



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:47 PM GMT

PDB ID : 1M3J  
Title : CRYSTAL form II of perfringolysin O  
Authors : Rossjohn, J.; Parker, M.; Polekhina, G.; Feil, S.; Tweten, R.  
Deposited on : 2002-06-28  
Resolution : 3.00 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) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

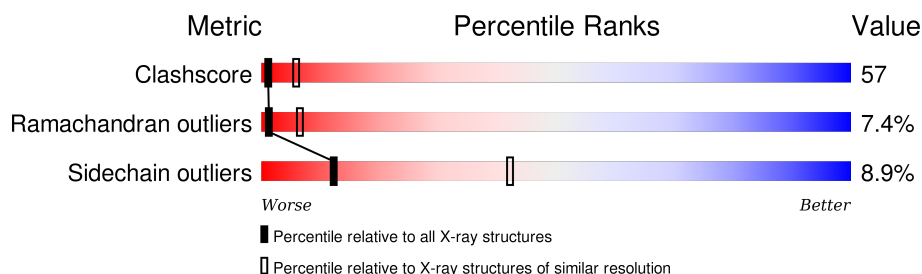
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 Å.


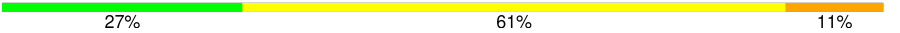
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| Clashscore            | 102246                      | 1912 (3.00-3.00)                                      |
| Ramachandran outliers | 100387                      | 1853 (3.00-3.00)                                      |
| Sidechain outliers    | 100360                      | 1856 (3.00-3.00)                                      |

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.

Note EDS was not executed.

| Mol | Chain | Length | Quality of chain  |
|-----|-------|--------|---|
| 1   | A     | 471    | <br>25% 64% 11% • |
| 1   | B     | 471    | <br>27% 61% 11%   |

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7467 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 perfringolysin o.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 1   | A     | 471      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 3705  | 2332 | 622 | 746 | 5 |         |         |       |
| 1   | B     | 471      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 3705  | 2332 | 622 | 746 | 5 |         |         |       |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| A     | 114     | LEU      | PHE    | see remark 999 | UNP P19995 |
| B     | 114     | LEU      | PHE    | see remark 999 | UNP P19995 |

- Molecule 2 is water.

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 2   | A     | 26       | Total | O  | 0       | 0       |
|     |       |          | 26    | 26 |         |         |
| 2   | B     | 31       | Total | O  | 0       | 0       |
|     |       |          | 31    | 31 |         |         |





## 4 Data and refinement statistics

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

| Property   | Value  | Source    |
|--|--|-----------|
| Space group  | P 21 21 2                                      | Depositor |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$ | 167.00Å 214.11Å 47.07Å<br>90.00° 90.00° 90.00° | Depositor |
| Resolution (Å)   | 20.00 – 3.00                                   | Depositor |
| % Data completeness<br>(in resolution range)             | (Not available) (20.00-3.00)                   | Depositor |
| $R_{merge}$  | 0.15   | Depositor |
| $R_{sym}$  | (Not available)                                | Depositor |
| Refinement program                                       | X-PLOR 3.1                                     | Depositor |
| R, $R_{free}$  | 0.247 , 0.337                                  | Depositor |
| Estimated twinning fraction                              | No twinning to report.                         | Xtriage   |
| Total number of atoms                                    | 7467   | wwPDB-VP  |
| Average B, all atoms (Å <sup>2</sup> )                   | 52.0   | wwPDB-VP  |

## 5 Model quality

### 5.1 Standard geometry

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

| Mol | Chain | Bond lengths |             | Bond angles |             |
|-----|-------|--------------|-------------|-------------|-------------|
|     |       | RMSZ         | $\# Z  > 5$ | RMSZ        | $\# Z  > 5$ |
| 1   | A     | 0.46         | 0/3776      | 0.70        | 0/5127      |
| 1   | B     | 0.48         | 0/3776      | 0.70        | 0/5127      |
| All | All   | 0.47         | 0/7552      | 0.70        | 0/10254     |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 3705  | 0        | 3656     | 427     | 0            |
| 1   | B     | 3705  | 0        | 3656     | 418     | 0            |
| 2   | A     | 26    | 0        | 0        | 3       | 0            |
| 2   | B     | 31    | 0        | 0        | 0       | 0            |
| All | All   | 7467  | 0        | 7312     | 845     | 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 57.

All (845) 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:B:96:ASP:HB2 | 1:B:100:ASP:HB2 | 1.22                     | 1.17              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:96:ASP:HB2   | 1:A:100:ASP:HB2  | 1.23                     | 1.16              |
| 1:A:481:ASN:HB2  | 1:A:500:ASN:ND2  | 1.62                     | 1.12              |
| 1:B:70:LYS:H     | 1:B:70:LYS:HD3   | 1.08                     | 1.10              |
| 1:A:70:LYS:HD3   | 1:A:70:LYS:H     | 1.15                     | 1.09              |
| 1:A:96:ASP:HB3   | 1:A:99:ASN:HB2   | 1.30                     | 1.08              |
| 1:B:163:SER:HA   | 1:B:166:ASN:HD22 | 1.20                     | 1.06              |
| 1:A:305:ASN:HA   | 1:A:310:LYS:HE2  | 1.41                     | 1.02              |
| 1:B:339:ASP:HA   | 1:B:342:ARG:HD2  | 1.37                     | 1.02              |
| 1:B:53:LEU:HD21  | 1:B:114:LEU:HD23 | 1.41                     | 1.01              |
| 1:A:468:ARG:HH11 | 1:A:468:ARG:HB3  | 1.25                     | 1.01              |
| 1:A:226:TYR:HB2  | 1:A:277:ILE:HB   | 1.42                     | 1.01              |
| 1:A:481:ASN:HB2  | 1:A:500:ASN:HD22 | 0.87                     | 1.00              |
| 1:A:38:ILE:HA    | 1:A:251:PHE:HB2  | 1.42                     | 1.00              |
| 1:A:462:LEU:HD22 | 1:A:466:TRP:HZ3  | 1.27                     | 0.99              |
| 1:A:335:THR:HG22 | 1:A:337:ASP:H    | 1.27                     | 0.98              |
| 1:A:449:ALA:C    | 1:A:450:ARG:HD2  | 1.84                     | 0.97              |
| 1:B:59:LYS:HB2   | 1:B:59:LYS:HZ2   | 1.29                     | 0.97              |
| 1:B:393:LYS:HD2  | 1:B:442:VAL:HG11 | 1.45                     | 0.97              |
| 1:B:130:ASN:HD21 | 1:B:145:LYS:HE2  | 1.31                     | 0.96              |
| 1:A:182:SER:HB2  | 1:A:225:ALA:HB3  | 1.48                     | 0.95              |
| 1:A:277:ILE:CD1  | 1:A:345:ILE:HA   | 1.97                     | 0.94              |
| 1:B:335:THR:HG22 | 1:B:337:ASP:H    | 1.30                     | 0.94              |
| 1:A:59:LYS:HZ2   | 1:A:59:LYS:HB2   | 1.34                     | 0.93              |
| 1:B:96:ASP:CB    | 1:B:100:ASP:H    | 1.82                     | 0.92              |
| 1:B:226:TYR:HB2  | 1:B:277:ILE:HB   | 1.48                     | 0.92              |
| 1:A:96:ASP:HB3   | 1:A:100:ASP:H    | 1.33                     | 0.92              |
| 1:A:479:THR:HG21 | 1:A:499:TYR:HB3  | 1.50                     | 0.92              |
| 1:A:462:LEU:HD22 | 1:A:466:TRP:CZ3  | 2.05                     | 0.90              |
| 1:A:96:ASP:CB    | 1:A:100:ASP:H    | 1.83                     | 0.90              |
| 1:A:418:GLU:HB2  | 1:A:420:ASN:ND2  | 1.88                     | 0.88              |
| 1:A:394:ILE:HD11 | 1:A:445:LEU:HD11 | 1.54                     | 0.88              |
| 1:A:96:ASP:HB2   | 1:A:100:ASP:CB   | 2.04                     | 0.87              |
| 1:B:107:LEU:HD11 | 1:B:126:ARG:HH11 | 1.37                     | 0.87              |
| 1:B:96:ASP:HB2   | 1:B:100:ASP:CB   | 2.03                     | 0.86              |
| 1:B:186:VAL:O    | 1:B:214:VAL:HG11 | 1.73                     | 0.86              |
| 1:A:343:LYS:HG2  | 1:A:347:ASP:OD2  | 1.75                     | 0.86              |
| 1:B:277:ILE:HD13 | 1:B:345:ILE:HA   | 1.58                     | 0.86              |
| 1:B:343:LYS:HA   | 1:B:346:LYS:HE3  | 1.58                     | 0.84              |
| 1:B:182:SER:HB2  | 1:B:225:ALA:HB3  | 1.57                     | 0.84              |
| 1:B:128:PRO:HG3  | 1:B:147:ASP:HA   | 1.59                     | 0.84              |
| 1:B:90:VAL:O     | 1:B:363:THR:HG22 | 1.78                     | 0.84              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:49:ARG:HG3   | 1:A:50:ASN:ND2   | 1.93                     | 0.84              |
| 1:B:412:GLU:HG3  | 1:B:426:LYS:HD2  | 1.60                     | 0.84              |
| 1:B:79:GLU:HB2   | 1:B:385:THR:OG1  | 1.77                     | 0.83              |
| 1:A:277:ILE:HD13 | 1:A:345:ILE:HA   | 1.60                     | 0.83              |
| 1:B:277:ILE:HG12 | 1:B:322:VAL:HG22 | 1.60                     | 0.83              |
| 1:B:239:LYS:H    | 1:B:239:LYS:HD2  | 1.42                     | 0.83              |
| 1:B:403:VAL:HG11 | 1:B:434:ASP:OD2  | 1.78                     | 0.83              |
| 1:B:398:HIS:HA   | 1:B:486:ILE:HD11 | 1.59                     | 0.83              |
| 1:B:43:SER:HA    | 1:B:368:LYS:HG3  | 1.60                     | 0.82              |
| 1:A:103:TYR:CD1  | 1:A:154:VAL:HG21 | 2.14                     | 0.82              |
| 1:A:95:ILE:HG22  | 1:A:96:ASP:N     | 1.95                     | 0.82              |
| 1:A:220:LYS:HD2  | 1:A:290:VAL:HG21 | 1.62                     | 0.82              |
| 1:B:104:PRO:HB2  | 1:B:235:ALA:HB2  | 1.61                     | 0.82              |
| 1:B:96:ASP:HB2   | 1:B:100:ASP:H    | 1.43                     | 0.82              |
| 1:A:224:LEU:HB2  | 1:A:279:VAL:HB   | 1.60                     | 0.82              |
| 1:B:456:ALA:HB3  | 1:B:471:ILE:HG22 | 1.60                     | 0.81              |
| 1:A:70:LYS:HD3   | 1:A:70:LYS:N     | 1.94                     | 0.81              |
| 1:A:101:ARG:NE   | 1:A:101:ARG:H    | 1.79                     | 0.81              |
| 1:A:232:THR:HB   | 1:A:271:VAL:O    | 1.81                     | 0.81              |
| 1:B:70:LYS:N     | 1:B:70:LYS:HD3   | 1.91                     | 0.81              |
| 1:B:95:ILE:HG12  | 1:B:117:ASN:HB2  | 1.63                     | 0.80              |
| 1:A:33:ASP:O     | 1:A:34:LYS:HG3   | 1.82                     | 0.80              |
| 1:A:398:HIS:ND1  | 1:A:486:ILE:HD11 | 1.97                     | 0.80              |
| 1:B:224:LEU:HB2  | 1:B:279:VAL:HB   | 1.64                     | 0.79              |
| 1:B:107:LEU:HD11 | 1:B:126:ARG:NH1  | 1.98                     | 0.79              |
| 1:B:38:ILE:HA    | 1:B:251:PHE:HB2  | 1.64                     | 0.79              |
| 1:A:491:LEU:HD22 | 1:A:492:TYR:CE1  | 2.18                     | 0.79              |
| 1:B:95:ILE:HG12  | 1:B:117:ASN:CB   | 2.13                     | 0.79              |
| 1:A:178:ARG:HB2  | 1:A:229:ILE:HB   | 1.62                     | 0.78              |
| 1:A:59:LYS:NZ    | 1:A:59:LYS:HB2   | 1.95                     | 0.78              |
| 1:B:148:ASP:O    | 1:B:153:LYS:HG2  | 1.83                     | 0.78              |
| 1:B:402:TYR:HB3  | 1:B:490:THR:OG1  | 1.84                     | 0.78              |
| 1:A:104:PRO:HG3  | 1:A:233:VAL:CG1  | 2.14                     | 0.78              |
| 1:B:449:ALA:C    | 1:B:450:ARG:HD2  | 2.03                     | 0.78              |
| 1:A:124:VAL:HG21 | 1:A:245:PHE:HD2  | 1.48                     | 0.78              |
| 1:A:413:VAL:HG11 | 1:A:450:ARG:NH1  | 1.99                     | 0.78              |
| 1:A:150:THR:O    | 1:A:154:VAL:HG23 | 1.83                     | 0.77              |
| 1:A:80:ARG:HG3   | 1:A:80:ARG:HH11  | 1.48                     | 0.77              |
| 1:A:458:GLU:O    | 1:A:467:TRP:HB3  | 1.84                     | 0.77              |
| 1:B:457:ARG:HD3  | 1:B:469:ASP:OD2  | 1.84                     | 0.77              |
| 1:A:418:GLU:HB2  | 1:A:420:ASN:HD22 | 1.48                     | 0.77              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:454:ILE:HG21 | 1:A:484:VAL:HG21 | 1.67                     | 0.77              |
| 1:A:306:SER:O    | 1:A:310:LYS:HG2  | 1.85                     | 0.76              |
| 1:A:49:ARG:HG3   | 1:A:50:ASN:HD22  | 1.49                     | 0.76              |
| 1:B:96:ASP:HB3   | 1:B:100:ASP:H    | 1.50                     | 0.76              |
| 1:B:129:ILE:HG12 | 1:B:130:ASN:H    | 1.49                     | 0.76              |
| 1:A:98:VAL:HG12  | 1:A:325:GLY:HA2  | 1.67                     | 0.76              |
| 1:B:135:LEU:HD23 | 1:B:136:PRO:HD2  | 1.66                     | 0.76              |
| 1:B:96:ASP:HB3   | 1:B:99:ASN:HB2   | 1.67                     | 0.76              |
| 1:A:101:ARG:HE   | 1:A:101:ARG:H    | 1.31                     | 0.76              |
| 1:A:104:PRO:HG3  | 1:A:233:VAL:HG11 | 1.68                     | 0.76              |
| 1:A:305:ASN:HA   | 1:A:310:LYS:CE   | 2.15                     | 0.75              |
| 1:A:210:ASP:OD2  | 1:A:213:ALA:HB2  | 1.87                     | 0.75              |
| 1:A:339:ASP:HA   | 1:A:342:ARG:HD2  | 1.69                     | 0.74              |
| 1:B:306:SER:O    | 1:B:310:LYS:HG2  | 1.88                     | 0.74              |
| 1:A:263:ALA:N    | 1:A:264:PRO:HD3  | 2.02                     | 0.74              |
| 1:A:144:ILE:HG13 | 1:A:145:LYS:H    | 1.52                     | 0.74              |
| 1:A:144:ILE:HB   | 1:A:161:LEU:HD21 | 1.67                     | 0.74              |
| 1:A:491:LEU:HD22 | 1:A:492:TYR:CD1  | 2.23                     | 0.74              |
| 1:A:465:GLU:CD   | 1:A:465:GLU:H    | 1.89                     | 0.74              |
| 1:B:457:ARG:NH2  | 1:B:465:GLU:HA   | 2.03                     | 0.73              |
| 1:B:163:SER:HA   | 1:B:166:ASN:ND2  | 1.99                     | 0.73              |
| 1:B:103:TYR:CD1  | 1:B:154:VAL:HG21 | 2.23                     | 0.73              |
| 1:B:263:ALA:N    | 1:B:264:PRO:HD3  | 2.03                     | 0.73              |
| 1:A:96:ASP:HB3   | 1:A:99:ASN:CB    | 2.14                     | 0.73              |
| 1:B:335:THR:HG22 | 1:B:337:ASP:N    | 2.04                     | 0.73              |
| 1:B:49:ARG:HG3   | 1:B:50:ASN:N     | 2.03                     | 0.73              |
| 1:B:91:ASP:OD1   | 1:B:361:SER:OG   | 2.06                     | 0.73              |
| 1:A:335:THR:HG21 | 1:A:340:GLU:HG3  | 1.69                     | 0.73              |
| 1:B:112:LYS:HA   | 1:B:115:VAL:HG23 | 1.70                     | 0.73              |
| 1:B:70:LYS:CD    | 1:B:70:LYS:H     | 1.93                     | 0.73              |
| 1:B:130:ASN:ND2  | 1:B:145:LYS:HE2  | 2.04                     | 0.72              |
| 1:A:121:ILE:HD13 | 1:A:122:LEU:H    | 1.54                     | 0.72              |
| 1:B:365:VAL:HG13 | 1:B:371:SER:O    | 1.88                     | 0.72              |
| 1:A:158:ILE:O    | 1:A:162:VAL:HG23 | 1.89                     | 0.72              |
| 1:B:398:HIS:ND1  | 1:B:486:ILE:HD11 | 2.04                     | 0.72              |
| 1:A:133:ILE:HG13 | 1:A:232:THR:O    | 1.89                     | 0.72              |
| 1:A:196:LEU:HD22 | 1:A:225:ALA:HB2  | 1.72                     | 0.72              |
| 1:B:230:PHE:HZ   | 1:B:275:ARG:NH1  | 1.88                     | 0.72              |
| 1:A:123:MET:H    | 1:A:257:LYS:HE2  | 1.51                     | 0.72              |
| 1:B:55:SER:HB3   | 1:B:115:VAL:HG11 | 1.70                     | 0.72              |
| 1:B:95:ILE:HG22  | 1:B:96:ASP:N     | 2.02                     | 0.72              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:98:VAL:HG12  | 1:B:358:TYR:HD1  | 1.56                     | 0.71              |
| 1:A:416:ASP:OD1  | 1:A:420:ASN:HB2  | 1.90                     | 0.71              |
| 1:B:230:PHE:HB3  | 1:B:351:PHE:CE1  | 2.25                     | 0.71              |
| 1:A:98:VAL:HG12  | 1:A:358:TYR:CD1  | 2.25                     | 0.71              |
| 1:A:41:GLY:HA3   | 1:A:251:PHE:CE2  | 2.25                     | 0.71              |
| 1:B:417:LYS:NZ   | 1:B:417:LYS:HB2  | 2.06                     | 0.71              |
| 1:A:403:VAL:HG11 | 1:A:434:ASP:OD2  | 1.91                     | 0.71              |
| 1:A:213:ALA:HB1  | 1:A:219:LYS:HG3  | 1.71                     | 0.71              |
| 1:A:266:LEU:HD23 | 1:A:366:PHE:HA   | 1.73                     | 0.71              |
| 1:A:468:ARG:CB   | 1:A:468:ARG:HH11 | 2.04                     | 0.70              |
| 1:B:104:PRO:HG3  | 1:B:233:VAL:HG12 | 1.73                     | 0.70              |
| 1:A:259:VAL:HG13 | 1:A:265:PRO:HD3  | 1.72                     | 0.70              |
| 1:B:476:VAL:HG13 | 1:B:499:TYR:OH   | 1.91                     | 0.70              |
| 1:B:458:GLU:O    | 1:B:467:TRP:HB3  | 1.92                     | 0.70              |
| 1:B:366:PHE:CE1  | 1:B:373:ALA:HA   | 2.26                     | 0.70              |
| 1:B:324:GLY:O    | 1:B:358:TYR:HB2  | 1.91                     | 0.70              |
| 1:B:129:ILE:HG12 | 1:B:130:ASN:N    | 2.06                     | 0.70              |
| 1:B:96:ASP:HB3   | 1:B:99:ASN:CB    | 2.22                     | 0.70              |
| 1:B:393:LYS:HD2  | 1:B:442:VAL:CG1  | 2.22                     | 0.70              |
| 1:A:393:LYS:HD2  | 1:A:442:VAL:HG11 | 1.74                     | 0.69              |
| 1:B:178:ARG:HB2  | 1:B:229:ILE:HB   | 1.73                     | 0.69              |
| 1:A:107:LEU:O    | 1:A:121:ILE:HD13 | 1.92                     | 0.69              |
| 1:B:53:LEU:HD21  | 1:B:114:LEU:CD2  | 2.20                     | 0.69              |
| 1:B:339:ASP:HA   | 1:B:342:ARG:CD   | 2.20                     | 0.69              |
| 1:A:158:ILE:HD13 | 1:A:233:VAL:HG21 | 1.73                     | 0.69              |
| 1:B:287:SER:O    | 1:B:290:VAL:HG23 | 1.93                     | 0.69              |
| 1:B:31:ILE:HD11  | 1:B:35:ASN:O     | 1.92                     | 0.69              |
| 1:B:123:MET:H    | 1:B:257:LYS:HE2  | 1.57                     | 0.69              |
| 1:B:199:ASN:HB3  | 1:B:202:VAL:HG23 | 1.72                     | 0.68              |
| 1:A:114:LEU:HA   | 1:A:119:PRO:HB3  | 1.74                     | 0.68              |
| 1:B:398:HIS:HA   | 1:B:486:ILE:CD1  | 2.23                     | 0.68              |
| 1:A:144:ILE:HG13 | 1:A:145:LYS:N    | 2.07                     | 0.68              |
| 1:B:452:ILE:HD11 | 1:B:478:LEU:HD13 | 1.75                     | 0.68              |
| 1:A:185:MET:SD   | 1:A:222:MET:HG3  | 2.34                     | 0.68              |
| 1:A:34:LYS:HE2   | 1:A:34:LYS:C     | 2.14                     | 0.68              |
| 1:B:192:ILE:HG12 | 1:B:223:ILE:HD12 | 1.76                     | 0.68              |
| 1:A:228:GLN:HA   | 1:A:228:GLN:HE21 | 1.57                     | 0.68              |
| 1:B:46:SER:O     | 1:B:47:TYR:HB3   | 1.93                     | 0.67              |
| 1:A:409:ALA:HB2  | 1:A:427:THR:HG22 | 1.75                     | 0.67              |
| 1:B:38:ILE:HG23  | 1:B:39:ASP:H     | 1.59                     | 0.67              |
| 1:B:96:ASP:CB    | 1:B:100:ASP:HB2  | 2.13                     | 0.67              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:98:VAL:CG1   | 1:A:325:GLY:HA2  | 2.24                     | 0.67              |
| 1:A:427:THR:HB   | 1:A:431:ASN:ND2  | 2.10                     | 0.67              |
| 1:B:30:ASP:CA    | 1:B:36:GLN:HG2   | 2.25                     | 0.67              |
| 1:B:479:THR:HG21 | 1:B:499:TYR:HB3  | 1.77                     | 0.67              |
| 1:A:85:LEU:HD23  | 1:A:194:SER:HB3  | 1.75                     | 0.67              |
| 1:A:94:ILE:HD12  | 1:A:359:PRO:HB2  | 1.76                     | 0.66              |
| 1:A:107:LEU:HD11 | 1:A:126:ARG:HH11 | 1.59                     | 0.66              |
| 1:A:110:ALA:HB2  | 1:A:266:LEU:HD11 | 1.77                     | 0.66              |
| 1:A:46:SER:O     | 1:A:47:TYR:HB3   | 1.95                     | 0.66              |
| 1:A:462:LEU:HB3  | 1:A:466:TRP:CE3  | 2.29                     | 0.66              |
| 1:B:449:ALA:O    | 1:B:450:ARG:HD2  | 1.95                     | 0.66              |
| 1:B:480:ASN:HB2  | 1:B:500:ASN:O    | 1.96                     | 0.66              |
| 1:B:394:ILE:HG12 | 1:B:482:ILE:HB   | 1.78                     | 0.66              |
| 1:A:144:ILE:HD11 | 2:A:506:HOH:O    | 1.96                     | 0.66              |
| 1:A:131:ILE:HG23 | 1:A:233:VAL:HG13 | 1.78                     | 0.66              |
| 1:B:230:PHE:CE1  | 1:B:351:PHE:HB2  | 2.31                     | 0.66              |
| 1:B:133:ILE:HD11 | 1:B:231:TYR:CD2  | 2.30                     | 0.66              |
| 1:B:391:LYS:HG2  | 1:B:447:ALA:H    | 1.60                     | 0.66              |
| 1:A:124:VAL:HG21 | 1:A:245:PHE:CD2  | 2.31                     | 0.66              |
| 1:A:457:ARG:HG2  | 1:A:467:TRP:HB2  | 1.76                     | 0.65              |
| 1:A:452:ILE:CD1  | 1:A:478:LEU:HD13 | 2.26                     | 0.65              |
| 1:A:452:ILE:HD11 | 1:A:478:LEU:HD13 | 1.78                     | 0.65              |
| 1:B:277:ILE:CD1  | 1:B:345:ILE:HA   | 2.27                     | 0.65              |
| 1:A:312:ILE:HA   | 2:A:524:HOH:O    | 1.95                     | 0.65              |
| 1:A:318:PHE:HD1  | 1:A:335:THR:O    | 1.79                     | 0.65              |
| 1:A:97:SER:HB3   | 1:A:324:GLY:HA2  | 1.79                     | 0.65              |
| 1:A:134:ASP:OD1  | 1:A:232:THR:HG23 | 1.97                     | 0.65              |
| 1:B:413:VAL:HG11 | 1:B:450:ARG:NH1  | 2.12                     | 0.64              |
| 1:B:49:ARG:HG3   | 1:B:50:ASN:H     | 1.62                     | 0.64              |
| 1:A:68:GLY:HA2   | 1:A:76:ILE:O     | 1.97                     | 0.64              |
| 1:A:98:VAL:HG12  | 1:A:358:TYR:HD1  | 1.62                     | 0.64              |
| 1:A:96:ASP:HB2   | 1:A:100:ASP:H    | 1.62                     | 0.64              |
| 1:A:366:PHE:CE1  | 1:A:373:ALA:HA   | 2.32                     | 0.64              |
| 1:B:30:ASP:HA    | 1:B:36:GLN:HG2   | 1.80                     | 0.64              |
| 1:B:135:LEU:CD2  | 1:B:136:PRO:HD2  | 2.26                     | 0.64              |
| 1:A:199:ASN:HB3  | 1:A:202:VAL:HG23 | 1.79                     | 0.64              |
| 1:A:309:TYR:HB3  | 1:A:313:TYR:CE1  | 2.32                     | 0.64              |
| 1:B:96:ASP:HB2   | 1:B:100:ASP:N    | 2.10                     | 0.64              |
| 1:B:128:PRO:HA   | 1:B:146:VAL:O    | 1.98                     | 0.64              |
| 1:A:477:PRO:O    | 1:A:482:ILE:HD11 | 1.98                     | 0.64              |
| 1:B:275:ARG:HD2  | 1:B:322:VAL:CG1  | 2.28                     | 0.64              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:259:VAL:HG13 | 1:B:265:PRO:HD3  | 1.79                     | 0.64              |
| 1:A:337:ASP:OD2  | 1:A:339:ASP:HB2  | 1.99                     | 0.64              |
| 1:A:182:SER:HB2  | 1:A:225:ALA:CB   | 2.24                     | 0.63              |
| 1:B:98:VAL:HG12  | 1:B:358:TYR:CD1  | 2.33                     | 0.63              |
| 1:A:95:ILE:HG12  | 1:A:117:ASN:CB   | 2.29                     | 0.63              |
| 1:A:305:ASN:CA   | 1:A:310:LYS:HE2  | 2.25                     | 0.63              |
| 1:B:305:ASN:HA   | 1:B:310:LYS:HE2  | 1.81                     | 0.63              |
| 1:B:45:LEU:O     | 1:B:368:LYS:NZ   | 2.22                     | 0.63              |
| 1:B:212:ASN:HA   | 1:B:215:ALA:HB3  | 1.80                     | 0.63              |
| 1:A:449:ALA:O    | 1:A:450:ARG:HD2  | 1.99                     | 0.63              |
| 1:A:339:ASP:HA   | 1:A:342:ARG:CD   | 2.29                     | 0.63              |
| 1:A:394:ILE:HG23 | 1:A:482:ILE:O    | 1.98                     | 0.63              |
| 1:B:457:ARG:HH21 | 1:B:465:GLU:HA   | 1.63                     | 0.63              |
| 1:A:134:ASP:CG   | 1:A:178:ARG:HH22 | 2.02                     | 0.62              |
| 1:A:31:ILE:HD11  | 1:A:35:ASN:O     | 1.98                     | 0.62              |
| 1:A:75:PHE:HB3   | 1:A:389:TYR:HB2  | 1.81                     | 0.62              |
| 1:B:291:GLN:O    | 1:B:295:LYS:HG3  | 2.00                     | 0.62              |
| 1:A:107:LEU:HD12 | 1:A:107:LEU:N    | 2.15                     | 0.62              |
| 1:A:187:TYR:HD1  | 1:A:381:TYR:HE1  | 1.46                     | 0.62              |
| 1:A:409:ALA:HB1  | 1:A:425:HIS:CE1  | 2.34                     | 0.62              |
| 1:B:60:ILE:HG12  | 1:B:61:GLU:N     | 2.14                     | 0.62              |
| 1:A:138:LEU:CD1  | 1:A:141:GLU:HG3  | 2.30                     | 0.62              |
| 1:B:319:THR:HA   | 1:B:333:VAL:O    | 2.00                     | 0.62              |
| 1:A:103:TYR:OH   | 1:A:150:THR:HA   | 2.00                     | 0.62              |
| 1:B:369:ASP:OD2  | 1:B:371:SER:HB3  | 1.99                     | 0.62              |
| 1:A:95:ILE:CG2   | 1:A:96:ASP:N     | 2.62                     | 0.61              |
| 1:A:269:SER:HB3  | 1:A:365:VAL:HG23 | 1.82                     | 0.61              |
| 1:A:129:ILE:C    | 1:A:130:ASN:HD22 | 2.02                     | 0.61              |
| 1:A:130:ASN:HD21 | 1:A:145:LYS:HE2  | 1.65                     | 0.61              |
| 1:A:138:LEU:HD12 | 1:A:141:GLU:HG3  | 1.82                     | 0.61              |
| 1:A:413:VAL:HG12 | 1:A:448:ASN:O    | 2.00                     | 0.61              |
| 1:A:222:MET:O    | 1:A:281:LEU:HD12 | 2.00                     | 0.61              |
| 1:B:394:ILE:HA   | 1:B:482:ILE:O    | 2.00                     | 0.61              |
| 1:B:486:ILE:O    | 1:B:486:ILE:HD12 | 2.01                     | 0.61              |
| 1:B:73:ASN:C     | 1:B:74:LYS:HG3   | 2.20                     | 0.61              |
| 1:A:89:PRO:HD2   | 1:A:375:VAL:O    | 2.01                     | 0.60              |
| 1:A:90:VAL:O     | 1:A:363:THR:HG22 | 2.00                     | 0.60              |
| 1:B:48:ASN:HD22  | 1:B:51:GLU:HB2   | 1.66                     | 0.60              |
| 1:B:230:PHE:CD1  | 1:B:351:PHE:HB2  | 2.36                     | 0.60              |
| 1:B:89:PRO:HD2   | 1:B:375:VAL:O    | 2.01                     | 0.60              |
| 1:A:107:LEU:HD11 | 1:A:126:ARG:NH1  | 2.17                     | 0.60              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:220:LYS:HD2  | 1:B:290:VAL:HG21 | 1.83                     | 0.60              |
| 1:B:263:ALA:N    | 1:B:264:PRO:CD   | 2.62                     | 0.60              |
| 1:B:401:ALA:HB3  | 1:B:489:THR:HA   | 1.84                     | 0.60              |
| 1:B:198:VAL:HG11 | 1:B:278:TYR:OH   | 2.01                     | 0.59              |
| 1:B:154:VAL:O    | 1:B:158:ILE:HG13 | 2.02                     | 0.59              |
| 1:B:291:GLN:HE21 | 1:B:295:LYS:HD2  | 1.65                     | 0.59              |
| 1:A:53:LEU:O     | 1:A:375:VAL:HA   | 2.02                     | 0.59              |
| 1:A:130:ASN:C    | 1:A:131:ILE:HD12 | 2.22                     | 0.59              |
| 1:A:397:ASP:HB3  | 1:A:485:SER:OG   | 2.02                     | 0.59              |
| 1:B:125:LYS:HD3  | 1:B:246:ASP:OD2  | 2.01                     | 0.59              |
| 1:B:263:ALA:H    | 1:B:264:PRO:HD3  | 1.67                     | 0.59              |
| 1:B:454:ILE:HG21 | 1:B:484:VAL:HG21 | 1.83                     | 0.59              |
| 1:B:33:ASP:O     | 1:B:34:LYS:HG3   | 2.01                     | 0.59              |
| 1:B:462:LEU:HD23 | 1:B:462:LEU:O    | 2.02                     | 0.59              |
| 1:A:30:ASP:CA    | 1:A:36:GLN:HG2   | 2.32                     | 0.59              |
| 1:B:259:VAL:HG12 | 1:B:260:SER:N    | 2.18                     | 0.59              |
| 1:A:95:ILE:HG22  | 1:A:96:ASP:H     | 1.66                     | 0.59              |
| 1:A:104:PRO:HG3  | 1:A:233:VAL:HG12 | 1.85                     | 0.59              |
| 1:B:293:ALA:HB1  | 1:B:313:TYR:CE2  | 2.38                     | 0.59              |
| 1:B:189:LYS:HG2  | 1:B:211:PHE:CZ   | 2.38                     | 0.59              |
| 1:B:207:LEU:HD22 | 1:B:280:LYS:HB2  | 1.85                     | 0.59              |
| 1:B:133:ILE:HD13 | 1:B:135:LEU:HD12 | 1.85                     | 0.59              |
| 1:B:461:GLY:C    | 1:B:467:TRP:HE1  | 2.06                     | 0.59              |
| 1:A:319:THR:HA   | 1:A:333:VAL:O    | 2.03                     | 0.59              |
| 1:A:462:LEU:O    | 1:A:462:LEU:HD23 | 2.03                     | 0.59              |
| 1:A:49:ARG:CG    | 1:A:50:ASN:ND2   | 2.64                     | 0.59              |
| 1:B:124:VAL:HG21 | 1:B:245:PHE:HD2  | 1.68                     | 0.59              |
| 1:B:68:GLY:HA2   | 1:B:76:ILE:O     | 2.03                     | 0.59              |
| 1:B:134:ASP:OD1  | 1:B:232:THR:HG23 | 2.03                     | 0.58              |
| 1:A:228:GLN:HA   | 1:A:228:GLN:NE2  | 2.17                     | 0.58              |
| 1:B:30:ASP:CG    | 1:B:36:GLN:HB3   | 2.23                     | 0.58              |
| 1:B:391:LYS:HG2  | 1:B:447:ALA:N    | 2.18                     | 0.58              |
| 1:B:491:LEU:HD22 | 1:B:492:TYR:CE1  | 2.38                     | 0.58              |
| 1:A:41:GLY:HA3   | 1:A:251:PHE:CD2  | 2.39                     | 0.58              |
| 1:A:114:LEU:O    | 1:A:114:LEU:HD12 | 2.04                     | 0.58              |
| 1:A:254:LEU:O    | 1:A:259:VAL:HG23 | 2.03                     | 0.58              |
| 1:B:60:ILE:CD1   | 1:B:382:ILE:HD11 | 2.34                     | 0.58              |
| 1:A:275:ARG:HB2  | 1:A:323:LEU:O    | 2.04                     | 0.58              |
| 1:B:275:ARG:HB2  | 1:B:323:LEU:O    | 2.04                     | 0.58              |
| 1:A:263:ALA:N    | 1:A:264:PRO:CD   | 2.67                     | 0.58              |
| 1:A:222:MET:HE1  | 1:A:281:LEU:HD13 | 1.84                     | 0.58              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:207:LEU:HD21 | 1:A:278:TYR:O    | 2.02                     | 0.58              |
| 1:B:83:ARG:NE    | 1:B:383:GLU:OE2  | 2.37                     | 0.58              |
| 1:A:79:GLU:HB2   | 1:A:385:THR:OG1  | 2.04                     | 0.58              |
| 1:A:275:ARG:HH21 | 1:A:348:ASN:CA   | 2.16                     | 0.57              |
| 1:B:111:ASP:O    | 1:B:114:LEU:HB3  | 2.04                     | 0.57              |
| 1:A:48:ASN:O     | 1:A:52:VAL:HG13  | 2.03                     | 0.57              |
| 1:A:30:ASP:CB    | 1:A:36:GLN:HG2   | 2.35                     | 0.57              |
| 1:A:38:ILE:HG23  | 1:A:39:ASP:H     | 1.69                     | 0.57              |
| 1:A:80:ARG:CG    | 1:A:80:ARG:HH11  | 2.17                     | 0.57              |
| 1:A:239:LYS:HD2  | 1:A:239:LYS:H    | 1.69                     | 0.57              |
| 1:A:230:PHE:CE1  | 1:A:351:PHE:HB2  | 2.40                     | 0.57              |
| 1:A:413:VAL:HG11 | 1:A:450:ARG:CZ   | 2.35                     | 0.57              |
| 1:A:484:VAL:CG2  | 1:A:497:ILE:HD12 | 2.34                     | 0.57              |
| 1:A:133:ILE:HD11 | 1:A:231:TYR:CD2  | 2.40                     | 0.57              |
| 1:A:432:TYR:O    | 1:A:433:GLN:HG3  | 2.04                     | 0.57              |
| 1:B:77:VAL:O     | 1:B:386:SER:HA   | 2.05                     | 0.57              |
| 1:B:284:THR:OG1  | 1:B:315:ASN:HB3  | 2.04                     | 0.57              |
| 1:A:98:VAL:HA    | 1:A:358:TYR:CD1  | 2.39                     | 0.57              |
| 1:A:287:SER:O    | 1:A:290:VAL:HG23 | 2.04                     | 0.57              |
| 1:A:409:ALA:CB   | 1:A:427:THR:HG22 | 2.34                     | 0.57              |
| 1:B:486:ILE:C    | 1:B:486:ILE:HD12 | 2.25                     | 0.56              |
| 1:B:104:PRO:CB   | 1:B:235:ALA:HB2  | 2.34                     | 0.56              |
| 1:B:103:TYR:HB2  | 1:B:104:PRO:HD2  | 1.87                     | 0.56              |
| 1:A:471:ILE:HD13 | 1:A:495:SER:HB2  | 1.85                     | 0.56              |
| 1:B:95:ILE:CG1   | 1:B:117:ASN:HB2  | 2.35                     | 0.56              |
| 1:A:158:ILE:CD1  | 1:A:233:VAL:HG21 | 2.35                     | 0.56              |
| 1:B:230:PHE:CE2  | 1:B:274:GLY:HA2  | 2.40                     | 0.56              |
| 1:A:394:ILE:HA   | 1:A:482:ILE:O    | 2.05                     | 0.56              |
| 1:A:365:VAL:HG13 | 1:A:371:SER:O    | 2.05                     | 0.56              |
| 1:B:468:ARG:HH11 | 1:B:468:ARG:HB3  | 1.69                     | 0.56              |
| 1:A:298:ILE:HG22 | 1:A:299:LYS:N    | 2.20                     | 0.56              |
| 1:A:134:ASP:OD2  | 1:A:231:TYR:HB2  | 2.04                     | 0.56              |
| 1:B:465:GLU:CD   | 1:B:465:GLU:H    | 2.08                     | 0.56              |
| 1:A:31:ILE:H     | 1:A:31:ILE:HD12  | 1.70                     | 0.56              |
| 1:B:96:ASP:HB3   | 1:B:99:ASN:OD1   | 2.04                     | 0.56              |
| 1:A:226:TYR:CB   | 1:A:277:ILE:HB   | 2.27                     | 0.56              |
| 1:A:491:LEU:C    | 1:A:493:PRO:HD3  | 2.25                     | 0.56              |
| 1:A:298:ILE:C    | 1:A:300:ASN:H    | 2.09                     | 0.56              |
| 1:B:230:PHE:CD2  | 1:B:274:GLY:HA2  | 2.41                     | 0.56              |
| 1:B:104:PRO:HG3  | 1:B:233:VAL:CG1  | 2.34                     | 0.56              |
| 1:A:401:ALA:HB3  | 1:A:489:THR:HA   | 1.87                     | 0.56              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:60:ILE:HD11  | 1:B:382:ILE:HD11 | 1.88                     | 0.56              |
| 1:B:150:THR:O    | 1:B:154:VAL:HG23 | 2.06                     | 0.55              |
| 1:B:101:ARG:NE   | 1:B:101:ARG:H    | 2.04                     | 0.55              |
| 1:A:275:ARG:HH21 | 1:A:348:ASN:C    | 2.09                     | 0.55              |
| 1:B:293:ALA:HB1  | 1:B:313:TYR:HE2  | 1.71                     | 0.55              |
| 1:B:369:ASP:CG   | 1:B:371:SER:HB3  | 2.27                     | 0.55              |
| 1:A:481:ASN:CB   | 1:A:500:ASN:ND2  | 2.54                     | 0.55              |
| 1:B:207:LEU:HD21 | 1:B:278:TYR:O    | 2.07                     | 0.55              |
| 1:A:189:LYS:O    | 1:A:193:SER:HB2  | 2.06                     | 0.55              |
| 1:A:238:PRO:HB3  | 1:A:244:LEU:HD21 | 1.88                     | 0.55              |
| 1:A:230:PHE:HZ   | 1:A:275:ARG:NH1  | 2.05                     | 0.55              |
| 1:B:209:VAL:HG12 | 1:B:211:PHE:H    | 1.72                     | 0.55              |
| 1:A:186:VAL:O    | 1:A:214:VAL:HG11 | 2.07                     | 0.54              |
| 1:B:138:LEU:HD12 | 1:B:141:GLU:HG3  | 1.89                     | 0.54              |
| 1:B:94:ILE:HD13  | 1:B:359:PRO:HB2  | 1.88                     | 0.54              |
| 1:B:452:ILE:O    | 1:B:476:VAL:N    | 2.37                     | 0.54              |
| 1:A:407:GLU:HA   | 1:A:431:ASN:OD1  | 2.08                     | 0.54              |
| 1:B:226:TYR:CE1  | 1:B:345:ILE:HD13 | 2.42                     | 0.54              |
| 1:A:163:SER:HA   | 1:A:166:ASN:ND2  | 2.22                     | 0.54              |
| 1:B:464:TRP:HA   | 1:B:467:TRP:CE3  | 2.42                     | 0.54              |
| 1:B:456:ALA:H    | 1:B:471:ILE:HG23 | 1.72                     | 0.54              |
| 1:B:189:LYS:HG2  | 1:B:211:PHE:CE1  | 2.42                     | 0.54              |
| 1:A:452:ILE:O    | 1:A:476:VAL:N    | 2.33                     | 0.54              |
| 1:B:259:VAL:O    | 1:B:260:SER:HB3  | 2.08                     | 0.54              |
| 1:B:72:GLY:O     | 1:B:74:LYS:N     | 2.38                     | 0.54              |
| 1:A:214:VAL:HA   | 1:A:219:LYS:O    | 2.09                     | 0.53              |
| 1:A:281:LEU:N    | 1:A:281:LEU:HD12 | 2.23                     | 0.53              |
| 1:A:156:GLY:O    | 1:A:159:ASP:HB2  | 2.08                     | 0.53              |
| 1:B:38:ILE:HG23  | 1:B:39:ASP:N     | 2.22                     | 0.53              |
| 1:B:457:ARG:CD   | 1:B:469:ASP:OD2  | 2.55                     | 0.53              |
| 1:B:304:LYS:HA   | 1:B:309:TYR:HD2  | 1.74                     | 0.53              |
| 1:A:97:SER:C     | 1:A:99:ASN:H     | 2.11                     | 0.53              |
| 1:A:42:ILE:O     | 1:A:45:LEU:HB2   | 2.09                     | 0.53              |
| 1:B:59:LYS:HB2   | 1:B:59:LYS:NZ    | 2.10                     | 0.53              |
| 1:A:186:VAL:HG22 | 1:A:192:ILE:HD13 | 1.89                     | 0.53              |
| 1:B:276:THR:CG2  | 1:B:278:TYR:CE1  | 2.92                     | 0.53              |
| 1:B:107:LEU:HB2  | 1:B:122:LEU:HB2  | 1.90                     | 0.53              |
| 1:A:187:TYR:HD1  | 1:A:381:TYR:CE1  | 2.25                     | 0.53              |
| 1:B:346:LYS:C    | 1:B:348:ASN:H    | 2.12                     | 0.53              |
| 1:B:456:ALA:HB3  | 1:B:471:ILE:CG2  | 2.34                     | 0.53              |
| 1:B:83:ARG:CB    | 1:B:381:TYR:CZ   | 2.91                     | 0.53              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:259:VAL:O    | 1:A:260:SER:HB3  | 2.09                     | 0.53              |
| 1:A:167:GLU:N    | 1:A:167:GLU:OE2  | 2.41                     | 0.53              |
| 1:A:394:ILE:HG23 | 1:A:482:ILE:HG22 | 1.89                     | 0.53              |
| 1:A:259:VAL:HG12 | 1:A:260:SER:N    | 2.23                     | 0.53              |
| 1:B:207:LEU:HD11 | 1:B:278:TYR:HB3  | 1.90                     | 0.53              |
| 1:B:58:ASP:OD2   | 1:B:190:SER:CB   | 2.56                     | 0.53              |
| 1:A:99:ASN:OD1   | 1:A:99:ASN:N     | 2.42                     | 0.53              |
| 1:B:391:LYS:HG3  | 1:B:447:ALA:HB2  | 1.90                     | 0.53              |
| 1:B:491:LEU:HD22 | 1:B:492:TYR:CD1  | 2.44                     | 0.53              |
| 1:A:129:ILE:HG12 | 1:A:130:ASN:H    | 1.74                     | 0.52              |
| 1:A:335:THR:HG22 | 1:A:337:ASP:N    | 2.10                     | 0.52              |
| 1:A:41:GLY:HA3   | 1:A:251:PHE:CZ   | 2.44                     | 0.52              |
| 1:A:457:ARG:HD3  | 1:A:469:ASP:OD2  | 2.08                     | 0.52              |
| 1:B:253:ASP:O    | 1:B:257:LYS:HG3  | 2.08                     | 0.52              |
| 1:A:113:ALA:HA   | 1:A:118:ARG:NH1  | 2.24                     | 0.52              |
| 1:B:96:ASP:HB3   | 1:B:99:ASN:CG    | 2.30                     | 0.52              |
| 1:B:189:LYS:O    | 1:B:193:SER:HB2  | 2.08                     | 0.52              |
| 1:B:491:LEU:O    | 1:B:493:PRO:HD3  | 2.09                     | 0.52              |
| 1:A:188:SER:O    | 1:A:192:ILE:HG22 | 2.09                     | 0.52              |
| 1:A:346:LYS:C    | 1:A:348:ASN:H    | 2.13                     | 0.52              |
| 1:A:107:LEU:HB2  | 1:A:122:LEU:HB2  | 1.91                     | 0.52              |
| 1:B:464:TRP:C    | 1:B:466:TRP:H    | 2.13                     | 0.52              |
| 1:B:366:PHE:CZ   | 1:B:373:ALA:HA   | 2.44                     | 0.52              |
| 1:B:93:SER:O     | 1:B:117:ASN:ND2  | 2.40                     | 0.52              |
| 1:B:48:ASN:ND2   | 1:B:51:GLU:HB2   | 2.24                     | 0.52              |
| 1:A:30:ASP:HA    | 1:A:36:GLN:HG2   | 1.90                     | 0.52              |
| 1:A:480:ASN:HB2  | 1:A:500:ASN:O    | 2.10                     | 0.52              |
| 1:B:433:GLN:O    | 1:B:435:LYS:NZ   | 2.41                     | 0.52              |
| 1:B:224:LEU:HD11 | 1:B:281:LEU:HD11 | 1.92                     | 0.52              |
| 1:B:427:THR:HB   | 1:B:431:ASN:ND2  | 2.25                     | 0.52              |
| 1:A:325:GLY:HA3  | 1:A:358:TYR:CD1  | 2.45                     | 0.52              |
| 1:A:103:TYR:CE1  | 1:A:154:VAL:HG21 | 2.45                     | 0.52              |
| 1:B:230:PHE:HB3  | 1:B:351:PHE:CZ   | 2.43                     | 0.52              |
| 1:B:150:THR:HB   | 1:B:153:LYS:HB2  | 1.92                     | 0.52              |
| 1:A:96:ASP:CB    | 1:A:99:ASN:HB2   | 2.22                     | 0.52              |
| 1:B:441:THR:CG2  | 1:B:442:VAL:N    | 2.72                     | 0.52              |
| 1:B:224:LEU:CD1  | 1:B:281:LEU:HD11 | 2.39                     | 0.52              |
| 1:B:269:SER:OG   | 1:B:365:VAL:HG23 | 2.09                     | 0.52              |
| 1:B:434:ASP:O    | 1:B:435:LYS:HD3  | 2.10                     | 0.52              |
| 1:A:77:VAL:O     | 1:A:386:SER:HA   | 2.09                     | 0.52              |
| 1:A:275:ARG:HD2  | 1:A:322:VAL:CG1  | 2.40                     | 0.52              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:277:ILE:HD12 | 1:A:345:ILE:HA   | 1.89                     | 0.52              |
| 1:B:365:VAL:HG13 | 1:B:371:SER:C    | 2.29                     | 0.52              |
| 1:B:144:ILE:HG13 | 1:B:145:LYS:H    | 1.75                     | 0.51              |
| 1:B:130:ASN:HB2  | 1:B:236:ASP:OD1  | 2.10                     | 0.51              |
| 1:A:85:LEU:CD2   | 1:A:194:SER:HB3  | 2.40                     | 0.51              |
| 1:B:112:LYS:O    | 1:B:113:ALA:C    | 2.47                     | 0.51              |
| 1:A:450:ARG:HD2  | 1:A:450:ARG:N    | 2.25                     | 0.51              |
| 1:B:78:VAL:HG11  | 1:B:80:ARG:HE    | 1.74                     | 0.51              |
| 1:B:403:VAL:CG1  | 1:B:434:ASP:OD2  | 2.55                     | 0.51              |
| 1:A:298:ILE:O    | 1:A:300:ASN:N    | 2.43                     | 0.51              |
| 1:A:60:ILE:HD11  | 1:A:382:ILE:HD11 | 1.92                     | 0.51              |
| 1:A:103:TYR:HB2  | 1:A:104:PRO:HD2  | 1.92                     | 0.51              |
| 1:A:133:ILE:HD13 | 1:A:135:LEU:HD12 | 1.93                     | 0.51              |
| 1:B:219:LYS:HA   | 1:B:283:THR:O    | 2.11                     | 0.51              |
| 1:A:57:GLY:HA3   | 1:A:379:THR:HB   | 1.93                     | 0.51              |
| 1:B:318:PHE:O    | 1:B:341:ILE:HD11 | 2.11                     | 0.51              |
| 1:A:340:GLU:O    | 1:A:344:VAL:HG23 | 2.10                     | 0.51              |
| 1:B:254:LEU:O    | 1:B:259:VAL:HG23 | 2.10                     | 0.51              |
| 1:A:228:GLN:CA   | 1:A:228:GLN:HE21 | 2.18                     | 0.51              |
| 1:B:481:ASN:HB2  | 1:B:500:ASN:HD22 | 1.74                     | 0.51              |
| 1:A:343:LYS:HA   | 1:A:346:LYS:HE3  | 1.93                     | 0.51              |
| 1:A:394:ILE:O    | 1:A:442:VAL:HA   | 2.11                     | 0.51              |
| 1:B:101:ARG:HB2  | 1:B:151:TYR:CE1  | 2.45                     | 0.51              |
| 1:B:131:ILE:HG23 | 1:B:233:VAL:HG13 | 1.93                     | 0.51              |
| 1:A:497:ILE:O    | 1:A:497:ILE:HG23 | 2.10                     | 0.51              |
| 1:B:112:LYS:HA   | 1:B:115:VAL:CG2  | 2.39                     | 0.51              |
| 1:B:95:ILE:O     | 1:B:97:SER:N     | 2.44                     | 0.51              |
| 1:B:214:VAL:HA   | 1:B:219:LYS:O    | 2.11                     | 0.51              |
| 1:A:409:ALA:HB1  | 1:A:425:HIS:HE1  | 1.76                     | 0.51              |
| 1:A:83:ARG:NE    | 1:A:383:GLU:OE2  | 2.44                     | 0.51              |
| 1:A:462:LEU:HB3  | 1:A:466:TRP:HE3  | 1.76                     | 0.51              |
| 1:B:128:PRO:HG3  | 1:B:147:ASP:CA   | 2.36                     | 0.51              |
| 1:A:366:PHE:O    | 1:A:370:ASN:HA   | 2.11                     | 0.51              |
| 1:B:222:MET:CE   | 1:B:224:LEU:HD21 | 2.41                     | 0.51              |
| 1:A:318:PHE:O    | 1:A:341:ILE:HD11 | 2.11                     | 0.50              |
| 1:B:126:ARG:HB3  | 1:B:149:PRO:HD2  | 1.92                     | 0.50              |
| 1:A:298:ILE:C    | 1:A:300:ASN:N    | 2.64                     | 0.50              |
| 1:B:256:GLN:HA   | 1:B:256:GLN:OE1  | 2.11                     | 0.50              |
| 1:A:324:GLY:O    | 1:A:358:TYR:HB2  | 2.11                     | 0.50              |
| 1:A:104:PRO:HB2  | 1:A:235:ALA:HB2  | 1.93                     | 0.50              |
| 1:B:42:ILE:O     | 1:B:45:LEU:HB2   | 2.11                     | 0.50              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:446:GLU:O    | 1:B:448:ASN:N    | 2.43                     | 0.50              |
| 1:B:114:LEU:HA   | 1:B:119:PRO:HB3  | 1.93                     | 0.50              |
| 1:A:458:GLU:OE1  | 1:A:460:THR:HB   | 2.12                     | 0.50              |
| 1:B:45:LEU:HD11  | 1:B:259:VAL:HG12 | 1.92                     | 0.50              |
| 1:A:134:ASP:OD1  | 1:A:178:ARG:NH2  | 2.45                     | 0.50              |
| 1:B:226:TYR:CB   | 1:B:277:ILE:HB   | 2.33                     | 0.50              |
| 1:B:107:LEU:N    | 1:B:107:LEU:HD12 | 2.27                     | 0.50              |
| 1:B:232:THR:HB   | 1:B:271:VAL:O    | 2.12                     | 0.50              |
| 1:A:130:ASN:HD22 | 1:A:130:ASN:N    | 2.08                     | 0.50              |
| 1:B:98:VAL:HG12  | 1:B:325:GLY:HA2  | 1.93                     | 0.50              |
| 1:B:409:ALA:HB1  | 1:B:425:HIS:CE1  | 2.46                     | 0.50              |
| 1:A:319:THR:OG1  | 1:A:334:VAL:HG13 | 2.12                     | 0.50              |
| 1:B:30:ASP:CB    | 1:B:36:GLN:HG2   | 2.41                     | 0.50              |
| 1:A:304:LYS:HA   | 1:A:309:TYR:HD2  | 1.76                     | 0.50              |
| 1:A:132:ASN:OD1  | 1:A:234:SER:O    | 2.30                     | 0.50              |
| 1:A:94:ILE:CD1   | 1:A:359:PRO:HB2  | 2.42                     | 0.50              |
| 1:A:133:ILE:HG23 | 1:A:135:LEU:H    | 1.77                     | 0.49              |
| 1:B:151:TYR:O    | 1:B:152:GLY:C    | 2.47                     | 0.49              |
| 1:B:30:ASP:HA    | 1:B:36:GLN:CG    | 2.41                     | 0.49              |
| 1:B:185:MET:SD   | 1:B:291:GLN:HG3  | 2.52                     | 0.49              |
| 1:A:186:VAL:HG13 | 1:A:192:ILE:HB   | 1.93                     | 0.49              |
| 1:B:417:LYS:HZ2  | 1:B:417:LYS:HB2  | 1.74                     | 0.49              |
| 1:A:112:LYS:HA   | 1:A:115:VAL:HG23 | 1.94                     | 0.49              |
| 1:B:277:ILE:HD11 | 1:B:348:ASN:HB2  | 1.94                     | 0.49              |
| 1:B:63:PHE:HD1   | 1:B:64:VAL:N     | 2.10                     | 0.49              |
| 1:B:441:THR:HG22 | 1:B:442:VAL:N    | 2.26                     | 0.49              |
| 1:B:166:ASN:O    | 1:B:169:TYR:C    | 2.51                     | 0.49              |
| 1:A:131:ILE:N    | 1:A:131:ILE:HD12 | 2.27                     | 0.49              |
| 1:A:464:TRP:O    | 1:A:466:TRP:N    | 2.46                     | 0.49              |
| 1:B:343:LYS:HG2  | 1:B:347:ASP:OD2  | 2.12                     | 0.49              |
| 1:B:138:LEU:HG   | 1:B:142:ASN:HB3  | 1.93                     | 0.49              |
| 1:B:224:LEU:HD12 | 1:B:279:VAL:HB   | 1.95                     | 0.49              |
| 1:A:182:SER:HB3  | 1:A:196:LEU:HD23 | 1.94                     | 0.49              |
| 1:A:63:PHE:CD1   | 1:A:63:PHE:C     | 2.85                     | 0.49              |
| 1:A:96:ASP:CB    | 1:A:100:ASP:HB2  | 2.16                     | 0.49              |
| 1:A:464:TRP:C    | 1:A:466:TRP:H    | 2.16                     | 0.49              |
| 1:B:335:THR:HG21 | 1:B:340:GLU:HG3  | 1.94                     | 0.49              |
| 1:B:232:THR:O    | 1:B:233:VAL:HG23 | 2.12                     | 0.49              |
| 1:B:228:GLN:HA   | 1:B:228:GLN:NE2  | 2.28                     | 0.49              |
| 1:B:407:GLU:HG3  | 1:B:432:TYR:CE2  | 2.48                     | 0.49              |
| 1:A:127:LYS:HD2  | 1:A:246:ASP:HA   | 1.94                     | 0.49              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:129:ILE:CG1  | 1:B:130:ASN:N    | 2.76                     | 0.49              |
| 1:A:222:MET:CE   | 1:A:281:LEU:HD13 | 2.43                     | 0.49              |
| 1:A:61:GLU:HG3   | 1:A:61:GLU:O     | 2.13                     | 0.49              |
| 1:B:320:ALA:HB2  | 1:B:341:ILE:HD12 | 1.94                     | 0.49              |
| 1:B:150:THR:O    | 1:B:154:VAL:N    | 2.39                     | 0.49              |
| 1:B:92:ILE:O     | 1:B:361:SER:HA   | 2.13                     | 0.49              |
| 1:A:457:ARG:NH2  | 1:A:464:TRP:CE2  | 2.81                     | 0.48              |
| 1:A:441:THR:HG22 | 1:A:442:VAL:N    | 2.27                     | 0.48              |
| 1:B:265:PRO:CG   | 1:B:367:LEU:HD12 | 2.43                     | 0.48              |
| 1:A:98:VAL:HG12  | 1:A:358:TYR:CE1  | 2.47                     | 0.48              |
| 1:A:219:LYS:HA   | 1:A:283:THR:O    | 2.12                     | 0.48              |
| 1:A:454:ILE:HD11 | 1:A:482:ILE:HG21 | 1.94                     | 0.48              |
| 1:B:265:PRO:HG2  | 1:B:367:LEU:HD12 | 1.95                     | 0.48              |
| 1:B:457:ARG:HG2  | 1:B:467:TRP:HB2  | 1.94                     | 0.48              |
| 1:B:112:LYS:O    | 1:B:115:VAL:HG23 | 2.13                     | 0.48              |
| 1:A:480:ASN:CB   | 1:A:500:ASN:O    | 2.61                     | 0.48              |
| 1:B:158:ILE:O    | 1:B:162:VAL:HG23 | 2.13                     | 0.48              |
| 1:A:433:GLN:HB3  | 1:A:435:LYS:NZ   | 2.28                     | 0.48              |
| 1:A:168:LYS:HD3  | 1:A:169:TYR:HE1  | 1.77                     | 0.48              |
| 1:A:491:LEU:O    | 1:A:493:PRO:HD3  | 2.13                     | 0.48              |
| 1:A:275:ARG:HD2  | 1:A:322:VAL:HG13 | 1.95                     | 0.48              |
| 1:A:318:PHE:CD1  | 1:A:335:THR:O    | 2.64                     | 0.48              |
| 1:B:356:PRO:HB2  | 1:B:358:TYR:CE2  | 2.49                     | 0.48              |
| 1:A:74:LYS:HA    | 1:A:389:TYR:O    | 2.13                     | 0.48              |
| 1:A:230:PHE:CD1  | 1:A:351:PHE:HB2  | 2.48                     | 0.48              |
| 1:B:275:ARG:HA   | 1:B:324:GLY:HA3  | 1.94                     | 0.48              |
| 1:B:259:VAL:HG12 | 1:B:260:SER:H    | 1.75                     | 0.48              |
| 1:B:41:GLY:HA3   | 1:B:251:PHE:CE1  | 2.49                     | 0.48              |
| 1:B:217:ASN:HB2  | 1:B:384:THR:HG21 | 1.94                     | 0.48              |
| 1:A:135:LEU:CD2  | 1:A:136:PRO:HD2  | 2.43                     | 0.48              |
| 1:B:398:HIS:NE2  | 1:B:435:LYS:O    | 2.46                     | 0.48              |
| 1:B:281:LEU:N    | 1:B:281:LEU:HD12 | 2.28                     | 0.48              |
| 1:B:427:THR:HB   | 1:B:431:ASN:HD21 | 1.79                     | 0.48              |
| 1:A:261:ASN:HB2  | 1:A:262:GLU:OE2  | 2.14                     | 0.48              |
| 1:A:101:ARG:N    | 1:A:101:ARG:CD   | 2.77                     | 0.48              |
| 1:A:453:ARG:HG2  | 1:A:453:ARG:HH11 | 1.78                     | 0.48              |
| 1:B:156:GLY:O    | 1:B:159:ASP:HB2  | 2.14                     | 0.48              |
| 1:A:196:LEU:HD22 | 1:A:225:ALA:CB   | 2.43                     | 0.47              |
| 1:B:230:PHE:CZ   | 1:B:275:ARG:NH1  | 2.77                     | 0.47              |
| 1:A:114:LEU:HD12 | 1:A:114:LEU:C    | 2.34                     | 0.47              |
| 1:A:74:LYS:NZ    | 1:A:388:GLU:HB3  | 2.27                     | 0.47              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:83:ARG:O     | 1:B:380:ASP:HA   | 2.13                     | 0.47              |
| 1:A:456:ALA:HB3  | 1:A:471:ILE:HG22 | 1.96                     | 0.47              |
| 1:A:163:SER:HA   | 1:A:166:ASN:HD22 | 1.77                     | 0.47              |
| 1:A:328:GLN:O    | 1:A:331:ASN:HB3  | 2.14                     | 0.47              |
| 1:A:70:LYS:H     | 1:A:70:LYS:CD    | 2.01                     | 0.47              |
| 1:B:226:TYR:CZ   | 1:B:345:ILE:HD13 | 2.48                     | 0.47              |
| 1:A:63:PHE:HD1   | 1:A:63:PHE:C     | 2.18                     | 0.47              |
| 1:A:453:ARG:HD2  | 1:A:474:TYR:HE2  | 1.78                     | 0.47              |
| 1:B:307:GLN:O    | 1:B:311:ASP:OD1  | 2.32                     | 0.47              |
| 1:A:88:SER:HA    | 1:A:375:VAL:O    | 2.14                     | 0.47              |
| 1:A:483:ASN:OD1  | 1:A:498:THR:O    | 2.32                     | 0.47              |
| 1:A:33:ASP:C     | 1:A:34:LYS:HG3   | 2.35                     | 0.47              |
| 1:A:60:ILE:CD1   | 1:A:382:ILE:HD11 | 2.43                     | 0.47              |
| 1:A:464:TRP:HA   | 1:A:467:TRP:CE3  | 2.50                     | 0.47              |
| 1:B:287:SER:O    | 1:B:289:ASP:N    | 2.47                     | 0.47              |
| 1:B:259:VAL:O    | 1:B:260:SER:CB   | 2.62                     | 0.47              |
| 1:A:290:VAL:O    | 1:A:291:GLN:C    | 2.51                     | 0.47              |
| 1:A:31:ILE:HD12  | 1:A:31:ILE:N     | 2.30                     | 0.47              |
| 1:A:286:SER:HB2  | 1:A:388:GLU:HG2  | 1.96                     | 0.47              |
| 1:B:332:LYS:HG2  | 1:B:333:VAL:N    | 2.30                     | 0.47              |
| 1:B:72:GLY:C     | 1:B:74:LYS:H     | 2.16                     | 0.47              |
| 1:A:212:ASN:HA   | 1:A:215:ALA:HB3  | 1.96                     | 0.47              |
| 1:B:56:ASN:HD21  | 1:B:59:LYS:NZ    | 2.13                     | 0.47              |
| 1:B:297:LEU:HD13 | 1:B:313:TYR:CZ   | 2.50                     | 0.47              |
| 1:A:96:ASP:HB2   | 1:A:100:ASP:N    | 2.30                     | 0.47              |
| 1:B:325:GLY:HA3  | 1:B:358:TYR:CD1  | 2.50                     | 0.47              |
| 1:B:133:ILE:HG13 | 1:B:232:THR:O    | 2.14                     | 0.46              |
| 1:B:266:LEU:HD23 | 1:B:366:PHE:HA   | 1.96                     | 0.46              |
| 1:A:253:ASP:O    | 1:A:257:LYS:HG3  | 2.14                     | 0.46              |
| 1:B:30:ASP:OD2   | 1:B:36:GLN:HB3   | 2.15                     | 0.46              |
| 1:A:31:ILE:HG13  | 1:A:252:ASN:CG   | 2.36                     | 0.46              |
| 1:B:297:LEU:HD12 | 1:B:304:LYS:HD2  | 1.97                     | 0.46              |
| 1:B:328:GLN:O    | 1:B:331:ASN:HB3  | 2.15                     | 0.46              |
| 1:A:124:VAL:HG11 | 1:A:254:LEU:CD2  | 2.45                     | 0.46              |
| 1:B:480:ASN:CB   | 1:B:500:ASN:O    | 2.63                     | 0.46              |
| 1:A:168:LYS:HG2  | 1:A:169:TYR:CE1  | 2.50                     | 0.46              |
| 1:A:174:THR:HB   | 1:A:350:THR:HG23 | 1.97                     | 0.46              |
| 1:A:343:LYS:HA   | 1:A:346:LYS:CE   | 2.45                     | 0.46              |
| 1:A:457:ARG:HB3  | 1:A:464:TRP:CZ3  | 2.50                     | 0.46              |
| 1:A:416:ASP:OD2  | 1:A:420:ASN:N    | 2.37                     | 0.46              |
| 1:B:78:VAL:HG12  | 1:B:79:GLU:N     | 2.30                     | 0.46              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:168:LYS:HD3  | 1:B:169:TYR:HE1  | 1.79                     | 0.46              |
| 1:A:54:ALA:HA    | 1:A:376:HIS:HB2  | 1.96                     | 0.46              |
| 1:B:464:TRP:O    | 1:B:466:TRP:N    | 2.48                     | 0.46              |
| 1:B:83:ARG:HB2   | 1:B:381:TYR:CZ   | 2.50                     | 0.46              |
| 1:A:454:ILE:O    | 1:A:455:LYS:HB2  | 2.16                     | 0.46              |
| 1:A:80:ARG:NH1   | 1:A:80:ARG:CG    | 2.78                     | 0.46              |
| 1:A:123:MET:N    | 1:A:257:LYS:HE2  | 2.25                     | 0.46              |
| 1:B:89:PRO:HG2   | 1:B:375:VAL:HB   | 1.97                     | 0.46              |
| 1:A:383:GLU:HG2  | 1:A:383:GLU:O    | 2.15                     | 0.46              |
| 1:A:174:THR:HB   | 1:A:350:THR:CG2  | 2.45                     | 0.46              |
| 1:A:405:GLN:HG3  | 1:A:459:CYS:SG   | 2.56                     | 0.46              |
| 1:A:281:LEU:H    | 1:A:281:LEU:HD12 | 1.80                     | 0.46              |
| 1:B:88:SER:HA    | 1:B:375:VAL:O    | 2.15                     | 0.46              |
| 1:B:106:ALA:HB1  | 1:B:121:ILE:HD11 | 1.97                     | 0.46              |
| 1:B:398:HIS:O    | 1:B:438:HIS:N    | 2.48                     | 0.46              |
| 1:B:45:LEU:HD11  | 1:B:259:VAL:CG1  | 2.46                     | 0.46              |
| 1:A:491:LEU:HD23 | 1:A:491:LEU:O    | 2.16                     | 0.46              |
| 1:B:453:ARG:O    | 1:B:453:ARG:HG3  | 2.15                     | 0.46              |
| 1:A:246:ASP:O    | 1:A:249:VAL:N    | 2.36                     | 0.46              |
| 1:A:165:TRP:CZ3  | 1:A:169:TYR:HB2  | 2.51                     | 0.46              |
| 1:A:173:HIS:CE1  | 1:A:354:LYS:NZ   | 2.83                     | 0.46              |
| 1:A:78:VAL:HG11  | 1:A:80:ARG:NH2   | 2.31                     | 0.45              |
| 1:B:32:THR:C     | 1:B:34:LYS:H     | 2.19                     | 0.45              |
| 1:B:172:THR:O    | 1:B:173:HIS:HD2  | 1.99                     | 0.45              |
| 1:A:204:GLU:O    | 1:A:204:GLU:HG2  | 2.15                     | 0.45              |
| 1:A:318:PHE:O    | 1:A:334:VAL:HA   | 2.16                     | 0.45              |
| 1:B:130:ASN:ND2  | 1:B:145:LYS:HG3  | 2.31                     | 0.45              |
| 1:A:436:THR:O    | 1:A:437:ALA:C    | 2.55                     | 0.45              |
| 1:B:417:LYS:HB2  | 1:B:417:LYS:HZ3  | 1.79                     | 0.45              |
| 1:B:418:GLU:HB2  | 1:B:420:ASN:ND2  | 2.31                     | 0.45              |
| 1:A:150:THR:HG22 | 1:A:151:TYR:N    | 2.31                     | 0.45              |
| 1:B:129:ILE:CG1  | 1:B:130:ASN:H    | 2.22                     | 0.45              |
| 1:A:224:LEU:HD12 | 1:A:279:VAL:HB   | 1.98                     | 0.45              |
| 1:A:101:ARG:H    | 1:A:101:ARG:CD   | 2.29                     | 0.45              |
| 1:A:356:PRO:HB2  | 1:A:358:TYR:HE2  | 1.82                     | 0.45              |
| 1:A:96:ASP:HB3   | 1:A:100:ASP:N    | 2.16                     | 0.45              |
| 1:A:458:GLU:HB2  | 1:A:470:VAL:CG2  | 2.46                     | 0.45              |
| 1:B:476:VAL:CG1  | 1:B:477:PRO:HD2  | 2.47                     | 0.45              |
| 1:A:321:VAL:HG12 | 1:A:332:LYS:HG3  | 1.97                     | 0.45              |
| 1:A:38:ILE:HA    | 1:A:251:PHE:CB   | 2.30                     | 0.45              |
| 1:B:125:LYS:HD3  | 1:B:246:ASP:CB   | 2.47                     | 0.45              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:228:GLN:HA   | 1:B:228:GLN:HE21 | 1.81                     | 0.45              |
| 1:A:453:ARG:HG2  | 1:A:453:ARG:NH1  | 2.32                     | 0.45              |
| 1:A:441:THR:CG2  | 1:A:442:VAL:N    | 2.79                     | 0.45              |
| 1:B:73:ASN:O     | 1:B:74:LYS:HG3   | 2.16                     | 0.45              |
| 1:B:210:ASP:O    | 1:B:211:PHE:C    | 2.55                     | 0.45              |
| 1:B:58:ASP:OD2   | 1:B:190:SER:HB3  | 2.16                     | 0.45              |
| 1:B:49:ARG:HG3   | 1:B:50:ASN:CG    | 2.36                     | 0.45              |
| 1:B:60:ILE:CG1   | 1:B:61:GLU:N     | 2.80                     | 0.45              |
| 1:A:30:ASP:HB3   | 1:A:36:GLN:HG2   | 1.98                     | 0.45              |
| 1:A:105:GLY:O    | 1:A:106:ALA:C    | 2.55                     | 0.45              |
| 1:B:102:THR:OG1  | 1:B:108:GLN:NE2  | 2.49                     | 0.45              |
| 1:B:96:ASP:CB    | 1:B:100:ASP:N    | 2.65                     | 0.45              |
| 1:B:433:GLN:HB3  | 1:B:435:LYS:HZ1  | 1.82                     | 0.45              |
| 1:A:58:ASP:OD2   | 1:A:190:SER:CB   | 2.64                     | 0.45              |
| 1:B:40:SER:O     | 1:B:44:SER:CB    | 2.65                     | 0.45              |
| 1:A:93:SER:O     | 1:A:117:ASN:ND2  | 2.50                     | 0.45              |
| 1:A:121:ILE:CD1  | 1:A:122:LEU:H    | 2.26                     | 0.45              |
| 1:B:49:ARG:HG3   | 1:B:50:ASN:ND2   | 2.32                     | 0.45              |
| 1:B:389:TYR:O    | 1:B:447:ALA:HB1  | 2.16                     | 0.45              |
| 1:B:212:ASN:HA   | 1:B:215:ALA:CB   | 2.45                     | 0.45              |
| 1:A:31:ILE:HG12  | 1:A:255:LYS:NZ   | 2.32                     | 0.45              |
| 1:A:269:SER:HB3  | 1:A:365:VAL:CG2  | 2.46                     | 0.45              |
| 1:A:283:THR:OG1  | 1:A:284:THR:N    | 2.48                     | 0.45              |
| 1:B:132:ASN:ND2  | 1:B:143:SER:OG   | 2.50                     | 0.45              |
| 1:A:73:ASN:C     | 1:A:74:LYS:HG3   | 2.36                     | 0.45              |
| 1:B:83:ARG:HB3   | 1:B:381:TYR:CZ   | 2.52                     | 0.45              |
| 1:B:446:GLU:C    | 1:B:448:ASN:H    | 2.21                     | 0.45              |
| 1:B:182:SER:HB3  | 1:B:196:LEU:CD2  | 2.48                     | 0.44              |
| 1:B:292:ALA:O    | 1:B:293:ALA:C    | 2.55                     | 0.44              |
| 1:B:187:TYR:HD1  | 1:B:381:TYR:CE1  | 2.36                     | 0.44              |
| 1:B:432:TYR:CD2  | 1:B:432:TYR:N    | 2.84                     | 0.44              |
| 1:B:40:SER:O     | 1:B:44:SER:HB3   | 2.17                     | 0.44              |
| 1:A:192:ILE:HD11 | 1:A:196:LEU:HD12 | 2.00                     | 0.44              |
| 1:B:214:VAL:HG22 | 1:B:221:VAL:HG23 | 1.99                     | 0.44              |
| 1:B:491:LEU:C    | 1:B:493:PRO:HD3  | 2.38                     | 0.44              |
| 1:B:468:ARG:CZ   | 1:B:493:PRO:HG2  | 2.47                     | 0.44              |
| 1:B:277:ILE:HG21 | 1:B:345:ILE:HG12 | 1.99                     | 0.44              |
| 1:B:222:MET:CE   | 1:B:298:ILE:HD11 | 2.48                     | 0.44              |
| 1:B:95:ILE:HG12  | 1:B:117:ASN:HB3  | 1.95                     | 0.44              |
| 1:B:163:SER:OG   | 1:B:164:LYS:N    | 2.50                     | 0.44              |
| 1:B:283:THR:HB   | 1:B:316:SER:OG   | 2.18                     | 0.44              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:42:ILE:HG22  | 1:B:368:LYS:HB2  | 1.99                     | 0.44              |
| 1:B:224:LEU:CB   | 1:B:279:VAL:HB   | 2.42                     | 0.44              |
| 1:A:189:LYS:O    | 1:A:193:SER:CB   | 2.66                     | 0.44              |
| 1:A:131:ILE:N    | 1:A:131:ILE:CD1  | 2.80                     | 0.44              |
| 1:A:210:ASP:OD2  | 1:A:213:ALA:CB   | 2.60                     | 0.44              |
| 1:B:113:ALA:HB1  | 1:B:118:ARG:O    | 2.17                     | 0.44              |
| 1:B:173:HIS:CE1  | 1:B:354:LYS:HZ1  | 2.36                     | 0.44              |
| 1:B:299:LYS:HB2  | 1:B:301:THR:HG22 | 2.00                     | 0.44              |
| 1:A:219:LYS:HD3  | 1:A:282:GLU:OE2  | 2.17                     | 0.44              |
| 1:B:150:THR:O    | 1:B:153:LYS:HB3  | 2.17                     | 0.44              |
| 1:B:319:THR:OG1  | 1:B:334:VAL:HG22 | 2.18                     | 0.44              |
| 1:B:189:LYS:NZ   | 1:B:204:GLU:OE1  | 2.40                     | 0.44              |
| 1:B:155:SER:O    | 1:B:159:ASP:OD2  | 2.36                     | 0.44              |
| 1:A:341:ILE:O    | 1:A:344:VAL:HB   | 2.17                     | 0.44              |
| 1:B:126:ARG:CB   | 1:B:149:PRO:HD2  | 2.46                     | 0.44              |
| 1:B:239:LYS:HE3  | 1:B:239:LYS:HB3  | 1.83                     | 0.44              |
| 1:B:118:ARG:HH11 | 1:B:118:ARG:HG3  | 1.81                     | 0.44              |
| 1:A:427:THR:HB   | 1:A:431:ASN:HD22 | 1.81                     | 0.44              |
| 1:A:132:ASN:HA   | 1:A:142:ASN:O    | 2.17                     | 0.44              |
| 1:B:96:ASP:HB2   | 1:B:100:ASP:CA   | 2.48                     | 0.44              |
| 1:B:138:LEU:CG   | 1:B:142:ASN:HB3  | 2.47                     | 0.44              |
| 1:B:49:ARG:NH2   | 1:B:369:ASP:OD2  | 2.51                     | 0.44              |
| 1:B:113:ALA:HA   | 1:B:118:ARG:NH1  | 2.33                     | 0.44              |
| 1:B:173:HIS:CD2  | 1:B:354:LYS:HZ1  | 2.35                     | 0.44              |
| 1:A:366:PHE:HB2  | 1:A:369:ASP:OD1  | 2.18                     | 0.44              |
| 1:B:78:VAL:HA    | 1:B:385:THR:O    | 2.17                     | 0.44              |
| 1:B:276:THR:N    | 1:B:323:LEU:O    | 2.46                     | 0.43              |
| 1:B:122:LEU:HA   | 1:B:122:LEU:HD23 | 1.82                     | 0.43              |
| 1:A:49:ARG:HB2   | 1:A:366:PHE:CZ   | 2.53                     | 0.43              |
| 1:B:405:GLN:HG2  | 1:B:433:GLN:C    | 2.38                     | 0.43              |
| 1:B:148:ASP:HB3  | 1:B:153:LYS:HE2  | 1.98                     | 0.43              |
| 1:A:285:SER:OG   | 1:A:286:SER:N    | 2.51                     | 0.43              |
| 1:A:198:VAL:HG11 | 1:A:278:TYR:OH   | 2.18                     | 0.43              |
| 1:A:163:SER:CA   | 1:A:166:ASN:HD22 | 2.30                     | 0.43              |
| 1:A:487:TRP:O    | 1:A:494:GLY:N    | 2.51                     | 0.43              |
| 1:A:175:LEU:HD22 | 1:A:176:PRO:HD2  | 2.00                     | 0.43              |
| 1:A:129:ILE:HG12 | 1:A:130:ASN:N    | 2.32                     | 0.43              |
| 1:A:144:ILE:CG1  | 1:A:145:LYS:H    | 2.27                     | 0.43              |
| 1:A:277:ILE:HD11 | 1:A:348:ASN:HB2  | 2.00                     | 0.43              |
| 1:A:301:THR:O    | 1:A:303:ILE:N    | 2.51                     | 0.43              |
| 1:B:433:GLN:CB   | 1:B:435:LYS:HZ1  | 2.31                     | 0.43              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:266:LEU:HD13 | 1:B:364:SER:OG   | 2.17                     | 0.43              |
| 1:B:124:VAL:HG12 | 1:B:257:LYS:HD2  | 2.00                     | 0.43              |
| 1:B:327:ALA:O    | 1:B:328:GLN:C    | 2.56                     | 0.43              |
| 1:B:436:THR:O    | 1:B:437:ALA:C    | 2.56                     | 0.43              |
| 1:B:150:THR:O    | 1:B:151:TYR:C    | 2.57                     | 0.43              |
| 1:B:453:ARG:NH1  | 1:B:453:ARG:HG2  | 2.33                     | 0.43              |
| 1:A:128:PRO:HA   | 1:A:146:VAL:O    | 2.18                     | 0.43              |
| 1:A:103:TYR:CE2  | 1:A:151:TYR:N    | 2.87                     | 0.43              |
| 1:B:398:HIS:CA   | 1:B:486:ILE:HD11 | 2.40                     | 0.43              |
| 1:B:39:ASP:OD1   | 1:B:241:PRO:HD2  | 2.18                     | 0.43              |
| 1:A:89:PRO:HG2   | 1:A:375:VAL:HB   | 2.01                     | 0.43              |
| 1:A:64:VAL:HA    | 1:A:65:PRO:HD2   | 1.65                     | 0.43              |
| 1:B:114:LEU:HD11 | 1:B:362:TYR:OH   | 2.19                     | 0.43              |
| 1:A:134:ASP:OD1  | 1:A:178:ARG:NH1  | 2.50                     | 0.43              |
| 1:B:132:ASN:HA   | 1:B:142:ASN:O    | 2.17                     | 0.43              |
| 1:A:293:ALA:HB1  | 1:A:313:TYR:CE2  | 2.54                     | 0.43              |
| 1:A:134:ASP:N    | 1:A:134:ASP:OD2  | 2.49                     | 0.43              |
| 1:A:83:ARG:HG3   | 1:A:383:GLU:HB2  | 2.01                     | 0.43              |
| 1:B:296:ALA:HA   | 1:B:301:THR:HG23 | 2.00                     | 0.43              |
| 1:B:346:LYS:O    | 1:B:348:ASN:N    | 2.52                     | 0.43              |
| 1:B:101:ARG:HE   | 1:B:101:ARG:H    | 1.67                     | 0.43              |
| 1:A:252:ASN:ND2  | 1:A:255:LYS:HD2  | 2.34                     | 0.43              |
| 1:A:151:TYR:O    | 1:A:152:GLY:C    | 2.56                     | 0.43              |
| 1:A:434:ASP:O    | 1:A:435:LYS:HD3  | 2.18                     | 0.43              |
| 1:A:358:TYR:HB3  | 1:A:359:PRO:HD2  | 1.99                     | 0.43              |
| 1:B:42:ILE:O     | 1:B:45:LEU:N     | 2.52                     | 0.43              |
| 1:A:288:LYS:HE3  | 1:A:387:THR:HG23 | 2.01                     | 0.43              |
| 1:B:483:ASN:OD1  | 1:B:498:THR:O    | 2.37                     | 0.43              |
| 1:A:104:PRO:HD3  | 1:A:271:VAL:CG2  | 2.49                     | 0.42              |
| 1:A:338:PHE:O    | 1:A:342:ARG:HG3  | 2.19                     | 0.42              |
| 1:B:283:THR:OG1  | 1:B:284:THR:N    | 2.52                     | 0.42              |
| 1:B:458:GLU:OE2  | 1:B:460:THR:N    | 2.52                     | 0.42              |
| 1:B:407:GLU:HG3  | 1:B:432:TYR:HE2  | 1.83                     | 0.42              |
| 1:A:95:ILE:HG12  | 1:A:117:ASN:HB2  | 2.01                     | 0.42              |
| 1:B:343:LYS:HA   | 1:B:346:LYS:CE   | 2.38                     | 0.42              |
| 1:B:452:ILE:HB   | 1:B:476:VAL:O    | 2.19                     | 0.42              |
| 1:B:125:LYS:HD3  | 1:B:246:ASP:HB3  | 2.00                     | 0.42              |
| 1:A:118:ARG:HG3  | 1:A:118:ARG:O    | 2.19                     | 0.42              |
| 1:A:95:ILE:HA    | 1:A:95:ILE:HD13  | 1.78                     | 0.42              |
| 1:A:130:ASN:ND2  | 1:A:145:LYS:HE2  | 2.33                     | 0.42              |
| 1:B:413:VAL:HG11 | 1:B:450:ARG:CZ   | 2.49                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:199:ASN:OD1  | 1:A:201:LYS:HB2  | 2.19                     | 0.42              |
| 1:A:207:LEU:HD22 | 1:A:280:LYS:HB2  | 2.01                     | 0.42              |
| 1:B:64:VAL:HA    | 1:B:65:PRO:HD2   | 1.60                     | 0.42              |
| 1:A:175:LEU:HA   | 1:A:175:LEU:HD23 | 1.74                     | 0.42              |
| 1:A:457:ARG:NH2  | 1:A:464:TRP:NE1  | 2.68                     | 0.42              |
| 1:A:484:VAL:HG23 | 1:A:497:ILE:HD12 | 2.00                     | 0.42              |
| 1:B:276:THR:HB   | 1:B:278:TYR:HE1  | 1.82                     | 0.42              |
| 1:A:32:THR:HG21  | 2:A:517:HOH:O    | 2.19                     | 0.42              |
| 1:B:305:ASN:HA   | 1:B:310:LYS:CE   | 2.48                     | 0.42              |
| 1:B:209:VAL:HG12 | 1:B:211:PHE:N    | 2.33                     | 0.42              |
| 1:A:128:PRO:HG3  | 1:A:147:ASP:HA   | 2.02                     | 0.42              |
| 1:A:418:GLU:CB   | 1:A:420:ASN:ND2  | 2.72                     | 0.42              |
| 1:A:50:ASN:N     | 1:A:50:ASN:HD22  | 2.17                     | 0.42              |
| 1:B:131:ILE:CG2  | 1:B:132:ASN:N    | 2.83                     | 0.42              |
| 1:A:276:THR:HG21 | 1:A:278:TYR:CZ   | 2.55                     | 0.42              |
| 1:B:409:ALA:CB   | 1:B:427:THR:HG22 | 2.50                     | 0.42              |
| 1:A:38:ILE:HG23  | 1:A:39:ASP:N     | 2.34                     | 0.42              |
| 1:B:227:LYS:HA   | 1:B:276:THR:HG23 | 2.01                     | 0.42              |
| 1:B:222:MET:HE2  | 1:B:224:LEU:HD21 | 2.01                     | 0.42              |
| 1:A:465:GLU:CD   | 1:A:465:GLU:N    | 2.65                     | 0.42              |
| 1:A:343:LYS:HA   | 1:A:346:LYS:NZ   | 2.35                     | 0.42              |
| 1:B:152:GLY:O    | 1:B:153:LYS:C    | 2.57                     | 0.42              |
| 1:A:34:LYS:HE2   | 1:A:34:LYS:O     | 2.19                     | 0.42              |
| 1:A:232:THR:CB   | 1:A:271:VAL:O    | 2.61                     | 0.42              |
| 1:B:220:LYS:HB2  | 1:B:283:THR:HG23 | 2.02                     | 0.42              |
| 1:A:50:ASN:HA    | 1:A:376:HIS:NE2  | 2.35                     | 0.42              |
| 1:B:271:VAL:HG12 | 1:B:273:TYR:CE1  | 2.55                     | 0.42              |
| 1:A:30:ASP:HA    | 1:A:36:GLN:CG    | 2.49                     | 0.42              |
| 1:A:165:TRP:O    | 1:A:168:LYS:N    | 2.52                     | 0.42              |
| 1:A:150:THR:C    | 1:A:154:VAL:HG23 | 2.40                     | 0.42              |
| 1:A:275:ARG:NH2  | 1:A:348:ASN:O    | 2.52                     | 0.42              |
| 1:A:450:ARG:O    | 1:A:451:ASN:HB2  | 2.20                     | 0.42              |
| 1:B:43:SER:O     | 1:B:368:LYS:HE3  | 2.20                     | 0.42              |
| 1:A:60:ILE:HG12  | 1:A:61:GLU:N     | 2.34                     | 0.42              |
| 1:A:83:ARG:CZ    | 1:A:383:GLU:OE2  | 2.67                     | 0.42              |
| 1:A:433:GLN:HB3  | 1:A:435:LYS:HZ3  | 1.85                     | 0.41              |
| 1:B:338:PHE:CE1  | 1:B:341:ILE:HG21 | 2.54                     | 0.41              |
| 1:A:351:PHE:C    | 1:A:351:PHE:CD1  | 2.93                     | 0.41              |
| 1:B:144:ILE:HG13 | 1:B:145:LYS:N    | 2.34                     | 0.41              |
| 1:B:239:LYS:H    | 1:B:239:LYS:CD   | 2.14                     | 0.41              |
| 1:B:303:ILE:C    | 1:B:305:ASN:H    | 2.23                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:424:THR:HG22 | 1:A:424:THR:O    | 2.19                     | 0.41              |
| 1:A:449:ALA:O    | 1:A:478:LEU:HD22 | 2.21                     | 0.41              |
| 1:B:127:LYS:HD2  | 1:B:246:ASP:HA   | 2.02                     | 0.41              |
| 1:A:287:SER:O    | 1:A:289:ASP:N    | 2.53                     | 0.41              |
| 1:B:273:TYR:CD1  | 1:B:273:TYR:N    | 2.87                     | 0.41              |
| 1:B:396:LEU:HA   | 1:B:484:VAL:O    | 2.19                     | 0.41              |
| 1:A:96:ASP:CB    | 1:A:100:ASP:N    | 2.66                     | 0.41              |
| 1:B:266:LEU:HA   | 1:B:365:VAL:O    | 2.20                     | 0.41              |
| 1:B:75:PHE:HB3   | 1:B:389:TYR:HB2  | 2.02                     | 0.41              |
| 1:B:487:TRP:O    | 1:B:494:GLY:N    | 2.53                     | 0.41              |
| 1:B:163:SER:O    | 1:B:167:GLU:OE1  | 2.39                     | 0.41              |
| 1:A:320:ALA:HB2  | 1:A:341:ILE:HG23 | 2.02                     | 0.41              |
| 1:A:182:SER:CB   | 1:A:225:ALA:HB3  | 2.35                     | 0.41              |
| 1:B:150:THR:HG22 | 1:B:151:TYR:N    | 2.36                     | 0.41              |
| 1:B:456:ALA:H    | 1:B:471:ILE:CG2  | 2.33                     | 0.41              |
| 1:B:461:GLY:CA   | 1:B:467:TRP:HE1  | 2.33                     | 0.41              |
| 1:B:319:THR:HG23 | 1:B:333:VAL:O    | 2.21                     | 0.41              |
| 1:A:113:ALA:HA   | 1:A:116:GLU:OE1  | 2.20                     | 0.41              |
| 1:B:63:PHE:CD1   | 1:B:63:PHE:C     | 2.94                     | 0.41              |
| 1:A:43:SER:HA    | 1:A:368:LYS:HG3  | 2.03                     | 0.41              |
| 1:A:103:TYR:CE2  | 1:A:151:TYR:CA   | 3.04                     | 0.41              |
| 1:A:398:HIS:HD2  | 1:A:436:THR:O    | 2.03                     | 0.41              |
| 1:A:75:PHE:O     | 1:A:389:TYR:HD1  | 2.03                     | 0.41              |
| 1:B:462:LEU:C    | 1:B:462:LEU:HD23 | 2.41                     | 0.41              |
| 1:A:37:SER:HB3   | 1:A:40:SER:CB    | 2.51                     | 0.41              |
| 1:B:95:ILE:HD11  | 1:B:199:ASN:HB2  | 2.03                     | 0.41              |
| 1:A:457:ARG:HD2  | 1:A:467:TRP:O    | 2.21                     | 0.41              |
| 1:A:196:LEU:O    | 1:A:197:ASN:HB3  | 2.21                     | 0.41              |
| 1:B:343:LYS:O    | 1:B:347:ASP:OD2  | 2.39                     | 0.41              |
| 1:B:398:HIS:HB3  | 1:B:439:TYR:H    | 1.86                     | 0.41              |
| 1:B:391:LYS:CG   | 1:B:447:ALA:H    | 2.29                     | 0.41              |
| 1:A:31:ILE:HG23  | 1:A:252:ASN:OD1  | 2.20                     | 0.41              |
| 1:B:74:LYS:HZ1   | 1:B:388:GLU:CD   | 2.24                     | 0.41              |
| 1:A:166:ASN:H    | 1:A:166:ASN:ND2  | 2.19                     | 0.41              |
| 1:A:55:SER:OG    | 1:A:377:ASN:HA   | 2.21                     | 0.41              |
| 1:A:342:ARG:O    | 1:A:346:LYS:HG2  | 2.21                     | 0.41              |
| 1:A:282:GLU:O    | 1:A:316:SER:HA   | 2.21                     | 0.41              |
| 1:A:107:LEU:HA   | 1:A:266:LEU:O    | 2.20                     | 0.41              |
| 1:B:405:GLN:HG2  | 1:B:434:ASP:N    | 2.35                     | 0.41              |
| 1:A:32:THR:C     | 1:A:34:LYS:H     | 2.25                     | 0.41              |
| 1:A:80:ARG:NH1   | 1:A:80:ARG:HG3   | 2.25                     | 0.41              |

*Continued on next page...*

Continued from previous page...

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:83:ARG:HG3   | 1:B:383:GLU:HB2  | 2.03                     | 0.41              |
| 1:B:94:ILE:HD12  | 1:B:360:ILE:N    | 2.36                     | 0.41              |
| 1:A:148:ASP:O    | 1:A:153:LYS:HG2  | 2.20                     | 0.41              |
| 1:A:230:PHE:O    | 1:A:231:TYR:HB3  | 2.21                     | 0.40              |
| 1:A:254:LEU:C    | 1:A:256:GLN:N    | 2.75                     | 0.40              |
| 1:A:191:GLN:HG3  | 1:A:381:TYR:CD1  | 2.55                     | 0.40              |
| 1:B:346:LYS:C    | 1:B:348:ASN:N    | 2.74                     | 0.40              |
| 1:B:192:ILE:HD11 | 1:B:196:LEU:CD1  | 2.51                     | 0.40              |
| 1:B:79:GLU:HB2   | 1:B:385:THR:HG1  | 1.83                     | 0.40              |
| 1:B:38:ILE:HA    | 1:B:251:PHE:CB   | 2.44                     | 0.40              |
| 1:A:138:LEU:HA   | 1:A:138:LEU:HD12 | 1.93                     | 0.40              |
| 1:A:439:TYR:CG   | 1:A:440:SER:N    | 2.90                     | 0.40              |
| 1:A:161:LEU:O    | 1:A:164:LYS:HB3  | 2.22                     | 0.40              |
| 1:B:78:VAL:CG1   | 1:B:80:ARG:HE    | 2.34                     | 0.40              |
| 1:A:72:GLY:C     | 1:A:74:LYS:H     | 2.24                     | 0.40              |
| 1:A:90:VAL:HG23  | 1:A:91:ASP:N     | 2.37                     | 0.40              |
| 1:B:57:GLY:HA3   | 1:B:379:THR:HB   | 2.03                     | 0.40              |
| 1:A:126:ARG:HB3  | 1:A:149:PRO:HD2  | 2.04                     | 0.40              |
| 1:B:101:ARG:CD   | 1:B:101:ARG:N    | 2.85                     | 0.40              |
| 1:B:298:ILE:C    | 1:B:300:ASN:H    | 2.24                     | 0.40              |
| 1:B:461:GLY:N    | 1:B:467:TRP:HE1  | 2.18                     | 0.40              |
| 1:B:318:PHE:CD1  | 1:B:318:PHE:N    | 2.89                     | 0.40              |
| 1:A:406:PHE:CD1  | 1:A:406:PHE:N    | 2.89                     | 0.40              |
| 1:A:217:ASN:OD1  | 1:A:384:THR:HG21 | 2.22                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

| Mol | Chain | Analysed       | Favoured  | Allowed  | Outliers | Percentiles       |
|-----|-------|----------------|-----------|----------|----------|-------------------|
| 1   | A     | 469/471 (100%) | 358 (76%) | 77 (16%) | 34 (7%)  | <b>1</b> <b>7</b> |

Continued on next page...

*Continued from previous page...*

| Mol | Chain | Analysed       | Favoured  | Allowed   | Outliers | Percentiles |   |
|-----|-------|----------------|-----------|-----------|----------|-------------|---|
| 1   | B     | 469/471 (100%) | 358 (76%) | 76 (16%)  | 35 (8%)  | 1           | 6 |
| All | All   | 938/942 (100%) | 716 (76%) | 153 (16%) | 69 (7%)  | 1           | 6 |

All (69) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 298 | ILE  |
| 1   | B     | 288 | LYS  |
| 1   | B     | 438 | HIS  |
| 1   | A     | 151 | TYR  |
| 1   | A     | 259 | VAL  |
| 1   | A     | 288 | LYS  |
| 1   | A     | 438 | HIS  |
| 1   | A     | 464 | TRP  |
| 1   | A     | 465 | GLU  |
| 1   | B     | 47  | TYR  |
| 1   | B     | 95  | ILE  |
| 1   | B     | 96  | ASP  |
| 1   | B     | 151 | TYR  |
| 1   | B     | 259 | VAL  |
| 1   | B     | 260 | SER  |
| 1   | B     | 347 | ASP  |
| 1   | B     | 447 | ALA  |
| 1   | B     | 464 | TRP  |
| 1   | B     | 465 | GLU  |
| 1   | A     | 47  | TYR  |
| 1   | A     | 97  | SER  |
| 1   | A     | 100 | ASP  |
| 1   | A     | 247 | ASP  |
| 1   | A     | 299 | LYS  |
| 1   | A     | 302 | ASP  |
| 1   | A     | 345 | ILE  |
| 1   | A     | 347 | ASP  |
| 1   | A     | 447 | ALA  |
| 1   | B     | 63  | PHE  |
| 1   | B     | 65  | PRO  |
| 1   | B     | 73  | ASN  |
| 1   | B     | 97  | SER  |
| 1   | B     | 100 | ASP  |
| 1   | B     | 128 | PRO  |
| 1   | B     | 153 | LYS  |
| 1   | B     | 211 | PHE  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 302 | ASP  |
| 1   | A     | 63  | PHE  |
| 1   | A     | 73  | ASN  |
| 1   | A     | 211 | PHE  |
| 1   | A     | 231 | TYR  |
| 1   | A     | 368 | LYS  |
| 1   | A     | 437 | ALA  |
| 1   | B     | 139 | LYS  |
| 1   | B     | 208 | GLY  |
| 1   | B     | 437 | ALA  |
| 1   | A     | 65  | PRO  |
| 1   | A     | 260 | SER  |
| 1   | A     | 328 | GLN  |
| 1   | A     | 455 | LYS  |
| 1   | B     | 51  | GLU  |
| 1   | B     | 57  | GLY  |
| 1   | B     | 327 | ALA  |
| 1   | B     | 368 | LYS  |
| 1   | A     | 95  | ILE  |
| 1   | A     | 208 | GLY  |
| 1   | B     | 162 | VAL  |
| 1   | B     | 231 | TYR  |
| 1   | B     | 310 | LYS  |
| 1   | B     | 328 | GLN  |
| 1   | B     | 298 | ILE  |
| 1   | B     | 345 | ILE  |
| 1   | A     | 52  | VAL  |
| 1   | A     | 104 | PRO  |
| 1   | A     | 202 | VAL  |
| 1   | A     | 128 | PRO  |
| 1   | A     | 98  | VAL  |
| 1   | A     | 497 | ILE  |
| 1   | B     | 149 | 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     | 418/418 (100%) | 379 (91%) | 39 (9%)  | 11          | 39 |
| 1   | B     | 418/418 (100%) | 383 (92%) | 35 (8%)  | 14          | 45 |
| All | All   | 836/836 (100%) | 762 (91%) | 74 (9%)  | 12          | 42 |

All (74) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 31  | ILE  |
| 1   | A     | 34  | LYS  |
| 1   | A     | 44  | SER  |
| 1   | A     | 45  | LEU  |
| 1   | A     | 46  | SER  |
| 1   | A     | 59  | LYS  |
| 1   | A     | 63  | PHE  |
| 1   | A     | 70  | LYS  |
| 1   | A     | 88  | SER  |
| 1   | A     | 90  | VAL  |
| 1   | A     | 95  | ILE  |
| 1   | A     | 99  | ASN  |
| 1   | A     | 100 | ASP  |
| 1   | A     | 101 | ARG  |
| 1   | A     | 102 | THR  |
| 1   | A     | 108 | GLN  |
| 1   | A     | 114 | LEU  |
| 1   | A     | 121 | ILE  |
| 1   | A     | 132 | ASN  |
| 1   | A     | 167 | GLU  |
| 1   | A     | 184 | SER  |
| 1   | A     | 198 | VAL  |
| 1   | A     | 239 | LYS  |
| 1   | A     | 245 | PHE  |
| 1   | A     | 247 | ASP  |
| 1   | A     | 250 | THR  |
| 1   | A     | 270 | ASN  |
| 1   | A     | 286 | SER  |
| 1   | A     | 301 | THR  |
| 1   | A     | 326 | ASP  |
| 1   | A     | 351 | PHE  |
| 1   | A     | 370 | ASN  |
| 1   | A     | 395 | ASN  |
| 1   | A     | 424 | THR  |
| 1   | A     | 434 | ASP  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 444 | PRO  |
| 1   | A     | 468 | ARG  |
| 1   | A     | 475 | ASP  |
| 1   | A     | 483 | ASN  |
| 1   | B     | 30  | ASP  |
| 1   | B     | 31  | ILE  |
| 1   | B     | 34  | LYS  |
| 1   | B     | 45  | LEU  |
| 1   | B     | 59  | LYS  |
| 1   | B     | 70  | LYS  |
| 1   | B     | 90  | VAL  |
| 1   | B     | 99  | ASN  |
| 1   | B     | 100 | ASP  |
| 1   | B     | 101 | ARG  |
| 1   | B     | 102 | THR  |
| 1   | B     | 107 | LEU  |
| 1   | B     | 115 | VAL  |
| 1   | B     | 121 | ILE  |
| 1   | B     | 128 | PRO  |
| 1   | B     | 147 | ASP  |
| 1   | B     | 163 | SER  |
| 1   | B     | 184 | SER  |
| 1   | B     | 239 | LYS  |
| 1   | B     | 250 | THR  |
| 1   | B     | 286 | SER  |
| 1   | B     | 289 | ASP  |
| 1   | B     | 301 | THR  |
| 1   | B     | 326 | ASP  |
| 1   | B     | 330 | HIS  |
| 1   | B     | 339 | ASP  |
| 1   | B     | 351 | PHE  |
| 1   | B     | 370 | ASN  |
| 1   | B     | 371 | SER  |
| 1   | B     | 395 | ASN  |
| 1   | B     | 453 | ARG  |
| 1   | B     | 457 | ARG  |
| 1   | B     | 468 | ARG  |
| 1   | B     | 475 | ASP  |
| 1   | B     | 497 | ILE  |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:



| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 50  | ASN  |
| 1   | A     | 56  | ASN  |
| 1   | A     | 130 | ASN  |
| 1   | A     | 132 | ASN  |
| 1   | A     | 166 | ASN  |
| 1   | A     | 173 | HIS  |
| 1   | A     | 197 | ASN  |
| 1   | A     | 228 | GLN  |
| 1   | A     | 252 | ASN  |
| 1   | A     | 270 | ASN  |
| 1   | A     | 291 | GLN  |
| 1   | A     | 308 | GLN  |
| 1   | A     | 420 | ASN  |
| 1   | A     | 433 | GLN  |
| 1   | A     | 451 | ASN  |
| 1   | A     | 500 | ASN  |
| 1   | B     | 48  | ASN  |
| 1   | B     | 50  | ASN  |
| 1   | B     | 56  | ASN  |
| 1   | B     | 108 | GLN  |
| 1   | B     | 130 | ASN  |
| 1   | B     | 132 | ASN  |
| 1   | B     | 197 | ASN  |
| 1   | B     | 205 | ASN  |
| 1   | B     | 228 | GLN  |
| 1   | B     | 252 | ASN  |
| 1   | B     | 291 | GLN  |
| 1   | B     | 405 | GLN  |
| 1   | B     | 420 | ASN  |
| 1   | B     | 433 | GLN  |
| 1   | B     | 451 | ASN  |
| 1   | B     | 500 | ASN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

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

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

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.