



# Full wwPDB NMR Structure Validation Report ⓘ

Feb 12, 2017 – 10:06 pm GMT

PDB ID : 2HHI  
Title : The solution structure of antigen MPT64 from Mycobacterium tuberculosis defines a novel class of beta-grasp proteins  
Authors : Wang, Z.; Potter, B.M.; Gray, A.M.; Sacksteder, K.A.; Geisbrecht, B.V.; Laity, J.H.  
Deposited on : 2006-06-28

This is a Full wwPDB NMR 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/NMRValidationReportHelp>

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:

Cyrange : Kirchner and Güntert (2011)  
NmrClust : Kelley et al. (1996)  
MolProbity : 4.02b-467  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
RCI : v\_1n\_11\_5\_13\_A (Berjanski et al., 2005)  
PANAV : Wang et al. (2010)  
ShiftChecker : trunk28760  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

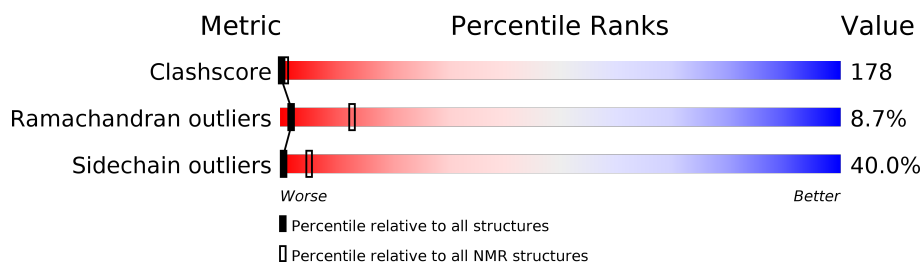
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment was not calculated.

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) | NMR archive<br>(#Entries) |
|-----------------------|-----------------------------|---------------------------|
| Clashscore            | 125131                      | 11601                     |
| Ramachandran outliers | 121729                      | 10391                     |
| Sidechain outliers    | 121581                      | 10367                     |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and 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  $\leq 5\%$

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | A     | 204    |                  |

## 2 Ensemble composition and analysis

This entry contains 24 models. Model 16 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *closest to the average*.

The following residues are included in the computation of the global validation metrics.

| Well-defined (core) protein residues |   |                   |              |
|--------------------------------------|---|-------------------|--------------|
| Well-defined core                    | Residue range (total)                   | Backbone RMSD (Å) | Medoid model |
| 1                                    | A:3-A:35, A:40-A:162, A:169-A:206 (194) | 0.15              | 16           |

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 5 clusters and 2 single-model clusters were found.

| Cluster number        | Models                         |
|-----------------------|--------------------------------|
| 1                     | 1, 2, 3, 7, 12, 13, 20, 21, 24 |
| 2                     | 11, 14, 16, 19, 22, 23         |
| 3                     | 4, 6, 9                        |
| 4                     | 10, 18                         |
| 5                     | 8, 17                          |
| Single-model clusters | 5; 15                          |

### 3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 3106 atoms, of which 1527 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Immunogenic protein MPT64.

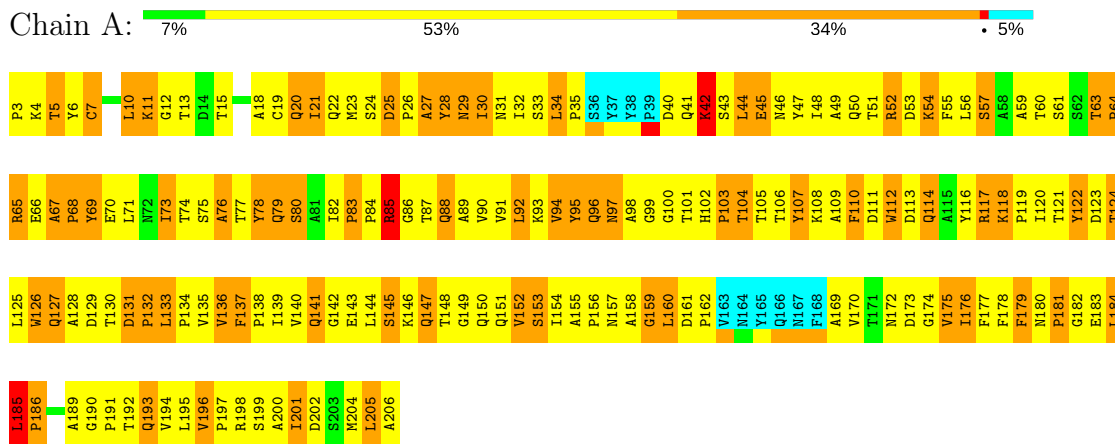
| Mol | Chain | Residues | Atoms |      |      |     |     |   | Trace |
|-----|-------|----------|-------|------|------|-----|-----|---|-------|
| 1   | A     | 204      | Total | C    | H    | N   | O   | S | 0     |
|     |       |          | 3106  | 1003 | 1527 | 257 | 315 | 4 |       |

## 4 Residue-property plots

### 4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA and DNA chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

- Molecule 1: Immunogenic protein MPT64



### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

#### 4.2.1 Score per residue for model 1

- Molecule 1: Immunogenic protein MPT64

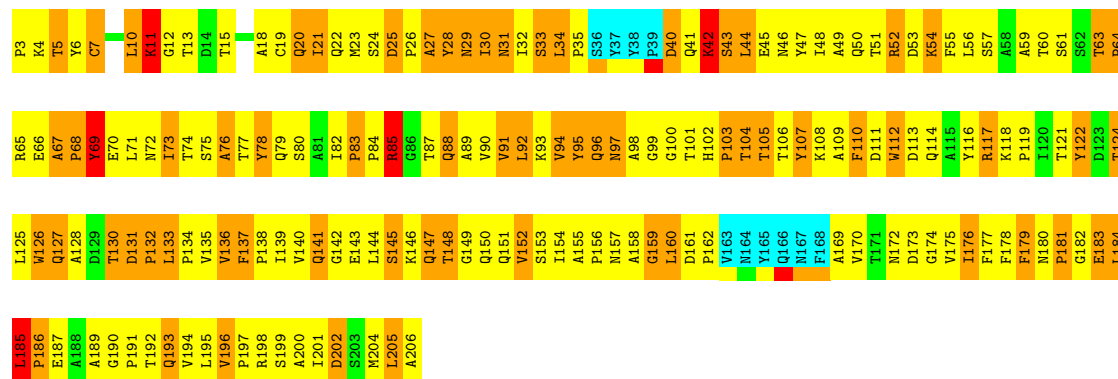




#### 4.2.2 Score per residue for model 2

- Molecule 1: Immunogenic protein MPT64

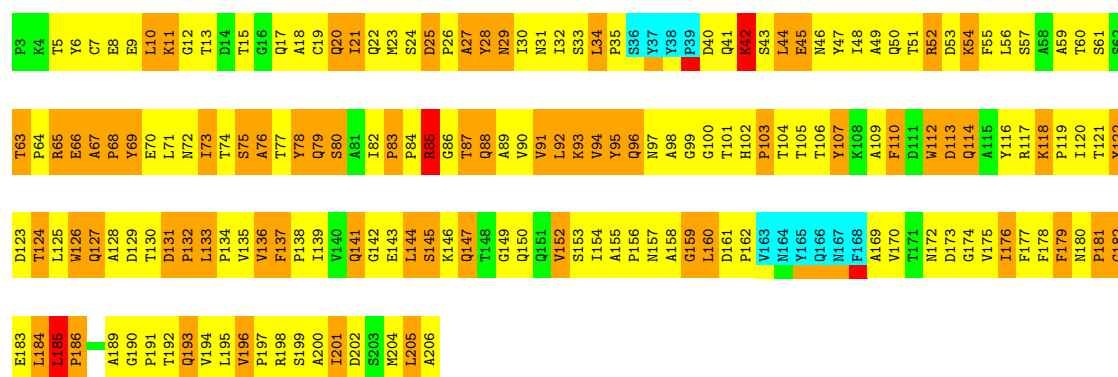
Chain A: 8% 52% 33% 5%



#### 4.2.3 Score per residue for model 3

- Molecule 1: Immunogenic protein MPT64

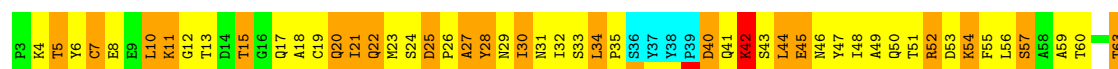
Chain A: 8% 52% 33% 5%

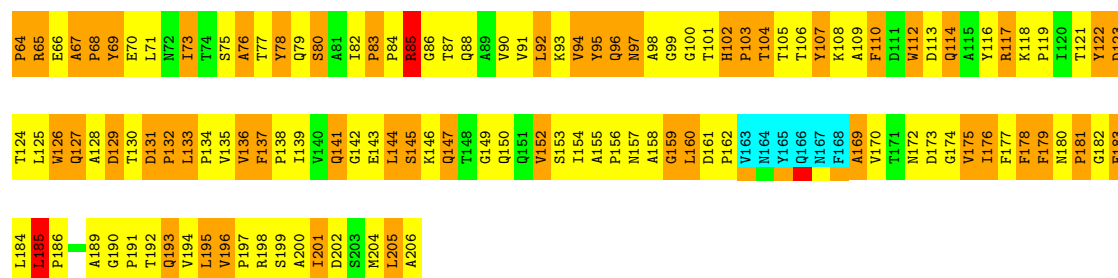


#### 4.2.4 Score per residue for model 4

- Molecule 1: Immunogenic protein MPT64

Chain A: 10% 48% 35% 5%

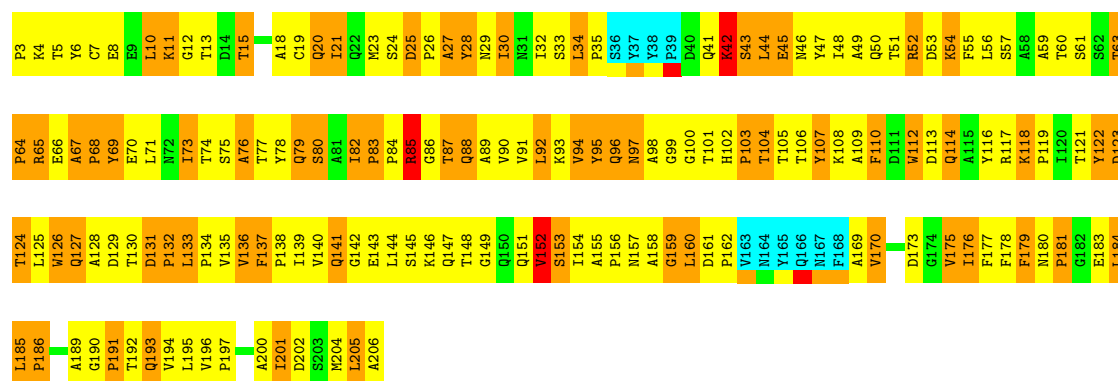




#### 4.2.5 Score per residue for model 5

- Molecule 1: Immunogenic protein MPT64

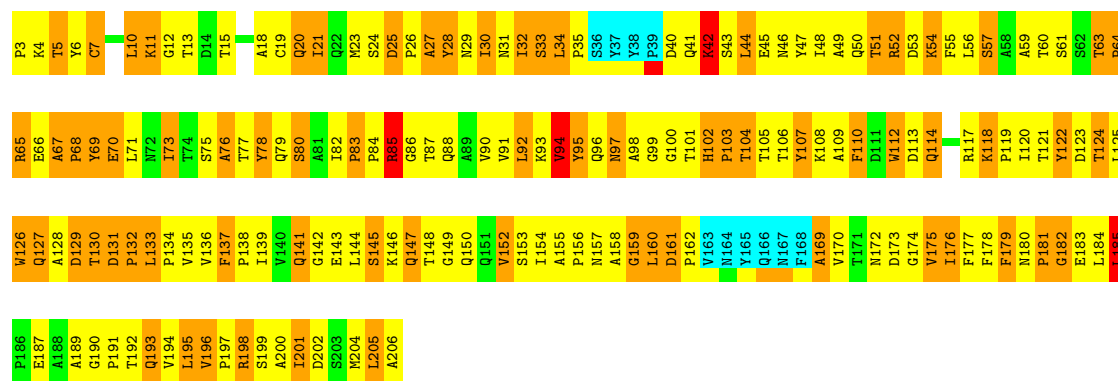
Chain A: 12% 49% 33% 5%



#### 4.2.6 Score per residue for model 6

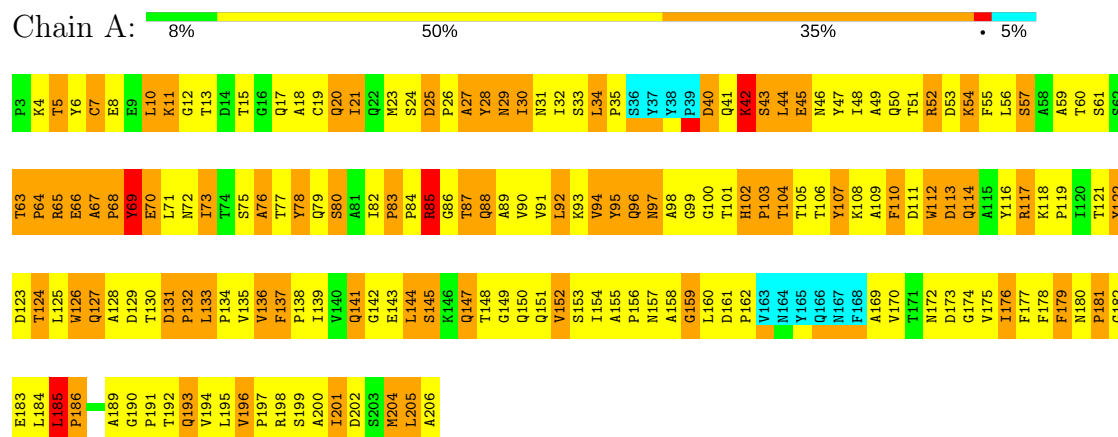
- Molecule 1: Immunogenic protein MPT64

Chain A: 10% 49% 34% 5%



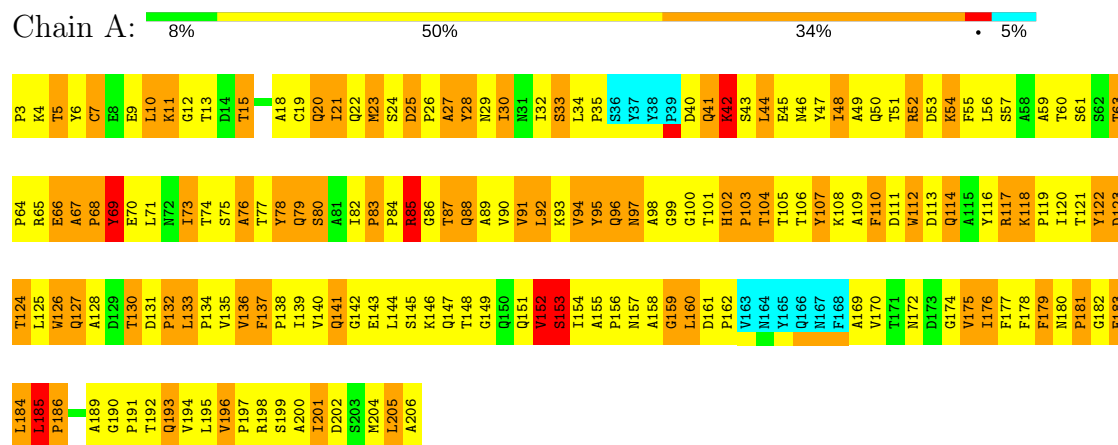
### 4.2.7 Score per residue for model 7

- Molecule 1: Immunogenic protein MPT64



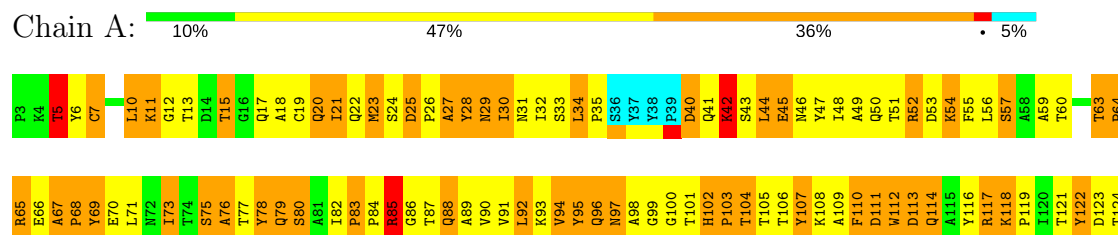
### 4.2.8 Score per residue for model 8

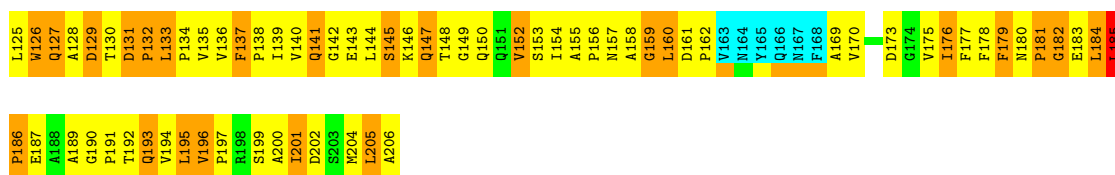
- Molecule 1: Immunogenic protein MPT64



### 4.2.9 Score per residue for model 9

- Molecule 1: Immunogenic protein MPT64

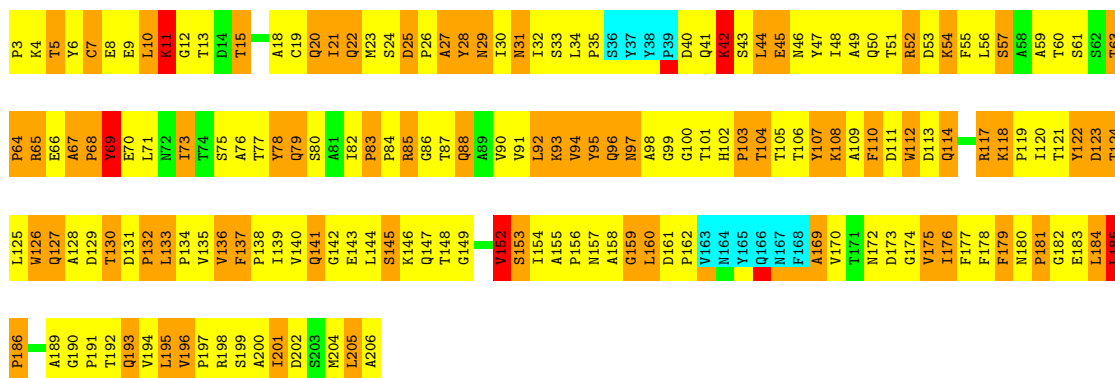




#### 4.2.10 Score per residue for model 10

- Molecule 1: Immunogenic protein MPT64

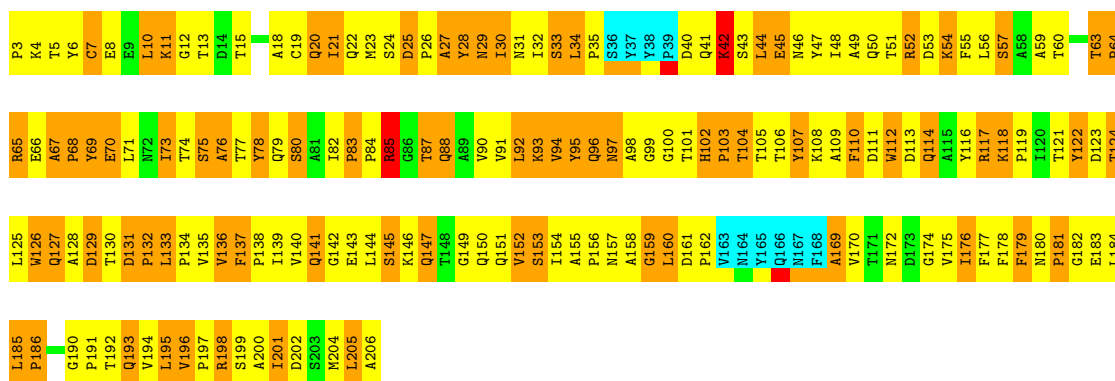
Chain A: 8% 50% 34% 5%



#### 4.2.11 Score per residue for model 11

- Molecule 1: Immunogenic protein MPT64

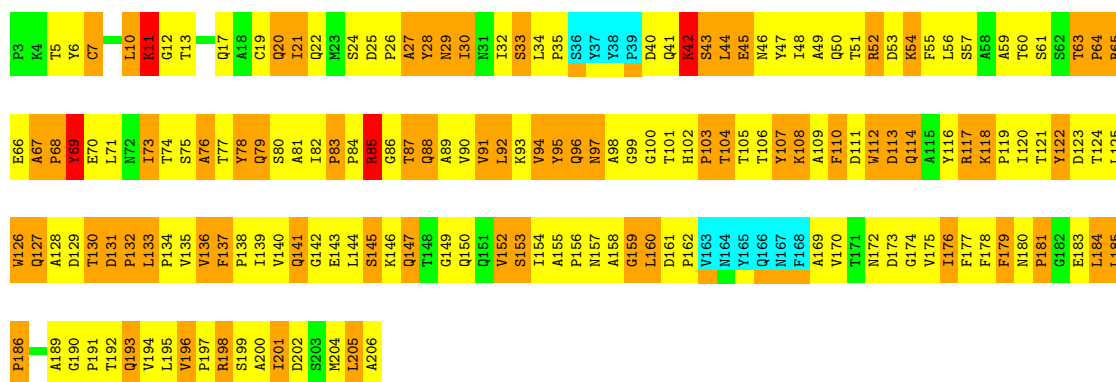
Chain A: 10% 47% 37% 5%



#### 4.2.12 Score per residue for model 12

- Molecule 1: Immunogenic protein MPT64

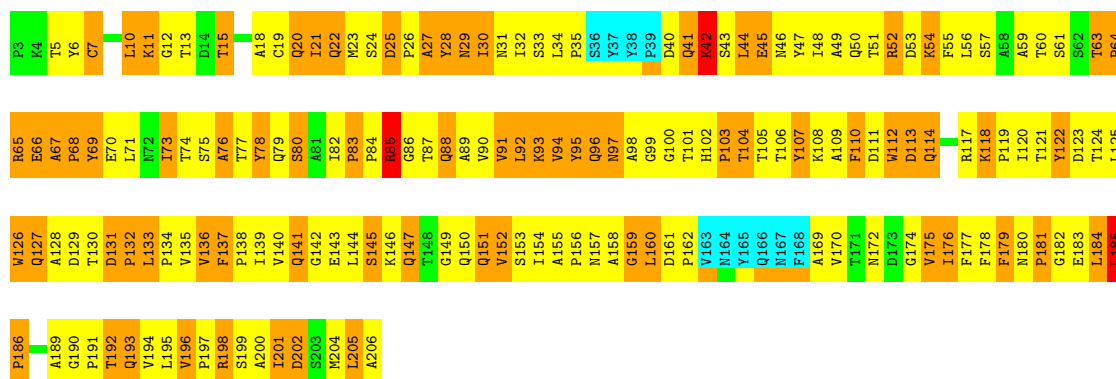
Chain A: 10% 49% 34% 5%



#### 4.2.13 Score per residue for model 13

- Molecule 1: Immunogenic protein MPT64

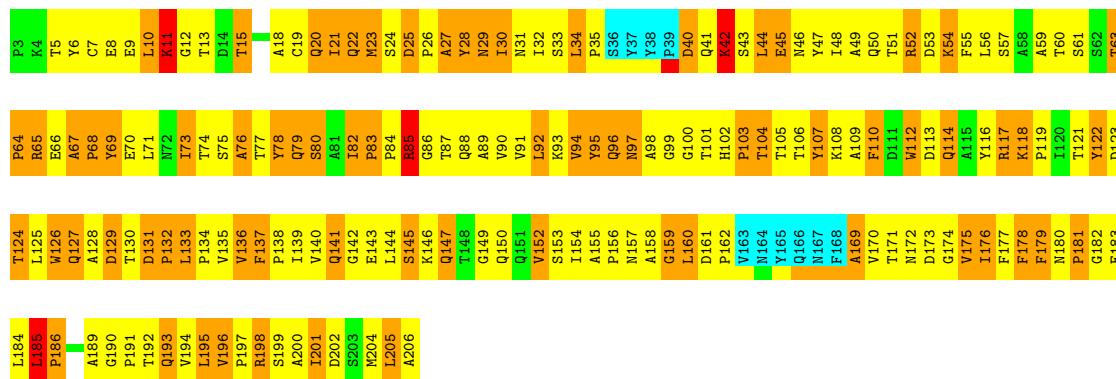
Chain A: 9% 49% 36% 5%



#### 4.2.14 Score per residue for model 14

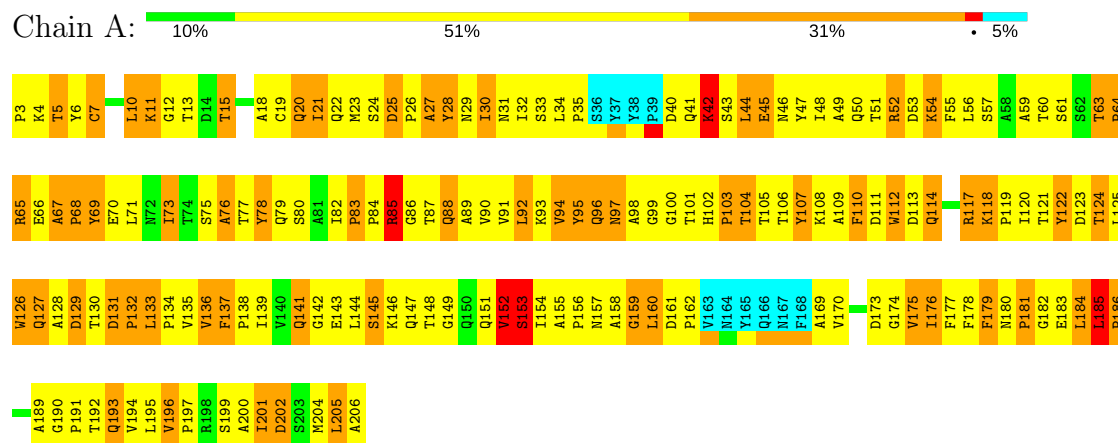
- Molecule 1: Immunogenic protein MPT64

Chain A: 8% 50% 35% 5%



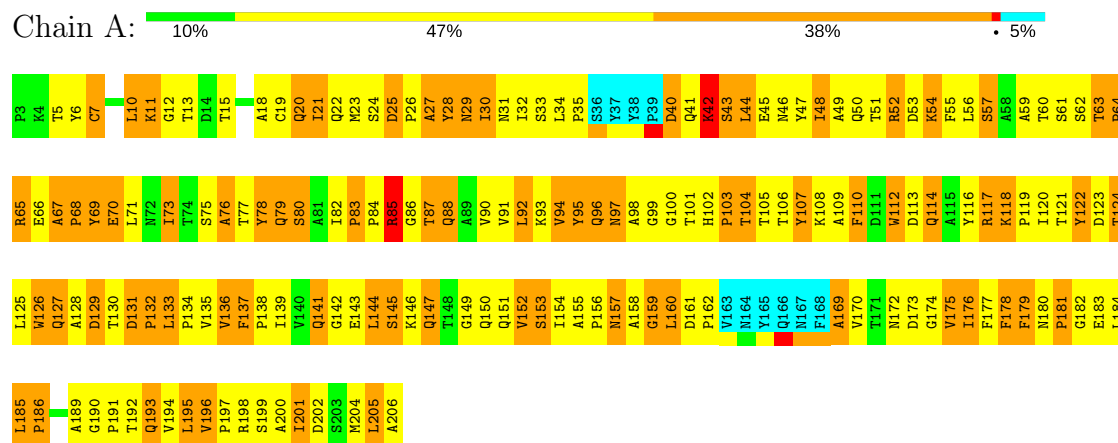
### 4.2.15 Score per residue for model 15

- Molecule 1: Immunogenic protein MPT64



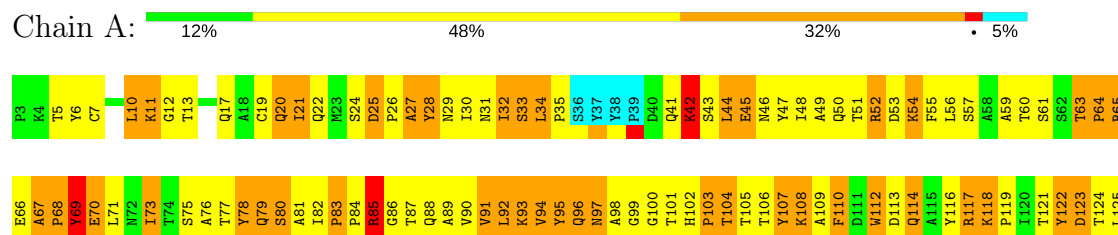
### 4.2.16 Score per residue for model 16 (medoid)

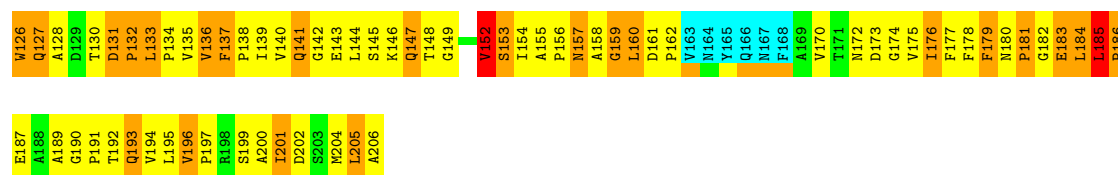
- Molecule 1: Immunogenic protein MPT64



### 4.2.17 Score per residue for model 17

- Molecule 1: Immunogenic protein MPT64

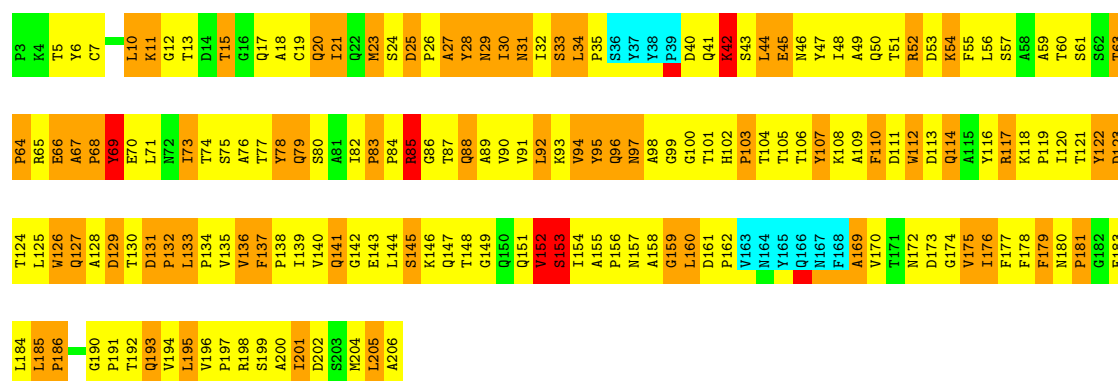




#### 4.2.18 Score per residue for model 18

- Molecule 1: Immunogenic protein MPT64

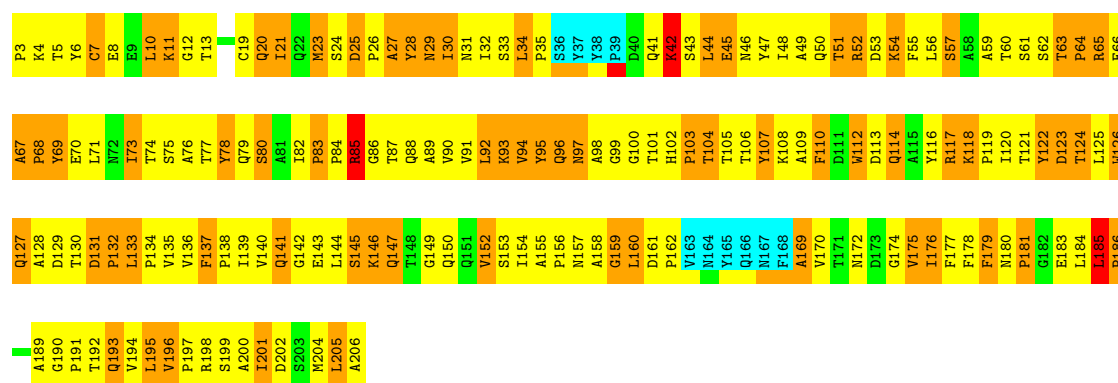
Chain A: 9% 52% 31% 5%



#### 4.2.19 Score per residue for model 19

- Molecule 1: Immunogenic protein MPT64

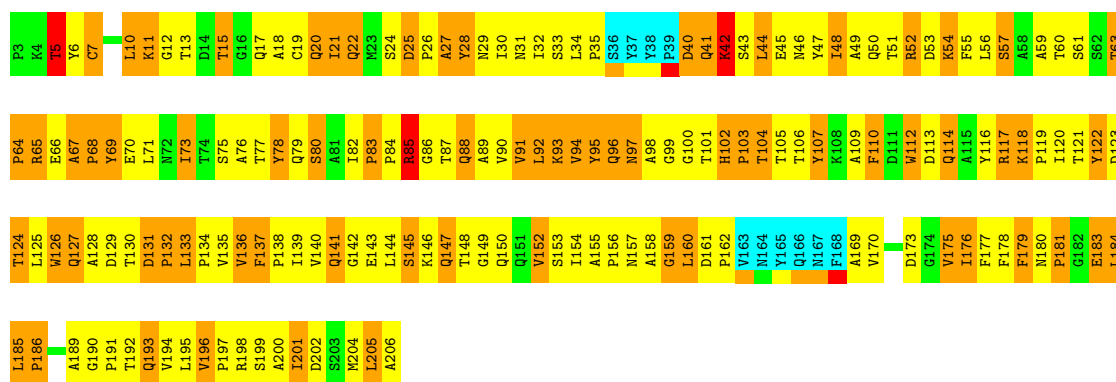
Chain A: 10% 50% 34% 5%



#### 4.2.20 Score per residue for model 20

- Molecule 1: Immunogenic protein MPT64

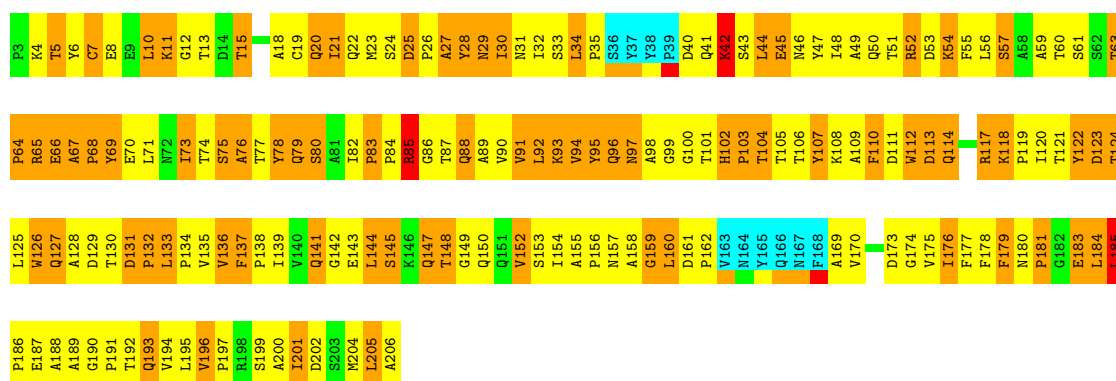
Chain A: 11% 48% 35% 5%



#### 4.2.21 Score per residue for model 21

- Molecule 1: Immunogenic protein MPT64

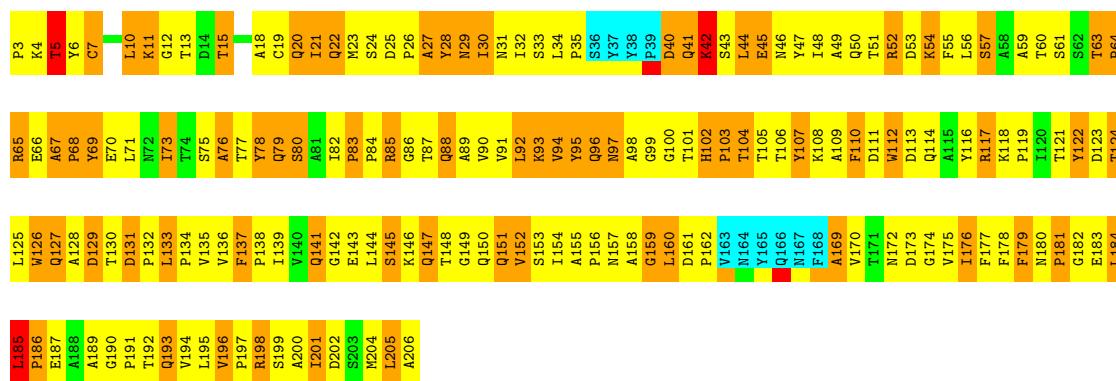
Chain A: 9% 47% 38% 5%



#### 4.2.22 Score per residue for model 22

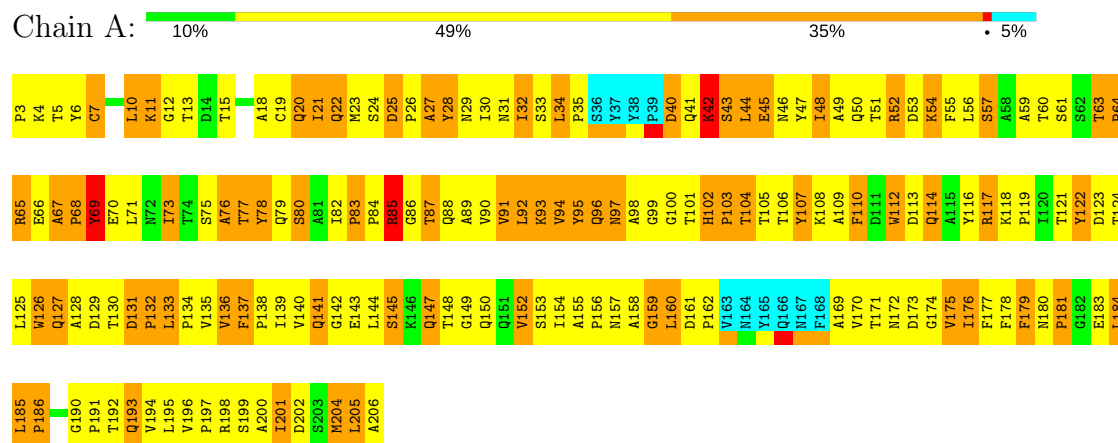
- Molecule 1: Immunogenic protein MPT64

Chain A: 8% 51% 35% 5%



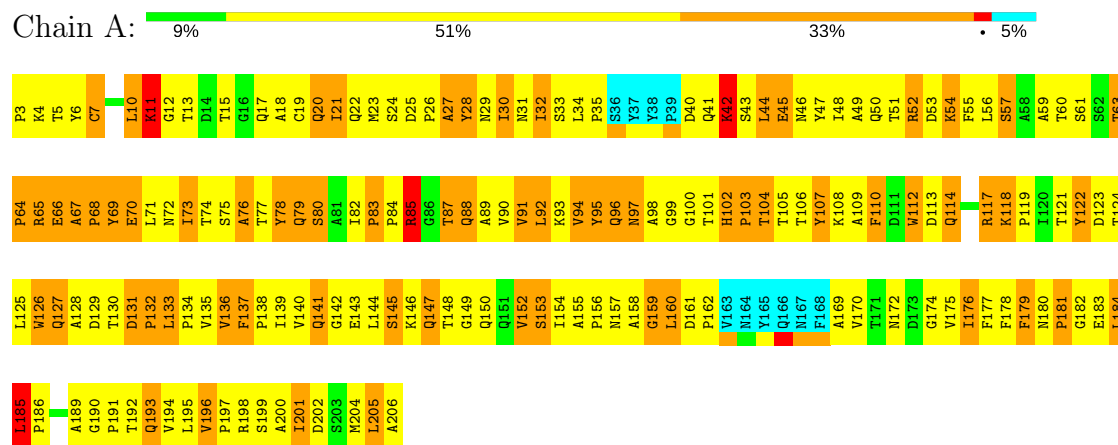
### 4.2.23 Score per residue for model 23

- Molecule 1: Immunogenic protein MPT64



### 4.2.24 Score per residue for model 24

- Molecule 1: Immunogenic protein MPT64



## 5 Refinement protocol and experimental data overview

The models were refined using the following method: *Torsion Angle Dynamics followed by RDC refinement using CNS 1.1.*

Of the 50 calculated structures, 24 were deposited, based on the following criterion: *structures with the lowest energy.*

The following table shows the software used for structure solution, optimisation and refinement.

| Software name | Classification | Version |
|---------------|----------------|---------|
| CNS           | refinement     | 1.1     |

No chemical shift data was provided. No validations of the models with respect to experimental NMR restraints is performed at this time.

## 6 Model quality i

### 6.1 Standard geometry i

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the (average) 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     | 0.59±0.01    | 0±0/1524 (0.0±0.0%) | 1.06±0.01   | 5±1/2087 (0.2±0.0%) |
| All | All   | 0.59         | 0/36576 (0.0%)      | 1.06        | 119/50088 (0.2%)    |

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

| Mol | Chain | Chirality | Planarity |
|-----|-------|-----------|-----------|
| 1   | A     | 0.0±0.0   | 1.0±0.0   |
| All | All   | 0         | 24        |

There are no bond-length outliers.

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) | Models |       |
|-----|-------|-----|------|-----------|-------|-------------|----------|--------|-------|
|     |       |     |      |           |       |             |          | Worst  | Total |
| 1   | A     | 76  | ALA  | CA-C-N    | 9.19  | 137.42      | 117.20   | 3      | 24    |
| 1   | A     | 94  | VAL  | CA-C-N    | -8.27 | 99.00       | 117.20   | 6      | 24    |
| 1   | A     | 76  | ALA  | O-C-N     | -5.74 | 113.51      | 122.70   | 3      | 24    |
| 1   | A     | 76  | ALA  | CA-C-O    | -5.44 | 108.68      | 120.10   | 3      | 24    |
| 1   | A     | 69  | TYR  | CB-CG-CD1 | 5.29  | 124.18      | 121.00   | 10     | 8     |
| 1   | A     | 153 | SER  | N-CA-C    | -5.26 | 96.80       | 111.00   | 17     | 6     |
| 1   | A     | 195 | LEU  | CA-C-N    | 5.24  | 128.72      | 117.20   | 18     | 9     |

There are no chirality outliers.

All unique planar outliers are listed below.

| Mol | Chain | Res | Type | Group     | Models (Total) |
|-----|-------|-----|------|-----------|----------------|
| 1   | A     | 126 | TRP  | Mainchain | 24             |

## 6.2 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 each 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 averaged over the ensemble.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes |
|-----|-------|-------|----------|----------|---------|
| 1   | A     | 1487  | 1450     | 1447     | 522±11  |
| All | All   | 35688 | 34800    | 34728    | 12538   |

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 178.

All unique clashes are listed below, sorted by their clash magnitude.

| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:66:GLU:HB3   | 1:A:99:GLY:O     | 1.29     | 1.26        | 16     | 24    |
| 1:A:184:LEU:O    | 1:A:185:LEU:HG   | 1.26     | 1.19        | 13     | 15    |
| 1:A:66:GLU:CB    | 1:A:99:GLY:O     | 1.25     | 1.84        | 15     | 24    |
| 1:A:94:VAL:O     | 1:A:106:THR:O    | 1.23     | 1.56        | 7      | 24    |
| 1:A:185:LEU:HD21 | 1:A:191:PRO:O    | 1.20     | 1.35        | 7      | 15    |
| 1:A:65:ARG:HA    | 1:A:98:ALA:O     | 1.19     | 1.38        | 8      | 24    |
| 1:A:185:LEU:HD13 | 1:A:185:LEU:O    | 1.17     | 1.34        | 21     | 5     |
| 1:A:155:ALA:HB3  | 1:A:158:ALA:HB3  | 1.14     | 1.15        | 17     | 24    |
| 1:A:44:LEU:HD22  | 1:A:92:LEU:HD21  | 1.12     | 1.16        | 7      | 24    |
| 1:A:30:ILE:HG22  | 1:A:32:ILE:HD11  | 1.12     | 1.12        | 14     | 16    |
| 1:A:156:PRO:HB3  | 1:A:160:LEU:HD12 | 1.11     | 1.14        | 24     | 24    |
| 1:A:160:LEU:HD13 | 1:A:194:VAL:HG12 | 1.11     | 1.21        | 7      | 24    |
| 1:A:42:LYS:O     | 1:A:46:ASN:HB2   | 1.08     | 1.48        | 12     | 24    |
| 1:A:178:PHE:CG   | 1:A:193:GLN:HB2  | 1.08     | 1.83        | 4      | 24    |
| 1:A:185:LEU:HD11 | 1:A:190:GLY:O    | 1.08     | 1.45        | 21     | 1     |
| 1:A:91:VAL:HG23  | 1:A:109:ALA:HB2  | 1.08     | 1.15        | 23     | 5     |
| 1:A:175:VAL:HG13 | 1:A:196:VAL:HG12 | 1.06     | 1.19        | 20     | 3     |
| 1:A:66:GLU:HB2   | 1:A:100:GLY:HA3  | 1.05     | 1.28        | 3      | 24    |
| 1:A:95:TYR:HB2   | 1:A:105:THR:HG23 | 1.05     | 1.26        | 18     | 22    |
| 1:A:196:VAL:HG13 | 1:A:201:ILE:HG21 | 1.04     | 1.24        | 13     | 3     |
| 1:A:196:VAL:HG12 | 1:A:201:ILE:HG21 | 1.04     | 1.29        | 23     | 21    |
| 1:A:185:LEU:HD11 | 1:A:191:PRO:C    | 1.04     | 1.73        | 10     | 14    |
| 1:A:69:TYR:HA    | 1:A:99:GLY:H     | 1.03     | 1.13        | 19     | 24    |
| 1:A:133:LEU:HD23 | 1:A:196:VAL:HG22 | 1.03     | 1.24        | 2      | 20    |
| 1:A:156:PRO:O    | 1:A:184:LEU:HD12 | 1.02     | 1.54        | 1      | 18    |
| 1:A:136:VAL:HG23 | 1:A:195:LEU:HD22 | 1.02     | 1.08        | 7      | 2     |
| 1:A:184:LEU:O    | 1:A:185:LEU:CG   | 1.01     | 2.07        | 13     | 15    |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:133:LEU:HD22 | 1:A:194:VAL:HG23 | 0.99     | 1.34        | 7      | 24    |
| 1:A:15:THR:CG2   | 1:A:18:ALA:HB3   | 0.98     | 1.88        | 24     | 19    |
| 1:A:185:LEU:HD21 | 1:A:190:GLY:N    | 0.98     | 1.73        | 21     | 1     |
| 1:A:155:ALA:O    | 1:A:159:GLY:N    | 0.98     | 1.97        | 14     | 24    |
| 1:A:91:VAL:CG2   | 1:A:109:ALA:HB2  | 0.96     | 1.90        | 23     | 13    |
| 1:A:127:GLN:CG   | 1:A:204:MET:O    | 0.96     | 2.14        | 8      | 24    |
| 1:A:197:PRO:HB2  | 1:A:200:ALA:HB3  | 0.96     | 1.37        | 17     | 24    |
| 1:A:44:LEU:CD2   | 1:A:92:LEU:HD21  | 0.96     | 1.90        | 12     | 24    |
| 1:A:155:ALA:HB3  | 1:A:158:ALA:CB   | 0.96     | 1.91        | 21     | 24    |
| 1:A:127:GLN:CB   | 1:A:204:MET:O    | 0.95     | 2.13        | 18     | 24    |
| 1:A:91:VAL:HG23  | 1:A:109:ALA:CB   | 0.95     | 1.91        | 23     | 3     |
| 1:A:53:ASP:O     | 1:A:57:SER:HB2   | 0.95     | 1.59        | 18     | 24    |
| 1:A:185:LEU:CD2  | 1:A:191:PRO:O    | 0.95     | 2.14        | 7      | 12    |
| 1:A:41:GLN:HE22  | 1:A:90:VAL:HG21  | 0.95     | 1.16        | 4      | 10    |
| 1:A:197:PRO:CB   | 1:A:200:ALA:HB3  | 0.95     | 1.90        | 11     | 24    |
| 1:A:127:GLN:HB3  | 1:A:204:MET:O    | 0.95     | 1.61        | 18     | 24    |
| 1:A:48:ILE:HD11  | 1:A:71:LEU:HD21  | 0.95     | 1.38        | 3      | 10    |
| 1:A:29:ASN:N     | 1:A:69:TYR:O     | 0.95     | 2.00        | 13     | 24    |
| 1:A:66:GLU:CA    | 1:A:99:GLY:O     | 0.95     | 2.14        | 3      | 24    |
| 1:A:178:PHE:CD1  | 1:A:193:GLN:HB2  | 0.95     | 1.97        | 5      | 24    |
| 1:A:91:VAL:HB    | 1:A:109:ALA:HB2  | 0.95     | 1.37        | 4      | 21    |
| 1:A:30:ILE:HG22  | 1:A:32:ILE:CD1   | 0.94     | 1.93        | 13     | 16    |
| 1:A:44:LEU:HD22  | 1:A:92:LEU:CD2   | 0.94     | 1.93        | 12     | 24    |
| 1:A:160:LEU:HD13 | 1:A:194:VAL:CG1  | 0.93     | 1.93        | 4      | 24    |
| 1:A:185:LEU:HD12 | 1:A:185:LEU:O    | 0.92     | 1.63        | 16     | 7     |
| 1:A:179:PHE:O    | 1:A:192:THR:N    | 0.92     | 2.01        | 15     | 24    |
| 1:A:67:ALA:HB3   | 1:A:68:PRO:HD3   | 0.92     | 1.39        | 21     | 24    |
| 1:A:176:ILE:HG23 | 1:A:178:PHE:CE1  | 0.92     | 1.99        | 4      | 10    |
| 1:A:133:LEU:N    | 1:A:134:PRO:HD3  | 0.92     | 1.80        | 22     | 24    |
| 1:A:68:PRO:O     | 1:A:99:GLY:CA    | 0.91     | 2.17        | 3      | 24    |
| 1:A:30:ILE:CG2   | 1:A:32:ILE:HD11  | 0.91     | 1.96        | 6      | 15    |
| 1:A:136:VAL:CG2  | 1:A:195:LEU:HD22 | 0.91     | 1.95        | 7      | 2     |
| 1:A:65:ARG:CA    | 1:A:98:ALA:O     | 0.91     | 2.19        | 20     | 24    |
| 1:A:15:THR:HG22  | 1:A:18:ALA:HB3   | 0.91     | 1.39        | 1      | 8     |
| 1:A:196:VAL:HG13 | 1:A:201:ILE:CG2  | 0.90     | 1.96        | 15     | 3     |
| 1:A:196:VAL:CG1  | 1:A:201:ILE:HG21 | 0.90     | 1.97        | 12     | 24    |
| 1:A:175:VAL:HG11 | 1:A:201:ILE:HD11 | 0.90     | 1.42        | 3      | 24    |
| 1:A:87:THR:CA    | 1:A:114:GLN:HB2  | 0.90     | 1.95        | 11     | 22    |
| 1:A:32:ILE:HG23  | 1:A:73:ILE:HG23  | 0.90     | 1.43        | 18     | 15    |
| 1:A:175:VAL:HG11 | 1:A:201:ILE:CD1  | 0.89     | 1.97        | 3      | 21    |
| 1:A:175:VAL:CG1  | 1:A:196:VAL:HG12 | 0.88     | 1.97        | 20     | 3     |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:32:ILE:HG13  | 1:A:73:ILE:HG23  | 0.88     | 1.43        | 10     | 22    |
| 1:A:91:VAL:CB    | 1:A:109:ALA:HB2  | 0.88     | 1.99        | 12     | 24    |
| 1:A:73:ILE:HA    | 1:A:93:LYS:O     | 0.88     | 1.68        | 8      | 24    |
| 1:A:44:LEU:HD23  | 1:A:110:PHE:CZ   | 0.88     | 2.04        | 13     | 19    |
| 1:A:185:LEU:HD13 | 1:A:185:LEU:C    | 0.88     | 1.89        | 21     | 2     |
| 1:A:176:ILE:HG21 | 1:A:193:GLN:OE1  | 0.87     | 1.69        | 20     | 24    |
| 1:A:42:LYS:O     | 1:A:46:ASN:CB    | 0.87     | 2.23        | 8      | 24    |
| 1:A:71:LEU:HA    | 1:A:96:GLN:HB2   | 0.87     | 1.46        | 19     | 24    |
| 1:A:87:THR:HA    | 1:A:114:GLN:HB2  | 0.87     | 1.43        | 24     | 16    |
| 1:A:184:LEU:HD23 | 1:A:184:LEU:O    | 0.87     | 1.68        | 16     | 5     |
| 1:A:178:PHE:CE2  | 1:A:193:GLN:HB3  | 0.87     | 2.05        | 21     | 24    |
| 1:A:34:LEU:HD13  | 1:A:35:PRO:HD2   | 0.86     | 1.44        | 5      | 8     |
| 1:A:82:ILE:O     | 1:A:85:ARG:O     | 0.86     | 1.93        | 14     | 24    |
| 1:A:6:TYR:CG     | 1:A:45:GLU:HG2   | 0.86     | 2.05        | 3      | 24    |
| 1:A:41:GLN:HB3   | 1:A:44:LEU:HD11  | 0.86     | 1.47        | 13     | 13    |
| 1:A:185:LEU:O    | 1:A:185:LEU:HD13 | 0.85     | 1.70        | 22     | 2     |
| 1:A:25:ASP:HB2   | 1:A:28:TYR:CE1   | 0.85     | 2.07        | 11     | 24    |
| 1:A:180:ASN:HA   | 1:A:191:PRO:HA   | 0.85     | 1.46        | 23     | 24    |
| 1:A:178:PHE:CD1  | 1:A:193:GLN:CB   | 0.85     | 2.59        | 17     | 21    |
| 1:A:32:ILE:HG23  | 1:A:73:ILE:HG12  | 0.85     | 1.46        | 3      | 22    |
| 1:A:23:MET:O     | 1:A:30:ILE:HD12  | 0.85     | 1.72        | 21     | 19    |
| 1:A:15:THR:HG23  | 1:A:18:ALA:HB3   | 0.85     | 1.48        | 13     | 9     |
| 1:A:77:THR:CB    | 1:A:90:VAL:HG12  | 0.85     | 2.02        | 12     | 23    |
| 1:A:178:PHE:CD2  | 1:A:193:GLN:HB2  | 0.84     | 2.07        | 4      | 7     |
| 1:A:44:LEU:O     | 1:A:48:ILE:N     | 0.84     | 2.10        | 4      | 24    |
| 1:A:136:VAL:HG23 | 1:A:195:LEU:CD2  | 0.84     | 2.00        | 7      | 2     |
| 1:A:69:TYR:HA    | 1:A:99:GLY:N     | 0.84     | 1.87        | 23     | 24    |
| 1:A:124:THR:HA   | 1:A:206:ALA:CB   | 0.84     | 2.02        | 11     | 24    |
| 1:A:47:TYR:O     | 1:A:51:THR:N     | 0.84     | 2.11        | 6      | 24    |
| 1:A:185:LEU:HD11 | 1:A:191:PRO:O    | 0.84     | 1.71        | 16     | 13    |
| 1:A:66:GLU:N     | 1:A:99:GLY:O     | 0.84     | 2.11        | 3      | 13    |
| 1:A:161:ASP:OD1  | 1:A:194:VAL:HA   | 0.84     | 1.73        | 6      | 23    |
| 1:A:200:ALA:O    | 1:A:204:MET:HB2  | 0.83     | 1.72        | 9      | 22    |
| 1:A:179:PHE:CE1  | 1:A:192:THR:HG22 | 0.83     | 2.08        | 13     | 17    |
| 1:A:41:GLN:OE1   | 1:A:44:LEU:HD21  | 0.83     | 1.73        | 24     | 6     |
| 1:A:116:TYR:O    | 1:A:117:ARG:HG3  | 0.83     | 1.73        | 23     | 12    |
| 1:A:196:VAL:HG22 | 1:A:197:PRO:HD2  | 0.83     | 1.50        | 13     | 3     |
| 1:A:133:LEU:HD23 | 1:A:196:VAL:CG2  | 0.83     | 2.01        | 23     | 16    |
| 1:A:34:LEU:HD23  | 1:A:44:LEU:HD11  | 0.83     | 1.49        | 11     | 8     |
| 1:A:184:LEU:O    | 1:A:184:LEU:HD23 | 0.83     | 1.73        | 14     | 2     |
| 1:A:185:LEU:O    | 1:A:185:LEU:CD1  | 0.83     | 2.25        | 21     | 9     |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:185:LEU:HD12 | 1:A:190:GLY:N    | 0.83     | 1.89        | 3      | 6     |
| 1:A:10:LEU:O     | 1:A:21:ILE:HG13  | 0.83     | 1.74        | 4      | 24    |
| 1:A:55:PHE:CD2   | 1:A:96:GLN:NE2   | 0.83     | 2.45        | 19     | 8     |
| 1:A:161:ASP:OD2  | 1:A:195:LEU:N    | 0.83     | 2.11        | 7      | 23    |
| 1:A:144:LEU:HD23 | 1:A:152:VAL:HG21 | 0.83     | 1.49        | 18     | 8     |
| 1:A:77:THR:HB    | 1:A:90:VAL:HG12  | 0.83     | 1.50        | 9      | 22    |
| 1:A:83:PRO:HB2   | 1:A:84:PRO:CD    | 0.82     | 2.04        | 21     | 24    |
| 1:A:56:LEU:HD22  | 1:A:69:TYR:CD2   | 0.82     | 2.10        | 8      | 24    |
| 1:A:71:LEU:HD11  | 1:A:94:VAL:HG23  | 0.82     | 1.50        | 17     | 23    |
| 1:A:34:LEU:HD21  | 1:A:41:GLN:OE1   | 0.82     | 1.75        | 19     | 4     |
| 1:A:184:LEU:CD1  | 1:A:192:THR:HG23 | 0.82     | 2.04        | 12     | 17    |
| 1:A:32:ILE:HG23  | 1:A:73:ILE:CG2   | 0.82     | 2.04        | 19     | 14    |
| 1:A:156:PRO:HB3  | 1:A:160:LEU:CD1  | 0.82     | 2.05        | 8      | 23    |
| 1:A:73:ILE:HB    | 1:A:94:VAL:HB    | 0.82     | 1.49        | 10     | 21    |
| 1:A:91:VAL:HG23  | 1:A:108:LYS:C    | 0.82     | 1.95        | 16     | 10    |
| 1:A:30:ILE:HG23  | 1:A:32:ILE:CD1   | 0.82     | 2.05        | 12     | 2     |
| 1:A:127:GLN:O    | 1:A:130:THR:HG23 | 0.81     | 1.75        | 23     | 20    |
| 1:A:178:PHE:CD2  | 1:A:193:GLN:CB   | 0.81     | 2.63        | 4      | 23    |
| 1:A:93:LYS:HA    | 1:A:107:TYR:CE1  | 0.81     | 2.10        | 10     | 23    |
| 1:A:73:ILE:HD11  | 1:A:92:LEU:HD22  | 0.81     | 1.50        | 12     | 18    |
| 1:A:136:VAL:HG21 | 1:A:176:ILE:HD12 | 0.81     | 1.52        | 7      | 4     |
| 1:A:185:LEU:O    | 1:A:185:LEU:HD12 | 0.81     | 1.74        | 23     | 1     |
| 1:A:92:LEU:HD11  | 1:A:110:PHE:CZ   | 0.81     | 2.10        | 7      | 18    |
| 1:A:49:ALA:O     | 1:A:53:ASP:HB2   | 0.81     | 1.76        | 1      | 24    |
| 1:A:176:ILE:CG2  | 1:A:193:GLN:OE1  | 0.81     | 2.28        | 20     | 24    |
| 1:A:161:ASP:O    | 1:A:184:LEU:HD21 | 0.81     | 1.76        | 21     | 17    |
| 1:A:66:GLU:N     | 1:A:99:GLY:C     | 0.81     | 2.34        | 3      | 24    |
| 1:A:87:THR:N     | 1:A:114:GLN:HG3  | 0.81     | 1.90        | 22     | 2     |
| 1:A:66:GLU:HB2   | 1:A:100:GLY:CA   | 0.80     | 2.06        | 12     | 24    |
| 1:A:185:LEU:HD11 | 1:A:191:PRO:N    | 0.80     | 1.92        | 1      | 8     |
| 1:A:28:TYR:HB3   | 1:A:69:TYR:CD2   | 0.80     | 2.10        | 20     | 24    |
| 1:A:63:THR:O     | 1:A:65:ARG:N     | 0.80     | 2.13        | 4      | 24    |
| 1:A:161:ASP:CB   | 1:A:193:GLN:NE2  | 0.80     | 2.45        | 15     | 24    |
| 1:A:87:THR:CA    | 1:A:114:GLN:HG3  | 0.80     | 2.05        | 2      | 1     |
| 1:A:156:PRO:CB   | 1:A:160:LEU:HD12 | 0.80     | 2.07        | 13     | 13    |
| 1:A:32:ILE:HD11  | 1:A:71:LEU:HD23  | 0.80     | 1.53        | 8      | 9     |
| 1:A:71:LEU:HD13  | 1:A:96:GLN:NE2   | 0.80     | 1.92        | 21     | 20    |
| 1:A:112:TRP:HA   | 1:A:119:PRO:HA   | 0.80     | 1.52        | 16     | 24    |
| 1:A:48:ILE:CD1   | 1:A:71:LEU:HD21  | 0.80     | 2.07        | 3      | 10    |
| 1:A:185:LEU:HD12 | 1:A:190:GLY:CA   | 0.80     | 2.07        | 17     | 6     |
| 1:A:112:TRP:CZ2  | 1:A:117:ARG:HA   | 0.80     | 2.12        | 2      | 24    |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:78:TYR:CE1   | 1:A:91:VAL:HG13  | 0.79     | 2.12        | 12     | 10    |
| 1:A:32:ILE:CG1   | 1:A:73:ILE:HG23  | 0.79     | 2.07        | 3      | 21    |
| 1:A:152:VAL:HG12 | 1:A:153:SER:H    | 0.79     | 1.35        | 21     | 24    |
| 1:A:44:LEU:HD23  | 1:A:110:PHE:CE1  | 0.79     | 2.13        | 12     | 17    |
| 1:A:64:PRO:O     | 1:A:101:THR:HB   | 0.79     | 1.76        | 14     | 24    |
| 1:A:41:GLN:OE1   | 1:A:90:VAL:HG21  | 0.79     | 1.78        | 10     | 6     |
| 1:A:155:ALA:CB   | 1:A:158:ALA:HB3  | 0.78     | 2.06        | 3      | 24    |
| 1:A:110:PHE:N    | 1:A:110:PHE:CD1  | 0.78     | 2.51        | 1      | 13    |
| 1:A:28:TYR:CB    | 1:A:69:TYR:CD2   | 0.78     | 2.67        | 13     | 24    |
| 1:A:176:ILE:N    | 1:A:195:LEU:HD12 | 0.78     | 1.93        | 9      | 24    |
| 1:A:120:ILE:CG2  | 1:A:124:THR:HG23 | 0.78     | 2.08        | 19     | 10    |
| 1:A:75:SER:CB    | 1:A:92:LEU:HD23  | 0.78     | 2.09        | 3      | 4     |
| 1:A:127:GLN:HG3  | 1:A:204:MET:O    | 0.78     | 1.77        | 5      | 24    |
| 1:A:120:ILE:HG23 | 1:A:124:THR:HG23 | 0.78     | 1.56        | 18     | 13    |
| 1:A:28:TYR:CD2   | 1:A:56:LEU:HD13  | 0.78     | 2.13        | 13     | 24    |
| 1:A:56:LEU:HD22  | 1:A:69:TYR:HD2   | 0.77     | 1.38        | 3      | 24    |
| 1:A:178:PHE:CD2  | 1:A:193:GLN:HB3  | 0.77     | 2.14        | 19     | 23    |
| 1:A:32:ILE:HD12  | 1:A:32:ILE:N     | 0.77     | 1.94        | 24     | 5     |
| 1:A:79:GLN:NE2   | 1:A:114:GLN:OE1  | 0.77     | 2.17        | 22     | 8     |
| 1:A:144:LEU:HD23 | 1:A:152:VAL:CG2  | 0.77     | 2.08        | 18     | 17    |
| 1:A:175:VAL:HG13 | 1:A:196:VAL:HB   | 0.77     | 1.55        | 18     | 2     |
| 1:A:138:PRO:O    | 1:A:142:GLY:N    | 0.77     | 2.18        | 10     | 24    |
| 1:A:48:ILE:HD13  | 1:A:73:ILE:HD13  | 0.77     | 1.56        | 4      | 12    |
| 1:A:41:GLN:HE21  | 1:A:44:LEU:HD21  | 0.77     | 1.40        | 6      | 10    |
| 1:A:31:ASN:C     | 1:A:32:ILE:HD12  | 0.77     | 2.00        | 20     | 14    |
| 1:A:161:ASP:HB2  | 1:A:193:GLN:NE2  | 0.77     | 1.95        | 17     | 24    |
| 1:A:91:VAL:HG12  | 1:A:109:ALA:CB   | 0.77     | 2.10        | 12     | 9     |
| 1:A:91:VAL:HG23  | 1:A:109:ALA:N    | 0.77     | 1.95        | 18     | 10    |
| 1:A:124:THR:HA   | 1:A:206:ALA:HB2  | 0.76     | 1.54        | 18     | 18    |
| 1:A:133:LEU:HD22 | 1:A:194:VAL:CG2  | 0.76     | 2.10        | 18     | 20    |
| 1:A:127:GLN:HA   | 1:A:206:ALA:C    | 0.76     | 1.99        | 18     | 24    |
| 1:A:178:PHE:CZ   | 1:A:193:GLN:CD   | 0.76     | 2.59        | 19     | 23    |
| 1:A:44:LEU:HB3   | 1:A:110:PHE:CZ   | 0.76     | 2.16        | 20     | 21    |
| 1:A:10:LEU:O     | 1:A:21:ILE:CG1   | 0.76     | 2.34        | 8      | 24    |
| 1:A:185:LEU:HD11 | 1:A:190:GLY:C    | 0.76     | 2.00        | 21     | 1     |
| 1:A:32:ILE:HG13  | 1:A:73:ILE:CG2   | 0.76     | 2.10        | 22     | 19    |
| 1:A:113:ASP:N    | 1:A:118:LYS:O    | 0.76     | 2.14        | 11     | 11    |
| 1:A:175:VAL:HG13 | 1:A:196:VAL:HG23 | 0.76     | 1.57        | 21     | 17    |
| 1:A:52:ARG:HB3   | 1:A:71:LEU:HD22  | 0.76     | 1.56        | 19     | 18    |
| 1:A:91:VAL:HG11  | 1:A:169:ALA:HB2  | 0.76     | 1.57        | 21     | 8     |
| 1:A:44:LEU:O     | 1:A:47:TYR:HB3   | 0.75     | 1.81        | 12     | 24    |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:159:GLY:N    | 1:A:184:LEU:HD12 | 0.75     | 1.96        | 19     | 5     |
| 1:A:41:GLN:O     | 1:A:44:LEU:HG    | 0.75     | 1.81        | 17     | 21    |
| 1:A:202:ASP:HA   | 1:A:205:LEU:HD22 | 0.75     | 1.56        | 5      | 23    |
| 1:A:184:LEU:C    | 1:A:185:LEU:HD12 | 0.75     | 2.02        | 10     | 6     |
| 1:A:185:LEU:C    | 1:A:189:ALA:HB3  | 0.75     | 2.02        | 19     | 11    |
| 1:A:34:LEU:CD1   | 1:A:41:GLN:HG3   | 0.75     | 2.11        | 19     | 16    |
| 1:A:34:LEU:HD11  | 1:A:41:GLN:HG3   | 0.75     | 1.59        | 19     | 9     |
| 1:A:184:LEU:HD22 | 1:A:184:LEU:O    | 0.75     | 1.80        | 21     | 8     |
| 1:A:196:VAL:HG12 | 1:A:201:ILE:CG2  | 0.74     | 2.11        | 18     | 21    |
| 1:A:92:LEU:HD12  | 1:A:108:LYS:O    | 0.74     | 1.81        | 7      | 8     |
| 1:A:19:CYS:O     | 1:A:33:SER:HA    | 0.74     | 1.82        | 2      | 24    |
| 1:A:77:THR:OG1   | 1:A:90:VAL:HG12  | 0.74     | 1.82        | 3      | 15    |
| 1:A:44:LEU:HB3   | 1:A:92:LEU:HD21  | 0.74     | 1.58        | 19     | 2     |
| 1:A:82:ILE:O     | 1:A:83:PRO:C     | 0.74     | 2.26        | 20     | 24    |
| 1:A:176:ILE:HG12 | 1:A:193:GLN:CG   | 0.74     | 2.13        | 15     | 24    |
| 1:A:89:ALA:HB2   | 1:A:170:VAL:HG13 | 0.74     | 1.60        | 5      | 1     |
| 1:A:43:SER:O     | 1:A:47:TYR:HB2   | 0.74     | 1.82        | 7      | 24    |
| 1:A:139:ILE:O    | 1:A:143:GLU:N    | 0.74     | 2.20        | 17     | 24    |
| 1:A:80:SER:N     | 1:A:87:THR:O     | 0.74     | 2.21        | 7      | 24    |
| 1:A:63:THR:O     | 1:A:65:ARG:HG3   | 0.74     | 1.83        | 13     | 12    |
| 1:A:110:PHE:CD1  | 1:A:110:PHE:N    | 0.74     | 2.56        | 8      | 11    |
| 1:A:41:GLN:C     | 1:A:43:SER:N     | 0.74     | 2.40        | 15     | 24    |
| 1:A:170:VAL:HG23 | 1:A:174:GLY:O    | 0.74     | 1.83        | 7      | 21    |
| 1:A:178:PHE:CE1  | 1:A:193:GLN:HB3  | 0.74     | 2.18        | 17     | 3     |
| 1:A:178:PHE:CZ   | 1:A:193:GLN:HB3  | 0.74     | 2.18        | 11     | 18    |
| 1:A:184:LEU:HD12 | 1:A:192:THR:HG23 | 0.74     | 1.60        | 12     | 6     |
| 1:A:133:LEU:N    | 1:A:134:PRO:CD   | 0.73     | 2.51        | 22     | 24    |
| 1:A:152:VAL:HG12 | 1:A:153:SER:N    | 0.73     | 1.98        | 21     | 18    |
| 1:A:55:PHE:CD1   | 1:A:104:THR:HG21 | 0.73     | 2.18        | 24     | 22    |
| 1:A:95:TYR:CD1   | 1:A:105:THR:HG22 | 0.73     | 2.18        | 8      | 2     |
| 1:A:124:THR:CA   | 1:A:206:ALA:HB2  | 0.73     | 2.14        | 11     | 24    |
| 1:A:44:LEU:HB3   | 1:A:110:PHE:HZ   | 0.73     | 1.43        | 17     | 21    |
| 1:A:32:ILE:CG2   | 1:A:73:ILE:HG23  | 0.73     | 2.14        | 18     | 15    |
| 1:A:27:ALA:O     | 1:A:69:TYR:CD1   | 0.72     | 2.42        | 20     | 24    |
| 1:A:92:LEU:O     | 1:A:107:TYR:CD1  | 0.72     | 2.41        | 17     | 22    |
| 1:A:78:TYR:CE1   | 1:A:91:VAL:HG12  | 0.72     | 2.19        | 9      | 11    |
| 1:A:6:TYR:CG     | 1:A:7:CYS:N      | 0.72     | 2.55        | 6      | 24    |
| 1:A:33:SER:O     | 1:A:34:LEU:HD22  | 0.72     | 1.84        | 24     | 10    |
| 1:A:6:TYR:OH     | 1:A:34:LEU:HD23  | 0.72     | 1.84        | 15     | 10    |
| 1:A:68:PRO:O     | 1:A:99:GLY:HA2   | 0.72     | 1.84        | 3      | 7     |
| 1:A:97:ASN:OD1   | 1:A:100:GLY:C    | 0.72     | 2.27        | 17     | 5     |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:144:LEU:HD23 | 1:A:152:VAL:HG23 | 0.72     | 1.61        | 6      | 16    |
| 1:A:53:ASP:O     | 1:A:57:SER:CB    | 0.72     | 2.37        | 24     | 24    |
| 1:A:107:TYR:HB2  | 1:A:191:PRO:HG3  | 0.72     | 1.60        | 21     | 9     |
| 1:A:185:LEU:CD1  | 1:A:190:GLY:C    | 0.72     | 2.58        | 20     | 8     |
| 1:A:44:LEU:HB3   | 1:A:92:LEU:HD11  | 0.72     | 1.59        | 5      | 18    |
| 1:A:21:ILE:CG2   | 1:A:32:ILE:HB    | 0.72     | 2.15        | 6      | 22    |
| 1:A:31:ASN:O     | 1:A:32:ILE:HD12  | 0.72     | 1.85        | 23     | 4     |
| 1:A:185:LEU:HD12 | 1:A:190:GLY:C    | 0.72     | 2.05        | 8      | 10    |
| 1:A:133:LEU:HD13 | 1:A:194:VAL:HG21 | 0.71     | 1.62        | 13     | 15    |
| 1:A:160:LEU:CD1  | 1:A:194:VAL:HG12 | 0.71     | 2.15        | 4      | 21    |
| 1:A:90:VAL:HG23  | 1:A:110:PHE:CE1  | 0.71     | 2.20        | 11     | 22    |
| 1:A:185:LEU:O    | 1:A:190:GLY:O    | 0.71     | 2.08        | 4      | 15    |
| 1:A:178:PHE:CG   | 1:A:193:GLN:CB   | 0.71     | 2.73        | 7      | 23    |
| 1:A:197:PRO:HB3  | 1:A:200:ALA:HB3  | 0.71     | 1.61        | 18     | 24    |
| 1:A:68:PRO:C     | 1:A:99:GLY:HA2   | 0.71     | 2.05        | 5      | 24    |
| 1:A:73:ILE:HB    | 1:A:94:VAL:CG2   | 0.71     | 2.14        | 6      | 23    |
| 1:A:32:ILE:N     | 1:A:32:ILE:HD12  | 0.71     | 2.01        | 11     | 7     |
| 1:A:159:GLY:CA   | 1:A:184:LEU:HD12 | 0.71     | 2.16        | 11     | 5     |
| 1:A:54:LYS:O     | 1:A:57:SER:HB3   | 0.71     | 1.86        | 8      | 16    |
| 1:A:102:HIS:CE1  | 1:A:104:THR:OG1  | 0.70     | 2.43        | 2      | 14    |
| 1:A:196:VAL:HG12 | 1:A:197:PRO:HD2  | 0.70     | 1.63        | 16     | 21    |
| 1:A:178:PHE:N    | 1:A:178:PHE:CD1  | 0.70     | 2.59        | 16     | 2     |
| 1:A:34:LEU:HD11  | 1:A:44:LEU:HD21  | 0.70     | 1.63        | 15     | 3     |
| 1:A:133:LEU:HD13 | 1:A:194:VAL:CG2  | 0.70     | 2.16        | 14     | 17    |
| 1:A:73:ILE:HB    | 1:A:94:VAL:CB    | 0.70     | 2.16        | 3      | 21    |
| 1:A:41:GLN:NE2   | 1:A:90:VAL:HG21  | 0.70     | 2.02        | 17     | 15    |
| 1:A:78:TYR:HE1   | 1:A:91:VAL:HG12  | 0.70     | 1.47        | 15     | 7     |
| 1:A:52:ARG:HA    | 1:A:96:GLN:HE22  | 0.70     | 1.46        | 6      | 5     |
| 1:A:44:LEU:CB    | 1:A:92:LEU:HD21  | 0.70     | 2.17        | 19     | 8     |
| 1:A:34:LEU:HD13  | 1:A:35:PRO:CD    | 0.70     | 2.17        | 5      | 6     |
| 1:A:6:TYR:CD2    | 1:A:7:CYS:N      | 0.70     | 2.60        | 19     | 24    |
| 1:A:41:GLN:NE2   | 1:A:44:LEU:HD21  | 0.70     | 2.00        | 9      | 7     |
| 1:A:133:LEU:HB2  | 1:A:194:VAL:HB   | 0.70     | 1.63        | 4      | 24    |
| 1:A:34:LEU:HD21  | 1:A:44:LEU:HD21  | 0.69     | 1.64        | 5      | 2     |
| 1:A:88:GLN:HB3   | 1:A:114:GLN:HG2  | 0.69     | 1.64        | 3      | 2     |
| 1:A:41:GLN:CD    | 1:A:44:LEU:HD21  | 0.69     | 2.08        | 3      | 4     |
| 1:A:75:SER:HB3   | 1:A:92:LEU:HD23  | 0.69     | 1.63        | 3      | 6     |
| 1:A:161:ASP:OD2  | 1:A:195:LEU:HB2  | 0.69     | 1.87        | 17     | 23    |
| 1:A:136:VAL:HG11 | 1:A:162:PRO:CD   | 0.69     | 2.17        | 7      | 23    |
| 1:A:95:TYR:CG    | 1:A:105:THR:HG22 | 0.69     | 2.22        | 1      | 2     |
| 1:A:116:TYR:O    | 1:A:117:ARG:HG2  | 0.69     | 1.86        | 12     | 2     |

*Continued on next page...*

Continued from previous page...

| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:134:PRO:O    | 1:A:138:PRO:HD3  | 0.69     | 1.88        | 5      | 24    |
| 1:A:42:LYS:HE3   | 1:A:42:LYS:HA    | 0.69     | 1.63        | 8      | 11    |
| 1:A:184:LEU:CD2  | 1:A:184:LEU:O    | 0.69     | 2.40        | 7      | 8     |
| 1:A:96:GLN:O     | 1:A:104:THR:O    | 0.69     | 2.11        | 18     | 24    |
| 1:A:93:LYS:CA    | 1:A:107:TYR:CE1  | 0.69     | 2.75        | 18     | 23    |
| 1:A:90:VAL:CG2   | 1:A:110:PHE:CE1  | 0.69     | 2.76        | 5      | 3     |
| 1:A:68:PRO:HD2   | 1:A:99:GLY:HA2   | 0.69     | 1.64        | 6      | 23    |
| 1:A:197:PRO:HB2  | 1:A:201:ILE:HG23 | 0.69     | 1.64        | 18     | 6     |
| 1:A:124:THR:HB   | 1:A:206:ALA:HB2  | 0.69     | 1.63        | 24     | 6     |
| 1:A:13:THR:N     | 1:A:20:GLN:O     | 0.68     | 2.24        | 2      | 24    |
| 1:A:176:ILE:HD13 | 1:A:193:GLN:OE1  | 0.68     | 1.88        | 19     | 24    |
| 1:A:71:LEU:HD11  | 1:A:94:VAL:CG2   | 0.68     | 2.16        | 17     | 23    |
| 1:A:68:PRO:O     | 1:A:99:GLY:N     | 0.68     | 2.26        | 20     | 24    |
| 1:A:161:ASP:OD2  | 1:A:176:ILE:CG1  | 0.68     | 2.41        | 6      | 24    |
| 1:A:181:PRO:CG   | 1:A:192:THR:OG1  | 0.68     | 2.42        | 1      | 24    |
| 1:A:41:GLN:O     | 1:A:43:SER:N     | 0.68     | 2.26        | 15     | 24    |
| 1:A:92:LEU:HD11  | 1:A:110:PHE:HZ   | 0.68     | 1.48        | 13     | 19    |
| 1:A:55:PHE:CD2   | 1:A:96:GLN:HG2   | 0.68     | 2.24        | 6      | 2     |
| 1:A:42:LYS:CA    | 1:A:42:LYS:HE3   | 0.68     | 2.17        | 2      | 10    |
| 1:A:178:PHE:CE1  | 1:A:193:GLN:CD   | 0.68     | 2.67        | 6      | 14    |
| 1:A:86:GLY:C     | 1:A:114:GLN:HB2  | 0.68     | 2.08        | 16     | 9     |
| 1:A:30:ILE:HG22  | 1:A:32:ILE:HD12  | 0.68     | 1.65        | 16     | 4     |
| 1:A:124:THR:CB   | 1:A:206:ALA:HB2  | 0.68     | 2.19        | 9      | 24    |
| 1:A:116:TYR:C    | 1:A:117:ARG:HG3  | 0.68     | 2.10        | 14     | 2     |
| 1:A:175:VAL:O    | 1:A:196:VAL:HG23 | 0.68     | 1.89        | 21     | 20    |
| 1:A:184:LEU:HD13 | 1:A:192:THR:HG23 | 0.67     | 1.65        | 1      | 10    |
| 1:A:44:LEU:HD12  | 1:A:45:GLU:H     | 0.67     | 1.50        | 15     | 10    |
| 1:A:122:TYR:HB3  | 1:A:126:TRP:CD1  | 0.67     | 2.23        | 5      | 24    |
| 1:A:133:LEU:N    | 1:A:133:LEU:HD12 | 0.67     | 2.05        | 19     | 13    |
| 1:A:184:LEU:HB3  | 1:A:192:THR:OG1  | 0.67     | 1.89        | 15     | 23    |
| 1:A:157:ASN:O    | 1:A:184:LEU:HB2  | 0.67     | 1.88        | 7      | 22    |
| 1:A:42:LYS:HE3   | 1:A:42:LYS:CA    | 0.67     | 2.18        | 16     | 9     |
| 1:A:59:ALA:HA    | 1:A:63:THR:OG1   | 0.67     | 1.89        | 3      | 24    |
| 1:A:96:GLN:O     | 1:A:104:THR:CB   | 0.67     | 2.42        | 6      | 19    |
| 1:A:28:TYR:HA    | 1:A:69:TYR:H     | 0.67     | 1.50        | 17     | 24    |
| 1:A:65:ARG:O     | 1:A:66:GLU:C     | 0.67     | 2.32        | 3      | 24    |
| 1:A:116:TYR:O    | 1:A:118:LYS:HG3  | 0.67     | 1.89        | 2      | 6     |
| 1:A:141:GLN:HA   | 1:A:144:LEU:HB2  | 0.67     | 1.66        | 21     | 24    |
| 1:A:184:LEU:O    | 1:A:185:LEU:HB2  | 0.67     | 1.88        | 17     | 7     |
| 1:A:178:PHE:CE1  | 1:A:193:GLN:CB   | 0.66     | 2.79        | 1      | 21    |
| 1:A:88:GLN:HB2   | 1:A:114:GLN:OE1  | 0.66     | 1.89        | 22     | 1     |

Continued on next page...

*Continued from previous page...*

| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:176:ILE:HG23 | 1:A:193:GLN:HG3  | 0.66     | 1.67        | 11     | 24    |
| 1:A:201:ILE:HA   | 1:A:204:MET:HB3  | 0.66     | 1.68        | 7      | 24    |
| 1:A:178:PHE:CE2  | 1:A:193:GLN:CB   | 0.66     | 2.78        | 21     | 17    |
| 1:A:48:ILE:CG1   | 1:A:71:LEU:HD21  | 0.66     | 2.20        | 7      | 23    |
| 1:A:91:VAL:CG1   | 1:A:109:ALA:HB2  | 0.66     | 2.20        | 12     | 9     |
| 1:A:28:TYR:C     | 1:A:28:TYR:HD1   | 0.66     | 1.92        | 5      | 13    |
| 1:A:66:GLU:HB2   | 1:A:99:GLY:O     | 0.66     | 1.87        | 3      | 2     |
| 1:A:75:SER:HA    | 1:A:92:LEU:HA    | 0.66     | 1.67        | 3      | 21    |
| 1:A:69:TYR:HB3   | 1:A:98:ALA:HA    | 0.66     | 1.68        | 17     | 24    |
| 1:A:21:ILE:HD13  | 1:A:21:ILE:C     | 0.66     | 2.12        | 14     | 10    |
| 1:A:48:ILE:CD1   | 1:A:73:ILE:HD13  | 0.66     | 2.21        | 4      | 6     |
| 1:A:48:ILE:HD13  | 1:A:73:ILE:CD1   | 0.66     | 2.21        | 2      | 12    |
| 1:A:77:THR:HG23  | 1:A:90:VAL:CG1   | 0.66     | 2.21        | 23     | 1     |
| 1:A:184:LEU:O    | 1:A:184:LEU:HD22 | 0.66     | 1.90        | 15     | 8     |
| 1:A:28:TYR:HD1   | 1:A:28:TYR:C     | 0.65     | 1.93        | 15     | 11    |
| 1:A:137:PHE:CE1  | 1:A:160:LEU:HA   | 0.65     | 2.25        | 15     | 24    |
| 1:A:170:VAL:HA   | 1:A:175:VAL:HA   | 0.65     | 1.68        | 4      | 21    |
| 1:A:133:LEU:HD12 | 1:A:133:LEU:N    | 0.65     | 2.05        | 10     | 11    |
| 1:A:15:THR:HG21  | 1:A:20:GLN:NE2   | 0.65     | 2.05        | 23     | 9     |
| 1:A:66:GLU:H     | 1:A:99:GLY:C     | 0.65     | 1.93        | 3      | 3     |
| 1:A:111:ASP:OD2  | 1:A:170:VAL:HG11 | 0.65     | 1.91        | 10     | 5     |
| 1:A:86:GLY:O     | 1:A:114:GLN:HB2  | 0.65     | 1.92        | 20     | 7     |
| 1:A:176:ILE:HG13 | 1:A:195:LEU:HB2  | 0.65     | 1.67        | 21     | 24    |
| 1:A:133:LEU:O    | 1:A:195:LEU:N    | 0.65     | 2.30        | 13     | 24    |
| 1:A:144:LEU:O    | 1:A:147:GLN:N    | 0.65     | 2.30        | 15     | 24    |
| 1:A:184:LEU:O    | 1:A:184:LEU:CD2  | 0.65     | 2.44        | 13     | 12    |
| 1:A:185:LEU:CB   | 1:A:191:PRO:O    | 0.65     | 2.45        | 17     | 8     |
| 1:A:125:LEU:C    | 1:A:125:LEU:HD13 | 0.65     | 2.12        | 18     | 16    |
| 1:A:141:GLN:O    | 1:A:145:SER:N    | 0.65     | 2.27        | 10     | 24    |
| 1:A:42:LYS:CE    | 1:A:42:LYS:HA    | 0.65     | 2.22        | 24     | 13    |
| 1:A:156:PRO:O    | 1:A:184:LEU:CD1  | 0.65     | 2.44        | 17     | 15    |
| 1:A:175:VAL:HG13 | 1:A:196:VAL:CG2  | 0.65     | 2.20        | 21     | 17    |
| 1:A:90:VAL:O     | 1:A:109:ALA:HA   | 0.65     | 1.92        | 23     | 9     |
| 1:A:82:ILE:O     | 1:A:83:PRO:O     | 0.65     | 2.15        | 20     | 24    |
| 1:A:28:TYR:HA    | 1:A:69:TYR:N     | 0.65     | 2.06        | 23     | 24    |
| 1:A:29:ASN:O     | 1:A:70:GLU:HA    | 0.65     | 1.91        | 19     | 24    |
| 1:A:160:LEU:HD22 | 1:A:161:ASP:OD1  | 0.65     | 1.92        | 17     | 14    |
| 1:A:176:ILE:HA   | 1:A:195:LEU:HA   | 0.65     | 1.68        | 5      | 24    |
| 1:A:80:SER:HB2   | 1:A:87:THR:N     | 0.65     | 2.05        | 2      | 3     |
| 1:A:141:GLN:NE2  | 1:A:154:ILE:HD12 | 0.64     | 2.07        | 18     | 20    |
| 1:A:28:TYR:CD1   | 1:A:28:TYR:C     | 0.64     | 2.70        | 15     | 11    |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:28:TYR:C     | 1:A:28:TYR:CD1   | 0.64     | 2.70        | 2      | 13    |
| 1:A:21:ILE:HG23  | 1:A:21:ILE:O     | 0.64     | 1.91        | 23     | 13    |
| 1:A:179:PHE:CD1  | 1:A:192:THR:HG22 | 0.64     | 2.26        | 13     | 1     |
| 1:A:152:VAL:CG1  | 1:A:153:SER:H    | 0.64     | 2.03        | 6      | 24    |
| 1:A:178:PHE:CA   | 1:A:192:THR:O    | 0.64     | 2.46        | 19     | 24    |
| 1:A:156:PRO:HA   | 1:A:160:LEU:HB2  | 0.64     | 1.69        | 14     | 15    |
| 1:A:6:TYR:CD1    | 1:A:45:GLU:HG2   | 0.64     | 2.26        | 13     | 16    |
| 1:A:32:ILE:CG1   | 1:A:73:ILE:CG2   | 0.64     | 2.75        | 13     | 22    |
| 1:A:184:LEU:O    | 1:A:185:LEU:HB3  | 0.64     | 1.92        | 21     | 1     |
| 1:A:87:THR:N     | 1:A:114:GLN:HB2  | 0.64     | 2.06        | 3      | 7     |
| 1:A:30:ILE:HG22  | 1:A:32:ILE:HD13  | 0.64     | 1.70        | 23     | 2     |
| 1:A:12:GLY:HA2   | 1:A:20:GLN:O     | 0.64     | 1.92        | 12     | 24    |
| 1:A:56:LEU:HB3   | 1:A:69:TYR:CE2   | 0.64     | 2.28        | 12     | 24    |
| 1:A:113:ASP:O    | 1:A:113:ASP:OD1  | 0.64     | 2.15        | 1      | 8     |
| 1:A:66:GLU:CB    | 1:A:99:GLY:C     | 0.64     | 2.65        | 24     | 23    |
| 1:A:91:VAL:HB    | 1:A:109:ALA:CB   | 0.64     | 2.21        | 9      | 9     |
| 1:A:88:GLN:OE1   | 1:A:112:TRP:HB3  | 0.64     | 1.93        | 6      | 20    |
| 1:A:21:ILE:C     | 1:A:21:ILE:HD13  | 0.63     | 2.12        | 6      | 12    |
| 1:A:136:VAL:CG1  | 1:A:161:ASP:HA   | 0.63     | 2.24        | 17     | 22    |
| 1:A:63:THR:HG22  | 1:A:64:PRO:HD2   | 0.63     | 1.70        | 18     | 23    |
| 1:A:134:PRO:HA   | 1:A:160:LEU:HD21 | 0.63     | 1.71        | 7      | 19    |
| 1:A:26:PRO:O     | 1:A:27:ALA:HB2   | 0.63     | 1.93        | 15     | 24    |
| 1:A:21:ILE:O     | 1:A:21:ILE:HG23  | 0.63     | 1.93        | 5      | 11    |
| 1:A:15:THR:HG21  | 1:A:18:ALA:HB3   | 0.63     | 1.70        | 15     | 12    |
| 1:A:32:ILE:HD11  | 1:A:71:LEU:CD2   | 0.63     | 2.24        | 20     | 5     |
| 1:A:21:ILE:HG22  | 1:A:32:ILE:O     | 0.63     | 1.93        | 6      | 13    |
| 1:A:41:GLN:N     | 1:A:41:GLN:OE1   | 0.63     | 2.31        | 8      | 8     |
| 1:A:52:ARG:O     | 1:A:56:LEU:HG    | 0.63     | 1.93        | 8      | 24    |
| 1:A:133:LEU:CD2  | 1:A:196:VAL:HG22 | 0.63     | 2.15        | 23     | 1     |
| 1:A:176:ILE:CA   | 1:A:195:LEU:HD12 | 0.63     | 2.23        | 9      | 24    |
| 1:A:185:LEU:HD21 | 1:A:190:GLY:CA   | 0.63     | 2.23        | 21     | 1     |
| 1:A:137:PHE:N    | 1:A:138:PRO:HD2  | 0.63     | 2.09        | 22     | 24    |
| 1:A:71:LEU:HD13  | 1:A:96:GLN:HE21  | 0.63     | 1.51        | 11     | 13    |
| 1:A:205:LEU:O    | 1:A:206:ALA:HB3  | 0.63     | 1.94        | 18     | 24    |
| 1:A:161:ASP:H    | 1:A:184:LEU:HD11 | 0.63     | 1.54        | 3      | 11    |
| 1:A:136:VAL:HG11 | 1:A:176:ILE:HD11 | 0.63     | 1.70        | 6      | 14    |
| 1:A:34:LEU:HD11  | 1:A:41:GLN:OE1   | 0.63     | 1.94        | 24     | 2     |
| 1:A:185:LEU:CD1  | 1:A:190:GLY:N    | 0.63     | 2.62        | 3      | 8     |
| 1:A:181:PRO:HG3  | 1:A:192:THR:CB   | 0.62     | 2.23        | 22     | 20    |
| 1:A:44:LEU:CG    | 1:A:92:LEU:HD21  | 0.62     | 2.24        | 11     | 9     |
| 1:A:156:PRO:HA   | 1:A:160:LEU:H    | 0.62     | 1.54        | 19     | 6     |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:89:ALA:CB    | 1:A:170:VAL:HG13 | 0.62     | 2.23        | 5      | 1     |
| 1:A:178:PHE:HA   | 1:A:192:THR:O    | 0.62     | 1.94        | 19     | 23    |
| 1:A:91:VAL:CA    | 1:A:109:ALA:HB2  | 0.62     | 2.24        | 12     | 3     |
| 1:A:135:VAL:C    | 1:A:195:LEU:HD23 | 0.62     | 2.15        | 8      | 23    |
| 1:A:107:TYR:HB2  | 1:A:191:PRO:CG   | 0.62     | 2.24        | 21     | 18    |
| 1:A:156:PRO:O    | 1:A:184:LEU:HD13 | 0.62     | 1.95        | 11     | 5     |
| 1:A:113:ASP:CB   | 1:A:118:LYS:O    | 0.62     | 2.48        | 24     | 6     |
| 1:A:30:ILE:HG23  | 1:A:32:ILE:HD12  | 0.62     | 1.71        | 12     | 1     |
| 1:A:87:THR:HA    | 1:A:114:GLN:HG3  | 0.62     | 1.69        | 2      | 1     |
| 1:A:145:SER:O    | 1:A:149:GLY:CA   | 0.62     | 2.47        | 4      | 24    |
| 1:A:136:VAL:C    | 1:A:138:PRO:HD2  | 0.62     | 2.15        | 7      | 24    |
| 1:A:178:PHE:CZ   | 1:A:193:GLN:CB   | 0.62     | 2.82        | 5      | 18    |
| 1:A:79:GLN:HA    | 1:A:87:THR:O     | 0.62     | 1.95        | 7      | 23    |
| 1:A:6:TYR:CD2    | 1:A:45:GLU:CB    | 0.62     | 2.83        | 6      | 16    |
| 1:A:97:ASN:OD1   | 1:A:100:GLY:CA   | 0.62     | 2.48        | 6      | 3     |
| 1:A:197:PRO:O    | 1:A:201:ILE:HG23 | 0.62     | 1.94        | 20     | 3     |
| 1:A:183:GLU:HA   | 1:A:186:PRO:HD3  | 0.62     | 1.72        | 11     | 20    |
| 1:A:47:TYR:O     | 1:A:50:GLN:HB2   | 0.62     | 1.95        | 15     | 24    |
| 1:A:30:ILE:HG23  | 1:A:71:LEU:HD23  | 0.62     | 1.71        | 22     | 9     |
| 1:A:177:PHE:O    | 1:A:193:GLN:HA   | 0.62     | 1.95        | 13     | 24    |
| 1:A:176:ILE:HG23 | 1:A:178:PHE:CZ   | 0.62     | 2.30        | 4      | 2     |
| 1:A:175:VAL:C    | 1:A:195:LEU:HD12 | 0.61     | 2.15        | 9      | 24    |
| 1:A:179:PHE:O    | 1:A:191:PRO:CA   | 0.61     | 2.48        | 10     | 10    |
| 1:A:88:GLN:CB    | 1:A:114:GLN:HG2  | 0.61     | 2.25        | 11     | 2     |
| 1:A:77:THR:OG1   | 1:A:90:VAL:CG1   | 0.61     | 2.49        | 3      | 1     |
| 1:A:125:LEU:HD13 | 1:A:125:LEU:C    | 0.61     | 2.15        | 23     | 8     |
| 1:A:124:THR:O    | 1:A:205:LEU:HB3  | 0.61     | 1.94        | 18     | 8     |
| 1:A:41:GLN:CD    | 1:A:41:GLN:N     | 0.61     | 2.54        | 22     | 8     |
| 1:A:112:TRP:CD1  | 1:A:112:TRP:C    | 0.61     | 2.74        | 5      | 14    |
| 1:A:91:VAL:HG12  | 1:A:109:ALA:HB2  | 0.61     | 1.73        | 2      | 5     |
| 1:A:34:LEU:HD23  | 1:A:44:LEU:CD1   | 0.61     | 2.24        | 11     | 6     |
| 1:A:30:ILE:CG2   | 1:A:71:LEU:HD23  | 0.61     | 2.25        | 21     | 9     |
| 1:A:175:VAL:HG11 | 1:A:201:ILE:CG1  | 0.61     | 2.26        | 1      | 4     |
| 1:A:176:ILE:CG2  | 1:A:178:PHE:CE1  | 0.61     | 2.82        | 4      | 3     |
| 1:A:134:PRO:O    | 1:A:138:PRO:CD   | 0.61     | 2.49        | 5      | 24    |
| 1:A:21:ILE:HG23  | 1:A:32:ILE:HD13  | 0.61     | 1.70        | 24     | 9     |
| 1:A:179:PHE:HE1  | 1:A:192:THR:HG22 | 0.61     | 1.55        | 15     | 18    |
| 1:A:78:TYR:HE1   | 1:A:91:VAL:HG13  | 0.61     | 1.55        | 12     | 7     |
| 1:A:31:ASN:C     | 1:A:32:ILE:CD1   | 0.61     | 2.69        | 17     | 3     |
| 1:A:77:THR:HG23  | 1:A:90:VAL:HG12  | 0.61     | 1.71        | 23     | 1     |
| 1:A:176:ILE:HG13 | 1:A:195:LEU:CB   | 0.61     | 2.26        | 20     | 24    |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:87:THR:C     | 1:A:114:GLN:HG3  | 0.61     | 2.17        | 21     | 9     |
| 1:A:83:PRO:HB2   | 1:A:84:PRO:HD3   | 0.61     | 1.73        | 21     | 24    |
| 1:A:97:ASN:ND2   | 1:A:100:GLY:C    | 0.61     | 2.55        | 24     | 5     |
| 1:A:185:LEU:HD12 | 1:A:185:LEU:C    | 0.61     | 2.15        | 9      | 2     |
| 1:A:181:PRO:HG3  | 1:A:192:THR:HB   | 0.60     | 1.73        | 22     | 15    |
| 1:A:185:LEU:CD2  | 1:A:189:ALA:HB3  | 0.60     | 2.26        | 21     | 1     |
| 1:A:89:ALA:HA    | 1:A:110:PHE:O    | 0.60     | 1.97        | 1      | 18    |
| 1:A:97:ASN:HB2   | 1:A:102:HIS:O    | 0.60     | 1.97        | 7      | 12    |
| 1:A:178:PHE:CZ   | 1:A:193:GLN:NE2  | 0.60     | 2.69        | 6      | 10    |
| 1:A:84:PRO:O     | 1:A:85:ARG:O     | 0.60     | 2.18        | 16     | 24    |
| 1:A:124:THR:HA   | 1:A:206:ALA:CA   | 0.60     | 2.26        | 6      | 24    |
| 1:A:53:ASP:O     | 1:A:57:SER:N     | 0.60     | 2.34        | 8      | 24    |
| 1:A:6:TYR:CG     | 1:A:45:GLU:CG    | 0.60     | 2.84        | 23     | 24    |
| 1:A:116:TYR:O    | 1:A:117:ARG:CG   | 0.60     | 2.49        | 4      | 11    |
| 1:A:91:VAL:CG2   | 1:A:91:VAL:O     | 0.60     | 2.49        | 12     | 4     |
| 1:A:136:VAL:CG1  | 1:A:162:PRO:HD3  | 0.60     | 2.27        | 22     | 24    |
| 1:A:42:LYS:HA    | 1:A:42:LYS:HE3   | 0.60     | 1.73        | 16     | 13    |
| 1:A:66:GLU:CB    | 1:A:100:GLY:HA3  | 0.60     | 2.25        | 18     | 23    |
| 1:A:112:TRP:CE3  | 1:A:119:PRO:HD3  | 0.60     | 2.32        | 6      | 18    |
| 1:A:56:LEU:HD22  | 1:A:69:TYR:HB2   | 0.60     | 1.74        | 24     | 21    |
| 1:A:175:VAL:HG13 | 1:A:196:VAL:CG1  | 0.60     | 2.18        | 13     | 2     |
| 1:A:10:LEU:O     | 1:A:21:ILE:HG12  | 0.60     | 1.97        | 16     | 24    |
| 1:A:47:TYR:CD2   | 1:A:51:THR:OG1   | 0.60     | 2.53        | 19     | 24    |
| 1:A:121:THR:O    | 1:A:125:LEU:N    | 0.60     | 2.35        | 10     | 24    |
| 1:A:41:GLN:HA    | 1:A:41:GLN:NE2   | 0.60     | 2.12        | 1      | 2     |
| 1:A:178:PHE:CD1  | 1:A:178:PHE:N    | 0.60     | 2.66        | 14     | 3     |
| 1:A:44:LEU:HD23  | 1:A:110:PHE:HE1  | 0.60     | 1.51        | 12     | 1     |
| 1:A:157:ASN:HD22 | 1:A:192:THR:HG21 | 0.60     | 1.57        | 15     | 10    |
| 1:A:77:THR:CG2   | 1:A:90:VAL:HG12  | 0.60     | 2.26        | 23     | 2     |
| 1:A:42:LYS:HA    | 1:A:42:LYS:CE    | 0.60     | 2.24        | 22     | 6     |
| 1:A:131:ASP:HB3  | 1:A:132:PRO:CD   | 0.60     | 2.25        | 22     | 3     |
| 1:A:47:TYR:CE2   | 1:A:51:THR:HG23  | 0.60     | 2.32        | 19     | 1     |
| 1:A:185:LEU:CD1  | 1:A:191:PRO:N    | 0.59     | 2.65        | 23     | 8     |
| 1:A:40:ASP:O     | 1:A:43:SER:N     | 0.59     | 2.34        | 8      | 16    |
| 1:A:161:ASP:HB3  | 1:A:176:ILE:HD11 | 0.59     | 1.74        | 22     | 10    |
| 1:A:145:SER:HA   | 1:A:150:GLN:C    | 0.59     | 2.18        | 3      | 18    |
| 1:A:90:VAL:O     | 1:A:110:PHE:CE1  | 0.59     | 2.54        | 3      | 17    |
| 1:A:48:ILE:HG13  | 1:A:71:LEU:HD21  | 0.59     | 1.74        | 21     | 12    |
| 1:A:95:TYR:C     | 1:A:95:TYR:CD1   | 0.59     | 2.73        | 15     | 9     |
| 1:A:42:LYS:HZ1   | 1:A:46:ASN:HA    | 0.59     | 1.57        | 5      | 4     |
| 1:A:101:THR:O    | 1:A:103:PRO:HD3  | 0.59     | 1.98        | 12     | 24    |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:136:VAL:HG11 | 1:A:162:PRO:HD3  | 0.59     | 1.74        | 7      | 15    |
| 1:A:41:GLN:O     | 1:A:44:LEU:N     | 0.59     | 2.36        | 15     | 20    |
| 1:A:112:TRP:NE1  | 1:A:113:ASP:O    | 0.59     | 2.36        | 11     | 22    |
| 1:A:32:ILE:HG23  | 1:A:73:ILE:CG1   | 0.59     | 2.26        | 6      | 21    |
| 1:A:185:LEU:CD1  | 1:A:191:PRO:O    | 0.59     | 2.51        | 18     | 11    |
| 1:A:94:VAL:O     | 1:A:94:VAL:HG13  | 0.59     | 1.97        | 20     | 10    |
| 1:A:161:ASP:HB3  | 1:A:193:GLN:NE2  | 0.59     | 2.10        | 12     | 24    |
| 1:A:131:ASP:CB   | 1:A:132:PRO:CD   | 0.59     | 2.80        | 22     | 4     |
| 1:A:91:VAL:O     | 1:A:91:VAL:CG2   | 0.59     | 2.50        | 2      | 6     |
| 1:A:196:VAL:HG13 | 1:A:201:ILE:HG12 | 0.59     | 1.74        | 13     | 3     |
| 1:A:78:TYR:O     | 1:A:79:GLN:HG2   | 0.59     | 1.97        | 7      | 5     |
| 1:A:73:ILE:HB    | 1:A:94:VAL:HG23  | 0.59     | 1.75        | 21     | 17    |
| 1:A:6:TYR:CE1    | 1:A:44:LEU:HD11  | 0.59     | 2.32        | 10     | 8     |
| 1:A:113:ASP:OD1  | 1:A:113:ASP:O    | 0.59     | 2.21        | 23     | 6     |
| 1:A:179:PHE:N    | 1:A:192:THR:O    | 0.59     | 2.33        | 6      | 24    |
| 1:A:70:GLU:O     | 1:A:96:GLN:HB2   | 0.59     | 1.97        | 6      | 2     |
| 1:A:42:LYS:CE    | 1:A:46:ASN:HB2   | 0.59     | 2.28        | 2      | 24    |
| 1:A:127:GLN:HA   | 1:A:206:ALA:OXT  | 0.59     | 1.97        | 5      | 24    |
| 1:A:178:PHE:CD2  | 1:A:192:THR:C    | 0.59     | 2.76        | 17     | 7     |
| 1:A:184:LEU:C    | 1:A:185:LEU:CG   | 0.59     | 2.71        | 13     | 2     |
| 1:A:91:VAL:O     | 1:A:91:VAL:HG13  | 0.59     | 1.96        | 7      | 5     |
| 1:A:185:LEU:HD11 | 1:A:192:THR:N    | 0.59     | 2.13        | 7      | 7     |
| 1:A:97:ASN:OD1   | 1:A:100:GLY:N    | 0.59     | 2.36        | 17     | 3     |
| 1:A:68:PRO:O     | 1:A:69:TYR:HD1   | 0.58     | 1.81        | 8      | 24    |
| 1:A:112:TRP:CZ2  | 1:A:117:ARG:CA   | 0.58     | 2.86        | 21     | 24    |
| 1:A:113:ASP:OD2  | 1:A:116:TYR:HB2  | 0.58     | 1.98        | 1      | 4     |
| 1:A:48:ILE:O     | 1:A:49:ALA:C     | 0.58     | 2.41        | 14     | 24    |
| 1:A:112:TRP:CD1  | 1:A:113:ASP:O    | 0.58     | 2.56        | 16     | 20    |
| 1:A:95:TYR:CD1   | 1:A:95:TYR:C     | 0.58     | 2.75        | 13     | 15    |
| 1:A:91:VAL:CG1   | 1:A:91:VAL:O     | 0.58     | 2.51        | 23     | 1     |
| 1:A:31:ASN:C     | 1:A:32:ILE:HD13  | 0.58     | 2.19        | 17     | 1     |
| 1:A:178:PHE:HD1  | 1:A:178:PHE:N    | 0.58     | 1.96        | 4      | 2     |
| 1:A:136:VAL:HG11 | 1:A:161:ASP:HA   | 0.58     | 1.75        | 5      | 22    |
| 1:A:127:GLN:H    | 1:A:127:GLN:NE2  | 0.58     | 1.96        | 2      | 16    |
| 1:A:145:SER:HA   | 1:A:150:GLN:O    | 0.58     | 1.98        | 6      | 18    |
| 1:A:28:TYR:CE1   | 1:A:30:ILE:HD11  | 0.58     | 2.34        | 5      | 12    |
| 1:A:185:LEU:HD22 | 1:A:190:GLY:CA   | 0.58     | 2.28        | 10     | 5     |
| 1:A:185:LEU:HD22 | 1:A:190:GLY:C    | 0.58     | 2.18        | 19     | 5     |
| 1:A:95:TYR:CB    | 1:A:105:THR:HG23 | 0.58     | 2.18        | 21     | 3     |
| 1:A:73:ILE:CG1   | 1:A:94:VAL:HG23  | 0.58     | 2.29        | 6      | 1     |
| 1:A:154:ILE:CG2  | 1:A:159:GLY:HA3  | 0.58     | 2.27        | 14     | 5     |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:112:TRP:CZ3  | 1:A:119:PRO:HD3  | 0.58     | 2.33        | 24     | 12    |
| 1:A:185:LEU:CD1  | 1:A:185:LEU:O    | 0.58     | 2.48        | 11     | 4     |
| 1:A:78:TYR:N     | 1:A:78:TYR:CD1   | 0.58     | 2.71        | 23     | 14    |
| 1:A:196:VAL:CB   | 1:A:201:ILE:HG21 | 0.58     | 2.28        | 7      | 18    |
| 1:A:86:GLY:C     | 1:A:114:GLN:HB3  | 0.58     | 2.18        | 23     | 7     |
| 1:A:122:TYR:HA   | 1:A:126:TRP:CD1  | 0.58     | 2.34        | 18     | 7     |
| 1:A:178:PHE:CD2  | 1:A:192:THR:O    | 0.58     | 2.56        | 17     | 8     |
| 1:A:32:ILE:CG2   | 1:A:73:ILE:HD13  | 0.58     | 2.29        | 6      | 2     |
| 1:A:28:TYR:HB2   | 1:A:69:TYR:CD2   | 0.58     | 2.33        | 15     | 24    |
| 1:A:94:VAL:HG13  | 1:A:94:VAL:O     | 0.58     | 1.99        | 12     | 13    |
| 1:A:96:GLN:O     | 1:A:104:THR:HG22 | 0.58     | 1.99        | 8      | 9     |
| 1:A:170:VAL:HB   | 1:A:175:VAL:HB   | 0.58     | 1.75        | 15     | 11    |
| 1:A:135:VAL:HB   | 1:A:195:LEU:HD23 | 0.58     | 1.76        | 7      | 12    |
| 1:A:41:GLN:N     | 1:A:41:GLN:CD    | 0.58     | 2.56        | 16     | 7     |
| 1:A:201:ILE:HA   | 1:A:204:MET:CB   | 0.58     | 2.28        | 5      | 18    |
| 1:A:178:PHE:CE1  | 1:A:193:GLN:HG3  | 0.58     | 2.33        | 4      | 3     |
| 1:A:140:VAL:O    | 1:A:144:LEU:HD13 | 0.58     | 1.98        | 11     | 11    |
| 1:A:22:GLN:HA    | 1:A:30:ILE:O     | 0.57     | 1.99        | 12     | 12    |
| 1:A:94:VAL:O     | 1:A:94:VAL:CG1   | 0.57     | 2.51        | 6      | 2     |
| 1:A:71:LEU:CD1   | 1:A:94:VAL:HG23  | 0.57     | 2.29        | 14     | 11    |
| 1:A:172:ASN:O    | 1:A:198:ARG:HG3  | 0.57     | 1.99        | 11     | 17    |
| 1:A:32:ILE:HG12  | 1:A:73:ILE:CG2   | 0.57     | 2.29        | 12     | 8     |
| 1:A:78:TYR:CD1   | 1:A:78:TYR:N     | 0.57     | 2.72        | 3      | 9     |
| 1:A:143:GLU:O    | 1:A:147:GLN:N    | 0.57     | 2.36        | 5      | 6     |
| 1:A:184:LEU:HD13 | 1:A:193:GLN:H    | 0.57     | 1.58        | 24     | 6     |
| 1:A:97:ASN:ND2   | 1:A:100:GLY:O    | 0.57     | 2.37        | 3      | 1     |
| 1:A:176:ILE:HG23 | 1:A:178:PHE:HE1  | 0.57     | 1.57        | 14     | 10    |
| 1:A:181:PRO:HG3  | 1:A:192:THR:OG1  | 0.57     | 1.99        | 15     | 7     |
| 1:A:54:LYS:CA    | 1:A:57:SER:HB2   | 0.57     | 2.30        | 22     | 19    |
| 1:A:185:LEU:HD22 | 1:A:189:ALA:HB3  | 0.57     | 1.76        | 21     | 1     |
| 1:A:152:VAL:CG1  | 1:A:153:SER:N    | 0.57     | 2.67        | 1      | 16    |
| 1:A:89:ALA:HB2   | 1:A:170:VAL:CG1  | 0.57     | 2.28        | 5      | 1     |
| 1:A:182:GLY:O    | 1:A:183:GLU:HG3  | 0.57     | 1.99        | 13     | 10    |
| 1:A:161:ASP:OD2  | 1:A:176:ILE:HD11 | 0.57     | 1.99        | 20     | 23    |
| 1:A:41:GLN:C     | 1:A:43:SER:H     | 0.57     | 2.02        | 15     | 23    |
| 1:A:55:PHE:CE1   | 1:A:104:THR:HG21 | 0.57     | 2.35        | 9      | 18    |
| 1:A:10:LEU:O     | 1:A:11:LYS:HB2   | 0.57     | 1.98        | 24     | 23    |
| 1:A:27:ALA:O     | 1:A:69:TYR:CE1   | 0.57     | 2.58        | 12     | 24    |
| 1:A:93:LYS:HB2   | 1:A:107:TYR:CE1  | 0.57     | 2.35        | 2      | 20    |
| 1:A:44:LEU:HD12  | 1:A:45:GLU:HB3   | 0.57     | 1.75        | 24     | 10    |
| 1:A:185:LEU:CD1  | 1:A:191:PRO:C    | 0.57     | 2.73        | 13     | 8     |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:29:ASN:ND2   | 1:A:31:ASN:OD1   | 0.57     | 2.38        | 9      | 3     |
| 1:A:73:ILE:CB    | 1:A:94:VAL:HG23  | 0.56     | 2.30        | 6      | 1     |
| 1:A:90:VAL:O     | 1:A:110:PHE:CD1  | 0.56     | 2.58        | 3      | 15    |
| 1:A:63:THR:HG22  | 1:A:102:HIS:HB2  | 0.56     | 1.76        | 21     | 12    |
| 1:A:112:TRP:C    | 1:A:112:TRP:CD1  | 0.56     | 2.78        | 1      | 10    |
| 1:A:101:THR:O    | 1:A:103:PRO:CD   | 0.56     | 2.53        | 3      | 23    |
| 1:A:178:PHE:CE1  | 1:A:193:GLN:CG   | 0.56     | 2.89        | 23     | 22    |
| 1:A:42:LYS:CE    | 1:A:42:LYS:CA    | 0.56     | 2.82        | 8      | 11    |
| 1:A:111:ASP:CG   | 1:A:170:VAL:HG11 | 0.56     | 2.20        | 8      | 5     |
| 1:A:185:LEU:HG   | 1:A:191:PRO:N    | 0.56     | 2.15        | 9      | 2     |
| 1:A:75:SER:HB2   | 1:A:92:LEU:HD23  | 0.56     | 1.76        | 19     | 6     |
| 1:A:178:PHE:CD1  | 1:A:193:GLN:HB3  | 0.56     | 2.31        | 17     | 1     |
| 1:A:91:VAL:HG12  | 1:A:109:ALA:HB1  | 0.56     | 1.77        | 8      | 7     |
| 1:A:102:HIS:CE1  | 1:A:104:THR:HG1  | 0.56     | 2.19        | 18     | 4     |
| 1:A:175:VAL:HG22 | 1:A:175:VAL:O    | 0.56     | 1.99        | 23     | 4     |
| 1:A:141:GLN:O    | 1:A:144:LEU:N    | 0.56     | 2.39        | 24     | 23    |
| 1:A:161:ASP:CB   | 1:A:193:GLN:CD   | 0.56     | 2.74        | 15     | 24    |
| 1:A:175:VAL:CG1  | 1:A:196:VAL:HB   | 0.56     | 2.31        | 18     | 2     |
| 1:A:185:LEU:HD13 | 1:A:189:ALA:CB   | 0.56     | 2.30        | 17     | 4     |
| 1:A:66:GLU:H     | 1:A:101:THR:H    | 0.56     | 1.42        | 18     | 24    |
| 1:A:88:GLN:OE1   | 1:A:112:TRP:CD1  | 0.56     | 2.58        | 8      | 13    |
| 1:A:34:LEU:CD2   | 1:A:44:LEU:HD11  | 0.56     | 2.27        | 11     | 2     |
| 1:A:129:ASP:HB2  | 1:A:204:MET:HG3  | 0.56     | 1.76        | 10     | 5     |
| 1:A:52:ARG:CB    | 1:A:71:LEU:HD22  | 0.56     | 2.30        | 19     | 7     |
| 1:A:55:PHE:CE1   | 1:A:104:THR:CG2  | 0.56     | 2.89        | 10     | 15    |
| 1:A:63:THR:HG21  | 1:A:102:HIS:CD2  | 0.56     | 2.36        | 18     | 2     |
| 1:A:94:VAL:O     | 1:A:94:VAL:HG12  | 0.56     | 2.00        | 6      | 1     |
| 1:A:30:ILE:CG2   | 1:A:32:ILE:CD1   | 0.56     | 2.84        | 3      | 4     |
| 1:A:113:ASP:HB3  | 1:A:118:LYS:O    | 0.55     | 2.02        | 8      | 5     |
| 1:A:34:LEU:HD21  | 1:A:44:LEU:HD13  | 0.55     | 1.78        | 13     | 2     |
| 1:A:133:LEU:HD13 | 1:A:194:VAL:HB   | 0.55     | 1.76        | 18     | 4     |
| 1:A:71:LEU:HG    | 1:A:73:ILE:CG2   | 0.55     | 2.31        | 20     | 5     |
| 1:A:185:LEU:HB3  | 1:A:191:PRO:O    | 0.55     | 2.00        | 24     | 7     |
| 1:A:95:TYR:HB2   | 1:A:105:THR:HG22 | 0.55     | 1.78        | 8      | 2     |
| 1:A:93:LYS:HB2   | 1:A:107:TYR:CZ   | 0.55     | 2.36        | 15     | 18    |
| 1:A:55:PHE:HD2   | 1:A:96:GLN:NE2   | 0.55     | 1.99        | 10     | 7     |
| 1:A:156:PRO:CA   | 1:A:160:LEU:HB2  | 0.55     | 2.31        | 19     | 16    |
| 1:A:159:GLY:O    | 1:A:160:LEU:C    | 0.55     | 2.44        | 4      | 9     |
| 1:A:124:THR:CA   | 1:A:206:ALA:CB   | 0.55     | 2.79        | 23     | 2     |
| 1:A:34:LEU:CD1   | 1:A:35:PRO:HD2   | 0.55     | 2.28        | 5      | 2     |
| 1:A:185:LEU:HD11 | 1:A:191:PRO:CA   | 0.55     | 2.32        | 20     | 5     |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:98:ALA:HB3   | 1:A:102:HIS:HB3  | 0.55     | 1.79        | 3      | 17    |
| 1:A:157:ASN:ND2  | 1:A:192:THR:HG21 | 0.55     | 2.17        | 15     | 2     |
| 1:A:41:GLN:OE1   | 1:A:41:GLN:N     | 0.55     | 2.38        | 16     | 7     |
| 1:A:48:ILE:HD13  | 1:A:73:ILE:HD12  | 0.55     | 1.79        | 22     | 3     |
| 1:A:41:GLN:O     | 1:A:42:LYS:C     | 0.55     | 2.45        | 18     | 24    |
| 1:A:145:SER:O    | 1:A:149:GLY:HA2  | 0.55     | 2.01        | 19     | 24    |
| 1:A:127:GLN:NE2  | 1:A:127:GLN:H    | 0.55     | 1.99        | 19     | 8     |
| 1:A:144:LEU:HD22 | 1:A:154:ILE:HD11 | 0.55     | 1.79        | 15     | 6     |
| 1:A:29:ASN:HB3   | 1:A:70:GLU:CG    | 0.55     | 2.32        | 21     | 2     |
| 1:A:44:LEU:O     | 1:A:47:TYR:CB    | 0.55     | 2.55        | 12     | 24    |
| 1:A:196:VAL:CG1  | 1:A:197:PRO:HD2  | 0.55     | 2.32        | 18     | 3     |
| 1:A:95:TYR:C     | 1:A:95:TYR:HD1   | 0.55     | 2.05        | 15     | 1     |
| 1:A:141:GLN:HE22 | 1:A:154:ILE:HD12 | 0.55     | 1.60        | 7      | 19    |
| 1:A:90:VAL:HG23  | 1:A:110:PHE:HE1  | 0.55     | 1.61        | 16     | 15    |
| 1:A:95:TYR:CB    | 1:A:105:THR:HG22 | 0.55     | 2.32        | 8      | 2     |
| 1:A:95:TYR:HD1   | 1:A:96:GLN:N     | 0.55     | 2.00        | 15     | 3     |
| 1:A:83:PRO:HB2   | 1:A:84:PRO:HD2   | 0.55     | 1.79        | 14     | 24    |
| 1:A:197:PRO:O    | 1:A:201:ILE:CG1  | 0.55     | 2.55        | 15     | 21    |
| 1:A:44:LEU:CD2   | 1:A:110:PHE:CZ   | 0.55     | 2.88        | 13     | 6     |
| 1:A:175:VAL:HG13 | 1:A:196:VAL:CB   | 0.55     | 2.32        | 11     | 17    |
| 1:A:185:LEU:CD1  | 1:A:189:ALA:CB   | 0.55     | 2.84        | 24     | 5     |
| 1:A:134:PRO:O    | 1:A:137:PHE:HB2  | 0.55     | 2.02        | 13     | 22    |
| 1:A:97:ASN:C     | 1:A:97:ASN:HD22  | 0.55     | 2.05        | 24     | 5     |
| 1:A:194:VAL:O    | 1:A:194:VAL:HG23 | 0.55     | 2.01        | 17     | 11    |
| 1:A:122:TYR:HB3  | 1:A:126:TRP:NE1  | 0.54     | 2.17        | 8      | 24    |
| 1:A:6:TYR:CE2    | 1:A:45:GLU:CB    | 0.54     | 2.90        | 23     | 24    |
| 1:A:6:TYR:CD2    | 1:A:45:GLU:CG    | 0.54     | 2.90        | 24     | 21    |
| 1:A:156:PRO:HA   | 1:A:160:LEU:N    | 0.54     | 2.17        | 19     | 21    |
| 1:A:181:PRO:HG2  | 1:A:192:THR:OG1  | 0.54     | 2.02        | 6      | 11    |
| 1:A:66:GLU:HB2   | 1:A:101:THR:N    | 0.54     | 2.17        | 7      | 7     |
| 1:A:91:VAL:HG13  | 1:A:91:VAL:O     | 0.54     | 2.02        | 15     | 4     |
| 1:A:52:ARG:HD3   | 1:A:53:ASP:N     | 0.54     | 2.17        | 12     | 6     |
| 1:A:93:LYS:HG3   | 1:A:107:TYR:CZ   | 0.54     | 2.37        | 5      | 4     |
| 1:A:6:TYR:CE1    | 1:A:41:GLN:HB3   | 0.54     | 2.38        | 6      | 20    |
| 1:A:136:VAL:HB   | 1:A:195:LEU:HB2  | 0.54     | 1.77        | 10     | 20    |
| 1:A:34:LEU:HD21  | 1:A:41:GLN:CG    | 0.54     | 2.32        | 18     | 2     |
| 1:A:170:VAL:O    | 1:A:170:VAL:HG13 | 0.54     | 2.02        | 9      | 1     |
| 1:A:34:LEU:HD12  | 1:A:41:GLN:HG3   | 0.54     | 1.78        | 12     | 3     |
| 1:A:78:TYR:C     | 1:A:79:GLN:HG2   | 0.54     | 2.21        | 17     | 9     |
| 1:A:42:LYS:CA    | 1:A:42:LYS:CE    | 0.54     | 2.86        | 22     | 9     |
| 1:A:178:PHE:CZ   | 1:A:193:GLN:OE1  | 0.54     | 2.61        | 4      | 4     |

*Continued on next page...*

Continued from previous page...

| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:30:ILE:CG2   | 1:A:32:ILE:HD13  | 0.54     | 2.32        | 20     | 2     |
| 1:A:46:ASN:O     | 1:A:50:GLN:HG2   | 0.54     | 2.03        | 10     | 24    |
| 1:A:131:ASP:HB3  | 1:A:132:PRO:HD2  | 0.54     | 1.78        | 22     | 7     |
| 1:A:157:ASN:C    | 1:A:184:LEU:HB2  | 0.54     | 2.23        | 21     | 4     |
| 1:A:161:ASP:HB3  | 1:A:193:GLN:CD   | 0.54     | 2.23        | 1      | 22    |
| 1:A:175:VAL:O    | 1:A:196:VAL:N    | 0.54     | 2.34        | 22     | 17    |
| 1:A:185:LEU:CD1  | 1:A:189:ALA:HB3  | 0.54     | 2.33        | 6      | 4     |
| 1:A:197:PRO:HD2  | 1:A:201:ILE:CG2  | 0.54     | 2.32        | 1      | 18    |
| 1:A:65:ARG:CB    | 1:A:99:GLY:HA3   | 0.54     | 2.32        | 3      | 1     |
| 1:A:69:TYR:CA    | 1:A:99:GLY:H     | 0.54     | 2.04        | 19     | 6     |
| 1:A:6:TYR:HE1    | 1:A:41:GLN:HB3   | 0.54     | 1.62        | 14     | 15    |
| 1:A:80:SER:HB3   | 1:A:87:THR:N     | 0.54     | 2.17        | 8      | 8     |
| 1:A:52:ARG:HA    | 1:A:96:GLN:NE2   | 0.54     | 2.17        | 6      | 9     |
| 1:A:65:ARG:HB3   | 1:A:99:GLY:HA3   | 0.54     | 1.78        | 3      | 1     |
| 1:A:28:TYR:CB    | 1:A:69:TYR:CG    | 0.54     | 2.90        | 23     | 24    |
| 1:A:136:VAL:HG21 | 1:A:176:ILE:CD1  | 0.54     | 2.33        | 17     | 19    |
| 1:A:67:ALA:HB3   | 1:A:68:PRO:CD    | 0.54     | 2.27        | 5      | 14    |
| 1:A:3:PRO:O      | 1:A:4:LYS:HG2    | 0.54     | 2.03        | 5      | 12    |
| 1:A:88:GLN:HG3   | 1:A:112:TRP:CD1  | 0.54     | 2.38        | 15     | 2     |
| 1:A:111:ASP:OD2  | 1:A:125:LEU:HD23 | 0.54     | 2.03        | 9      | 1     |
| 1:A:161:ASP:HB2  | 1:A:193:GLN:O    | 0.54     | 2.03        | 14     | 21    |
| 1:A:113:ASP:OD1  | 1:A:118:LYS:N    | 0.54     | 2.41        | 16     | 9     |
| 1:A:32:ILE:CB    | 1:A:73:ILE:HG23  | 0.54     | 2.33        | 2      | 13    |
| 1:A:55:PHE:CG    | 1:A:104:THR:HG21 | 0.54     | 2.38        | 15     | 12    |
| 1:A:110:PHE:HD1  | 1:A:110:PHE:N    | 0.54     | 2.00        | 1      | 1     |
| 1:A:170:VAL:HG13 | 1:A:170:VAL:O    | 0.54     | 2.03        | 20     | 4     |
| 1:A:28:TYR:HB3   | 1:A:69:TYR:CG    | 0.54     | 2.38        | 10     | 24    |
| 1:A:42:LYS:CD    | 1:A:45:GLU:OE2   | 0.54     | 2.56        | 5      | 8     |
| 1:A:126:TRP:O    | 1:A:206:ALA:CA   | 0.53     | 2.56        | 18     | 24    |
| 1:A:90:VAL:O     | 1:A:90:VAL:HG23  | 0.53     | 2.04        | 23     | 13    |
| 1:A:131:ASP:CB   | 1:A:132:PRO:HD2  | 0.53     | 2.33        | 22     | 22    |
| 1:A:34:LEU:CG    | 1:A:41:GLN:HG3   | 0.53     | 2.33        | 4      | 10    |
| 1:A:91:VAL:HG22  | 1:A:91:VAL:O     | 0.53     | 2.04        | 1      | 1     |
| 1:A:113:ASP:CG   | 1:A:116:TYR:HB2  | 0.53     | 2.22        | 22     | 3     |
| 1:A:64:PRO:O     | 1:A:102:HIS:N    | 0.53     | 2.42        | 4      | 4     |
| 1:A:6:TYR:CE2    | 1:A:45:GLU:HB3   | 0.53     | 2.39        | 20     | 6     |
| 1:A:181:PRO:HD3  | 1:A:192:THR:H    | 0.53     | 1.63        | 23     | 14    |
| 1:A:113:ASP:OD2  | 1:A:118:LYS:HG2  | 0.53     | 2.04        | 18     | 1     |
| 1:A:144:LEU:CD2  | 1:A:152:VAL:HG21 | 0.53     | 2.28        | 18     | 3     |
| 1:A:41:GLN:NE2   | 1:A:41:GLN:HA    | 0.53     | 2.18        | 18     | 2     |
| 1:A:175:VAL:O    | 1:A:175:VAL:CG2  | 0.53     | 2.57        | 23     | 1     |

Continued on next page...

*Continued from previous page...*

| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:202:ASP:O    | 1:A:205:LEU:HB2  | 0.53     | 2.03        | 14     | 24    |
| 1:A:175:VAL:CG2  | 1:A:177:PHE:CE1  | 0.53     | 2.92        | 1      | 18    |
| 1:A:71:LEU:HG    | 1:A:73:ILE:HG22  | 0.53     | 1.79        | 17     | 10    |
| 1:A:41:GLN:N     | 1:A:41:GLN:NE2   | 0.53     | 2.56        | 12     | 3     |
| 1:A:73:ILE:HD11  | 1:A:92:LEU:HD13  | 0.53     | 1.81        | 21     | 2     |
| 1:A:29:ASN:HB3   | 1:A:70:GLU:HG3   | 0.53     | 1.79        | 2      | 2     |
| 1:A:55:PHE:CE1   | 1:A:104:THR:HB   | 0.53     | 2.39        | 19     | 1     |
| 1:A:179:PHE:N    | 1:A:179:PHE:CD1  | 0.53     | 2.77        | 13     | 11    |
| 1:A:185:LEU:HD12 | 1:A:191:PRO:C    | 0.53     | 2.24        | 21     | 1     |
| 1:A:40:ASP:C     | 1:A:42:LYS:N     | 0.53     | 2.61        | 8      | 20    |
| 1:A:82:ILE:N     | 1:A:85:ARG:O     | 0.53     | 2.42        | 3      | 24    |
| 1:A:54:LYS:O     | 1:A:57:SER:CB    | 0.53     | 2.57        | 23     | 23    |
| 1:A:179:PHE:CD1  | 1:A:179:PHE:N    | 0.53     | 2.77        | 23     | 11    |
| 1:A:82:ILE:HG23  | 1:A:83:PRO:HD2   | 0.53     | 1.79        | 16     | 12    |
| 1:A:96:GLN:O     | 1:A:104:THR:HB   | 0.53     | 2.03        | 6      | 7     |
| 1:A:32:ILE:CD1   | 1:A:32:ILE:N     | 0.53     | 2.66        | 24     | 8     |
| 1:A:97:ASN:CG    | 1:A:102:HIS:O    | 0.53     | 2.47        | 21     | 2     |
| 1:A:29:ASN:OD1   | 1:A:30:ILE:N     | 0.53     | 2.42        | 17     | 2     |
| 1:A:90:VAL:HG23  | 1:A:110:PHE:CD1  | 0.53     | 2.38        | 4      | 4     |
| 1:A:185:LEU:HD21 | 1:A:191:PRO:HD2  | 0.53     | 1.81        | 10     | 3     |
| 1:A:178:PHE:HB3  | 1:A:192:THR:O    | 0.53     | 2.03        | 4      | 4     |
| 1:A:71:LEU:CD1   | 1:A:73:ILE:HG22  | 0.53     | 2.34        | 23     | 1     |
| 1:A:180:ASN:CA   | 1:A:191:PRO:HA   | 0.53     | 2.30        | 20     | 4     |
| 1:A:184:LEU:O    | 1:A:185:LEU:HD23 | 0.53     | 2.03        | 1      | 7     |
| 1:A:160:LEU:CD2  | 1:A:161:ASP:OD1  | 0.53     | 2.57        | 15     | 17    |
| 1:A:87:THR:C     | 1:A:114:GLN:CG   | 0.53     | 2.77        | 16     | 8     |
| 1:A:41:GLN:OE1   | 1:A:44:LEU:CD2   | 0.53     | 2.53        | 24     | 4     |
| 1:A:113:ASP:CG   | 1:A:118:LYS:O    | 0.53     | 2.48        | 7      | 3     |
| 1:A:86:GLY:O     | 1:A:114:GLN:HB3  | 0.53     | 2.03        | 1      | 6     |
| 1:A:34:LEU:HD21  | 1:A:44:LEU:CD2   | 0.53     | 2.34        | 5      | 1     |
| 1:A:91:VAL:HG23  | 1:A:107:TYR:CE1  | 0.53     | 2.39        | 17     | 1     |
| 1:A:128:ALA:C    | 1:A:130:THR:H    | 0.53     | 2.07        | 1      | 24    |
| 1:A:197:PRO:CB   | 1:A:201:ILE:HG23 | 0.53     | 2.34        | 18     | 6     |
| 1:A:141:GLN:NE2  | 1:A:154:ILE:CD1  | 0.53     | 2.71        | 18     | 23    |
| 1:A:80:SER:HB2   | 1:A:87:THR:HB    | 0.53     | 1.81        | 13     | 10    |
| 1:A:33:SER:HB2   | 1:A:74:THR:HG23  | 0.53     | 1.79        | 14     | 8     |
| 1:A:32:ILE:HD11  | 1:A:71:LEU:HG    | 0.53     | 1.81        | 23     | 1     |
| 1:A:179:PHE:CE1  | 1:A:181:PRO:HG3  | 0.53     | 2.39        | 17     | 1     |
| 1:A:32:ILE:HD12  | 1:A:73:ILE:CG2   | 0.53     | 2.34        | 17     | 1     |
| 1:A:45:GLU:HA    | 1:A:48:ILE:HB    | 0.53     | 1.80        | 15     | 1     |
| 1:A:131:ASP:O    | 1:A:132:PRO:O    | 0.52     | 2.27        | 8      | 18    |

*Continued on next page...*

Continued from previous page...

| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:6:TYR:CZ     | 1:A:45:GLU:HB3   | 0.52     | 2.38        | 13     | 12    |
| 1:A:124:THR:OG1  | 1:A:206:ALA:HB2  | 0.52     | 2.04        | 8      | 5     |
| 1:A:55:PHE:CE2   | 1:A:104:THR:HB   | 0.52     | 2.38        | 6      | 1     |
| 1:A:176:ILE:HG13 | 1:A:195:LEU:CA   | 0.52     | 2.34        | 20     | 18    |
| 1:A:48:ILE:C     | 1:A:50:GLN:N     | 0.52     | 2.62        | 13     | 24    |
| 1:A:196:VAL:HG13 | 1:A:201:ILE:CG1  | 0.52     | 2.34        | 20     | 3     |
| 1:A:68:PRO:C     | 1:A:99:GLY:CA    | 0.52     | 2.76        | 19     | 8     |
| 1:A:175:VAL:O    | 1:A:175:VAL:HG22 | 0.52     | 2.03        | 13     | 1     |
| 1:A:19:CYS:O     | 1:A:33:SER:CA    | 0.52     | 2.56        | 6      | 10    |
| 1:A:88:GLN:OE1   | 1:A:112:TRP:CG   | 0.52     | 2.63        | 10     | 15    |
| 1:A:132:PRO:C    | 1:A:134:PRO:HD3  | 0.52     | 2.25        | 11     | 19    |
| 1:A:184:LEU:O    | 1:A:185:LEU:CB   | 0.52     | 2.58        | 9      | 4     |
| 1:A:185:LEU:CG   | 1:A:191:PRO:O    | 0.52     | 2.57        | 23     | 5     |
| 1:A:91:VAL:HG23  | 1:A:109:ALA:CA   | 0.52     | 2.34        | 16     | 3     |
| 1:A:48:ILE:HD12  | 1:A:51:THR:HB    | 0.52     | 1.81        | 11     | 3     |
| 1:A:6:TYR:CD2    | 1:A:45:GLU:HB2   | 0.52     | 2.38        | 6      | 4     |
| 1:A:32:ILE:HG12  | 1:A:73:ILE:HG23  | 0.52     | 1.79        | 3      | 1     |
| 1:A:176:ILE:N    | 1:A:195:LEU:CD1  | 0.52     | 2.71        | 9      | 19    |
| 1:A:141:GLN:NE2  | 1:A:154:ILE:CG1  | 0.52     | 2.73        | 15     | 17    |
| 1:A:90:VAL:HG23  | 1:A:90:VAL:O     | 0.52     | 2.04        | 4      | 8     |
| 1:A:175:VAL:CG1  | 1:A:201:ILE:HD11 | 0.52     | 2.34        | 5      | 2     |
| 1:A:88:GLN:CG    | 1:A:112:TRP:CD1  | 0.52     | 2.92        | 15     | 1     |
| 1:A:19:CYS:CB    | 1:A:34:LEU:O     | 0.52     | 2.58        | 17     | 8     |
| 1:A:116:TYR:HB2  | 1:A:118:LYS:HD2  | 0.52     | 1.82        | 11     | 1     |
| 1:A:75:SER:HB3   | 1:A:92:LEU:CD2   | 0.52     | 2.34        | 23     | 3     |
| 1:A:68:PRO:O     | 1:A:99:GLY:HA3   | 0.52     | 2.04        | 3      | 3     |
| 1:A:34:LEU:HD11  | 1:A:41:GLN:CG    | 0.52     | 2.32        | 19     | 1     |
| 1:A:73:ILE:HB    | 1:A:94:VAL:HG22  | 0.52     | 1.80        | 6      | 1     |
| 1:A:83:PRO:CB    | 1:A:84:PRO:CD    | 0.52     | 2.87        | 1      | 20    |
| 1:A:179:PHE:O    | 1:A:181:PRO:HD3  | 0.52     | 2.05        | 23     | 16    |
| 1:A:90:VAL:CG2   | 1:A:90:VAL:O     | 0.52     | 2.58        | 3      | 5     |
| 1:A:176:ILE:CD1  | 1:A:193:GLN:OE1  | 0.52     | 2.56        | 19     | 17    |
| 1:A:43:SER:CB    | 1:A:110:PHE:CE2  | 0.52     | 2.93        | 5      | 2     |
| 1:A:73:ILE:CD1   | 1:A:92:LEU:HD13  | 0.52     | 2.34        | 21     | 1     |
| 1:A:65:ARG:CB    | 1:A:98:ALA:O     | 0.52     | 2.58        | 20     | 13    |
| 1:A:97:ASN:ND2   | 1:A:100:GLY:CA   | 0.52     | 2.72        | 2      | 17    |
| 1:A:26:PRO:O     | 1:A:27:ALA:CB    | 0.52     | 2.58        | 18     | 24    |
| 1:A:97:ASN:HD21  | 1:A:101:THR:N    | 0.52     | 2.01        | 24     | 4     |
| 1:A:113:ASP:OD2  | 1:A:118:LYS:HB3  | 0.52     | 2.05        | 21     | 10    |
| 1:A:178:PHE:CB   | 1:A:192:THR:O    | 0.52     | 2.58        | 19     | 12    |
| 1:A:75:SER:HB3   | 1:A:92:LEU:CG    | 0.52     | 2.35        | 1      | 5     |

Continued on next page...

Continued from previous page...

| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:88:GLN:O     | 1:A:88:GLN:OE1   | 0.52     | 2.28        | 24     | 5     |
| 1:A:184:LEU:O    | 1:A:185:LEU:HD12 | 0.52     | 2.04        | 10     | 2     |
| 1:A:161:ASP:HB3  | 1:A:176:ILE:CD1  | 0.51     | 2.35        | 22     | 7     |
| 1:A:51:THR:O     | 1:A:55:PHE:HD2   | 0.51     | 1.88        | 19     | 1     |
| 1:A:44:LEU:HD12  | 1:A:45:GLU:N     | 0.51     | 2.20        | 12     | 9     |
| 1:A:137:PHE:CE1  | 1:A:159:GLY:O    | 0.51     | 2.63        | 14     | 21    |
| 1:A:51:THR:O     | 1:A:55:PHE:CD2   | 0.51     | 2.63        | 19     | 2     |
| 1:A:68:PRO:C     | 1:A:69:TYR:CD1   | 0.51     | 2.83        | 3      | 24    |
| 1:A:48:ILE:HG13  | 1:A:71:LEU:CD2   | 0.51     | 2.36        | 24     | 17    |
| 1:A:6:TYR:HD2    | 1:A:10:LEU:HG    | 0.51     | 1.65        | 12     | 17    |
| 1:A:67:ALA:N     | 1:A:99:GLY:O     | 0.51     | 2.43        | 22     | 18    |
| 1:A:178:PHE:CE1  | 1:A:193:GLN:HB2  | 0.51     | 2.39        | 21     | 4     |
| 1:A:93:LYS:CB    | 1:A:107:TYR:CZ   | 0.51     | 2.94        | 5      | 14    |
| 1:A:35:PRO:CG    | 1:A:75:SER:O     | 0.51     | 2.58        | 14     | 7     |
| 1:A:179:PHE:O    | 1:A:191:PRO:CB   | 0.51     | 2.58        | 22     | 7     |
| 1:A:186:PRO:O    | 1:A:190:GLY:N    | 0.51     | 2.38        | 17     | 7     |
| 1:A:129:ASP:HB3  | 1:A:204:MET:HG3  | 0.51     | 1.81        | 16     | 5     |
| 1:A:185:LEU:HD11 | 1:A:189:ALA:C    | 0.51     | 2.25        | 9      | 1     |
| 1:A:91:VAL:CG1   | 1:A:109:ALA:CB   | 0.51     | 2.89        | 8      | 2     |
| 1:A:87:THR:N     | 1:A:114:GLN:CG   | 0.51     | 2.70        | 22     | 1     |
| 1:A:113:ASP:OD2  | 1:A:118:LYS:HB2  | 0.51     | 2.05        | 14     | 8     |
| 1:A:79:GLN:HB3   | 1:A:114:GLN:HE22 | 0.51     | 1.65        | 5      | 4     |
| 1:A:73:ILE:HG13  | 1:A:94:VAL:HG23  | 0.51     | 1.83        | 6      | 1     |
| 1:A:125:LEU:CD1  | 1:A:126:TRP:CE3  | 0.51     | 2.94        | 5      | 13    |
| 1:A:48:ILE:O     | 1:A:51:THR:N     | 0.51     | 2.44        | 13     | 24    |
| 1:A:136:VAL:HG11 | 1:A:161:ASP:CB   | 0.51     | 2.35        | 6      | 17    |
| 1:A:125:LEU:HD12 | 1:A:126:TRP:CE2  | 0.51     | 2.41        | 5      | 23    |
| 1:A:96:GLN:O     | 1:A:104:THR:OG1  | 0.51     | 2.29        | 17     | 6     |
| 1:A:13:THR:HB    | 1:A:20:GLN:HG3   | 0.51     | 1.83        | 7      | 9     |
| 1:A:185:LEU:CD1  | 1:A:190:GLY:CA   | 0.51     | 2.88        | 8      | 2     |
| 1:A:76:ALA:O     | 1:A:78:TYR:CE1   | 0.51     | 2.64        | 3      | 18    |
| 1:A:21:ILE:CD1   | 1:A:21:ILE:C     | 0.51     | 2.79        | 14     | 9     |
| 1:A:145:SER:O    | 1:A:149:GLY:N    | 0.51     | 2.44        | 15     | 6     |
| 1:A:97:ASN:ND2   | 1:A:97:ASN:C     | 0.51     | 2.64        | 24     | 2     |
| 1:A:15:THR:CG2   | 1:A:20:GLN:NE2   | 0.51     | 2.74        | 23     | 6     |
| 1:A:141:GLN:CA   | 1:A:144:LEU:HB2  | 0.51     | 2.35        | 21     | 23    |
| 1:A:93:LYS:HA    | 1:A:107:TYR:CD1  | 0.51     | 2.41        | 6      | 22    |
| 1:A:35:PRO:HG2   | 1:A:75:SER:O     | 0.51     | 2.05        | 14     | 7     |
| 1:A:169:ALA:N    | 1:A:176:ILE:O    | 0.51     | 2.44        | 6      | 8     |
| 1:A:185:LEU:HB3  | 1:A:191:PRO:C    | 0.51     | 2.26        | 8      | 5     |
| 1:A:32:ILE:HG12  | 1:A:48:ILE:HG12  | 0.51     | 1.83        | 20     | 1     |

Continued on next page...

Continued from previous page...

| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:160:LEU:HD22 | 1:A:194:VAL:HA   | 0.51     | 1.82        | 7      | 14    |
| 1:A:21:ILE:CG2   | 1:A:21:ILE:O     | 0.51     | 2.58        | 8      | 10    |
| 1:A:19:CYS:HB3   | 1:A:34:LEU:O     | 0.51     | 2.06        | 19     | 9     |
| 1:A:178:PHE:CD2  | 1:A:191:PRO:O    | 0.51     | 2.63        | 7      | 3     |
| 1:A:184:LEU:O    | 1:A:185:LEU:CD2  | 0.50     | 2.59        | 1      | 6     |
| 1:A:59:ALA:HB2   | 1:A:98:ALA:HB1   | 0.50     | 1.83        | 3      | 2     |
| 1:A:91:VAL:HG23  | 1:A:91:VAL:O     | 0.50     | 2.06        | 2      | 1     |
| 1:A:133:LEU:HB2  | 1:A:194:VAL:C    | 0.50     | 2.27        | 13     | 10    |
| 1:A:97:ASN:ND2   | 1:A:100:GLY:HA2  | 0.50     | 2.22        | 3      | 8     |
| 1:A:45:GLU:HG3   | 1:A:46:ASN:N     | 0.50     | 2.21        | 10     | 19    |
| 1:A:91:VAL:CG1   | 1:A:169:ALA:HB2  | 0.50     | 2.32        | 21     | 2     |
| 1:A:32:ILE:HG12  | 1:A:73:ILE:HD13  | 0.50     | 1.82        | 10     | 1     |
| 1:A:82:ILE:HB    | 1:A:86:GLY:HA2   | 0.50     | 1.83        | 23     | 14    |
| 1:A:6:TYR:CE1    | 1:A:41:GLN:CB    | 0.50     | 2.94        | 8      | 19    |
| 1:A:112:TRP:HZ2  | 1:A:117:ARG:HA   | 0.50     | 1.66        | 7      | 1     |
| 1:A:77:THR:HB    | 1:A:90:VAL:CG1   | 0.50     | 2.32        | 15     | 12    |
| 1:A:178:PHE:CG   | 1:A:193:GLN:HB3  | 0.50     | 2.40        | 7      | 1     |
| 1:A:84:PRO:O     | 1:A:85:ARG:C     | 0.50     | 2.50        | 10     | 24    |
| 1:A:67:ALA:CB    | 1:A:68:PRO:HD3   | 0.50     | 2.24        | 22     | 15    |
| 1:A:137:PHE:CD1  | 1:A:160:LEU:HA   | 0.50     | 2.42        | 17     | 4     |
| 1:A:185:LEU:N    | 1:A:185:LEU:HD12 | 0.50     | 2.21        | 14     | 3     |
| 1:A:157:ASN:O    | 1:A:183:GLU:C    | 0.50     | 2.50        | 3      | 13    |
| 1:A:133:LEU:HD13 | 1:A:194:VAL:CB   | 0.50     | 2.36        | 18     | 3     |
| 1:A:42:LYS:O     | 1:A:42:LYS:HE3   | 0.50     | 2.06        | 5      | 8     |
| 1:A:184:LEU:O    | 1:A:185:LEU:CD1  | 0.50     | 2.59        | 10     | 3     |
| 1:A:87:THR:CA    | 1:A:114:GLN:CG   | 0.50     | 2.89        | 22     | 2     |
| 1:A:97:ASN:CB    | 1:A:102:HIS:O    | 0.50     | 2.60        | 18     | 17    |
| 1:A:113:ASP:OD2  | 1:A:118:LYS:CB   | 0.50     | 2.59        | 19     | 10    |
| 1:A:80:SER:HB2   | 1:A:87:THR:CB    | 0.50     | 2.37        | 21     | 12    |
| 1:A:32:ILE:CG2   | 1:A:73:ILE:CG2   | 0.50     | 2.89        | 22     | 10    |
| 1:A:87:THR:HA    | 1:A:114:GLN:CB   | 0.50     | 2.37        | 4      | 2     |
| 1:A:55:PHE:CE2   | 1:A:104:THR:CG2  | 0.50     | 2.94        | 6      | 2     |
| 1:A:88:GLN:N     | 1:A:114:GLN:HG2  | 0.50     | 2.22        | 16     | 4     |
| 1:A:124:THR:HA   | 1:A:206:ALA:HA   | 0.50     | 1.84        | 17     | 24    |
| 1:A:34:LEU:HG    | 1:A:41:GLN:HG3   | 0.50     | 1.82        | 5      | 2     |
| 1:A:157:ASN:HA   | 1:A:184:LEU:HB2  | 0.50     | 1.84        | 8      | 4     |
| 1:A:87:THR:CG2   | 1:A:112:TRP:O    | 0.50     | 2.60        | 15     | 4     |
| 1:A:6:TYR:CD2    | 1:A:45:GLU:CD    | 0.50     | 2.85        | 15     | 5     |
| 1:A:159:GLY:HA2  | 1:A:184:LEU:HD12 | 0.50     | 1.83        | 11     | 2     |
| 1:A:127:GLN:O    | 1:A:130:THR:CG2  | 0.50     | 2.58        | 3      | 8     |
| 1:A:32:ILE:HD11  | 1:A:71:LEU:CG    | 0.50     | 2.37        | 23     | 2     |

Continued on next page...

*Continued from previous page...*

| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:19:CYS:N     | 1:A:34:LEU:O     | 0.50     | 2.45        | 21     | 3     |
| 1:A:4:LYS:HE3    | 1:A:8:GLU:CG     | 0.50     | 2.37        | 19     | 1     |
| 1:A:40:ASP:HB2   | 1:A:112:TRP:HZ3  | 0.50     | 1.67        | 15     | 1     |
| 1:A:178:PHE:CZ   | 1:A:193:GLN:CG   | 0.49     | 2.94        | 4      | 6     |
| 1:A:34:LEU:HD21  | 1:A:41:GLN:CD    | 0.49     | 2.28        | 3      | 2     |
| 1:A:97:ASN:ND2   | 1:A:98:ALA:N     | 0.49     | 2.59        | 24     | 4     |
| 1:A:71:LEU:HA    | 1:A:96:GLN:CB    | 0.49     | 2.36        | 6      | 1     |
| 1:A:133:LEU:HB2  | 1:A:194:VAL:CB   | 0.49     | 2.35        | 20     | 14    |
| 1:A:6:TYR:CE2    | 1:A:45:GLU:HB2   | 0.49     | 2.42        | 1      | 9     |
| 1:A:196:VAL:HG22 | 1:A:197:PRO:CD   | 0.49     | 2.32        | 13     | 1     |
| 1:A:34:LEU:HD11  | 1:A:44:LEU:CD2   | 0.49     | 2.35        | 15     | 1     |
| 1:A:68:PRO:C     | 1:A:69:TYR:HD1   | 0.49     | 2.11        | 19     | 24    |
| 1:A:52:ARG:HA    | 1:A:96:GLN:OE1   | 0.49     | 2.07        | 10     | 7     |
| 1:A:117:ARG:O    | 1:A:118:LYS:HG2  | 0.49     | 2.07        | 14     | 1     |
| 1:A:179:PHE:CZ   | 1:A:181:PRO:HB3  | 0.49     | 2.42        | 17     | 1     |
| 1:A:59:ALA:CA    | 1:A:63:THR:OG1   | 0.49     | 2.58        | 3      | 11    |
| 1:A:6:TYR:OH     | 1:A:34:LEU:CD2   | 0.49     | 2.60        | 15     | 5     |
| 1:A:34:LEU:HD21  | 1:A:41:GLN:HG3   | 0.49     | 1.84        | 2      | 4     |
| 1:A:140:VAL:HG12 | 1:A:154:ILE:HD12 | 0.49     | 1.84        | 17     | 5     |
| 1:A:156:PRO:HA   | 1:A:160:LEU:CB   | 0.49     | 2.38        | 14     | 5     |
| 1:A:97:ASN:HD21  | 1:A:100:GLY:HA2  | 0.49     | 1.67        | 3      | 1     |
| 1:A:185:LEU:O    | 1:A:186:PRO:O    | 0.49     | 2.31        | 7      | 8     |
| 1:A:32:ILE:N     | 1:A:32:ILE:CD1   | 0.49     | 2.75        | 17     | 4     |
| 1:A:185:LEU:C    | 1:A:185:LEU:CD1  | 0.49     | 2.65        | 21     | 1     |
| 1:A:21:ILE:O     | 1:A:21:ILE:CG2   | 0.49     | 2.60        | 5      | 11    |
| 1:A:133:LEU:N    | 1:A:133:LEU:CD1  | 0.49     | 2.76        | 2      | 8     |
| 1:A:134:PRO:HA   | 1:A:160:LEU:CD2  | 0.49     | 2.37        | 4      | 14    |
| 1:A:21:ILE:HG22  | 1:A:32:ILE:HB    | 0.49     | 1.85        | 8      | 7     |
| 1:A:40:ASP:HB2   | 1:A:112:TRP:CZ3  | 0.49     | 2.43        | 3      | 3     |
| 1:A:77:THR:HG23  | 1:A:88:GLN:OE1   | 0.49     | 2.07        | 3      | 1     |
| 1:A:74:THR:O     | 1:A:92:LEU:HA    | 0.49     | 2.07        | 3      | 2     |
| 1:A:89:ALA:CB    | 1:A:170:VAL:HG12 | 0.49     | 2.38        | 9      | 1     |
| 1:A:185:LEU:HD11 | 1:A:190:GLY:N    | 0.49     | 2.23        | 9      | 1     |
| 1:A:97:ASN:ND2   | 1:A:100:GLY:H    | 0.49     | 2.06        | 15     | 16    |
| 1:A:161:ASP:HB2  | 1:A:193:GLN:HE21 | 0.49     | 1.65        | 22     | 17    |
| 1:A:30:ILE:HD13  | 1:A:52:ARG:NH2   | 0.49     | 2.23        | 1      | 1     |
| 1:A:43:SER:HB2   | 1:A:110:PHE:CE2  | 0.49     | 2.43        | 5      | 1     |
| 1:A:15:THR:HG23  | 1:A:18:ALA:CB    | 0.49     | 2.35        | 21     | 3     |
| 1:A:197:PRO:O    | 1:A:201:ILE:HG13 | 0.49     | 2.08        | 2      | 9     |
| 1:A:113:ASP:C    | 1:A:113:ASP:OD1  | 0.49     | 2.51        | 1      | 3     |
| 1:A:30:ILE:HG23  | 1:A:32:ILE:HD11  | 0.49     | 1.83        | 12     | 1     |

*Continued on next page...*

Continued from previous page...

| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:75:SER:HB2   | 1:A:92:LEU:HG    | 0.49     | 1.85        | 6      | 3     |
| 1:A:54:LYS:HA    | 1:A:57:SER:HB2   | 0.49     | 1.84        | 19     | 18    |
| 1:A:122:TYR:CB   | 1:A:126:TRP:CD1  | 0.49     | 2.96        | 19     | 22    |
| 1:A:177:PHE:O    | 1:A:193:GLN:CA   | 0.49     | 2.60        | 15     | 8     |
| 1:A:75:SER:HB2   | 1:A:92:LEU:CD2   | 0.49     | 2.38        | 7      | 1     |
| 1:A:136:VAL:CG1  | 1:A:176:ILE:HD11 | 0.49     | 2.38        | 19     | 5     |
| 1:A:87:THR:O     | 1:A:114:GLN:NE2  | 0.49     | 2.46        | 6      | 4     |
| 1:A:117:ARG:O    | 1:A:117:ARG:HG3  | 0.49     | 2.08        | 5      | 1     |
| 1:A:74:THR:O     | 1:A:93:LYS:N     | 0.49     | 2.37        | 21     | 8     |
| 1:A:81:ALA:HB3   | 1:A:172:ASN:ND2  | 0.49     | 2.23        | 12     | 1     |
| 1:A:28:TYR:CD2   | 1:A:56:LEU:CD1   | 0.48     | 2.93        | 13     | 13    |
| 1:A:192:THR:CG2  | 1:A:193:GLN:N    | 0.48     | 2.76        | 16     | 7     |
| 1:A:21:ILE:HG23  | 1:A:32:ILE:CD1   | 0.48     | 2.38        | 6      | 4     |
| 1:A:63:THR:O     | 1:A:65:ARG:CG    | 0.48     | 2.62        | 10     | 3     |
| 1:A:136:VAL:HG11 | 1:A:162:PRO:HD2  | 0.48     | 1.84        | 7      | 2     |
| 1:A:178:PHE:HD2  | 1:A:191:PRO:O    | 0.48     | 1.90        | 7      | 2     |
| 1:A:185:LEU:CA   | 1:A:189:ALA:HB3  | 0.48     | 2.37        | 19     | 3     |
| 1:A:21:ILE:C     | 1:A:21:ILE:CD1   | 0.48     | 2.82        | 21     | 9     |
| 1:A:42:LYS:HE3   | 1:A:42:LYS:O     | 0.48     | 2.08        | 11     | 5     |
| 1:A:185:LEU:HG   | 1:A:191:PRO:O    | 0.48     | 2.08        | 21     | 1     |
| 1:A:178:PHE:CE2  | 1:A:191:PRO:O    | 0.48     | 2.66        | 17     | 1     |
| 1:A:196:VAL:CG1  | 1:A:201:ILE:HG12 | 0.48     | 2.37        | 13     | 3     |
| 1:A:75:SER:CA    | 1:A:92:LEU:HA    | 0.48     | 2.38        | 2      | 11    |
| 1:A:175:VAL:HG22 | 1:A:196:VAL:HG23 | 0.48     | 1.85        | 1      | 1     |
| 1:A:135:VAL:C    | 1:A:138:PRO:HD2  | 0.48     | 2.28        | 15     | 21    |
| 1:A:89:ALA:CB    | 1:A:170:VAL:CG1  | 0.48     | 2.91        | 5      | 1     |
| 1:A:33:SER:C     | 1:A:34:LEU:HD22  | 0.48     | 2.28        | 13     | 1     |
| 1:A:121:THR:HG23 | 1:A:123:ASP:H    | 0.48     | 1.68        | 14     | 17    |
| 1:A:34:LEU:HD21  | 1:A:92:LEU:CD2   | 0.48     | 2.38        | 16     | 1     |
| 1:A:56:LEU:HD22  | 1:A:69:TYR:CB    | 0.48     | 2.36        | 24     | 12    |
| 1:A:141:GLN:NE2  | 1:A:154:ILE:HG13 | 0.48     | 2.23        | 11     | 22    |
| 1:A:56:LEU:HB3   | 1:A:69:TYR:CD2   | 0.48     | 2.43        | 24     | 16    |
| 1:A:54:LYS:C     | 1:A:57:SER:HB2   | 0.48     | 2.28        | 23     | 6     |
| 1:A:137:PHE:CZ   | 1:A:160:LEU:HA   | 0.48     | 2.44        | 16     | 5     |
| 1:A:161:ASP:CG   | 1:A:176:ILE:HD11 | 0.48     | 2.29        | 7      | 1     |
| 1:A:117:ARG:O    | 1:A:117:ARG:CG   | 0.48     | 2.62        | 12     | 1     |
| 1:A:176:ILE:CG2  | 1:A:178:PHE:CZ   | 0.48     | 2.96        | 4      | 1     |
| 1:A:44:LEU:HD13  | 1:A:92:LEU:CD2   | 0.48     | 2.39        | 11     | 1     |
| 1:A:137:PHE:CD1  | 1:A:160:LEU:O    | 0.48     | 2.66        | 22     | 5     |
| 1:A:18:ALA:HB1   | 1:A:20:GLN:NE2   | 0.48     | 2.24        | 20     | 1     |
| 1:A:97:ASN:C     | 1:A:97:ASN:ND2   | 0.48     | 2.67        | 21     | 2     |

Continued on next page...

*Continued from previous page...*

| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:40:ASP:HB3   | 1:A:112:TRP:CZ3  | 0.48     | 2.43        | 21     | 2     |
| 1:A:102:HIS:NE2  | 1:A:104:THR:HG23 | 0.48     | 2.24        | 4      | 1     |
| 1:A:47:TYR:O     | 1:A:50:GLN:CB    | 0.48     | 2.62        | 8      | 24    |
| 1:A:127:GLN:N    | 1:A:127:GLN:NE2  | 0.48     | 2.62        | 2      | 18    |
| 1:A:136:VAL:CG1  | 1:A:161:ASP:OD2  | 0.48     | 2.62        | 4      | 18    |
| 1:A:126:TRP:O    | 1:A:206:ALA:HA   | 0.47     | 2.08        | 18     | 19    |
| 1:A:143:GLU:O    | 1:A:146:LYS:HB3  | 0.47     | 2.09        | 17     | 4     |
| 1:A:93:LYS:HB2   | 1:A:107:TYR:OH   | 0.47     | 2.09        | 4      | 8     |
| 1:A:68:PRO:O     | 1:A:69:TYR:CD1   | 0.47     | 2.66        | 8      | 24    |
| 1:A:41:GLN:CA    | 1:A:41:GLN:NE2   | 0.47     | 2.77        | 18     | 3     |
| 1:A:116:TYR:C    | 1:A:117:ARG:CG   | 0.47     | 2.82        | 1      | 6     |
| 1:A:32:ILE:N     | 1:A:32:ILE:HD13  | 0.47     | 2.24        | 17     | 1     |
| 1:A:113:ASP:HB3  | 1:A:118:LYS:CG   | 0.47     | 2.39        | 8      | 1     |
| 1:A:80:SER:HB3   | 1:A:87:THR:CB    | 0.47     | 2.39        | 8      | 1     |
| 1:A:107:TYR:H    | 1:A:191:PRO:HG3  | 0.47     | 1.68        | 13     | 1     |
| 1:A:125:LEU:O    | 1:A:125:LEU:HD22 | 0.47     | 2.09        | 16     | 12    |
| 1:A:136:VAL:CG1  | 1:A:137:PHE:N    | 0.47     | 2.78        | 4      | 17    |
| 1:A:86:GLY:C     | 1:A:114:GLN:CB   | 0.47     | 2.81        | 16     | 7     |
| 1:A:43:SER:HB3   | 1:A:110:PHE:CD2  | 0.47     | 2.44        | 23     | 3     |
| 1:A:73:ILE:CB    | 1:A:94:VAL:CG2   | 0.47     | 2.91        | 6      | 1     |
| 1:A:113:ASP:OD2  | 1:A:116:TYR:N    | 0.47     | 2.45        | 8      | 1     |
| 1:A:194:VAL:HG23 | 1:A:194:VAL:O    | 0.47     | 2.10        | 12     | 10    |
| 1:A:112:TRP:CZ2  | 1:A:117:ARG:C    | 0.47     | 2.87        | 18     | 3     |
| 1:A:112:TRP:CA   | 1:A:119:PRO:HA   | 0.47     | 2.36        | 6      | 3     |
| 1:A:176:ILE:CG1  | 1:A:195:LEU:HD13 | 0.47     | 2.39        | 18     | 12    |
| 1:A:141:GLN:O    | 1:A:144:LEU:HB2  | 0.47     | 2.09        | 24     | 14    |
| 1:A:91:VAL:O     | 1:A:91:VAL:HG23  | 0.47     | 2.09        | 12     | 1     |
| 1:A:13:THR:O     | 1:A:20:GLN:HG2   | 0.47     | 2.10        | 6      | 3     |
| 1:A:161:ASP:OD2  | 1:A:176:ILE:CD1  | 0.47     | 2.63        | 22     | 20    |
| 1:A:59:ALA:HB2   | 1:A:98:ALA:CB    | 0.47     | 2.39        | 8      | 15    |
| 1:A:133:LEU:HB3  | 1:A:195:LEU:C    | 0.47     | 2.30        | 2      | 15    |
| 1:A:135:VAL:O    | 1:A:138:PRO:CG   | 0.47     | 2.63        | 18     | 10    |
| 1:A:72:ASN:O     | 1:A:94:VAL:HA    | 0.47     | 2.09        | 2      | 4     |
| 1:A:80:SER:CB    | 1:A:87:THR:N     | 0.47     | 2.78        | 7      | 5     |
| 1:A:42:LYS:HZ1   | 1:A:46:ASN:CA    | 0.47     | 2.23        | 5      | 2     |
| 1:A:67:ALA:H     | 1:A:68:PRO:CD    | 0.47     | 2.23        | 3      | 1     |
| 1:A:8:GLU:CG     | 1:A:9:GLU:N      | 0.47     | 2.77        | 3      | 3     |
| 1:A:185:LEU:HD21 | 1:A:191:PRO:CD   | 0.47     | 2.39        | 10     | 2     |
| 1:A:196:VAL:HB   | 1:A:201:ILE:HG12 | 0.47     | 1.85        | 7      | 2     |
| 1:A:32:ILE:HG23  | 1:A:73:ILE:HD13  | 0.47     | 1.86        | 6      | 1     |
| 1:A:44:LEU:O     | 1:A:47:TYR:CA    | 0.47     | 2.63        | 9      | 24    |

*Continued on next page...*

Continued from previous page...

| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:192:THR:HG22 | 1:A:193:GLN:N    | 0.47     | 2.25        | 19     | 4     |
| 1:A:133:LEU:CD1  | 1:A:133:LEU:N    | 0.47     | 2.74        | 10     | 9     |
| 1:A:79:GLN:CA    | 1:A:87:THR:O     | 0.47     | 2.62        | 15     | 7     |
| 1:A:136:VAL:CB   | 1:A:176:ILE:HD11 | 0.47     | 2.40        | 15     | 7     |
| 1:A:93:LYS:CB    | 1:A:107:TYR:CE1  | 0.47     | 2.97        | 2      | 11    |
| 1:A:6:TYR:CE1    | 1:A:44:LEU:CD1   | 0.47     | 2.97        | 10     | 3     |
| 1:A:185:LEU:HD12 | 1:A:185:LEU:N    | 0.47     | 2.25        | 22     | 3     |
| 1:A:22:GLN:HB3   | 1:A:31:ASN:ND2   | 0.47     | 2.25        | 4      | 9     |
| 1:A:75:SER:HB2   | 1:A:92:LEU:CA    | 0.47     | 2.40        | 8      | 2     |
| 1:A:10:LEU:HD21  | 1:A:45:GLU:OE1   | 0.47     | 2.10        | 22     | 1     |
| 1:A:75:SER:HG    | 1:A:90:VAL:HB    | 0.47     | 1.69        | 20     | 2     |
| 1:A:32:ILE:HG23  | 1:A:73:ILE:CD1   | 0.47     | 2.40        | 6      | 2     |
| 1:A:177:PHE:O    | 1:A:194:VAL:N    | 0.47     | 2.46        | 15     | 10    |
| 1:A:196:VAL:HB   | 1:A:201:ILE:HG21 | 0.47     | 1.85        | 1      | 8     |
| 1:A:135:VAL:CB   | 1:A:195:LEU:HD23 | 0.47     | 2.40        | 22     | 5     |
| 1:A:44:LEU:HA    | 1:A:47:TYR:HB3   | 0.47     | 1.87        | 11     | 4     |
| 1:A:196:VAL:HG13 | 1:A:201:ILE:CB   | 0.46     | 2.40        | 20     | 3     |
| 1:A:47:TYR:O     | 1:A:50:GLN:CA    | 0.46     | 2.64        | 14     | 24    |
| 1:A:125:LEU:HD22 | 1:A:125:LEU:O    | 0.46     | 2.10        | 8      | 10    |
| 1:A:92:LEU:C     | 1:A:107:TYR:CE1  | 0.46     | 2.88        | 17     | 1     |
| 1:A:94:VAL:HG12  | 1:A:106:THR:O    | 0.46     | 2.10        | 6      | 1     |
| 1:A:127:GLN:OE1  | 1:A:130:THR:HG23 | 0.46     | 2.10        | 8      | 1     |
| 1:A:170:VAL:CG1  | 1:A:170:VAL:O    | 0.46     | 2.63        | 20     | 1     |
| 1:A:42:LYS:HE2   | 1:A:46:ASN:HB2   | 0.46     | 1.87        | 2      | 3     |
| 1:A:28:TYR:HB3   | 1:A:69:TYR:CE2   | 0.46     | 2.45        | 14     | 12    |
| 1:A:137:PHE:N    | 1:A:138:PRO:CD   | 0.46     | 2.78        | 4      | 24    |
| 1:A:73:ILE:CG2   | 1:A:94:VAL:HG23  | 0.46     | 2.40        | 3      | 4     |
| 1:A:160:LEU:C    | 1:A:161:ASP:OD1  | 0.46     | 2.53        | 22     | 5     |
| 1:A:143:GLU:O    | 1:A:146:LYS:N    | 0.46     | 2.49        | 17     | 20    |
| 1:A:185:LEU:HD11 | 1:A:192:THR:CA   | 0.46     | 2.40        | 7      | 2     |
| 1:A:127:GLN:NE2  | 1:A:205:LEU:HD12 | 0.46     | 2.25        | 13     | 15    |
| 1:A:7:CYS:HA     | 1:A:10:LEU:HB2   | 0.46     | 1.87        | 19     | 9     |
| 1:A:6:TYR:CD1    | 1:A:41:GLN:HB2   | 0.46     | 2.44        | 6      | 4     |
| 1:A:121:THR:HG23 | 1:A:123:ASP:HB2  | 0.46     | 1.87        | 19     | 6     |
| 1:A:89:ALA:CA    | 1:A:110:PHE:O    | 0.46     | 2.63        | 2      | 6     |
| 1:A:175:VAL:CG1  | 1:A:201:ILE:HG12 | 0.46     | 2.41        | 1      | 12    |
| 1:A:160:LEU:O    | 1:A:161:ASP:OD1  | 0.46     | 2.34        | 7      | 1     |
| 1:A:87:THR:HG22  | 1:A:112:TRP:O    | 0.46     | 2.10        | 1      | 5     |
| 1:A:136:VAL:N    | 1:A:195:LEU:HD23 | 0.46     | 2.26        | 8      | 7     |
| 1:A:185:LEU:HD13 | 1:A:189:ALA:HB3  | 0.46     | 1.87        | 4      | 4     |
| 1:A:63:THR:CG2   | 1:A:102:HIS:HB2  | 0.46     | 2.41        | 8      | 8     |

Continued on next page...

Continued from previous page...

| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:136:VAL:HG11 | 1:A:161:ASP:CA   | 0.46     | 2.41        | 18     | 12    |
| 1:A:78:TYR:HD1   | 1:A:89:ALA:O     | 0.46     | 1.93        | 18     | 3     |
| 1:A:137:PHE:HZ   | 1:A:154:ILE:O    | 0.46     | 1.94        | 14     | 2     |
| 1:A:70:GLU:O     | 1:A:96:GLN:HG3   | 0.46     | 2.11        | 19     | 1     |
| 1:A:15:THR:HB    | 1:A:18:ALA:HB3   | 0.46     | 1.86        | 16     | 2     |
| 1:A:116:TYR:O    | 1:A:117:ARG:CD   | 0.46     | 2.64        | 20     | 1     |
| 1:A:186:PRO:O    | 1:A:189:ALA:N    | 0.46     | 2.48        | 3      | 12    |
| 1:A:127:GLN:CD   | 1:A:204:MET:O    | 0.46     | 2.53        | 2      | 15    |
| 1:A:48:ILE:O     | 1:A:52:ARG:HG3   | 0.46     | 2.11        | 6      | 5     |
| 1:A:64:PRO:O     | 1:A:101:THR:CB   | 0.46     | 2.60        | 3      | 1     |
| 1:A:135:VAL:HG21 | 1:A:197:PRO:N    | 0.46     | 2.26        | 10     | 1     |
| 1:A:185:LEU:CD2  | 1:A:190:GLY:N    | 0.46     | 2.64        | 21     | 1     |
| 1:A:6:TYR:OH     | 1:A:44:LEU:HD11  | 0.46     | 2.10        | 21     | 1     |
| 1:A:133:LEU:CD2  | 1:A:194:VAL:HG23 | 0.46     | 2.27        | 1      | 4     |
| 1:A:181:PRO:CD   | 1:A:192:THR:OG1  | 0.46     | 2.63        | 1      | 1     |
| 1:A:180:ASN:O    | 1:A:180:ASN:OD1  | 0.46     | 2.34        | 19     | 1     |
| 1:A:185:LEU:O    | 1:A:190:GLY:N    | 0.46     | 2.49        | 19     | 1     |
| 1:A:94:VAL:C     | 1:A:106:THR:O    | 0.46     | 2.51        | 6      | 1     |
| 1:A:205:LEU:O    | 1:A:206:ALA:CB   | 0.46     | 2.64        | 13     | 1     |
| 1:A:44:LEU:CD1   | 1:A:92:LEU:HD21  | 0.46     | 2.41        | 11     | 1     |
| 1:A:92:LEU:HD21  | 1:A:110:PHE:CZ   | 0.46     | 2.46        | 21     | 1     |
| 1:A:156:PRO:O    | 1:A:184:LEU:HG   | 0.45     | 2.11        | 2      | 1     |
| 1:A:126:TRP:O    | 1:A:206:ALA:O    | 0.45     | 2.34        | 21     | 22    |
| 1:A:143:GLU:O    | 1:A:146:LYS:CB   | 0.45     | 2.64        | 10     | 6     |
| 1:A:162:PRO:O    | 1:A:193:GLN:NE2  | 0.45     | 2.48        | 21     | 3     |
| 1:A:141:GLN:HE22 | 1:A:154:ILE:CD1  | 0.45     | 2.24        | 7      | 8     |
| 1:A:184:LEU:HB3  | 1:A:192:THR:HG23 | 0.45     | 1.88        | 2      | 4     |
| 1:A:185:LEU:HD22 | 1:A:185:LEU:C    | 0.45     | 2.32        | 21     | 1     |
| 1:A:81:ALA:O     | 1:A:172:ASN:ND2  | 0.45     | 2.49        | 17     | 1     |
| 1:A:133:LEU:HG   | 1:A:196:VAL:HG23 | 0.45     | 1.87        | 13     | 1     |
| 1:A:113:ASP:OD1  | 1:A:117:ARG:N    | 0.45     | 2.48        | 13     | 6     |
| 1:A:78:TYR:HB3   | 1:A:171:THR:HG22 | 0.45     | 1.88        | 23     | 2     |
| 1:A:87:THR:C     | 1:A:114:GLN:NE2  | 0.45     | 2.70        | 6      | 1     |
| 1:A:43:SER:O     | 1:A:47:TYR:CB    | 0.45     | 2.63        | 6      | 14    |
| 1:A:176:ILE:HG12 | 1:A:193:GLN:CD   | 0.45     | 2.32        | 6      | 12    |
| 1:A:48:ILE:CG1   | 1:A:71:LEU:CD2   | 0.45     | 2.94        | 15     | 5     |
| 1:A:113:ASP:OD1  | 1:A:113:ASP:C    | 0.45     | 2.55        | 3      | 2     |
| 1:A:29:ASN:ND2   | 1:A:30:ILE:N     | 0.45     | 2.65        | 7      | 3     |
| 1:A:10:LEU:CD1   | 1:A:10:LEU:O     | 0.45     | 2.65        | 13     | 1     |
| 1:A:44:LEU:HB3   | 1:A:110:PHE:CE2  | 0.45     | 2.45        | 20     | 1     |
| 1:A:49:ALA:O     | 1:A:53:ASP:CB    | 0.45     | 2.64        | 4      | 6     |

Continued on next page...

Continued from previous page...

| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:82:ILE:CG2   | 1:A:83:PRO:HD2   | 0.45     | 2.42        | 13     | 5     |
| 1:A:77:THR:CG2   | 1:A:88:GLN:HG2   | 0.45     | 2.41        | 23     | 1     |
| 1:A:77:THR:CG2   | 1:A:88:GLN:OE1   | 0.45     | 2.65        | 3      | 1     |
| 1:A:117:ARG:HG2  | 1:A:117:ARG:O    | 0.45     | 2.11        | 12     | 1     |
| 1:A:78:TYR:O     | 1:A:79:GLN:OE1   | 0.45     | 2.35        | 6      | 1     |
| 1:A:97:ASN:OD1   | 1:A:100:GLY:HA2  | 0.45     | 2.12        | 6      | 1     |
| 1:A:27:ALA:C     | 1:A:68:PRO:HB2   | 0.45     | 2.31        | 18     | 7     |
| 1:A:176:ILE:HG12 | 1:A:193:GLN:HG2  | 0.45     | 1.88        | 7      | 11    |
| 1:A:97:ASN:ND2   | 1:A:101:THR:N    | 0.45     | 2.65        | 21     | 2     |
| 1:A:75:SER:HB2   | 1:A:92:LEU:CG    | 0.45     | 2.41        | 15     | 8     |
| 1:A:185:LEU:CD2  | 1:A:191:PRO:N    | 0.45     | 2.80        | 19     | 4     |
| 1:A:44:LEU:HD13  | 1:A:92:LEU:HD21  | 0.45     | 1.88        | 11     | 1     |
| 1:A:95:TYR:HB2   | 1:A:105:THR:CG2  | 0.45     | 2.24        | 19     | 2     |
| 1:A:52:ARG:CG    | 1:A:71:LEU:HD22  | 0.45     | 2.42        | 12     | 9     |
| 1:A:29:ASN:OD1   | 1:A:70:GLU:CG    | 0.45     | 2.64        | 6      | 1     |
| 1:A:97:ASN:ND2   | 1:A:100:GLY:N    | 0.45     | 2.65        | 12     | 16    |
| 1:A:97:ASN:O     | 1:A:97:ASN:ND2   | 0.45     | 2.48        | 8      | 7     |
| 1:A:34:LEU:CD1   | 1:A:41:GLN:OE1   | 0.45     | 2.65        | 24     | 1     |
| 1:A:140:VAL:O    | 1:A:144:LEU:CD1  | 0.45     | 2.65        | 11     | 4     |
| 1:A:185:LEU:HD11 | 1:A:191:PRO:CD   | 0.45     | 2.40        | 23     | 2     |
| 1:A:127:GLN:HG2  | 1:A:129:ASP:H    | 0.45     | 1.70        | 5      | 8     |
| 1:A:113:ASP:OD1  | 1:A:116:TYR:N    | 0.45     | 2.50        | 3      | 2     |
| 1:A:75:SER:HB3   | 1:A:92:LEU:HG    | 0.45     | 1.89        | 12     | 3     |
| 1:A:48:ILE:HD11  | 1:A:73:ILE:HG21  | 0.45     | 1.88        | 12     | 2     |
| 1:A:34:LEU:HD21  | 1:A:41:GLN:HE21  | 0.45     | 1.72        | 23     | 2     |
| 1:A:87:THR:C     | 1:A:114:GLN:HG2  | 0.45     | 2.32        | 22     | 1     |
| 1:A:127:GLN:NE2  | 1:A:127:GLN:N    | 0.44     | 2.64        | 18     | 6     |
| 1:A:144:LEU:O    | 1:A:147:GLN:CB   | 0.44     | 2.66        | 15     | 6     |
| 1:A:161:ASP:OD2  | 1:A:195:LEU:CB   | 0.44     | 2.64        | 24     | 4     |
| 1:A:4:LYS:HD2    | 1:A:8:GLU:HB2    | 0.44     | 1.88        | 21     | 5     |
| 1:A:134:PRO:O    | 1:A:137:PHE:CB   | 0.44     | 2.65        | 22     | 7     |
| 1:A:161:ASP:CB   | 1:A:176:ILE:HD11 | 0.44     | 2.41        | 7      | 1     |
| 1:A:97:ASN:HD22  | 1:A:97:ASN:C     | 0.44     | 2.15        | 5      | 3     |
| 1:A:77:THR:CG2   | 1:A:90:VAL:CG1   | 0.44     | 2.92        | 23     | 1     |
| 1:A:32:ILE:HG13  | 1:A:73:ILE:HG21  | 0.44     | 1.88        | 17     | 1     |
| 1:A:6:TYR:CD2    | 1:A:45:GLU:HG2   | 0.44     | 2.47        | 15     | 1     |
| 1:A:92:LEU:O     | 1:A:107:TYR:HD1  | 0.44     | 1.96        | 18     | 1     |
| 1:A:184:LEU:C    | 1:A:185:LEU:CD1  | 0.44     | 2.82        | 22     | 4     |
| 1:A:6:TYR:HE1    | 1:A:41:GLN:CB    | 0.44     | 2.26        | 12     | 4     |
| 1:A:170:VAL:O    | 1:A:170:VAL:CG1  | 0.44     | 2.65        | 9      | 1     |
| 1:A:94:VAL:O     | 1:A:106:THR:N    | 0.44     | 2.44        | 6      | 1     |

Continued on next page...

*Continued from previous page...*

| Atom-1          | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|-----------------|------------------|----------|-------------|--------|-------|
|                 |                  |          |             | Worst  | Total |
| 1:A:141:GLN:NE2 | 1:A:141:GLN:N    | 0.44     | 2.65        | 10     | 3     |
| 1:A:29:ASN:ND2  | 1:A:70:GLU:HG3   | 0.44     | 2.28        | 5      | 2     |
| 1:A:43:SER:HB3  | 1:A:110:PHE:CE2  | 0.44     | 2.48        | 12     | 1     |
| 1:A:47:TYR:O    | 1:A:51:THR:OG1   | 0.44     | 2.35        | 19     | 1     |
| 1:A:63:THR:HG21 | 1:A:102:HIS:CG   | 0.44     | 2.48        | 19     | 4     |
| 1:A:34:LEU:CD2  | 1:A:41:GLN:HG3   | 0.44     | 2.43        | 2      | 3     |
| 1:A:179:PHE:CZ  | 1:A:194:VAL:CG2  | 0.44     | 3.00        | 9      | 3     |
| 1:A:66:GLU:CB   | 1:A:100:GLY:CA   | 0.44     | 2.93        | 7      | 1     |
| 1:A:161:ASP:OD2 | 1:A:176:ILE:HG13 | 0.44     | 2.11        | 6      | 5     |
| 1:A:107:TYR:HB2 | 1:A:191:PRO:HG2  | 0.44     | 1.88        | 16     | 1     |
| 1:A:97:ASN:ND2  | 1:A:102:HIS:N    | 0.44     | 2.66        | 6      | 1     |
| 1:A:97:ASN:HD22 | 1:A:100:GLY:H    | 0.44     | 1.56        | 18     | 8     |
| 1:A:102:HIS:CE1 | 1:A:104:THR:CG2  | 0.44     | 3.00        | 4      | 3     |
| 1:A:98:ALA:H    | 1:A:102:HIS:HB3  | 0.44     | 1.73        | 18     | 3     |
| 1:A:141:GLN:N   | 1:A:141:GLN:NE2  | 0.44     | 2.66        | 18     | 3     |
| 1:A:56:LEU:CD2  | 1:A:69:TYR:HD2   | 0.44     | 2.18        | 8      | 12    |
| 1:A:175:VAL:CG2 | 1:A:175:VAL:O    | 0.44     | 2.65        | 5      | 1     |
| 1:A:75:SER:OG   | 1:A:90:VAL:HB    | 0.44     | 2.13        | 21     | 1     |
| 1:A:185:LEU:H   | 1:A:186:PRO:CD   | 0.44     | 2.26        | 19     | 1     |
| 1:A:10:LEU:HD12 | 1:A:21:ILE:HG13  | 0.44     | 1.90        | 13     | 1     |
| 1:A:48:ILE:CG2  | 1:A:49:ALA:N     | 0.44     | 2.81        | 3      | 8     |
| 1:A:182:GLY:O   | 1:A:183:GLU:HG2  | 0.44     | 2.12        | 3      | 1     |
| 1:A:6:TYR:OH    | 1:A:44:LEU:CD1   | 0.44     | 2.66        | 19     | 2     |
| 1:A:181:PRO:HD3 | 1:A:192:THR:HB   | 0.44     | 1.89        | 21     | 1     |
| 1:A:66:GLU:HB2  | 1:A:99:GLY:C     | 0.44     | 2.30        | 23     | 2     |
| 1:A:77:THR:HG21 | 1:A:88:GLN:HG2   | 0.44     | 1.88        | 23     | 1     |
| 1:A:178:PHE:HB3 | 1:A:191:PRO:HB2  | 0.44     | 1.90        | 23     | 3     |
| 1:A:33:SER:O    | 1:A:74:THR:HA    | 0.44     | 2.13        | 21     | 3     |
| 1:A:42:LYS:CE   | 1:A:46:ASN:CB    | 0.44     | 2.95        | 12     | 4     |
| 1:A:77:THR:CA   | 1:A:90:VAL:HG12  | 0.44     | 2.42        | 1      | 1     |
| 1:A:15:THR:CG2  | 1:A:18:ALA:CB    | 0.44     | 2.86        | 13     | 4     |
| 1:A:88:GLN:OE1  | 1:A:88:GLN:O     | 0.44     | 2.34        | 21     | 3     |
| 1:A:185:LEU:CD1 | 1:A:189:ALA:C    | 0.44     | 2.86        | 2      | 3     |
| 1:A:34:LEU:HD21 | 1:A:44:LEU:HD22  | 0.44     | 1.88        | 15     | 1     |
| 1:A:113:ASP:OD2 | 1:A:118:LYS:CG   | 0.44     | 2.66        | 16     | 4     |
| 1:A:181:PRO:CG  | 1:A:192:THR:CB   | 0.44     | 2.96        | 3      | 8     |
| 1:A:129:ASP:HB3 | 1:A:204:MET:CG   | 0.44     | 2.43        | 16     | 3     |
| 1:A:32:ILE:CG1  | 1:A:73:ILE:HD13  | 0.44     | 2.42        | 10     | 1     |
| 1:A:178:PHE:N   | 1:A:178:PHE:HD1  | 0.44     | 2.08        | 14     | 1     |
| 1:A:30:ILE:CG2  | 1:A:32:ILE:HD12  | 0.43     | 2.39        | 3      | 1     |
| 1:A:90:VAL:HG22 | 1:A:110:PHE:CD1  | 0.43     | 2.47        | 3      | 1     |

*Continued on next page...*

Continued from previous page...

| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:125:LEU:CD1  | 1:A:126:TRP:CD2  | 0.43     | 3.01        | 5      | 1     |
| 1:A:51:THR:O     | 1:A:55:PHE:CD1   | 0.43     | 2.71        | 6      | 1     |
| 1:A:90:VAL:O     | 1:A:90:VAL:CG2   | 0.43     | 2.67        | 20     | 3     |
| 1:A:205:LEU:HD12 | 1:A:205:LEU:HA   | 0.43     | 1.72        | 24     | 6     |
| 1:A:157:ASN:HA   | 1:A:192:THR:HG21 | 0.43     | 1.88        | 11     | 2     |
| 1:A:89:ALA:CB    | 1:A:110:PHE:O    | 0.43     | 2.66        | 2      | 4     |
| 1:A:42:LYS:HA    | 1:A:42:LYS:HD2   | 0.43     | 1.69        | 22     | 3     |
| 1:A:102:HIS:NE2  | 1:A:104:THR:CG2  | 0.43     | 2.81        | 4      | 2     |
| 1:A:176:ILE:CG1  | 1:A:193:GLN:OE1  | 0.43     | 2.66        | 19     | 2     |
| 1:A:15:THR:OG1   | 1:A:20:GLN:NE2   | 0.43     | 2.51        | 16     | 1     |
| 1:A:197:PRO:CA   | 1:A:201:ILE:HG23 | 0.43     | 2.42        | 20     | 2     |
| 1:A:159:GLY:CA   | 1:A:184:LEU:CD1  | 0.43     | 2.96        | 19     | 4     |
| 1:A:116:TYR:CB   | 1:A:118:LYS:HD2  | 0.43     | 2.43        | 11     | 1     |
| 1:A:136:VAL:CG1  | 1:A:161:ASP:CG   | 0.43     | 2.86        | 6      | 4     |
| 1:A:97:ASN:ND2   | 1:A:97:ASN:O     | 0.43     | 2.51        | 15     | 5     |
| 1:A:55:PHE:CZ    | 1:A:104:THR:CG2  | 0.43     | 3.01        | 23     | 2     |
| 1:A:32:ILE:CD1   | 1:A:73:ILE:CG2   | 0.43     | 2.97        | 17     | 1     |
| 1:A:87:THR:HA    | 1:A:114:GLN:CG   | 0.43     | 2.42        | 2      | 1     |
| 1:A:176:ILE:CB   | 1:A:195:LEU:HD13 | 0.43     | 2.43        | 20     | 3     |
| 1:A:73:ILE:CD1   | 1:A:92:LEU:HD22  | 0.43     | 2.42        | 9      | 1     |
| 1:A:178:PHE:HA   | 1:A:193:GLN:HA   | 0.43     | 1.91        | 21     | 3     |
| 1:A:185:LEU:HD21 | 1:A:190:GLY:C    | 0.43     | 2.34        | 21     | 1     |
| 1:A:10:LEU:CD2   | 1:A:45:GLU:OE1   | 0.43     | 2.67        | 22     | 1     |
| 1:A:91:VAL:HA    | 1:A:109:ALA:HA   | 0.43     | 1.89        | 20     | 1     |
| 1:A:125:LEU:CD1  | 1:A:125:LEU:C    | 0.43     | 2.82        | 18     | 2     |
| 1:A:96:GLN:N     | 1:A:104:THR:O    | 0.43     | 2.51        | 9      | 11    |
| 1:A:41:GLN:NE2   | 1:A:41:GLN:CA    | 0.43     | 2.81        | 24     | 1     |
| 1:A:137:PHE:CE1  | 1:A:154:ILE:CG2  | 0.43     | 3.01        | 22     | 2     |
| 1:A:87:THR:HG23  | 1:A:112:TRP:O    | 0.43     | 2.13        | 19     | 1     |
| 1:A:178:PHE:CE1  | 1:A:193:GLN:OE1  | 0.43     | 2.72        | 7      | 2     |
| 1:A:52:ARG:CA    | 1:A:96:GLN:HE22  | 0.43     | 2.20        | 6      | 1     |
| 1:A:53:ASP:O     | 1:A:57:SER:CA    | 0.43     | 2.67        | 8      | 1     |
| 1:A:176:ILE:HB   | 1:A:195:LEU:HD13 | 0.43     | 1.89        | 16     | 2     |
| 1:A:89:ALA:HB3   | 1:A:170:VAL:HG12 | 0.43     | 1.90        | 9      | 1     |
| 1:A:48:ILE:CD1   | 1:A:73:ILE:CD1   | 0.43     | 2.96        | 14     | 4     |
| 1:A:126:TRP:O    | 1:A:206:ALA:C    | 0.43     | 2.57        | 2      | 18    |
| 1:A:185:LEU:HD12 | 1:A:189:ALA:HB3  | 0.43     | 1.90        | 24     | 1     |
| 1:A:41:GLN:HE21  | 1:A:41:GLN:N     | 0.43     | 2.11        | 24     | 1     |
| 1:A:170:VAL:HB   | 1:A:175:VAL:CB   | 0.43     | 2.44        | 11     | 1     |
| 1:A:186:PRO:HD2  | 1:A:189:ALA:HB3  | 0.43     | 1.91        | 21     | 1     |
| 1:A:44:LEU:CB    | 1:A:92:LEU:CD2   | 0.43     | 2.94        | 19     | 1     |

Continued on next page...

Continued from previous page...

| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:94:VAL:HG13  | 1:A:106:THR:O    | 0.43     | 2.14        | 24     | 1     |
| 1:A:133:LEU:H    | 1:A:133:LEU:HD12 | 0.43     | 1.70        | 10     | 1     |
| 1:A:91:VAL:O     | 1:A:91:VAL:CG1   | 0.43     | 2.67        | 7      | 2     |
| 1:A:78:TYR:CE1   | 1:A:91:VAL:CG1   | 0.43     | 3.00        | 15     | 2     |
| 1:A:156:PRO:CG   | 1:A:160:LEU:HD12 | 0.43     | 2.44        | 19     | 3     |
| 1:A:125:LEU:HD12 | 1:A:126:TRP:CD2  | 0.42     | 2.49        | 5      | 1     |
| 1:A:55:PHE:CD2   | 1:A:104:THR:HB   | 0.42     | 2.49        | 6      | 1     |
| 1:A:64:PRO:HB2   | 1:A:101:THR:HB   | 0.42     | 1.89        | 3      | 1     |
| 1:A:97:ASN:OD1   | 1:A:101:THR:N    | 0.42     | 2.52        | 9      | 1     |
| 1:A:201:ILE:HD12 | 1:A:205:LEU:HD13 | 0.42     | 1.90        | 15     | 2     |
| 1:A:15:THR:CG2   | 1:A:15:THR:O     | 0.42     | 2.67        | 4      | 3     |
| 1:A:185:LEU:HG   | 1:A:190:GLY:C    | 0.42     | 2.34        | 24     | 2     |
| 1:A:170:VAL:CG2  | 1:A:174:GLY:O    | 0.42     | 2.63        | 15     | 6     |
| 1:A:133:LEU:O    | 1:A:160:LEU:CD2  | 0.42     | 2.67        | 17     | 4     |
| 1:A:48:ILE:HD11  | 1:A:71:LEU:CD2   | 0.42     | 2.28        | 3      | 1     |
| 1:A:90:VAL:HG22  | 1:A:110:PHE:CE1  | 0.42     | 2.47        | 5      | 1     |
| 1:A:179:PHE:CE1  | 1:A:192:THR:HB   | 0.42     | 2.49        | 17     | 1     |
| 1:A:184:LEU:HB3  | 1:A:192:THR:HG1  | 0.42     | 1.72        | 13     | 1     |
| 1:A:6:TYR:HD2    | 1:A:10:LEU:CG    | 0.42     | 2.27        | 9      | 1     |
| 1:A:29:ASN:ND2   | 1:A:70:GLU:HG2   | 0.42     | 2.30        | 2      | 1     |
| 1:A:184:LEU:HD22 | 1:A:192:THR:HA   | 0.42     | 1.92        | 14     | 3     |
| 1:A:54:LYS:HA    | 1:A:57:SER:CB    | 0.42     | 2.44        | 12     | 3     |
| 1:A:102:HIS:NE2  | 1:A:104:THR:OG1  | 0.42     | 2.52        | 5      | 2     |
| 1:A:184:LEU:HB3  | 1:A:192:THR:CB   | 0.42     | 2.44        | 4      | 2     |
| 1:A:185:LEU:CD2  | 1:A:191:PRO:HD2  | 0.42     | 2.44        | 15     | 1     |
| 1:A:111:ASP:OD2  | 1:A:125:LEU:CD2  | 0.42     | 2.65        | 9      | 1     |
| 1:A:205:LEU:HA   | 1:A:205:LEU:HD12 | 0.42     | 1.74        | 21     | 2     |
| 1:A:157:ASN:CA   | 1:A:184:LEU:HB2  | 0.42     | 2.44        | 21     | 1     |
| 1:A:111:ASP:OD1  | 1:A:170:VAL:HG11 | 0.42     | 2.13        | 15     | 2     |
| 1:A:112:TRP:HB2  | 1:A:119:PRO:HA   | 0.42     | 1.91        | 2      | 1     |
| 1:A:41:GLN:NE2   | 1:A:41:GLN:N     | 0.42     | 2.67        | 24     | 1     |
| 1:A:136:VAL:CG2  | 1:A:176:ILE:HD12 | 0.42     | 2.36        | 7      | 1     |
| 1:A:91:VAL:HA    | 1:A:109:ALA:CB   | 0.42     | 2.45        | 12     | 1     |
| 1:A:129:ASP:CB   | 1:A:204:MET:HG3  | 0.42     | 2.45        | 22     | 3     |
| 1:A:42:LYS:HD2   | 1:A:42:LYS:HA    | 0.42     | 1.74        | 21     | 3     |
| 1:A:90:VAL:CG2   | 1:A:110:PHE:CZ   | 0.42     | 3.03        | 5      | 1     |
| 1:A:186:PRO:C    | 1:A:188:ALA:N    | 0.42     | 2.73        | 21     | 1     |
| 1:A:95:TYR:HA    | 1:A:105:THR:HA   | 0.42     | 1.92        | 22     | 2     |
| 1:A:55:PHE:CD2   | 1:A:104:THR:CG2  | 0.42     | 3.02        | 6      | 1     |
| 1:A:87:THR:HG22  | 1:A:111:ASP:OD1  | 0.42     | 2.14        | 8      | 1     |
| 1:A:183:GLU:CA   | 1:A:186:PRO:HD3  | 0.42     | 2.45        | 19     | 2     |

Continued on next page...

*Continued from previous page...*

| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:170:VAL:CA   | 1:A:175:VAL:HA   | 0.42     | 2.43        | 3      | 5     |
| 1:A:34:LEU:O     | 1:A:35:PRO:O     | 0.42     | 2.37        | 5      | 4     |
| 1:A:112:TRP:CE2  | 1:A:117:ARG:HA   | 0.42     | 2.48        | 10     | 1     |
| 1:A:25:ASP:CG    | 1:A:26:PRO:CD    | 0.42     | 2.88        | 7      | 1     |
| 1:A:133:LEU:H    | 1:A:134:PRO:HD3  | 0.42     | 1.67        | 22     | 1     |
| 1:A:122:TYR:HB3  | 1:A:126:TRP:HE1  | 0.42     | 1.73        | 10     | 1     |
| 1:A:88:GLN:OE1   | 1:A:112:TRP:CB   | 0.42     | 2.68        | 4      | 3     |
| 1:A:75:SER:HB3   | 1:A:92:LEU:CA    | 0.42     | 2.45        | 12     | 1     |
| 1:A:66:GLU:HA    | 1:A:101:THR:OG1  | 0.42     | 2.14        | 4      | 2     |
| 1:A:44:LEU:HG    | 1:A:45:GLU:H     | 0.42     | 1.75        | 19     | 1     |
| 1:A:141:GLN:HB3  | 1:A:151:GLN:HB2  | 0.42     | 1.91        | 22     | 2     |
| 1:A:172:ASN:O    | 1:A:198:ARG:NE   | 0.42     | 2.53        | 22     | 2     |
| 1:A:87:THR:CA    | 1:A:114:GLN:HG2  | 0.42     | 2.45        | 22     | 1     |
| 1:A:65:ARG:O     | 1:A:67:ALA:N     | 0.41     | 2.53        | 3      | 1     |
| 1:A:185:LEU:HD21 | 1:A:189:ALA:C    | 0.41     | 2.34        | 21     | 1     |
| 1:A:67:ALA:CB    | 1:A:68:PRO:CD    | 0.41     | 2.95        | 21     | 1     |
| 1:A:85:ARG:CD    | 1:A:85:ARG:N     | 0.41     | 2.83        | 8      | 1     |
| 1:A:156:PRO:O    | 1:A:160:LEU:N    | 0.41     | 2.51        | 4      | 1     |
| 1:A:105:THR:O    | 1:A:106:THR:CG2  | 0.41     | 2.68        | 12     | 5     |
| 1:A:180:ASN:CG   | 1:A:191:PRO:HB3  | 0.41     | 2.35        | 7      | 3     |
| 1:A:30:ILE:CD1   | 1:A:52:ARG:NH2   | 0.41     | 2.83        | 1      | 1     |
| 1:A:185:LEU:HD12 | 1:A:191:PRO:N    | 0.41     | 2.30        | 8      | 1     |
| 1:A:6:TYR:CD2    | 1:A:10:LEU:HG    | 0.41     | 2.50        | 13     | 1     |
| 1:A:170:VAL:CB   | 1:A:175:VAL:HB   | 0.41     | 2.45        | 15     | 1     |
| 1:A:55:PHE:CG    | 1:A:96:GLN:NE2   | 0.41     | 2.87        | 19     | 1     |
| 1:A:66:GLU:N     | 1:A:101:THR:H    | 0.41     | 2.13        | 20     | 2     |
| 1:A:127:GLN:N    | 1:A:127:GLN:HE21 | 0.41     | 2.14        | 18     | 1     |
| 1:A:159:GLY:N    | 1:A:184:LEU:HG   | 0.41     | 2.30        | 9      | 2     |
| 1:A:56:LEU:HD23  | 1:A:56:LEU:N     | 0.41     | 2.31        | 17     | 1     |
| 1:A:69:TYR:HA    | 1:A:99:GLY:CA    | 0.41     | 2.44        | 3      | 3     |
| 1:A:91:VAL:HA    | 1:A:109:ALA:HB2  | 0.41     | 1.90        | 12     | 1     |
| 1:A:44:LEU:H     | 1:A:44:LEU:HG    | 0.41     | 1.48        | 14     | 1     |
| 1:A:32:ILE:CD1   | 1:A:73:ILE:HG23  | 0.41     | 2.45        | 23     | 1     |
| 1:A:32:ILE:HG13  | 1:A:48:ILE:HG12  | 0.41     | 1.92        | 17     | 1     |
| 1:A:176:ILE:CB   | 1:A:195:LEU:CD1  | 0.41     | 2.99        | 16     | 3     |
| 1:A:144:LEU:CD2  | 1:A:154:ILE:HD11 | 0.41     | 2.45        | 10     | 1     |
| 1:A:137:PHE:CZ   | 1:A:154:ILE:O    | 0.41     | 2.73        | 14     | 1     |
| 1:A:137:PHE:CE1  | 1:A:160:LEU:CA   | 0.41     | 3.02        | 17     | 1     |
| 1:A:68:PRO:HD2   | 1:A:99:GLY:CA    | 0.41     | 2.42        | 6      | 1     |
| 1:A:184:LEU:CB   | 1:A:192:THR:HG23 | 0.41     | 2.46        | 2      | 2     |
| 1:A:170:VAL:CG2  | 1:A:175:VAL:HB   | 0.41     | 2.46        | 22     | 2     |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:52:ARG:HG2   | 1:A:71:LEU:CD2   | 0.41     | 2.45        | 22     | 1     |
| 1:A:196:VAL:CG1  | 1:A:201:ILE:CG1  | 0.41     | 2.98        | 20     | 1     |
| 1:A:10:LEU:HD21  | 1:A:45:GLU:OE2   | 0.41     | 2.16        | 3      | 1     |
| 1:A:44:LEU:CB    | 1:A:110:PHE:CZ   | 0.41     | 3.03        | 6      | 1     |
| 1:A:55:PHE:CD2   | 1:A:104:THR:HG21 | 0.41     | 2.50        | 6      | 1     |
| 1:A:32:ILE:CA    | 1:A:73:ILE:HG23  | 0.41     | 2.45        | 6      | 1     |
| 1:A:48:ILE:O     | 1:A:52:ARG:CD    | 0.41     | 2.69        | 8      | 3     |
| 1:A:23:MET:O     | 1:A:30:ILE:CD1   | 0.41     | 2.67        | 24     | 1     |
| 1:A:78:TYR:OH    | 1:A:91:VAL:CG1   | 0.41     | 2.68        | 10     | 1     |
| 1:A:78:TYR:OH    | 1:A:91:VAL:HG12  | 0.41     | 2.16        | 10     | 1     |
| 1:A:43:SER:CB    | 1:A:110:PHE:CD2  | 0.41     | 3.03        | 23     | 2     |
| 1:A:141:GLN:O    | 1:A:144:LEU:CB   | 0.41     | 2.69        | 22     | 2     |
| 1:A:113:ASP:OD2  | 1:A:118:LYS:HD3  | 0.41     | 2.16        | 11     | 1     |
| 1:A:197:PRO:CD   | 1:A:201:ILE:CG2  | 0.41     | 2.98        | 1      | 2     |
| 1:A:148:THR:C    | 1:A:150:GLN:H    | 0.41     | 2.19        | 21     | 3     |
| 1:A:42:LYS:HD2   | 1:A:45:GLU:OE2   | 0.41     | 2.16        | 5      | 1     |
| 1:A:90:VAL:CG2   | 1:A:110:PHE:CD1  | 0.41     | 3.04        | 23     | 1     |
| 1:A:42:LYS:HA    | 1:A:45:GLU:OE2   | 0.41     | 2.15        | 6      | 1     |
| 1:A:43:SER:HG    | 1:A:110:PHE:HD2  | 0.41     | 1.57        | 8      | 1     |
| 1:A:116:TYR:O    | 1:A:118:LYS:CG   | 0.41     | 2.69        | 22     | 1     |
| 1:A:137:PHE:CZ   | 1:A:154:ILE:HB   | 0.41     | 2.51        | 22     | 1     |
| 1:A:185:LEU:HD22 | 1:A:191:PRO:N    | 0.41     | 2.29        | 15     | 1     |
| 1:A:65:ARG:HB3   | 1:A:99:GLY:CA    | 0.41     | 2.45        | 3      | 1     |
| 1:A:88:GLN:OE1   | 1:A:89:ALA:N     | 0.41     | 2.53        | 3      | 1     |
| 1:A:88:GLN:N     | 1:A:114:GLN:CG   | 0.41     | 2.84        | 8      | 1     |
| 1:A:94:VAL:CG1   | 1:A:106:THR:O    | 0.41     | 2.69        | 8      | 1     |
| 1:A:86:GLY:C     | 1:A:114:GLN:HG3  | 0.41     | 2.35        | 22     | 1     |
| 1:A:87:THR:CA    | 1:A:114:GLN:CB   | 0.41     | 2.99        | 4      | 1     |
| 1:A:185:LEU:CD1  | 1:A:185:LEU:C    | 0.40     | 2.88        | 9      | 1     |
| 1:A:15:THR:O     | 1:A:15:THR:CG2   | 0.40     | 2.68        | 14     | 1     |
| 1:A:185:LEU:CD2  | 1:A:189:ALA:CB   | 0.40     | 2.99        | 21     | 1     |
| 1:A:40:ASP:CG    | 1:A:40:ASP:O     | 0.40     | 2.60        | 21     | 1     |
| 1:A:32:ILE:HA    | 1:A:73:ILE:HG23  | 0.40     | 1.91        | 6      | 2     |
| 1:A:175:VAL:CG1  | 1:A:196:VAL:CG1  | 0.40     | 2.90        | 13     | 1     |
| 1:A:93:LYS:HG3   | 1:A:107:TYR:OH   | 0.40     | 2.15        | 5      | 1     |
| 1:A:34:LEU:HD21  | 1:A:92:LEU:HD23  | 0.40     | 1.93        | 16     | 1     |
| 1:A:185:LEU:HD13 | 1:A:190:GLY:O    | 0.40     | 2.16        | 15     | 1     |
| 1:A:77:THR:HG22  | 1:A:78:TYR:N     | 0.40     | 2.31        | 3      | 1     |
| 1:A:97:ASN:OD1   | 1:A:102:HIS:O    | 0.40     | 2.39        | 21     | 1     |
| 1:A:34:LEU:HD13  | 1:A:34:LEU:C     | 0.40     | 2.35        | 4      | 1     |
| 1:A:156:PRO:O    | 1:A:184:LEU:CG   | 0.40     | 2.70        | 2      | 1     |

*Continued on next page...*

Continued from previous page...

| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:48:ILE:O     | 1:A:52:ARG:HD2   | 0.40     | 2.16        | 24     | 1     |
| 1:A:185:LEU:HD21 | 1:A:191:PRO:N    | 0.40     | 2.31        | 10     | 1     |
| 1:A:6:TYR:HB2    | 1:A:10:LEU:HD23  | 0.40     | 1.92        | 9      | 1     |
| 1:A:43:SER:OG    | 1:A:110:PHE:CD2  | 0.40     | 2.75        | 23     | 1     |
| 1:A:193:GLN:HG2  | 1:A:194:VAL:N    | 0.40     | 2.30        | 23     | 1     |
| 1:A:21:ILE:N     | 1:A:32:ILE:O     | 0.40     | 2.53        | 6      | 1     |
| 1:A:182:GLY:O    | 1:A:183:GLU:CG   | 0.40     | 2.70        | 3      | 1     |
| 1:A:79:GLN:HB2   | 1:A:114:GLN:HE22 | 0.40     | 1.76        | 10     | 1     |
| 1:A:148:THR:C    | 1:A:150:GLN:N    | 0.40     | 2.75        | 7      | 1     |
| 1:A:89:ALA:HB2   | 1:A:111:ASP:HA   | 0.40     | 1.92        | 9      | 1     |
| 1:A:20:GLN:HA    | 1:A:32:ILE:O     | 0.40     | 2.17        | 9      | 1     |
| 1:A:82:ILE:CA    | 1:A:85:ARG:O     | 0.40     | 2.69        | 9      | 1     |
| 1:A:179:PHE:HE1  | 1:A:192:THR:CG2  | 0.40     | 2.29        | 16     | 1     |
| 1:A:136:VAL:HG12 | 1:A:160:LEU:O    | 0.40     | 2.16        | 8      | 1     |
| 1:A:134:PRO:N    | 1:A:160:LEU:HD21 | 0.40     | 2.31        | 4      | 1     |

## 6.3 Torsion angles ⓘ

### 6.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. 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     | 192/204 (94%)   | 150±1 (78±1%) | 25±1 (13±1%) | 17±1 (9±0%) | 2           | 13 |
| All | All   | 4608/4896 (94%) | 3604 (78%)    | 602 (13%)    | 402 (9%)    | 2           | 13 |

All 22 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 27  | ALA  | 24             |
| 1   | A     | 159 | GLY  | 24             |
| 1   | A     | 185 | LEU  | 24             |
| 1   | A     | 152 | VAL  | 24             |
| 1   | A     | 67  | ALA  | 24             |
| 1   | A     | 103 | PRO  | 24             |
| 1   | A     | 85  | ARG  | 24             |

Continued on next page...

*Continued from previous page...*

| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 11  | LYS  | 24             |
| 1   | A     | 68  | PRO  | 24             |
| 1   | A     | 181 | PRO  | 24             |
| 1   | A     | 83  | PRO  | 24             |
| 1   | A     | 42  | LYS  | 24             |
| 1   | A     | 132 | PRO  | 23             |
| 1   | A     | 64  | PRO  | 22             |
| 1   | A     | 186 | PRO  | 20             |
| 1   | A     | 7   | CYS  | 19             |
| 1   | A     | 182 | GLY  | 9              |
| 1   | A     | 169 | ALA  | 9              |
| 1   | A     | 5   | THR  | 9              |
| 1   | A     | 66  | GLU  | 1              |
| 1   | A     | 131 | ASP  | 1              |
| 1   | A     | 183 | GLU  | 1              |

### 6.3.2 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 PDB entries followed by that with respect to all NMR entries. 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     | 163/173 (94%)   | 98±2 (60±2%) | 65±2 (40±2%) | 0           | 5 |
| All | All   | 3912/4152 (94%) | 2347 (60%)   | 1565 (40%)   | 0           | 5 |

All 110 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 21  | ILE  | 24             |
| 1   | A     | 5   | THR  | 24             |
| 1   | A     | 54  | LYS  | 24             |
| 1   | A     | 60  | THR  | 24             |
| 1   | A     | 42  | LYS  | 24             |
| 1   | A     | 63  | THR  | 24             |
| 1   | A     | 52  | ARG  | 24             |
| 1   | A     | 107 | TYR  | 24             |
| 1   | A     | 205 | LEU  | 24             |
| 1   | A     | 73  | ILE  | 24             |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 179 | PHE  | 24             |
| 1   | A     | 122 | TYR  | 24             |
| 1   | A     | 10  | LEU  | 24             |
| 1   | A     | 44  | LEU  | 24             |
| 1   | A     | 95  | TYR  | 24             |
| 1   | A     | 110 | PHE  | 24             |
| 1   | A     | 127 | GLN  | 24             |
| 1   | A     | 141 | GLN  | 24             |
| 1   | A     | 69  | TYR  | 24             |
| 1   | A     | 28  | TYR  | 24             |
| 1   | A     | 24  | SER  | 24             |
| 1   | A     | 176 | ILE  | 24             |
| 1   | A     | 112 | TRP  | 24             |
| 1   | A     | 137 | PHE  | 24             |
| 1   | A     | 133 | LEU  | 24             |
| 1   | A     | 92  | LEU  | 24             |
| 1   | A     | 20  | GLN  | 24             |
| 1   | A     | 193 | GLN  | 24             |
| 1   | A     | 199 | SER  | 23             |
| 1   | A     | 96  | GLN  | 23             |
| 1   | A     | 78  | TYR  | 23             |
| 1   | A     | 201 | ILE  | 23             |
| 1   | A     | 97  | ASN  | 23             |
| 1   | A     | 160 | LEU  | 23             |
| 1   | A     | 104 | THR  | 22             |
| 1   | A     | 85  | ARG  | 22             |
| 1   | A     | 114 | GLN  | 22             |
| 1   | A     | 25  | ASP  | 21             |
| 1   | A     | 196 | VAL  | 21             |
| 1   | A     | 61  | SER  | 21             |
| 1   | A     | 145 | SER  | 21             |
| 1   | A     | 65  | ARG  | 20             |
| 1   | A     | 136 | VAL  | 20             |
| 1   | A     | 117 | ARG  | 20             |
| 1   | A     | 131 | ASP  | 20             |
| 1   | A     | 173 | ASP  | 19             |
| 1   | A     | 45  | GLU  | 19             |
| 1   | A     | 80  | SER  | 19             |
| 1   | A     | 30  | ILE  | 19             |
| 1   | A     | 147 | GLN  | 19             |
| 1   | A     | 88  | GLN  | 18             |
| 1   | A     | 118 | LYS  | 17             |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 185 | LEU  | 16             |
| 1   | A     | 124 | THR  | 16             |
| 1   | A     | 123 | ASP  | 15             |
| 1   | A     | 34  | LEU  | 15             |
| 1   | A     | 184 | LEU  | 15             |
| 1   | A     | 148 | THR  | 14             |
| 1   | A     | 129 | ASP  | 14             |
| 1   | A     | 29  | ASN  | 14             |
| 1   | A     | 175 | VAL  | 14             |
| 1   | A     | 79  | GLN  | 13             |
| 1   | A     | 57  | SER  | 13             |
| 1   | A     | 15  | THR  | 12             |
| 1   | A     | 102 | HIS  | 12             |
| 1   | A     | 22  | GLN  | 11             |
| 1   | A     | 151 | GLN  | 10             |
| 1   | A     | 93  | LYS  | 10             |
| 1   | A     | 87  | THR  | 10             |
| 1   | A     | 17  | GLN  | 10             |
| 1   | A     | 91  | VAL  | 10             |
| 1   | A     | 40  | ASP  | 9              |
| 1   | A     | 198 | ARG  | 8              |
| 1   | A     | 33  | SER  | 7              |
| 1   | A     | 153 | SER  | 7              |
| 1   | A     | 113 | ASP  | 7              |
| 1   | A     | 11  | LYS  | 6              |
| 1   | A     | 152 | VAL  | 6              |
| 1   | A     | 70  | GLU  | 6              |
| 1   | A     | 66  | GLU  | 6              |
| 1   | A     | 130 | THR  | 6              |
| 1   | A     | 187 | GLU  | 6              |
| 1   | A     | 43  | SER  | 6              |
| 1   | A     | 23  | MET  | 6              |
| 1   | A     | 108 | LYS  | 5              |
| 1   | A     | 144 | LEU  | 5              |
| 1   | A     | 183 | GLU  | 5              |
| 1   | A     | 202 | ASP  | 4              |
| 1   | A     | 32  | ILE  | 4              |
| 1   | A     | 41  | GLN  | 4              |
| 1   | A     | 48  | ILE  | 4              |
| 1   | A     | 31  | ASN  | 4              |
| 1   | A     | 75  | SER  | 4              |
| 1   | A     | 178 | PHE  | 3              |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 157 | ASN  | 3              |
| 1   | A     | 82  | ILE  | 2              |
| 1   | A     | 62  | SER  | 2              |
| 1   | A     | 51  | THR  | 2              |
| 1   | A     | 204 | MET  | 2              |
| 1   | A     | 146 | LYS  | 2              |
| 1   | A     | 170 | VAL  | 1              |
| 1   | A     | 94  | VAL  | 1              |
| 1   | A     | 111 | ASP  | 1              |
| 1   | A     | 105 | THR  | 1              |
| 1   | A     | 161 | ASP  | 1              |
| 1   | A     | 192 | THR  | 1              |
| 1   | A     | 53  | ASP  | 1              |
| 1   | A     | 77  | THR  | 1              |
| 1   | A     | 191 | PRO  | 1              |
| 1   | A     | 9   | GLU  | 1              |

### 6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 6.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 6.6 Ligand geometry ⓘ

There are no ligands in this entry.

### 6.7 Other polymers ⓘ

There are no such molecules in this entry.

## 6.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 7 Chemical shift validation

No chemical shift data were provided