 | 1:C:265:LEU:C    | 2.44                     | 0.43              |
| 1:C:299:ALA:O    | 1:C:300:ILE:C    | 2.59                     | 0.43              |
| 1:C:373:THR:C    | 1:C:374:GLU:O    | 2.60                     | 0.43              |
| 1:D:142:THR:HG23 | 1:D:158:MSE:CG   | 2.48                     | 0.43              |
| 1:D:149:ILE:HG22 | 1:D:150:SER:HB3  | 2.00                     | 0.43              |
| 1:B:195:ALA:H    | 1:B:217:TRP:HH2  | 1.65                     | 0.43              |
| 1:C:236:LEU:HD12 | 1:C:441:VAL:HG11 | 2.01                     | 0.43              |
| 1:C:349:LEU:HD12 | 1:C:353:VAL:HG13 | 2.01                     | 0.43              |
| 1:C:406:LEU:O    | 1:C:407:ILE:C    | 2.62                     | 0.43              |
| 1:D:146:SER:O    | 1:D:148:TRP:N    | 2.52                     | 0.43              |
| 1:D:289:LYS:O    | 1:D:290:SER:HB2  | 2.18                     | 0.43              |
| 1:B:259:LYS:C    | 1:B:261:LYS:H    | 2.27                     | 0.43              |
| 1:B:374:GLU:HB3  | 1:B:417:LEU:HD21 | 2.01                     | 0.43              |
| 1:A:114:GLY:O    | 1:A:118:VAL:HG13 | 2.19                     | 0.43              |
| 1:A:123:VAL:HG11 | 1:A:141:VAL:HG22 | 2.00                     | 0.43              |
| 1:A:435:GLN:HB3  | 1:A:439:MSE:SE   | 2.69                     | 0.43              |
| 1:C:376:ALA:O    | 1:C:377:SER:HB3  | 2.19                     | 0.43              |
| 1:C:379:THR:HG1  | 4:C:501:CIT:H22  | 1.84                     | 0.43              |
| 1:D:51:MSE:HE1   | 1:D:82:ILE:CD1   | 2.48                     | 0.42              |
| 1:B:78:VAL:HG12  | 1:B:79:PHE:H     | 1.84                     | 0.42              |
| 1:B:78:VAL:O     | 1:B:81:GLY:N     | 2.40                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:330:LEU:HD23 | 1:B:330:LEU:HA   | 1.89                     | 0.42              |
| 1:C:311:TRP:CZ3  | 1:C:314:ILE:HG21 | 2.54                     | 0.42              |
| 1:C:387:PRO:O    | 1:C:391:THR:HG23 | 2.18                     | 0.42              |
| 1:B:26:LEU:HD23  | 1:A:305:PHE:HZ   | 1.84                     | 0.42              |
| 1:A:115:LEU:HA   | 1:A:118:VAL:HG22 | 2.01                     | 0.42              |
| 1:A:236:LEU:HD12 | 1:A:236:LEU:HA   | 1.83                     | 0.42              |
| 1:A:447:ILE:CA   | 1:A:450:ILE:HG23 | 2.47                     | 0.42              |
| 1:C:44:ASN:O     | 1:C:339:THR:HB   | 2.19                     | 0.42              |
| 1:C:167:SER:C    | 1:C:169:VAL:H    | 2.27                     | 0.42              |
| 1:D:194:ILE:CD1  | 1:D:224:THR:HG22 | 2.49                     | 0.42              |
| 1:B:61:THR:O     | 1:B:62:GLU:C     | 2.61                     | 0.42              |
| 1:B:144:LEU:O    | 1:B:144:LEU:HD13 | 2.19                     | 0.42              |
| 1:B:281:ILE:O    | 1:B:285:LEU:HG   | 2.18                     | 0.42              |
| 1:A:159:LEU:HB3  | 1:A:160:PRO:CD   | 2.45                     | 0.42              |
| 1:C:263:VAL:HG22 | 1:C:264:THR:N    | 2.34                     | 0.42              |
| 1:B:96:ILE:HD13  | 1:B:96:ILE:HA    | 1.73                     | 0.42              |
| 1:B:416:MSE:HB3  | 1:B:417:LEU:H    | 1.53                     | 0.42              |
| 1:C:76:MSE:O     | 1:C:79:PHE:O     | 2.38                     | 0.42              |
| 1:C:77:ALA:O     | 1:C:78:VAL:CB    | 2.66                     | 0.42              |
| 1:C:135:VAL:CG2  | 1:C:136:PHE:N    | 2.82                     | 0.42              |
| 1:D:218:MSE:CG   | 1:D:222:LEU:HB2  | 2.49                     | 0.42              |
| 1:D:358:ILE:HD13 | 1:D:461:TRP:CH2  | 2.54                     | 0.42              |
| 1:B:104:PHE:O    | 1:B:107:ALA:N    | 2.53                     | 0.42              |
| 1:B:123:VAL:HB   | 1:B:141:VAL:HG21 | 2.01                     | 0.42              |
| 1:B:182:LEU:O    | 1:B:185:VAL:HG12 | 2.19                     | 0.42              |
| 1:C:356:MSE:HG3  | 1:C:361:VAL:HG23 | 2.02                     | 0.42              |
| 1:D:432:HIS:O    | 1:D:434:LYS:N    | 2.52                     | 0.42              |
| 1:D:445:LEU:HD12 | 1:D:445:LEU:HA   | 1.82                     | 0.42              |
| 1:B:65:HIS:O     | 1:B:66:VAL:C     | 2.63                     | 0.42              |
| 1:B:229:LEU:HB3  | 1:B:230:PRO:CD   | 2.40                     | 0.42              |
| 1:B:367:THR:O    | 1:B:370:VAL:HG22 | 2.20                     | 0.42              |
| 1:A:76:MSE:C     | 1:A:77:ALA:O     | 2.60                     | 0.42              |
| 1:A:99:LEU:O     | 1:A:99:LEU:HD13  | 2.19                     | 0.42              |
| 1:A:143:ALA:O    | 1:A:144:LEU:C    | 2.61                     | 0.42              |
| 1:C:70:ALA:O     | 1:C:74:PRO:HD3   | 2.19                     | 0.42              |
| 1:B:60:LEU:C     | 1:B:61:THR:HG23  | 2.45                     | 0.42              |
| 1:B:104:PHE:O    | 1:B:105:ALA:C    | 2.62                     | 0.42              |
| 1:A:105:ALA:HB1  | 1:A:314:ILE:HD13 | 2.02                     | 0.42              |
| 1:A:166:LEU:HD22 | 1:A:166:LEU:H    | 1.85                     | 0.42              |
| 1:B:74:PRO:HG2   | 1:B:92:PHE:CE1   | 2.55                     | 0.42              |
| 1:B:116:ASP:N    | 1:B:116:ASP:OD1  | 2.52                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:139:PHE:CE2  | 1:B:184:GLY:C    | 2.97                     | 0.42              |
| 1:B:362:ILE:HD11 | 1:B:454:THR:HA   | 2.01                     | 0.42              |
| 1:A:201:PRO:O    | 1:A:202:PRO:C    | 2.62                     | 0.42              |
| 1:A:221:GLY:O    | 1:A:224:THR:HB   | 2.19                     | 0.42              |
| 1:C:48:GLY:O     | 1:C:52:LEU:N     | 2.45                     | 0.42              |
| 1:C:66:VAL:HG13  | 1:C:325:LEU:HD13 | 2.00                     | 0.42              |
| 1:C:284:ALA:C    | 1:C:285:LEU:HD23 | 2.45                     | 0.42              |
| 1:C:424:ASN:ND2  | 1:C:438:MSE:HE1  | 2.35                     | 0.42              |
| 1:D:186:ALA:HB2  | 1:D:427:VAL:CG1  | 2.49                     | 0.42              |
| 1:A:152:THR:CG2  | 4:A:501:CIT:H41  | 2.49                     | 0.42              |
| 1:A:433:ILE:CD1  | 1:A:436:SER:HB2  | 2.49                     | 0.42              |
| 1:D:97:ILE:N     | 1:D:97:ILE:CD1   | 2.83                     | 0.42              |
| 1:D:101:LEU:HA   | 1:D:101:LEU:HD12 | 1.52                     | 0.42              |
| 1:D:151:ASN:O    | 1:D:152:THR:C    | 2.62                     | 0.42              |
| 1:D:204:ALA:HB3  | 1:D:326:PHE:CE1  | 2.54                     | 0.42              |
| 1:D:232:ALA:O    | 1:D:236:LEU:HB2  | 2.20                     | 0.42              |
| 1:D:362:ILE:HD13 | 1:D:458:MSE:HE3  | 2.02                     | 0.42              |
| 1:A:49:ILE:HG13  | 1:A:341:THR:HG23 | 2.00                     | 0.42              |
| 1:A:320:TRP:O    | 1:A:323:LEU:N    | 2.53                     | 0.42              |
| 1:C:196:THR:HG22 | 1:C:198:VAL:O    | 2.19                     | 0.42              |
| 1:C:223:PRO:HA   | 1:C:226:MSE:HG2  | 2.01                     | 0.42              |
| 1:D:297:LEU:HA   | 1:D:297:LEU:HD23 | 1.30                     | 0.41              |
| 1:C:99:LEU:CD2   | 1:C:197:LEU:HD13 | 2.50                     | 0.41              |
| 1:D:110:MSE:HE1  | 1:D:148:TRP:CB   | 2.50                     | 0.41              |
| 1:D:115:LEU:HA   | 1:D:118:VAL:HG12 | 2.02                     | 0.41              |
| 1:B:222:LEU:N    | 1:B:223:PRO:HD2  | 2.35                     | 0.41              |
| 1:B:363:LEU:HD12 | 1:B:454:THR:OG1  | 2.21                     | 0.41              |
| 1:A:369:VAL:C    | 1:A:370:VAL:O    | 2.58                     | 0.41              |
| 1:A:372:LEU:O    | 1:A:376:ALA:CB   | 2.68                     | 0.41              |
| 1:C:89:LEU:C     | 1:C:91:ASN:H     | 2.28                     | 0.41              |
| 1:B:93:ALA:O     | 1:B:94:ASN:C     | 2.61                     | 0.41              |
| 1:B:416:MSE:O    | 1:B:418:PRO:HD3  | 2.20                     | 0.41              |
| 1:A:56:ALA:HB2   | 1:A:384:LEU:HD11 | 2.01                     | 0.41              |
| 1:D:157:MSE:O    | 1:D:160:PRO:HD2  | 2.21                     | 0.41              |
| 1:D:239:LEU:HD13 | 1:D:441:VAL:CG2  | 2.50                     | 0.41              |
| 1:D:324:LEU:HA   | 1:D:324:LEU:HD12 | 1.67                     | 0.41              |
| 1:B:151:ASN:HD22 | 1:B:200:SER:HB3  | 1.86                     | 0.41              |
| 1:B:177:THR:O    | 1:B:180:PHE:N    | 2.50                     | 0.41              |
| 1:B:334:ASN:O    | 1:B:337:LYS:N    | 2.53                     | 0.41              |
| 1:D:66:VAL:HG13  | 1:D:325:LEU:HD23 | 2.02                     | 0.41              |
| 1:D:289:LYS:HD3  | 1:D:289:LYS:HA   | 1.82                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:310:HIS:O    | 1:D:314:ILE:HG13 | 2.20                     | 0.41              |
| 1:D:386:ILE:O    | 1:D:390:ALA:CB   | 2.68                     | 0.41              |
| 1:D:415:PHE:O    | 1:D:416:MSE:HB2  | 2.20                     | 0.41              |
| 1:D:438:MSE:O    | 1:D:439:MSE:C    | 2.64                     | 0.41              |
| 1:B:186:ALA:HB2  | 1:B:427:VAL:HG13 | 2.03                     | 0.41              |
| 1:B:446:ASN:O    | 1:B:450:ILE:HG13 | 2.20                     | 0.41              |
| 1:C:89:LEU:O     | 1:C:91:ASN:N     | 2.54                     | 0.41              |
| 1:C:195:ALA:HA   | 1:C:222:LEU:N    | 2.35                     | 0.41              |
| 1:D:41:PHE:O     | 1:D:46:VAL:HG23  | 2.21                     | 0.41              |
| 1:D:42:GLU:CG    | 1:D:43:HIS:N     | 2.73                     | 0.41              |
| 1:D:49:ILE:O     | 1:D:50:SER:C     | 2.64                     | 0.41              |
| 1:D:373:THR:CG2  | 1:D:374:GLU:N    | 2.75                     | 0.41              |
| 1:B:344:PHE:CD2  | 1:B:344:PHE:C    | 2.98                     | 0.41              |
| 1:A:122:LYS:HE3  | 1:A:122:LYS:HB2  | 1.87                     | 0.41              |
| 1:A:301:LEU:O    | 1:A:302:MSE:C    | 2.63                     | 0.41              |
| 1:C:183:LEU:HD11 | 1:C:438:MSE:CG   | 2.48                     | 0.41              |
| 1:C:261:LYS:C    | 1:C:263:VAL:N    | 2.76                     | 0.41              |
| 1:C:285:LEU:HD23 | 1:C:285:LEU:N    | 2.35                     | 0.41              |
| 1:D:416:MSE:O    | 1:D:438:MSE:SE   | 2.89                     | 0.41              |
| 1:B:146:SER:HB2  | 1:B:154:THR:HG21 | 2.03                     | 0.41              |
| 1:B:149:ILE:HD11 | 1:B:154:THR:OG1  | 2.21                     | 0.41              |
| 1:B:297:LEU:HA   | 1:B:297:LEU:HD23 | 1.75                     | 0.41              |
| 1:B:372:LEU:O    | 1:B:414:ALA:HB2  | 2.20                     | 0.41              |
| 1:A:22:SER:O     | 1:A:23:LEU:C     | 2.64                     | 0.41              |
| 1:C:41:PHE:CE2   | 1:C:344:PHE:HZ   | 2.39                     | 0.41              |
| 1:D:73:VAL:CB    | 1:D:74:PRO:HD3   | 2.49                     | 0.41              |
| 1:D:100:PHE:HE1  | 1:D:197:LEU:O    | 2.04                     | 0.41              |
| 1:D:267:ILE:HG22 | 1:D:268:PHE:N    | 2.36                     | 0.41              |
| 1:B:278:SER:HB2  | 1:B:291:PHE:HD2  | 1.85                     | 0.41              |
| 1:B:418:PRO:HA   | 1:B:419:VAL:HA   | 1.91                     | 0.41              |
| 1:A:116:ASP:OD1  | 1:A:117:LYS:N    | 2.49                     | 0.41              |
| 1:A:232:ALA:HA   | 1:A:445:LEU:HD11 | 2.01                     | 0.41              |
| 1:A:239:LEU:CD1  | 1:A:441:VAL:HA   | 2.51                     | 0.41              |
| 1:C:416:MSE:HE2  | 1:C:416:MSE:HB3  | 1.97                     | 0.41              |
| 1:C:447:ILE:CA   | 1:C:450:ILE:HG22 | 2.49                     | 0.41              |
| 1:D:368:PHE:HD1  | 1:D:368:PHE:HA   | 1.69                     | 0.41              |
| 1:D:399:SER:HA   | 1:D:400:PRO:HD3  | 1.89                     | 0.41              |
| 1:B:105:ALA:O    | 1:B:106:LEU:C    | 2.64                     | 0.41              |
| 1:B:113:GLN:OE1  | 1:B:261:LYS:CB   | 2.69                     | 0.41              |
| 1:B:152:THR:HG21 | 1:B:422:PRO:HB2  | 2.03                     | 0.41              |
| 1:B:159:LEU:HB3  | 1:B:160:PRO:CD   | 2.44                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:194:ILE:CB   | 1:B:217:TRP:HH2  | 2.34                     | 0.41              |
| 1:B:294:LEU:O    | 1:B:298:GLY:N    | 2.53                     | 0.41              |
| 1:B:392:VAL:O    | 1:B:393:ALA:C    | 2.63                     | 0.41              |
| 1:C:31:LEU:HD12  | 1:C:31:LEU:C     | 2.46                     | 0.41              |
| 1:C:48:GLY:O     | 1:C:52:LEU:HB2   | 2.21                     | 0.41              |
| 1:C:67:THR:O     | 1:C:70:ALA:HB3   | 2.21                     | 0.41              |
| 1:C:73:VAL:CB    | 1:C:74:PRO:HD3   | 2.48                     | 0.41              |
| 1:C:322:VAL:HG12 | 1:C:323:LEU:N    | 2.36                     | 0.41              |
| 1:D:131:MSE:O    | 1:D:132:SER:C    | 2.63                     | 0.41              |
| 1:D:195:ALA:O    | 1:D:218:MSE:HG3  | 2.21                     | 0.41              |
| 1:B:394:GLU:CG   | 1:B:400:PRO:HG3  | 2.42                     | 0.41              |
| 1:B:460:PHE:O    | 1:B:461:TRP:C    | 2.63                     | 0.41              |
| 1:C:134:ALA:O    | 1:C:138:LEU:HD23 | 2.22                     | 0.41              |
| 1:C:402:LEU:HD12 | 1:C:402:LEU:HA   | 1.69                     | 0.41              |
| 1:D:40:PRO:HD2   | 1:D:41:PHE:CE2   | 2.56                     | 0.40              |
| 1:D:47:LEU:HD23  | 1:D:82:ILE:HD11  | 2.02                     | 0.40              |
| 1:D:175:ARG:O    | 1:D:176:SER:CB   | 2.68                     | 0.40              |
| 1:B:76:MSE:HE2   | 1:B:76:MSE:HB3   | 1.90                     | 0.40              |
| 1:B:79:PHE:HA    | 1:A:288:PHE:CZ   | 2.57                     | 0.40              |
| 1:B:387:PRO:O    | 1:B:391:THR:OG1  | 2.27                     | 0.40              |
| 1:A:183:LEU:HD12 | 1:A:183:LEU:HA   | 1.79                     | 0.40              |
| 1:A:325:LEU:HD23 | 1:A:379:THR:CG2  | 2.50                     | 0.40              |
| 1:C:23:LEU:O     | 1:C:24:ILE:C     | 2.64                     | 0.40              |
| 1:A:192:GLY:O    | 1:A:194:ILE:O    | 2.39                     | 0.40              |
| 1:A:402:LEU:HA   | 1:A:402:LEU:HD22 | 1.83                     | 0.40              |
| 1:C:19:HIS:O     | 1:C:20:ARG:C     | 2.63                     | 0.40              |
| 1:C:74:PRO:O     | 1:C:78:VAL:HG23  | 2.22                     | 0.40              |
| 1:C:107:ALA:O    | 1:C:108:ALA:C    | 2.62                     | 0.40              |
| 1:C:123:VAL:HG11 | 1:C:141:VAL:HG22 | 2.01                     | 0.40              |
| 1:C:194:ILE:HB   | 1:C:217:TRP:HH2  | 1.86                     | 0.40              |
| 1:C:367:THR:HA   | 1:C:450:ILE:HD12 | 2.03                     | 0.40              |
| 1:D:113:GLN:OE1  | 1:D:261:LYS:HA   | 2.21                     | 0.40              |
| 1:D:200:SER:CB   | 1:D:201:PRO:CD   | 2.95                     | 0.40              |
| 1:D:287:GLY:HA3  | 1:D:288:PHE:HA   | 1.43                     | 0.40              |
| 1:D:460:PHE:HD1  | 1:D:460:PHE:HA   | 1.78                     | 0.40              |
| 1:B:42:GLU:O     | 1:B:43:HIS:C     | 2.64                     | 0.40              |
| 1:B:215:THR:OG1  | 1:B:276:ILE:HA   | 2.20                     | 0.40              |
| 1:B:415:PHE:O    | 1:B:416:MSE:CB   | 2.69                     | 0.40              |
| 1:C:166:LEU:HG   | 1:C:177:THR:HA   | 2.03                     | 0.40              |
| 1:C:194:ILE:HA   | 1:C:217:TRP:CH2  | 2.55                     | 0.40              |
| 1:C:264:THR:OG1  | 1:C:308:VAL:CG2  | 2.69                     | 0.40              |

*Continued on next page...*

Continued from previous page...

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:329:GLY:O    | 1:D:332:LEU:HB3  | 2.21                     | 0.40              |
| 1:D:352:MSE:O    | 1:D:356:MSE:HB2  | 2.21                     | 0.40              |
| 1:D:362:ILE:CD1  | 1:D:457:ALA:HB3  | 2.51                     | 0.40              |
| 1:B:26:LEU:HA    | 1:B:29:VAL:HB    | 2.03                     | 0.40              |
| 1:B:39:LEU:HD13  | 1:B:40:PRO:CD    | 2.52                     | 0.40              |
| 1:B:66:VAL:HG12  | 1:B:325:LEU:HD13 | 2.02                     | 0.40              |
| 1:B:239:LEU:CD1  | 1:B:441:VAL:HA   | 2.52                     | 0.40              |
| 1:B:367:THR:HA   | 1:B:450:ILE:CD1  | 2.43                     | 0.40              |
| 1:A:362:ILE:CG1  | 1:A:454:THR:HG23 | 2.50                     | 0.40              |
| 1:C:47:LEU:HD13  | 1:C:47:LEU:HA    | 1.70                     | 0.40              |
| 1:C:287:GLY:HA3  | 1:C:288:PHE:HA   | 1.60                     | 0.40              |
| 1:C:369:VAL:HG13 | 1:C:370:VAL:N    | 2.35                     | 0.40              |
| 1:C:393:ALA:HB1  | 1:C:398:MSE:CG   | 2.52                     | 0.40              |
| 1:D:61:THR:C     | 1:D:62:GLU:HG3   | 2.44                     | 0.40              |
| 1:D:274:LEU:HD23 | 1:D:281:ILE:HD13 | 2.03                     | 0.40              |
| 1:C:18:LEU:C     | 1:C:20:ARG:H     | 2.26                     | 0.40              |
| 1:C:197:LEU:HD21 | 1:C:207:ALA:CB   | 2.52                     | 0.40              |
| 1:C:323:LEU:HD23 | 1:C:323:LEU:HA   | 1.80                     | 0.40              |
| 1:C:416:MSE:N    | 1:C:438:MSE:HE2  | 2.37                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

| Mol | Chain | Analysed        | Favoured   | Allowed   | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|-----------|----------|-------------|----|
| 1   | A     | 430/449 (96%)   | 355 (83%)  | 72 (17%)  | 3 (1%)   | 18          | 52 |
| 1   | B     | 404/449 (90%)   | 360 (89%)  | 40 (10%)  | 4 (1%)   | 12          | 45 |
| 1   | C     | 426/449 (95%)   | 369 (87%)  | 53 (12%)  | 4 (1%)   | 14          | 47 |
| 1   | D     | 426/449 (95%)   | 356 (84%)  | 68 (16%)  | 2 (0%)   | 24          | 59 |
| All | All   | 1686/1796 (94%) | 1440 (85%) | 233 (14%) | 13 (1%)  | 16          | 50 |

All (13) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 78  | VAL  |
| 1   | B     | 78  | VAL  |
| 1   | C     | 78  | VAL  |
| 1   | B     | 40  | PRO  |
| 1   | A     | 376 | ALA  |
| 1   | B     | 82  | ILE  |
| 1   | C     | 149 | ILE  |
| 1   | C     | 433 | ILE  |
| 1   | D     | 181 | VAL  |
| 1   | C     | 241 | LYS  |
| 1   | A     | 194 | ILE  |
| 1   | D     | 194 | ILE  |
| 1   | B     | 25  | 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     | 307/334 (92%)   | 240 (78%) | 67 (22%)  | 1           | 6 |
| 1   | B     | 297/334 (89%)   | 239 (80%) | 58 (20%)  | 1           | 8 |
| 1   | C     | 310/334 (93%)   | 246 (79%) | 64 (21%)  | 1           | 7 |
| 1   | D     | 303/334 (91%)   | 248 (82%) | 55 (18%)  | 2           | 9 |
| All | All   | 1217/1336 (91%) | 973 (80%) | 244 (20%) | 1           | 7 |

All (244) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 22  | SER  |
| 1   | D     | 41  | PHE  |
| 1   | D     | 45  | VAL  |
| 1   | D     | 47  | LEU  |
| 1   | D     | 50  | SER  |
| 1   | D     | 55  | ILE  |
| 1   | D     | 59  | TRP  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 61  | THR  |
| 1   | D     | 64  | LEU  |
| 1   | D     | 71  | ILE  |
| 1   | D     | 78  | VAL  |
| 1   | D     | 84  | GLU  |
| 1   | D     | 89  | LEU  |
| 1   | D     | 106 | LEU  |
| 1   | D     | 118 | VAL  |
| 1   | D     | 119 | ILE  |
| 1   | D     | 137 | MSE  |
| 1   | D     | 144 | LEU  |
| 1   | D     | 151 | ASN  |
| 1   | D     | 183 | LEU  |
| 1   | D     | 185 | VAL  |
| 1   | D     | 194 | ILE  |
| 1   | D     | 197 | LEU  |
| 1   | D     | 198 | VAL  |
| 1   | D     | 203 | ASN  |
| 1   | D     | 209 | GLU  |
| 1   | D     | 210 | VAL  |
| 1   | D     | 214 | PHE  |
| 1   | D     | 215 | THR  |
| 1   | D     | 231 | MSE  |
| 1   | D     | 239 | LEU  |
| 1   | D     | 262 | VAL  |
| 1   | D     | 267 | ILE  |
| 1   | D     | 288 | PHE  |
| 1   | D     | 308 | VAL  |
| 1   | D     | 313 | GLU  |
| 1   | D     | 324 | LEU  |
| 1   | D     | 335 | VAL  |
| 1   | D     | 353 | VAL  |
| 1   | D     | 358 | ILE  |
| 1   | D     | 360 | VAL  |
| 1   | D     | 362 | ILE  |
| 1   | D     | 368 | PHE  |
| 1   | D     | 369 | VAL  |
| 1   | D     | 372 | LEU  |
| 1   | D     | 379 | THR  |
| 1   | D     | 381 | SER  |
| 1   | D     | 386 | ILE  |
| 1   | D     | 402 | LEU  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 404 | SER  |
| 1   | D     | 412 | SER  |
| 1   | D     | 441 | VAL  |
| 1   | D     | 456 | ILE  |
| 1   | D     | 458 | MSE  |
| 1   | D     | 460 | PHE  |
| 1   | B     | 22  | SER  |
| 1   | B     | 26  | LEU  |
| 1   | B     | 29  | VAL  |
| 1   | B     | 39  | LEU  |
| 1   | B     | 47  | LEU  |
| 1   | B     | 58  | LEU  |
| 1   | B     | 59  | TRP  |
| 1   | B     | 66  | VAL  |
| 1   | B     | 69  | THR  |
| 1   | B     | 84  | GLU  |
| 1   | B     | 86  | GLN  |
| 1   | B     | 89  | LEU  |
| 1   | B     | 96  | ILE  |
| 1   | B     | 106 | LEU  |
| 1   | B     | 112 | HIS  |
| 1   | B     | 115 | LEU  |
| 1   | B     | 118 | VAL  |
| 1   | B     | 119 | ILE  |
| 1   | B     | 149 | ILE  |
| 1   | B     | 154 | THR  |
| 1   | B     | 157 | MSE  |
| 1   | B     | 161 | LEU  |
| 1   | B     | 180 | PHE  |
| 1   | B     | 185 | VAL  |
| 1   | B     | 187 | TYR  |
| 1   | B     | 190 | SER  |
| 1   | B     | 194 | ILE  |
| 1   | B     | 201 | PRO  |
| 1   | B     | 213 | SER  |
| 1   | B     | 224 | THR  |
| 1   | B     | 263 | VAL  |
| 1   | B     | 274 | LEU  |
| 1   | B     | 279 | SER  |
| 1   | B     | 288 | PHE  |
| 1   | B     | 289 | LYS  |
| 1   | B     | 300 | ILE  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 304 | SER  |
| 1   | B     | 308 | VAL  |
| 1   | B     | 335 | VAL  |
| 1   | B     | 343 | VAL  |
| 1   | B     | 345 | LEU  |
| 1   | B     | 351 | ASP  |
| 1   | B     | 353 | VAL  |
| 1   | B     | 362 | ILE  |
| 1   | B     | 371 | PHE  |
| 1   | B     | 372 | LEU  |
| 1   | B     | 384 | LEU  |
| 1   | B     | 398 | MSE  |
| 1   | B     | 399 | SER  |
| 1   | B     | 403 | LEU  |
| 1   | B     | 417 | LEU  |
| 1   | B     | 419 | VAL  |
| 1   | B     | 426 | ILE  |
| 1   | B     | 441 | VAL  |
| 1   | B     | 445 | LEU  |
| 1   | B     | 450 | ILE  |
| 1   | B     | 458 | MSE  |
| 1   | B     | 461 | TRP  |
| 1   | A     | 22  | SER  |
| 1   | A     | 24  | ILE  |
| 1   | A     | 25  | VAL  |
| 1   | A     | 42  | GLU  |
| 1   | A     | 58  | LEU  |
| 1   | A     | 66  | VAL  |
| 1   | A     | 69  | THR  |
| 1   | A     | 71  | ILE  |
| 1   | A     | 89  | LEU  |
| 1   | A     | 95  | SER  |
| 1   | A     | 97  | ILE  |
| 1   | A     | 99  | LEU  |
| 1   | A     | 104 | PHE  |
| 1   | A     | 122 | LYS  |
| 1   | A     | 133 | VAL  |
| 1   | A     | 142 | THR  |
| 1   | A     | 144 | LEU  |
| 1   | A     | 145 | LEU  |
| 1   | A     | 149 | ILE  |
| 1   | A     | 152 | THR  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 165 | VAL  |
| 1   | A     | 166 | LEU  |
| 1   | A     | 183 | LEU  |
| 1   | A     | 185 | VAL  |
| 1   | A     | 194 | ILE  |
| 1   | A     | 196 | THR  |
| 1   | A     | 197 | LEU  |
| 1   | A     | 198 | VAL  |
| 1   | A     | 200 | SER  |
| 1   | A     | 203 | ASN  |
| 1   | A     | 205 | ILE  |
| 1   | A     | 215 | THR  |
| 1   | A     | 222 | LEU  |
| 1   | A     | 239 | LEU  |
| 1   | A     | 261 | LYS  |
| 1   | A     | 285 | LEU  |
| 1   | A     | 288 | PHE  |
| 1   | A     | 300 | ILE  |
| 1   | A     | 304 | SER  |
| 1   | A     | 308 | VAL  |
| 1   | A     | 322 | VAL  |
| 1   | A     | 324 | LEU  |
| 1   | A     | 343 | VAL  |
| 1   | A     | 345 | LEU  |
| 1   | A     | 351 | ASP  |
| 1   | A     | 353 | VAL  |
| 1   | A     | 358 | ILE  |
| 1   | A     | 363 | LEU  |
| 1   | A     | 364 | VAL  |
| 1   | A     | 365 | VAL  |
| 1   | A     | 367 | THR  |
| 1   | A     | 370 | VAL  |
| 1   | A     | 372 | LEU  |
| 1   | A     | 373 | THR  |
| 1   | A     | 377 | SER  |
| 1   | A     | 402 | LEU  |
| 1   | A     | 403 | LEU  |
| 1   | A     | 412 | SER  |
| 1   | A     | 428 | PHE  |
| 1   | A     | 434 | LYS  |
| 1   | A     | 438 | MSE  |
| 1   | A     | 439 | MSE  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 445 | LEU  |
| 1   | A     | 450 | ILE  |
| 1   | A     | 456 | ILE  |
| 1   | A     | 458 | MSE  |
| 1   | A     | 459 | LEU  |
| 1   | C     | 19  | HIS  |
| 1   | C     | 47  | LEU  |
| 1   | C     | 49  | ILE  |
| 1   | C     | 50  | SER  |
| 1   | C     | 59  | TRP  |
| 1   | C     | 61  | THR  |
| 1   | C     | 62  | GLU  |
| 1   | C     | 66  | VAL  |
| 1   | C     | 69  | THR  |
| 1   | C     | 75  | VAL  |
| 1   | C     | 76  | MSE  |
| 1   | C     | 85  | THR  |
| 1   | C     | 89  | LEU  |
| 1   | C     | 97  | ILE  |
| 1   | C     | 101 | LEU  |
| 1   | C     | 110 | MSE  |
| 1   | C     | 112 | HIS  |
| 1   | C     | 118 | VAL  |
| 1   | C     | 130 | LYS  |
| 1   | C     | 131 | MSE  |
| 1   | C     | 137 | MSE  |
| 1   | C     | 157 | MSE  |
| 1   | C     | 165 | VAL  |
| 1   | C     | 166 | LEU  |
| 1   | C     | 177 | THR  |
| 1   | C     | 181 | VAL  |
| 1   | C     | 190 | SER  |
| 1   | C     | 191 | ILE  |
| 1   | C     | 194 | ILE  |
| 1   | C     | 197 | LEU  |
| 1   | C     | 203 | ASN  |
| 1   | C     | 205 | ILE  |
| 1   | C     | 213 | SER  |
| 1   | C     | 215 | THR  |
| 1   | C     | 222 | LEU  |
| 1   | C     | 261 | LYS  |
| 1   | C     | 263 | VAL  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 272 | VAL  |
| 1   | C     | 274 | LEU  |
| 1   | C     | 288 | PHE  |
| 1   | C     | 290 | SER  |
| 1   | C     | 300 | ILE  |
| 1   | C     | 307 | ARG  |
| 1   | C     | 308 | VAL  |
| 1   | C     | 313 | GLU  |
| 1   | C     | 322 | VAL  |
| 1   | C     | 324 | LEU  |
| 1   | C     | 343 | VAL  |
| 1   | C     | 349 | LEU  |
| 1   | C     | 358 | ILE  |
| 1   | C     | 360 | VAL  |
| 1   | C     | 362 | ILE  |
| 1   | C     | 370 | VAL  |
| 1   | C     | 374 | GLU  |
| 1   | C     | 388 | VAL  |
| 1   | C     | 412 | SER  |
| 1   | C     | 419 | VAL  |
| 1   | C     | 438 | MSE  |
| 1   | C     | 439 | MSE  |
| 1   | C     | 443 | LEU  |
| 1   | C     | 447 | ILE  |
| 1   | C     | 456 | ILE  |
| 1   | C     | 458 | MSE  |
| 1   | C     | 459 | LEU  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 65  | HIS  |
| 1   | B     | 37  | HIS  |
| 1   | B     | 90  | ASN  |
| 1   | B     | 203 | ASN  |
| 1   | B     | 282 | ASN  |
| 1   | A     | 94  | ASN  |
| 1   | C     | 37  | HIS  |
| 1   | C     | 44  | ASN  |
| 1   | C     | 151 | ASN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 10 ligands modelled in this entry, 4 are monoatomic - leaving 6 for Mogul analysis.

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

| Mol | Type | Chain | Res | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |     |      | Counts       | RMSZ | # $ Z  > 2$ | Counts      | RMSZ | # $ Z  > 2$ |
| 3   | BNG  | B     | 503 | -    | 21,21,21     | 1.33 | 3 (14%)     | 26,26,26    | 1.85 | 4 (15%)     |
| 4   | CIT  | B     | 501 | -    | 12,12,12     | 1.12 | 0           | 17,17,17    | 1.39 | 2 (11%)     |
| 4   | CIT  | A     | 501 | -    | 12,12,12     | 1.11 | 0           | 17,17,17    | 1.27 | 1 (5%)      |
| 3   | BNG  | D     | 502 | -    | 21,21,21     | 1.22 | 2 (9%)      | 26,26,26    | 1.89 | 8 (30%)     |
| 4   | CIT  | C     | 501 | -    | 12,12,12     | 1.08 | 0           | 17,17,17    | 1.60 | 6 (35%)     |
| 3   | BNG  | C     | 503 | -    | 21,21,21     | 1.21 | 3 (14%)     | 26,26,26    | 1.23 | 2 (7%)      |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions    | Rings   |
|-----|------|-------|-----|------|---------|-------------|---------|
| 3   | BNG  | B     | 503 | -    | -       | 7/12/32/32  | 0/1/1/1 |
| 4   | CIT  | B     | 501 | -    | -       | 10/16/16/16 | -       |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res | Link | Chirals | Torsions    | Rings   |
|-----|------|-------|-----|------|---------|-------------|---------|
| 4   | CIT  | A     | 501 | -    | -       | 11/16/16/16 | -       |
| 3   | BNG  | D     | 502 | -    | -       | 6/12/32/32  | 0/1/1/1 |
| 4   | CIT  | C     | 501 | -    | -       | 5/16/16/16  | -       |
| 3   | BNG  | C     | 503 | -    | -       | 4/12/32/32  | 0/1/1/1 |

All (8) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 3   | B     | 503 | BNG  | C3-C2 | -4.08 | 1.41        | 1.52     |
| 3   | D     | 502 | BNG  | C3-C2 | -3.92 | 1.42        | 1.52     |
| 3   | C     | 503 | BNG  | C3-C2 | -3.58 | 1.43        | 1.52     |
| 3   | C     | 503 | BNG  | O5-C1 | 2.68  | 1.48        | 1.41     |
| 3   | B     | 503 | BNG  | O5-C1 | 2.34  | 1.47        | 1.41     |
| 3   | D     | 502 | BNG  | O5-C1 | 2.30  | 1.47        | 1.41     |
| 3   | B     | 503 | BNG  | C4-C3 | -2.13 | 1.46        | 1.52     |
| 3   | C     | 503 | BNG  | C4-C3 | -2.01 | 1.47        | 1.52     |

All (23) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 3   | B     | 503 | BNG  | C1'-O1-C1  | 5.28  | 122.70      | 113.68   |
| 3   | B     | 503 | BNG  | O1-C1'-C2' | 3.69  | 121.88      | 109.37   |
| 3   | D     | 502 | BNG  | C1'-O1-C1  | 3.62  | 119.87      | 113.68   |
| 3   | D     | 502 | BNG  | C1-C2-C3   | 3.60  | 117.58      | 110.01   |
| 3   | B     | 503 | BNG  | O1-C1-C2   | 3.60  | 113.73      | 108.27   |
| 4   | B     | 501 | CIT  | O6-C6-C3   | 3.47  | 119.80      | 113.14   |
| 4   | C     | 501 | CIT  | O6-C6-C3   | 3.45  | 119.76      | 113.14   |
| 3   | D     | 502 | BNG  | O2-C2-C3   | -3.36 | 102.45      | 110.38   |
| 4   | A     | 501 | CIT  | O6-C6-C3   | 3.21  | 119.30      | 113.14   |
| 3   | D     | 502 | BNG  | C4-C3-C2   | 3.20  | 116.45      | 110.83   |
| 3   | D     | 502 | BNG  | O1-C1'-C2' | 3.04  | 119.69      | 109.37   |
| 3   | B     | 503 | BNG  | O2-C2-C3   | -2.80 | 103.77      | 110.38   |
| 3   | C     | 503 | BNG  | O1-C1'-C2' | 2.76  | 118.75      | 109.37   |
| 3   | C     | 503 | BNG  | O1-C1-C2   | 2.66  | 112.31      | 108.27   |
| 3   | D     | 502 | BNG  | O6-C6-C5   | 2.65  | 120.36      | 111.33   |
| 3   | D     | 502 | BNG  | O5-C1-C2   | 2.55  | 115.61      | 110.37   |
| 4   | C     | 501 | CIT  | O7-C3-C6   | -2.37 | 105.59      | 108.96   |
| 4   | C     | 501 | CIT  | O4-C5-C4   | 2.37  | 121.87      | 114.35   |
| 3   | D     | 502 | BNG  | O1-C1-C2   | 2.08  | 111.44      | 108.27   |
| 4   | C     | 501 | CIT  | O2-C1-C2   | 2.07  | 120.92      | 114.35   |
| 4   | C     | 501 | CIT  | O2-C1-O1   | -2.07 | 118.02      | 123.33   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 4   | B     | 501 | CIT  | O2-C1-C2 | 2.03  | 120.77      | 114.35   |
| 4   | C     | 501 | CIT  | O4-C5-O3 | -2.01 | 118.16      | 123.33   |

There are no chirality outliers.

All (43) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 3   | B     | 503 | BNG  | O5-C1-O1-C1'    |
| 3   | C     | 503 | BNG  | C2-C1-O1-C1'    |
| 3   | C     | 503 | BNG  | O5-C1-O1-C1'    |
| 4   | B     | 501 | CIT  | C2-C3-C6-O5     |
| 4   | B     | 501 | CIT  | C2-C3-C6-O6     |
| 4   | B     | 501 | CIT  | O7-C3-C6-O5     |
| 4   | B     | 501 | CIT  | O7-C3-C6-O6     |
| 4   | A     | 501 | CIT  | C6-C3-C4-C5     |
| 4   | A     | 501 | CIT  | O7-C3-C6-O5     |
| 4   | A     | 501 | CIT  | O7-C3-C6-O6     |
| 4   | A     | 501 | CIT  | C4-C3-C6-O5     |
| 4   | A     | 501 | CIT  | C4-C3-C6-O6     |
| 4   | C     | 501 | CIT  | O7-C3-C6-O5     |
| 4   | C     | 501 | CIT  | O7-C3-C6-O6     |
| 4   | C     | 501 | CIT  | C4-C3-C6-O5     |
| 4   | C     | 501 | CIT  | C4-C3-C6-O6     |
| 4   | B     | 501 | CIT  | C2-C3-C4-C5     |
| 4   | B     | 501 | CIT  | C6-C3-C4-C5     |
| 4   | A     | 501 | CIT  | C2-C3-C4-C5     |
| 3   | D     | 502 | BNG  | O5-C5-C6-O6     |
| 3   | C     | 503 | BNG  | O1-C1'-C2'-C3'  |
| 3   | D     | 502 | BNG  | O1-C1'-C2'-C3'  |
| 4   | A     | 501 | CIT  | C2-C3-C6-O5     |
| 3   | B     | 503 | BNG  | C5'-C6'-C7'-C8' |
| 3   | B     | 503 | BNG  | C1'-C2'-C3'-C4' |
| 4   | A     | 501 | CIT  | O7-C3-C4-C5     |
| 3   | B     | 503 | BNG  | C2'-C3'-C4'-C5' |
| 3   | B     | 503 | BNG  | C2-C1-O1-C1'    |
| 3   | B     | 503 | BNG  | O5-C5-C6-O6     |
| 4   | B     | 501 | CIT  | O7-C3-C4-C5     |
| 3   | B     | 503 | BNG  | C4'-C5'-C6'-C7' |
| 3   | D     | 502 | BNG  | C6'-C7'-C8'-C9' |
| 4   | A     | 501 | CIT  | C2-C3-C6-O6     |
| 4   | C     | 501 | CIT  | C1-C2-C3-O7     |
| 3   | C     | 503 | BNG  | C3'-C4'-C5'-C6' |

*Continued on next page...*

*Continued from previous page...*

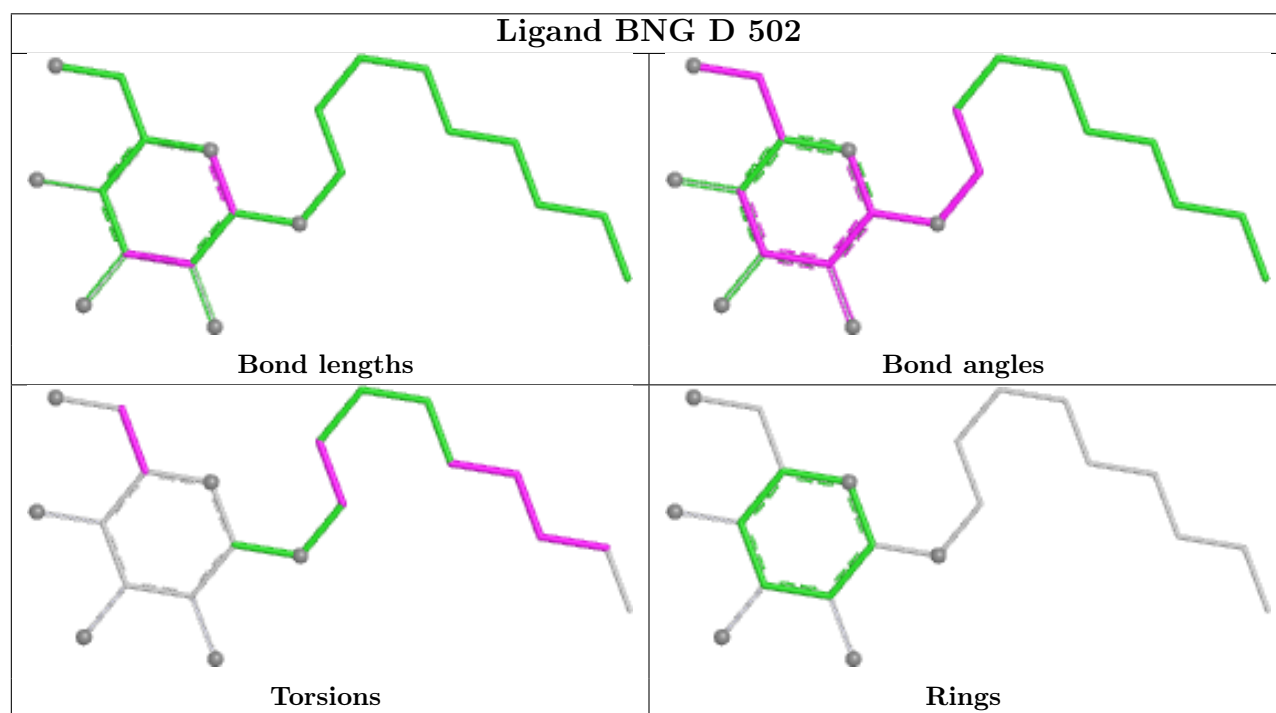
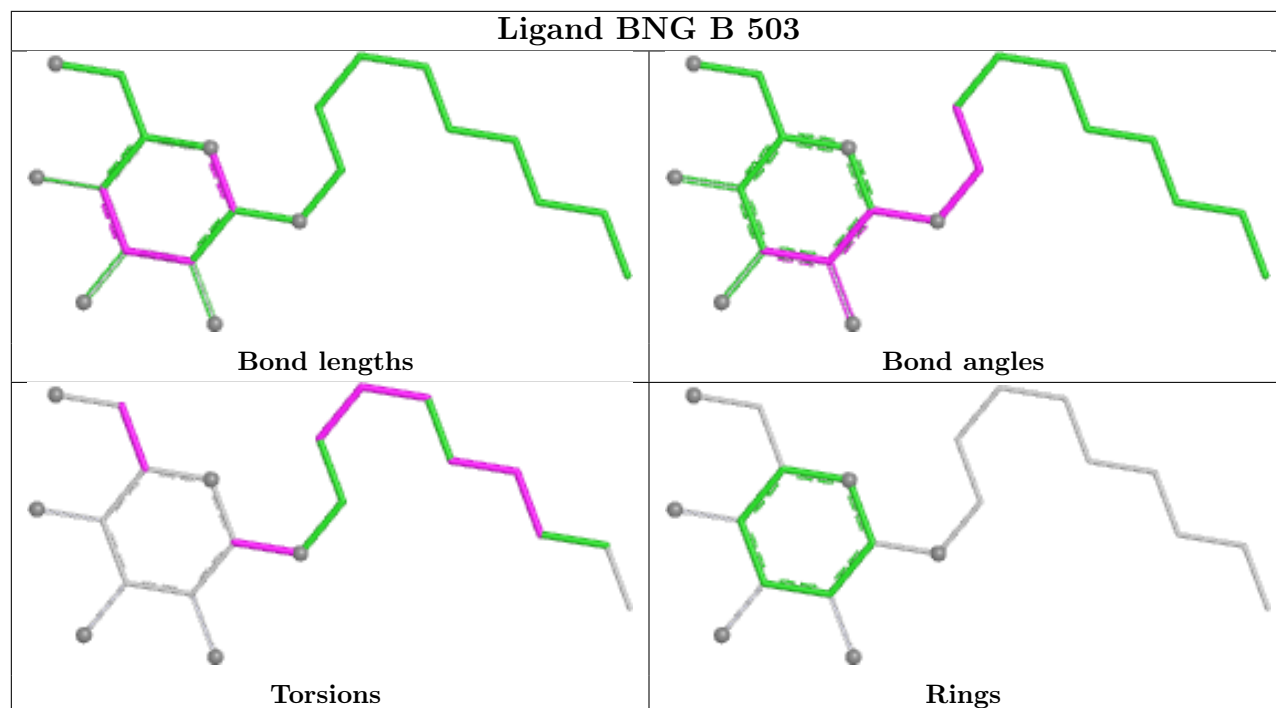
| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 4   | B     | 501 | CIT  | C4-C3-C6-O6     |
| 3   | D     | 502 | BNG  | C5'-C6'-C7'-C8' |
| 4   | A     | 501 | CIT  | C1-C2-C3-O7     |
| 3   | D     | 502 | BNG  | C4'-C5'-C6'-C7' |
| 3   | D     | 502 | BNG  | C4-C5-C6-O6     |
| 4   | A     | 501 | CIT  | C1-C2-C3-C4     |
| 4   | B     | 501 | CIT  | C1-C2-C3-O7     |
| 4   | B     | 501 | CIT  | C4-C3-C6-O5     |

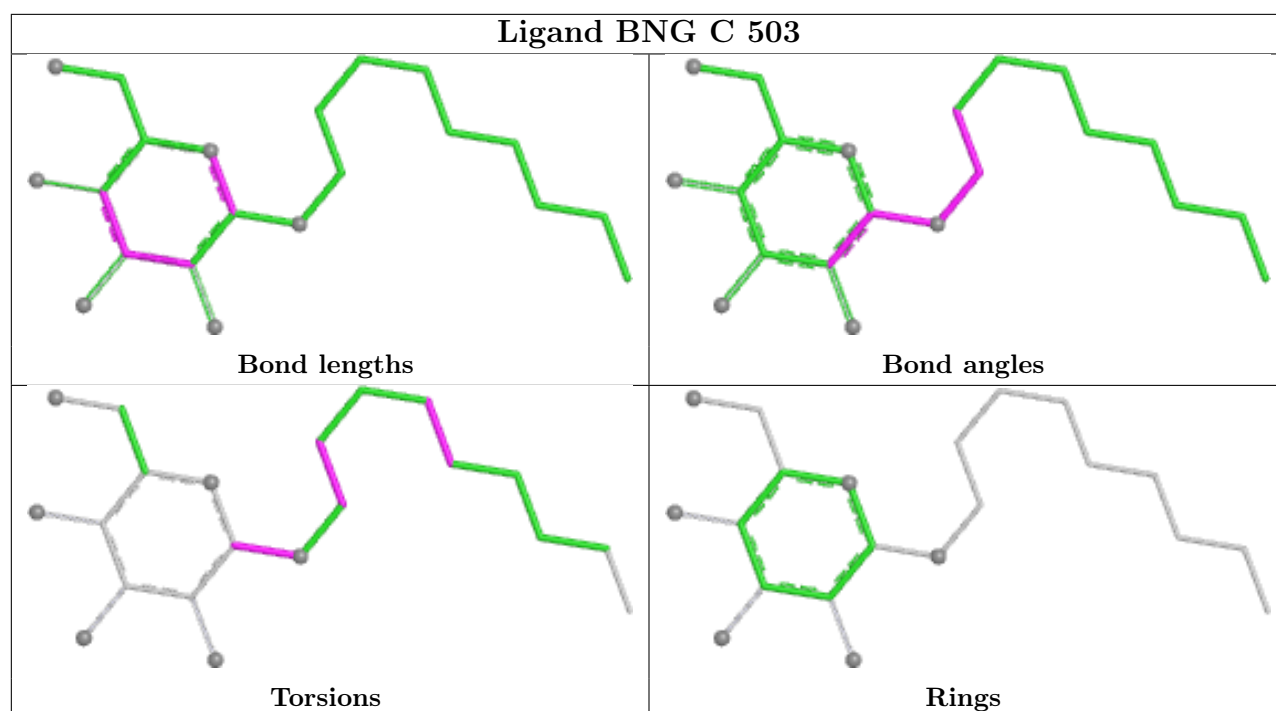
There are no ring outliers.

6 monomers are involved in 23 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 3   | B     | 503 | BNG  | 5       | 0            |
| 4   | B     | 501 | CIT  | 6       | 0            |
| 4   | A     | 501 | CIT  | 3       | 0            |
| 3   | D     | 502 | BNG  | 3       | 0            |
| 4   | C     | 501 | CIT  | 5       | 0            |
| 3   | C     | 503 | BNG  | 1       | 0            |

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





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

| Mol | Chain | Analysed        | <RSRZ> | #RSRZ > 2 |       | OWAB(Å <sup>2</sup> ) | Q < 0.9 |
|-----|-------|-----------------|--------|-----------|-------|-----------------------|---------|
| 1   | A     | 412/449 (91%)   | 0.16   | 26 (6%)   | 26 17 | 56, 93, 150, 196      | 0       |
| 1   | B     | 393/449 (87%)   | 0.24   | 30 (7%)   | 20 13 | 61, 103, 160, 188     | 0       |
| 1   | C     | 408/449 (90%)   | -0.02  | 13 (3%)   | 50 31 | 53, 87, 139, 187      | 0       |
| 1   | D     | 408/449 (90%)   | 0.16   | 15 (3%)   | 45 28 | 48, 89, 142, 229      | 1 (0%)  |
| All | All   | 1621/1796 (90%) | 0.13   | 84 (5%)   | 33 21 | 48, 93, 150, 229      | 1 (0%)  |

All (84) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | C     | 178 | TYR  | 5.5  |
| 1   | B     | 260 | GLY  | 5.0  |
| 1   | C     | 443 | LEU  | 4.8  |
| 1   | A     | 132 | SER  | 4.4  |
| 1   | C     | 177 | THR  | 4.3  |
| 1   | D     | 114 | GLY  | 4.2  |
| 1   | D     | 432 | HIS  | 4.1  |
| 1   | B     | 134 | ALA  | 4.0  |
| 1   | D     | 164 | GLY  | 4.0  |
| 1   | C     | 81  | GLY  | 4.0  |
| 1   | B     | 111 | HIS  | 3.7  |
| 1   | C     | 289 | LYS  | 3.7  |
| 1   | C     | 370 | VAL  | 3.6  |
| 1   | B     | 61  | THR  | 3.3  |
| 1   | A     | 429 | ALA  | 3.2  |
| 1   | B     | 153 | ALA  | 3.2  |
| 1   | A     | 242 | PRO  | 3.2  |
| 1   | D     | 433 | ILE  | 3.0  |
| 1   | D     | 193 | GLY  | 3.0  |
| 1   | C     | 420 | ALA  | 2.9  |
| 1   | B     | 412 | SER  | 2.9  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | A     | 258 | ASP  | 2.9  |
| 1   | B     | 334 | ASN  | 2.8  |
| 1   | B     | 136 | PHE  | 2.8  |
| 1   | B     | 220 | PHE  | 2.8  |
| 1   | A     | 125 | ALA  | 2.7  |
| 1   | B     | 268 | PHE  | 2.7  |
| 1   | B     | 289 | LYS  | 2.7  |
| 1   | B     | 178 | TYR  | 2.7  |
| 1   | B     | 306 | ALA  | 2.7  |
| 1   | A     | 80  | PHE  | 2.6  |
| 1   | D     | 381 | SER  | 2.6  |
| 1   | A     | 420 | ALA  | 2.6  |
| 1   | C     | 132 | SER  | 2.6  |
| 1   | A     | 417 | LEU  | 2.6  |
| 1   | A     | 241 | LYS  | 2.6  |
| 1   | C     | 430 | SER  | 2.6  |
| 1   | C     | 176 | SER  | 2.5  |
| 1   | C     | 130 | LYS  | 2.5  |
| 1   | B     | 370 | VAL  | 2.5  |
| 1   | A     | 49  | ILE  | 2.5  |
| 1   | D     | 179 | VAL  | 2.5  |
| 1   | C     | 374 | GLU  | 2.4  |
| 1   | D     | 429 | ALA  | 2.4  |
| 1   | A     | 174 | GLN  | 2.4  |
| 1   | A     | 373 | THR  | 2.4  |
| 1   | D     | 177 | THR  | 2.4  |
| 1   | A     | 433 | ILE  | 2.4  |
| 1   | D     | 176 | SER  | 2.4  |
| 1   | B     | 414 | ALA  | 2.4  |
| 1   | C     | 358 | ILE  | 2.4  |
| 1   | B     | 462 | GLN  | 2.4  |
| 1   | B     | 338 | GLN  | 2.3  |
| 1   | D     | 260 | GLY  | 2.3  |
| 1   | A     | 260 | GLY  | 2.3  |
| 1   | B     | 176 | SER  | 2.3  |
| 1   | D     | 417 | LEU  | 2.3  |
| 1   | A     | 368 | PHE  | 2.3  |
| 1   | A     | 430 | SER  | 2.3  |
| 1   | A     | 128 | GLN  | 2.3  |
| 1   | A     | 307 | ARG  | 2.3  |
| 1   | A     | 28  | ASP  | 2.3  |
| 1   | B     | 375 | PHE  | 2.2  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | A     | 412 | SER  | 2.2  |
| 1   | A     | 121 | ASP  | 2.2  |
| 1   | D     | 214 | PHE  | 2.2  |
| 1   | B     | 152 | THR  | 2.2  |
| 1   | A     | 36  | TYR  | 2.2  |
| 1   | A     | 257 | TRP  | 2.2  |
| 1   | B     | 112 | HIS  | 2.2  |
| 1   | B     | 167 | SER  | 2.1  |
| 1   | B     | 259 | LYS  | 2.1  |
| 1   | B     | 40  | PRO  | 2.1  |
| 1   | B     | 211 | GLY  | 2.1  |
| 1   | B     | 367 | THR  | 2.1  |
| 1   | A     | 265 | LEU  | 2.1  |
| 1   | D     | 452 | LEU  | 2.1  |
| 1   | B     | 360 | VAL  | 2.1  |
| 1   | B     | 376 | ALA  | 2.1  |
| 1   | B     | 409 | VAL  | 2.0  |
| 1   | A     | 183 | LEU  | 2.0  |
| 1   | A     | 176 | SER  | 2.0  |
| 1   | D     | 428 | PHE  | 2.0  |
| 1   | B     | 402 | LEU  | 2.0  |

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

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

## 6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 6.4 Ligands ⓘ

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

| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 3   | BNG  | B     | 503 | 21/21 | 0.83 | 0.18 | 62,175,190,333              | 0     |
| 3   | BNG  | D     | 502 | 21/21 | 0.84 | 0.12 | 75,100,143,143              | 0     |

*Continued on next page...*

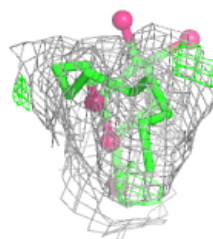
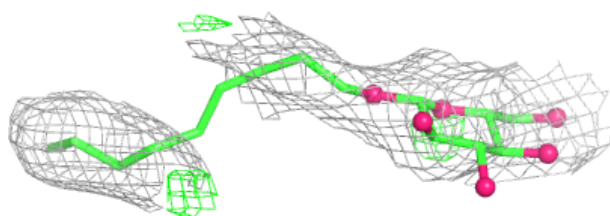
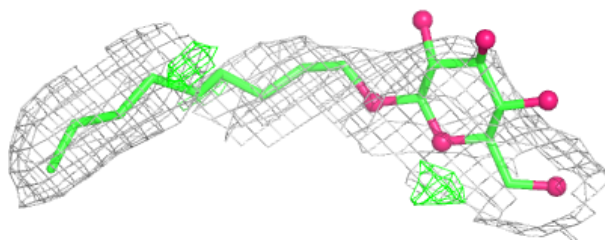
*Continued from previous page...*

| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 4   | CIT  | B     | 501 | 13/13 | 0.86 | 0.14 | 127,135,161,164             | 0     |
| 3   | BNG  | C     | 503 | 21/21 | 0.87 | 0.13 | 58,111,159,160              | 0     |
| 4   | CIT  | C     | 501 | 13/13 | 0.87 | 0.16 | 88,110,139,149              | 0     |
| 4   | CIT  | A     | 501 | 13/13 | 0.88 | 0.15 | 101,117,130,136             | 0     |
| 2   | NA   | B     | 502 | 1/1   | 0.94 | 0.21 | 71,71,71,71                 | 0     |
| 2   | NA   | D     | 501 | 1/1   | 0.96 | 0.10 | 63,63,63,63                 | 0     |
| 2   | NA   | A     | 502 | 1/1   | 0.97 | 0.32 | 77,77,77,77                 | 0     |
| 2   | NA   | C     | 502 | 1/1   | 0.97 | 0.15 | 53,53,53,53                 | 0     |

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

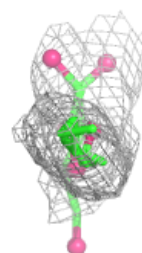
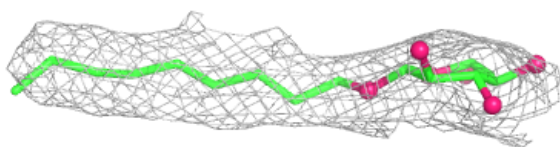
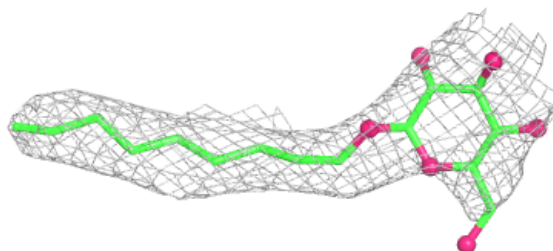
**Electron density around BNG B 503:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)

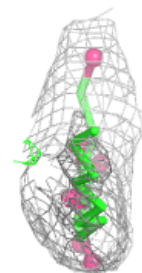
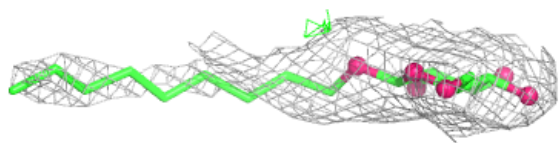


**Electron density around BNG D 502:**

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

**Electron density around BNG C 503:**

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



## 6.5 Other polymers [i](#)

There are no such residues in this entry.