



# Full wwPDB NMR Structure Validation Report ⓘ

Mar 5, 2026 – 07:20 PM UTC

PDB ID : 2JXY / pdb\_00002jxy  
Title : Solution structure of the hemopexin-like domain of MMP12  
Authors : Bertini, I.; Calderone, V.; Fragai, M.; Jaiswal, R.; Luchinat, C.; Melikian, M.  
Deposited on : 2007-12-01

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

<https://www.wwpdb.org/validation/2017/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

---

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

|                                |   |                                                                  |
|--------------------------------|---|------------------------------------------------------------------|
| MolProbity                     | : | 4-5-2 with Phenix2.0                                             |
| Percentile statistics          | : | 20250101.v01 (using entries in the PDB archive January 1st 2025) |
| wwPDB-RCI                      | : | v_1n_11_5_13_A (Berjanski et al., 2005)                          |
| PANAV                          | : | Wang et al. (2010)                                               |
| wwPDB-ShiftChecker             | : | v1.2                                                             |
| Ideal geometry (proteins)      | : | Engh & Huber (2001)                                              |
| Ideal geometry (DNA, RNA)      | : | Parkinson et al. (1996)                                          |
| Validation Pipeline (wwPDB-VP) | : | 2.49                                                             |

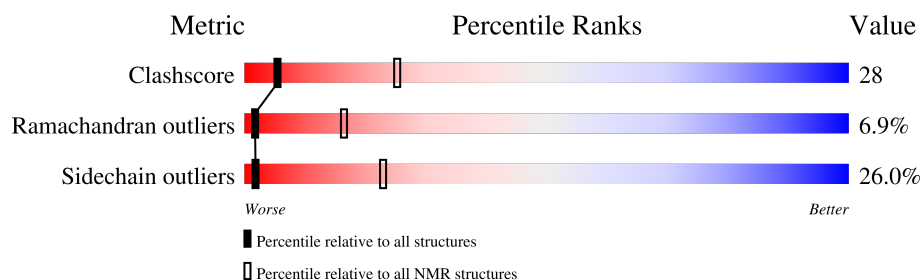
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*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            | 229148                      | 14424                     |
| Ramachandran outliers | 224038                      | 12848                     |
| Sidechain outliers    | 223484                      | 12823                     |

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     | 194    | <div> <div></div> <div>34%</div> <div>57%</div> <div>7%</div> <div></div> </div> |

## 2 Ensemble composition and analysis

This entry contains 20 models. Model 1 is the overall representative, medoid model (most similar to other models).

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:281-A:470 (190)     | 1.22              | 1            |

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 3 clusters and 4 single-model clusters were found.

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

### 3 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 3243 atoms, of which 1595 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Macrophage metalloelastase.

| Mol | Chain | Residues | Atoms |      |      |     |     |   | Trace |
|-----|-------|----------|-------|------|------|-----|-----|---|-------|
| 1   | A     | 194      | Total | C    | H    | N   | O   | S | 0     |
|     |       |          | 3242  | 1089 | 1595 | 267 | 286 | 5 |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| A     | 277     | MET      | -      | expression tag | UNP P39900 |

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

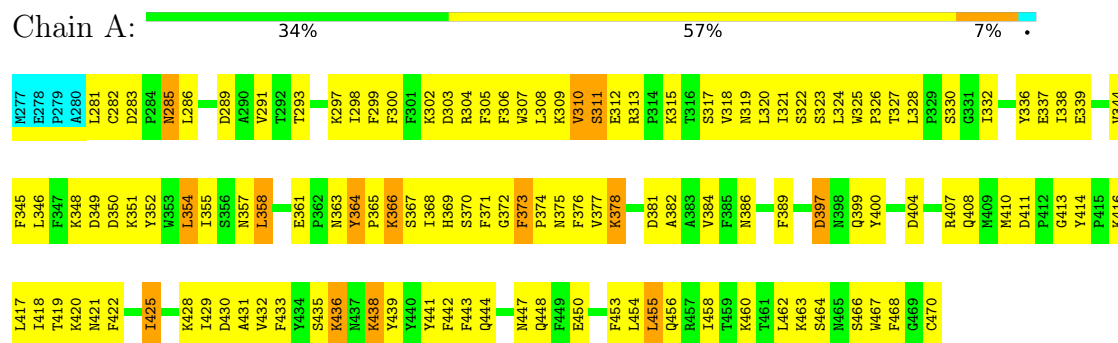
| Mol | Chain | Residues | Atoms |    |
|-----|-------|----------|-------|----|
| 2   | A     | 1        | Total | Ca |
|     |       |          | 1     | 1  |

## 4 Residue-property plots

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

These plots are provided for all protein, RNA, DNA and oligosaccharide 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: Macrophage metalloelastase



### 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 (medoid)

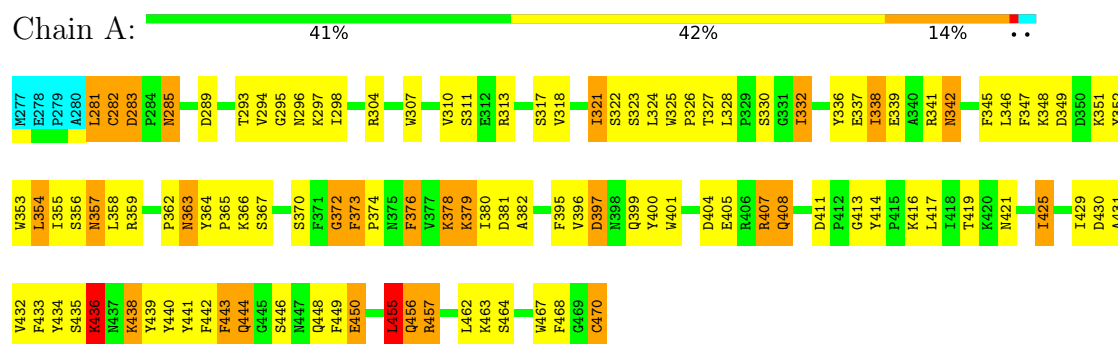
- Molecule 1: Macrophage metalloelastase



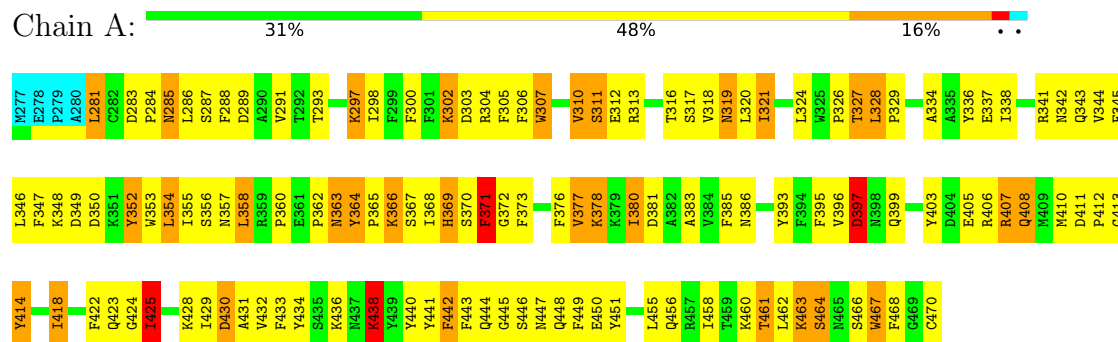


### 4.2.5 Score per residue for model 5

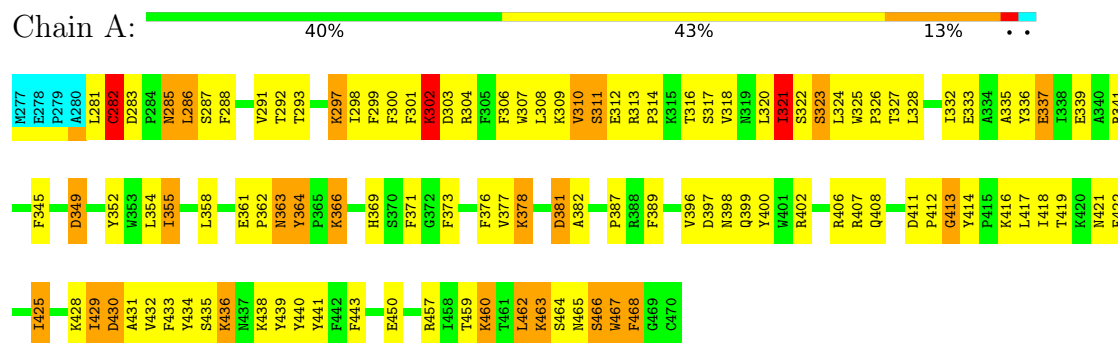
- Molecule 1: Macrophage metalloelastase



- Molecule 1: Macrophage metalloelastase

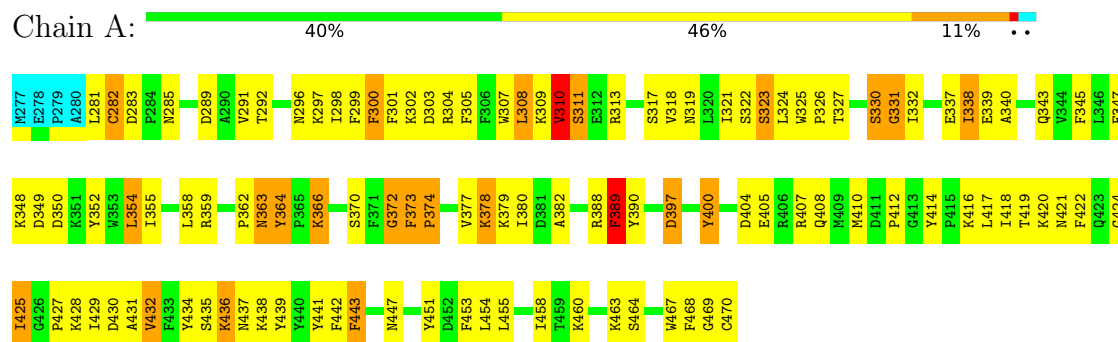


- Molecule 1: Macrophage metalloelastase



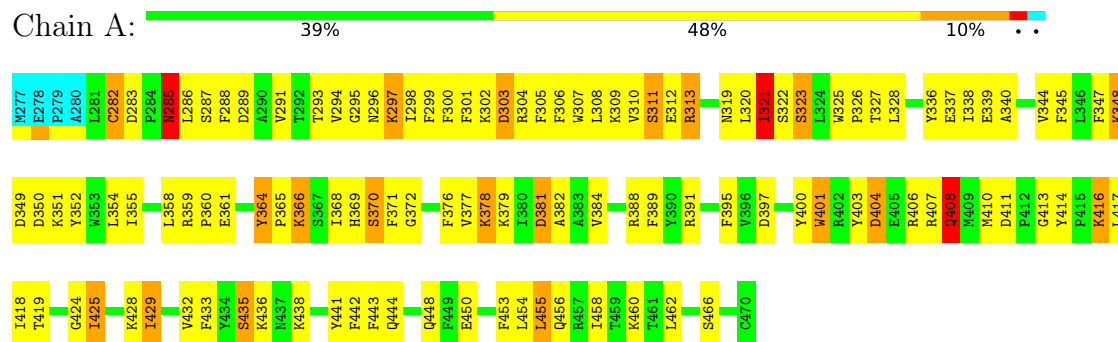
### 4.2.8 Score per residue for model 8

- Molecule 1: Macrophage metalloelastase



### 4.2.9 Score per residue for model 9

- Molecule 1: Macrophage metalloelastase



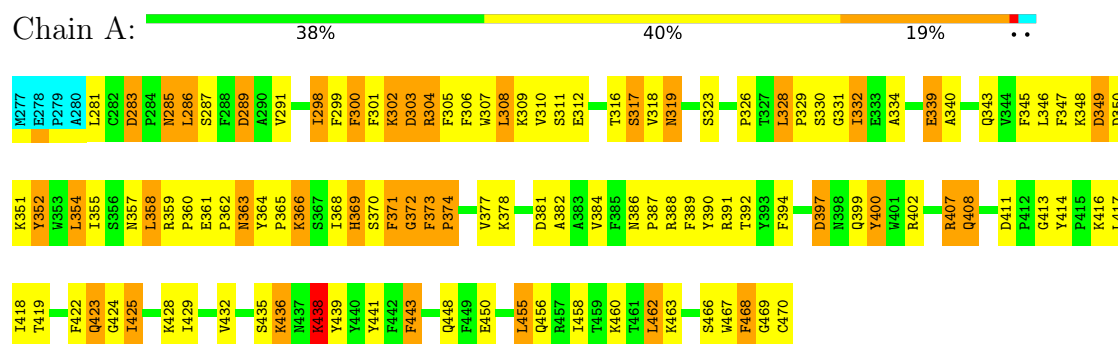
### 4.2.10 Score per residue for model 10

- Molecule 1: Macrophage metalloelastase



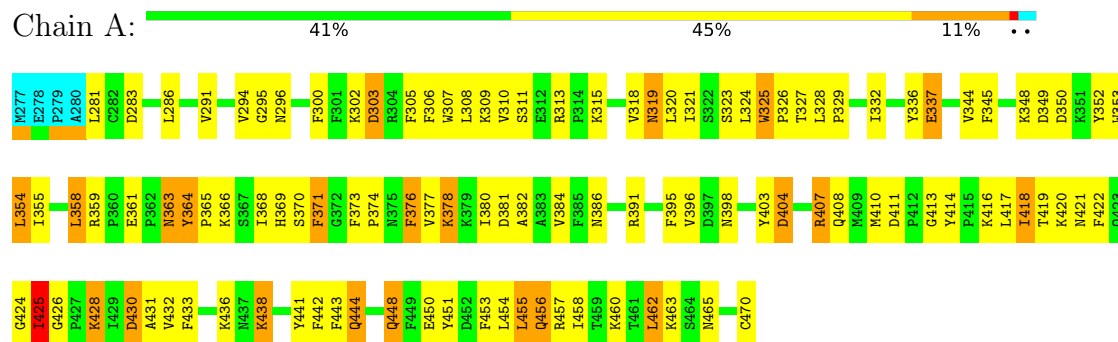
### 4.2.11 Score per residue for model 11

- Molecule 1: Macrophage metalloelastase



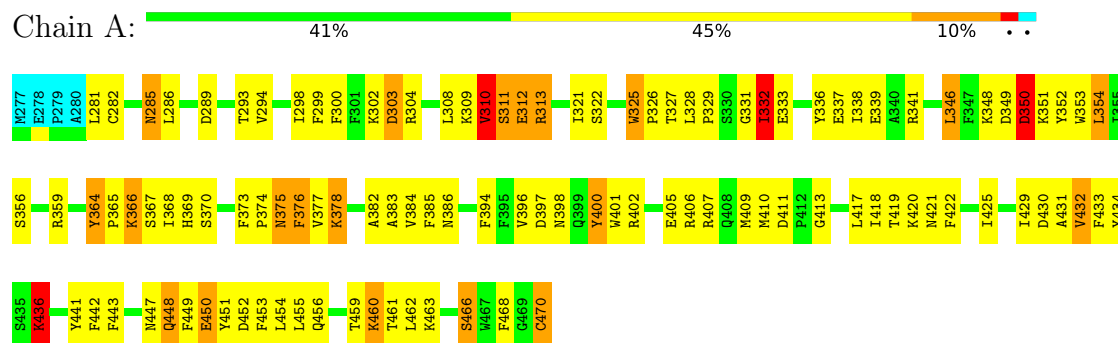
### 4.2.12 Score per residue for model 12

- Molecule 1: Macrophage metalloelastase



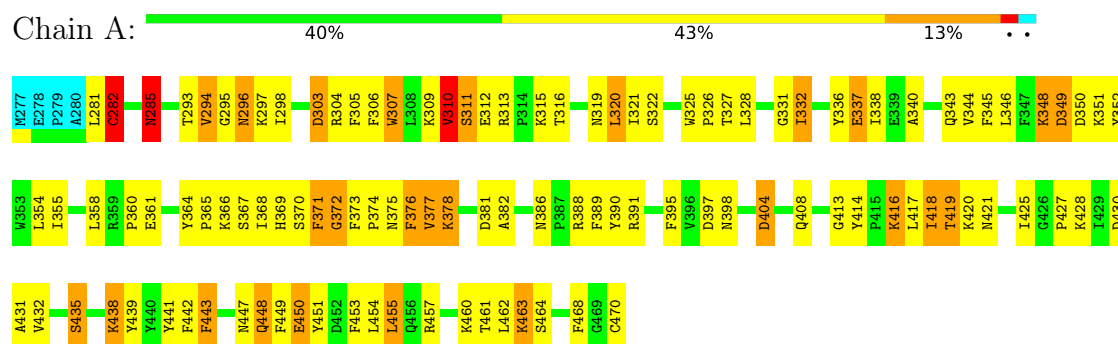
### 4.2.13 Score per residue for model 13

- Molecule 1: Macrophage metalloelastase



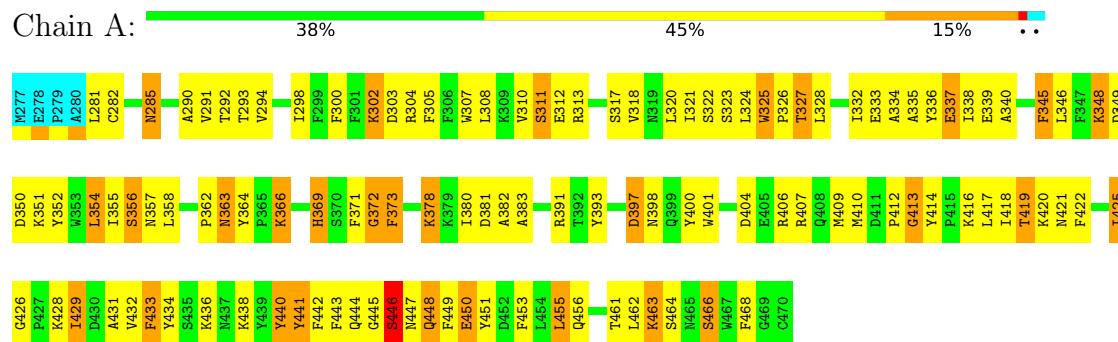
## 4.2.14 Score per residue for model 14

## • Molecule 1: Macrophage metalloelastase



## 4.2.15 Score per residue for model 15

## • Molecule 1: Macrophage metalloelastase



## 4.2.16 Score per residue for model 16

## • Molecule 1: Macrophage metalloelastase



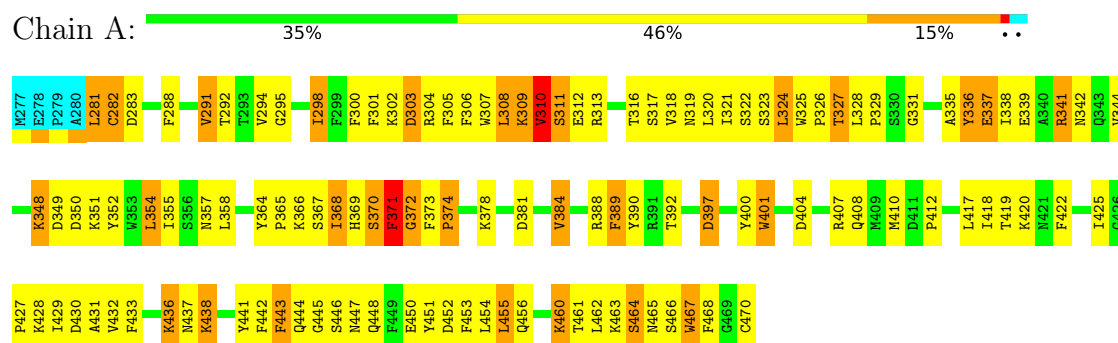
## 4.2.17 Score per residue for model 17

- Molecule 1: Macrophage metalloelastase



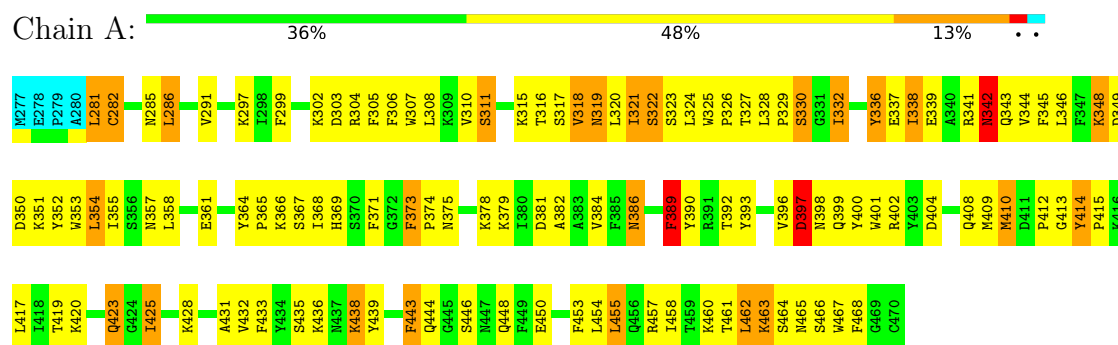
## 4.2.18 Score per residue for model 18

- Molecule 1: Macrophage metalloelastase



## 4.2.19 Score per residue for model 19

- Molecule 1: Macrophage metalloelastase



## 4.2.20 Score per residue for model 20

## ● Molecule 1: Macrophage metalloelastase



## 5 Refinement protocol and experimental data overview

The models were refined using the following method: *simulated annealing*.

Of the 1600 calculated structures, 20 were deposited, based on the following criterion: *lowest target function*.

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

| Software name | Classification | Version |
|---------------|----------------|---------|
| DYANA         | refinement     |         |

No chemical shift data was provided.

## 6 Model quality [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: CA

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     | 0.69±0.00    | 0±0/1675 ( 0.0± 0.0%) | 1.11±0.01   | 2±1/2268 ( 0.1± 0.0%) |
| All | All   | 0.69         | 0/33500 ( 0.0%)       | 1.11        | 38/45360 ( 0.1%)      |

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     | 373 | PHE  | O-C-N   | 6.62  | 124.58      | 121.53   | 15     | 3     |
| 1   | A     | 397 | ASP  | CB-CA-C | -6.59 | 107.95      | 115.79   | 10     | 15    |
| 1   | A     | 349 | ASP  | CB-CA-C | -6.58 | 107.96      | 115.79   | 7      | 18    |
| 1   | A     | 414 | TYR  | O-C-N   | 6.42  | 124.48      | 121.53   | 6      | 1     |
| 1   | A     | 414 | TYR  | N-CA-CB | -5.11 | 105.98      | 111.66   | 6      | 1     |

There are no chirality outliers.

There are no planarity outliers.

### 6.2 Too-close contacts [i](#)

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     | 1618  | 1568     | 1565     | 89±16   |
| All | All   | 32380 | 31360    | 31324    | 1775    |

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 28.

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

| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:281:LEU:HD11 | 1:A:307:TRP:CZ3  | 1.00     | 1.91        | 17     | 1     |
| 1:A:328:LEU:HD21 | 1:A:355:ILE:HD11 | 0.94     | 1.40        | 10     | 3     |
| 1:A:346:LEU:HD23 | 1:A:355:ILE:HD13 | 0.92     | 1.37        | 2      | 2     |
| 1:A:291:VAL:HG21 | 1:A:442:PHE:CZ   | 0.91     | 2.01        | 15     | 1     |
| 1:A:298:ILE:HD13 | 1:A:300:PHE:CZ   | 0.90     | 2.01        | 13     | 1     |
| 1:A:432:VAL:HG21 | 1:A:442:PHE:CE1  | 0.88     | 2.02        | 8      | 3     |
| 1:A:368:ILE:HD12 | 1:A:377:VAL:HG13 | 0.88     | 1.45        | 2      | 1     |
| 1:A:286:LEU:HD11 | 1:A:307:TRP:CZ2  | 0.88     | 2.04        | 16     | 2     |
| 1:A:336:TYR:OH   | 1:A:338:ILE:HD11 | 0.87     | 1.69        | 10     | 1     |
| 1:A:327:THR:O    | 1:A:328:LEU:HD22 | 0.87     | 1.70        | 6      | 13    |
| 1:A:334:ALA:HB1  | 1:A:383:ALA:HB2  | 0.86     | 1.46        | 15     | 1     |
| 1:A:281:LEU:HD11 | 1:A:316:THR:OG1  | 0.85     | 1.71        | 18     | 1     |
| 1:A:450:GLU:O    | 1:A:458:ILE:HG23 | 0.84     | 1.72        | 1      | 3     |
| 1:A:382:ALA:HB1  | 1:A:432:VAL:HG12 | 0.84     | 1.50        | 1      | 5     |
| 1:A:354:LEU:HD23 | 1:A:364:TYR:CE2  | 0.83     | 2.08        | 18     | 3     |
| 1:A:350:ASP:O    | 1:A:368:ILE:HG23 | 0.82     | 1.74        | 13     | 1     |
| 1:A:338:ILE:HD12 | 1:A:345:PHE:CE1  | 0.82     | 2.10        | 10     | 2     |
| 1:A:291:VAL:HG22 | 1:A:431:ALA:HB1  | 0.81     | 1.50        | 4      | 5     |
| 1:A:291:VAL:HG21 | 1:A:442:PHE:CE1  | 0.81     | 2.11        | 15     | 1     |
| 1:A:291:VAL:HG21 | 1:A:300:PHE:CE2  | 0.80     | 2.11        | 16     | 1     |
| 1:A:424:GLY:CA   | 1:A:458:ILE:HD11 | 0.80     | 2.06        | 12     | 2     |
| 1:A:337:GLU:OE1  | 1:A:344:VAL:HG22 | 0.80     | 1.75        | 19     | 1     |
| 1:A:462:LEU:HD11 | 1:A:466:SER:CB   | 0.79     | 2.07        | 15     | 3     |
| 1:A:364:TYR:N    | 1:A:365:PRO:CD   | 0.79     | 2.46        | 12     | 3     |
| 1:A:328:LEU:HD13 | 1:A:329:PRO:HD2  | 0.79     | 1.54        | 10     | 6     |
| 1:A:290:ALA:HB2  | 1:A:333:GLU:O    | 0.78     | 1.77        | 15     | 2     |
| 1:A:429:ILE:HD11 | 1:A:440:TYR:OH   | 0.78     | 1.77        | 15     | 1     |
| 1:A:336:TYR:CZ   | 1:A:338:ILE:HD11 | 0.77     | 2.14        | 10     | 1     |
| 1:A:347:PHE:CZ   | 1:A:380:ILE:HD12 | 0.77     | 2.15        | 5      | 1     |
| 1:A:288:PHE:CE2  | 1:A:300:PHE:CD1  | 0.77     | 2.72        | 4      | 2     |
| 1:A:281:LEU:HD13 | 1:A:316:THR:OG1  | 0.77     | 1.80        | 17     | 1     |
| 1:A:354:LEU:C    | 1:A:354:LEU:HD12 | 0.76     | 2.05        | 18     | 3     |
| 1:A:396:VAL:HG22 | 1:A:397:ASP:OD1  | 0.76     | 1.79        | 19     | 1     |
| 1:A:298:ILE:HD12 | 1:A:310:VAL:HG23 | 0.76     | 1.58        | 20     | 1     |
| 1:A:345:PHE:C    | 1:A:346:LEU:HD22 | 0.76     | 2.06        | 2      | 8     |
| 1:A:345:PHE:C    | 1:A:346:LEU:HD23 | 0.76     | 2.05        | 10     | 1     |
| 1:A:462:LEU:HD12 | 1:A:466:SER:CB   | 0.74     | 2.10        | 13     | 7     |
| 1:A:428:LYS:C    | 1:A:429:ILE:HD12 | 0.74     | 2.07        | 1      | 2     |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:449:PHE:CE1  | 1:A:461:THR:HG22 | 0.74     | 2.16        | 14     | 1     |
| 1:A:462:LEU:HD12 | 1:A:466:SER:HB3  | 0.74     | 1.57        | 1      | 7     |
| 1:A:347:PHE:CE1  | 1:A:380:ILE:HD12 | 0.74     | 2.18        | 5      | 1     |
| 1:A:299:PHE:CD1  | 1:A:308:LEU:HD23 | 0.73     | 2.18        | 9      | 1     |
| 1:A:432:VAL:HG23 | 1:A:441:TYR:O    | 0.73     | 1.82        | 16     | 2     |
| 1:A:425:ILE:HD13 | 1:A:425:ILE:N    | 0.72     | 2.00        | 10     | 4     |
| 1:A:281:LEU:HD21 | 1:A:307:TRP:CD1  | 0.72     | 2.20        | 5      | 1     |
| 1:A:425:ILE:HG21 | 1:A:442:PHE:CD2  | 0.72     | 2.20        | 16     | 2     |
| 1:A:364:TYR:C    | 1:A:364:TYR:CD1  | 0.72     | 2.67        | 12     | 1     |
| 1:A:354:LEU:HD12 | 1:A:355:ILE:N    | 0.72     | 1.98        | 8      | 5     |
| 1:A:346:LEU:HD23 | 1:A:355:ILE:CD1  | 0.71     | 2.16        | 2      | 1     |
| 1:A:354:LEU:C    | 1:A:354:LEU:HD13 | 0.71     | 2.09        | 17     | 3     |
| 1:A:334:ALA:HB1  | 1:A:383:ALA:CB   | 0.71     | 2.15        | 15     | 2     |
| 1:A:327:THR:C    | 1:A:328:LEU:HD22 | 0.71     | 2.09        | 9      | 6     |
| 1:A:297:LYS:HA   | 1:A:310:VAL:HG11 | 0.71     | 1.62        | 5      | 3     |
| 1:A:384:VAL:HG11 | 1:A:432:VAL:HG12 | 0.70     | 1.62        | 18     | 1     |
| 1:A:425:ILE:CG2  | 1:A:429:ILE:HD13 | 0.70     | 2.17        | 5      | 1     |
| 1:A:353:TRP:NE1  | 1:A:364:TYR:CE1  | 0.69     | 2.60        | 12     | 1     |
| 1:A:298:ILE:O    | 1:A:298:ILE:HD12 | 0.69     | 1.86        | 13     | 1     |
| 1:A:396:VAL:HG12 | 1:A:397:ASP:OD2  | 0.69     | 1.88        | 6      | 1     |
| 1:A:281:LEU:HD13 | 1:A:468:PHE:CE2  | 0.69     | 2.23        | 1      | 1     |
| 1:A:418:ILE:HG22 | 1:A:425:ILE:HD11 | 0.69     | 1.63        | 14     | 2     |
| 1:A:346:LEU:HD23 | 1:A:346:LEU:N    | 0.69     | 2.03        | 10     | 1     |
| 1:A:297:LYS:HA   | 1:A:310:VAL:HG21 | 0.68     | 1.65        | 20     | 4     |
| 1:A:382:ALA:HB1  | 1:A:432:VAL:HG22 | 0.68     | 1.64        | 14     | 3     |
| 1:A:304:ARG:O    | 1:A:320:LEU:HD12 | 0.68     | 1.89        | 20     | 1     |
| 1:A:424:GLY:HA3  | 1:A:458:ILE:HD11 | 0.68     | 1.64        | 12     | 3     |
| 1:A:429:ILE:HD11 | 1:A:442:PHE:HB3  | 0.68     | 1.66        | 3      | 3     |
| 1:A:281:LEU:HD22 | 1:A:468:PHE:HB3  | 0.67     | 1.65        | 15     | 1     |
| 1:A:432:VAL:CG2  | 1:A:442:PHE:CE1  | 0.67     | 2.77        | 1      | 2     |
| 1:A:461:THR:HG22 | 1:A:461:THR:O    | 0.67     | 1.89        | 6      | 2     |
| 1:A:432:VAL:HG21 | 1:A:442:PHE:CZ   | 0.67     | 2.24        | 8      | 2     |
| 1:A:346:LEU:CD2  | 1:A:355:ILE:HD13 | 0.67     | 2.18        | 2      | 1     |
| 1:A:357:ASN:O    | 1:A:358:LEU:HD23 | 0.67     | 1.88        | 4      | 5     |
| 1:A:418:ILE:HD13 | 1:A:427:PRO:O    | 0.67     | 1.90        | 18     | 2     |
| 1:A:281:LEU:HD23 | 1:A:307:TRP:CH2  | 0.66     | 2.25        | 19     | 2     |
| 1:A:328:LEU:HD11 | 1:A:346:LEU:HD11 | 0.66     | 1.66        | 10     | 1     |
| 1:A:354:LEU:HD23 | 1:A:354:LEU:O    | 0.66     | 1.90        | 13     | 2     |
| 1:A:462:LEU:HD11 | 1:A:466:SER:HB3  | 0.66     | 1.67        | 15     | 1     |
| 1:A:399:GLN:O    | 1:A:418:ILE:HD11 | 0.65     | 1.91        | 20     | 5     |
| 1:A:338:ILE:HD11 | 1:A:385:PHE:HB3  | 0.65     | 1.66        | 20     | 1     |

*Continued on next page...*

Continued from previous page...

| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:281:LEU:HD13 | 1:A:468:PHE:CD2  | 0.65     | 2.26        | 1      | 1     |
| 1:A:421:ASN:ND2  | 1:A:422:PHE:CZ   | 0.65     | 2.65        | 15     | 1     |
| 1:A:281:LEU:CD2  | 1:A:468:PHE:CD1  | 0.65     | 2.79        | 11     | 1     |
| 1:A:299:PHE:CE2  | 1:A:308:LEU:HD23 | 0.65     | 2.26        | 8      | 2     |
| 1:A:433:PHE:CE1  | 1:A:443:PHE:CZ   | 0.65     | 2.85        | 7      | 1     |
| 1:A:294:VAL:HG22 | 1:A:337:GLU:CD   | 0.65     | 2.16        | 17     | 1     |
| 1:A:443:PHE:CE2  | 1:A:448:GLN:NE2  | 0.64     | 2.65        | 2      | 3     |
| 1:A:373:PHE:O    | 1:A:373:PHE:CD2  | 0.64     | 2.50        | 20     | 3     |
| 1:A:336:TYR:C    | 1:A:336:TYR:CD1  | 0.64     | 2.75        | 18     | 3     |
| 1:A:372:GLY:O    | 1:A:373:PHE:C    | 0.64     | 2.40        | 11     | 10    |
| 1:A:328:LEU:HD11 | 1:A:355:ILE:HD11 | 0.64     | 1.66        | 14     | 2     |
| 1:A:299:PHE:CD2  | 1:A:308:LEU:HD21 | 0.64     | 2.27        | 3      | 1     |
| 1:A:291:VAL:HG23 | 1:A:299:PHE:O    | 0.64     | 1.93        | 7      | 1     |
| 1:A:354:LEU:C    | 1:A:355:ILE:HD12 | 0.64     | 2.18        | 15     | 3     |
| 1:A:382:ALA:HB2  | 1:A:431:ALA:HA   | 0.64     | 1.69        | 16     | 5     |
| 1:A:432:VAL:HG13 | 1:A:441:TYR:O    | 0.64     | 1.93        | 12     | 1     |
| 1:A:327:THR:O    | 1:A:327:THR:HG23 | 0.64     | 1.93        | 2      | 8     |
| 1:A:310:VAL:HG13 | 1:A:311:SER:N    | 0.64     | 2.08        | 16     | 1     |
| 1:A:384:VAL:CG2  | 1:A:432:VAL:HG13 | 0.63     | 2.23        | 10     | 2     |
| 1:A:449:PHE:CE2  | 1:A:461:THR:CG2  | 0.63     | 2.81        | 20     | 1     |
| 1:A:336:TYR:CE2  | 1:A:338:ILE:HD11 | 0.63     | 2.28        | 2      | 1     |
| 1:A:355:ILE:N    | 1:A:355:ILE:HD12 | 0.63     | 2.09        | 11     | 5     |
| 1:A:443:PHE:CD1  | 1:A:443:PHE:C    | 0.63     | 2.75        | 1      | 6     |
| 1:A:443:PHE:CE1  | 1:A:448:GLN:CG   | 0.63     | 2.81        | 15     | 2     |
| 1:A:281:LEU:CD2  | 1:A:468:PHE:CE1  | 0.63     | 2.82        | 11     | 1     |
| 1:A:336:TYR:CZ   | 1:A:345:PHE:CB   | 0.63     | 2.81        | 9      | 2     |
| 1:A:336:TYR:CE1  | 1:A:345:PHE:CB   | 0.63     | 2.81        | 2      | 3     |
| 1:A:290:ALA:HB2  | 1:A:333:GLU:C    | 0.63     | 2.19        | 15     | 1     |
| 1:A:369:HIS:CE1  | 1:A:373:PHE:CD2  | 0.63     | 2.87        | 16     | 1     |
| 1:A:369:HIS:NE2  | 1:A:373:PHE:CD1  | 0.63     | 2.66        | 16     | 1     |
| 1:A:384:VAL:O    | 1:A:392:THR:HG23 | 0.63     | 1.93        | 20     | 6     |
| 1:A:357:ASN:C    | 1:A:358:LEU:HD23 | 0.63     | 2.19        | 2      | 5     |
| 1:A:338:ILE:HD12 | 1:A:345:PHE:CD1  | 0.63     | 2.28        | 10     | 1     |
| 1:A:443:PHE:CD2  | 1:A:448:GLN:NE2  | 0.62     | 2.67        | 2      | 1     |
| 1:A:369:HIS:CE1  | 1:A:373:PHE:CG   | 0.62     | 2.87        | 16     | 1     |
| 1:A:389:PHE:C    | 1:A:390:TYR:CG   | 0.62     | 2.75        | 14     | 4     |
| 1:A:352:TYR:CD1  | 1:A:352:TYR:C    | 0.62     | 2.77        | 12     | 4     |
| 1:A:307:TRP:CD1  | 1:A:317:SER:O    | 0.62     | 2.52        | 18     | 1     |
| 1:A:291:VAL:HG22 | 1:A:431:ALA:CB   | 0.62     | 2.23        | 20     | 1     |
| 1:A:328:LEU:HD21 | 1:A:360:PRO:HG3  | 0.62     | 1.71        | 9      | 1     |
| 1:A:298:ILE:H    | 1:A:310:VAL:HG11 | 0.62     | 1.55        | 15     | 4     |

Continued on next page...

*Continued from previous page...*

| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:364:TYR:N    | 1:A:365:PRO:HD2  | 0.62     | 2.10        | 12     | 1     |
| 1:A:332:ILE:HG23 | 1:A:347:PHE:O    | 0.62     | 1.94        | 5      | 1     |
| 1:A:425:ILE:HG21 | 1:A:442:PHE:CG   | 0.62     | 2.30        | 17     | 1     |
| 1:A:316:THR:CG2  | 1:A:468:PHE:CD1  | 0.62     | 2.82        | 6      | 1     |
| 1:A:281:LEU:HD22 | 1:A:468:PHE:CD1  | 0.62     | 2.29        | 11     | 1     |
| 1:A:400:TYR:C    | 1:A:400:TYR:CD1  | 0.61     | 2.78        | 10     | 7     |
| 1:A:468:PHE:C    | 1:A:468:PHE:CD1  | 0.61     | 2.79        | 3      | 3     |
| 1:A:425:ILE:HG22 | 1:A:429:ILE:HD13 | 0.61     | 1.71        | 5      | 1     |
| 1:A:400:TYR:CD1  | 1:A:400:TYR:O    | 0.61     | 2.53        | 20     | 1     |
| 1:A:338:ILE:HG23 | 1:A:338:ILE:O    | 0.61     | 1.95        | 4      | 7     |
| 1:A:292:THR:HG21 | 1:A:337:GLU:CD   | 0.61     | 2.20        | 3      | 1     |
| 1:A:422:PHE:O    | 1:A:425:ILE:HD11 | 0.61     | 1.95        | 6      | 2     |
| 1:A:448:GLN:NE2  | 1:A:462:LEU:HD21 | 0.61     | 2.09        | 13     | 1     |
| 1:A:434:TYR:O    | 1:A:434:TYR:CD2  | 0.61     | 2.53        | 6      | 3     |
| 1:A:330:SER:O    | 1:A:331:GLY:C    | 0.61     | 2.42        | 8      | 2     |
| 1:A:298:ILE:HD13 | 1:A:300:PHE:CE2  | 0.61     | 2.31        | 13     | 1     |
| 1:A:325:TRP:HB3  | 1:A:328:LEU:HD23 | 0.61     | 1.72        | 9      | 8     |
| 1:A:282:CYS:SG   | 1:A:470:CYS:CB   | 0.61     | 2.89        | 5      | 1     |
| 1:A:329:PRO:O    | 1:A:332:ILE:HD11 | 0.61     | 1.94        | 12     | 1     |
| 1:A:467:TRP:O    | 1:A:468:PHE:CD1  | 0.61     | 2.54        | 18     | 1     |
| 1:A:395:PHE:CE2  | 1:A:432:VAL:HG21 | 0.61     | 2.30        | 14     | 1     |
| 1:A:462:LEU:HD11 | 1:A:466:SER:OG   | 0.61     | 1.95        | 2      | 2     |
| 1:A:291:VAL:HG11 | 1:A:443:PHE:CE1  | 0.61     | 2.31        | 6      | 1     |
| 1:A:316:THR:HG22 | 1:A:468:PHE:CD1  | 0.61     | 2.31        | 6      | 1     |
| 1:A:294:VAL:HG23 | 1:A:297:LYS:HB2  | 0.61     | 1.72        | 14     | 1     |
| 1:A:308:LEU:HD23 | 1:A:309:LYS:N    | 0.61     | 2.10        | 20     | 1     |
| 1:A:299:PHE:CE1  | 1:A:308:LEU:HD23 | 0.61     | 2.30        | 9      | 1     |
| 1:A:443:PHE:CZ   | 1:A:448:GLN:CD   | 0.60     | 2.78        | 10     | 2     |
| 1:A:429:ILE:HD11 | 1:A:442:PHE:CD1  | 0.60     | 2.31        | 16     | 2     |
| 1:A:361:GLU:OE2  | 1:A:364:TYR:CE1  | 0.60     | 2.54        | 3      | 1     |
| 1:A:332:ILE:HG13 | 1:A:346:LEU:HD12 | 0.60     | 1.74        | 14     | 1     |
| 1:A:368:ILE:HD12 | 1:A:377:VAL:CG1  | 0.60     | 2.25        | 2      | 1     |
| 1:A:369:HIS:CD2  | 1:A:369:HIS:C    | 0.60     | 2.79        | 20     | 6     |
| 1:A:337:GLU:HG2  | 1:A:344:VAL:HG22 | 0.60     | 1.74        | 6      | 1     |
| 1:A:297:LYS:HA   | 1:A:310:VAL:HG23 | 0.60     | 1.73        | 19     | 3     |
| 1:A:332:ILE:HD13 | 1:A:346:LEU:HD12 | 0.60     | 1.72        | 5      | 2     |
| 1:A:361:GLU:OE1  | 1:A:364:TYR:CE1  | 0.60     | 2.54        | 10     | 1     |
| 1:A:336:TYR:CZ   | 1:A:345:PHE:CG   | 0.60     | 2.90        | 2      | 1     |
| 1:A:403:TYR:CE1  | 1:A:404:ASP:O    | 0.60     | 2.55        | 12     | 3     |
| 1:A:286:LEU:CD1  | 1:A:307:TRP:CZ2  | 0.60     | 2.83        | 16     | 1     |
| 1:A:298:ILE:CD1  | 1:A:310:VAL:HG23 | 0.60     | 2.27        | 20     | 1     |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:305:PHE:CE1  | 1:A:320:LEU:HD12 | 0.59     | 2.31        | 4      | 3     |
| 1:A:347:PHE:N    | 1:A:347:PHE:CD1  | 0.59     | 2.70        | 10     | 1     |
| 1:A:400:TYR:CE1  | 1:A:401:TRP:O    | 0.59     | 2.55        | 5      | 2     |
| 1:A:443:PHE:CZ   | 1:A:448:GLN:OE1  | 0.59     | 2.55        | 6      | 2     |
| 1:A:466:SER:O    | 1:A:467:TRP:CD1  | 0.59     | 2.55        | 19     | 2     |
| 1:A:293:THR:HG21 | 1:A:434:TYR:O    | 0.59     | 1.97        | 5      | 1     |
| 1:A:306:PHE:C    | 1:A:306:PHE:CD1  | 0.59     | 2.79        | 18     | 5     |
| 1:A:358:LEU:HD23 | 1:A:359:ARG:HG2  | 0.59     | 1.73        | 17     | 1     |
| 1:A:281:LEU:O    | 1:A:468:PHE:CZ   | 0.59     | 2.55        | 5      | 1     |
| 1:A:361:GLU:OE1  | 1:A:364:TYR:CD1  | 0.59     | 2.55        | 10     | 1     |
| 1:A:441:TYR:CD1  | 1:A:441:TYR:N    | 0.59     | 2.68        | 15     | 1     |
| 1:A:438:LYS:O    | 1:A:439:TYR:CD1  | 0.59     | 2.55        | 14     | 3     |
| 1:A:296:ASN:O    | 1:A:310:VAL:HG21 | 0.59     | 1.98        | 8      | 2     |
| 1:A:421:ASN:O    | 1:A:422:PHE:CD1  | 0.59     | 2.56        | 2      | 2     |
| 1:A:371:PHE:CD1  | 1:A:371:PHE:C    | 0.59     | 2.81        | 12     | 1     |
| 1:A:432:VAL:HG22 | 1:A:442:PHE:HB3  | 0.59     | 1.75        | 6      | 1     |
| 1:A:306:PHE:O    | 1:A:306:PHE:CD1  | 0.59     | 2.56        | 7      | 1     |
| 1:A:395:PHE:CD2  | 1:A:429:ILE:HG21 | 0.59     | 2.33        | 2      | 3     |
| 1:A:368:ILE:CD1  | 1:A:377:VAL:HG21 | 0.59     | 2.28        | 9      | 1     |
| 1:A:462:LEU:HD22 | 1:A:466:SER:HB2  | 0.58     | 1.73        | 10     | 1     |
| 1:A:336:TYR:CG   | 1:A:336:TYR:O    | 0.58     | 2.56        | 18     | 10    |
| 1:A:312:GLU:O    | 1:A:313:ARG:C    | 0.58     | 2.46        | 9      | 3     |
| 1:A:281:LEU:HD21 | 1:A:468:PHE:CE1  | 0.58     | 2.33        | 11     | 1     |
| 1:A:346:LEU:HD22 | 1:A:346:LEU:N    | 0.58     | 2.13        | 2      | 2     |
| 1:A:299:PHE:CZ   | 1:A:308:LEU:HD23 | 0.58     | 2.34        | 13     | 1     |
| 1:A:377:VAL:HG22 | 1:A:396:VAL:HG11 | 0.58     | 1.76        | 13     | 1     |
| 1:A:425:ILE:HG22 | 1:A:442:PHE:CZ   | 0.58     | 2.33        | 20     | 1     |
| 1:A:382:ALA:HB3  | 1:A:432:VAL:HG12 | 0.58     | 1.75        | 4      | 1     |
| 1:A:290:ALA:HB2  | 1:A:332:ILE:O    | 0.58     | 1.97        | 10     | 1     |
| 1:A:286:LEU:CD2  | 1:A:288:PHE:CZ   | 0.58     | 2.86        | 10     | 1     |
| 1:A:298:ILE:HD11 | 1:A:309:LYS:O    | 0.58     | 1.98        | 13     | 1     |
| 1:A:396:VAL:HG21 | 1:A:401:TRP:CZ3  | 0.58     | 2.33        | 20     | 1     |
| 1:A:421:ASN:OD1  | 1:A:422:PHE:CE2  | 0.58     | 2.57        | 7      | 4     |
| 1:A:372:GLY:O    | 1:A:373:PHE:CD2  | 0.58     | 2.57        | 6      | 1     |
| 1:A:412:PRO:O    | 1:A:413:GLY:C    | 0.58     | 2.46        | 16     | 1     |
| 1:A:433:PHE:CD1  | 1:A:433:PHE:C    | 0.58     | 2.81        | 17     | 3     |
| 1:A:294:VAL:HG23 | 1:A:294:VAL:O    | 0.58     | 1.98        | 18     | 2     |
| 1:A:306:PHE:C    | 1:A:307:TRP:CE3  | 0.58     | 2.82        | 18     | 1     |
| 1:A:298:ILE:HD12 | 1:A:298:ILE:C    | 0.58     | 2.23        | 13     | 1     |
| 1:A:454:LEU:HD23 | 1:A:455:LEU:CD2  | 0.58     | 2.29        | 16     | 1     |
| 1:A:334:ALA:HB1  | 1:A:383:ALA:HB3  | 0.57     | 1.74        | 10     | 2     |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:364:TYR:CD2  | 1:A:365:PRO:HD3  | 0.57     | 2.34        | 12     | 1     |
| 1:A:288:PHE:CD2  | 1:A:300:PHE:CE1  | 0.57     | 2.92        | 18     | 1     |
| 1:A:434:TYR:O    | 1:A:434:TYR:CG   | 0.57     | 2.57        | 6      | 3     |
| 1:A:380:ILE:HG23 | 1:A:395:PHE:O    | 0.57     | 1.98        | 5      | 1     |
| 1:A:373:PHE:CZ   | 1:A:375:ASN:O    | 0.57     | 2.57        | 17     | 1     |
| 1:A:352:TYR:CD1  | 1:A:368:ILE:HG23 | 0.57     | 2.34        | 19     | 2     |
| 1:A:281:LEU:O    | 1:A:468:PHE:CE1  | 0.57     | 2.57        | 5      | 1     |
| 1:A:425:ILE:HD13 | 1:A:425:ILE:H    | 0.57     | 1.58        | 19     | 3     |
| 1:A:300:PHE:CD1  | 1:A:300:PHE:N    | 0.57     | 2.73        | 8      | 3     |
| 1:A:307:TRP:CZ3  | 1:A:468:PHE:CE1  | 0.57     | 2.92        | 7      | 1     |
| 1:A:401:TRP:CH2  | 1:A:411:ASP:O    | 0.57     | 2.57        | 9      | 1     |
| 1:A:432:VAL:HG21 | 1:A:442:PHE:CE2  | 0.57     | 2.35        | 5      | 2     |
| 1:A:328:LEU:HD12 | 1:A:346:LEU:HD12 | 0.57     | 1.76        | 4      | 1     |
| 1:A:308:LEU:C    | 1:A:308:LEU:HD13 | 0.57     | 2.25        | 9      | 1     |
| 1:A:343:GLN:NE2  | 1:A:354:LEU:HD21 | 0.57     | 2.15        | 3      | 2     |
| 1:A:425:ILE:CG2  | 1:A:442:PHE:CZ   | 0.57     | 2.87        | 6      | 1     |
| 1:A:362:PRO:O    | 1:A:363:ASN:CB   | 0.57     | 2.53        | 6      | 9     |
| 1:A:309:LYS:HB2  | 1:A:316:THR:HG22 | 0.57     | 1.76        | 16     | 1     |
| 1:A:308:LEU:HD23 | 1:A:308:LEU:C    | 0.57     | 2.24        | 20     | 1     |
| 1:A:310:VAL:O    | 1:A:311:SER:C    | 0.57     | 2.47        | 18     | 6     |
| 1:A:281:LEU:HD22 | 1:A:468:PHE:CB   | 0.57     | 2.30        | 15     | 1     |
| 1:A:332:ILE:HD12 | 1:A:346:LEU:HB3  | 0.57     | 1.75        | 16     | 1     |
| 1:A:316:THR:HG21 | 1:A:468:PHE:CE2  | 0.57     | 2.35        | 18     | 1     |
| 1:A:433:PHE:CZ   | 1:A:441:TYR:CB   | 0.57     | 2.88        | 9      | 3     |
| 1:A:337:GLU:CB   | 1:A:344:VAL:HA   | 0.57     | 2.29        | 18     | 1     |
| 1:A:332:ILE:CG2  | 1:A:335:ALA:HB2  | 0.56     | 2.30        | 2      | 1     |
| 1:A:281:LEU:HD22 | 1:A:468:PHE:CE2  | 0.56     | 2.34        | 14     | 1     |
| 1:A:309:LYS:HG2  | 1:A:316:THR:HG22 | 0.56     | 1.77        | 18     | 1     |
| 1:A:306:PHE:CD2  | 1:A:319:ASN:O    | 0.56     | 2.58        | 12     | 2     |
| 1:A:467:TRP:O    | 1:A:468:PHE:CG   | 0.56     | 2.58        | 7      | 2     |
| 1:A:384:VAL:HB   | 1:A:432:VAL:HG23 | 0.56     | 1.76        | 19     | 2     |
| 1:A:327:THR:HG22 | 1:A:327:THR:O    | 0.56     | 2.00        | 1      | 1     |
| 1:A:441:TYR:CE1  | 1:A:450:GLU:CG   | 0.56     | 2.88        | 10     | 2     |
| 1:A:301:PHE:CD1  | 1:A:332:ILE:HD13 | 0.56     | 2.35        | 11     | 2     |
| 1:A:309:LYS:C    | 1:A:310:VAL:HG12 | 0.56     | 2.24        | 8      | 1     |
| 1:A:298:ILE:HG21 | 1:A:300:PHE:CZ   | 0.56     | 2.35        | 9      | 1     |
| 1:A:373:PHE:O    | 1:A:373:PHE:CG   | 0.56     | 2.56        | 20     | 1     |
| 1:A:292:THR:HG21 | 1:A:337:GLU:OE1  | 0.56     | 2.00        | 3      | 1     |
| 1:A:281:LEU:CD2  | 1:A:307:TRP:CH2  | 0.56     | 2.88        | 19     | 1     |
| 1:A:328:LEU:HD13 | 1:A:329:PRO:CD   | 0.56     | 2.29        | 16     | 3     |
| 1:A:370:SER:O    | 1:A:371:PHE:CG   | 0.56     | 2.59        | 1      | 3     |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:382:ALA:CB   | 1:A:432:VAL:HG12 | 0.56     | 2.31        | 20     | 7     |
| 1:A:353:TRP:CH2  | 1:A:365:PRO:HA   | 0.56     | 2.35        | 5      | 1     |
| 1:A:425:ILE:N    | 1:A:425:ILE:CD1  | 0.56     | 2.68        | 10     | 3     |
| 1:A:434:TYR:CG   | 1:A:434:TYR:O    | 0.56     | 2.58        | 15     | 1     |
| 1:A:433:PHE:CD1  | 1:A:433:PHE:O    | 0.56     | 2.59        | 15     | 2     |
| 1:A:371:PHE:CG   | 1:A:371:PHE:O    | 0.56     | 2.58        | 15     | 1     |
| 1:A:281:LEU:HD11 | 1:A:307:TRP:CE3  | 0.56     | 2.33        | 17     | 1     |
| 1:A:332:ILE:HG21 | 1:A:346:LEU:HD12 | 0.56     | 1.78        | 11     | 3     |
| 1:A:294:VAL:HG22 | 1:A:337:GLU:OE1  | 0.56     | 2.00        | 15     | 1     |
| 1:A:369:HIS:CE1  | 1:A:373:PHE:CD1  | 0.56     | 2.94        | 16     | 1     |
| 1:A:364:TYR:CD1  | 1:A:366:LYS:CE   | 0.56     | 2.88        | 4      | 3     |
| 1:A:336:TYR:OH   | 1:A:345:PHE:CD2  | 0.56     | 2.59        | 9      | 1     |
| 1:A:453:PHE:CD1  | 1:A:453:PHE:O    | 0.55     | 2.60        | 4      | 3     |
| 1:A:348:LYS:O    | 1:A:349:ASP:C    | 0.55     | 2.49        | 13     | 1     |
| 1:A:288:PHE:CE1  | 1:A:443:PHE:CZ   | 0.55     | 2.93        | 18     | 1     |
| 1:A:443:PHE:CE2  | 1:A:448:GLN:CG   | 0.55     | 2.89        | 20     | 1     |
| 1:A:299:PHE:CE2  | 1:A:308:LEU:HD21 | 0.55     | 2.36        | 11     | 2     |
| 1:A:325:TRP:CH2  | 1:A:346:LEU:HD21 | 0.55     | 2.36        | 19     | 1     |
| 1:A:293:THR:HG22 | 1:A:298:ILE:HG22 | 0.55     | 1.78        | 5      | 1     |
| 1:A:307:TRP:CZ3  | 1:A:468:PHE:CE2  | 0.55     | 2.95        | 6      | 1     |
| 1:A:369:HIS:CE1  | 1:A:373:PHE:CE2  | 0.55     | 2.94        | 16     | 1     |
| 1:A:432:VAL:CG2  | 1:A:442:PHE:CZ   | 0.55     | 2.90        | 1      | 1     |
| 1:A:299:PHE:CE2  | 1:A:308:LEU:CD2  | 0.55     | 2.90        | 11     | 2     |
| 1:A:337:GLU:CD   | 1:A:344:VAL:HG22 | 0.55     | 2.26        | 19     | 1     |
| 1:A:462:LEU:HD21 | 1:A:466:SER:OG   | 0.55     | 2.00        | 2      | 1     |
| 1:A:372:GLY:O    | 1:A:373:PHE:CG   | 0.55     | 2.59        | 6      | 1     |
| 1:A:347:PHE:CD2  | 1:A:352:TYR:CB   | 0.55     | 2.90        | 10     | 1     |
| 1:A:461:THR:C    | 1:A:462:LEU:HD13 | 0.55     | 2.27        | 19     | 1     |
| 1:A:288:PHE:CD2  | 1:A:300:PHE:CD1  | 0.55     | 2.95        | 18     | 2     |
| 1:A:301:PHE:CD2  | 1:A:332:ILE:CG1  | 0.55     | 2.90        | 7      | 1     |
| 1:A:364:TYR:CG   | 1:A:365:PRO:HD3  | 0.55     | 2.37        | 12     | 1     |
| 1:A:286:LEU:C    | 1:A:286:LEU:HD23 | 0.55     | 2.27        | 1      | 1     |
| 1:A:453:PHE:C    | 1:A:453:PHE:CD1  | 0.55     | 2.84        | 13     | 1     |
| 1:A:286:LEU:HD22 | 1:A:307:TRP:CZ2  | 0.55     | 2.37        | 2      | 1     |
| 1:A:344:VAL:CG1  | 1:A:346:LEU:CD2  | 0.55     | 2.85        | 14     | 1     |
| 1:A:384:VAL:HG13 | 1:A:432:VAL:HG13 | 0.54     | 1.78        | 16     | 2     |
| 1:A:286:LEU:HD11 | 1:A:307:TRP:CH2  | 0.54     | 2.37        | 7      | 1     |
| 1:A:369:HIS:CD2  | 1:A:369:HIS:O    | 0.54     | 2.60        | 20     | 1     |
| 1:A:344:VAL:HG12 | 1:A:346:LEU:CD2  | 0.54     | 2.32        | 14     | 3     |
| 1:A:395:PHE:CD1  | 1:A:418:ILE:HG23 | 0.54     | 2.37        | 6      | 1     |
| 1:A:288:PHE:CE2  | 1:A:443:PHE:CE2  | 0.54     | 2.95        | 9      | 2     |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:389:PHE:O    | 1:A:390:TYR:CD2  | 0.54     | 2.60        | 1      | 4     |
| 1:A:466:SER:O    | 1:A:467:TRP:CG   | 0.54     | 2.61        | 6      | 1     |
| 1:A:354:LEU:HD12 | 1:A:355:ILE:H    | 0.54     | 1.60        | 7      | 2     |
| 1:A:292:THR:HB   | 1:A:335:ALA:HB3  | 0.54     | 1.78        | 18     | 1     |
| 1:A:368:ILE:N    | 1:A:368:ILE:HD13 | 0.54     | 2.18        | 18     | 1     |
| 1:A:301:PHE:CE2  | 1:A:332:ILE:HD13 | 0.54     | 2.38        | 1      | 1     |
| 1:A:355:ILE:N    | 1:A:355:ILE:CD1  | 0.54     | 2.70        | 1      | 3     |
| 1:A:439:TYR:CD1  | 1:A:450:GLU:OE2  | 0.54     | 2.60        | 2      | 3     |
| 1:A:293:THR:HG21 | 1:A:435:SER:CB   | 0.54     | 2.32        | 9      | 3     |
| 1:A:441:TYR:CE1  | 1:A:450:GLU:OE1  | 0.54     | 2.61        | 3      | 1     |
| 1:A:281:LEU:CD2  | 1:A:307:TRP:CZ2  | 0.54     | 2.91        | 6      | 1     |
| 1:A:289:ASP:O    | 1:A:431:ALA:HB2  | 0.54     | 2.02        | 6      | 1     |
| 1:A:291:VAL:CG2  | 1:A:431:ALA:HB1  | 0.54     | 2.32        | 8      | 1     |
| 1:A:301:PHE:CE1  | 1:A:332:ILE:HD13 | 0.54     | 2.38        | 8      | 1     |
| 1:A:306:PHE:CD2  | 1:A:319:ASN:ND2  | 0.54     | 2.76        | 9      | 1     |
| 1:A:444:GLN:CG   | 1:A:444:GLN:O    | 0.54     | 2.56        | 4      | 1     |
| 1:A:414:TYR:N    | 1:A:415:PRO:HD3  | 0.54     | 2.18        | 19     | 3     |
| 1:A:288:PHE:CE2  | 1:A:300:PHE:CG   | 0.54     | 2.96        | 18     | 1     |
| 1:A:336:TYR:CZ   | 1:A:345:PHE:CD2  | 0.54     | 2.96        | 2      | 1     |
| 1:A:370:SER:O    | 1:A:371:PHE:CD2  | 0.53     | 2.61        | 6      | 2     |
| 1:A:352:TYR:N    | 1:A:352:TYR:CD1  | 0.53     | 2.76        | 13     | 3     |
| 1:A:374:PRO:O    | 1:A:375:ASN:CB   | 0.53     | 2.57        | 10     | 2     |
| 1:A:288:PHE:CG   | 1:A:443:PHE:CD2  | 0.53     | 2.96        | 18     | 1     |
| 1:A:336:TYR:CE1  | 1:A:345:PHE:HB3  | 0.53     | 2.39        | 9      | 1     |
| 1:A:455:LEU:HD23 | 1:A:455:LEU:N    | 0.53     | 2.18        | 14     | 1     |
| 1:A:429:ILE:CD1  | 1:A:442:PHE:CD1  | 0.53     | 2.91        | 16     | 1     |
| 1:A:467:TRP:C    | 1:A:468:PHE:CD2  | 0.53     | 2.87        | 7      | 2     |
| 1:A:337:GLU:HG3  | 1:A:344:VAL:HG22 | 0.53     | 1.80        | 12     | 1     |
| 1:A:443:PHE:CD1  | 1:A:448:GLN:HG2  | 0.53     | 2.38        | 15     | 1     |
| 1:A:463:LYS:N    | 1:A:463:LYS:CD   | 0.53     | 2.72        | 18     | 1     |
| 1:A:364:TYR:CD2  | 1:A:366:LYS:HD2  | 0.53     | 2.38        | 17     | 6     |
| 1:A:440:TYR:C    | 1:A:440:TYR:CD1  | 0.53     | 2.84        | 15     | 1     |
| 1:A:400:TYR:CE2  | 1:A:416:LYS:HB2  | 0.53     | 2.39        | 20     | 1     |
| 1:A:323:SER:HB3  | 1:A:324:LEU:HD12 | 0.53     | 1.80        | 16     | 1     |
| 1:A:371:PHE:O    | 1:A:371:PHE:CD2  | 0.53     | 2.62        | 20     | 3     |
| 1:A:371:PHE:O    | 1:A:371:PHE:CG   | 0.52     | 2.62        | 12     | 2     |
| 1:A:286:LEU:CD2  | 1:A:307:TRP:CZ2  | 0.52     | 2.92        | 2      | 1     |
| 1:A:336:TYR:CD2  | 1:A:338:ILE:HD11 | 0.52     | 2.39        | 2      | 1     |
| 1:A:310:VAL:HG13 | 1:A:311:SER:H    | 0.52     | 1.62        | 18     | 2     |
| 1:A:298:ILE:HD12 | 1:A:300:PHE:CZ   | 0.52     | 2.39        | 6      | 3     |
| 1:A:439:TYR:CG   | 1:A:450:GLU:OE2  | 0.52     | 2.63        | 2      | 1     |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:431:ALA:HB3  | 1:A:442:PHE:CE2  | 0.52     | 2.40        | 15     | 1     |
| 1:A:433:PHE:CE2  | 1:A:441:TYR:HB2  | 0.52     | 2.40        | 17     | 1     |
| 1:A:447:ASN:OD1  | 1:A:449:PHE:CD2  | 0.52     | 2.63        | 2      | 1     |
| 1:A:288:PHE:CD1  | 1:A:443:PHE:CD2  | 0.52     | 2.98        | 6      | 1     |
| 1:A:364:TYR:CE2  | 1:A:366:LYS:HD3  | 0.52     | 2.40        | 17     | 5     |
| 1:A:299:PHE:CZ   | 1:A:308:LEU:CD2  | 0.52     | 2.92        | 13     | 1     |
| 1:A:332:ILE:HD12 | 1:A:332:ILE:N    | 0.52     | 2.19        | 2      | 1     |
| 1:A:305:PHE:CD2  | 1:A:319:ASN:O    | 0.52     | 2.62        | 8      | 1     |
| 1:A:418:ILE:HD12 | 1:A:427:PRO:O    | 0.52     | 2.05        | 17     | 1     |
| 1:A:390:TYR:O    | 1:A:405:GLU:CB   | 0.52     | 2.58        | 20     | 1     |
| 1:A:311:SER:O    | 1:A:312:GLU:C    | 0.52     | 2.51        | 17     | 4     |
| 1:A:328:LEU:CD1  | 1:A:346:LEU:HD11 | 0.52     | 2.33        | 10     | 1     |
| 1:A:393:TYR:CD1  | 1:A:393:TYR:N    | 0.52     | 2.76        | 6      | 2     |
| 1:A:310:VAL:HG22 | 1:A:311:SER:H    | 0.52     | 1.65        | 17     | 5     |
| 1:A:318:VAL:HG12 | 1:A:318:VAL:O    | 0.52     | 2.03        | 10     | 3     |
| 1:A:336:TYR:HB2  | 1:A:383:ALA:HB3  | 0.52     | 1.82        | 4      | 1     |
| 1:A:449:PHE:CE2  | 1:A:461:THR:HG23 | 0.52     | 2.40        | 20     | 1     |
| 1:A:462:LEU:CD2  | 1:A:467:TRP:CZ2  | 0.52     | 2.92        | 2      | 1     |
| 1:A:338:ILE:HD12 | 1:A:340:ALA:HB3  | 0.52     | 1.82        | 3      | 1     |
| 1:A:433:PHE:CE2  | 1:A:441:TYR:HB3  | 0.52     | 2.40        | 3      | 1     |
| 1:A:353:TRP:CZ3  | 1:A:361:GLU:O    | 0.52     | 2.63        | 20     | 2     |
| 1:A:300:PHE:CD1  | 1:A:300:PHE:C    | 0.52     | 2.87        | 18     | 1     |
| 1:A:336:TYR:CE1  | 1:A:347:PHE:CE2  | 0.52     | 2.98        | 9      | 1     |
| 1:A:449:PHE:CD1  | 1:A:449:PHE:N    | 0.52     | 2.78        | 15     | 1     |
| 1:A:291:VAL:CG2  | 1:A:300:PHE:CD2  | 0.52     | 2.94        | 16     | 1     |
| 1:A:421:ASN:ND2  | 1:A:422:PHE:CE2  | 0.52     | 2.78        | 17     | 1     |
| 1:A:462:LEU:CD1  | 1:A:466:SER:CB   | 0.51     | 2.88        | 2      | 1     |
| 1:A:400:TYR:O    | 1:A:400:TYR:CG   | 0.51     | 2.63        | 10     | 5     |
| 1:A:325:TRP:CE3  | 1:A:328:LEU:HD12 | 0.51     | 2.41        | 10     | 1     |
| 1:A:364:TYR:CD1  | 1:A:366:LYS:HE3  | 0.51     | 2.40        | 3      | 10    |
| 1:A:281:LEU:HD23 | 1:A:307:TRP:CZ2  | 0.51     | 2.40        | 6      | 1     |
| 1:A:433:PHE:CZ   | 1:A:441:TYR:HB2  | 0.51     | 2.39        | 9      | 1     |
| 1:A:375:ASN:O    | 1:A:376:PHE:C    | 0.51     | 2.54        | 13     | 1     |
| 1:A:354:LEU:C    | 1:A:354:LEU:CD1  | 0.51     | 2.81        | 17     | 5     |
| 1:A:433:PHE:CZ   | 1:A:441:TYR:CG   | 0.51     | 2.98        | 3      | 1     |
| 1:A:337:GLU:CG   | 1:A:344:VAL:HG22 | 0.51     | 2.36        | 12     | 2     |
| 1:A:384:VAL:HG11 | 1:A:432:VAL:CG1  | 0.51     | 2.35        | 12     | 1     |
| 1:A:354:LEU:C    | 1:A:354:LEU:HD22 | 0.51     | 2.30        | 15     | 1     |
| 1:A:281:LEU:HD23 | 1:A:307:TRP:CZ3  | 0.51     | 2.40        | 19     | 1     |
| 1:A:310:VAL:HG13 | 1:A:312:GLU:H    | 0.51     | 1.66        | 11     | 1     |
| 1:A:328:LEU:HD11 | 1:A:346:LEU:CD1  | 0.51     | 2.36        | 16     | 1     |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:364:TYR:CD1  | 1:A:366:LYS:HE2  | 0.51     | 2.40        | 4      | 3     |
| 1:A:281:LEU:O    | 1:A:282:CYS:CB   | 0.51     | 2.59        | 14     | 2     |
| 1:A:307:TRP:CZ3  | 1:A:318:VAL:N    | 0.51     | 2.78        | 15     | 1     |
| 1:A:443:PHE:CE1  | 1:A:448:GLN:HG3  | 0.51     | 2.40        | 15     | 1     |
| 1:A:364:TYR:CG   | 1:A:366:LYS:CE   | 0.51     | 2.94        | 1      | 1     |
| 1:A:395:PHE:CE1  | 1:A:418:ILE:HG23 | 0.51     | 2.41        | 6      | 1     |
| 1:A:462:LEU:CG   | 1:A:466:SER:OG   | 0.51     | 2.59        | 2      | 1     |
| 1:A:308:LEU:C    | 1:A:308:LEU:CD2  | 0.51     | 2.84        | 20     | 1     |
| 1:A:310:VAL:O    | 1:A:313:ARG:CD   | 0.51     | 2.59        | 13     | 1     |
| 1:A:443:PHE:CZ   | 1:A:448:GLN:HG3  | 0.51     | 2.40        | 16     | 2     |
| 1:A:468:PHE:CD1  | 1:A:468:PHE:N    | 0.51     | 2.74        | 17     | 1     |
| 1:A:400:TYR:CE2  | 1:A:416:LYS:CB   | 0.51     | 2.94        | 20     | 1     |
| 1:A:422:PHE:O    | 1:A:425:ILE:CD1  | 0.51     | 2.59        | 2      | 6     |
| 1:A:286:LEU:CD1  | 1:A:307:TRP:CH2  | 0.51     | 2.93        | 7      | 1     |
| 1:A:301:PHE:CE2  | 1:A:332:ILE:HG13 | 0.51     | 2.41        | 7      | 1     |
| 1:A:374:PRO:HG2  | 1:A:377:VAL:HG13 | 0.51     | 1.82        | 8      | 1     |
| 1:A:354:LEU:HD11 | 1:A:356:SER:OG   | 0.51     | 2.06        | 10     | 1     |
| 1:A:364:TYR:CE2  | 1:A:366:LYS:HG3  | 0.51     | 2.41        | 18     | 1     |
| 1:A:364:TYR:N    | 1:A:365:PRO:HD3  | 0.51     | 2.21        | 20     | 12    |
| 1:A:357:ASN:O    | 1:A:358:LEU:CD2  | 0.51     | 2.59        | 16     | 5     |
| 1:A:364:TYR:CE1  | 1:A:366:LYS:HE3  | 0.51     | 2.41        | 3      | 1     |
| 1:A:338:ILE:O    | 1:A:338:ILE:CG2  | 0.51     | 2.59        | 5      | 3     |
| 1:A:347:PHE:CG   | 1:A:380:ILE:HD12 | 0.51     | 2.41        | 8      | 1     |
| 1:A:385:PHE:C    | 1:A:385:PHE:CD1  | 0.50     | 2.89        | 1      | 1     |
| 1:A:347:PHE:CZ   | 1:A:380:ILE:CD1  | 0.50     | 2.94        | 5      | 1     |
| 1:A:449:PHE:CZ   | 1:A:461:THR:HG23 | 0.50     | 2.41        | 20     | 1     |
| 1:A:389:PHE:O    | 1:A:390:TYR:CB   | 0.50     | 2.59        | 14     | 4     |
| 1:A:364:TYR:CD2  | 1:A:366:LYS:CD   | 0.50     | 2.94        | 9      | 4     |
| 1:A:367:SER:O    | 1:A:370:SER:CB   | 0.50     | 2.59        | 20     | 1     |
| 1:A:391:ARG:CG   | 1:A:392:THR:N    | 0.50     | 2.74        | 20     | 1     |
| 1:A:442:PHE:CZ   | 1:A:449:PHE:CB   | 0.50     | 2.94        | 20     | 1     |
| 1:A:394:PHE:CD1  | 1:A:403:TYR:CD1  | 0.50     | 2.99        | 4      | 1     |
| 1:A:387:PRO:HG3  | 1:A:434:TYR:CE2  | 0.50     | 2.41        | 7      | 1     |
| 1:A:372:GLY:C    | 1:A:373:PHE:CD1  | 0.50     | 2.89        | 20     | 1     |
| 1:A:399:GLN:OE1  | 1:A:415:PRO:CB   | 0.50     | 2.60        | 20     | 1     |
| 1:A:443:PHE:CE1  | 1:A:448:GLN:HG2  | 0.50     | 2.41        | 2      | 2     |
| 1:A:467:TRP:O    | 1:A:468:PHE:C    | 0.50     | 2.55        | 10     | 6     |
| 1:A:291:VAL:HG12 | 1:A:300:PHE:HA   | 0.50     | 1.82        | 15     | 2     |
| 1:A:328:LEU:HD11 | 1:A:355:ILE:HG12 | 0.50     | 1.83        | 12     | 1     |
| 1:A:460:LYS:C    | 1:A:461:THR:CG2  | 0.50     | 2.84        | 13     | 1     |
| 1:A:350:ASP:O    | 1:A:351:LYS:CG   | 0.50     | 2.60        | 15     | 10    |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:370:SER:O    | 1:A:371:PHE:CB   | 0.50     | 2.58        | 6      | 2     |
| 1:A:393:TYR:C    | 1:A:394:PHE:CD1  | 0.50     | 2.89        | 1      | 1     |
| 1:A:362:PRO:C    | 1:A:363:ASN:CG   | 0.50     | 2.79        | 3      | 4     |
| 1:A:438:LYS:CG   | 1:A:438:LYS:O    | 0.50     | 2.60        | 15     | 2     |
| 1:A:307:TRP:CZ2  | 1:A:316:THR:OG1  | 0.50     | 2.57        | 14     | 1     |
| 1:A:422:PHE:HB2  | 1:A:425:ILE:HD11 | 0.50     | 1.82        | 18     | 1     |
| 1:A:338:ILE:HG13 | 1:A:385:PHE:CD2  | 0.50     | 2.42        | 20     | 1     |
| 1:A:352:TYR:HD2  | 1:A:368:ILE:HG23 | 0.50     | 1.66        | 4      | 2     |
| 1:A:288:PHE:CE2  | 1:A:443:PHE:CZ   | 0.50     | 3.00        | 9      | 1     |
| 1:A:329:PRO:O    | 1:A:332:ILE:CD1  | 0.50     | 2.60        | 12     | 1     |
| 1:A:384:VAL:CG1  | 1:A:432:VAL:HG13 | 0.50     | 2.36        | 16     | 1     |
| 1:A:281:LEU:HD11 | 1:A:307:TRP:HZ3  | 0.50     | 1.58        | 17     | 1     |
| 1:A:443:PHE:CE2  | 1:A:448:GLN:HG2  | 0.50     | 2.42        | 20     | 1     |
| 1:A:360:PRO:O    | 1:A:361:GLU:C    | 0.50     | 2.54        | 16     | 6     |
| 1:A:292:THR:HG21 | 1:A:337:GLU:OE2  | 0.50     | 2.07        | 3      | 1     |
| 1:A:336:TYR:O    | 1:A:336:TYR:CG   | 0.50     | 2.65        | 3      | 2     |
| 1:A:433:PHE:CE2  | 1:A:441:TYR:CB   | 0.50     | 2.94        | 3      | 2     |
| 1:A:301:PHE:O    | 1:A:302:LYS:C    | 0.50     | 2.54        | 7      | 1     |
| 1:A:455:LEU:C    | 1:A:456:GLN:CD   | 0.50     | 2.80        | 16     | 2     |
| 1:A:432:VAL:CG2  | 1:A:433:PHE:N    | 0.50     | 2.75        | 13     | 1     |
| 1:A:443:PHE:CD1  | 1:A:464:SER:HA   | 0.50     | 2.42        | 15     | 1     |
| 1:A:298:ILE:HD12 | 1:A:310:VAL:HB   | 0.50     | 1.84        | 18     | 1     |
| 1:A:418:ILE:O    | 1:A:419:THR:C    | 0.49     | 2.53        | 14     | 10    |
| 1:A:315:LYS:C    | 1:A:316:THR:HG23 | 0.49     | 2.32        | 3      | 1     |
| 1:A:285:ASN:ND2  | 1:A:285:ASN:N    | 0.49     | 2.58        | 9      | 2     |
| 1:A:377:VAL:CG1  | 1:A:378:LYS:N    | 0.49     | 2.74        | 6      | 2     |
| 1:A:298:ILE:C    | 1:A:299:PHE:CD1  | 0.49     | 2.90        | 11     | 3     |
| 1:A:429:ILE:CD1  | 1:A:431:ALA:O    | 0.49     | 2.60        | 7      | 1     |
| 1:A:299:PHE:C    | 1:A:300:PHE:CG   | 0.49     | 2.90        | 11     | 1     |
| 1:A:374:PRO:HB3  | 1:A:401:TRP:CZ2  | 0.49     | 2.42        | 13     | 1     |
| 1:A:288:PHE:CE1  | 1:A:443:PHE:CE2  | 0.49     | 3.00        | 18     | 1     |
| 1:A:463:LYS:O    | 1:A:464:SER:C    | 0.49     | 2.55        | 17     | 8     |
| 1:A:338:ILE:CG2  | 1:A:338:ILE:O    | 0.49     | 2.60        | 3      | 1     |
| 1:A:304:ARG:HG2  | 1:A:305:PHE:CD2  | 0.49     | 2.42        | 11     | 1     |
| 1:A:422:PHE:CE2  | 1:A:456:GLN:HG2  | 0.49     | 2.43        | 13     | 1     |
| 1:A:352:TYR:CZ   | 1:A:366:LYS:HB2  | 0.49     | 2.42        | 5      | 2     |
| 1:A:298:ILE:CG2  | 1:A:300:PHE:CZ   | 0.49     | 2.95        | 9      | 1     |
| 1:A:336:TYR:CZ   | 1:A:345:PHE:HB2  | 0.49     | 2.42        | 9      | 2     |
| 1:A:443:PHE:CD1  | 1:A:448:GLN:CG   | 0.49     | 2.95        | 15     | 1     |
| 1:A:350:ASP:OD1  | 1:A:368:ILE:HD11 | 0.49     | 2.08        | 1      | 1     |
| 1:A:309:LYS:CB   | 1:A:316:THR:HG22 | 0.49     | 2.37        | 10     | 1     |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:281:LEU:HD11 | 1:A:307:TRP:CH2  | 0.49     | 2.42        | 11     | 1     |
| 1:A:310:VAL:HG22 | 1:A:311:SER:N    | 0.49     | 2.23        | 15     | 8     |
| 1:A:302:LYS:O    | 1:A:305:PHE:O    | 0.49     | 2.30        | 20     | 2     |
| 1:A:425:ILE:HG22 | 1:A:442:PHE:CE1  | 0.49     | 2.43        | 20     | 2     |
| 1:A:395:PHE:CD1  | 1:A:418:ILE:HG12 | 0.49     | 2.43        | 9      | 1     |
| 1:A:431:ALA:O    | 1:A:432:VAL:HG13 | 0.49     | 2.08        | 14     | 1     |
| 1:A:310:VAL:HG13 | 1:A:311:SER:OG   | 0.49     | 2.07        | 16     | 1     |
| 1:A:467:TRP:C    | 1:A:468:PHE:CG   | 0.49     | 2.91        | 19     | 2     |
| 1:A:294:VAL:HG12 | 1:A:294:VAL:O    | 0.49     | 2.07        | 9      | 2     |
| 1:A:425:ILE:CG2  | 1:A:442:PHE:CG   | 0.49     | 2.96        | 17     | 1     |
| 1:A:374:PRO:CB   | 1:A:401:TRP:CZ2  | 0.49     | 2.96        | 20     | 1     |
| 1:A:374:PRO:HB2  | 1:A:401:TRP:CZ2  | 0.49     | 2.42        | 20     | 1     |
| 1:A:306:PHE:CE2  | 1:A:319:ASN:C    | 0.49     | 2.91        | 2      | 2     |
| 1:A:458:ILE:HG22 | 1:A:458:ILE:O    | 0.49     | 2.07        | 11     | 1     |
| 1:A:429:ILE:HG12 | 1:A:442:PHE:CD1  | 0.49     | 2.42        | 13     | 2     |
| 1:A:355:ILE:HG22 | 1:A:355:ILE:O    | 0.49     | 2.07        | 7      | 1     |
| 1:A:421:ASN:OD1  | 1:A:422:PHE:CD2  | 0.49     | 2.66        | 7      | 2     |
| 1:A:345:PHE:C    | 1:A:346:LEU:CD2  | 0.49     | 2.85        | 10     | 1     |
| 1:A:345:PHE:CE2  | 1:A:352:TYR:CE1  | 0.49     | 3.01        | 11     | 1     |
| 1:A:436:LYS:HG2  | 1:A:441:TYR:CE1  | 0.49     | 2.43        | 13     | 1     |
| 1:A:462:LEU:CD1  | 1:A:466:SER:OG   | 0.49     | 2.61        | 2      | 1     |
| 1:A:288:PHE:CE2  | 1:A:300:PHE:CE1  | 0.49     | 3.01        | 4      | 2     |
| 1:A:398:ASN:O    | 1:A:417:LEU:CD1  | 0.49     | 2.61        | 14     | 2     |
| 1:A:422:PHE:CE2  | 1:A:451:TYR:CD1  | 0.49     | 3.01        | 1      | 1     |
| 1:A:432:VAL:HG23 | 1:A:442:PHE:CD1  | 0.49     | 2.43        | 1      | 1     |
| 1:A:462:LEU:HD11 | 1:A:466:SER:HB2  | 0.49     | 1.83        | 2      | 1     |
| 1:A:393:TYR:CE2  | 1:A:400:TYR:OH   | 0.49     | 2.58        | 15     | 2     |
| 1:A:441:TYR:CZ   | 1:A:450:GLU:CG   | 0.49     | 2.96        | 5      | 2     |
| 1:A:286:LEU:HD13 | 1:A:287:SER:N    | 0.49     | 2.22        | 9      | 1     |
| 1:A:441:TYR:CE1  | 1:A:450:GLU:HG3  | 0.48     | 2.43        | 14     | 7     |
| 1:A:300:PHE:C    | 1:A:301:PHE:CD1  | 0.48     | 2.91        | 9      | 1     |
| 1:A:344:VAL:C    | 1:A:345:PHE:CD1  | 0.48     | 2.91        | 9      | 1     |
| 1:A:428:LYS:O    | 1:A:444:GLN:CG   | 0.48     | 2.61        | 9      | 1     |
| 1:A:387:PRO:O    | 1:A:390:TYR:CE1  | 0.48     | 2.66        | 11     | 1     |
| 1:A:449:PHE:HB2  | 1:A:451:TYR:CE1  | 0.48     | 2.43        | 13     | 1     |
| 1:A:373:PHE:CZ   | 1:A:377:VAL:O    | 0.48     | 2.66        | 14     | 1     |
| 1:A:373:PHE:HA   | 1:A:377:VAL:HG12 | 0.48     | 1.85        | 1      | 1     |
| 1:A:453:PHE:C    | 1:A:455:LEU:N    | 0.48     | 2.70        | 13     | 3     |
| 1:A:284:PRO:C    | 1:A:285:ASN:CG   | 0.48     | 2.80        | 6      | 1     |
| 1:A:350:ASP:O    | 1:A:350:ASP:CG   | 0.48     | 2.54        | 9      | 5     |
| 1:A:441:TYR:CZ   | 1:A:450:GLU:HG2  | 0.48     | 2.43        | 13     | 1     |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:431:ALA:O    | 1:A:432:VAL:CG1  | 0.48     | 2.61        | 14     | 1     |
| 1:A:443:PHE:CZ   | 1:A:448:GLN:CG   | 0.48     | 2.96        | 16     | 2     |
| 1:A:288:PHE:CZ   | 1:A:443:PHE:CE2  | 0.48     | 3.01        | 18     | 1     |
| 1:A:291:VAL:HG23 | 1:A:433:PHE:HB3  | 0.48     | 1.86        | 19     | 1     |
| 1:A:367:SER:HB3  | 1:A:369:HIS:CE1  | 0.48     | 2.43        | 19     | 1     |
| 1:A:306:PHE:CD1  | 1:A:306:PHE:C    | 0.48     | 2.91        | 7      | 3     |
| 1:A:374:PRO:HD2  | 1:A:377:VAL:HG21 | 0.48     | 1.85        | 12     | 1     |
| 1:A:306:PHE:HB3  | 1:A:321:ILE:HD11 | 0.48     | 1.84        | 19     | 1     |
| 1:A:373:PHE:CZ   | 1:A:375:ASN:HA   | 0.48     | 2.44        | 10     | 2     |
| 1:A:455:LEU:O    | 1:A:456:GLN:C    | 0.48     | 2.56        | 15     | 9     |
| 1:A:338:ILE:HD11 | 1:A:385:PHE:CB   | 0.48     | 2.38        | 20     | 1     |
| 1:A:368:ILE:C    | 1:A:370:SER:N    | 0.48     | 2.71        | 1      | 4     |
| 1:A:315:LYS:O    | 1:A:316:THR:CG2  | 0.48     | 2.62        | 3      | 1     |
| 1:A:364:TYR:CE1  | 1:A:366:LYS:CE   | 0.48     | 2.97        | 4      | 3     |
| 1:A:433:PHE:CZ   | 1:A:441:TYR:HB3  | 0.48     | 2.43        | 5      | 1     |
| 1:A:441:TYR:CZ   | 1:A:450:GLU:OE1  | 0.48     | 2.66        | 17     | 1     |
| 1:A:443:PHE:CE1  | 1:A:464:SER:HB2  | 0.48     | 2.44        | 18     | 1     |
| 1:A:374:PRO:HG2  | 1:A:401:TRP:CH2  | 0.48     | 2.42        | 1      | 1     |
| 1:A:336:TYR:O    | 1:A:336:TYR:CD2  | 0.48     | 2.67        | 5      | 2     |
| 1:A:307:TRP:CZ3  | 1:A:468:PHE:CZ   | 0.48     | 3.02        | 6      | 2     |
| 1:A:303:ASP:O    | 1:A:305:PHE:N    | 0.48     | 2.44        | 16     | 2     |
| 1:A:403:TYR:C    | 1:A:403:TYR:CD1  | 0.48     | 2.91        | 1      | 2     |
| 1:A:421:ASN:OD1  | 1:A:422:PHE:CZ   | 0.48     | 2.67        | 4      | 1     |
| 1:A:369:HIS:CE1  | 1:A:373:PHE:CE1  | 0.48     | 3.01        | 16     | 1     |
| 1:A:412:PRO:O    | 1:A:414:TYR:N    | 0.48     | 2.46        | 19     | 1     |
| 1:A:449:PHE:CE2  | 1:A:461:THR:HG21 | 0.48     | 2.43        | 20     | 1     |
| 1:A:425:ILE:HG21 | 1:A:442:PHE:CE2  | 0.48     | 2.44        | 6      | 2     |
| 1:A:291:VAL:CG2  | 1:A:300:PHE:CE2  | 0.48     | 2.94        | 16     | 1     |
| 1:A:429:ILE:HD12 | 1:A:444:GLN:OE1  | 0.48     | 2.08        | 16     | 1     |
| 1:A:464:SER:O    | 1:A:465:ASN:C    | 0.48     | 2.57        | 18     | 1     |
| 1:A:462:LEU:HD13 | 1:A:462:LEU:N    | 0.48     | 2.24        | 19     | 1     |
| 1:A:449:PHE:CZ   | 1:A:461:THR:CG2  | 0.48     | 2.96        | 20     | 1     |
| 1:A:297:LYS:CA   | 1:A:310:VAL:HG11 | 0.48     | 2.36        | 5      | 1     |
| 1:A:298:ILE:O    | 1:A:308:LEU:CD2  | 0.48     | 2.61        | 9      | 1     |
| 1:A:344:VAL:HG12 | 1:A:346:LEU:HD22 | 0.48     | 1.86        | 10     | 1     |
| 1:A:424:GLY:C    | 1:A:425:ILE:CG2  | 0.48     | 2.86        | 12     | 1     |
| 1:A:281:LEU:HB3  | 1:A:468:PHE:CZ   | 0.48     | 2.44        | 2      | 1     |
| 1:A:301:PHE:CD1  | 1:A:301:PHE:N    | 0.48     | 2.82        | 9      | 2     |
| 1:A:336:TYR:CG   | 1:A:337:GLU:N    | 0.48     | 2.81        | 19     | 2     |
| 1:A:374:PRO:O    | 1:A:376:PHE:N    | 0.48     | 2.47        | 13     | 1     |
| 1:A:354:LEU:HD22 | 1:A:354:LEU:O    | 0.48     | 2.09        | 15     | 1     |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:327:THR:O    | 1:A:327:THR:CG2  | 0.47     | 2.62        | 2      | 4     |
| 1:A:422:PHE:HB2  | 1:A:425:ILE:HD12 | 0.47     | 1.86        | 2      | 1     |
| 1:A:455:LEU:O    | 1:A:456:GLN:CB   | 0.47     | 2.62        | 5      | 2     |
| 1:A:295:GLY:O    | 1:A:296:ASN:CB   | 0.47     | 2.62        | 9      | 2     |
| 1:A:419:THR:O    | 1:A:423:GLN:N    | 0.47     | 2.47        | 19     | 2     |
| 1:A:285:ASN:N    | 1:A:285:ASN:HD22 | 0.47     | 2.07        | 14     | 1     |
| 1:A:337:GLU:CD   | 1:A:338:ILE:N    | 0.47     | 2.72        | 16     | 1     |
| 1:A:310:VAL:HG13 | 1:A:312:GLU:N    | 0.47     | 2.24        | 11     | 1     |
| 1:A:354:LEU:HD23 | 1:A:361:GLU:CG   | 0.47     | 2.38        | 16     | 1     |
| 1:A:374:PRO:HD2  | 1:A:377:VAL:HG12 | 0.47     | 1.85        | 16     | 1     |
| 1:A:281:LEU:CD1  | 1:A:307:TRP:CZ3  | 0.47     | 2.83        | 17     | 1     |
| 1:A:321:ILE:O    | 1:A:322:SER:C    | 0.47     | 2.56        | 5      | 11    |
| 1:A:328:LEU:CD1  | 1:A:346:LEU:HD12 | 0.47     | 2.39        | 4      | 1     |
| 1:A:440:TYR:HB3  | 1:A:442:PHE:CE1  | 0.47     | 2.43        | 5      | 1     |
| 1:A:368:ILE:O    | 1:A:372:GLY:N    | 0.47     | 2.47        | 6      | 2     |
| 1:A:288:PHE:CD1  | 1:A:443:PHE:CE2  | 0.47     | 3.01        | 18     | 1     |
| 1:A:291:VAL:HG12 | 1:A:431:ALA:HB1  | 0.47     | 1.86        | 18     | 1     |
| 1:A:338:ILE:CG2  | 1:A:339:GLU:N    | 0.47     | 2.77        | 18     | 1     |
| 1:A:418:ILE:CG2  | 1:A:425:ILE:HD11 | 0.47     | 2.39        | 14     | 2     |
| 1:A:434:TYR:CD1  | 1:A:439:TYR:O    | 0.47     | 2.67        | 2      | 1     |
| 1:A:307:TRP:CE2  | 1:A:318:VAL:HG12 | 0.47     | 2.44        | 5      | 1     |
| 1:A:348:LYS:O    | 1:A:350:ASP:N    | 0.47     | 2.47        | 10     | 1     |
| 1:A:352:TYR:CE2  | 1:A:366:LYS:HB2  | 0.47     | 2.45        | 12     | 1     |
| 1:A:364:TYR:CD1  | 1:A:365:PRO:N    | 0.47     | 2.83        | 12     | 1     |
| 1:A:288:PHE:CD2  | 1:A:443:PHE:CE2  | 0.47     | 3.03        | 18     | 1     |
| 1:A:407:ARG:O    | 1:A:408:GLN:CB   | 0.47     | 2.62        | 12     | 9     |
| 1:A:368:ILE:CD1  | 1:A:377:VAL:HG13 | 0.47     | 2.30        | 2      | 1     |
| 1:A:298:ILE:HD12 | 1:A:300:PHE:HZ   | 0.47     | 1.69        | 3      | 1     |
| 1:A:307:TRP:CH2  | 1:A:318:VAL:HG13 | 0.47     | 2.45        | 8      | 1     |
| 1:A:344:VAL:O    | 1:A:345:PHE:CD1  | 0.47     | 2.68        | 9      | 1     |
| 1:A:346:LEU:N    | 1:A:346:LEU:CD2  | 0.47     | 2.74        | 10     | 1     |
| 1:A:352:TYR:CD2  | 1:A:366:LYS:HB3  | 0.47     | 2.44        | 11     | 1     |
| 1:A:307:TRP:NE1  | 1:A:318:VAL:HG22 | 0.47     | 2.24        | 18     | 1     |
| 1:A:414:TYR:CE2  | 1:A:416:LYS:HG3  | 0.47     | 2.45        | 4      | 11    |
| 1:A:315:LYS:HG2  | 1:A:468:PHE:CE2  | 0.47     | 2.45        | 3      | 1     |
| 1:A:305:PHE:CD2  | 1:A:318:VAL:CG1  | 0.47     | 2.98        | 6      | 1     |
| 1:A:316:THR:HG21 | 1:A:468:PHE:CD1  | 0.47     | 2.43        | 11     | 3     |
| 1:A:301:PHE:CD2  | 1:A:332:ILE:HB   | 0.47     | 2.45        | 8      | 1     |
| 1:A:352:TYR:CZ   | 1:A:366:LYS:HB3  | 0.47     | 2.45        | 18     | 8     |
| 1:A:372:GLY:O    | 1:A:374:PRO:N    | 0.47     | 2.47        | 11     | 6     |
| 1:A:306:PHE:CZ   | 1:A:319:ASN:HB2  | 0.47     | 2.44        | 10     | 4     |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:293:THR:HG21 | 1:A:435:SER:HB2  | 0.47     | 1.86        | 3      | 2     |
| 1:A:418:ILE:HD12 | 1:A:418:ILE:H    | 0.47     | 1.68        | 8      | 2     |
| 1:A:298:ILE:C    | 1:A:298:ILE:HD12 | 0.47     | 2.35        | 4      | 1     |
| 1:A:322:SER:O    | 1:A:323:SER:C    | 0.47     | 2.57        | 9      | 7     |
| 1:A:347:PHE:CE2  | 1:A:380:ILE:HB   | 0.47     | 2.45        | 5      | 1     |
| 1:A:448:GLN:O    | 1:A:462:LEU:CD2  | 0.47     | 2.63        | 5      | 1     |
| 1:A:347:PHE:CE2  | 1:A:352:TYR:CE1  | 0.47     | 3.02        | 6      | 1     |
| 1:A:461:THR:O    | 1:A:461:THR:CG2  | 0.47     | 2.60        | 6      | 1     |
| 1:A:459:THR:OG1  | 1:A:460:LYS:N    | 0.47     | 2.47        | 7      | 1     |
| 1:A:293:THR:HG21 | 1:A:435:SER:OG   | 0.47     | 2.09        | 9      | 1     |
| 1:A:286:LEU:HD23 | 1:A:287:SER:H    | 0.47     | 1.69        | 11     | 1     |
| 1:A:343:GLN:NE2  | 1:A:354:LEU:HD11 | 0.47     | 2.25        | 14     | 1     |
| 1:A:369:HIS:CE1  | 1:A:373:PHE:CZ   | 0.47     | 3.02        | 16     | 1     |
| 1:A:362:PRO:O    | 1:A:363:ASN:CG   | 0.47     | 2.58        | 8      | 3     |
| 1:A:418:ILE:HG22 | 1:A:425:ILE:CD1  | 0.47     | 2.39        | 14     | 1     |
| 1:A:437:ASN:O    | 1:A:438:LYS:C    | 0.47     | 2.58        | 17     | 1     |
| 1:A:339:GLU:O    | 1:A:342:ASN:N    | 0.47     | 2.48        | 18     | 1     |
| 1:A:460:LYS:HE2  | 1:A:462:LEU:HD22 | 0.47     | 1.86        | 18     | 1     |
| 1:A:364:TYR:CD2  | 1:A:366:LYS:HD3  | 0.47     | 2.44        | 6      | 2     |
| 1:A:434:TYR:CE1  | 1:A:439:TYR:O    | 0.47     | 2.68        | 2      | 1     |
| 1:A:341:ARG:O    | 1:A:342:ASN:CB   | 0.47     | 2.63        | 19     | 2     |
| 1:A:400:TYR:CE1  | 1:A:402:ARG:HG3  | 0.47     | 2.45        | 7      | 1     |
| 1:A:448:GLN:CB   | 1:A:462:LEU:CD2  | 0.47     | 2.92        | 16     | 1     |
| 1:A:322:SER:C    | 1:A:324:LEU:N    | 0.47     | 2.70        | 19     | 4     |
| 1:A:300:PHE:O    | 1:A:307:TRP:CE3  | 0.47     | 2.68        | 8      | 1     |
| 1:A:395:PHE:HE2  | 1:A:432:VAL:HG21 | 0.47     | 1.69        | 9      | 2     |
| 1:A:439:TYR:CE1  | 1:A:452:ASP:HB2  | 0.47     | 2.44        | 10     | 1     |
| 1:A:467:TRP:C    | 1:A:469:GLY:N    | 0.47     | 2.73        | 11     | 1     |
| 1:A:433:PHE:CD1  | 1:A:433:PHE:N    | 0.46     | 2.83        | 5      | 5     |
| 1:A:301:PHE:CE1  | 1:A:321:ILE:HG12 | 0.46     | 2.45        | 2      | 1     |
| 1:A:403:TYR:CE2  | 1:A:405:GLU:OE2  | 0.46     | 2.67        | 6      | 1     |
| 1:A:292:THR:HB   | 1:A:335:ALA:HB1  | 0.46     | 1.86        | 7      | 2     |
| 1:A:301:PHE:CD2  | 1:A:332:ILE:HG12 | 0.46     | 2.45        | 7      | 1     |
| 1:A:298:ILE:CG2  | 1:A:300:PHE:CE1  | 0.46     | 2.98        | 9      | 1     |
| 1:A:307:TRP:CE2  | 1:A:316:THR:CB   | 0.46     | 2.98        | 14     | 1     |
| 1:A:418:ILE:CD1  | 1:A:427:PRO:O    | 0.46     | 2.63        | 17     | 3     |
| 1:A:374:PRO:O    | 1:A:375:ASN:CG   | 0.46     | 2.58        | 16     | 1     |
| 1:A:301:PHE:CZ   | 1:A:332:ILE:HD13 | 0.46     | 2.45        | 1      | 1     |
| 1:A:418:ILE:O    | 1:A:420:LYS:N    | 0.46     | 2.48        | 1      | 4     |
| 1:A:460:LYS:O    | 1:A:461:THR:HG23 | 0.46     | 2.10        | 3      | 1     |
| 1:A:444:GLN:CD   | 1:A:444:GLN:O    | 0.46     | 2.59        | 15     | 3     |

*Continued on next page...*

Continued from previous page...

| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:451:TYR:CE1  | 1:A:456:GLN:HA   | 0.46     | 2.45        | 6      | 1     |
| 1:A:306:PHE:CE2  | 1:A:319:ASN:HB3  | 0.46     | 2.45        | 14     | 1     |
| 1:A:429:ILE:CD1  | 1:A:444:GLN:OE1  | 0.46     | 2.64        | 16     | 1     |
| 1:A:418:ILE:C    | 1:A:420:LYS:N    | 0.46     | 2.72        | 3      | 6     |
| 1:A:430:ASP:CB   | 1:A:443:PHE:O    | 0.46     | 2.64        | 2      | 5     |
| 1:A:364:TYR:CD2  | 1:A:366:LYS:HE3  | 0.46     | 2.45        | 8      | 3     |
| 1:A:433:PHE:CE1  | 1:A:441:TYR:O    | 0.46     | 2.69        | 9      | 1     |
| 1:A:373:PHE:C    | 1:A:373:PHE:CD1  | 0.46     | 2.92        | 3      | 1     |
| 1:A:391:ARG:CZ   | 1:A:404:ASP:OD1  | 0.46     | 2.63        | 9      | 1     |
| 1:A:436:LYS:HD3  | 1:A:441:TYR:CE1  | 0.46     | 2.46        | 10     | 2     |
| 1:A:431:ALA:C    | 1:A:432:VAL:HG13 | 0.46     | 2.35        | 14     | 1     |
| 1:A:448:GLN:CB   | 1:A:462:LEU:HD21 | 0.46     | 2.40        | 14     | 1     |
| 1:A:432:VAL:HG23 | 1:A:440:TYR:CD1  | 0.46     | 2.44        | 15     | 1     |
| 1:A:307:TRP:CE3  | 1:A:318:VAL:HB   | 0.46     | 2.46        | 17     | 1     |
| 1:A:288:PHE:CG   | 1:A:443:PHE:CE2  | 0.46     | 3.03        | 18     | 1     |
| 1:A:321:ILE:C    | 1:A:323:SER:N    | 0.46     | 2.74        | 2      | 4     |
| 1:A:299:PHE:HB3  | 1:A:301:PHE:CE1  | 0.46     | 2.45        | 3      | 1     |
| 1:A:356:SER:O    | 1:A:358:LEU:N    | 0.46     | 2.49        | 6      | 3     |
| 1:A:422:PHE:HB3  | 1:A:451:TYR:CE2  | 0.46     | 2.46        | 8      | 2     |
| 1:A:311:SER:OG   | 1:A:312:GLU:N    | 0.46     | 2.49        | 9      | 1     |
| 1:A:388:ARG:O    | 1:A:390:TYR:CE2  | 0.46     | 2.68        | 11     | 1     |
| 1:A:296:ASN:OD1  | 1:A:296:ASN:C    | 0.46     | 2.56        | 14     | 1     |
| 1:A:352:TYR:CZ   | 1:A:366:LYS:CB   | 0.46     | 2.99        | 18     | 2     |
| 1:A:329:PRO:HG3  | 1:A:353:TRP:CZ3  | 0.46     | 2.46        | 1      | 1     |
| 1:A:380:ILE:HG22 | 1:A:381:ASP:N    | 0.46     | 2.26        | 12     | 3     |
| 1:A:296:ASN:O    | 1:A:296:ASN:CG   | 0.46     | 2.58        | 3      | 1     |
| 1:A:334:ALA:HB1  | 1:A:382:ALA:HA   | 0.46     | 1.88        | 4      | 1     |
| 1:A:430:ASP:N    | 1:A:430:ASP:OD1  | 0.46     | 2.49        | 6      | 2     |
| 1:A:432:VAL:HB   | 1:A:442:PHE:CD1  | 0.46     | 2.45        | 13     | 3     |
| 1:A:377:VAL:HG12 | 1:A:378:LYS:N    | 0.46     | 2.24        | 10     | 1     |
| 1:A:382:ALA:HB3  | 1:A:395:PHE:HD2  | 0.46     | 1.70        | 12     | 1     |
| 1:A:455:LEU:N    | 1:A:455:LEU:CD2  | 0.46     | 2.78        | 14     | 1     |
| 1:A:285:ASN:O    | 1:A:285:ASN:CG   | 0.46     | 2.58        | 14     | 3     |
| 1:A:302:LYS:O    | 1:A:304:ARG:N    | 0.46     | 2.49        | 6      | 3     |
| 1:A:299:PHE:HB3  | 1:A:301:PHE:CZ   | 0.46     | 2.46        | 3      | 2     |
| 1:A:364:TYR:CG   | 1:A:366:LYS:HE3  | 0.46     | 2.46        | 7      | 4     |
| 1:A:381:ASP:CG   | 1:A:429:ILE:O    | 0.46     | 2.59        | 4      | 7     |
| 1:A:352:TYR:CD2  | 1:A:368:ILE:HG23 | 0.46     | 2.45        | 4      | 1     |
| 1:A:445:GLY:O    | 1:A:447:ASN:ND2  | 0.46     | 2.49        | 16     | 3     |
| 1:A:325:TRP:CG   | 1:A:328:LEU:CB   | 0.46     | 2.99        | 10     | 1     |
| 1:A:429:ILE:CD1  | 1:A:442:PHE:CD2  | 0.46     | 2.98        | 20     | 1     |

Continued on next page...

*Continued from previous page...*

| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:336:TYR:CE1  | 1:A:345:PHE:CG   | 0.46     | 3.04        | 2      | 1     |
| 1:A:441:TYR:CD1  | 1:A:450:GLU:HG3  | 0.46     | 2.46        | 6      | 1     |
| 1:A:437:ASN:O    | 1:A:439:TYR:CD2  | 0.46     | 2.69        | 17     | 2     |
| 1:A:293:THR:O    | 1:A:337:GLU:CG   | 0.46     | 2.63        | 13     | 1     |
| 1:A:293:THR:HG21 | 1:A:435:SER:HA   | 0.46     | 1.86        | 14     | 1     |
| 1:A:386:ASN:ND2  | 1:A:393:TYR:CE1  | 0.46     | 2.83        | 17     | 2     |
| 1:A:449:PHE:CD1  | 1:A:461:THR:HG23 | 0.46     | 2.46        | 17     | 1     |
| 1:A:419:THR:HG23 | 1:A:420:LYS:N    | 0.46     | 2.26        | 18     | 2     |
| 1:A:293:THR:HG21 | 1:A:435:SER:HB3  | 0.46     | 1.87        | 20     | 1     |
| 1:A:447:ASN:OD1  | 1:A:449:PHE:CE2  | 0.46     | 2.69        | 2      | 1     |
| 1:A:431:ALA:HB3  | 1:A:443:PHE:HB2  | 0.46     | 1.87        | 3      | 1     |
| 1:A:321:ILE:O    | 1:A:324:LEU:N    | 0.46     | 2.47        | 10     | 5     |
| 1:A:445:GLY:O    | 1:A:447:ASN:CG   | 0.46     | 2.59        | 16     | 3     |
| 1:A:352:TYR:CE1  | 1:A:366:LYS:HB3  | 0.46     | 2.47        | 9      | 2     |
| 1:A:318:VAL:O    | 1:A:318:VAL:HG13 | 0.46     | 2.11        | 15     | 1     |
| 1:A:400:TYR:CD1  | 1:A:400:TYR:C    | 0.46     | 2.94        | 15     | 4     |
| 1:A:337:GLU:CD   | 1:A:337:GLU:C    | 0.46     | 2.84        | 16     | 1     |
| 1:A:463:LYS:O    | 1:A:466:SER:N    | 0.46     | 2.49        | 17     | 1     |
| 1:A:392:THR:HG22 | 1:A:393:TYR:H    | 0.46     | 1.70        | 19     | 1     |
| 1:A:397:ASP:OD1  | 1:A:397:ASP:N    | 0.46     | 2.49        | 19     | 1     |
| 1:A:299:PHE:CD1  | 1:A:308:LEU:HD21 | 0.45     | 2.47        | 2      | 1     |
| 1:A:345:PHE:O    | 1:A:346:LEU:HD22 | 0.45     | 2.11        | 5      | 2     |
| 1:A:441:TYR:CE2  | 1:A:450:GLU:HG3  | 0.45     | 2.47        | 5      | 1     |
| 1:A:463:LYS:C    | 1:A:465:ASN:N    | 0.45     | 2.72        | 7      | 3     |
| 1:A:432:VAL:HG12 | 1:A:442:PHE:HD1  | 0.45     | 1.71        | 9      | 1     |
| 1:A:298:ILE:CD1  | 1:A:300:PHE:CZ   | 0.45     | 2.90        | 13     | 1     |
| 1:A:433:PHE:CE2  | 1:A:435:SER:HB3  | 0.45     | 2.46        | 19     | 1     |
| 1:A:453:PHE:O    | 1:A:454:LEU:C    | 0.45     | 2.59        | 19     | 10    |
| 1:A:338:ILE:CD1  | 1:A:340:ALA:HB3  | 0.45     | 2.40        | 3      | 1     |
| 1:A:403:TYR:CD2  | 1:A:410:MET:HB3  | 0.45     | 2.46        | 4      | 1     |
| 1:A:387:PRO:HG2  | 1:A:434:TYR:CZ   | 0.45     | 2.47        | 7      | 1     |
| 1:A:464:SER:O    | 1:A:465:ASN:CG   | 0.45     | 2.59        | 10     | 1     |
| 1:A:354:LEU:HD13 | 1:A:354:LEU:O    | 0.45     | 2.11        | 11     | 1     |
| 1:A:391:ARG:NH1  | 1:A:404:ASP:OD2  | 0.45     | 2.50        | 14     | 1     |
| 1:A:403:TYR:CE2  | 1:A:410:MET:HB3  | 0.45     | 2.45        | 10     | 2     |
| 1:A:293:THR:HG22 | 1:A:433:PHE:CE2  | 0.45     | 2.46        | 6      | 1     |
| 1:A:321:ILE:HG22 | 1:A:322:SER:N    | 0.45     | 2.27        | 7      | 3     |
| 1:A:420:LYS:O    | 1:A:421:ASN:C    | 0.45     | 2.59        | 15     | 4     |
| 1:A:355:ILE:HD12 | 1:A:355:ILE:N    | 0.45     | 2.27        | 15     | 1     |
| 1:A:281:LEU:HD21 | 1:A:307:TRP:CE3  | 0.45     | 2.46        | 17     | 1     |
| 1:A:395:PHE:CE2  | 1:A:432:VAL:HG11 | 0.45     | 2.46        | 17     | 1     |

*Continued on next page...*

Continued from previous page...

| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:455:LEU:C    | 1:A:456:GLN:OE1  | 0.45     | 2.60        | 2      | 1     |
| 1:A:307:TRP:CZ3  | 1:A:318:VAL:HB   | 0.45     | 2.47        | 11     | 2     |
| 1:A:468:PHE:CD1  | 1:A:470:CYS:HB2  | 0.45     | 2.47        | 20     | 2     |
| 1:A:291:VAL:HG11 | 1:A:442:PHE:HZ   | 0.45     | 1.71        | 15     | 1     |
| 1:A:324:LEU:O    | 1:A:325:TRP:C    | 0.45     | 2.60        | 16     | 2     |
| 1:A:281:LEU:HA   | 1:A:286:LEU:HD12 | 0.45     | 1.89        | 17     | 1     |
| 1:A:307:TRP:HE1  | 1:A:318:VAL:HG22 | 0.45     | 1.72        | 18     | 1     |
| 1:A:297:LYS:HG2  | 1:A:299:PHE:CZ   | 0.45     | 2.47        | 19     | 1     |
| 1:A:302:LYS:N    | 1:A:305:PHE:O    | 0.45     | 2.49        | 1      | 4     |
| 1:A:373:PHE:CD1  | 1:A:377:VAL:HG21 | 0.45     | 2.46        | 6      | 1     |
| 1:A:455:LEU:O    | 1:A:456:GLN:CD   | 0.45     | 2.59        | 6      | 1     |
| 1:A:436:LYS:HE3  | 1:A:441:TYR:CE2  | 0.45     | 2.46        | 8      | 1     |
| 1:A:336:TYR:OH   | 1:A:345:PHE:CG   | 0.45     | 2.64        | 9      | 1     |
| 1:A:465:ASN:O    | 1:A:470:CYS:C    | 0.45     | 2.60        | 20     | 2     |
| 1:A:448:GLN:HB3  | 1:A:462:LEU:HD21 | 0.45     | 1.87        | 11     | 1     |
| 1:A:433:PHE:CE2  | 1:A:443:PHE:CE1  | 0.45     | 3.05        | 12     | 1     |
| 1:A:400:TYR:CE2  | 1:A:418:ILE:HA   | 0.45     | 2.46        | 13     | 1     |
| 1:A:376:PHE:O    | 1:A:377:VAL:C    | 0.45     | 2.59        | 16     | 2     |
| 1:A:288:PHE:CD2  | 1:A:443:PHE:CD1  | 0.45     | 3.04        | 7      | 1     |
| 1:A:419:THR:O    | 1:A:422:PHE:C    | 0.45     | 2.60        | 13     | 3     |
| 1:A:308:LEU:HD21 | 1:A:313:ARG:CZ   | 0.45     | 2.41        | 16     | 1     |
| 1:A:463:LYS:O    | 1:A:466:SER:CB   | 0.45     | 2.65        | 16     | 1     |
| 1:A:414:TYR:N    | 1:A:415:PRO:CD   | 0.45     | 2.79        | 19     | 1     |
| 1:A:462:LEU:CD2  | 1:A:466:SER:OG   | 0.45     | 2.65        | 2      | 1     |
| 1:A:296:ASN:O    | 1:A:296:ASN:ND2  | 0.45     | 2.50        | 20     | 2     |
| 1:A:344:VAL:N    | 1:A:355:ILE:O    | 0.45     | 2.49        | 3      | 1     |
| 1:A:393:TYR:CD2  | 1:A:400:TYR:CE1  | 0.45     | 3.05        | 4      | 2     |
| 1:A:294:VAL:O    | 1:A:296:ASN:N    | 0.45     | 2.49        | 12     | 2     |
| 1:A:307:TRP:CE3  | 1:A:317:SER:O    | 0.45     | 2.69        | 11     | 1     |
| 1:A:441:TYR:CD2  | 1:A:448:GLN:OE1  | 0.45     | 2.69        | 16     | 1     |
| 1:A:369:HIS:C    | 1:A:371:PHE:N    | 0.45     | 2.74        | 1      | 3     |
| 1:A:433:PHE:O    | 1:A:441:TYR:N    | 0.45     | 2.49        | 6      | 1     |
| 1:A:418:ILE:O    | 1:A:421:ASN:N    | 0.45     | 2.50        | 16     | 1     |
| 1:A:447:ASN:N    | 1:A:447:ASN:ND2  | 0.45     | 2.64        | 20     | 1     |
| 1:A:428:LYS:O    | 1:A:444:GLN:CD   | 0.45     | 2.60        | 12     | 2     |
| 1:A:338:ILE:CD1  | 1:A:385:PHE:CD2  | 0.45     | 3.00        | 6      | 1     |
| 1:A:299:PHE:C    | 1:A:300:PHE:CD1  | 0.45     | 2.95        | 8      | 2     |
| 1:A:352:TYR:O    | 1:A:352:TYR:CG   | 0.45     | 2.67        | 11     | 1     |
| 1:A:286:LEU:HD23 | 1:A:287:SER:N    | 0.45     | 2.27        | 20     | 1     |
| 1:A:352:TYR:C    | 1:A:353:TRP:CE3  | 0.45     | 2.95        | 10     | 1     |
| 1:A:432:VAL:HG21 | 1:A:442:PHE:CD2  | 0.44     | 2.47        | 5      | 1     |

Continued on next page...

*Continued from previous page...*

| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:443:PHE:CZ   | 1:A:448:GLN:NE2  | 0.44     | 2.84        | 9      | 1     |
| 1:A:328:LEU:HD23 | 1:A:360:PRO:HB3  | 0.44     | 1.90        | 10     | 1     |
| 1:A:336:TYR:CE2  | 1:A:338:ILE:CG1  | 0.44     | 3.00        | 10     | 1     |
| 1:A:364:TYR:CZ   | 1:A:366:LYS:HD3  | 0.44     | 2.47        | 15     | 2     |
| 1:A:345:PHE:CE2  | 1:A:354:LEU:HD13 | 0.44     | 2.48        | 12     | 1     |
| 1:A:425:ILE:O    | 1:A:444:GLN:NE2  | 0.44     | 2.49        | 12     | 1     |
| 1:A:354:LEU:N    | 1:A:354:LEU:CD1  | 0.44     | 2.80        | 15     | 1     |
| 1:A:368:ILE:O    | 1:A:369:HIS:C    | 0.44     | 2.60        | 1      | 2     |
| 1:A:380:ILE:CG2  | 1:A:381:ASP:N    | 0.44     | 2.81        | 1      | 1     |
| 1:A:448:GLN:HG2  | 1:A:462:LEU:HD23 | 0.44     | 1.88        | 3      | 1     |
| 1:A:428:LYS:O    | 1:A:444:GLN:NE2  | 0.44     | 2.50        | 4      | 1     |
| 1:A:281:LEU:HB2  | 1:A:468:PHE:CE2  | 0.44     | 2.47        | 5      | 1     |
| 1:A:440:TYR:CD1  | 1:A:440:TYR:N    | 0.44     | 2.84        | 7      | 2     |
| 1:A:425:ILE:HD13 | 1:A:426:GLY:H    | 0.44     | 1.73        | 12     | 1     |
| 1:A:305:PHE:HB3  | 1:A:307:TRP:CH2  | 0.44     | 2.47        | 18     | 1     |
| 1:A:419:THR:O    | 1:A:420:LYS:C    | 0.44     | 2.60        | 19     | 1     |
| 1:A:286:LEU:HD11 | 1:A:307:TRP:CZ3  | 0.44     | 2.47        | 1      | 1     |
| 1:A:373:PHE:CZ   | 1:A:376:PHE:HA   | 0.44     | 2.47        | 1      | 1     |
| 1:A:384:VAL:HG11 | 1:A:432:VAL:HG22 | 0.44     | 1.88        | 4      | 1     |
| 1:A:291:VAL:HG13 | 1:A:300:PHE:CE1  | 0.44     | 2.47        | 9      | 1     |
| 1:A:409:MET:O    | 1:A:410:MET:C    | 0.44     | 2.59        | 19     | 2     |
| 1:A:468:PHE:CD1  | 1:A:468:PHE:C    | 0.44     | 2.95        | 1      | 3     |
| 1:A:315:LYS:C    | 1:A:316:THR:CG2  | 0.44     | 2.91        | 3      | 1     |
| 1:A:292:THR:OG1  | 1:A:335:ALA:CB   | 0.44     | 2.66        | 4      | 1     |
| 1:A:356:SER:O    | 1:A:357:ASN:CB   | 0.44     | 2.65        | 17     | 2     |
| 1:A:430:ASP:CG   | 1:A:443:PHE:O    | 0.44     | 2.60        | 6      | 2     |
| 1:A:303:ASP:O    | 1:A:331:GLY:N    | 0.44     | 2.49        | 11     | 2     |
| 1:A:320:LEU:HD23 | 1:A:320:LEU:H    | 0.44     | 1.71        | 19     | 1     |
| 1:A:368:ILE:O    | 1:A:371:PHE:CD1  | 0.44     | 2.69        | 20     | 1     |
| 1:A:444:GLN:O    | 1:A:447:ASN:ND2  | 0.44     | 2.50        | 3      | 3     |
| 1:A:379:LYS:O    | 1:A:396:VAL:HG23 | 0.44     | 2.13        | 5      | 1     |
| 1:A:447:ASN:HB3  | 1:A:449:PHE:CD1  | 0.44     | 2.47        | 6      | 1     |
| 1:A:309:LYS:NZ   | 1:A:313:ARG:O    | 0.44     | 2.49        | 9      | 1     |
| 1:A:325:TRP:CZ3  | 1:A:328:LEU:HD12 | 0.44     | 2.48        | 10     | 1     |
| 1:A:384:VAL:HG23 | 1:A:432:VAL:HG13 | 0.44     | 1.88        | 10     | 1     |
| 1:A:448:GLN:O    | 1:A:462:LEU:HD23 | 0.44     | 2.12        | 11     | 2     |
| 1:A:462:LEU:HD12 | 1:A:466:SER:OG   | 0.44     | 2.12        | 11     | 1     |
| 1:A:449:PHE:CD1  | 1:A:461:THR:HG22 | 0.44     | 2.47        | 14     | 1     |
| 1:A:338:ILE:HD12 | 1:A:385:PHE:CE2  | 0.44     | 2.47        | 6      | 1     |
| 1:A:447:ASN:HB3  | 1:A:449:PHE:CE1  | 0.44     | 2.47        | 6      | 1     |
| 1:A:464:SER:C    | 1:A:466:SER:N    | 0.44     | 2.74        | 18     | 1     |

*Continued on next page...*

Continued from previous page...

| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:286:LEU:HD22 | 1:A:307:TRP:CZ3  | 0.44     | 2.48        | 19     | 1     |
| 1:A:391:ARG:NH1  | 1:A:411:ASP:OD2  | 0.44     | 2.51        | 3      | 1     |
| 1:A:306:PHE:CB   | 1:A:319:ASN:O    | 0.44     | 2.66        | 6      | 1     |
| 1:A:312:GLU:O    | 1:A:314:PRO:N    | 0.44     | 2.51        | 7      | 1     |
| 1:A:394:PHE:CD2  | 1:A:403:TYR:CD1  | 0.44     | 3.05        | 10     | 1     |
| 1:A:281:LEU:CB   | 1:A:468:PHE:CD2  | 0.44     | 3.01        | 5      | 1     |
| 1:A:283:ASP:O    | 1:A:285:ASN:ND2  | 0.44     | 2.50        | 9      | 2     |
| 1:A:440:TYR:HB3  | 1:A:442:PHE:CE2  | 0.44     | 2.48        | 10     | 1     |
| 1:A:395:PHE:HE2  | 1:A:432:VAL:HG11 | 0.44     | 1.73        | 17     | 1     |
| 1:A:425:ILE:CG1  | 1:A:426:GLY:N    | 0.44     | 2.81        | 1      | 1     |
| 1:A:301:PHE:CD1  | 1:A:321:ILE:HD11 | 0.44     | 2.47        | 2      | 1     |
| 1:A:352:TYR:O    | 1:A:352:TYR:CD2  | 0.44     | 2.71        | 9      | 1     |
| 1:A:449:PHE:CD2  | 1:A:461:THR:CG2  | 0.44     | 3.01        | 13     | 1     |
| 1:A:448:GLN:HB3  | 1:A:462:LEU:CD2  | 0.44     | 2.43        | 16     | 1     |
| 1:A:306:PHE:CD1  | 1:A:319:ASN:O    | 0.44     | 2.70        | 19     | 1     |
| 1:A:329:PRO:O    | 1:A:330:SER:CB   | 0.43     | 2.66        | 19     | 2     |
| 1:A:425:ILE:CG2  | 1:A:442:PHE:CE1  | 0.43     | 3.01        | 6      | 1     |
| 1:A:442:PHE:CD1  | 1:A:442:PHE:N    | 0.43     | 2.86        | 6      | 1     |
| 1:A:350:ASP:OD1  | 1:A:369:HIS:ND1  | 0.43     | 2.50        | 11     | 1     |
| 1:A:353:TRP:CD1  | 1:A:364:TYR:CD1  | 0.43     | 3.06        | 12     | 1     |
| 1:A:393:TYR:CB   | 1:A:401:TRP:O    | 0.43     | 2.66        | 1      | 1     |
| 1:A:348:LYS:O    | 1:A:351:LYS:O    | 0.43     | 2.37        | 16     | 11    |
| 1:A:305:PHE:CD2  | 1:A:318:VAL:HG12 | 0.43     | 2.48        | 8      | 1     |
| 1:A:313:ARG:CG   | 1:A:315:LYS:O    | 0.43     | 2.66        | 12     | 1     |
| 1:A:310:VAL:CG2  | 1:A:311:SER:N    | 0.43     | 2.81        | 1      | 1     |
| 1:A:438:LYS:C    | 1:A:439:TYR:CG   | 0.43     | 2.96        | 11     | 1     |
| 1:A:358:LEU:O    | 1:A:358:LEU:CG   | 0.43     | 2.66        | 12     | 1     |
| 1:A:429:ILE:CG1  | 1:A:442:PHE:CD1  | 0.43     | 3.01        | 16     | 1     |
| 1:A:465:ASN:O    | 1:A:468:PHE:N    | 0.43     | 2.51        | 18     | 1     |
| 1:A:299:PHE:CD2  | 1:A:308:LEU:CD2  | 0.43     | 3.01        | 1      | 2     |
| 1:A:438:LYS:O    | 1:A:438:LYS:CG   | 0.43     | 2.67        | 4      | 3     |
| 1:A:367:SER:C    | 1:A:369:HIS:N    | 0.43     | 2.75        | 16     | 3     |
| 1:A:303:ASP:O    | 1:A:304:ARG:CB   | 0.43     | 2.64        | 8      | 1     |
| 1:A:299:PHE:CD1  | 1:A:299:PHE:N    | 0.43     | 2.86        | 11     | 1     |
| 1:A:339:GLU:O    | 1:A:340:ALA:C    | 0.43     | 2.61        | 11     | 1     |
| 1:A:419:THR:O    | 1:A:423:GLN:CA   | 0.43     | 2.67        | 11     | 1     |
| 1:A:283:ASP:O    | 1:A:465:ASN:ND2  | 0.43     | 2.52        | 12     | 1     |
| 1:A:291:VAL:CG2  | 1:A:442:PHE:CZ   | 0.43     | 2.90        | 15     | 1     |
| 1:A:425:ILE:HG21 | 1:A:442:PHE:CD1  | 0.43     | 2.48        | 17     | 1     |
| 1:A:292:THR:OG1  | 1:A:335:ALA:HB1  | 0.43     | 2.13        | 4      | 1     |
| 1:A:435:SER:O    | 1:A:436:LYS:CB   | 0.43     | 2.66        | 20     | 2     |

Continued on next page...

*Continued from previous page...*

| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:441:TYR:CZ   | 1:A:450:GLU:CD   | 0.43     | 2.97        | 6      | 1     |
| 1:A:291:VAL:HG21 | 1:A:300:PHE:CZ   | 0.43     | 2.46        | 16     | 1     |
| 1:A:295:GLY:CA   | 1:A:339:GLU:OE1  | 0.43     | 2.66        | 18     | 1     |
| 1:A:390:TYR:O    | 1:A:405:GLU:N    | 0.43     | 2.50        | 20     | 1     |
| 1:A:421:ASN:C    | 1:A:422:PHE:CG   | 0.43     | 2.96        | 2      | 1     |
| 1:A:293:THR:O    | 1:A:337:GLU:CD   | 0.43     | 2.62        | 7      | 2     |
| 1:A:310:VAL:O    | 1:A:311:SER:O    | 0.43     | 2.36        | 18     | 2     |
| 1:A:425:ILE:HD11 | 1:A:451:TYR:CD1  | 0.43     | 2.49        | 15     | 1     |
| 1:A:300:PHE:O    | 1:A:306:PHE:CB   | 0.43     | 2.67        | 16     | 1     |
| 1:A:384:VAL:CG1  | 1:A:432:VAL:HG12 | 0.43     | 2.41        | 18     | 1     |
| 1:A:332:ILE:CG2  | 1:A:334:ALA:O    | 0.43     | 2.66        | 4      | 1     |
| 1:A:438:LYS:HA   | 1:A:438:LYS:CE   | 0.43     | 2.43        | 5      | 2     |
| 1:A:304:ARG:N    | 1:A:304:ARG:CD   | 0.43     | 2.81        | 10     | 1     |
| 1:A:294:VAL:O    | 1:A:294:VAL:HG13 | 0.43     | 2.14        | 13     | 1     |
| 1:A:346:LEU:CD2  | 1:A:346:LEU:N    | 0.43     | 2.81        | 2      | 1     |
| 1:A:309:LYS:CD   | 1:A:315:LYS:O    | 0.43     | 2.67        | 3      | 1     |
| 1:A:293:THR:CG2  | 1:A:435:SER:OG   | 0.43     | 2.67        | 9      | 1     |
| 1:A:425:ILE:H    | 1:A:425:ILE:HD13 | 0.43     | 1.72        | 16     | 2     |
| 1:A:364:TYR:CG   | 1:A:365:PRO:CD   | 0.43     | 3.02        | 12     | 1     |
| 1:A:329:PRO:HG3  | 1:A:353:TRP:CE3  | 0.43     | 2.49        | 13     | 1     |
| 1:A:295:GLY:O    | 1:A:296:ASN:OD1  | 0.43     | 2.37        | 14     | 1     |
| 1:A:425:ILE:HD12 | 1:A:442:PHE:CE2  | 0.43     | 2.48        | 14     | 1     |
| 1:A:393:TYR:N    | 1:A:393:TYR:CD1  | 0.43     | 2.86        | 16     | 1     |
| 1:A:433:PHE:CE1  | 1:A:441:TYR:CB   | 0.43     | 3.02        | 18     | 1     |
| 1:A:403:TYR:O    | 1:A:403:TYR:CG   | 0.43     | 2.70        | 20     | 1     |
| 1:A:325:TRP:CE3  | 1:A:328:LEU:HG   | 0.43     | 2.48        | 15     | 1     |
| 1:A:442:PHE:CZ   | 1:A:449:PHE:HB2  | 0.43     | 2.49        | 20     | 1     |
| 1:A:374:PRO:CG   | 1:A:401:TRP:CH2  | 0.43     | 3.01        | 1      | 1     |
| 1:A:373:PHE:CZ   | 1:A:380:ILE:HG12 | 0.43     | 2.49        | 6      | 1     |
| 1:A:352:TYR:CE1  | 1:A:366:LYS:HB2  | 0.43     | 2.48        | 10     | 1     |
| 1:A:414:TYR:CZ   | 1:A:416:LYS:HG3  | 0.42     | 2.49        | 5      | 1     |
| 1:A:430:ASP:N    | 1:A:443:PHE:O    | 0.42     | 2.51        | 10     | 1     |
| 1:A:292:THR:CG2  | 1:A:293:THR:N    | 0.42     | 2.81        | 17     | 1     |
| 1:A:389:PHE:O    | 1:A:390:TYR:C    | 0.42     | 2.62        | 20     | 2     |
| 1:A:306:PHE:CD1  | 1:A:321:ILE:HG13 | 0.42     | 2.49        | 19     | 1     |
| 1:A:331:GLY:O    | 1:A:332:ILE:C    | 0.42     | 2.62        | 14     | 3     |
| 1:A:412:PRO:O    | 1:A:413:GLY:O    | 0.42     | 2.37        | 16     | 4     |
| 1:A:373:PHE:N    | 1:A:374:PRO:HD3  | 0.42     | 2.28        | 20     | 3     |
| 1:A:336:TYR:CD1  | 1:A:336:TYR:C    | 0.42     | 2.96        | 7      | 1     |
| 1:A:467:TRP:O    | 1:A:469:GLY:N    | 0.42     | 2.52        | 11     | 1     |
| 1:A:298:ILE:C    | 1:A:298:ILE:CD1  | 0.42     | 2.93        | 13     | 1     |

*Continued on next page...*

*Continued from previous page...*

| Atom-1          | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|-----------------|------------------|----------|-------------|--------|-------|
|                 |                  |          |             | Worst  | Total |
| 1:A:442:PHE:HB2 | 1:A:449:PHE:CZ   | 0.42     | 2.49        | 5      | 1     |
| 1:A:437:ASN:C   | 1:A:439:TYR:N    | 0.42     | 2.76        | 8      | 1     |
| 1:A:320:LEU:O   | 1:A:321:ILE:C    | 0.42     | 2.62        | 10     | 1     |
| 1:A:350:ASP:C   | 1:A:351:LYS:CG   | 0.42     | 2.93        | 15     | 1     |
| 1:A:401:TRP:CZ2 | 1:A:412:PRO:HA   | 0.42     | 2.49        | 18     | 1     |
| 1:A:338:ILE:O   | 1:A:341:ARG:N    | 0.42     | 2.52        | 20     | 1     |
| 1:A:344:VAL:O   | 1:A:355:ILE:HG22 | 0.42     | 2.13        | 4      | 1     |
| 1:A:336:TYR:CE1 | 1:A:345:PHE:HB2  | 0.42     | 2.49        | 6      | 2     |
| 1:A:325:TRP:HB3 | 1:A:328:LEU:CB   | 0.42     | 2.44        | 10     | 1     |
| 1:A:306:PHE:CZ  | 1:A:319:ASN:CB   | 0.42     | 3.03        | 12     | 1     |
| 1:A:349:ASP:C   | 1:A:378:LYS:O    | 0.42     | 2.62        | 13     | 1     |
| 1:A:384:VAL:CG1 | 1:A:385:PHE:N    | 0.42     | 2.82        | 13     | 1     |
| 1:A:440:TYR:CD1 | 1:A:441:TYR:N    | 0.42     | 2.87        | 15     | 1     |
| 1:A:322:SER:O   | 1:A:324:LEU:N    | 0.42     | 2.53        | 19     | 1     |
| 1:A:380:ILE:HA  | 1:A:396:VAL:HG22 | 0.42     | 1.90        | 20     | 1     |
| 1:A:282:CYS:O   | 1:A:283:ASP:CG   | 0.42     | 2.62        | 7      | 1     |
| 1:A:363:ASN:C   | 1:A:365:PRO:HD2  | 0.42     | 2.39        | 12     | 1     |
| 1:A:383:ALA:HB1 | 1:A:394:PHE:CE1  | 0.42     | 2.48        | 13     | 1     |
| 1:A:389:PHE:O   | 1:A:390:TYR:CG   | 0.42     | 2.72        | 14     | 2     |
| 1:A:431:ALA:CB  | 1:A:442:PHE:CE2  | 0.42     | 3.03        | 15     | 1     |
| 1:A:451:TYR:CD2 | 1:A:458:ILE:HG13 | 0.42     | 2.50        | 17     | 1     |
| 1:A:399:GLN:CB  | 1:A:416:LYS:O    | 0.42     | 2.67        | 20     | 1     |
| 1:A:333:GLU:CD  | 1:A:380:ILE:O    | 0.42     | 2.63        | 3      | 1     |
| 1:A:344:VAL:CG1 | 1:A:346:LEU:HD21 | 0.42     | 2.45        | 3      | 2     |
| 1:A:338:ILE:O   | 1:A:340:ALA:N    | 0.42     | 2.53        | 8      | 4     |
| 1:A:373:PHE:CE1 | 1:A:375:ASN:HA   | 0.42     | 2.50        | 4      | 1     |
| 1:A:281:LEU:O   | 1:A:468:PHE:CE2  | 0.42     | 2.72        | 5      | 1     |
| 1:A:354:LEU:O   | 1:A:360:PRO:CB   | 0.42     | 2.67        | 6      | 1     |
| 1:A:373:PHE:CE2 | 1:A:380:ILE:HG12 | 0.42     | 2.50        | 6      | 1     |
| 1:A:396:VAL:O   | 1:A:398:ASN:N    | 0.42     | 2.53        | 13     | 3     |
| 1:A:424:GLY:HA3 | 1:A:458:ILE:HD12 | 0.42     | 1.91        | 9      | 1     |
| 1:A:367:SER:O   | 1:A:370:SER:N    | 0.42     | 2.51        | 14     | 1     |
| 1:A:307:TRP:CD2 | 1:A:318:VAL:HB   | 0.42     | 2.50        | 17     | 1     |
| 1:A:337:GLU:HB3 | 1:A:344:VAL:HG12 | 0.42     | 1.92        | 20     | 1     |
| 1:A:343:GLN:CG  | 1:A:355:ILE:O    | 0.42     | 2.67        | 1      | 1     |
| 1:A:389:PHE:O   | 1:A:391:ARG:CG   | 0.42     | 2.67        | 11     | 1     |
| 1:A:455:LEU:O   | 1:A:456:GLN:NE2  | 0.42     | 2.53        | 11     | 1     |
| 1:A:307:TRP:CE2 | 1:A:316:THR:OG1  | 0.42     | 2.72        | 14     | 1     |
| 1:A:329:PRO:CB  | 1:A:348:LYS:HD3  | 0.42     | 2.44        | 16     | 1     |
| 1:A:442:PHE:CZ  | 1:A:449:PHE:HB3  | 0.42     | 2.49        | 20     | 1     |
| 1:A:396:VAL:O   | 1:A:397:ASP:CB   | 0.42     | 2.68        | 1      | 1     |

*Continued on next page...*

Continued from previous page...

| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:354:LEU:HD13 | 1:A:355:ILE:N    | 0.42     | 2.30        | 3      | 1     |
| 1:A:443:PHE:CE1  | 1:A:448:GLN:HB3  | 0.42     | 2.50        | 3      | 1     |
| 1:A:400:TYR:CD1  | 1:A:401:TRP:N    | 0.42     | 2.87        | 5      | 1     |
| 1:A:443:PHE:CD1  | 1:A:444:GLN:N    | 0.42     | 2.87        | 5      | 1     |
| 1:A:354:LEU:HD12 | 1:A:354:LEU:O    | 0.42     | 2.12        | 18     | 1     |
| 1:A:425:ILE:CG2  | 1:A:442:PHE:CD1  | 0.42     | 3.03        | 18     | 1     |
| 1:A:443:PHE:CZ   | 1:A:464:SER:HB2  | 0.42     | 2.49        | 18     | 1     |
| 1:A:368:ILE:O    | 1:A:370:SER:N    | 0.42     | 2.53        | 1      | 1     |
| 1:A:362:PRO:O    | 1:A:363:ASN:HB2  | 0.42     | 2.14        | 5      | 2     |
| 1:A:436:LYS:HD3  | 1:A:439:TYR:CD1  | 0.42     | 2.50        | 5      | 1     |
| 1:A:445:GLY:O    | 1:A:446:SER:C    | 0.42     | 2.62        | 6      | 3     |
| 1:A:303:ASP:C    | 1:A:304:ARG:HG2  | 0.42     | 2.40        | 8      | 1     |
| 1:A:301:PHE:CZ   | 1:A:306:PHE:CE1  | 0.42     | 3.08        | 9      | 1     |
| 1:A:410:MET:O    | 1:A:411:ASP:C    | 0.42     | 2.63        | 10     | 1     |
| 1:A:448:GLN:HG3  | 1:A:462:LEU:HD23 | 0.42     | 1.91        | 12     | 1     |
| 1:A:348:LYS:N    | 1:A:351:LYS:O    | 0.42     | 2.49        | 13     | 1     |
| 1:A:376:PHE:O    | 1:A:377:VAL:O    | 0.42     | 2.38        | 14     | 1     |
| 1:A:421:ASN:C    | 1:A:421:ASN:OD1  | 0.42     | 2.63        | 15     | 1     |
| 1:A:354:LEU:HD23 | 1:A:361:GLU:HG2  | 0.42     | 1.90        | 16     | 1     |
| 1:A:337:GLU:OE1  | 1:A:337:GLU:C    | 0.42     | 2.63        | 17     | 1     |
| 1:A:398:ASN:CG   | 1:A:398:ASN:O    | 0.42     | 2.59        | 19     | 1     |
| 1:A:332:ILE:HG12 | 1:A:346:LEU:HD12 | 0.42     | 1.90        | 2      | 1     |
| 1:A:455:LEU:HD11 | 1:A:457:ARG:HB2  | 0.42     | 1.91        | 5      | 1     |
| 1:A:386:ASN:CG   | 1:A:440:TYR:OH   | 0.42     | 2.63        | 6      | 1     |
| 1:A:469:GLY:O    | 1:A:470:CYS:SG   | 0.42     | 2.78        | 8      | 1     |
| 1:A:286:LEU:HD22 | 1:A:288:PHE:CZ   | 0.42     | 2.50        | 10     | 1     |
| 1:A:307:TRP:CD1  | 1:A:318:VAL:HG22 | 0.42     | 2.50        | 12     | 1     |
| 1:A:380:ILE:HG22 | 1:A:381:ASP:H    | 0.42     | 1.75        | 15     | 1     |
| 1:A:419:THR:OG1  | 1:A:426:GLY:C    | 0.42     | 2.63        | 15     | 1     |
| 1:A:367:SER:O    | 1:A:368:ILE:C    | 0.41     | 2.64        | 18     | 2     |
| 1:A:385:PHE:CG   | 1:A:386:ASN:N    | 0.41     | 2.87        | 2      | 1     |
| 1:A:352:TYR:CD1  | 1:A:352:TYR:O    | 0.41     | 2.73        | 3      | 2     |
| 1:A:399:GLN:O    | 1:A:418:ILE:CD1  | 0.41     | 2.68        | 10     | 1     |
| 1:A:422:PHE:CB   | 1:A:425:ILE:HD11 | 0.41     | 2.45        | 11     | 1     |
| 1:A:369:HIS:HB2  | 1:A:373:PHE:CG   | 0.41     | 2.50        | 12     | 1     |
| 1:A:468:PHE:CE1  | 1:A:470:CYS:HB2  | 0.41     | 2.50        | 20     | 2     |
| 1:A:450:GLU:OE1  | 1:A:450:GLU:C    | 0.41     | 2.63        | 15     | 1     |
| 1:A:381:ASP:O    | 1:A:430:ASP:O    | 0.41     | 2.38        | 17     | 1     |
| 1:A:419:THR:O    | 1:A:423:GLN:CD   | 0.41     | 2.63        | 17     | 1     |
| 1:A:300:PHE:CD1  | 1:A:301:PHE:N    | 0.41     | 2.88        | 18     | 1     |
| 1:A:422:PHE:CE1  | 1:A:451:TYR:CE2  | 0.41     | 3.08        | 18     | 1     |

Continued on next page...

*Continued from previous page...*

| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:433:PHE:CE1  | 1:A:441:TYR:HB3  | 0.41     | 2.50        | 18     | 1     |
| 1:A:338:ILE:O    | 1:A:338:ILE:HG23 | 0.41     | 2.15        | 3      | 1     |
| 1:A:377:VAL:O    | 1:A:378:LYS:CB   | 0.41     | 2.68        | 3      | 1     |
| 1:A:424:GLY:H    | 1:A:425:ILE:HD13 | 0.41     | 1.75        | 10     | 2     |
| 1:A:343:GLN:OE1  | 1:A:345:PHE:CE1  | 0.41     | 2.72        | 8      | 1     |
| 1:A:356:SER:N    | 1:A:359:ARG:O    | 0.41     | 2.52        | 10     | 1     |
| 1:A:350:ASP:CG   | 1:A:350:ASP:O    | 0.41     | 2.62        | 12     | 1     |
| 1:A:281:LEU:HB3  | 1:A:468:PHE:CE2  | 0.41     | 2.50        | 16     | 1     |
| 1:A:357:ASN:O    | 1:A:358:LEU:CG   | 0.41     | 2.68        | 16     | 1     |
| 1:A:436:LYS:HG3  | 1:A:441:TYR:CE1  | 0.41     | 2.50        | 2      | 1     |
| 1:A:302:LYS:O    | 1:A:303:ASP:C    | 0.41     | 2.63        | 20     | 2     |
| 1:A:413:GLY:O    | 1:A:414:TYR:C    | 0.41     | 2.63        | 6      | 1     |
| 1:A:425:ILE:HG12 | 1:A:442:PHE:CD2  | 0.41     | 2.50        | 9      | 1     |
| 1:A:289:ASP:CG   | 1:A:302:LYS:O    | 0.41     | 2.63        | 11     | 1     |
| 1:A:322:SER:O    | 1:A:325:TRP:O    | 0.41     | 2.38        | 15     | 1     |
| 1:A:296:ASN:OD1  | 1:A:296:ASN:N    | 0.41     | 2.53        | 16     | 1     |
| 1:A:391:ARG:HG2  | 1:A:392:THR:N    | 0.41     | 2.30        | 20     | 1     |
| 1:A:462:LEU:CB   | 1:A:466:SER:HB3  | 0.41     | 2.45        | 7      | 1     |
| 1:A:349:ASP:O    | 1:A:378:LYS:O    | 0.41     | 2.39        | 10     | 1     |
| 1:A:358:LEU:O    | 1:A:358:LEU:HD12 | 0.41     | 2.16        | 12     | 1     |
| 1:A:351:LYS:CB   | 1:A:366:LYS:O    | 0.41     | 2.69        | 13     | 1     |
| 1:A:307:TRP:CE3  | 1:A:307:TRP:HA   | 0.41     | 2.51        | 15     | 1     |
| 1:A:354:LEU:N    | 1:A:354:LEU:HD13 | 0.41     | 2.31        | 15     | 1     |
| 1:A:393:TYR:CE1  | 1:A:402:ARG:NE   | 0.41     | 2.88        | 16     | 1     |
| 1:A:439:TYR:CD1  | 1:A:450:GLU:CD   | 0.41     | 2.98        | 16     | 1     |
| 1:A:363:ASN:C    | 1:A:365:PRO:HD3  | 0.41     | 2.41        | 16     | 3     |
| 1:A:432:VAL:CG2  | 1:A:442:PHE:CD2  | 0.41     | 3.04        | 5      | 1     |
| 1:A:352:TYR:CE2  | 1:A:366:LYS:HB3  | 0.41     | 2.50        | 11     | 1     |
| 1:A:372:GLY:O    | 1:A:373:PHE:CD1  | 0.41     | 2.73        | 20     | 1     |
| 1:A:432:VAL:HG23 | 1:A:442:PHE:CE1  | 0.41     | 2.48        | 1      | 1     |
| 1:A:374:PRO:O    | 1:A:375:ASN:C    | 0.41     | 2.63        | 2      | 1     |
| 1:A:364:TYR:CZ   | 1:A:366:LYS:HE3  | 0.41     | 2.49        | 3      | 1     |
| 1:A:442:PHE:HB2  | 1:A:451:TYR:CE1  | 0.41     | 2.50        | 13     | 1     |
| 1:A:433:PHE:O    | 1:A:433:PHE:CG   | 0.41     | 2.73        | 18     | 1     |
| 1:A:389:PHE:CD2  | 1:A:402:ARG:NH1  | 0.41     | 2.88        | 19     | 1     |
| 1:A:330:SER:O    | 1:A:332:ILE:N    | 0.41     | 2.54        | 20     | 1     |
| 1:A:453:PHE:O    | 1:A:453:PHE:CD1  | 0.41     | 2.73        | 1      | 1     |
| 1:A:421:ASN:OD1  | 1:A:421:ASN:C    | 0.41     | 2.63        | 5      | 1     |
| 1:A:430:ASP:OD1  | 1:A:430:ASP:N    | 0.41     | 2.54        | 7      | 1     |
| 1:A:321:ILE:HD12 | 1:A:330:SER:HB3  | 0.41     | 1.93        | 10     | 1     |
| 1:A:354:LEU:CD2  | 1:A:361:GLU:CG   | 0.41     | 2.99        | 16     | 1     |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:339:GLU:C    | 1:A:341:ARG:N    | 0.41     | 2.77        | 18     | 1     |
| 1:A:305:PHE:CD2  | 1:A:318:VAL:HB   | 0.41     | 2.50        | 19     | 1     |
| 1:A:321:ILE:O    | 1:A:323:SER:N    | 0.41     | 2.53        | 2      | 1     |
| 1:A:396:VAL:CG1  | 1:A:401:TRP:CZ3  | 0.41     | 3.03        | 5      | 1     |
| 1:A:287:SER:O    | 1:A:302:LYS:CE   | 0.41     | 2.68        | 6      | 1     |
| 1:A:352:TYR:CE2  | 1:A:368:ILE:HG22 | 0.41     | 2.51        | 6      | 1     |
| 1:A:368:ILE:O    | 1:A:373:PHE:N    | 0.41     | 2.54        | 6      | 1     |
| 1:A:436:LYS:HD3  | 1:A:441:TYR:CD1  | 0.41     | 2.50        | 7      | 1     |
| 1:A:332:ILE:CG2  | 1:A:346:LEU:HD12 | 0.41     | 2.45        | 11     | 1     |
| 1:A:419:THR:O    | 1:A:423:GLN:CG   | 0.41     | 2.69        | 11     | 1     |
| 1:A:398:ASN:O    | 1:A:398:ASN:OD1  | 0.41     | 2.38        | 17     | 1     |
| 1:A:305:PHE:CB   | 1:A:307:TRP:CH2  | 0.41     | 3.04        | 18     | 1     |
| 1:A:302:LYS:O    | 1:A:305:PHE:N    | 0.41     | 2.54        | 1      | 1     |
| 1:A:286:LEU:CD2  | 1:A:307:TRP:CH2  | 0.41     | 3.04        | 2      | 1     |
| 1:A:467:TRP:CE3  | 1:A:467:TRP:HA   | 0.41     | 2.50        | 4      | 1     |
| 1:A:281:LEU:HB3  | 1:A:468:PHE:CD2  | 0.41     | 2.50        | 5      | 1     |
| 1:A:424:GLY:HA3  | 1:A:458:ILE:CD1  | 0.41     | 2.46        | 8      | 1     |
| 1:A:306:PHE:O    | 1:A:319:ASN:O    | 0.41     | 2.38        | 9      | 1     |
| 1:A:436:LYS:HE2  | 1:A:441:TYR:CE1  | 0.41     | 2.51        | 9      | 1     |
| 1:A:306:PHE:CE1  | 1:A:319:ASN:HB2  | 0.41     | 2.51        | 10     | 1     |
| 1:A:329:PRO:HG3  | 1:A:353:TRP:CH2  | 0.41     | 2.51        | 10     | 1     |
| 1:A:328:LEU:CD1  | 1:A:329:PRO:HD2  | 0.41     | 2.46        | 11     | 1     |
| 1:A:282:CYS:CA   | 1:A:470:CYS:SG   | 0.41     | 3.08        | 13     | 1     |
| 1:A:349:ASP:O    | 1:A:350:ASP:CB   | 0.41     | 2.68        | 13     | 1     |
| 1:A:452:ASP:C    | 1:A:454:LEU:N    | 0.41     | 2.76        | 13     | 1     |
| 1:A:350:ASP:C    | 1:A:351:LYS:HG3  | 0.41     | 2.41        | 15     | 1     |
| 1:A:374:PRO:HD2  | 1:A:377:VAL:CG1  | 0.41     | 2.45        | 16     | 1     |
| 1:A:445:GLY:C    | 1:A:447:ASN:N    | 0.41     | 2.75        | 16     | 1     |
| 1:A:393:TYR:CE1  | 1:A:402:ARG:NH1  | 0.41     | 2.89        | 19     | 1     |
| 1:A:350:ASP:O    | 1:A:350:ASP:OD2  | 0.41     | 2.39        | 20     | 1     |
| 1:A:399:GLN:CG   | 1:A:416:LYS:O    | 0.41     | 2.69        | 20     | 1     |
| 1:A:395:PHE:CE1  | 1:A:432:VAL:HG11 | 0.41     | 2.50        | 2      | 1     |
| 1:A:290:ALA:O    | 1:A:291:VAL:HG13 | 0.41     | 2.15        | 10     | 1     |
| 1:A:304:ARG:O    | 1:A:320:LEU:CD1  | 0.41     | 2.66        | 20     | 1     |
| 1:A:338:ILE:C    | 1:A:338:ILE:CD1  | 0.40     | 2.94        | 5      | 1     |
| 1:A:450:GLU:OE1  | 1:A:451:TYR:O    | 0.40     | 2.40        | 14     | 1     |
| 1:A:368:ILE:HD11 | 1:A:377:VAL:HG21 | 0.40     | 1.93        | 9      | 1     |
| 1:A:286:LEU:CD2  | 1:A:288:PHE:CE2  | 0.40     | 3.05        | 10     | 1     |
| 1:A:357:ASN:C    | 1:A:359:ARG:N    | 0.40     | 2.77        | 10     | 1     |
| 1:A:334:ALA:HB3  | 1:A:347:PHE:HB2  | 0.40     | 1.91        | 11     | 1     |
| 1:A:402:ARG:HB3  | 1:A:402:ARG:CZ   | 0.40     | 2.46        | 11     | 1     |

*Continued on next page...*

Continued from previous page...

| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:344:VAL:HG12 | 1:A:346:LEU:HD23 | 0.40     | 1.93        | 14     | 1     |
| 1:A:462:LEU:HG   | 1:A:463:LYS:N    | 0.40     | 2.32        | 15     | 1     |
| 1:A:308:LEU:HD23 | 1:A:317:SER:CB   | 0.40     | 2.46        | 16     | 1     |
| 1:A:299:PHE:CZ   | 1:A:308:LEU:HD11 | 0.40     | 2.51        | 20     | 1     |
| 1:A:400:TYR:CZ   | 1:A:416:LYS:HB2  | 0.40     | 2.51        | 20     | 1     |
| 1:A:433:PHE:CG   | 1:A:434:TYR:N    | 0.40     | 2.89        | 6      | 1     |
| 1:A:383:ALA:CB   | 1:A:394:PHE:CE1  | 0.40     | 3.05        | 13     | 1     |
| 1:A:432:VAL:HA   | 1:A:442:PHE:CG   | 0.40     | 2.51        | 15     | 1     |
| 1:A:452:ASP:OD1  | 1:A:454:LEU:CB   | 0.40     | 2.69        | 18     | 1     |
| 1:A:345:PHE:CE1  | 1:A:354:LEU:HD13 | 0.40     | 2.50        | 20     | 1     |
| 1:A:434:TYR:CD1  | 1:A:434:TYR:C    | 0.40     | 2.99        | 3      | 1     |
| 1:A:296:ASN:ND2  | 1:A:296:ASN:O    | 0.40     | 2.55        | 4      | 1     |
| 1:A:330:SER:C    | 1:A:332:ILE:N    | 0.40     | 2.78        | 5      | 1     |
| 1:A:337:GLU:OE2  | 1:A:338:ILE:C    | 0.40     | 2.64        | 14     | 1     |
| 1:A:291:VAL:O    | 1:A:335:ALA:O    | 0.40     | 2.40        | 15     | 1     |
| 1:A:445:GLY:O    | 1:A:446:SER:CB   | 0.40     | 2.68        | 15     | 1     |
| 1:A:303:ASP:O    | 1:A:304:ARG:HB2  | 0.40     | 2.17        | 16     | 2     |
| 1:A:429:ILE:HD11 | 1:A:442:PHE:CG   | 0.40     | 2.51        | 16     | 1     |
| 1:A:462:LEU:HD12 | 1:A:466:SER:HB2  | 0.40     | 1.92        | 16     | 1     |
| 1:A:290:ALA:HA   | 1:A:431:ALA:HB2  | 0.40     | 1.93        | 17     | 1     |
| 1:A:298:ILE:O    | 1:A:308:LEU:HD12 | 0.40     | 2.15        | 18     | 1     |
| 1:A:439:TYR:CD2  | 1:A:452:ASP:OD1  | 0.40     | 2.74        | 20     | 1     |
| 1:A:298:ILE:HD12 | 1:A:300:PHE:CE2  | 0.40     | 2.52        | 10     | 1     |
| 1:A:294:VAL:HG23 | 1:A:297:LYS:CB   | 0.40     | 2.45        | 14     | 1     |
| 1:A:364:TYR:CD2  | 1:A:366:LYS:HG2  | 0.40     | 2.51        | 14     | 1     |
| 1:A:432:VAL:HG23 | 1:A:440:TYR:CE1  | 0.40     | 2.51        | 15     | 1     |
| 1:A:300:PHE:CE1  | 1:A:301:PHE:O    | 0.40     | 2.75        | 18     | 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     | 189/194 (97%)   | 138±5 (73±3%) | 38±5 (20±3%) | 13±3 (7±1%) | 2           | 16 |
| All | All   | 3780/3880 (97%) | 2753 (73%)    | 767 (20%)    | 260 (7%)    | 2           | 16 |

All 48 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     | 326 | PRO  | 20             |
| 1   | A     | 378 | LYS  | 16             |
| 1   | A     | 413 | GLY  | 15             |
| 1   | A     | 455 | LEU  | 14             |
| 1   | A     | 303 | ASP  | 13             |
| 1   | A     | 311 | SER  | 12             |
| 1   | A     | 372 | GLY  | 12             |
| 1   | A     | 436 | LYS  | 11             |
| 1   | A     | 373 | PHE  | 10             |
| 1   | A     | 282 | CYS  | 10             |
| 1   | A     | 285 | ASN  | 9              |
| 1   | A     | 310 | VAL  | 9              |
| 1   | A     | 376 | PHE  | 9              |
| 1   | A     | 371 | PHE  | 8              |
| 1   | A     | 374 | PRO  | 8              |
| 1   | A     | 425 | ILE  | 7              |
| 1   | A     | 438 | LYS  | 6              |
| 1   | A     | 363 | ASN  | 6              |
| 1   | A     | 467 | TRP  | 6              |
| 1   | A     | 377 | VAL  | 5              |
| 1   | A     | 295 | GLY  | 4              |
| 1   | A     | 332 | ILE  | 4              |
| 1   | A     | 419 | THR  | 3              |
| 1   | A     | 446 | SER  | 3              |
| 1   | A     | 321 | ILE  | 3              |
| 1   | A     | 412 | PRO  | 3              |
| 1   | A     | 375 | ASN  | 3              |
| 1   | A     | 358 | LEU  | 3              |
| 1   | A     | 418 | ILE  | 2              |
| 1   | A     | 342 | ASN  | 2              |
| 1   | A     | 408 | GLN  | 2              |
| 1   | A     | 397 | ASP  | 2              |
| 1   | A     | 468 | PHE  | 2              |
| 1   | A     | 331 | GLY  | 2              |
| 1   | A     | 389 | PHE  | 2              |
| 1   | A     | 465 | ASN  | 2              |
| 1   | A     | 430 | ASP  | 1              |
| 1   | A     | 314 | PRO  | 1              |
| 1   | A     | 456 | GLN  | 1              |
| 1   | A     | 302 | LYS  | 1              |
| 1   | A     | 432 | VAL  | 1              |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 349 | ASP  | 1              |
| 1   | A     | 330 | SER  | 1              |
| 1   | A     | 350 | ASP  | 1              |
| 1   | A     | 294 | VAL  | 1              |
| 1   | A     | 340 | ALA  | 1              |
| 1   | A     | 312 | GLU  | 1              |
| 1   | A     | 359 | ARG  | 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     | 175/178 (98%)   | 129±4 (74±2%) | 46±4 (26±2%) | 2           | 23 |
| All | All   | 3500/3560 (98%) | 2589 (74%)    | 911 (26%)    | 2           | 23 |

All 140 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     | 378 | LYS  | 19             |
| 1   | A     | 354 | LEU  | 17             |
| 1   | A     | 358 | LEU  | 17             |
| 1   | A     | 460 | LYS  | 17             |
| 1   | A     | 285 | ASN  | 16             |
| 1   | A     | 304 | ARG  | 16             |
| 1   | A     | 417 | LEU  | 16             |
| 1   | A     | 438 | LYS  | 15             |
| 1   | A     | 302 | LYS  | 14             |
| 1   | A     | 348 | LYS  | 14             |
| 1   | A     | 366 | LYS  | 14             |
| 1   | A     | 428 | LYS  | 14             |
| 1   | A     | 320 | LEU  | 13             |
| 1   | A     | 404 | ASP  | 13             |
| 1   | A     | 463 | LYS  | 13             |
| 1   | A     | 470 | CYS  | 13             |
| 1   | A     | 317 | SER  | 13             |
| 1   | A     | 308 | LEU  | 12             |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 407 | ARG  | 12             |
| 1   | A     | 411 | ASP  | 12             |
| 1   | A     | 397 | ASP  | 12             |
| 1   | A     | 313 | ARG  | 11             |
| 1   | A     | 325 | TRP  | 11             |
| 1   | A     | 381 | ASP  | 11             |
| 1   | A     | 408 | GLN  | 11             |
| 1   | A     | 436 | LYS  | 11             |
| 1   | A     | 443 | PHE  | 11             |
| 1   | A     | 339 | GLU  | 11             |
| 1   | A     | 369 | HIS  | 11             |
| 1   | A     | 410 | MET  | 11             |
| 1   | A     | 337 | GLU  | 11             |
| 1   | A     | 289 | ASP  | 10             |
| 1   | A     | 323 | SER  | 10             |
| 1   | A     | 364 | TYR  | 10             |
| 1   | A     | 450 | GLU  | 10             |
| 1   | A     | 425 | ILE  | 10             |
| 1   | A     | 286 | LEU  | 9              |
| 1   | A     | 315 | LYS  | 9              |
| 1   | A     | 430 | ASP  | 9              |
| 1   | A     | 447 | ASN  | 9              |
| 1   | A     | 448 | GLN  | 9              |
| 1   | A     | 457 | ARG  | 9              |
| 1   | A     | 379 | LYS  | 9              |
| 1   | A     | 282 | CYS  | 9              |
| 1   | A     | 309 | LYS  | 8              |
| 1   | A     | 371 | PHE  | 8              |
| 1   | A     | 386 | ASN  | 8              |
| 1   | A     | 399 | GLN  | 8              |
| 1   | A     | 321 | ILE  | 8              |
| 1   | A     | 370 | SER  | 8              |
| 1   | A     | 281 | LEU  | 8              |
| 1   | A     | 319 | ASN  | 7              |
| 1   | A     | 324 | LEU  | 7              |
| 1   | A     | 367 | SER  | 7              |
| 1   | A     | 388 | ARG  | 7              |
| 1   | A     | 389 | PHE  | 7              |
| 1   | A     | 435 | SER  | 7              |
| 1   | A     | 283 | ASP  | 7              |
| 1   | A     | 359 | ARG  | 7              |
| 1   | A     | 328 | LEU  | 6              |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 333 | GLU  | 6              |
| 1   | A     | 338 | ILE  | 6              |
| 1   | A     | 462 | LEU  | 6              |
| 1   | A     | 464 | SER  | 6              |
| 1   | A     | 405 | GLU  | 6              |
| 1   | A     | 406 | ARG  | 6              |
| 1   | A     | 444 | GLN  | 6              |
| 1   | A     | 341 | ARG  | 6              |
| 1   | A     | 297 | LYS  | 6              |
| 1   | A     | 357 | ASN  | 6              |
| 1   | A     | 429 | ILE  | 6              |
| 1   | A     | 310 | VAL  | 6              |
| 1   | A     | 312 | GLU  | 5              |
| 1   | A     | 330 | SER  | 5              |
| 1   | A     | 343 | GLN  | 5              |
| 1   | A     | 466 | SER  | 5              |
| 1   | A     | 361 | GLU  | 5              |
| 1   | A     | 409 | MET  | 5              |
| 1   | A     | 455 | LEU  | 5              |
| 1   | A     | 303 | ASP  | 5              |
| 1   | A     | 363 | ASN  | 5              |
| 1   | A     | 376 | PHE  | 5              |
| 1   | A     | 327 | THR  | 5              |
| 1   | A     | 322 | SER  | 5              |
| 1   | A     | 377 | VAL  | 4              |
| 1   | A     | 346 | LEU  | 4              |
| 1   | A     | 351 | LYS  | 4              |
| 1   | A     | 419 | THR  | 4              |
| 1   | A     | 292 | THR  | 4              |
| 1   | A     | 368 | ILE  | 4              |
| 1   | A     | 467 | TRP  | 4              |
| 1   | A     | 418 | ILE  | 4              |
| 1   | A     | 423 | GLN  | 4              |
| 1   | A     | 349 | ASP  | 4              |
| 1   | A     | 400 | TYR  | 4              |
| 1   | A     | 311 | SER  | 4              |
| 1   | A     | 307 | TRP  | 3              |
| 1   | A     | 402 | ARG  | 3              |
| 1   | A     | 375 | ASN  | 3              |
| 1   | A     | 446 | SER  | 3              |
| 1   | A     | 336 | TYR  | 3              |
| 1   | A     | 355 | ILE  | 3              |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 332 | ILE  | 3              |
| 1   | A     | 345 | PHE  | 3              |
| 1   | A     | 401 | TRP  | 3              |
| 1   | A     | 356 | SER  | 3              |
| 1   | A     | 298 | ILE  | 3              |
| 1   | A     | 391 | ARG  | 3              |
| 1   | A     | 394 | PHE  | 2              |
| 1   | A     | 421 | ASN  | 2              |
| 1   | A     | 432 | VAL  | 2              |
| 1   | A     | 468 | PHE  | 2              |
| 1   | A     | 342 | ASN  | 2              |
| 1   | A     | 352 | TYR  | 2              |
| 1   | A     | 461 | THR  | 2              |
| 1   | A     | 300 | PHE  | 2              |
| 1   | A     | 416 | LYS  | 2              |
| 1   | A     | 291 | VAL  | 2              |
| 1   | A     | 384 | VAL  | 2              |
| 1   | A     | 396 | VAL  | 1              |
| 1   | A     | 353 | TRP  | 1              |
| 1   | A     | 380 | ILE  | 1              |
| 1   | A     | 442 | PHE  | 1              |
| 1   | A     | 287 | SER  | 1              |
| 1   | A     | 305 | PHE  | 1              |
| 1   | A     | 347 | PHE  | 1              |
| 1   | A     | 456 | GLN  | 1              |
| 1   | A     | 350 | ASP  | 1              |
| 1   | A     | 459 | THR  | 1              |
| 1   | A     | 296 | ASN  | 1              |
| 1   | A     | 293 | THR  | 1              |
| 1   | A     | 433 | PHE  | 1              |
| 1   | A     | 440 | TYR  | 1              |
| 1   | A     | 441 | TYR  | 1              |
| 1   | A     | 301 | PHE  | 1              |
| 1   | A     | 452 | ASP  | 1              |
| 1   | A     | 437 | ASN  | 1              |
| 1   | A     | 318 | VAL  | 1              |
| 1   | A     | 414 | TYR  | 1              |
| 1   | A     | 458 | ILE  | 1              |

### 6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.6 Ligand geometry [i](#)

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

## 6.7 Other polymers [i](#)

There are no such molecules in this entry.

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

There are no chain breaks in this entry.

## 7 Chemical shift validation

No chemical shift data were provided