



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:17 PM GMT

PDB ID : 4HUL  
Title : MATE transporter NorM-NG in complex with Cs<sup>+</sup> and monobody  
Authors : Lu, M.  
Deposited on : 2012-11-02  
Resolution : 3.81 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  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

---

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

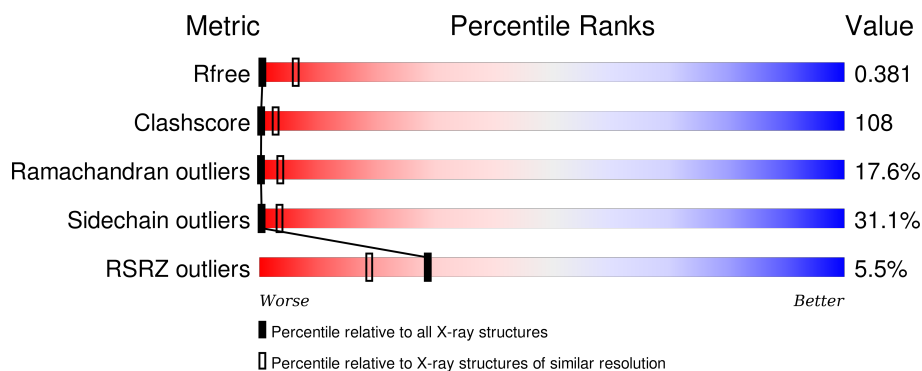
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.81 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)) |
|-----------------------|-----------------------------|---|
| $R_{free}$            | 91344                       | 1324 (4.14-3.50)                                      |
| Clashscore            | 102246                      | 1028 (4.12-3.52)                                      |
| Ramachandran outliers | 100387                      | 1404 (4.14-3.50)                                      |
| Sidechain outliers    | 100360                      | 1399 (4.14-3.50)                                      |
| RSRZ outliers         | 91569                       | 1332 (4.14-3.50)                                      |

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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     | 459    |                  |
| 2   | B     | 99     |                  |

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4216 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 Multidrug efflux protein.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | A     | 459      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3508  | 2338 | 558 | 589 | 23 |         |         |       |

There are 4 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| A     | 460     | SER      | -      | EXPRESSION TAG | UNP E8SM44 |
| A     | 461     | SER      | -      | EXPRESSION TAG | UNP E8SM44 |
| A     | 462     | GLY      | -      | EXPRESSION TAG | UNP E8SM44 |
| A     | 463     | LEU      | -      | EXPRESSION TAG | UNP E8SM44 |

- Molecule 2 is a protein called Protein B.

| Mol | Chain | Residues | Atoms |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 2   | B     | 91       | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 707   | 457 | 110 | 140 |         |         |       |

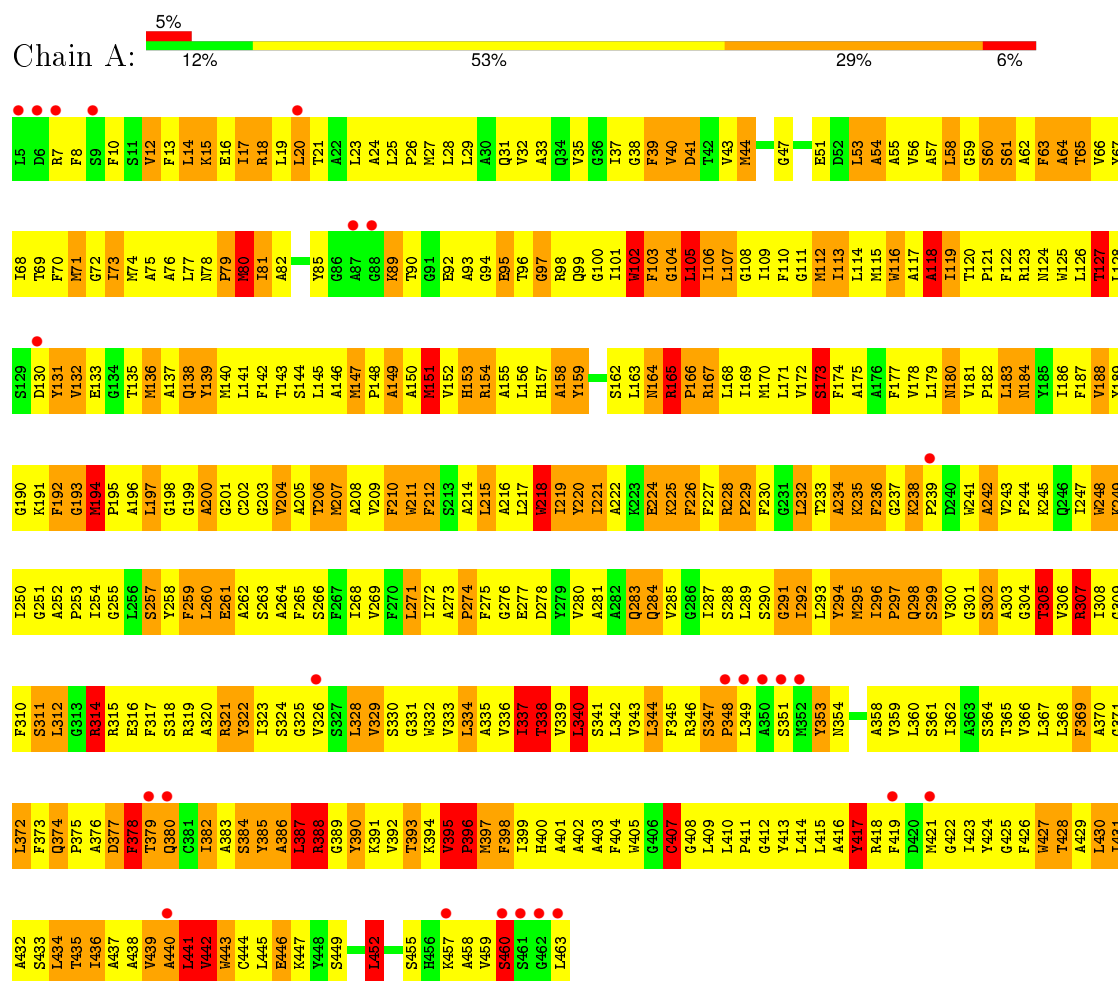
- Molecule 3 is CESIUM ION (three-letter code: CS) (formula: Cs).

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 3   | A     | 1        | Total | Cs | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

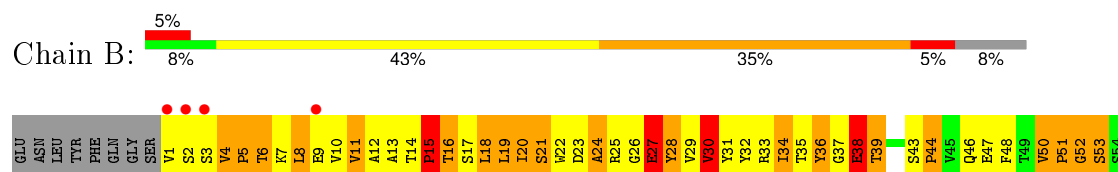
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: Multidrug efflux protein



#### • Molecule 2: Protein B



|     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| S55 | T56 | A57 | T58 | I59 | S60 | G61 | L62 | S63 | P64 | G65 | Y66 | D67 | Y68 | T69 | I70 | T71 | V72 | Y73 | A74 | R75 | S76 | Y77 | Y78 | W79 | G80 | W81 | Y82 | S83 | P84 | I85 | S86 | I87 | N88 | Y89 | F90 | T91 |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

## 4 Data and refinement statistics

| Property  | Value   | Source           |
|---|---|------------------|
| Space group   | P 32 2 1  | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 118.33Å 118.33Å 227.32Å<br>90.00° 90.00° 120.00°            | Depositor        |
| Resolution (Å)  | 20.00 – 3.81<br>52.48 – 3.81                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 98.3 (20.00-3.81)<br>98.3 (52.48-3.81)                      | Depositor<br>EDS |
| $R_{merge}$   | (Not available)   | Depositor        |
| $R_{sym}$   | (Not available)   | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.81 (at 3.77Å)   | Xtriage          |
| Refinement program  | REFMAC 5.6.0117   | Depositor        |
| R, $R_{free}$   | 0.311 , 0.376<br>0.313 , 0.381                              | Depositor<br>DCC |
| $R_{free}$ test set   | 926 reflections (5.37%)                                     | DCC              |
| Wilson B-factor (Å <sup>2</sup> )                                       | 119.9   | Xtriage          |
| Anisotropy  | 0.437   | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.17 , 135.6  | EDS              |
| Estimated twinning fraction   | 0.197 for -h,-k,l   | Xtriage          |
| L-test for twinning <sup>2</sup>  | $\langle  L  \rangle = 0.33$ , $\langle L^2 \rangle = 0.16$ | Xtriage          |
| Outliers  | 3 of 18305 reflections (0.016%)                             | Xtriage          |
| $F_o, F_c$ correlation  | 0.82  | EDS              |
| Total number of atoms   | 4216  | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 215.0   | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.05% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: CS

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     | 0.92         | 5/3605 (0.1%) | 1.08        | 10/4898 (0.2%) |
| 2   | B     | 0.95         | 0/729         | 1.19        | 2/1004 (0.2%)  |
| All | All   | 0.92         | 5/4334 (0.1%) | 1.10        | 12/5902 (0.2%) |

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                   | 24                  |
| 2   | B     | 0                   | 4                   |
| All | All   | 0                   | 28                  |

All (5) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 1   | A     | 125 | TRP  | CD2-CE2 | 5.48 | 1.48        | 1.41     |
| 1   | A     | 211 | TRP  | CD2-CE2 | 5.37 | 1.47        | 1.41     |
| 1   | A     | 102 | TRP  | CD2-CE2 | 5.32 | 1.47        | 1.41     |
| 1   | A     | 218 | TRP  | CD2-CE2 | 5.25 | 1.47        | 1.41     |
| 1   | A     | 443 | TRP  | CD2-CE2 | 5.22 | 1.47        | 1.41     |

All (12) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 2   | B     | 30  | VAL  | CB-CA-C  | -8.80 | 94.68       | 111.40   |
| 1   | A     | 340 | LEU  | CA-CB-CG | 6.67  | 130.64      | 115.30   |
| 1   | A     | 221 | ILE  | N-CA-C   | -6.12 | 94.49       | 111.00   |
| 1   | A     | 441 | LEU  | CA-CB-CG | 6.07  | 129.26      | 115.30   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | A     | 328 | LEU  | CA-CB-CG  | 5.96  | 129.01      | 115.30   |
| 1   | A     | 312 | LEU  | CA-CB-CG  | 5.86  | 128.77      | 115.30   |
| 2   | B     | 27  | GLU  | C-N-CA    | -5.65 | 107.57      | 121.70   |
| 1   | A     | 407 | CYS  | CA-CB-SG  | 5.51  | 123.92      | 114.00   |
| 1   | A     | 105 | LEU  | CA-CB-CG  | -5.33 | 103.03      | 115.30   |
| 1   | A     | 340 | LEU  | CB-CG-CD1 | 5.09  | 119.65      | 111.00   |
| 1   | A     | 218 | TRP  | CA-CB-CG  | -5.01 | 104.18      | 113.70   |
| 1   | A     | 388 | ARG  | NE-CZ-NH1 | 5.01  | 122.80      | 120.30   |

There are no chirality outliers.

All (28) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 1   | A     | 118 | ALA  | Peptide |
| 1   | A     | 131 | TYR  | Peptide |
| 1   | A     | 138 | GLN  | Peptide |
| 1   | A     | 165 | ARG  | Peptide |
| 1   | A     | 188 | VAL  | Peptide |
| 1   | A     | 194 | MET  | Peptide |
| 1   | A     | 220 | TYR  | Peptide |
| 1   | A     | 226 | PHE  | Peptide |
| 1   | A     | 249 | LYS  | Peptide |
| 1   | A     | 273 | ALA  | Peptide |
| 1   | A     | 314 | ARG  | Peptide |
| 1   | A     | 322 | TYR  | Peptide |
| 1   | A     | 337 | ILE  | Peptide |
| 1   | A     | 338 | THR  | Peptide |
| 1   | A     | 387 | LEU  | Peptide |
| 1   | A     | 393 | THR  | Peptide |
| 1   | A     | 395 | VAL  | Peptide |
| 1   | A     | 396 | PRO  | Peptide |
| 1   | A     | 40  | VAL  | Peptide |
| 1   | A     | 430 | LEU  | Peptide |
| 1   | A     | 442 | VAL  | Peptide |
| 1   | A     | 446 | GLU  | Peptide |
| 1   | A     | 452 | LEU  | Peptide |
| 1   | A     | 54  | ALA  | Peptide |
| 2   | B     | 15  | PRO  | Peptide |
| 2   | B     | 27  | GLU  | Peptide |
| 2   | B     | 4   | VAL  | Peptide |
| 2   | B     | 82  | TYR  | 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     | 3508  | 0        | 3586     | 744     | 0            |
| 2   | B     | 707   | 0        | 681      | 189     | 0            |
| 3   | A     | 1     | 0        | 0        | 0       | 0            |
| All | All   | 4216  | 0        | 4267     | 918     | 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 108.

All (918) 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:158:ALA:HB2  | 1:A:217:LEU:CD1  | 1.28                     | 1.62              |
| 1:A:158:ALA:CB   | 1:A:217:LEU:HD11 | 1.47                     | 1.43              |
| 1:A:144:SER:CB   | 1:A:204:VAL:HG12 | 1.58                     | 1.31              |
| 1:A:78:ASN:HA    | 1:A:163:LEU:CD1  | 1.65                     | 1.24              |
| 1:A:343:VAL:HG13 | 1:A:367:LEU:O    | 1.35                     | 1.23              |
| 1:A:268:ILE:HD13 | 1:A:287:ILE:CD1  | 1.72                     | 1.20              |
| 2:B:4:VAL:HG22   | 2:B:6:THR:HG23   | 1.19                     | 1.17              |
| 1:A:78:ASN:HA    | 1:A:163:LEU:HD11 | 1.27                     | 1.16              |
| 2:B:19:LEU:HD11  | 2:B:21:SER:OG    | 1.46                     | 1.13              |
| 1:A:387:LEU:HD12 | 1:A:393:THR:CG2  | 1.78                     | 1.11              |
| 1:A:65:THR:O     | 1:A:69:THR:HG22  | 1.50                     | 1.11              |
| 1:A:149:ALA:HA   | 1:A:152:VAL:HG21 | 1.32                     | 1.10              |
| 2:B:30:VAL:O     | 2:B:30:VAL:HG13  | 1.40                     | 1.09              |
| 1:A:268:ILE:CD1  | 1:A:287:ILE:HD11 | 1.81                     | 1.09              |
| 1:A:149:ALA:HA   | 1:A:152:VAL:CG2  | 1.82                     | 1.09              |
| 1:A:183:LEU:HA   | 1:A:186:ILE:HD12 | 1.36                     | 1.08              |
| 1:A:73:ILE:O     | 1:A:76:ALA:HB3   | 1.51                     | 1.08              |
| 1:A:288:SER:O    | 1:A:292:ILE:HG23 | 1.50                     | 1.08              |
| 1:A:369:PHE:HB3  | 1:A:372:LEU:HD12 | 1.34                     | 1.08              |
| 1:A:372:LEU:HB3  | 1:A:431:ILE:HG21 | 1.36                     | 1.07              |
| 2:B:12:ALA:O     | 2:B:18:LEU:HD23  | 1.54                     | 1.06              |
| 2:B:4:VAL:CG2    | 2:B:6:THR:HG23   | 1.87                     | 1.05              |
| 2:B:19:LEU:HA    | 2:B:58:THR:HG22  | 1.38                     | 1.05              |
| 1:A:418:ARG:HG2  | 1:A:422:GLY:HA3  | 1.38                     | 1.04              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:144:SER:HB3  | 1:A:204:VAL:CG1  | 1.88                     | 1.04              |
| 1:A:339:VAL:HG21 | 1:A:375:PRO:HD3  | 1.40                     | 1.04              |
| 1:A:411:PRO:CB   | 1:A:428:THR:HG23 | 1.87                     | 1.03              |
| 1:A:395:VAL:HG13 | 1:A:396:PRO:HD3  | 1.37                     | 1.01              |
| 1:A:387:LEU:HD12 | 1:A:393:THR:HG22 | 1.40                     | 1.01              |
| 1:A:105:LEU:O    | 1:A:109:ILE:HG23 | 1.60                     | 1.00              |
| 1:A:158:ALA:CB   | 1:A:217:LEU:CD1  | 2.17                     | 1.00              |
| 1:A:394:LYS:HA   | 1:A:397:MET:HB2  | 1.41                     | 1.00              |
| 1:A:145:LEU:HD13 | 1:A:203:GLY:O    | 1.62                     | 0.99              |
| 1:A:289:LEU:HD13 | 1:A:292:ILE:HG12 | 1.43                     | 0.99              |
| 1:A:411:PRO:HB3  | 1:A:428:THR:CG2  | 1.92                     | 0.99              |
| 1:A:339:VAL:HA   | 1:A:342:LEU:CD1  | 1.94                     | 0.98              |
| 1:A:308:ILE:CD1  | 1:A:386:ALA:HA   | 1.94                     | 0.98              |
| 1:A:141:LEU:CD1  | 1:A:145:LEU:HD23 | 1.93                     | 0.98              |
| 1:A:218:TRP:HA   | 1:A:218:TRP:CE3  | 1.94                     | 0.97              |
| 1:A:411:PRO:HB3  | 1:A:428:THR:HG23 | 0.98                     | 0.97              |
| 1:A:268:ILE:HD13 | 1:A:287:ILE:HD11 | 0.97                     | 0.96              |
| 2:B:65:GLY:HA2   | 2:B:91:THR:CB    | 1.96                     | 0.96              |
| 1:A:214:ALA:C    | 1:A:215:LEU:HD23 | 1.86                     | 0.95              |
| 2:B:30:VAL:O     | 2:B:30:VAL:CG1   | 2.12                     | 0.95              |
| 1:A:144:SER:HB3  | 1:A:204:VAL:HG12 | 0.97                     | 0.95              |
| 1:A:333:VAL:HG12 | 1:A:334:LEU:HD13 | 1.44                     | 0.95              |
| 1:A:107:LEU:HD23 | 1:A:108:GLY:N    | 1.82                     | 0.95              |
| 1:A:158:ALA:HB2  | 1:A:217:LEU:HD12 | 1.46                     | 0.94              |
| 1:A:168:LEU:HA   | 1:A:171:LEU:HD13 | 1.47                     | 0.94              |
| 1:A:78:ASN:HA    | 1:A:163:LEU:HD13 | 1.48                     | 0.94              |
| 1:A:372:LEU:CD1  | 1:A:427:TRP:HB2  | 1.99                     | 0.93              |
| 1:A:260:LEU:HD21 | 1:A:404:PHE:O    | 1.69                     | 0.92              |
| 1:A:460:SER:O    | 2:B:8:LEU:CD1    | 2.17                     | 0.92              |
| 1:A:260:LEU:HD11 | 1:A:404:PHE:HB2  | 1.52                     | 0.92              |
| 1:A:115:MET:O    | 1:A:118:ALA:HB3  | 1.70                     | 0.91              |
| 1:A:290:SER:O    | 1:A:294:TYR:HB3  | 1.71                     | 0.91              |
| 1:A:164:ASN:O    | 1:A:166:PRO:HD3  | 1.71                     | 0.91              |
| 1:A:254:ILE:HB   | 1:A:394:LYS:NZ   | 1.85                     | 0.91              |
| 1:A:460:SER:O    | 2:B:8:LEU:HD12   | 1.69                     | 0.91              |
| 1:A:261:GLU:HA   | 1:A:264:ALA:HB3  | 1.53                     | 0.90              |
| 1:A:306:VAL:O    | 1:A:308:ILE:N    | 2.04                     | 0.90              |
| 1:A:251:GLY:O    | 1:A:254:ILE:HG22 | 1.71                     | 0.90              |
| 1:A:410:LEU:O    | 1:A:414:LEU:HD13 | 1.72                     | 0.90              |
| 1:A:339:VAL:HG23 | 1:A:342:LEU:HD12 | 1.53                     | 0.90              |
| 1:A:349:LEU:HD21 | 1:A:360:LEU:HD11 | 1.50                     | 0.90              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:272:ILE:HG22 | 1:A:280:VAL:O    | 1.71                     | 0.90              |
| 1:A:372:LEU:HD13 | 1:A:427:TRP:HB2  | 1.53                     | 0.90              |
| 1:A:351:SER:O    | 1:A:359:VAL:HG11 | 1.72                     | 0.90              |
| 1:A:372:LEU:HD13 | 1:A:427:TRP:CB   | 2.01                     | 0.89              |
| 2:B:67:ASP:HA    | 2:B:90:ARG:HG2   | 1.51                     | 0.89              |
| 1:A:107:LEU:HD23 | 1:A:108:GLY:H    | 1.37                     | 0.89              |
| 2:B:4:VAL:HG22   | 2:B:6:THR:CG2    | 2.01                     | 0.89              |
| 2:B:67:ASP:HA    | 2:B:90:ARG:CG    | 2.02                     | 0.88              |
| 1:A:254:ILE:HD11 | 1:A:388:ARG:HH11 | 1.37                     | 0.88              |
| 2:B:36:TYR:HA    | 2:B:70:ILE:HD11  | 1.55                     | 0.88              |
| 1:A:145:LEU:HD12 | 1:A:207:MET:HB3  | 1.52                     | 0.88              |
| 2:B:24:ALA:O     | 2:B:53:SER:OG    | 1.92                     | 0.87              |
| 1:A:254:ILE:HD11 | 1:A:388:ARG:NH1  | 1.89                     | 0.87              |
| 1:A:158:ALA:CA   | 1:A:217:LEU:HD11 | 2.04                     | 0.87              |
| 1:A:113:ILE:HG22 | 1:A:114:LEU:HD23 | 1.57                     | 0.87              |
| 1:A:44:MET:SD    | 1:A:206:THR:HG23 | 2.15                     | 0.86              |
| 1:A:218:TRP:HE3  | 1:A:218:TRP:HA   | 1.36                     | 0.86              |
| 1:A:368:LEU:HD12 | 1:A:423:ILE:CG2  | 2.05                     | 0.86              |
| 1:A:339:VAL:HA   | 1:A:342:LEU:HD12 | 1.56                     | 0.86              |
| 1:A:73:ILE:O     | 1:A:76:ALA:CB    | 2.23                     | 0.86              |
| 1:A:159:TYR:HB3  | 1:A:169:ILE:HD13 | 1.56                     | 0.86              |
| 1:A:168:LEU:HD23 | 1:A:171:LEU:HD22 | 1.58                     | 0.86              |
| 2:B:19:LEU:C     | 2:B:20:ILE:HD13  | 1.96                     | 0.86              |
| 1:A:387:LEU:HD12 | 1:A:393:THR:HG21 | 1.57                     | 0.86              |
| 1:A:337:ILE:O    | 1:A:337:ILE:HD12 | 1.73                     | 0.86              |
| 1:A:425:GLY:O    | 1:A:428:THR:CG2  | 2.23                     | 0.86              |
| 1:A:188:VAL:HA   | 1:A:198:GLY:HA2  | 1.58                     | 0.85              |
| 1:A:141:LEU:HD11 | 1:A:145:LEU:HD23 | 1.57                     | 0.85              |
| 1:A:346:ARG:CD   | 1:A:367:LEU:HD11 | 2.07                     | 0.84              |
| 2:B:65:GLY:HA2   | 2:B:91:THR:HB    | 1.59                     | 0.83              |
| 1:A:259:PHE:HA   | 1:A:262:ALA:HB3  | 1.60                     | 0.83              |
| 1:A:425:GLY:O    | 1:A:428:THR:HG22 | 1.78                     | 0.83              |
| 2:B:19:LEU:HD13  | 2:B:19:LEU:C     | 1.99                     | 0.82              |
| 1:A:63:PHE:O     | 1:A:65:THR:N     | 2.12                     | 0.82              |
| 1:A:395:VAL:CG1  | 1:A:396:PRO:HD3  | 2.07                     | 0.82              |
| 1:A:301:GLY:O    | 1:A:305:THR:HG22 | 1.79                     | 0.82              |
| 1:A:58:LEU:HD12  | 1:A:138:GLN:CD   | 2.00                     | 0.82              |
| 2:B:12:ALA:O     | 2:B:18:LEU:CD2   | 2.27                     | 0.81              |
| 2:B:20:ILE:HD11  | 2:B:59:ILE:HG23  | 1.60                     | 0.81              |
| 2:B:87:ILE:HG22  | 2:B:88:ASN:H     | 1.45                     | 0.81              |
| 1:A:53:LEU:HD22  | 1:A:135:THR:HG21 | 1.60                     | 0.81              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:340:LEU:HD12 | 1:A:341:SER:H    | 1.44                     | 0.81              |
| 1:A:394:LYS:HA   | 1:A:397:MET:CB   | 2.10                     | 0.81              |
| 1:A:172:VAL:HG21 | 1:A:216:ALA:CB   | 2.10                     | 0.81              |
| 1:A:137:ALA:O    | 1:A:199:GLY:O    | 1.98                     | 0.80              |
| 1:A:44:MET:CE    | 1:A:180:ASN:HD21 | 1.94                     | 0.80              |
| 1:A:215:LEU:N    | 1:A:215:LEU:HD23 | 1.92                     | 0.80              |
| 1:A:63:PHE:C     | 1:A:65:THR:H     | 1.81                     | 0.80              |
| 1:A:397:MET:O    | 1:A:400:HIS:N    | 2.15                     | 0.80              |
| 1:A:115:MET:O    | 1:A:118:ALA:CB   | 2.30                     | 0.80              |
| 1:A:441:LEU:O    | 1:A:444:CYS:N    | 2.15                     | 0.79              |
| 1:A:329:VAL:HA   | 1:A:332:TRP:HB3  | 1.64                     | 0.79              |
| 2:B:35:THR:HG23  | 2:B:73:TYR:HE1   | 1.48                     | 0.78              |
| 1:A:415:LEU:HD11 | 1:A:423:ILE:HD12 | 1.64                     | 0.78              |
| 1:A:442:VAL:HG23 | 1:A:445:LEU:HD22 | 1.64                     | 0.78              |
| 2:B:38:GLU:HA    | 2:B:68:TYR:HA    | 1.64                     | 0.78              |
| 1:A:141:LEU:HD13 | 1:A:145:LEU:HD23 | 1.64                     | 0.78              |
| 1:A:132:VAL:HG13 | 1:A:133:GLU:H    | 1.49                     | 0.78              |
| 1:A:31:GLN:NE2   | 1:A:296:ILE:O    | 2.17                     | 0.78              |
| 1:A:55:ALA:O     | 1:A:58:LEU:HD11  | 1.83                     | 0.78              |
| 1:A:429:ALA:O    | 1:A:433:SER:CB   | 2.32                     | 0.78              |
| 1:A:149:ALA:HA   | 1:A:152:VAL:HG22 | 1.65                     | 0.78              |
| 2:B:86:SER:O     | 2:B:87:ILE:HD13  | 1.84                     | 0.77              |
| 1:A:40:VAL:HG12  | 1:A:44:MET:HE3   | 1.66                     | 0.77              |
| 2:B:76:SER:HB3   | 2:B:82:TYR:CD2   | 2.19                     | 0.77              |
| 1:A:411:PRO:HG3  | 1:A:429:ALA:HB3  | 1.64                     | 0.77              |
| 1:A:463:LEU:O    | 2:B:3:SER:OG     | 2.02                     | 0.77              |
| 2:B:31:TYR:HB3   | 2:B:75:ARG:HB3   | 1.67                     | 0.77              |
| 1:A:297:PRO:O    | 1:A:299:SER:N    | 2.18                     | 0.76              |
| 1:A:305:THR:HB   | 1:A:385:TYR:O    | 1.86                     | 0.76              |
| 1:A:172:VAL:HG21 | 1:A:216:ALA:HB1  | 1.66                     | 0.76              |
| 1:A:148:PRO:O    | 1:A:150:ALA:N    | 2.19                     | 0.76              |
| 1:A:151:MET:HB2  | 1:A:211:TRP:CE2  | 2.20                     | 0.76              |
| 1:A:78:ASN:CA    | 1:A:163:LEU:CD1  | 2.58                     | 0.76              |
| 1:A:77:LEU:HD11  | 1:A:247:ILE:HG12 | 1.67                     | 0.76              |
| 1:A:180:ASN:O    | 1:A:184:ASN:N    | 2.19                     | 0.75              |
| 2:B:39:THR:HG1   | 2:B:69:THR:HG1   | 1.32                     | 0.75              |
| 1:A:404:PHE:HA   | 1:A:433:SER:OG   | 1.86                     | 0.75              |
| 1:A:55:ALA:HB1   | 1:A:58:LEU:HD21  | 1.69                     | 0.75              |
| 1:A:144:SER:CB   | 1:A:204:VAL:CG1  | 2.53                     | 0.75              |
| 1:A:148:PRO:HB2  | 1:A:152:VAL:HG11 | 1.67                     | 0.75              |
| 1:A:334:LEU:HD12 | 1:A:337:ILE:HD11 | 1.66                     | 0.75              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:184:ASN:HA   | 1:A:205:ALA:HB1  | 1.67                     | 0.74              |
| 1:A:82:ALA:HB1   | 1:A:310:PHE:HB2  | 1.68                     | 0.74              |
| 2:B:35:THR:O     | 2:B:70:ILE:HG12  | 1.86                     | 0.74              |
| 1:A:399:ILE:HG23 | 1:A:402:ALA:HB3  | 1.70                     | 0.74              |
| 1:A:359:VAL:HG12 | 1:A:360:LEU:HD22 | 1.70                     | 0.74              |
| 1:A:168:LEU:HD23 | 1:A:171:LEU:CD2  | 2.17                     | 0.74              |
| 2:B:36:TYR:HA    | 2:B:70:ILE:CD1   | 2.18                     | 0.73              |
| 2:B:87:ILE:HG22  | 2:B:88:ASN:N     | 2.03                     | 0.73              |
| 1:A:78:ASN:CA    | 1:A:163:LEU:HD13 | 2.18                     | 0.73              |
| 2:B:30:VAL:CG2   | 2:B:51:PRO:O     | 2.36                     | 0.73              |
| 1:A:102:TRP:CD1  | 1:A:233:THR:OG1  | 2.41                     | 0.73              |
| 1:A:259:PHE:HA   | 1:A:262:ALA:CB   | 2.18                     | 0.73              |
| 1:A:339:VAL:CG2  | 1:A:375:PRO:HD3  | 2.17                     | 0.73              |
| 1:A:230:PHE:CE1  | 1:A:233:THR:HG21 | 2.23                     | 0.73              |
| 1:A:260:LEU:O    | 1:A:262:ALA:N    | 2.22                     | 0.73              |
| 1:A:247:ILE:HG23 | 1:A:250:ILE:CD1  | 2.18                     | 0.73              |
| 1:A:332:TRP:HA   | 1:A:335:ALA:CB   | 2.19                     | 0.73              |
| 1:A:12:VAL:HG23  | 1:A:13:PHE:H     | 1.54                     | 0.73              |
| 1:A:395:VAL:CG1  | 1:A:396:PRO:CD   | 2.67                     | 0.72              |
| 1:A:168:LEU:CD2  | 1:A:171:LEU:HD22 | 2.20                     | 0.72              |
| 1:A:61:SER:O     | 1:A:265:PHE:HZ   | 1.71                     | 0.72              |
| 1:A:344:LEU:HD22 | 1:A:345:PHE:CD2  | 2.24                     | 0.72              |
| 1:A:188:VAL:HA   | 1:A:198:GLY:CA   | 2.20                     | 0.72              |
| 1:A:79:PRO:O     | 1:A:80:MET:C     | 2.27                     | 0.72              |
| 1:A:334:LEU:HA   | 1:A:337:ILE:HG13 | 1.72                     | 0.72              |
| 1:A:58:LEU:HD12  | 1:A:138:GLN:NE2  | 2.04                     | 0.72              |
| 1:A:300:VAL:O    | 1:A:304:GLY:N    | 2.23                     | 0.71              |
| 1:A:365:THR:HA   | 1:A:368:LEU:HD11 | 1.72                     | 0.71              |
| 1:A:247:ILE:HG23 | 1:A:250:ILE:HD11 | 1.69                     | 0.71              |
| 2:B:31:TYR:CD1   | 2:B:75:ARG:NH1   | 2.58                     | 0.71              |
| 1:A:255:GLY:O    | 1:A:258:TYR:N    | 2.24                     | 0.71              |
| 1:A:458:ALA:HB3  | 2:B:8:LEU:C      | 2.10                     | 0.71              |
| 1:A:61:SER:O     | 1:A:265:PHE:CZ   | 2.44                     | 0.71              |
| 1:A:296:ILE:HG22 | 1:A:297:PRO:HD3  | 1.73                     | 0.71              |
| 2:B:16:THR:O     | 2:B:61:GLY:O     | 2.08                     | 0.71              |
| 1:A:337:ILE:O    | 1:A:338:THR:OG1  | 2.08                     | 0.71              |
| 1:A:408:GLY:HA2  | 1:A:411:PRO:HG2  | 1.72                     | 0.71              |
| 1:A:432:ALA:O    | 1:A:436:ILE:HG23 | 1.91                     | 0.71              |
| 1:A:439:VAL:CG2  | 1:A:440:ALA:N    | 2.54                     | 0.71              |
| 1:A:44:MET:HE1   | 1:A:180:ASN:HD21 | 1.55                     | 0.71              |
| 1:A:151:MET:SD   | 1:A:211:TRP:CE3  | 2.84                     | 0.70              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:429:ALA:O    | 1:A:433:SER:HB2  | 1.89                     | 0.70              |
| 1:A:365:THR:HB   | 1:A:423:ILE:HG21 | 1.72                     | 0.70              |
| 1:A:306:VAL:C    | 1:A:308:ILE:H    | 1.95                     | 0.70              |
| 1:A:333:VAL:HG12 | 1:A:334:LEU:CD1  | 2.20                     | 0.70              |
| 1:A:308:ILE:HD13 | 1:A:386:ALA:HA   | 1.71                     | 0.70              |
| 1:A:250:ILE:HA   | 1:A:394:LYS:HD2  | 1.72                     | 0.70              |
| 1:A:349:LEU:CD2  | 1:A:360:LEU:HD11 | 2.20                     | 0.70              |
| 1:A:159:TYR:CB   | 1:A:169:ILE:HD13 | 2.21                     | 0.70              |
| 1:A:51:GLU:O     | 1:A:54:ALA:HB3   | 1.91                     | 0.70              |
| 1:A:343:VAL:HG22 | 1:A:370:ALA:C    | 2.12                     | 0.70              |
| 1:A:387:LEU:CD1  | 1:A:393:THR:CG2  | 2.66                     | 0.70              |
| 1:A:400:HIS:CE1  | 1:A:401:ALA:HB2  | 2.26                     | 0.70              |
| 1:A:340:LEU:HD13 | 1:A:341:SER:OG   | 1.92                     | 0.70              |
| 1:A:442:VAL:HG23 | 1:A:445:LEU:CD2  | 2.20                     | 0.70              |
| 1:A:297:PRO:O    | 1:A:298:GLN:C    | 2.30                     | 0.70              |
| 1:A:435:THR:HG22 | 1:A:438:ALA:HB2  | 1.74                     | 0.70              |
| 1:A:318:SER:HA   | 1:A:321:ARG:H    | 1.56                     | 0.70              |
| 1:A:346:ARG:HD3  | 1:A:367:LEU:HD11 | 1.73                     | 0.70              |
| 2:B:78:TYR:O     | 2:B:80:GLY:N     | 2.25                     | 0.70              |
| 1:A:116:TRP:HH2  | 1:A:147:MET:HA   | 1.57                     | 0.69              |
| 1:A:372:LEU:HD11 | 1:A:427:TRP:HB2  | 1.74                     | 0.69              |
| 1:A:158:ALA:HB2  | 1:A:217:LEU:HD11 | 0.70                     | 0.69              |
| 1:A:339:VAL:CG2  | 1:A:342:LEU:HD12 | 2.21                     | 0.69              |
| 1:A:393:THR:O    | 1:A:393:THR:HG22 | 1.91                     | 0.69              |
| 1:A:268:ILE:CD1  | 1:A:269:VAL:HG23 | 2.23                     | 0.69              |
| 1:A:424:TYR:HA   | 1:A:427:TRP:CD1  | 2.28                     | 0.69              |
| 2:B:20:ILE:CD1   | 2:B:59:ILE:HG23  | 2.22                     | 0.69              |
| 1:A:302:SER:HA   | 1:A:305:THR:CG2  | 2.22                     | 0.69              |
| 2:B:50:VAL:HG12  | 2:B:51:PRO:HD3   | 1.75                     | 0.69              |
| 1:A:59:GLY:O     | 1:A:63:PHE:N     | 2.26                     | 0.69              |
| 1:A:141:LEU:HD22 | 1:A:203:GLY:HA3  | 1.74                     | 0.69              |
| 1:A:260:LEU:CD2  | 1:A:404:PHE:O    | 2.40                     | 0.69              |
| 1:A:103:PHE:O    | 1:A:105:LEU:N    | 2.24                     | 0.68              |
| 2:B:72:VAL:HG22  | 2:B:73:TYR:H     | 1.57                     | 0.68              |
| 1:A:144:SER:HB2  | 1:A:204:VAL:HG12 | 1.69                     | 0.68              |
| 1:A:53:LEU:HD22  | 1:A:135:THR:CG2  | 2.23                     | 0.68              |
| 2:B:57:ALA:O     | 2:B:58:THR:HG23  | 1.92                     | 0.68              |
| 1:A:321:ARG:HH22 | 1:A:391:LYS:HB2  | 1.59                     | 0.68              |
| 1:A:7:ARG:NH1    | 1:A:12:VAL:HG21  | 2.08                     | 0.68              |
| 1:A:178:VAL:O    | 1:A:182:PRO:HD2  | 1.94                     | 0.68              |
| 1:A:103:PHE:HA   | 1:A:106:ILE:HG22 | 1.76                     | 0.68              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:141:LEU:O    | 1:A:145:LEU:HB3  | 1.94                     | 0.68              |
| 1:A:148:PRO:O    | 1:A:152:VAL:HG13 | 1.94                     | 0.68              |
| 1:A:16:GLU:HA    | 1:A:19:LEU:HD12  | 1.76                     | 0.68              |
| 1:A:23:LEU:O     | 1:A:23:LEU:HD23  | 1.95                     | 0.67              |
| 1:A:103:PHE:O    | 1:A:107:LEU:HD22 | 1.93                     | 0.67              |
| 2:B:10:VAL:HG12  | 2:B:18:LEU:CD2   | 2.25                     | 0.67              |
| 1:A:329:VAL:HA   | 1:A:332:TRP:CB   | 2.25                     | 0.67              |
| 1:A:372:LEU:HD11 | 1:A:424:TYR:HB2  | 1.77                     | 0.67              |
| 1:A:328:LEU:O    | 1:A:332:TRP:HB2  | 1.95                     | 0.66              |
| 1:A:235:LYS:HB2  | 1:A:241:TRP:HB3  | 1.75                     | 0.66              |
| 2:B:31:TYR:C     | 2:B:32:TYR:CD2   | 2.68                     | 0.66              |
| 1:A:340:LEU:HD12 | 1:A:341:SER:N    | 2.11                     | 0.66              |
| 1:A:27:MET:HG3   | 1:A:303:ALA:O    | 1.95                     | 0.66              |
| 1:A:118:ALA:HB3  | 1:A:119:ILE:HG13 | 1.78                     | 0.66              |
| 1:A:177:PHE:O    | 1:A:181:VAL:HG23 | 1.95                     | 0.66              |
| 1:A:216:ALA:HA   | 1:A:219:ILE:HG12 | 1.77                     | 0.66              |
| 2:B:75:ARG:NE    | 2:B:79:TRP:O     | 2.28                     | 0.66              |
| 1:A:33:ALA:HB2   | 1:A:170:MET:HA   | 1.78                     | 0.66              |
| 1:A:372:LEU:HD22 | 1:A:431:ILE:HG12 | 1.76                     | 0.66              |
| 1:A:308:ILE:HD11 | 1:A:386:ALA:HA   | 1.78                     | 0.66              |
| 1:A:387:LEU:CD1  | 1:A:393:THR:HG21 | 2.24                     | 0.66              |
| 1:A:372:LEU:HD13 | 1:A:427:TRP:HB3  | 1.76                     | 0.66              |
| 1:A:346:ARG:CG   | 1:A:367:LEU:HD11 | 2.26                     | 0.65              |
| 1:A:458:ALA:HB1  | 2:B:8:LEU:HB2    | 1.77                     | 0.65              |
| 2:B:63:SER:HB2   | 2:B:68:TYR:OH    | 1.97                     | 0.65              |
| 1:A:193:GLY:O    | 1:A:195:PRO:CD   | 2.45                     | 0.65              |
| 1:A:145:LEU:CD1  | 1:A:207:MET:HB3  | 2.27                     | 0.65              |
| 1:A:254:ILE:HB   | 1:A:394:LYS:CE   | 2.27                     | 0.65              |
| 2:B:38:GLU:CD    | 2:B:38:GLU:H     | 2.00                     | 0.65              |
| 2:B:69:THR:HA    | 2:B:88:ASN:HA    | 1.77                     | 0.65              |
| 1:A:302:SER:HA   | 1:A:305:THR:HG22 | 1.77                     | 0.65              |
| 1:A:290:SER:O    | 1:A:291:GLY:C    | 2.34                     | 0.65              |
| 2:B:19:LEU:HD13  | 2:B:20:ILE:N     | 2.12                     | 0.65              |
| 1:A:132:VAL:O    | 1:A:133:GLU:HG2  | 1.96                     | 0.65              |
| 2:B:51:PRO:O     | 2:B:52:GLY:O     | 2.15                     | 0.65              |
| 1:A:158:ALA:CB   | 1:A:217:LEU:HD12 | 2.13                     | 0.65              |
| 1:A:147:MET:HE1  | 1:A:207:MET:SD   | 2.37                     | 0.65              |
| 2:B:27:GLU:HG2   | 2:B:30:VAL:HG23  | 1.77                     | 0.64              |
| 2:B:71:THR:OG1   | 2:B:86:SER:HB2   | 1.97                     | 0.64              |
| 1:A:340:LEU:CD1  | 1:A:341:SER:OG   | 2.45                     | 0.64              |
| 1:A:180:ASN:ND2  | 1:A:180:ASN:C    | 2.49                     | 0.64              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:294:TYR:CE2  | 1:A:298:GLN:HB2  | 2.31                     | 0.64              |
| 1:A:318:SER:HA   | 1:A:321:ARG:N    | 2.11                     | 0.64              |
| 1:A:294:TYR:C    | 1:A:294:TYR:CD2  | 2.71                     | 0.64              |
| 2:B:87:ILE:CG2   | 2:B:88:ASN:H     | 2.09                     | 0.64              |
| 1:A:268:ILE:CD1  | 1:A:287:ILE:CD1  | 2.55                     | 0.64              |
| 2:B:17:SER:HA    | 2:B:61:GLY:HA3   | 1.80                     | 0.64              |
| 2:B:59:ILE:HD12  | 2:B:61:GLY:CA    | 2.27                     | 0.64              |
| 2:B:27:GLU:O     | 2:B:28:TYR:CD2   | 2.50                     | 0.64              |
| 1:A:144:SER:O    | 1:A:207:MET:HG2  | 1.97                     | 0.64              |
| 1:A:290:SER:O    | 1:A:294:TYR:CB   | 2.46                     | 0.64              |
| 1:A:411:PRO:HA   | 1:A:414:LEU:HB2  | 1.78                     | 0.64              |
| 1:A:332:TRP:HA   | 1:A:335:ALA:HB2  | 1.77                     | 0.64              |
| 1:A:372:LEU:CB   | 1:A:431:ILE:HG21 | 2.22                     | 0.64              |
| 1:A:458:ALA:HB3  | 2:B:8:LEU:O      | 1.97                     | 0.64              |
| 1:A:417:TYR:O    | 1:A:417:TYR:CG   | 2.50                     | 0.64              |
| 1:A:149:ALA:CA   | 1:A:152:VAL:HG22 | 2.27                     | 0.64              |
| 1:A:141:LEU:CD2  | 1:A:203:GLY:HA3  | 2.29                     | 0.63              |
| 1:A:372:LEU:CD1  | 1:A:427:TRP:CB   | 2.69                     | 0.63              |
| 2:B:78:TYR:C     | 2:B:80:GLY:H     | 2.01                     | 0.63              |
| 2:B:67:ASP:CA    | 2:B:90:ARG:HG2   | 2.28                     | 0.63              |
| 1:A:97:GLY:HA3   | 1:A:227:PHE:CZ   | 2.34                     | 0.63              |
| 1:A:65:THR:HG23  | 1:A:66:VAL:HG13  | 1.79                     | 0.63              |
| 1:A:44:MET:SD    | 1:A:206:THR:CG2  | 2.87                     | 0.63              |
| 1:A:147:MET:SD   | 1:A:148:PRO:HD3  | 2.38                     | 0.63              |
| 1:A:460:SER:O    | 2:B:8:LEU:CG     | 2.45                     | 0.63              |
| 2:B:50:VAL:HG12  | 2:B:51:PRO:CD    | 2.28                     | 0.63              |
| 1:A:65:THR:CG2   | 1:A:66:VAL:HG13  | 2.29                     | 0.63              |
| 1:A:40:VAL:O     | 1:A:43:VAL:HG12  | 1.99                     | 0.63              |
| 1:A:439:VAL:HG23 | 1:A:440:ALA:N    | 2.12                     | 0.62              |
| 1:A:441:LEU:O    | 1:A:443:TRP:N    | 2.32                     | 0.62              |
| 2:B:19:LEU:HD22  | 2:B:20:ILE:H     | 1.64                     | 0.62              |
| 1:A:297:PRO:HB3  | 1:A:378:PHE:CE2  | 2.34                     | 0.62              |
| 1:A:68:ILE:HA    | 1:A:71:MET:HB2   | 1.79                     | 0.62              |
| 1:A:78:ASN:O     | 1:A:163:LEU:HD13 | 1.99                     | 0.62              |
| 1:A:73:ILE:HG13  | 1:A:251:GLY:CA   | 2.30                     | 0.62              |
| 1:A:346:ARG:HG2  | 1:A:367:LEU:HD11 | 1.81                     | 0.62              |
| 1:A:368:LEU:HD12 | 1:A:423:ILE:HG22 | 1.79                     | 0.62              |
| 1:A:33:ALA:CB    | 1:A:170:MET:HA   | 2.30                     | 0.62              |
| 2:B:13:ALA:HA    | 2:B:18:LEU:HA    | 1.80                     | 0.62              |
| 1:A:455:SER:O    | 2:B:11:VAL:HA    | 1.99                     | 0.62              |
| 2:B:65:GLY:HA2   | 2:B:91:THR:CG2   | 2.29                     | 0.62              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:67:ASP:HA    | 2:B:90:ARG:CB    | 2.29                     | 0.62              |
| 1:A:408:GLY:HA3  | 1:A:430:LEU:HG   | 1.80                     | 0.62              |
| 1:A:98:ARG:O     | 1:A:101:ILE:N    | 2.32                     | 0.62              |
| 1:A:194:MET:O    | 1:A:196:ALA:N    | 2.33                     | 0.62              |
| 1:A:149:ALA:C    | 1:A:152:VAL:HG22 | 2.20                     | 0.62              |
| 1:A:187:PHE:HD1  | 1:A:205:ALA:HB2  | 1.65                     | 0.62              |
| 1:A:379:THR:O    | 1:A:382:ILE:N    | 2.33                     | 0.61              |
| 1:A:149:ALA:CA   | 1:A:152:VAL:CG2  | 2.70                     | 0.61              |
| 1:A:184:ASN:HA   | 1:A:205:ALA:CB   | 2.31                     | 0.61              |
| 1:A:369:PHE:CB   | 1:A:372:LEU:HD12 | 2.23                     | 0.61              |
| 1:A:429:ALA:HA   | 1:A:432:ALA:HB3  | 1.83                     | 0.61              |
| 1:A:254:ILE:HG23 | 1:A:255:GLY:H    | 1.64                     | 0.61              |
| 1:A:368:LEU:HD12 | 1:A:423:ILE:HG21 | 1.81                     | 0.61              |
| 2:B:19:LEU:HD11  | 2:B:21:SER:CB    | 2.30                     | 0.61              |
| 1:A:414:LEU:O    | 1:A:418:ARG:NH1  | 2.32                     | 0.61              |
| 1:A:369:PHE:HD2  | 1:A:424:TYR:CB   | 2.14                     | 0.61              |
| 1:A:382:ILE:HA   | 1:A:385:TYR:CD2  | 2.35                     | 0.61              |
| 1:A:435:THR:HG22 | 1:A:438:ALA:CB   | 2.31                     | 0.61              |
| 1:A:413:TYR:O    | 1:A:414:LEU:HD12 | 2.01                     | 0.61              |
| 1:A:33:ALA:HB2   | 1:A:170:MET:CA   | 2.30                     | 0.61              |
| 2:B:10:VAL:HG12  | 2:B:18:LEU:HD22  | 1.82                     | 0.61              |
| 1:A:103:PHE:O    | 1:A:107:LEU:CD2  | 2.48                     | 0.60              |
| 1:A:375:PRO:HA   | 1:A:378:PHE:HB2  | 1.83                     | 0.60              |
| 1:A:344:LEU:HD22 | 1:A:345:PHE:CG   | 2.36                     | 0.60              |
| 1:A:340:LEU:CD1  | 1:A:341:SER:N    | 2.64                     | 0.60              |
| 1:A:294:TYR:O    | 1:A:297:PRO:HB2  | 2.01                     | 0.60              |
| 2:B:8:LEU:HD13   | 2:B:87:ILE:HD11  | 1.83                     | 0.60              |
| 1:A:388:ARG:N    | 1:A:393:THR:O    | 2.35                     | 0.60              |
| 2:B:33:ARG:NE    | 2:B:47:GLU:OE2   | 2.35                     | 0.60              |
| 2:B:1:VAL:O      | 2:B:1:VAL:HG13   | 2.01                     | 0.60              |
| 1:A:98:ARG:CD    | 1:A:229:PRO:O    | 2.49                     | 0.60              |
| 1:A:98:ARG:HD2   | 1:A:229:PRO:O    | 2.02                     | 0.60              |
| 2:B:19:LEU:HD22  | 2:B:20:ILE:N     | 2.16                     | 0.60              |
| 1:A:183:LEU:HD21 | 1:A:209:VAL:HG23 | 1.82                     | 0.60              |
| 1:A:308:ILE:HD13 | 1:A:386:ALA:CB   | 2.32                     | 0.59              |
| 1:A:53:LEU:CD2   | 1:A:135:THR:CG2  | 2.80                     | 0.59              |
| 1:A:218:TRP:CA   | 1:A:218:TRP:CE3  | 2.79                     | 0.59              |
| 1:A:441:LEU:C    | 1:A:443:TRP:N    | 2.56                     | 0.59              |
| 1:A:81:ILE:HD12  | 1:A:81:ILE:O     | 2.02                     | 0.59              |
| 2:B:19:LEU:HD11  | 2:B:21:SER:HG    | 1.63                     | 0.59              |
| 1:A:248:TRP:CZ3  | 1:A:252:ALA:HB2  | 2.37                     | 0.59              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:394:LYS:CA   | 1:A:397:MET:HB2  | 2.24                     | 0.59              |
| 1:A:458:ALA:CB   | 2:B:8:LEU:HB2    | 2.32                     | 0.59              |
| 1:A:260:LEU:HD21 | 1:A:404:PHE:C    | 2.22                     | 0.59              |
| 1:A:159:TYR:HA   | 1:A:162:SER:OG   | 2.03                     | 0.59              |
| 1:A:242:ALA:O    | 1:A:243:VAL:HG22 | 2.03                     | 0.59              |
| 2:B:4:VAL:HG12   | 2:B:83:SER:OG    | 2.02                     | 0.59              |
| 1:A:218:TRP:CZ3  | 1:A:221:ILE:HD11 | 2.38                     | 0.59              |
| 1:A:305:THR:HA   | 1:A:308:ILE:HD11 | 1.85                     | 0.59              |
| 1:A:31:GLN:HG3   | 1:A:296:ILE:HA   | 1.84                     | 0.59              |
| 1:A:339:VAL:HG11 | 1:A:375:PRO:HG3  | 1.85                     | 0.59              |
| 1:A:332:TRP:HD1  | 1:A:379:THR:HG21 | 1.67                     | 0.59              |
| 1:A:172:VAL:HG21 | 1:A:216:ALA:HB2  | 1.82                     | 0.59              |
| 1:A:71:MET:HG2   | 1:A:156:LEU:HD22 | 1.84                     | 0.59              |
| 1:A:338:THR:HG23 | 1:A:340:LEU:HD12 | 1.84                     | 0.58              |
| 1:A:212:PHE:CD2  | 1:A:212:PHE:C    | 2.76                     | 0.58              |
| 1:A:339:VAL:HA   | 1:A:342:LEU:CG   | 2.32                     | 0.58              |
| 1:A:122:PHE:HA   | 1:A:133:GLU:OE2  | 2.02                     | 0.58              |
| 1:A:193:GLY:O    | 1:A:195:PRO:N    | 2.37                     | 0.58              |
| 1:A:127:THR:HG22 | 1:A:128:LEU:H    | 1.68                     | 0.58              |
| 1:A:102:TRP:O    | 1:A:106:ILE:N    | 2.36                     | 0.58              |
| 1:A:374:GLN:HB3  | 1:A:375:PRO:HD3  | 1.86                     | 0.58              |
| 2:B:14:THR:O     | 2:B:16:THR:N     | 2.34                     | 0.58              |
| 1:A:119:ILE:HG12 | 1:A:142:PHE:CD2  | 2.39                     | 0.58              |
| 2:B:4:VAL:CG2    | 2:B:6:THR:CG2    | 2.71                     | 0.58              |
| 1:A:100:GLY:O    | 1:A:104:GLY:N    | 2.29                     | 0.58              |
| 1:A:332:TRP:HA   | 1:A:335:ALA:HB3  | 1.86                     | 0.58              |
| 2:B:4:VAL:HG11   | 2:B:84:PRO:O     | 2.03                     | 0.58              |
| 1:A:308:ILE:HD13 | 1:A:386:ALA:CA   | 2.34                     | 0.58              |
| 1:A:379:THR:HG22 | 1:A:382:ILE:HG12 | 1.85                     | 0.58              |
| 1:A:55:ALA:O     | 1:A:58:LEU:CD1   | 2.51                     | 0.57              |
| 1:A:193:GLY:O    | 1:A:195:PRO:HD3  | 2.04                     | 0.57              |
| 1:A:373:PHE:HB2  | 1:A:434:LEU:CD1  | 2.33                     | 0.57              |
| 1:A:387:LEU:HD21 | 1:A:444:CYS:O    | 2.04                     | 0.57              |
| 2:B:67:ASP:HA    | 2:B:90:ARG:HB3   | 1.84                     | 0.57              |
| 1:A:66:VAL:HG23  | 1:A:66:VAL:O     | 2.03                     | 0.57              |
| 1:A:102:TRP:O    | 1:A:106:ILE:HB   | 2.03                     | 0.57              |
| 1:A:460:SER:O    | 2:B:8:LEU:HG     | 2.04                     | 0.57              |
| 1:A:250:ILE:HA   | 1:A:394:LYS:CD   | 2.35                     | 0.57              |
| 1:A:429:ALA:O    | 1:A:433:SER:HB3  | 2.03                     | 0.57              |
| 1:A:38:GLY:O     | 1:A:41:ASP:OD2   | 2.22                     | 0.57              |
| 1:A:112:MET:CG   | 1:A:147:MET:O    | 2.52                     | 0.57              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:403:ALA:O    | 1:A:407:CYS:HB2  | 2.05                     | 0.57              |
| 1:A:411:PRO:HG3  | 1:A:429:ALA:CB   | 2.34                     | 0.57              |
| 1:A:411:PRO:HB2  | 1:A:426:PHE:O    | 2.05                     | 0.57              |
| 1:A:377:ASP:O    | 1:A:378:PHE:C    | 2.43                     | 0.57              |
| 1:A:395:VAL:HG12 | 1:A:396:PRO:CD   | 2.34                     | 0.57              |
| 2:B:29:VAL:O     | 2:B:30:VAL:HG12  | 2.05                     | 0.57              |
| 2:B:43:SER:O     | 2:B:44:PRO:O     | 2.22                     | 0.57              |
| 1:A:318:SER:C    | 1:A:320:ALA:N    | 2.58                     | 0.57              |
| 2:B:10:VAL:HG12  | 2:B:10:VAL:O     | 2.04                     | 0.57              |
| 1:A:260:LEU:C    | 1:A:262:ALA:H    | 2.08                     | 0.57              |
| 1:A:415:LEU:CD1  | 1:A:423:ILE:HA   | 2.35                     | 0.57              |
| 1:A:439:VAL:CG2  | 1:A:440:ALA:H    | 2.17                     | 0.57              |
| 1:A:289:LEU:HD13 | 1:A:292:ILE:CG1  | 2.28                     | 0.56              |
| 2:B:5:PRO:CD     | 2:B:74:ALA:HB2   | 2.35                     | 0.56              |
| 1:A:274:PRO:C    | 1:A:276:GLY:H    | 2.09                     | 0.56              |
| 2:B:19:LEU:CD1   | 2:B:21:SER:OG    | 2.38                     | 0.56              |
| 1:A:346:ARG:O    | 1:A:348:PRO:HD3  | 2.05                     | 0.56              |
| 2:B:63:SER:HB3   | 2:B:64:PRO:HD2   | 1.87                     | 0.56              |
| 1:A:156:LEU:CD1  | 1:A:159:TYR:CE1  | 2.88                     | 0.56              |
| 1:A:191:LYS:O    | 1:A:192:PHE:C    | 2.41                     | 0.56              |
| 1:A:302:SER:CA   | 1:A:305:THR:HG22 | 2.36                     | 0.56              |
| 2:B:9:GLU:O      | 2:B:22:TRP:NE1   | 2.38                     | 0.56              |
| 2:B:78:TYR:C     | 2:B:80:GLY:N     | 2.59                     | 0.56              |
| 1:A:116:TRP:CH2  | 1:A:147:MET:HA   | 2.40                     | 0.56              |
| 1:A:148:PRO:HG3  | 1:A:207:MET:HB2  | 1.88                     | 0.56              |
| 1:A:33:ALA:HB2   | 1:A:170:MET:CB   | 2.35                     | 0.56              |
| 1:A:268:ILE:HD12 | 1:A:269:VAL:HG23 | 1.87                     | 0.56              |
| 2:B:32:TYR:HB2   | 2:B:50:VAL:HG23  | 1.87                     | 0.56              |
| 1:A:322:TYR:HE1  | 1:A:449:SER:HB2  | 1.71                     | 0.56              |
| 2:B:27:GLU:O     | 2:B:28:TYR:HD2   | 1.88                     | 0.56              |
| 1:A:57:ALA:O     | 1:A:60:SER:N     | 2.39                     | 0.56              |
| 1:A:384:SER:C    | 1:A:386:ALA:H    | 2.08                     | 0.56              |
| 1:A:321:ARG:NH2  | 1:A:391:LYS:HB2  | 2.20                     | 0.56              |
| 1:A:43:VAL:HG13  | 1:A:44:MET:HE3   | 1.88                     | 0.56              |
| 1:A:292:ILE:HD12 | 1:A:293:LEU:HG   | 1.87                     | 0.56              |
| 1:A:430:LEU:HA   | 1:A:433:SER:HB3  | 1.87                     | 0.56              |
| 1:A:99:GLN:NE2   | 1:A:234:ALA:O    | 2.38                     | 0.56              |
| 1:A:304:GLY:O    | 1:A:306:VAL:N    | 2.39                     | 0.56              |
| 1:A:90:THR:O     | 1:A:94:GLY:N     | 2.39                     | 0.56              |
| 2:B:87:ILE:CG2   | 2:B:88:ASN:N     | 2.68                     | 0.56              |
| 1:A:27:MET:O     | 1:A:303:ALA:HB3  | 2.06                     | 0.56              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:364:SER:HA   | 1:A:366:VAL:HG22 | 1.87                     | 0.55              |
| 1:A:415:LEU:HD12 | 1:A:423:ILE:HA   | 1.88                     | 0.55              |
| 1:A:108:GLY:O    | 1:A:112:MET:HB2  | 2.05                     | 0.55              |
| 1:A:205:ALA:O    | 1:A:208:ALA:HB3  | 2.06                     | 0.55              |
| 1:A:292:ILE:HG13 | 1:A:293:LEU:H    | 1.71                     | 0.55              |
| 2:B:7:LYS:O      | 2:B:8:LEU:HD23   | 2.06                     | 0.55              |
| 1:A:365:THR:O    | 1:A:423:ILE:HG21 | 2.07                     | 0.55              |
| 2:B:19:LEU:CD1   | 2:B:19:LEU:C     | 2.70                     | 0.55              |
| 2:B:22:TRP:HZ3   | 2:B:85:ILE:HG23  | 1.72                     | 0.55              |
| 1:A:109:ILE:HA   | 1:A:112:MET:HB2  | 1.88                     | 0.55              |
| 1:A:217:LEU:O    | 1:A:218:TRP:C    | 2.43                     | 0.55              |
| 1:A:155:ALA:HB2  | 1:A:214:ALA:HA   | 1.89                     | 0.55              |
| 1:A:40:VAL:HG22  | 1:A:177:PHE:HB2  | 1.88                     | 0.55              |
| 1:A:372:LEU:CD1  | 1:A:424:TYR:HB2  | 2.37                     | 0.55              |
| 1:A:457:LYS:HB3  | 2:B:10:VAL:HB    | 1.89                     | 0.55              |
| 2:B:65:GLY:HA2   | 2:B:91:THR:HG21  | 1.89                     | 0.55              |
| 1:A:411:PRO:CG   | 1:A:429:ALA:HB3  | 2.37                     | 0.54              |
| 1:A:459:VAL:O    | 1:A:460:SER:OG   | 2.24                     | 0.54              |
| 1:A:292:ILE:HD12 | 1:A:293:LEU:CG   | 2.37                     | 0.54              |
| 1:A:315:ARG:HH21 | 2:B:11:VAL:HG11  | 1.73                     | 0.54              |
| 1:A:15:LYS:HG2   | 1:A:322:TYR:HA   | 1.88                     | 0.54              |
| 1:A:145:LEU:HD22 | 1:A:203:GLY:HA3  | 1.87                     | 0.54              |
| 1:A:218:TRP:CE3  | 1:A:221:ILE:HD11 | 2.42                     | 0.54              |
| 2:B:4:VAL:HG21   | 2:B:85:ILE:HB    | 1.88                     | 0.54              |
| 1:A:63:PHE:C     | 1:A:65:THR:N     | 2.54                     | 0.54              |
| 1:A:427:TRP:N    | 1:A:427:TRP:CD1  | 2.76                     | 0.54              |
| 1:A:112:MET:SD   | 1:A:147:MET:HA   | 2.48                     | 0.54              |
| 1:A:335:ALA:O    | 1:A:375:PRO:HB3  | 2.07                     | 0.54              |
| 1:A:65:THR:O     | 1:A:69:THR:CG2   | 2.40                     | 0.54              |
| 1:A:103:PHE:O    | 1:A:106:ILE:N    | 2.41                     | 0.54              |
| 1:A:76:ALA:O     | 1:A:250:ILE:HD13 | 2.08                     | 0.54              |
| 1:A:109:ILE:HD11 | 1:A:110:PHE:CE2  | 2.43                     | 0.54              |
| 2:B:68:TYR:O     | 2:B:88:ASN:O     | 2.26                     | 0.54              |
| 2:B:37:GLY:N     | 2:B:70:ILE:HD11  | 2.23                     | 0.54              |
| 1:A:109:ILE:O    | 1:A:113:ILE:HB   | 2.08                     | 0.54              |
| 1:A:97:GLY:HA2   | 1:A:157:HIS:HE1  | 1.73                     | 0.54              |
| 1:A:97:GLY:HA3   | 1:A:227:PHE:CE2  | 2.42                     | 0.54              |
| 1:A:74:MET:C     | 1:A:76:ALA:H     | 2.12                     | 0.54              |
| 2:B:38:GLU:CD    | 2:B:38:GLU:N     | 2.61                     | 0.54              |
| 1:A:156:LEU:HD12 | 1:A:159:TYR:CE1  | 2.43                     | 0.54              |
| 2:B:16:THR:C     | 2:B:61:GLY:O     | 2.47                     | 0.53              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:5:PRO:HD3    | 2:B:74:ALA:HB2   | 1.90                     | 0.53              |
| 1:A:203:GLY:HA2  | 1:A:206:THR:OG1  | 2.08                     | 0.53              |
| 1:A:263:SER:C    | 1:A:265:PHE:H    | 2.10                     | 0.53              |
| 1:A:31:GLN:OE1   | 1:A:299:SER:O    | 2.27                     | 0.53              |
| 1:A:325:GLY:O    | 1:A:328:LEU:N    | 2.42                     | 0.53              |
| 1:A:269:VAL:HG12 | 1:A:269:VAL:O    | 2.08                     | 0.53              |
| 2:B:20:ILE:HD13  | 2:B:20:ILE:N     | 2.23                     | 0.53              |
| 1:A:369:PHE:HA   | 1:A:372:LEU:HB2  | 1.89                     | 0.53              |
| 1:A:369:PHE:HD2  | 1:A:424:TYR:HB3  | 1.73                     | 0.53              |
| 1:A:316:GLU:HB3  | 1:A:319:ARG:HB2  | 1.91                     | 0.53              |
| 2:B:71:THR:HG23  | 2:B:85:ILE:C     | 2.29                     | 0.53              |
| 1:A:44:MET:CE    | 1:A:180:ASN:ND2  | 2.70                     | 0.53              |
| 2:B:20:ILE:HG12  | 2:B:58:THR:HA    | 1.91                     | 0.53              |
| 2:B:65:GLY:CA    | 2:B:91:THR:HB    | 2.36                     | 0.53              |
| 1:A:106:ILE:CG2  | 1:A:107:LEU:N    | 2.72                     | 0.53              |
| 1:A:151:MET:HB2  | 1:A:211:TRP:CZ2  | 2.43                     | 0.53              |
| 2:B:27:GLU:HG2   | 2:B:30:VAL:CG2   | 2.38                     | 0.53              |
| 1:A:141:LEU:HB2  | 1:A:200:ALA:HA   | 1.91                     | 0.53              |
| 1:A:154:ARG:HH21 | 1:A:215:LEU:HD22 | 1.74                     | 0.53              |
| 1:A:89:LYS:O     | 1:A:89:LYS:HG2   | 2.09                     | 0.52              |
| 1:A:384:SER:HA   | 1:A:387:LEU:HB2  | 1.91                     | 0.52              |
| 1:A:434:LEU:O    | 1:A:434:LEU:HD23 | 2.08                     | 0.52              |
| 1:A:442:VAL:HA   | 1:A:445:LEU:HB3  | 1.92                     | 0.52              |
| 1:A:103:PHE:HD2  | 1:A:106:ILE:CG2  | 2.22                     | 0.52              |
| 1:A:78:ASN:CA    | 1:A:163:LEU:HD11 | 2.19                     | 0.52              |
| 1:A:318:SER:C    | 1:A:320:ALA:H    | 2.10                     | 0.52              |
| 1:A:364:SER:C    | 1:A:366:VAL:H    | 2.11                     | 0.52              |
| 1:A:339:VAL:HG23 | 1:A:374:GLN:HB3  | 1.91                     | 0.52              |
| 1:A:425:GLY:O    | 1:A:428:THR:HG21 | 2.09                     | 0.52              |
| 1:A:439:VAL:HG22 | 1:A:440:ALA:H    | 1.74                     | 0.52              |
| 2:B:26:GLY:O     | 2:B:53:SER:OG    | 2.27                     | 0.52              |
| 1:A:12:VAL:HG23  | 1:A:13:PHE:N     | 2.23                     | 0.52              |
| 1:A:27:MET:O     | 1:A:303:ALA:CB   | 2.57                     | 0.52              |
| 1:A:294:TYR:CZ   | 1:A:298:GLN:HB2  | 2.45                     | 0.52              |
| 1:A:373:PHE:HB2  | 1:A:434:LEU:HD11 | 1.90                     | 0.52              |
| 1:A:268:ILE:HD11 | 1:A:269:VAL:HG23 | 1.91                     | 0.52              |
| 2:B:27:GLU:HG3   | 2:B:52:GLY:C     | 2.30                     | 0.52              |
| 2:B:4:VAL:HG12   | 2:B:83:SER:CB    | 2.40                     | 0.52              |
| 1:A:127:THR:HG22 | 1:A:128:LEU:N    | 2.24                     | 0.52              |
| 1:A:15:LYS:NZ    | 1:A:446:GLU:OE1  | 2.42                     | 0.52              |
| 1:A:215:LEU:N    | 1:A:215:LEU:CD2  | 2.65                     | 0.52              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:251:GLY:O    | 1:A:254:ILE:CG2  | 2.53                     | 0.52              |
| 1:A:302:SER:HA   | 1:A:305:THR:HG21 | 1.92                     | 0.52              |
| 2:B:31:TYR:CB    | 2:B:75:ARG:HB3   | 2.37                     | 0.52              |
| 1:A:38:GLY:O     | 1:A:41:ASP:CB    | 2.58                     | 0.52              |
| 1:A:143:THR:HA   | 1:A:146:ALA:HB3  | 1.91                     | 0.52              |
| 1:A:156:LEU:HD13 | 1:A:159:TYR:CZ   | 2.44                     | 0.52              |
| 1:A:28:LEU:O     | 1:A:32:VAL:HG23  | 2.10                     | 0.52              |
| 1:A:112:MET:SD   | 1:A:147:MET:O    | 2.68                     | 0.52              |
| 1:A:415:LEU:O    | 1:A:418:ARG:HB2  | 2.10                     | 0.52              |
| 1:A:77:LEU:HD12  | 1:A:250:ILE:CD1  | 2.39                     | 0.52              |
| 1:A:261:GLU:HA   | 1:A:264:ALA:CB   | 2.34                     | 0.52              |
| 1:A:151:MET:SD   | 1:A:211:TRP:HA   | 2.50                     | 0.51              |
| 1:A:365:THR:HA   | 1:A:368:LEU:CD1  | 2.40                     | 0.51              |
| 1:A:132:VAL:HG13 | 1:A:133:GLU:N    | 2.20                     | 0.51              |
| 1:A:383:ALA:HB3  | 1:A:441:LEU:HD12 | 1.92                     | 0.51              |
| 2:B:13:ALA:HA    | 2:B:18:LEU:HD23  | 1.92                     | 0.51              |
| 1:A:40:VAL:CG1   | 1:A:180:ASN:ND2  | 2.73                     | 0.51              |
| 1:A:418:ARG:HG2  | 1:A:422:GLY:CA   | 2.25                     | 0.51              |
| 1:A:44:MET:HE1   | 1:A:180:ASN:ND2  | 2.24                     | 0.51              |
| 1:A:29:LEU:N     | 1:A:29:LEU:HD23  | 2.25                     | 0.51              |
| 1:A:247:ILE:HG23 | 1:A:250:ILE:HD12 | 1.93                     | 0.51              |
| 1:A:254:ILE:HG23 | 1:A:255:GLY:N    | 2.25                     | 0.51              |
| 1:A:329:VAL:CA   | 1:A:332:TRP:HB3  | 2.35                     | 0.51              |
| 1:A:388:ARG:O    | 1:A:390:TYR:N    | 2.44                     | 0.51              |
| 1:A:151:MET:HB2  | 1:A:211:TRP:CD2  | 2.46                     | 0.51              |
| 1:A:73:ILE:HA    | 1:A:254:ILE:HG21 | 1.93                     | 0.51              |
| 1:A:151:MET:O    | 1:A:214:ALA:HB2  | 2.09                     | 0.51              |
| 1:A:221:ILE:HD13 | 1:A:228:ARG:HG3  | 1.93                     | 0.51              |
| 1:A:119:ILE:HG23 | 1:A:142:PHE:CG   | 2.46                     | 0.50              |
| 1:A:202:CYS:O    | 1:A:205:ALA:HB3  | 2.11                     | 0.50              |
| 1:A:191:LYS:C    | 1:A:193:GLY:N    | 2.64                     | 0.50              |
| 1:A:150:ALA:C    | 1:A:152:VAL:H    | 2.14                     | 0.50              |
| 1:A:40:VAL:HG22  | 1:A:177:PHE:HD1  | 1.76                     | 0.50              |
| 1:A:321:ARG:HA   | 1:A:324:SER:HB3  | 1.94                     | 0.50              |
| 1:A:366:VAL:HA   | 1:A:369:PHE:CZ   | 2.46                     | 0.50              |
| 2:B:24:ALA:HB1   | 2:B:53:SER:HA    | 1.94                     | 0.50              |
| 1:A:191:LYS:O    | 1:A:193:GLY:N    | 2.43                     | 0.50              |
| 1:A:103:PHE:HD2  | 1:A:106:ILE:HG22 | 1.77                     | 0.50              |
| 1:A:253:PRO:O    | 1:A:257:SER:HB2  | 2.11                     | 0.50              |
| 2:B:9:GLU:O      | 2:B:22:TRP:CD1   | 2.65                     | 0.50              |
| 1:A:337:ILE:O    | 1:A:337:ILE:CD1  | 2.52                     | 0.50              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:376:ALA:HB1  | 1:A:435:THR:CG2  | 2.41                     | 0.50              |
| 1:A:221:ILE:HD13 | 1:A:228:ARG:HB2  | 1.92                     | 0.50              |
| 1:A:207:MET:SD   | 1:A:207:MET:C    | 2.90                     | 0.50              |
| 2:B:10:VAL:HG12  | 2:B:18:LEU:HD21  | 1.93                     | 0.50              |
| 1:A:344:LEU:HD13 | 1:A:345:PHE:CE2  | 2.46                     | 0.50              |
| 1:A:119:ILE:HG23 | 1:A:142:PHE:CD2  | 2.47                     | 0.50              |
| 1:A:136:MET:HG2  | 1:A:136:MET:O    | 2.11                     | 0.50              |
| 1:A:101:ILE:HD11 | 1:A:217:LEU:CD2  | 2.42                     | 0.50              |
| 1:A:397:MET:O    | 1:A:400:HIS:CB   | 2.60                     | 0.50              |
| 2:B:35:THR:HG23  | 2:B:73:TYR:CE1   | 2.38                     | 0.50              |
| 1:A:18:ARG:O     | 1:A:18:ARG:HD3   | 2.11                     | 0.50              |
| 1:A:19:LEU:HB3   | 1:A:326:VAL:HG21 | 1.94                     | 0.50              |
| 1:A:197:LEU:O    | 1:A:201:GLY:HA3  | 2.12                     | 0.50              |
| 2:B:13:ALA:HB1   | 2:B:17:SER:O     | 2.12                     | 0.50              |
| 2:B:85:ILE:O     | 2:B:85:ILE:HG23  | 2.12                     | 0.50              |
| 1:A:147:MET:CE   | 1:A:207:MET:CE   | 2.90                     | 0.50              |
| 1:A:331:GLY:O    | 1:A:335:ALA:N    | 2.45                     | 0.50              |
| 1:A:68:ILE:HA    | 1:A:71:MET:CB    | 2.42                     | 0.50              |
| 1:A:411:PRO:HG3  | 1:A:429:ALA:C    | 2.32                     | 0.49              |
| 2:B:82:TYR:O     | 2:B:83:SER:HB2   | 2.12                     | 0.49              |
| 1:A:141:LEU:CD2  | 1:A:145:LEU:HD22 | 2.42                     | 0.49              |
| 1:A:151:MET:CG   | 1:A:211:TRP:CE3  | 2.95                     | 0.49              |
| 1:A:242:ALA:HA   | 1:A:245:LYS:H    | 1.77                     | 0.49              |
| 1:A:301:GLY:O    | 1:A:305:THR:N    | 2.31                     | 0.49              |
| 2:B:30:VAL:O     | 2:B:31:TYR:HB2   | 2.11                     | 0.49              |
| 2:B:29:VAL:O     | 2:B:30:VAL:CB    | 2.60                     | 0.49              |
| 1:A:180:ASN:CA   | 1:A:209:VAL:HG21 | 2.42                     | 0.49              |
| 1:A:377:ASP:O    | 1:A:379:THR:N    | 2.45                     | 0.49              |
| 1:A:374:GLN:OE1  | 1:A:378:PHE:CE1  | 2.66                     | 0.49              |
| 1:A:393:THR:CG2  | 1:A:393:THR:O    | 2.60                     | 0.49              |
| 1:A:441:LEU:C    | 1:A:443:TRP:H    | 2.14                     | 0.49              |
| 1:A:79:PRO:O     | 1:A:81:ILE:N     | 2.44                     | 0.49              |
| 1:A:73:ILE:HA    | 1:A:251:GLY:HA2  | 1.93                     | 0.49              |
| 2:B:22:TRP:O     | 2:B:56:THR:CG2   | 2.61                     | 0.49              |
| 2:B:29:VAL:HG23  | 2:B:77:TYR:N     | 2.28                     | 0.49              |
| 1:A:172:VAL:HG11 | 1:A:216:ALA:HB1  | 1.94                     | 0.49              |
| 1:A:115:MET:HB3  | 1:A:146:ALA:HB1  | 1.94                     | 0.49              |
| 2:B:29:VAL:H     | 2:B:76:SER:HA    | 1.78                     | 0.49              |
| 2:B:30:VAL:HG22  | 2:B:51:PRO:O     | 2.11                     | 0.49              |
| 1:A:224:GLU:HG2  | 1:A:225:LYS:N    | 2.28                     | 0.49              |
| 1:A:179:LEU:O    | 1:A:183:LEU:HB3  | 2.13                     | 0.49              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:289:LEU:HA   | 1:A:292:ILE:HG12 | 1.94                     | 0.49              |
| 1:A:272:ILE:HA   | 1:A:280:VAL:HG12 | 1.94                     | 0.49              |
| 2:B:24:ALA:HB3   | 2:B:53:SER:O     | 2.12                     | 0.49              |
| 1:A:377:ASP:O    | 1:A:380:GLN:N    | 2.46                     | 0.49              |
| 1:A:397:MET:O    | 1:A:398:PHE:C    | 2.50                     | 0.49              |
| 1:A:440:ALA:O    | 1:A:443:TRP:HB3  | 2.12                     | 0.49              |
| 1:A:156:LEU:CD1  | 1:A:159:TYR:CZ   | 2.96                     | 0.49              |
| 2:B:1:VAL:O      | 2:B:1:VAL:CG1    | 2.60                     | 0.49              |
| 1:A:89:LYS:CG    | 1:A:92:GLU:HB3   | 2.43                     | 0.49              |
| 1:A:247:ILE:O    | 1:A:247:ILE:HG22 | 2.13                     | 0.49              |
| 2:B:27:GLU:OE1   | 2:B:27:GLU:N     | 2.45                     | 0.49              |
| 2:B:4:VAL:HA     | 2:B:83:SER:HB3   | 1.95                     | 0.49              |
| 1:A:59:GLY:O     | 1:A:62:ALA:N     | 2.39                     | 0.49              |
| 1:A:73:ILE:HA    | 1:A:254:ILE:CG2  | 2.43                     | 0.49              |
| 1:A:418:ARG:NH1  | 1:A:425:GLY:O    | 2.46                     | 0.49              |
| 1:A:189:TYR:HA   | 1:A:195:PRO:O    | 2.13                     | 0.49              |
| 1:A:103:PHE:C    | 1:A:107:LEU:HD22 | 2.32                     | 0.48              |
| 1:A:108:GLY:HA2  | 1:A:153:HIS:HD2  | 1.78                     | 0.48              |
| 2:B:27:GLU:HB3   | 2:B:30:VAL:HA    | 1.95                     | 0.48              |
| 1:A:81:ILE:HG13  | 1:A:163:LEU:HB2  | 1.95                     | 0.48              |
| 2:B:22:TRP:O     | 2:B:56:THR:HG23  | 2.13                     | 0.48              |
| 1:A:65:THR:CG2   | 1:A:66:VAL:N     | 2.77                     | 0.48              |
| 1:A:56:VAL:HA    | 1:A:138:GLN:HE22 | 1.78                     | 0.48              |
| 1:A:339:VAL:CG2  | 1:A:370:ALA:O    | 2.61                     | 0.48              |
| 1:A:288:SER:O    | 1:A:292:ILE:CG2  | 2.42                     | 0.48              |
| 1:A:68:ILE:HD13  | 1:A:71:MET:HG3   | 1.96                     | 0.48              |
| 1:A:73:ILE:N     | 1:A:254:ILE:CG2  | 2.76                     | 0.48              |
| 1:A:259:PHE:CD2  | 1:A:262:ALA:HB3  | 2.48                     | 0.48              |
| 1:A:55:ALA:CB    | 1:A:58:LEU:HD21  | 2.42                     | 0.48              |
| 1:A:180:ASN:OD1  | 1:A:206:THR:HA   | 2.14                     | 0.48              |
| 1:A:74:MET:CE    | 1:A:103:PHE:HB3  | 2.44                     | 0.48              |
| 1:A:65:THR:HG23  | 1:A:66:VAL:CG1   | 2.44                     | 0.48              |
| 1:A:66:VAL:HA    | 1:A:69:THR:CG2   | 2.44                     | 0.48              |
| 1:A:292:ILE:HD12 | 1:A:293:LEU:HD12 | 1.96                     | 0.48              |
| 1:A:26:PRO:HB3   | 1:A:167:ARG:CZ   | 2.44                     | 0.48              |
| 1:A:365:THR:CA   | 1:A:368:LEU:HD11 | 2.43                     | 0.48              |
| 2:B:19:LEU:HD22  | 2:B:57:ALA:O     | 2.14                     | 0.48              |
| 2:B:67:ASP:OD2   | 2:B:68:TYR:N     | 2.46                     | 0.48              |
| 1:A:230:PHE:CD1  | 1:A:233:THR:HG21 | 2.48                     | 0.48              |
| 1:A:82:ALA:HB1   | 1:A:306:VAL:HG13 | 1.95                     | 0.48              |
| 1:A:343:VAL:HG22 | 1:A:371:GLY:N    | 2.28                     | 0.48              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:271:LEU:HD13 | 1:A:415:LEU:HD13 | 1.95                     | 0.48              |
| 1:A:338:THR:HG23 | 1:A:340:LEU:CD1  | 2.44                     | 0.48              |
| 1:A:103:PHE:HA   | 1:A:106:ILE:CG2  | 2.40                     | 0.48              |
| 1:A:163:LEU:HD22 | 1:A:306:VAL:CG2  | 2.44                     | 0.48              |
| 1:A:180:ASN:HD22 | 1:A:181:VAL:N    | 2.11                     | 0.48              |
| 1:A:199:GLY:O    | 1:A:200:ALA:HB2  | 2.14                     | 0.48              |
| 1:A:73:ILE:N     | 1:A:254:ILE:HG23 | 2.29                     | 0.48              |
| 1:A:102:TRP:CZ3  | 1:A:235:LYS:HG2  | 2.49                     | 0.48              |
| 1:A:96:THR:O     | 1:A:99:GLN:N     | 2.47                     | 0.48              |
| 2:B:4:VAL:CG1    | 2:B:84:PRO:O     | 2.61                     | 0.48              |
| 2:B:31:TYR:HB3   | 2:B:75:ARG:CB    | 2.40                     | 0.47              |
| 2:B:17:SER:OG    | 2:B:18:LEU:N     | 2.48                     | 0.47              |
| 2:B:65:GLY:HA2   | 2:B:91:THR:OG1   | 2.14                     | 0.47              |
| 1:A:143:THR:CG2  | 1:A:144:SER:N    | 2.77                     | 0.47              |
| 1:A:143:THR:HG23 | 1:A:144:SER:N    | 2.28                     | 0.47              |
| 1:A:71:MET:CE    | 1:A:159:TYR:OH   | 2.63                     | 0.47              |
| 1:A:116:TRP:O    | 1:A:117:ALA:C    | 2.52                     | 0.47              |
| 1:A:17:ILE:HG22  | 1:A:18:ARG:H     | 1.80                     | 0.47              |
| 1:A:339:VAL:HA   | 1:A:342:LEU:HG   | 1.95                     | 0.47              |
| 1:A:372:LEU:HB3  | 1:A:431:ILE:CG2  | 2.27                     | 0.47              |
| 2:B:8:LEU:HD13   | 2:B:87:ILE:CG1   | 2.45                     | 0.47              |
| 1:A:142:PHE:O    | 1:A:146:ALA:HB3  | 2.15                     | 0.47              |
| 1:A:268:ILE:CG1  | 1:A:287:ILE:CD1  | 2.92                     | 0.47              |
| 1:A:317:PHE:O    | 1:A:318:SER:HB2  | 2.15                     | 0.47              |
| 1:A:241:TRP:NE1  | 1:A:243:VAL:HG22 | 2.30                     | 0.47              |
| 1:A:364:SER:C    | 1:A:366:VAL:N    | 2.68                     | 0.47              |
| 1:A:372:LEU:HD22 | 1:A:431:ILE:HG21 | 1.97                     | 0.47              |
| 1:A:333:VAL:O    | 1:A:337:ILE:HG23 | 2.15                     | 0.47              |
| 1:A:416:ALA:O    | 1:A:417:TYR:CB   | 2.62                     | 0.47              |
| 1:A:314:ARG:O    | 1:A:316:GLU:N    | 2.47                     | 0.47              |
| 1:A:369:PHE:CD2  | 1:A:424:TYR:HB3  | 2.49                     | 0.47              |
| 1:A:43:VAL:HG13  | 1:A:44:MET:CE    | 2.44                     | 0.47              |
| 2:B:36:TYR:CA    | 2:B:70:ILE:HD11  | 2.36                     | 0.47              |
| 1:A:132:VAL:O    | 1:A:133:GLU:CG   | 2.60                     | 0.47              |
| 1:A:32:VAL:O     | 1:A:32:VAL:HG12  | 2.13                     | 0.47              |
| 1:A:106:ILE:HG22 | 1:A:107:LEU:N    | 2.30                     | 0.47              |
| 1:A:151:MET:CB   | 1:A:211:TRP:CD2  | 2.98                     | 0.47              |
| 1:A:463:LEU:O    | 2:B:3:SER:CB     | 2.62                     | 0.47              |
| 1:A:272:ILE:HD12 | 1:A:281:ALA:HB2  | 1.95                     | 0.47              |
| 1:A:164:ASN:O    | 1:A:165:ARG:HD3  | 2.14                     | 0.47              |
| 1:A:372:LEU:HD22 | 1:A:427:TRP:O    | 2.15                     | 0.47              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:30:VAL:HG23  | 2:B:51:PRO:O     | 2.13                     | 0.47              |
| 1:A:317:PHE:HB3  | 1:A:452:LEU:HG   | 1.96                     | 0.46              |
| 2:B:76:SER:O     | 2:B:77:TYR:C     | 2.54                     | 0.46              |
| 1:A:16:GLU:C     | 1:A:17:ILE:HD12  | 2.36                     | 0.46              |
| 1:A:110:PHE:O    | 1:A:111:GLY:C    | 2.51                     | 0.46              |
| 1:A:260:LEU:C    | 1:A:262:ALA:N    | 2.65                     | 0.46              |
| 1:A:40:VAL:HG11  | 1:A:180:ASN:ND2  | 2.30                     | 0.46              |
| 1:A:72:GLY:O     | 1:A:73:ILE:C     | 2.54                     | 0.46              |
| 1:A:98:ARG:HD3   | 1:A:229:PRO:O    | 2.16                     | 0.46              |
| 1:A:183:LEU:CD2  | 1:A:209:VAL:HG23 | 2.46                     | 0.46              |
| 1:A:26:PRO:HB3   | 1:A:167:ARG:NH1  | 2.30                     | 0.46              |
| 1:A:339:VAL:HG21 | 1:A:375:PRO:CD   | 2.27                     | 0.46              |
| 1:A:343:VAL:HA   | 1:A:367:LEU:HB3  | 1.98                     | 0.46              |
| 1:A:410:LEU:C    | 1:A:412:GLY:H    | 2.19                     | 0.46              |
| 2:B:63:SER:CB    | 2:B:64:PRO:HD2   | 2.45                     | 0.46              |
| 1:A:225:LYS:HE2  | 1:A:226:PHE:CE2  | 2.51                     | 0.46              |
| 1:A:372:LEU:HD22 | 1:A:431:ILE:CG1  | 2.45                     | 0.46              |
| 1:A:141:LEU:HD21 | 1:A:145:LEU:HD22 | 1.97                     | 0.46              |
| 1:A:418:ARG:CG   | 1:A:422:GLY:HA3  | 2.27                     | 0.46              |
| 1:A:439:VAL:O    | 1:A:441:LEU:N    | 2.49                     | 0.46              |
| 2:B:13:ALA:HB3   | 2:B:15:PRO:HG3   | 1.97                     | 0.46              |
| 1:A:216:ALA:HA   | 1:A:219:ILE:CG1  | 2.43                     | 0.46              |
| 1:A:89:LYS:HG3   | 1:A:92:GLU:CB    | 2.46                     | 0.46              |
| 1:A:283:GLN:O    | 1:A:283:GLN:NE2  | 2.47                     | 0.46              |
| 1:A:388:ARG:HB3  | 1:A:394:LYS:HB3  | 1.98                     | 0.46              |
| 1:A:40:VAL:HG22  | 1:A:177:PHE:CD1  | 2.51                     | 0.46              |
| 2:B:7:LYS:C      | 2:B:8:LEU:HD23   | 2.36                     | 0.46              |
| 1:A:329:VAL:C    | 1:A:332:TRP:HB3  | 2.36                     | 0.46              |
| 2:B:31:TYR:O     | 2:B:32:TYR:CD2   | 2.68                     | 0.46              |
| 1:A:138:GLN:O    | 1:A:139:TYR:C    | 2.54                     | 0.46              |
| 1:A:145:LEU:HD22 | 1:A:203:GLY:CA   | 2.46                     | 0.46              |
| 2:B:50:VAL:CG1   | 2:B:51:PRO:HD3   | 2.45                     | 0.46              |
| 1:A:136:MET:O    | 1:A:139:TYR:HB2  | 2.15                     | 0.46              |
| 1:A:230:PHE:CD1  | 1:A:233:THR:CG2  | 2.99                     | 0.46              |
| 1:A:257:SER:OG   | 1:A:398:PHE:HA   | 2.15                     | 0.46              |
| 1:A:95:GLU:HA    | 1:A:98:ARG:HD3   | 1.98                     | 0.46              |
| 2:B:36:TYR:HA    | 2:B:70:ILE:CG1   | 2.46                     | 0.46              |
| 1:A:40:VAL:HG22  | 1:A:177:PHE:CB   | 2.45                     | 0.45              |
| 1:A:268:ILE:HB   | 1:A:287:ILE:HD13 | 1.98                     | 0.45              |
| 1:A:94:GLY:HA2   | 1:A:227:PHE:CZ   | 2.51                     | 0.45              |
| 2:B:18:LEU:HB2   | 2:B:59:ILE:HD11  | 1.97                     | 0.45              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:24:ALA:HB1   | 2:B:53:SER:CA    | 2.46                     | 0.45              |
| 1:A:103:PHE:CD2  | 1:A:106:ILE:HG22 | 2.51                     | 0.45              |
| 1:A:409:LEU:HD23 | 1:A:410:LEU:HD11 | 1.98                     | 0.45              |
| 1:A:415:LEU:HA   | 1:A:418:ARG:HD3  | 1.98                     | 0.45              |
| 1:A:77:LEU:C     | 1:A:79:PRO:HD2   | 2.37                     | 0.45              |
| 2:B:4:VAL:HG23   | 2:B:6:THR:HG23   | 1.89                     | 0.45              |
| 1:A:192:PHE:O    | 1:A:193:GLY:O    | 2.34                     | 0.45              |
| 1:A:109:ILE:CD1  | 1:A:110:PHE:CE2  | 2.99                     | 0.45              |
| 1:A:397:MET:O    | 1:A:400:HIS:ND1  | 2.47                     | 0.45              |
| 1:A:317:PHE:HD2  | 1:A:455:SER:HB2  | 1.82                     | 0.45              |
| 2:B:28:TYR:O     | 2:B:29:VAL:C     | 2.51                     | 0.45              |
| 1:A:340:LEU:O    | 1:A:344:LEU:HB2  | 2.16                     | 0.45              |
| 1:A:163:LEU:HB3  | 1:A:306:VAL:HG22 | 1.99                     | 0.45              |
| 1:A:298:GLN:O    | 1:A:382:ILE:CG2  | 2.64                     | 0.45              |
| 1:A:426:PHE:CA   | 1:A:428:THR:HG22 | 2.47                     | 0.45              |
| 2:B:27:GLU:HG3   | 2:B:52:GLY:O     | 2.16                     | 0.45              |
| 1:A:106:ILE:O    | 1:A:109:ILE:HG13 | 2.16                     | 0.45              |
| 1:A:227:PHE:CD2  | 1:A:227:PHE:O    | 2.70                     | 0.45              |
| 1:A:271:LEU:HD13 | 1:A:426:PHE:CE2  | 2.52                     | 0.45              |
| 1:A:70:PHE:O     | 1:A:73:ILE:HB    | 2.15                     | 0.45              |
| 1:A:180:ASN:HA   | 1:A:209:VAL:HG21 | 1.98                     | 0.45              |
| 1:A:95:GLU:O     | 1:A:99:GLN:CG    | 2.65                     | 0.45              |
| 2:B:69:THR:O     | 2:B:70:ILE:HG13  | 2.17                     | 0.45              |
| 1:A:109:ILE:HD12 | 1:A:109:ILE:O    | 2.17                     | 0.45              |
| 1:A:113:ILE:O    | 1:A:113:ILE:HG23 | 2.16                     | 0.45              |
| 1:A:73:ILE:CA    | 1:A:254:ILE:HG21 | 2.46                     | 0.45              |
| 1:A:104:GLY:HA2  | 1:A:153:HIS:HB3  | 1.99                     | 0.45              |
| 1:A:31:GLN:CG    | 1:A:296:ILE:HA   | 2.47                     | 0.45              |
| 2:B:24:ALA:C     | 2:B:53:SER:OG    | 2.54                     | 0.45              |
| 1:A:147:MET:N    | 1:A:148:PRO:HD2  | 2.32                     | 0.44              |
| 1:A:201:GLY:HA2  | 1:A:204:VAL:HG13 | 1.99                     | 0.44              |
| 1:A:292:ILE:HG13 | 1:A:293:LEU:N    | 2.32                     | 0.44              |
| 1:A:136:MET:C    | 1:A:138:GLN:H    | 2.20                     | 0.44              |
| 1:A:133:GLU:O    | 1:A:133:GLU:CG   | 2.66                     | 0.44              |
| 1:A:322:TYR:HE1  | 1:A:449:SER:CB   | 2.31                     | 0.44              |
| 1:A:150:ALA:O    | 1:A:152:VAL:N    | 2.48                     | 0.44              |
| 1:A:388:ARG:O    | 1:A:391:LYS:N    | 2.50                     | 0.44              |
| 1:A:359:VAL:CG1  | 1:A:360:LEU:HD22 | 2.42                     | 0.44              |
| 1:A:133:GLU:O    | 1:A:133:GLU:HG2  | 2.18                     | 0.44              |
| 1:A:116:TRP:HH2  | 1:A:147:MET:CA   | 2.27                     | 0.44              |
| 1:A:147:MET:CE   | 1:A:207:MET:SD   | 3.06                     | 0.44              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:120:THR:N    | 1:A:121:PRO:CD   | 2.81                     | 0.44              |
| 1:A:40:VAL:O     | 1:A:43:VAL:N     | 2.49                     | 0.44              |
| 2:B:27:GLU:HB3   | 2:B:30:VAL:HG23  | 2.00                     | 0.44              |
| 2:B:35:THR:C     | 2:B:70:ILE:HG12  | 2.36                     | 0.44              |
| 2:B:75:ARG:NH2   | 2:B:79:TRP:CE2   | 2.86                     | 0.44              |
| 1:A:95:GLU:HA    | 1:A:98:ARG:CD    | 2.48                     | 0.44              |
| 1:A:94:GLY:O     | 1:A:98:ARG:N     | 2.50                     | 0.44              |
| 2:B:68:TYR:H     | 2:B:90:ARG:HB3   | 1.82                     | 0.44              |
| 1:A:364:SER:OG   | 1:A:367:LEU:HD12 | 2.18                     | 0.44              |
| 1:A:397:MET:O    | 1:A:400:HIS:HB3  | 2.17                     | 0.44              |
| 1:A:71:MET:HE2   | 1:A:159:TYR:OH   | 2.18                     | 0.44              |
| 1:A:224:GLU:HG2  | 1:A:225:LYS:H    | 1.82                     | 0.44              |
| 1:A:183:LEU:CD2  | 1:A:209:VAL:CG2  | 2.95                     | 0.44              |
| 1:A:332:TRP:CE3  | 1:A:332:TRP:O    | 2.71                     | 0.44              |
| 1:A:342:LEU:CD1  | 1:A:374:GLN:OE1  | 2.66                     | 0.44              |
| 1:A:40:VAL:HG11  | 1:A:180:ASN:CG   | 2.39                     | 0.44              |
| 1:A:216:ALA:HA   | 1:A:219:ILE:CD1  | 2.47                     | 0.44              |
| 1:A:416:ALA:O    | 1:A:417:TYR:HB3  | 2.16                     | 0.44              |
| 1:A:103:PHE:C    | 1:A:105:LEU:H    | 2.16                     | 0.44              |
| 1:A:372:LEU:HD11 | 1:A:424:TYR:O    | 2.18                     | 0.44              |
| 1:A:391:LYS:C    | 1:A:393:THR:H    | 2.21                     | 0.44              |
| 1:A:315:ARG:NH2  | 2:B:11:VAL:HG11  | 2.32                     | 0.44              |
| 1:A:225:LYS:HG2  | 1:A:226:PHE:HD2  | 1.82                     | 0.44              |
| 1:A:260:LEU:O    | 1:A:263:SER:N    | 2.49                     | 0.43              |
| 1:A:403:ALA:O    | 1:A:407:CYS:CB   | 2.66                     | 0.43              |
| 2:B:17:SER:HA    | 2:B:61:GLY:CA    | 2.47                     | 0.43              |
| 2:B:11:VAL:HG12  | 2:B:19:LEU:HD12  | 1.99                     | 0.43              |
| 2:B:71:THR:HG22  | 2:B:72:VAL:N     | 2.33                     | 0.43              |
| 1:A:17:ILE:HG22  | 1:A:18:ARG:N     | 2.33                     | 0.43              |
| 1:A:268:ILE:HD13 | 1:A:287:ILE:HD13 | 1.86                     | 0.43              |
| 2:B:5:PRO:HD2    | 2:B:83:SER:O     | 2.18                     | 0.43              |
| 1:A:330:SER:O    | 1:A:333:VAL:HB   | 2.18                     | 0.43              |
| 1:A:339:VAL:HG22 | 1:A:370:ALA:O    | 2.19                     | 0.43              |
| 1:A:411:PRO:HG3  | 1:A:429:ALA:CA   | 2.49                     | 0.43              |
| 1:A:428:THR:C    | 1:A:430:LEU:H    | 2.21                     | 0.43              |
| 1:A:373:PHE:HB3  | 1:A:431:ILE:HG22 | 2.00                     | 0.43              |
| 2:B:29:VAL:O     | 2:B:30:VAL:CG1   | 2.67                     | 0.43              |
| 1:A:132:VAL:CG1  | 1:A:133:GLU:H    | 2.25                     | 0.43              |
| 1:A:339:VAL:CA   | 1:A:342:LEU:HD12 | 2.39                     | 0.43              |
| 1:A:437:ALA:C    | 1:A:439:VAL:N    | 2.71                     | 0.43              |
| 2:B:19:LEU:HD13  | 2:B:19:LEU:O     | 2.17                     | 0.43              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:3:SER:OG     | 2:B:4:VAL:N      | 2.52                     | 0.43              |
| 1:A:411:PRO:O    | 1:A:426:PHE:O    | 2.36                     | 0.43              |
| 1:A:418:ARG:CZ   | 1:A:425:GLY:HA3  | 2.48                     | 0.43              |
| 1:A:372:LEU:HD22 | 1:A:431:ILE:CG2  | 2.48                     | 0.43              |
| 1:A:78:ASN:N     | 1:A:79:PRO:CD    | 2.82                     | 0.43              |
| 1:A:285:VAL:O    | 1:A:289:LEU:HD23 | 2.18                     | 0.43              |
| 2:B:26:GLY:O     | 2:B:53:SER:CB    | 2.67                     | 0.43              |
| 1:A:172:VAL:HG13 | 1:A:173:SER:N    | 2.34                     | 0.43              |
| 1:A:418:ARG:HG3  | 1:A:419:PHE:H    | 1.82                     | 0.43              |
| 1:A:180:ASN:HD22 | 1:A:180:ASN:C    | 2.23                     | 0.43              |
| 2:B:64:PRO:HB2   | 2:B:65:GLY:H     | 1.66                     | 0.43              |
| 1:A:78:ASN:C     | 1:A:163:LEU:HD13 | 2.38                     | 0.43              |
| 1:A:183:LEU:HD12 | 1:A:183:LEU:O    | 2.19                     | 0.43              |
| 1:A:186:ILE:O    | 1:A:190:GLY:HA3  | 2.19                     | 0.43              |
| 1:A:268:ILE:HD12 | 1:A:268:ILE:C    | 2.39                     | 0.43              |
| 1:A:346:ARG:O    | 1:A:348:PRO:CD   | 2.67                     | 0.43              |
| 1:A:424:TYR:O    | 1:A:427:TRP:HB2  | 2.19                     | 0.43              |
| 1:A:442:VAL:HG23 | 1:A:445:LEU:HD23 | 2.01                     | 0.43              |
| 1:A:308:ILE:HD12 | 1:A:390:TYR:CA   | 2.49                     | 0.42              |
| 2:B:76:SER:O     | 2:B:78:TYR:O     | 2.36                     | 0.42              |
| 1:A:89:LYS:HG3   | 1:A:92:GLU:HB2   | 1.99                     | 0.42              |
| 1:A:154:ARG:NH2  | 1:A:215:LEU:CD2  | 2.82                     | 0.42              |
| 1:A:265:PHE:O    | 1:A:269:VAL:HB   | 2.19                     | 0.42              |
| 1:A:51:GLU:HB3   | 1:A:54:ALA:HB2   | 2.00                     | 0.42              |
| 1:A:115:MET:O    | 1:A:118:ALA:HB2  | 2.13                     | 0.42              |
| 1:A:207:MET:SD   | 1:A:207:MET:O    | 2.77                     | 0.42              |
| 1:A:426:PHE:HA   | 1:A:428:THR:HG22 | 2.01                     | 0.42              |
| 1:A:90:THR:HA    | 1:A:93:ALA:HB3   | 1.99                     | 0.42              |
| 1:A:292:ILE:HD12 | 1:A:293:LEU:CD1  | 2.49                     | 0.42              |
| 1:A:155:ALA:HB2  | 1:A:214:ALA:CA   | 2.48                     | 0.42              |
| 1:A:317:PHE:CD2  | 1:A:455:SER:HB2  | 2.55                     | 0.42              |
| 2:B:16:THR:HG23  | 2:B:17:SER:H     | 1.83                     | 0.42              |
| 1:A:254:ILE:CD1  | 1:A:388:ARG:HD2  | 2.50                     | 0.42              |
| 2:B:50:VAL:CB    | 2:B:51:PRO:CD    | 2.98                     | 0.42              |
| 1:A:65:THR:CG2   | 1:A:66:VAL:H     | 2.32                     | 0.42              |
| 1:A:172:VAL:C    | 1:A:174:PHE:H    | 2.22                     | 0.42              |
| 1:A:32:VAL:O     | 1:A:35:VAL:HG12  | 2.19                     | 0.42              |
| 1:A:252:ALA:HB3  | 1:A:253:PRO:HD3  | 2.02                     | 0.42              |
| 1:A:301:GLY:O    | 1:A:305:THR:CG2  | 2.61                     | 0.42              |
| 1:A:418:ARG:HG3  | 1:A:419:PHE:N    | 2.35                     | 0.42              |
| 1:A:74:MET:C     | 1:A:76:ALA:N     | 2.72                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:77:LEU:HD12  | 1:A:250:ILE:HD13 | 2.02                     | 0.42              |
| 2:B:34:ILE:HA    | 2:B:71:THR:O     | 2.20                     | 0.42              |
| 1:A:295:MET:HG2  | 1:A:296:ILE:N    | 2.34                     | 0.42              |
| 1:A:339:VAL:CG2  | 1:A:374:GLN:HB3  | 2.49                     | 0.42              |
| 2:B:23:ASP:O     | 2:B:55:SER:OG    | 2.26                     | 0.42              |
| 1:A:117:ALA:O    | 1:A:118:ALA:C    | 2.57                     | 0.42              |
| 1:A:143:THR:O    | 1:A:147:MET:HB3  | 2.20                     | 0.42              |
| 1:A:85:TYR:HD1   | 1:A:310:PHE:CE1  | 2.37                     | 0.42              |
| 2:B:13:ALA:C     | 2:B:15:PRO:HD3   | 2.41                     | 0.42              |
| 2:B:13:ALA:HB2   | 2:B:18:LEU:HG    | 2.01                     | 0.42              |
| 1:A:292:ILE:CD1  | 1:A:293:LEU:HD12 | 2.49                     | 0.42              |
| 2:B:60:SER:O     | 2:B:62:LEU:N     | 2.52                     | 0.42              |
| 1:A:210:PHE:O    | 1:A:214:ALA:N    | 2.53                     | 0.41              |
| 1:A:209:VAL:O    | 1:A:209:VAL:HG12 | 2.20                     | 0.41              |
| 1:A:308:ILE:HD12 | 1:A:390:TYR:N    | 2.35                     | 0.41              |
| 2:B:69:THR:OG1   | 2:B:88:ASN:HB2   | 2.20                     | 0.41              |
| 1:A:376:ALA:HB1  | 1:A:435:THR:HG21 | 2.02                     | 0.41              |
| 1:A:118:ALA:O    | 1:A:120:THR:N    | 2.53                     | 0.41              |
| 1:A:43:VAL:O     | 1:A:43:VAL:HG22  | 2.20                     | 0.41              |
| 2:B:29:VAL:O     | 2:B:30:VAL:HB    | 2.19                     | 0.41              |
| 1:A:19:LEU:C     | 1:A:21:THR:N     | 2.74                     | 0.41              |
| 1:A:247:ILE:HA   | 1:A:250:ILE:HG13 | 2.02                     | 0.41              |
| 1:A:76:ALA:HB1   | 1:A:394:LYS:HZ1  | 1.85                     | 0.41              |
| 1:A:175:ALA:HA   | 1:A:178:VAL:HG12 | 2.03                     | 0.41              |
| 1:A:236:PHE:HE2  | 1:A:239:PRO:O    | 2.03                     | 0.41              |
| 1:A:116:TRP:N    | 1:A:116:TRP:HE3  | 2.18                     | 0.41              |
| 1:A:364:SER:OG   | 1:A:367:LEU:CD1  | 2.68                     | 0.41              |
| 1:A:384:SER:O    | 1:A:386:ALA:N    | 2.43                     | 0.41              |
| 2:B:67:ASP:OD2   | 2:B:67:ASP:C     | 2.59                     | 0.41              |
| 1:A:68:ILE:HG22  | 1:A:68:ILE:O     | 2.19                     | 0.41              |
| 1:A:37:ILE:C     | 1:A:39:PHE:N     | 2.73                     | 0.41              |
| 2:B:81:TRP:CD1   | 2:B:81:TRP:N     | 2.89                     | 0.41              |
| 1:A:100:GLY:C    | 1:A:157:HIS:CD2  | 2.93                     | 0.41              |
| 1:A:407:CYS:HB3  | 1:A:433:SER:HB2  | 2.02                     | 0.41              |
| 2:B:8:LEU:HD13   | 2:B:87:ILE:CD1   | 2.48                     | 0.41              |
| 1:A:152:VAL:HG12 | 1:A:210:PHE:CG   | 2.56                     | 0.41              |
| 1:A:371:GLY:O    | 1:A:375:PRO:HD2  | 2.21                     | 0.41              |
| 1:A:391:LYS:C    | 1:A:393:THR:N    | 2.74                     | 0.41              |
| 2:B:34:ILE:HG12  | 2:B:48:PHE:HB2   | 2.02                     | 0.41              |
| 1:A:24:ALA:HB1   | 1:A:27:MET:HB2   | 2.03                     | 0.41              |
| 1:A:274:PRO:C    | 1:A:276:GLY:N    | 2.74                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:311:SER:HA   | 1:A:314:ARG:HB2  | 2.03                     | 0.41              |
| 1:A:308:ILE:HG13 | 1:A:309:GLY:H    | 1.86                     | 0.41              |
| 1:A:209:VAL:HA   | 1:A:212:PHE:HB3  | 2.02                     | 0.41              |
| 1:A:306:VAL:C    | 1:A:308:ILE:N    | 2.63                     | 0.41              |
| 1:A:40:VAL:HG12  | 1:A:44:MET:CE    | 2.44                     | 0.41              |
| 1:A:304:GLY:O    | 1:A:307:ARG:N    | 2.54                     | 0.41              |
| 1:A:396:PRO:HA   | 1:A:398:PHE:HB3  | 2.03                     | 0.41              |
| 1:A:458:ALA:HB1  | 2:B:8:LEU:CB     | 2.48                     | 0.41              |
| 2:B:75:ARG:HD2   | 2:B:80:GLY:O     | 2.21                     | 0.41              |
| 1:A:334:LEU:N    | 1:A:334:LEU:HD22 | 2.36                     | 0.41              |
| 2:B:31:TYR:CE1   | 2:B:75:ARG:NH1   | 2.88                     | 0.40              |
| 1:A:272:ILE:CG2  | 1:A:281:ALA:HA   | 2.51                     | 0.40              |
| 1:A:76:ALA:HB2   | 1:A:254:ILE:HG21 | 2.02                     | 0.40              |
| 2:B:85:ILE:CG2   | 2:B:85:ILE:O     | 2.68                     | 0.40              |
| 1:A:64:ALA:HA    | 1:A:67:TYR:HB3   | 2.03                     | 0.40              |
| 1:A:254:ILE:HB   | 1:A:394:LYS:HE2  | 2.03                     | 0.40              |
| 1:A:255:GLY:O    | 1:A:259:PHE:N    | 2.54                     | 0.40              |
| 1:A:284:GLN:HA   | 1:A:287:ILE:HG12 | 2.03                     | 0.40              |
| 2:B:27:GLU:CG    | 2:B:30:VAL:HG23  | 2.46                     | 0.40              |
| 1:A:148:PRO:HG3  | 1:A:207:MET:CB   | 2.51                     | 0.40              |
| 1:A:387:LEU:HA   | 1:A:387:LEU:HD13 | 1.82                     | 0.40              |
| 1:A:395:VAL:HG12 | 1:A:396:PRO:HD2  | 2.04                     | 0.40              |
| 1:A:428:THR:OG1  | 1:A:429:ALA:N    | 2.55                     | 0.40              |
| 1:A:55:ALA:O     | 1:A:138:GLN:NE2  | 2.54                     | 0.40              |
| 1:A:220:TYR:HD2  | 1:A:222:ALA:HB3  | 1.86                     | 0.40              |
| 1:A:163:LEU:O    | 1:A:164:ASN:CB   | 2.69                     | 0.40              |
| 1:A:230:PHE:HE1  | 1:A:233:THR:HG21 | 1.80                     | 0.40              |
| 1:A:268:ILE:HD12 | 1:A:269:VAL:CG2  | 2.49                     | 0.40              |
| 1:A:82:ALA:CB    | 1:A:306:VAL:HG13 | 2.51                     | 0.40              |
| 1:A:321:ARG:HH21 | 1:A:390:TYR:HB3  | 1.86                     | 0.40              |
| 1:A:436:ILE:HG13 | 1:A:436:ILE:O    | 2.21                     | 0.40              |
| 2:B:4:VAL:HG12   | 2:B:83:SER:HB3   | 2.02                     | 0.40              |
| 1:A:266:SER:OG   | 1:A:266:SER:O    | 2.39                     | 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     | 457/459 (100%) | 258 (56%) | 121 (26%) | 78 (17%) | 0           | 4 |
| 2   | B     | 89/99 (90%)    | 52 (58%)  | 19 (21%)  | 18 (20%) | 0           | 2 |
| All | All   | 546/558 (98%)  | 310 (57%) | 140 (26%) | 96 (18%) | 0           | 3 |

All (96) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 10  | PHE  |
| 1   | A     | 41  | ASP  |
| 1   | A     | 58  | LEU  |
| 1   | A     | 64  | ALA  |
| 1   | A     | 80  | MET  |
| 1   | A     | 105 | LEU  |
| 1   | A     | 118 | ALA  |
| 1   | A     | 139 | TYR  |
| 1   | A     | 164 | ASN  |
| 1   | A     | 166 | PRO  |
| 1   | A     | 192 | PHE  |
| 1   | A     | 193 | GLY  |
| 1   | A     | 194 | MET  |
| 1   | A     | 234 | ALA  |
| 1   | A     | 236 | PHE  |
| 1   | A     | 238 | LYS  |
| 1   | A     | 261 | GLU  |
| 1   | A     | 277 | GLU  |
| 1   | A     | 278 | ASP  |
| 1   | A     | 297 | PRO  |
| 1   | A     | 298 | GLN  |
| 1   | A     | 305 | THR  |
| 1   | A     | 307 | ARG  |
| 1   | A     | 347 | SER  |
| 1   | A     | 354 | ASN  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 361 | SER  |
| 1   | A     | 372 | LEU  |
| 1   | A     | 378 | PHE  |
| 1   | A     | 386 | ALA  |
| 1   | A     | 392 | VAL  |
| 1   | A     | 398 | PHE  |
| 1   | A     | 417 | TYR  |
| 2   | B     | 11  | VAL  |
| 2   | B     | 15  | PRO  |
| 2   | B     | 30  | VAL  |
| 2   | B     | 44  | PRO  |
| 2   | B     | 51  | PRO  |
| 2   | B     | 61  | GLY  |
| 2   | B     | 77  | TYR  |
| 2   | B     | 79  | TRP  |
| 2   | B     | 90  | ARG  |
| 1   | A     | 14  | LEU  |
| 1   | A     | 17  | ILE  |
| 1   | A     | 20  | LEU  |
| 1   | A     | 75  | ALA  |
| 1   | A     | 79  | PRO  |
| 1   | A     | 104 | GLY  |
| 1   | A     | 127 | THR  |
| 1   | A     | 130 | ASP  |
| 1   | A     | 131 | TYR  |
| 1   | A     | 132 | VAL  |
| 1   | A     | 149 | ALA  |
| 1   | A     | 158 | ALA  |
| 1   | A     | 200 | ALA  |
| 1   | A     | 229 | PRO  |
| 1   | A     | 244 | PHE  |
| 1   | A     | 275 | PHE  |
| 1   | A     | 291 | GLY  |
| 1   | A     | 348 | PRO  |
| 1   | A     | 380 | GLN  |
| 1   | A     | 388 | ARG  |
| 1   | A     | 389 | GLY  |
| 1   | A     | 396 | PRO  |
| 1   | A     | 405 | TRP  |
| 1   | A     | 442 | VAL  |
| 2   | B     | 5   | PRO  |
| 2   | B     | 38  | GLU  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 52  | GLY  |
| 2   | B     | 62  | LEU  |
| 2   | B     | 64  | PRO  |
| 1   | A     | 12  | VAL  |
| 1   | A     | 237 | GLY  |
| 1   | A     | 242 | ALA  |
| 1   | A     | 385 | TYR  |
| 1   | A     | 460 | SER  |
| 2   | B     | 56  | THR  |
| 1   | A     | 151 | MET  |
| 1   | A     | 165 | ARG  |
| 1   | A     | 173 | SER  |
| 1   | A     | 232 | LEU  |
| 1   | A     | 358 | ALA  |
| 1   | A     | 421 | MET  |
| 1   | A     | 440 | ALA  |
| 1   | A     | 97  | GLY  |
| 1   | A     | 314 | ARG  |
| 1   | A     | 344 | LEU  |
| 1   | A     | 353 | TYR  |
| 2   | B     | 24  | ALA  |
| 2   | B     | 83  | SER  |
| 1   | A     | 284 | GLN  |
| 1   | A     | 73  | ILE  |
| 1   | A     | 219 | ILE  |
| 2   | B     | 84  | PRO  |
| 1   | A     | 47  | GLY  |
| 1   | A     | 119 | ILE  |
| 1   | A     | 274 | PRO  |

### 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     | 353/353 (100%) | 243 (69%) | 110 (31%) | 0           | 3 |
| 2   | B     | 78/85 (92%)    | 54 (69%)  | 24 (31%)  | 0           | 3 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Analysed      | Rotameric | Outliers  | Percentiles       |
|-----|-------|---------------|-----------|-----------|-------------------|
| All | All   | 431/438 (98%) | 297 (69%) | 134 (31%) | <b>0</b> <b>3</b> |

All (134) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 8   | PHE  |
| 1   | A     | 14  | LEU  |
| 1   | A     | 15  | LYS  |
| 1   | A     | 18  | ARG  |
| 1   | A     | 20  | LEU  |
| 1   | A     | 25  | LEU  |
| 1   | A     | 39  | PHE  |
| 1   | A     | 44  | MET  |
| 1   | A     | 53  | LEU  |
| 1   | A     | 60  | SER  |
| 1   | A     | 61  | SER  |
| 1   | A     | 63  | PHE  |
| 1   | A     | 65  | THR  |
| 1   | A     | 71  | MET  |
| 1   | A     | 80  | MET  |
| 1   | A     | 81  | ILE  |
| 1   | A     | 89  | LYS  |
| 1   | A     | 95  | GLU  |
| 1   | A     | 102 | TRP  |
| 1   | A     | 103 | PHE  |
| 1   | A     | 105 | LEU  |
| 1   | A     | 106 | ILE  |
| 1   | A     | 107 | LEU  |
| 1   | A     | 112 | MET  |
| 1   | A     | 113 | ILE  |
| 1   | A     | 116 | TRP  |
| 1   | A     | 123 | ARG  |
| 1   | A     | 124 | ASN  |
| 1   | A     | 126 | LEU  |
| 1   | A     | 127 | THR  |
| 1   | A     | 136 | MET  |
| 1   | A     | 140 | MET  |
| 1   | A     | 147 | MET  |
| 1   | A     | 151 | MET  |
| 1   | A     | 153 | HIS  |
| 1   | A     | 154 | ARG  |
| 1   | A     | 159 | TYR  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 165 | ARG  |
| 1   | A     | 167 | ARG  |
| 1   | A     | 173 | SER  |
| 1   | A     | 180 | ASN  |
| 1   | A     | 183 | LEU  |
| 1   | A     | 184 | ASN  |
| 1   | A     | 197 | LEU  |
| 1   | A     | 204 | VAL  |
| 1   | A     | 206 | THR  |
| 1   | A     | 207 | MET  |
| 1   | A     | 210 | PHE  |
| 1   | A     | 212 | PHE  |
| 1   | A     | 215 | LEU  |
| 1   | A     | 218 | TRP  |
| 1   | A     | 224 | GLU  |
| 1   | A     | 225 | LYS  |
| 1   | A     | 228 | ARG  |
| 1   | A     | 232 | LEU  |
| 1   | A     | 235 | LYS  |
| 1   | A     | 238 | LYS  |
| 1   | A     | 248 | TRP  |
| 1   | A     | 249 | LYS  |
| 1   | A     | 257 | SER  |
| 1   | A     | 259 | PHE  |
| 1   | A     | 260 | LEU  |
| 1   | A     | 271 | LEU  |
| 1   | A     | 283 | GLN  |
| 1   | A     | 292 | ILE  |
| 1   | A     | 294 | TYR  |
| 1   | A     | 295 | MET  |
| 1   | A     | 296 | ILE  |
| 1   | A     | 299 | SER  |
| 1   | A     | 302 | SER  |
| 1   | A     | 305 | THR  |
| 1   | A     | 307 | ARG  |
| 1   | A     | 311 | SER  |
| 1   | A     | 312 | LEU  |
| 1   | A     | 321 | ARG  |
| 1   | A     | 323 | ILE  |
| 1   | A     | 329 | VAL  |
| 1   | A     | 334 | LEU  |
| 1   | A     | 336 | VAL  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 337 | ILE  |
| 1   | A     | 338 | THR  |
| 1   | A     | 340 | LEU  |
| 1   | A     | 347 | SER  |
| 1   | A     | 353 | TYR  |
| 1   | A     | 362 | ILE  |
| 1   | A     | 369 | PHE  |
| 1   | A     | 374 | GLN  |
| 1   | A     | 377 | ASP  |
| 1   | A     | 378 | PHE  |
| 1   | A     | 379 | THR  |
| 1   | A     | 382 | ILE  |
| 1   | A     | 384 | SER  |
| 1   | A     | 387 | LEU  |
| 1   | A     | 388 | ARG  |
| 1   | A     | 390 | TYR  |
| 1   | A     | 395 | VAL  |
| 1   | A     | 397 | MET  |
| 1   | A     | 407 | CYS  |
| 1   | A     | 417 | TYR  |
| 1   | A     | 427 | TRP  |
| 1   | A     | 428 | THR  |
| 1   | A     | 431 | ILE  |
| 1   | A     | 434 | LEU  |
| 1   | A     | 435 | THR  |
| 1   | A     | 436 | ILE  |
| 1   | A     | 439 | VAL  |
| 1   | A     | 441 | LEU  |
| 1   | A     | 447 | LYS  |
| 1   | A     | 452 | LEU  |
| 1   | A     | 460 | SER  |
| 2   | B     | 2   | SER  |
| 2   | B     | 6   | THR  |
| 2   | B     | 8   | LEU  |
| 2   | B     | 16  | THR  |
| 2   | B     | 18  | LEU  |
| 2   | B     | 19  | LEU  |
| 2   | B     | 20  | ILE  |
| 2   | B     | 21  | SER  |
| 2   | B     | 25  | ARG  |
| 2   | B     | 28  | TYR  |
| 2   | B     | 34  | ILE  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 36  | TYR  |
| 2   | B     | 38  | GLU  |
| 2   | B     | 39  | THR  |
| 2   | B     | 46  | GLN  |
| 2   | B     | 50  | VAL  |
| 2   | B     | 53  | SER  |
| 2   | B     | 55  | SER  |
| 2   | B     | 58  | THR  |
| 2   | B     | 70  | ILE  |
| 2   | B     | 75  | ARG  |
| 2   | B     | 78  | TYR  |
| 2   | B     | 90  | ARG  |
| 2   | B     | 91  | THR  |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 180 | ASN  |
| 1   | A     | 184 | ASN  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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     | 459/459 (100%) | -0.27  | 25 (5%) | 29 | 19 | 93, 203, 346, 432     | 0     |
| 2   | B     | 91/99 (91%)    | -0.32  | 5 (5%)  | 29 | 19 | 104, 179, 267, 302    | 0     |
| All | All   | 550/558 (98%)  | -0.28  | 30 (5%) | 29 | 19 | 93, 200, 342, 432     | 0     |

All (30) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2   | B     | 2   | SER  | 11.8 |
| 2   | B     | 1   | VAL  | 9.4  |
| 1   | A     | 350 | ALA  | 7.8  |
| 1   | A     | 349 | LEU  | 7.4  |
| 1   | A     | 463 | LEU  | 6.5  |
| 1   | A     | 9   | SER  | 6.1  |
| 1   | A     | 5   | LEU  | 4.6  |
| 1   | A     | 239 | PRO  | 4.3  |
| 1   | A     | 6   | ASP  | 4.3  |
| 1   | A     | 352 | MET  | 4.0  |
| 1   | A     | 462 | GLY  | 3.7  |
| 1   | A     | 351 | SER  | 3.6  |
| 1   | A     | 87  | ALA  | 3.6  |
| 1   | A     | 380 | GLN  | 3.5  |
| 1   | A     | 88  | GLY  | 3.2  |
| 1   | A     | 379 | THR  | 3.1  |
| 2   | B     | 89  | TYR  | 3.0  |
| 1   | A     | 130 | ASP  | 2.9  |
| 1   | A     | 348 | PRO  | 2.6  |
| 1   | A     | 421 | MET  | 2.6  |
| 1   | A     | 7   | ARG  | 2.5  |
| 1   | A     | 326 | VAL  | 2.4  |
| 2   | B     | 3   | SER  | 2.4  |
| 1   | A     | 419 | PHE  | 2.4  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | A     | 20  | LEU  | 2.3  |
| 1   | A     | 457 | LYS  | 2.3  |
| 1   | A     | 440 | ALA  | 2.2  |
| 2   | B     | 9   | GLU  | 2.2  |
| 1   | A     | 460 | SER  | 2.1  |
| 1   | A     | 461 | SER  | 2.0  |

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|------|-----------------------------|-------|
| 3   | CS   | A     | 501 | 1/1   | 0.98 | 0.06 | -    | 127,127,127,127             | 0     |

## 6.5 Other polymers [i](#)

There are no such residues in this entry.