



# Full wwPDB NMR Structure Validation Report ⓘ

Mar 15, 2026 – 01:53 PM UTC

PDB ID : 1ULP / pdb\_00001ulp  
Title : N-TERMINAL CELLULOSE-BINDING DOMAIN FROM CELLULOMONAS FIMI BETA-1,4-GLUCANASE C, NMR, 25 STRUCTURES  
Authors : Johnson, P.E.; McIntosh, L.P.  
Deposited on : 1996-07-27

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>.

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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

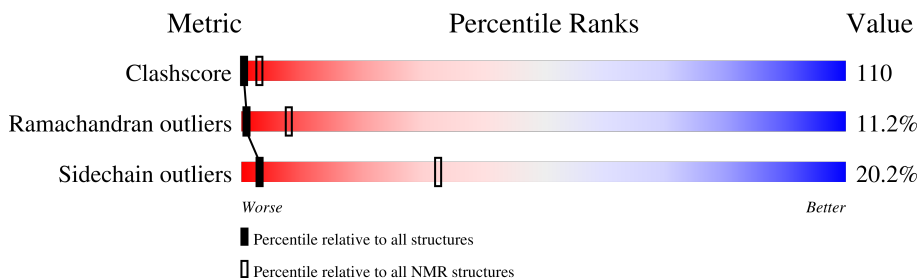
# 1 Overall quality at a glance i

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 (#Entries) | NMR archive (#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     | 152    |                  |

## 2 Ensemble composition and analysis i

This entry contains 25 models. Model 24 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:3-A:114, A:122-A:148<br>(139) | 0.93              | 24           |

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 6 clusters and 2 single-model clusters were found.

| Cluster number        | Models                           |
|-----------------------|----------------------------------|
| 1                     | 2, 8, 10, 11, 13, 19, 20, 23, 24 |
| 2                     | 3, 7, 14, 16, 25                 |
| 3                     | 17, 18, 21                       |
| 4                     | 4, 6                             |
| 5                     | 1, 22                            |
| 6                     | 5, 15                            |
| Single-model clusters | 9; 12                            |

### 3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2105 atoms, of which 1018 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called ENDOGLUCANASE C.

| Mol | Chain | Residues | Atoms |     |      |     |     |   | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|-------|
|     |       |          | Total | C   | H    | N   | O   | S |       |
| 1   | A     | 152      | 2105  | 678 | 1018 | 170 | 237 | 2 | 0     |

There is a discrepancy between the modelled and reference sequences:

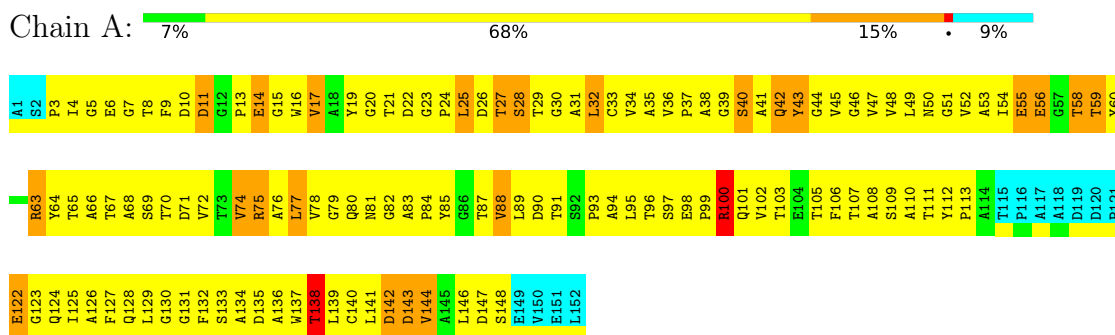
| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| A     | 139     | LEU      | PHE    | conflict | UNP P14090 |

## 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: ENDOGLUCANASE C

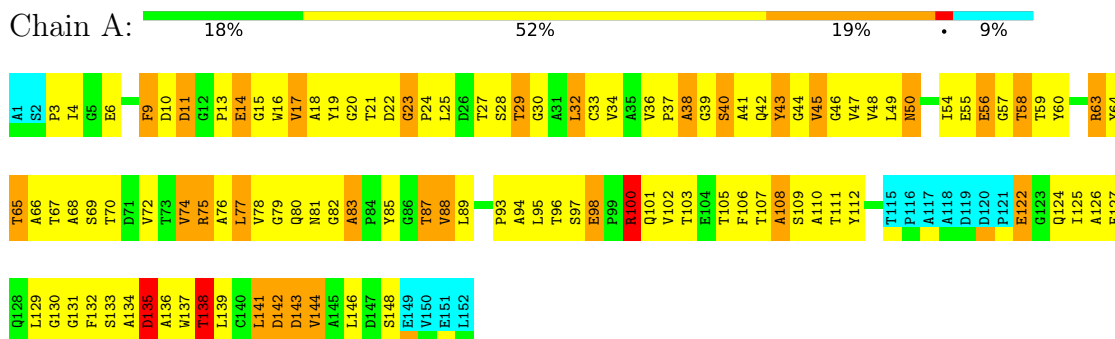


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

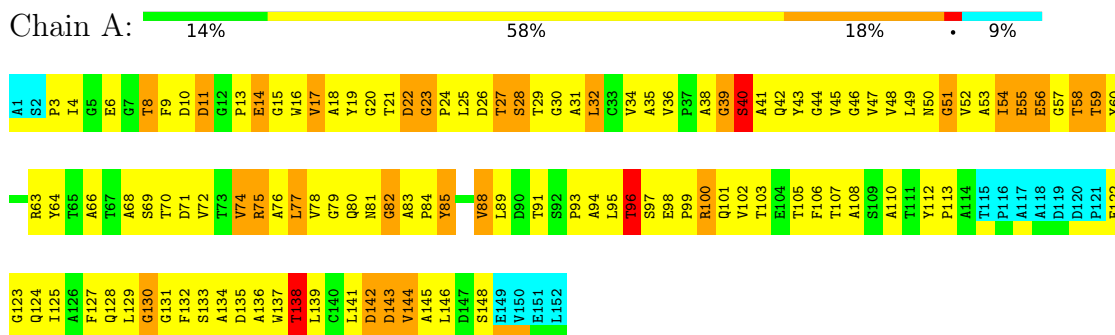
#### 4.2.1 Score per residue for model 1

- Molecule 1: ENDOGLUCANASE C



### 4.2.2 Score per residue for model 2

- Molecule 1: ENDOGLUCANASE C



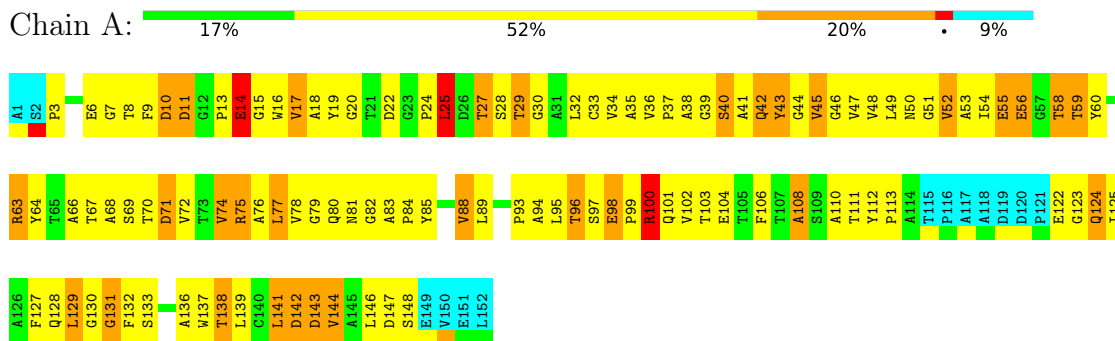
### 4.2.3 Score per residue for model 3

- Molecule 1: ENDOGLUCANASE C



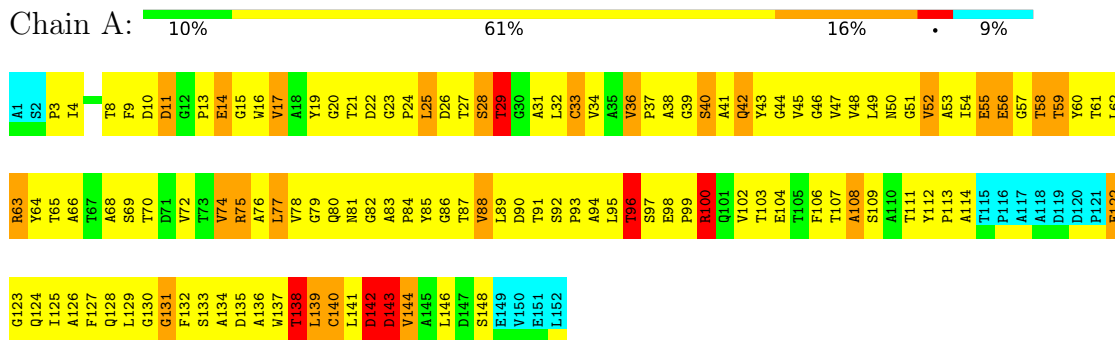
### 4.2.4 Score per residue for model 4

- Molecule 1: ENDOGLUCANASE C



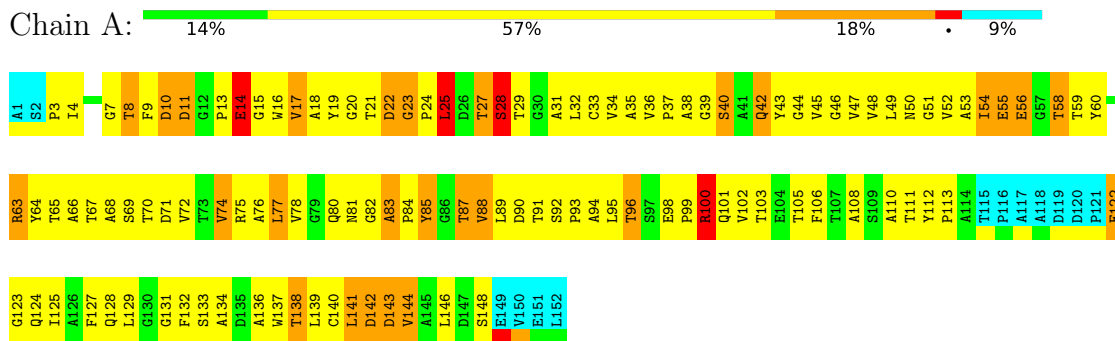
### 4.2.5 Score per residue for model 5

- Molecule 1: ENDOGLUCANASE C



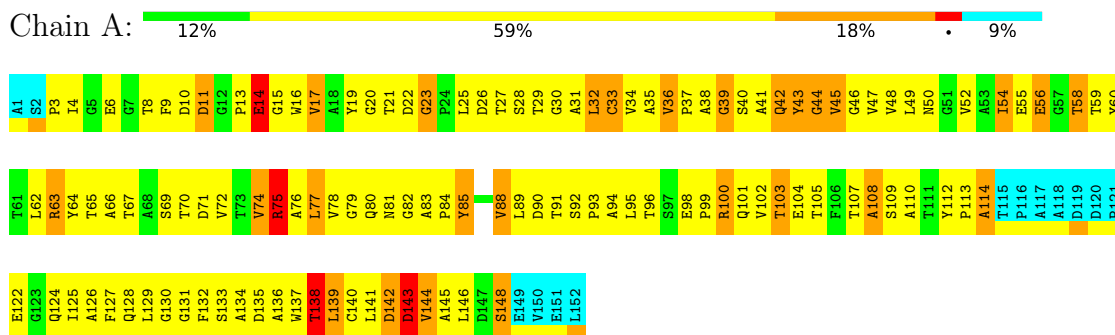
#### 4.2.6 Score per residue for model 6

- Molecule 1: ENDOGLUCANASE C



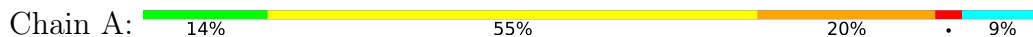
#### 4.2.7 Score per residue for model 7

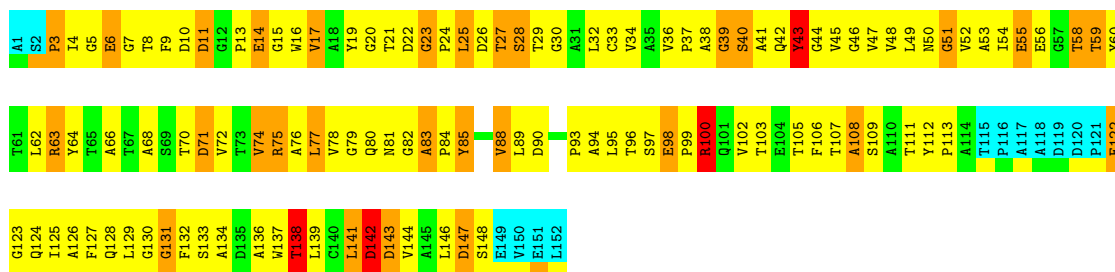
- Molecule 1: ENDOGLUCANASE C



#### 4.2.8 Score per residue for model 8

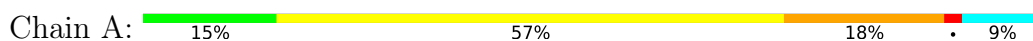
- Molecule 1: ENDOGLUCANASE C





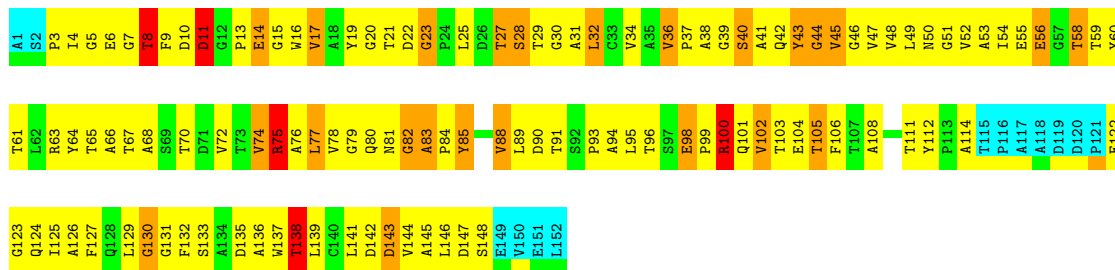
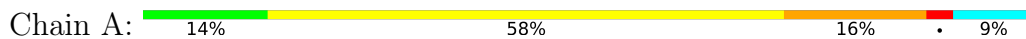
#### 4.2.9 Score per residue for model 9

- Molecule 1: ENDOGLUCANASE C



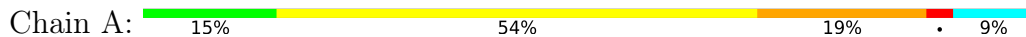
#### 4.2.10 Score per residue for model 10

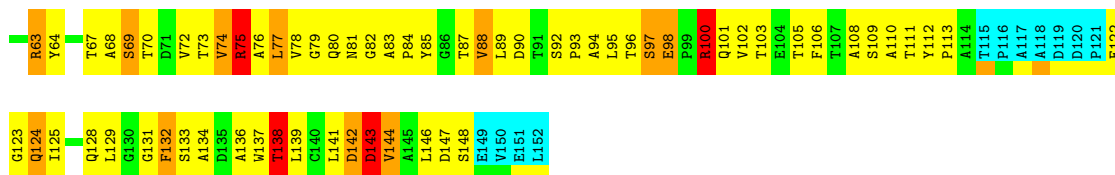
- Molecule 1: ENDOGLUCANASE C



#### 4.2.11 Score per residue for model 11

- Molecule 1: ENDOGLUCANASE C

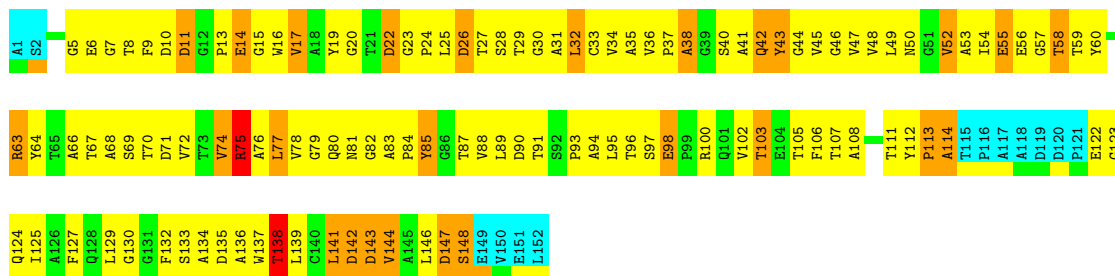




#### 4.2.12 Score per residue for model 12

- Molecule 1: ENDOGLUCANASE C

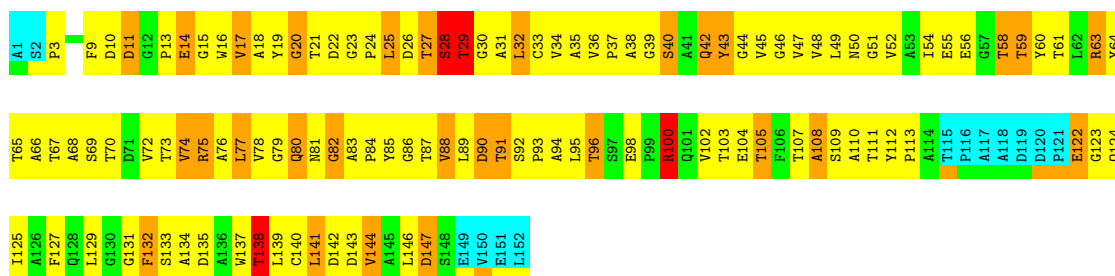
Chain A: 15% 58% 17% 9%



#### 4.2.13 Score per residue for model 13

- Molecule 1: ENDOGLUCANASE C

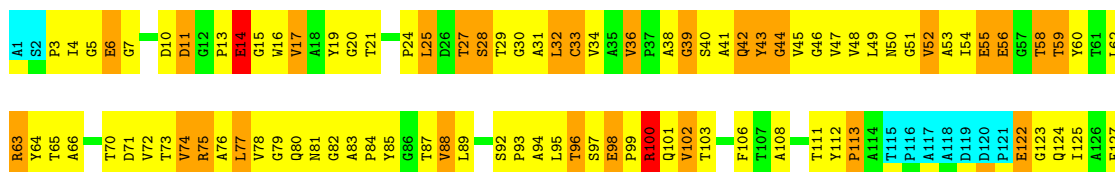
Chain A: 14% 55% 19% 9%



#### 4.2.14 Score per residue for model 14

- Molecule 1: ENDOGLUCANASE C

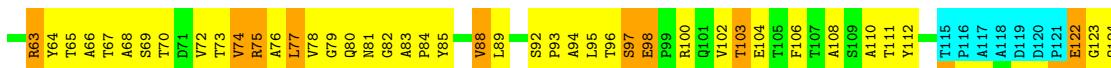
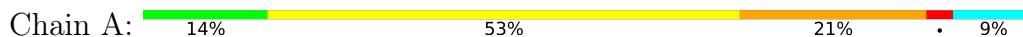
Chain A: 17% 50% 21% 9%





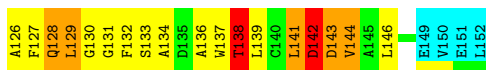
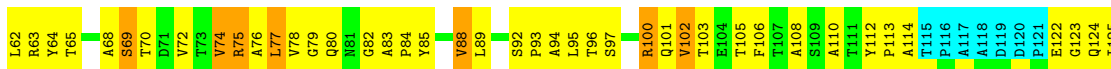
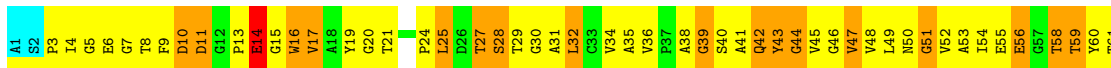
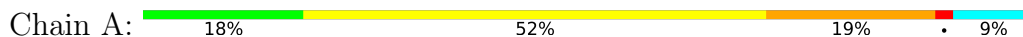
#### 4.2.15 Score per residue for model 15

- Molecule 1: ENDOGLUCANASE C



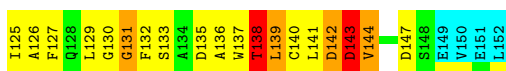
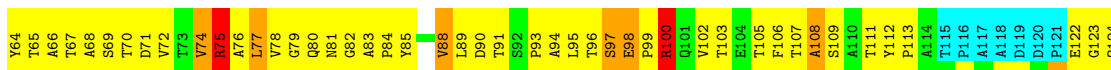
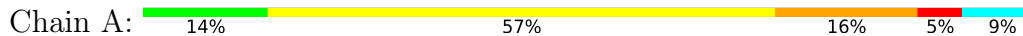
#### 4.2.16 Score per residue for model 16

- Molecule 1: ENDOGLUCANASE C



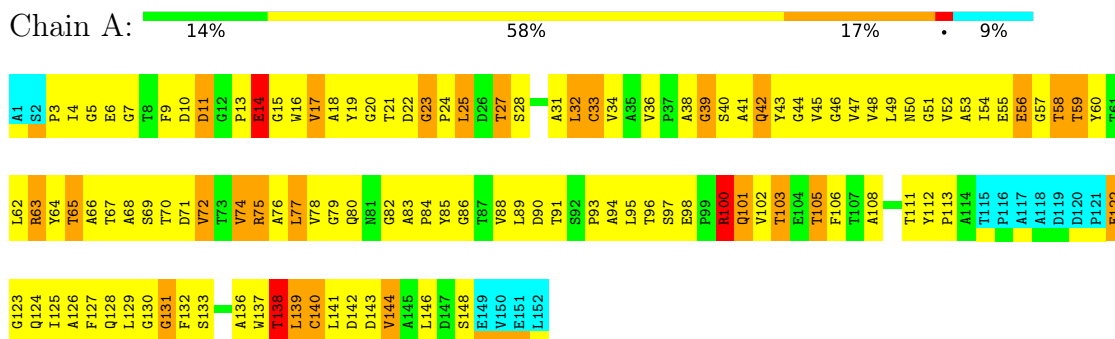
#### 4.2.17 Score per residue for model 17

- Molecule 1: ENDOGLUCANASE C



## 4.2.18 Score per residue for model 18

- Molecule 1: ENDOGLUCANASE C



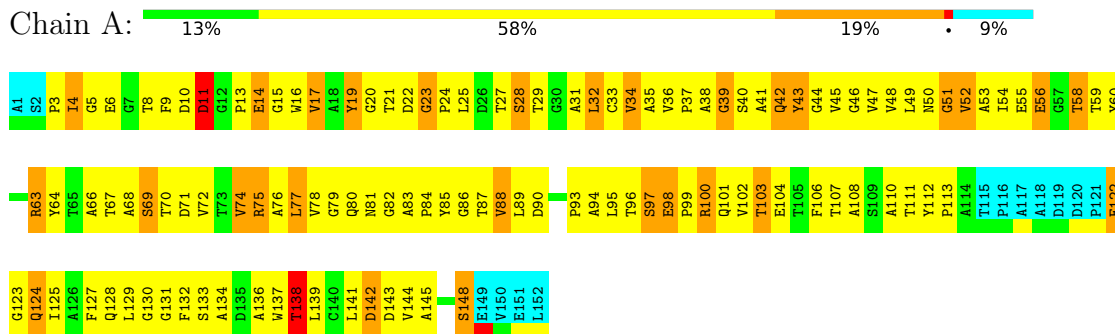
## 4.2.19 Score per residue for model 19

- Molecule 1: ENDOGLUCANASE C



## 4.2.20 Score per residue for model 20

- Molecule 1: ENDOGLUCANASE C



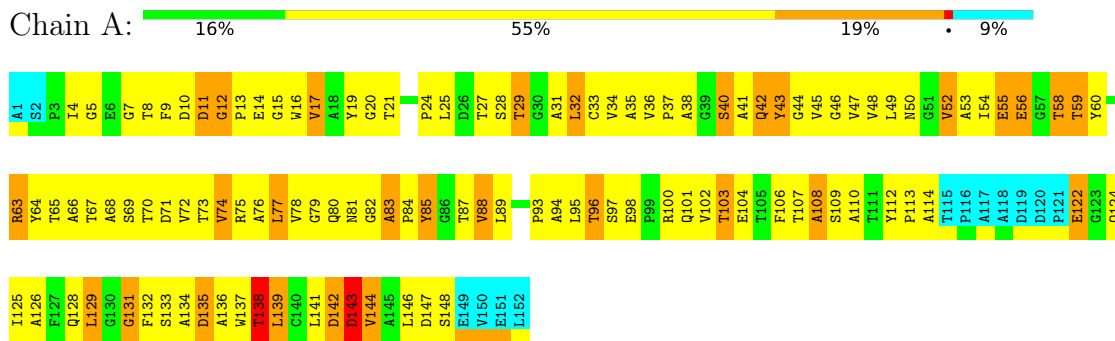
## 4.2.21 Score per residue for model 21

- Molecule 1: ENDOGLUCANASE C



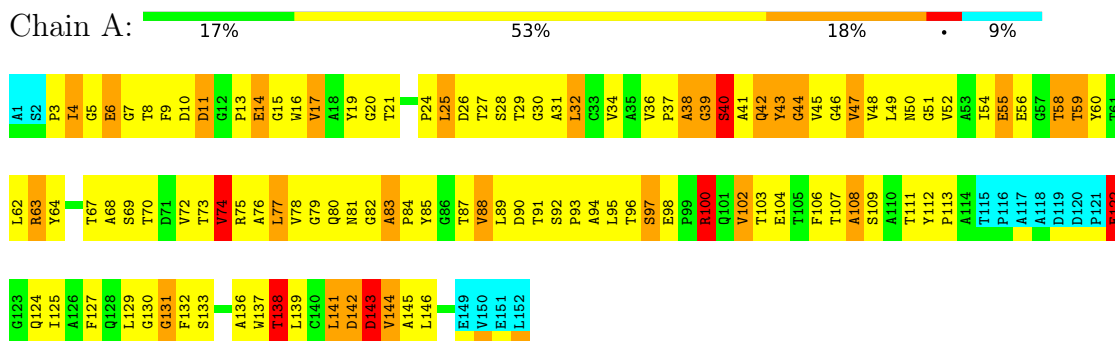
#### 4.2.22 Score per residue for model 22

- Molecule 1: ENDOGLUCANASE C



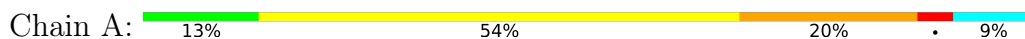
#### 4.2.23 Score per residue for model 23

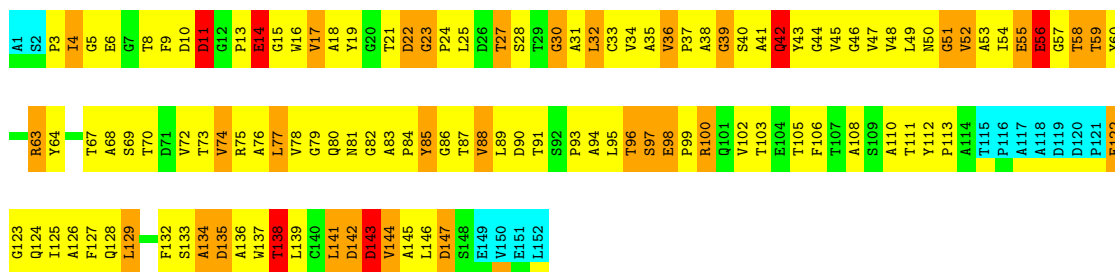
- Molecule 1: ENDOGLUCANASE C



#### 4.2.24 Score per residue for model 24 (medoid)

- Molecule 1: ENDOGLUCANASE C

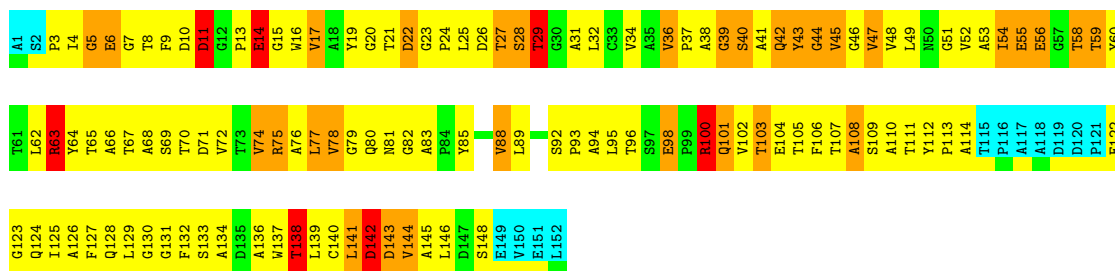




#### 4.2.25 Score per residue for model 25

- Molecule 1: ENDOGLUCANASE C

Chain A: 12% 55% 20% 5% 9%



## 5 Refinement protocol and experimental data overview

The models were refined using the following method: *XPLOR V3.1*.

Of the ? calculated structures, 25 were deposited, based on the following criterion: ?.

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

| Software name | Classification     | Version |
|---------------|--------------------|---------|
| X-PLOR        | refinement         | 3.1     |
| NMRPipe       | structure solution |         |
| PIPP          | structure solution |         |

No chemical shift data was provided.

## 6 Model quality i

### 6.1 Standard geometry i

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

| Mol | Chain | Bond lengths |                       | Bond angles |                       |
|-----|-------|--------------|-----------------------|-------------|-----------------------|
|     |       | RMSZ         | #Z>5                  | RMSZ        | #Z>5                  |
| 1   | A     | 1.46±0.01    | 0±0/1017 ( 0.0± 0.0%) | 1.51±0.01   | 4±1/1401 ( 0.3± 0.1%) |
| All | All   | 1.46         | 0/25425 ( 0.0%)       | 1.51        | 101/35025 ( 0.3%)     |

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

| Mol | Chain | Chirality | Planarity |
|-----|-------|-----------|-----------|
| 1   | A     | 0.0±0.0   | 2.8±0.4   |
| All | All   | 0         | 70        |

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     | 36  | VAL  | N-CA-CB | -6.78 | 105.19      | 112.37   | 15     | 10    |
| 1   | A     | 78  | VAL  | N-CA-CB | -6.49 | 104.86      | 112.32   | 9      | 2     |
| 1   | A     | 4   | ILE  | N-CA-CB | -6.43 | 104.87      | 112.39   | 23     | 3     |
| 1   | A     | 88  | VAL  | N-CA-CB | -6.13 | 105.03      | 112.33   | 13     | 22    |
| 1   | A     | 52  | VAL  | N-CA-CB | -5.97 | 104.89      | 112.60   | 12     | 11    |
| 1   | A     | 45  | VAL  | N-CA-CB | -5.86 | 105.58      | 112.32   | 10     | 3     |
| 1   | A     | 138 | THR  | N-CA-CB | -5.81 | 102.52      | 111.46   | 2      | 23    |
| 1   | A     | 34  | VAL  | N-CA-CB | -5.78 | 105.14      | 112.60   | 20     | 1     |
| 1   | A     | 54  | ILE  | N-CA-CB | -5.76 | 105.16      | 112.60   | 2      | 6     |
| 1   | A     | 114 | ALA  | N-CA-CB | -5.66 | 105.00      | 111.79   | 22     | 2     |
| 1   | A     | 47  | VAL  | N-CA-CB | -5.49 | 104.54      | 111.46   | 16     | 3     |
| 1   | A     | 102 | VAL  | N-CA-CB | -5.37 | 104.87      | 110.72   | 16     | 7     |
| 1   | A     | 144 | VAL  | N-CA-CB | -5.24 | 105.01      | 110.72   | 4      | 5     |
| 1   | A     | 72  | VAL  | N-CA-CB | -5.11 | 105.15      | 110.72   | 18     | 1     |
| 1   | A     | 9   | PHE  | N-CA-CB | -5.10 | 104.98      | 112.78   | 1      | 1     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) | Models |       |
|-----|-------|-----|------|---------|-------|-------------|----------|--------|-------|
|     |       |     |      |         |       |             |          | Worst  | Total |
| 1   | A     | 71  | ASP  | N-CA-CB | -5.02 | 104.45      | 111.62   | 8      | 1     |

There are no chirality outliers.

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

| Mol | Chain | Res | Type | Group     | Models (Total) |
|-----|-------|-----|------|-----------|----------------|
| 1   | A     | 75  | ARG  | Sidechain | 25             |
| 1   | A     | 63  | ARG  | Sidechain | 23             |
| 1   | A     | 100 | ARG  | Sidechain | 22             |

## 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     | 995   | 935      | 935      | 213±16  |
| All | All   | 24875 | 23375    | 23375    | 5318    |

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 110.

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

| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:129:LEU:HD13 | 1:A:139:LEU:HD13 | 1.10     | 1.11        | 2      | 16    |
| 1:A:25:LEU:HD22  | 1:A:34:VAL:HG12  | 1.08     | 1.25        | 24     | 5     |
| 1:A:64:TYR:CZ    | 1:A:102:VAL:HG21 | 1.07     | 1.84        | 15     | 18    |
| 1:A:36:VAL:HG11  | 1:A:137:TRP:CZ2  | 1.04     | 1.88        | 11     | 25    |
| 1:A:88:VAL:HG23  | 1:A:89:LEU:HD12  | 1.00     | 1.31        | 13     | 24    |
| 1:A:74:VAL:HG21  | 1:A:129:LEU:CD2  | 1.00     | 1.85        | 25     | 22    |
| 1:A:25:LEU:CD1   | 1:A:32:LEU:HD11  | 0.99     | 1.86        | 3      | 11    |
| 1:A:16:TRP:NE1   | 1:A:49:LEU:HD22  | 0.98     | 1.71        | 9      | 22    |
| 1:A:21:THR:HG22  | 1:A:45:VAL:CG1   | 0.97     | 1.90        | 16     | 9     |
| 1:A:88:VAL:HG23  | 1:A:89:LEU:CD1   | 0.97     | 1.88        | 13     | 24    |
| 1:A:77:LEU:CD1   | 1:A:126:ALA:HB3  | 0.97     | 1.88        | 18     | 12    |
| 1:A:54:ILE:HD11  | 1:A:146:LEU:HD21 | 0.97     | 1.28        | 21     | 13    |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:74:VAL:HG21  | 1:A:129:LEU:HD23 | 0.96     | 1.32        | 7      | 7     |
| 1:A:21:THR:HG22  | 1:A:45:VAL:HG13  | 0.96     | 1.33        | 14     | 2     |
| 1:A:128:GLN:O    | 1:A:129:LEU:HD23 | 0.95     | 1.61        | 14     | 4     |
| 1:A:77:LEU:HD11  | 1:A:126:ALA:HB3  | 0.95     | 1.36        | 18     | 11    |
| 1:A:129:LEU:CD1  | 1:A:139:LEU:HD13 | 0.95     | 1.90        | 2      | 8     |
| 1:A:16:TRP:CE2   | 1:A:49:LEU:HD22  | 0.94     | 1.98        | 6      | 21    |
| 1:A:64:TYR:CE2   | 1:A:102:VAL:HG21 | 0.94     | 1.97        | 15     | 11    |
| 1:A:58:THR:HG22  | 1:A:60:TYR:CE1   | 0.94     | 1.97        | 12     | 1     |
| 1:A:36:VAL:HG11  | 1:A:137:TRP:CE2  | 0.93     | 1.97        | 24     | 25    |
| 1:A:25:LEU:CD2   | 1:A:34:VAL:HG12  | 0.93     | 1.92        | 12     | 7     |
| 1:A:8:THR:HG22   | 1:A:142:ASP:O    | 0.93     | 1.61        | 5      | 11    |
| 1:A:4:ILE:HD11   | 1:A:144:VAL:O    | 0.93     | 1.61        | 8      | 6     |
| 1:A:94:ALA:HB3   | 1:A:100:ARG:NE   | 0.92     | 1.80        | 2      | 2     |
| 1:A:60:TYR:CD1   | 1:A:108:ALA:HB3  | 0.92     | 1.98        | 12     | 1     |
| 1:A:129:LEU:HD13 | 1:A:139:LEU:CD1  | 0.91     | 1.94        | 2      | 9     |
| 1:A:94:ALA:HB3   | 1:A:100:ARG:NH1  | 0.90     | 1.80        | 4      | 3     |
| 1:A:27:THR:HG22  | 1:A:31:ALA:O     | 0.89     | 1.67        | 19     | 3     |
| 1:A:49:LEU:HD23  | 1:A:125:ILE:HD12 | 0.88     | 1.45        | 2      | 5     |
| 1:A:27:THR:O     | 1:A:29:THR:HG22  | 0.88     | 1.69        | 16     | 8     |
| 1:A:18:ALA:HB3   | 1:A:25:LEU:HD21  | 0.87     | 1.44        | 24     | 2     |
| 1:A:128:GLN:C    | 1:A:129:LEU:HD23 | 0.87     | 1.94        | 19     | 7     |
| 1:A:40:SER:OG    | 1:A:45:VAL:HG21  | 0.87     | 1.67        | 13     | 4     |
| 1:A:89:LEU:HD11  | 1:A:106:PHE:CZ   | 0.87     | 2.05        | 22     | 23    |
| 1:A:22:ASP:O     | 1:A:35:ALA:HB3   | 0.87     | 1.70        | 15     | 2     |
| 1:A:40:SER:OG    | 1:A:45:VAL:HG23  | 0.86     | 1.70        | 17     | 7     |
| 1:A:25:LEU:HD12  | 1:A:32:LEU:HD11  | 0.86     | 1.45        | 3      | 5     |
| 1:A:53:ALA:O     | 1:A:54:ILE:HD13  | 0.86     | 1.69        | 5      | 8     |
| 1:A:89:LEU:HD11  | 1:A:106:PHE:CE1  | 0.85     | 2.06        | 2      | 12    |
| 1:A:62:LEU:HD22  | 1:A:89:LEU:CD2   | 0.85     | 1.99        | 23     | 8     |
| 1:A:22:ASP:HA    | 1:A:35:ALA:HB3   | 0.85     | 1.49        | 7      | 3     |
| 1:A:16:TRP:CH2   | 1:A:125:ILE:HG21 | 0.85     | 2.06        | 17     | 21    |
| 1:A:20:GLY:HA3   | 1:A:45:VAL:HG13  | 0.84     | 1.49        | 12     | 6     |
| 1:A:72:VAL:HG23  | 1:A:133:SER:HB2  | 0.84     | 1.46        | 25     | 23    |
| 1:A:72:VAL:HG21  | 1:A:137:TRP:CE2  | 0.84     | 2.08        | 19     | 14    |
| 1:A:111:THR:HG22 | 1:A:113:PRO:HD3  | 0.84     | 1.50        | 24     | 9     |
| 1:A:36:VAL:HG12  | 1:A:40:SER:OG    | 0.84     | 1.73        | 4      | 1     |
| 1:A:22:ASP:CB    | 1:A:35:ALA:HB3   | 0.84     | 2.01        | 6      | 4     |
| 1:A:8:THR:HG22   | 1:A:143:ASP:CA   | 0.83     | 2.03        | 3      | 2     |
| 1:A:19:TYR:CE1   | 1:A:48:VAL:HG13  | 0.83     | 2.08        | 10     | 2     |
| 1:A:74:VAL:HG11  | 1:A:129:LEU:HD22 | 0.83     | 1.50        | 13     | 9     |
| 1:A:16:TRP:CZ2   | 1:A:49:LEU:HD22  | 0.83     | 2.06        | 12     | 3     |

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| Atom-1          | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|-----------------|------------------|----------|-------------|--------|-------|
|                 |                  |          |             | Worst  | Total |
| 1:A:77:LEU:HD12 | 1:A:78:VAL:N     | 0.83     | 1.89        | 14     | 18    |
| 1:A:25:LEU:HD23 | 1:A:34:VAL:HG12  | 0.82     | 1.51        | 2      | 3     |
| 1:A:89:LEU:HD11 | 1:A:106:PHE:CE2  | 0.82     | 2.10        | 23     | 11    |
| 1:A:16:TRP:N    | 1:A:49:LEU:HD13  | 0.81     | 1.90        | 21     | 9     |
| 1:A:20:GLY:CA   | 1:A:45:VAL:HG13  | 0.81     | 2.05        | 4      | 3     |
| 1:A:18:ALA:HB3  | 1:A:25:LEU:CD2   | 0.81     | 2.04        | 1      | 2     |
| 1:A:142:ASP:O   | 1:A:144:VAL:HG23 | 0.80     | 1.74        | 19     | 2     |
| 1:A:78:VAL:CG2  | 1:A:89:LEU:HD22  | 0.80     | 2.06        | 18     | 24    |
| 1:A:15:GLY:C    | 1:A:49:LEU:HD13  | 0.79     | 2.01        | 23     | 13    |
| 1:A:64:TYR:HB2  | 1:A:144:VAL:HG22 | 0.79     | 1.54        | 11     | 2     |
| 1:A:20:GLY:O    | 1:A:45:VAL:HG13  | 0.79     | 1.78        | 21     | 4     |
| 1:A:95:LEU:CD1  | 1:A:139:LEU:HD21 | 0.79     | 2.08        | 21     | 8     |
| 1:A:25:LEU:HD13 | 1:A:32:LEU:HD11  | 0.78     | 1.56        | 18     | 13    |
| 1:A:66:ALA:HB1  | 1:A:95:LEU:HD21  | 0.78     | 1.56        | 25     | 11    |
| 1:A:17:VAL:O    | 1:A:47:VAL:HG13  | 0.77     | 1.78        | 12     | 24    |
| 1:A:78:VAL:HG23 | 1:A:89:LEU:HD22  | 0.77     | 1.54        | 22     | 24    |
| 1:A:95:LEU:HD11 | 1:A:139:LEU:HD21 | 0.77     | 1.55        | 21     | 7     |
| 1:A:60:TYR:O    | 1:A:105:THR:HG22 | 0.77     | 1.77        | 19     | 1     |
| 1:A:65:THR:HG23 | 1:A:101:GLN:CA   | 0.77     | 2.10        | 1      | 3     |
| 1:A:67:THR:HG23 | 1:A:98:GLU:O     | 0.77     | 1.79        | 24     | 18    |
| 1:A:61:THR:OG1  | 1:A:105:THR:HG22 | 0.77     | 1.79        | 10     | 2     |
| 1:A:72:VAL:HG23 | 1:A:133:SER:CB   | 0.76     | 2.10        | 22     | 21    |
| 1:A:13:PRO:HG3  | 1:A:27:THR:HG21  | 0.76     | 1.57        | 11     | 3     |
| 1:A:25:LEU:HD21 | 1:A:34:VAL:HG12  | 0.76     | 1.58        | 5      | 2     |
| 1:A:60:TYR:HB3  | 1:A:146:LEU:HD11 | 0.76     | 1.55        | 8      | 12    |
| 1:A:72:VAL:HG21 | 1:A:137:TRP:NE1  | 0.76     | 1.94        | 16     | 7     |
| 1:A:16:TRP:CD1  | 1:A:49:LEU:HD22  | 0.76     | 2.16        | 16     | 11    |
| 1:A:37:PRO:HD2  | 1:A:45:VAL:HG21  | 0.75     | 1.59        | 7      | 3     |
| 1:A:41:ALA:HB2  | 1:A:131:GLY:HA3  | 0.75     | 1.58        | 9      | 3     |
| 1:A:66:ALA:CB   | 1:A:95:LEU:HD21  | 0.75     | 2.12        | 25     | 21    |
| 1:A:25:LEU:HD22 | 1:A:34:VAL:CG1   | 0.75     | 2.11        | 24     | 1     |
| 1:A:22:ASP:HB2  | 1:A:35:ALA:HB3   | 0.74     | 1.56        | 13     | 1     |
| 1:A:17:VAL:HA   | 1:A:25:LEU:HD11  | 0.74     | 1.57        | 25     | 2     |
| 1:A:77:LEU:HD11 | 1:A:126:ALA:CB   | 0.73     | 2.13        | 8      | 6     |
| 1:A:42:GLN:NE2  | 1:A:45:VAL:HG22  | 0.73     | 1.98        | 17     | 1     |
| 1:A:65:THR:HG23 | 1:A:101:GLN:HA   | 0.73     | 1.60        | 1      | 2     |
| 1:A:20:GLY:C    | 1:A:21:THR:HG23  | 0.73     | 2.06        | 15     | 14    |
| 1:A:40:SER:HB2  | 1:A:45:VAL:HG23  | 0.73     | 1.61        | 23     | 2     |
| 1:A:88:VAL:HG12 | 1:A:109:SER:N    | 0.73     | 1.97        | 9      | 3     |
| 1:A:4:ILE:HB    | 1:A:49:LEU:HD21  | 0.73     | 1.61        | 14     | 1     |
| 1:A:54:ILE:HG23 | 1:A:60:TYR:CE2   | 0.72     | 2.19        | 24     | 7     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:60:TYR:O     | 1:A:105:THR:HG23 | 0.72     | 1.84        | 2      | 3     |
| 1:A:38:ALA:HB2   | 1:A:136:ALA:HB2  | 0.72     | 1.60        | 1      | 4     |
| 1:A:77:LEU:HD12  | 1:A:77:LEU:C     | 0.72     | 2.09        | 1      | 24    |
| 1:A:40:SER:HB2   | 1:A:45:VAL:HG21  | 0.72     | 1.59        | 9      | 6     |
| 1:A:17:VAL:HG22  | 1:A:48:VAL:O     | 0.72     | 1.83        | 21     | 12    |
| 1:A:74:VAL:HG23  | 1:A:75:ARG:N     | 0.72     | 2.00        | 25     | 15    |
| 1:A:66:ALA:HB2   | 1:A:141:LEU:HD23 | 0.72     | 1.60        | 4      | 12    |
| 1:A:13:PRO:HB3   | 1:A:32:LEU:HD12  | 0.72     | 1.58        | 2      | 15    |
| 1:A:25:LEU:O     | 1:A:27:THR:HG23  | 0.72     | 1.85        | 7      | 1     |
| 1:A:66:ALA:HB2   | 1:A:141:LEU:CD2  | 0.71     | 2.14        | 4      | 10    |
| 1:A:94:ALA:HB3   | 1:A:100:ARG:HH11 | 0.71     | 1.45        | 4      | 3     |
| 1:A:54:ILE:HG21  | 1:A:108:ALA:HB1  | 0.71     | 1.62        | 24     | 15    |
| 1:A:55:GLU:HA    | 1:A:111:THR:HG23 | 0.71     | 1.61        | 5      | 5     |
| 1:A:15:GLY:O     | 1:A:17:VAL:HG13  | 0.71     | 1.85        | 16     | 9     |
| 1:A:25:LEU:CB    | 1:A:34:VAL:HG12  | 0.71     | 2.14        | 16     | 3     |
| 1:A:74:VAL:HG21  | 1:A:129:LEU:HD22 | 0.71     | 1.61        | 4      | 9     |
| 1:A:16:TRP:CZ2   | 1:A:144:VAL:HG11 | 0.70     | 2.21        | 9      | 19    |
| 1:A:76:ALA:HB2   | 1:A:93:PRO:HG3   | 0.70     | 1.63        | 16     | 16    |
| 1:A:25:LEU:HD22  | 1:A:32:LEU:HD11  | 0.70     | 1.62        | 22     | 2     |
| 1:A:21:THR:CG2   | 1:A:45:VAL:HG13  | 0.70     | 2.16        | 14     | 3     |
| 1:A:129:LEU:HD23 | 1:A:129:LEU:N    | 0.70     | 2.00        | 4      | 5     |
| 1:A:42:GLN:O     | 1:A:43:TYR:CD2   | 0.70     | 2.45        | 15     | 2     |
| 1:A:25:LEU:HD12  | 1:A:32:LEU:CD1   | 0.70     | 2.17        | 21     | 3     |
| 1:A:74:VAL:HG12  | 1:A:132:PHE:CD2  | 0.70     | 2.22        | 15     | 6     |
| 1:A:6:GLU:HG2    | 1:A:145:ALA:HB1  | 0.70     | 1.64        | 14     | 3     |
| 1:A:58:THR:HG23  | 1:A:59:THR:N     | 0.70     | 2.01        | 12     | 1     |
| 1:A:64:TYR:CE2   | 1:A:102:VAL:HG11 | 0.69     | 2.21        | 5      | 16    |
| 1:A:16:TRP:HH2   | 1:A:125:ILE:HG21 | 0.69     | 1.45        | 25     | 16    |
| 1:A:62:LEU:HD22  | 1:A:89:LEU:HD23  | 0.69     | 1.64        | 23     | 4     |
| 1:A:54:ILE:CD1   | 1:A:146:LEU:HD21 | 0.69     | 2.16        | 12     | 3     |
| 1:A:28:SER:C     | 1:A:29:THR:HG22  | 0.69     | 2.12        | 5      | 4     |
| 1:A:13:PRO:CG    | 1:A:27:THR:HG21  | 0.69     | 2.18        | 11     | 1     |
| 1:A:18:ALA:CB    | 1:A:34:VAL:HG11  | 0.69     | 2.17        | 18     | 4     |
| 1:A:63:ARG:HD2   | 1:A:103:THR:HG23 | 0.69     | 1.62        | 25     | 1     |
| 1:A:60:TYR:CE2   | 1:A:108:ALA:HB3  | 0.69     | 2.23        | 19     | 24    |
| 1:A:20:GLY:C     | 1:A:45:VAL:HG13  | 0.69     | 2.13        | 21     | 2     |
| 1:A:54:ILE:CG2   | 1:A:108:ALA:HB1  | 0.69     | 2.18        | 12     | 17    |
| 1:A:16:TRP:CD1   | 1:A:49:LEU:HD13  | 0.68     | 2.23        | 14     | 7     |
| 1:A:78:VAL:CG2   | 1:A:89:LEU:HD13  | 0.68     | 2.18        | 21     | 17    |
| 1:A:94:ALA:O     | 1:A:95:LEU:HD23  | 0.68     | 1.89        | 11     | 2     |
| 1:A:90:ASP:O     | 1:A:91:THR:HG23  | 0.68     | 1.89        | 23     | 10    |

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| Atom-1          | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|-----------------|------------------|----------|-------------|--------|-------|
|                 |                  |          |             | Worst  | Total |
| 1:A:8:THR:HG22  | 1:A:143:ASP:HA   | 0.67     | 1.66        | 3      | 2     |
| 1:A:19:TYR:HE1  | 1:A:48:VAL:HG13  | 0.67     | 1.45        | 10     | 3     |
| 1:A:88:VAL:CG1  | 1:A:110:ALA:HB3  | 0.67     | 2.19        | 2      | 1     |
| 1:A:19:TYR:O    | 1:A:45:VAL:HG13  | 0.67     | 1.90        | 20     | 2     |
| 1:A:36:VAL:CG1  | 1:A:137:TRP:CZ2  | 0.67     | 2.78        | 7      | 19    |
| 1:A:74:VAL:HG22 | 1:A:93:PRO:HG2   | 0.67     | 1.66        | 23     | 12    |
| 1:A:13:PRO:HG3  | 1:A:32:LEU:HD12  | 0.67     | 1.67        | 20     | 2     |
| 1:A:88:VAL:HG13 | 1:A:112:TYR:OH   | 0.67     | 1.90        | 23     | 8     |
| 1:A:25:LEU:HB3  | 1:A:34:VAL:HG12  | 0.67     | 1.67        | 21     | 3     |
| 1:A:95:LEU:HD13 | 1:A:139:LEU:HG   | 0.66     | 1.67        | 19     | 9     |
| 1:A:18:ALA:CB   | 1:A:34:VAL:HG12  | 0.66     | 2.20        | 17     | 4     |
| 1:A:78:VAL:HG12 | 1:A:112:TYR:CE2  | 0.66     | 2.25        | 13     | 17    |
| 1:A:54:ILE:HD13 | 1:A:60:TYR:CE1   | 0.66     | 2.26        | 2      | 14    |
| 1:A:72:VAL:CG1  | 1:A:95:LEU:HD12  | 0.65     | 2.21        | 8      | 8     |
| 1:A:13:PRO:HD3  | 1:A:27:THR:HG21  | 0.65     | 1.66        | 5      | 2     |
| 1:A:58:THR:HG22 | 1:A:60:TYR:CE2   | 0.65     | 2.26        | 6      | 24    |
| 1:A:54:ILE:CG1  | 1:A:112:TYR:CD2  | 0.65     | 2.79        | 9      | 18    |
| 1:A:58:THR:HG22 | 1:A:60:TYR:CD1   | 0.65     | 2.26        | 12     | 1     |
| 1:A:60:TYR:CD2  | 1:A:108:ALA:CB   | 0.65     | 2.80        | 6      | 24    |
| 1:A:16:TRP:CZ2  | 1:A:125:ILE:HD13 | 0.65     | 2.26        | 25     | 2     |
| 1:A:16:TRP:CB   | 1:A:32:LEU:HD13  | 0.65     | 2.21        | 16     | 1     |
| 1:A:43:TYR:CD1  | 1:A:44:GLY:N     | 0.65     | 2.65        | 13     | 9     |
| 1:A:94:ALA:HB3  | 1:A:100:ARG:HD2  | 0.65     | 1.69        | 1      | 1     |
| 1:A:8:THR:HG22  | 1:A:143:ASP:HB2  | 0.65     | 1.68        | 2      | 2     |
| 1:A:6:GLU:CG    | 1:A:145:ALA:HB1  | 0.65     | 2.22        | 24     | 1     |
| 1:A:19:TYR:HE2  | 1:A:48:VAL:HG13  | 0.65     | 1.52        | 15     | 11    |
| 1:A:41:ALA:O    | 1:A:42:GLN:CG    | 0.64     | 2.46        | 20     | 8     |
| 1:A:43:TYR:CD1  | 1:A:43:TYR:C     | 0.64     | 2.75        | 15     | 6     |
| 1:A:16:TRP:CE2  | 1:A:49:LEU:CD2   | 0.64     | 2.81        | 15     | 5     |
| 1:A:16:TRP:HZ2  | 1:A:144:VAL:HG11 | 0.64     | 1.51        | 9      | 18    |
| 1:A:21:THR:CG2  | 1:A:43:TYR:CE2   | 0.64     | 2.80        | 7      | 3     |
| 1:A:19:TYR:CD1  | 1:A:19:TYR:N     | 0.64     | 2.66        | 17     | 6     |
| 1:A:54:ILE:CD1  | 1:A:60:TYR:CE1   | 0.64     | 2.81        | 18     | 17    |
| 1:A:16:TRP:O    | 1:A:25:LEU:HD11  | 0.64     | 1.93        | 20     | 4     |
| 1:A:60:TYR:CD1  | 1:A:108:ALA:CB   | 0.64     | 2.79        | 12     | 1     |
| 1:A:70:THR:HG22 | 1:A:137:TRP:HB2  | 0.63     | 1.69        | 6      | 17    |
| 1:A:22:ASP:CB   | 1:A:35:ALA:HB1   | 0.63     | 2.22        | 17     | 1     |
| 1:A:83:ALA:N    | 1:A:85:TYR:CE1   | 0.63     | 2.67        | 14     | 12    |
| 1:A:65:THR:HG23 | 1:A:101:GLN:HG2  | 0.63     | 1.70        | 18     | 2     |
| 1:A:43:TYR:N    | 1:A:43:TYR:CD1   | 0.63     | 2.64        | 8      | 1     |
| 1:A:60:TYR:CB   | 1:A:106:PHE:CZ   | 0.63     | 2.81        | 19     | 6     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:9:PHE:CE1    | 1:A:144:VAL:HG21 | 0.62     | 2.28        | 22     | 1     |
| 1:A:61:THR:HG23  | 1:A:104:GLU:O    | 0.62     | 1.94        | 5      | 1     |
| 1:A:39:GLY:O     | 1:A:40:SER:C     | 0.62     | 2.42        | 5      | 13    |
| 1:A:21:THR:HG23  | 1:A:45:VAL:HG13  | 0.62     | 1.69        | 5      | 1     |
| 1:A:4:ILE:HG22   | 1:A:51:GLY:O     | 0.62     | 1.95        | 16     | 7     |
| 1:A:8:THR:HG22   | 1:A:143:ASP:CG   | 0.62     | 2.18        | 23     | 3     |
| 1:A:43:TYR:OH    | 1:A:45:VAL:HG22  | 0.61     | 1.95        | 22     | 4     |
| 1:A:6:GLU:OE1    | 1:A:145:ALA:HB1  | 0.61     | 1.94        | 2      | 1     |
| 1:A:22:ASP:HB3   | 1:A:35:ALA:HB3   | 0.61     | 1.72        | 6      | 2     |
| 1:A:21:THR:HG22  | 1:A:45:VAL:HG11  | 0.61     | 1.71        | 21     | 3     |
| 1:A:54:ILE:CD1   | 1:A:60:TYR:CZ    | 0.61     | 2.84        | 3      | 11    |
| 1:A:74:VAL:HG12  | 1:A:132:PHE:HB2  | 0.61     | 1.71        | 9      | 2     |
| 1:A:42:GLN:O     | 1:A:42:GLN:CG    | 0.61     | 2.48        | 15     | 2     |
| 1:A:70:THR:HG21  | 1:A:137:TRP:CB   | 0.61     | 2.25        | 3      | 16    |
| 1:A:95:LEU:HD11  | 1:A:139:LEU:CD2  | 0.61     | 2.25        | 9      | 11    |
| 1:A:74:VAL:HG12  | 1:A:132:PHE:CB   | 0.60     | 2.25        | 9      | 6     |
| 1:A:32:LEU:HD23  | 1:A:141:LEU:HD12 | 0.60     | 1.72        | 16     | 3     |
| 1:A:9:PHE:N      | 1:A:9:PHE:CD1    | 0.60     | 2.67        | 9      | 6     |
| 1:A:18:ALA:HB2   | 1:A:34:VAL:HG11  | 0.60     | 1.72        | 18     | 3     |
| 1:A:27:THR:HG22  | 1:A:32:LEU:HA    | 0.60     | 1.72        | 9      | 3     |
| 1:A:95:LEU:C     | 1:A:96:THR:HG22  | 0.60     | 2.21        | 2      | 2     |
| 1:A:43:TYR:CD1   | 1:A:44:GLY:O     | 0.60     | 2.54        | 1      | 5     |
| 1:A:129:LEU:HD11 | 1:A:139:LEU:HD22 | 0.60     | 1.72        | 13     | 2     |
| 1:A:17:VAL:CG2   | 1:A:48:VAL:CG2   | 0.60     | 2.80        | 4      | 17    |
| 1:A:70:THR:CG2   | 1:A:137:TRP:CB   | 0.60     | 2.80        | 7      | 20    |
| 1:A:54:ILE:HD11  | 1:A:146:LEU:CD2  | 0.60     | 2.27        | 23     | 3     |
| 1:A:42:GLN:CD    | 1:A:43:TYR:CE2   | 0.60     | 2.80        | 11     | 3     |
| 1:A:128:GLN:O    | 1:A:132:PHE:CE2  | 0.60     | 2.55        | 16     | 9     |
| 1:A:60:TYR:CD2   | 1:A:108:ALA:HB2  | 0.60     | 2.32        | 9      | 17    |
| 1:A:19:TYR:CZ    | 1:A:46:GLY:C     | 0.60     | 2.80        | 6      | 12    |
| 1:A:22:ASP:CB    | 1:A:35:ALA:CB    | 0.60     | 2.80        | 17     | 2     |
| 1:A:39:GLY:O     | 1:A:41:ALA:N     | 0.59     | 2.35        | 23     | 6     |
| 1:A:13:PRO:CB    | 1:A:32:LEU:HD12  | 0.59     | 2.26        | 16     | 2     |
| 1:A:23:GLY:N     | 1:A:24:PRO:CD    | 0.59     | 2.65        | 12     | 3     |
| 1:A:74:VAL:CG2   | 1:A:129:LEU:HD23 | 0.59     | 2.22        | 17     | 3     |
| 1:A:64:TYR:CD1   | 1:A:64:TYR:C     | 0.59     | 2.81        | 9      | 25    |
| 1:A:60:TYR:CD2   | 1:A:108:ALA:HB3  | 0.59     | 2.31        | 6      | 22    |
| 1:A:82:GLY:C     | 1:A:85:TYR:CE1   | 0.59     | 2.81        | 5      | 11    |
| 1:A:6:GLU:CG     | 1:A:145:ALA:HB2  | 0.59     | 2.27        | 25     | 2     |
| 1:A:79:GLY:C     | 1:A:112:TYR:CE1  | 0.59     | 2.81        | 17     | 14    |
| 1:A:137:TRP:CD1  | 1:A:138:THR:N    | 0.59     | 2.71        | 22     | 15    |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:18:ALA:CB    | 1:A:34:VAL:CG1   | 0.59     | 2.81        | 13     | 6     |
| 1:A:95:LEU:CD1   | 1:A:139:LEU:CD2  | 0.59     | 2.81        | 17     | 9     |
| 1:A:42:GLN:O     | 1:A:43:TYR:CG    | 0.59     | 2.55        | 10     | 3     |
| 1:A:31:ALA:HB1   | 1:A:141:LEU:O    | 0.59     | 1.97        | 15     | 7     |
| 1:A:19:TYR:CZ    | 1:A:46:GLY:O     | 0.59     | 2.56        | 9      | 13    |
| 1:A:42:GLN:C     | 1:A:43:TYR:CD2   | 0.59     | 2.80        | 10     | 1     |
| 1:A:79:GLY:C     | 1:A:112:TYR:CZ   | 0.59     | 2.81        | 11     | 3     |
| 1:A:54:ILE:O     | 1:A:54:ILE:HG22  | 0.59     | 1.97        | 12     | 1     |
| 1:A:13:PRO:CD    | 1:A:27:THR:HG21  | 0.59     | 2.28        | 5      | 1     |
| 1:A:42:GLN:CD    | 1:A:43:TYR:CD2   | 0.59     | 2.81        | 11     | 1     |
| 1:A:21:THR:CG2   | 1:A:45:VAL:CG1   | 0.59     | 2.81        | 21     | 6     |
| 1:A:138:THR:C    | 1:A:139:LEU:HD12 | 0.59     | 2.22        | 18     | 9     |
| 1:A:72:VAL:CG2   | 1:A:133:SER:CB   | 0.58     | 2.81        | 13     | 9     |
| 1:A:82:GLY:O     | 1:A:85:TYR:CZ    | 0.58     | 2.56        | 19     | 6     |
| 1:A:58:THR:CG2   | 1:A:59:THR:N     | 0.58     | 2.66        | 8      | 25    |
| 1:A:88:VAL:CG1   | 1:A:110:ALA:CB   | 0.58     | 2.81        | 2      | 1     |
| 1:A:43:TYR:CZ    | 1:A:45:VAL:HG22  | 0.58     | 2.33        | 4      | 1     |
| 1:A:74:VAL:HG21  | 1:A:129:LEU:HD21 | 0.58     | 1.71        | 13     | 2     |
| 1:A:63:ARG:HG2   | 1:A:103:THR:HG23 | 0.58     | 1.75        | 23     | 3     |
| 1:A:43:TYR:CE1   | 1:A:44:GLY:O     | 0.58     | 2.56        | 12     | 5     |
| 1:A:59:THR:O     | 1:A:60:TYR:CG    | 0.58     | 2.57        | 1      | 23    |
| 1:A:82:GLY:O     | 1:A:83:ALA:HB2   | 0.58     | 1.97        | 17     | 5     |
| 1:A:52:VAL:HG23  | 1:A:124:GLN:HA   | 0.58     | 1.74        | 24     | 8     |
| 1:A:60:TYR:CE1   | 1:A:148:SER:CB   | 0.58     | 2.86        | 7      | 3     |
| 1:A:59:THR:O     | 1:A:60:TYR:CD2   | 0.58     | 2.57        | 23     | 15    |
| 1:A:105:THR:HG23 | 1:A:105:THR:O    | 0.58     | 1.97        | 1      | 2     |
| 1:A:84:PRO:C     | 1:A:85:TYR:CD2   | 0.58     | 2.81        | 13     | 9     |
| 1:A:74:VAL:CG2   | 1:A:129:LEU:CD2  | 0.58     | 2.79        | 10     | 2     |
| 1:A:83:ALA:N     | 1:A:85:TYR:CZ    | 0.58     | 2.71        | 24     | 7     |
| 1:A:60:TYR:CD1   | 1:A:147:ASP:O    | 0.58     | 2.57        | 8      | 2     |
| 1:A:77:LEU:CD1   | 1:A:78:VAL:N     | 0.58     | 2.66        | 12     | 12    |
| 1:A:82:GLY:O     | 1:A:85:TYR:CD2   | 0.58     | 2.57        | 18     | 2     |
| 1:A:9:PHE:CG     | 1:A:142:ASP:O    | 0.58     | 2.57        | 20     | 1     |
| 1:A:40:SER:HB3   | 1:A:45:VAL:HG23  | 0.58     | 1.73        | 25     | 2     |
| 1:A:131:GLY:O    | 1:A:132:PHE:CG   | 0.58     | 2.57        | 13     | 6     |
| 1:A:131:GLY:O    | 1:A:132:PHE:CD1  | 0.58     | 2.56        | 15     | 3     |
| 1:A:82:GLY:O     | 1:A:85:TYR:CE1   | 0.58     | 2.57        | 13     | 5     |
| 1:A:94:ALA:HB3   | 1:A:100:ARG:CD   | 0.58     | 2.28        | 2      | 1     |
| 1:A:42:GLN:CD    | 1:A:43:TYR:CZ    | 0.58     | 2.82        | 21     | 2     |
| 1:A:42:GLN:O     | 1:A:43:TYR:C     | 0.58     | 2.47        | 12     | 11    |
| 1:A:19:TYR:CE2   | 1:A:46:GLY:O     | 0.58     | 2.57        | 14     | 14    |

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| Atom-1          | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|-----------------|------------------|----------|-------------|--------|-------|
|                 |                  |          |             | Worst  | Total |
| 1:A:9:PHE:HB3   | 1:A:27:THR:HG21  | 0.58     | 1.74        | 20     | 2     |
| 1:A:19:TYR:CE1  | 1:A:46:GLY:O     | 0.58     | 2.57        | 20     | 4     |
| 1:A:18:ALA:HB2  | 1:A:34:VAL:HG12  | 0.58     | 1.76        | 17     | 1     |
| 1:A:54:ILE:HG13 | 1:A:112:TYR:CD2  | 0.58     | 2.34        | 25     | 23    |
| 1:A:133:SER:O   | 1:A:137:TRP:CZ3  | 0.58     | 2.57        | 1      | 2     |
| 1:A:45:VAL:O    | 1:A:129:LEU:CB   | 0.58     | 2.51        | 3      | 3     |
| 1:A:82:GLY:O    | 1:A:85:TYR:CG    | 0.58     | 2.56        | 18     | 2     |
| 1:A:82:GLY:O    | 1:A:85:TYR:CE2   | 0.57     | 2.57        | 19     | 2     |
| 1:A:23:GLY:N    | 1:A:24:PRO:HD3   | 0.57     | 2.14        | 5      | 3     |
| 1:A:42:GLN:OE1  | 1:A:43:TYR:CE2   | 0.57     | 2.57        | 21     | 2     |
| 1:A:79:GLY:O    | 1:A:112:TYR:CE2  | 0.57     | 2.57        | 13     | 1     |
| 1:A:79:GLY:O    | 1:A:112:TYR:CE1  | 0.57     | 2.57        | 15     | 2     |
| 1:A:25:LEU:HD23 | 1:A:25:LEU:N     | 0.57     | 2.14        | 21     | 6     |
| 1:A:78:VAL:HG13 | 1:A:124:GLN:O    | 0.57     | 1.99        | 14     | 13    |
| 1:A:15:GLY:C    | 1:A:49:LEU:HD12  | 0.57     | 2.23        | 2      | 4     |
| 1:A:17:VAL:HG22 | 1:A:48:VAL:CG2   | 0.57     | 2.29        | 22     | 16    |
| 1:A:21:THR:HG22 | 1:A:43:TYR:CE2   | 0.57     | 2.35        | 25     | 4     |
| 1:A:40:SER:CB   | 1:A:45:VAL:HG21  | 0.57     | 2.29        | 4      | 3     |
| 1:A:19:TYR:O    | 1:A:19:TYR:CD1   | 0.57     | 2.57        | 9      | 3     |
| 1:A:142:ASP:O   | 1:A:143:ASP:CB   | 0.57     | 2.52        | 9      | 13    |
| 1:A:72:VAL:HG13 | 1:A:95:LEU:HD12  | 0.57     | 1.74        | 21     | 3     |
| 1:A:82:GLY:C    | 1:A:85:TYR:CD1   | 0.57     | 2.82        | 9      | 4     |
| 1:A:20:GLY:O    | 1:A:45:VAL:HG22  | 0.57     | 1.99        | 8      | 3     |
| 1:A:40:SER:OG   | 1:A:137:TRP:CH2  | 0.57     | 2.57        | 24     | 4     |
| 1:A:7:GLY:C     | 1:A:8:THR:HG23   | 0.57     | 2.23        | 17     | 1     |
| 1:A:10:ASP:O    | 1:A:11:ASP:CB    | 0.57     | 2.52        | 16     | 25    |
| 1:A:18:ALA:CB   | 1:A:25:LEU:HD21  | 0.57     | 2.26        | 24     | 3     |
| 1:A:64:TYR:CE2  | 1:A:102:VAL:CG2  | 0.57     | 2.81        | 15     | 5     |
| 1:A:68:ALA:CB   | 1:A:72:VAL:HG12  | 0.57     | 2.29        | 21     | 3     |
| 1:A:130:GLY:O   | 1:A:132:PHE:CD2  | 0.57     | 2.57        | 7      | 6     |
| 1:A:9:PHE:O     | 1:A:10:ASP:CB    | 0.57     | 2.53        | 6      | 1     |
| 1:A:18:ALA:HB2  | 1:A:34:VAL:CG1   | 0.57     | 2.29        | 6      | 3     |
| 1:A:77:LEU:C    | 1:A:78:VAL:HG23  | 0.57     | 2.25        | 3      | 21    |
| 1:A:62:LEU:HD22 | 1:A:89:LEU:HD21  | 0.57     | 1.74        | 7      | 2     |
| 1:A:27:THR:CG2  | 1:A:32:LEU:HD12  | 0.57     | 2.30        | 13     | 1     |
| 1:A:41:ALA:O    | 1:A:42:GLN:O     | 0.57     | 2.23        | 15     | 1     |
| 1:A:42:GLN:HE21 | 1:A:45:VAL:HG22  | 0.57     | 1.60        | 17     | 1     |
| 1:A:56:GLU:CG   | 1:A:57:GLY:N     | 0.56     | 2.68        | 17     | 3     |
| 1:A:77:LEU:HG   | 1:A:126:ALA:HB3  | 0.56     | 1.77        | 24     | 1     |
| 1:A:82:GLY:O    | 1:A:85:TYR:CD1   | 0.56     | 2.57        | 3      | 2     |
| 1:A:55:GLU:HG3  | 1:A:111:THR:HG23 | 0.56     | 1.77        | 8      | 2     |

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| Atom-1          | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|-----------------|------------------|----------|-------------|--------|-------|
|                 |                  |          |             | Worst  | Total |
| 1:A:31:ALA:HB3  | 1:A:140:CYS:SG   | 0.56     | 2.40        | 18     | 3     |
| 1:A:20:GLY:C    | 1:A:21:THR:CG2   | 0.56     | 2.78        | 17     | 13    |
| 1:A:42:GLN:CG   | 1:A:42:GLN:O     | 0.56     | 2.53        | 7      | 5     |
| 1:A:20:GLY:HA2  | 1:A:45:VAL:HG13  | 0.56     | 1.74        | 4      | 1     |
| 1:A:60:TYR:HB2  | 1:A:106:PHE:CZ   | 0.56     | 2.35        | 8      | 9     |
| 1:A:70:THR:HG23 | 1:A:71:ASP:N     | 0.56     | 2.14        | 4      | 2     |
| 1:A:74:VAL:CG1  | 1:A:129:LEU:HD22 | 0.56     | 2.30        | 10     | 1     |
| 1:A:60:TYR:CE1  | 1:A:148:SER:OG   | 0.56     | 2.57        | 19     | 1     |
| 1:A:59:THR:C    | 1:A:60:TYR:CD2   | 0.56     | 2.84        | 23     | 10    |
| 1:A:60:TYR:O    | 1:A:106:PHE:CE2  | 0.56     | 2.57        | 12     | 1     |
| 1:A:96:THR:HG23 | 1:A:98:GLU:H     | 0.56     | 1.60        | 17     | 2     |
| 1:A:66:ALA:HB3  | 1:A:95:LEU:HD21  | 0.56     | 1.77        | 21     | 11    |
| 1:A:9:PHE:CE2   | 1:A:144:VAL:CG2  | 0.56     | 2.88        | 2      | 2     |
| 1:A:19:TYR:CE2  | 1:A:48:VAL:HG13  | 0.56     | 2.35        | 6      | 3     |
| 1:A:25:LEU:CD1  | 1:A:32:LEU:CD1   | 0.56     | 2.84        | 8      | 3     |
| 1:A:54:ILE:CD1  | 1:A:60:TYR:CD1   | 0.56     | 2.89        | 6      | 1     |
| 1:A:43:TYR:O    | 1:A:45:VAL:HG23  | 0.56     | 2.00        | 14     | 2     |
| 1:A:42:GLN:NE2  | 1:A:45:VAL:CG2   | 0.56     | 2.69        | 17     | 1     |
| 1:A:10:ASP:O    | 1:A:11:ASP:HB2   | 0.56     | 2.01        | 6      | 18    |
| 1:A:72:VAL:HG23 | 1:A:133:SER:N    | 0.56     | 2.16        | 15     | 2     |
| 1:A:77:LEU:HD12 | 1:A:126:ALA:HB3  | 0.56     | 1.74        | 18     | 3     |
| 1:A:47:VAL:O    | 1:A:48:VAL:HG13  | 0.56     | 2.00        | 9      | 1     |
| 1:A:9:PHE:CD2   | 1:A:142:ASP:HA   | 0.56     | 2.36        | 20     | 3     |
| 1:A:60:TYR:CE1  | 1:A:108:ALA:HB3  | 0.55     | 2.35        | 12     | 1     |
| 1:A:25:LEU:HD22 | 1:A:32:LEU:CD1   | 0.55     | 2.30        | 22     | 2     |
| 1:A:16:TRP:O    | 1:A:25:LEU:HD13  | 0.55     | 2.01        | 23     | 2     |
| 1:A:36:VAL:HG22 | 1:A:45:VAL:HG11  | 0.55     | 1.78        | 17     | 1     |
| 1:A:40:SER:O    | 1:A:131:GLY:CA   | 0.55     | 2.55        | 23     | 1     |
| 1:A:60:TYR:CE1  | 1:A:148:SER:HB3  | 0.55     | 2.37        | 7      | 8     |
| 1:A:41:ALA:O    | 1:A:42:GLN:CB    | 0.55     | 2.54        | 7      | 5     |
| 1:A:40:SER:HB2  | 1:A:137:TRP:CH2  | 0.55     | 2.36        | 1      | 3     |
| 1:A:58:THR:CG2  | 1:A:60:TYR:CE2   | 0.55     | 2.90        | 18     | 22    |
| 1:A:54:ILE:HD12 | 1:A:60:TYR:CZ    | 0.55     | 2.36        | 3      | 10    |
| 1:A:78:VAL:HB   | 1:A:89:LEU:HD13  | 0.55     | 1.79        | 3      | 2     |
| 1:A:25:LEU:H    | 1:A:25:LEU:HD23  | 0.55     | 1.62        | 11     | 10    |
| 1:A:9:PHE:CZ    | 1:A:142:ASP:O    | 0.55     | 2.60        | 10     | 2     |
| 1:A:18:ALA:CB   | 1:A:25:LEU:CD2   | 0.55     | 2.82        | 1      | 1     |
| 1:A:40:SER:O    | 1:A:130:GLY:CA   | 0.55     | 2.54        | 10     | 1     |
| 1:A:15:GLY:C    | 1:A:49:LEU:CD1   | 0.55     | 2.80        | 22     | 16    |
| 1:A:40:SER:OG   | 1:A:131:GLY:N    | 0.55     | 2.40        | 5      | 2     |
| 1:A:9:PHE:CZ    | 1:A:144:VAL:CG2  | 0.55     | 2.90        | 10     | 4     |

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| Atom-1          | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|-----------------|------------------|----------|-------------|--------|-------|
|                 |                  |          |             | Worst  | Total |
| 1:A:40:SER:HB3  | 1:A:45:VAL:HG21  | 0.55     | 1.78        | 10     | 1     |
| 1:A:52:VAL:HG12 | 1:A:54:ILE:HG12  | 0.55     | 1.78        | 23     | 2     |
| 1:A:6:GLU:CB    | 1:A:145:ALA:HB2  | 0.55     | 2.31        | 19     | 1     |
| 1:A:16:TRP:CG   | 1:A:49:LEU:HD13  | 0.55     | 2.36        | 11     | 8     |
| 1:A:22:ASP:CG   | 1:A:35:ALA:CB    | 0.55     | 2.80        | 6      | 1     |
| 1:A:32:LEU:CD2  | 1:A:141:LEU:HD12 | 0.55     | 2.31        | 16     | 2     |
| 1:A:94:ALA:C    | 1:A:95:LEU:HD12  | 0.55     | 2.27        | 16     | 1     |
| 1:A:133:SER:OG  | 1:A:137:TRP:CE3  | 0.54     | 2.57        | 1      | 3     |
| 1:A:25:LEU:CD2  | 1:A:34:VAL:CG1   | 0.54     | 2.81        | 2      | 4     |
| 1:A:74:VAL:HG11 | 1:A:129:LEU:CD2  | 0.54     | 2.30        | 6      | 2     |
| 1:A:96:THR:HG23 | 1:A:97:SER:N     | 0.54     | 2.17        | 23     | 5     |
| 1:A:16:TRP:CH2  | 1:A:125:ILE:HD13 | 0.54     | 2.37        | 25     | 3     |
| 1:A:133:SER:HB3 | 1:A:137:TRP:CE3  | 0.54     | 2.37        | 24     | 19    |
| 1:A:27:THR:O    | 1:A:29:THR:N     | 0.54     | 2.40        | 25     | 11    |
| 1:A:13:PRO:O    | 1:A:15:GLY:N     | 0.54     | 2.41        | 8      | 6     |
| 1:A:52:VAL:HG12 | 1:A:53:ALA:N     | 0.54     | 2.18        | 16     | 13    |
| 1:A:122:GLU:CG  | 1:A:123:GLY:N    | 0.54     | 2.69        | 24     | 6     |
| 1:A:138:THR:CG2 | 1:A:139:LEU:N    | 0.54     | 2.70        | 12     | 11    |
| 1:A:9:PHE:CE2   | 1:A:32:LEU:HB2   | 0.54     | 2.38        | 4      | 3     |
| 1:A:22:ASP:C    | 1:A:24:PRO:CD    | 0.54     | 2.81        | 15     | 3     |
| 1:A:81:ASN:ND2  | 1:A:124:GLN:NE2  | 0.54     | 2.54        | 1      | 2     |
| 1:A:88:VAL:HG22 | 1:A:112:TYR:OH   | 0.54     | 2.03        | 14     | 4     |
| 1:A:29:THR:HG23 | 1:A:30:GLY:N     | 0.54     | 2.18        | 15     | 6     |
| 1:A:66:ALA:C    | 1:A:95:LEU:CD2   | 0.54     | 2.81        | 12     | 8     |
| 1:A:42:GLN:O    | 1:A:43:TYR:CB    | 0.54     | 2.54        | 8      | 2     |
| 1:A:73:THR:O    | 1:A:132:PHE:CD1  | 0.54     | 2.60        | 11     | 4     |
| 1:A:129:LEU:N   | 1:A:129:LEU:HD23 | 0.54     | 2.17        | 16     | 1     |
| 1:A:74:VAL:HA   | 1:A:132:PHE:CZ   | 0.54     | 2.38        | 12     | 7     |
| 1:A:31:ALA:HB3  | 1:A:140:CYS:HB3  | 0.54     | 1.78        | 15     | 1     |
| 1:A:88:VAL:CG1  | 1:A:109:SER:N    | 0.54     | 2.69        | 9      | 5     |
| 1:A:42:GLN:C    | 1:A:43:TYR:CG    | 0.54     | 2.81        | 8      | 2     |
| 1:A:64:TYR:OH   | 1:A:102:VAL:HG21 | 0.54     | 2.03        | 8      | 2     |
| 1:A:13:PRO:CB   | 1:A:25:LEU:HD11  | 0.54     | 2.33        | 9      | 1     |
| 1:A:15:GLY:O    | 1:A:17:VAL:CG1   | 0.54     | 2.56        | 21     | 8     |
| 1:A:17:VAL:O    | 1:A:47:VAL:CG1   | 0.54     | 2.56        | 2      | 24    |
| 1:A:77:LEU:C    | 1:A:78:VAL:CG2   | 0.54     | 2.81        | 24     | 25    |
| 1:A:8:THR:CG2   | 1:A:144:VAL:O    | 0.54     | 2.56        | 9      | 1     |
| 1:A:9:PHE:CE1   | 1:A:16:TRP:CD1   | 0.54     | 2.96        | 4      | 11    |
| 1:A:43:TYR:CG   | 1:A:44:GLY:N     | 0.54     | 2.75        | 1      | 3     |
| 1:A:78:VAL:HG21 | 1:A:89:LEU:HD13  | 0.54     | 1.80        | 21     | 5     |
| 1:A:8:THR:CG2   | 1:A:142:ASP:O    | 0.54     | 2.56        | 16     | 7     |

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| Atom-1          | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|-----------------|------------------|----------|-------------|--------|-------|
|                 |                  |          |             | Worst  | Total |
| 1:A:11:ASP:CG   | 1:A:11:ASP:O     | 0.54     | 2.50        | 6      | 3     |
| 1:A:20:GLY:CA   | 1:A:43:TYR:OH    | 0.54     | 2.56        | 9      | 5     |
| 1:A:40:SER:O    | 1:A:131:GLY:N    | 0.54     | 2.41        | 10     | 2     |
| 1:A:9:PHE:CD2   | 1:A:32:LEU:HB2   | 0.54     | 2.37        | 3      | 7     |
| 1:A:94:ALA:O    | 1:A:100:ARG:CD   | 0.54     | 2.56        | 9      | 25    |
| 1:A:112:TYR:N   | 1:A:112:TYR:CD1  | 0.54     | 2.74        | 9      | 12    |
| 1:A:9:PHE:CZ    | 1:A:144:VAL:HG21 | 0.54     | 2.38        | 18     | 5     |
| 1:A:17:VAL:HG22 | 1:A:48:VAL:HG23  | 0.53     | 1.80        | 22     | 17    |
| 1:A:107:THR:O   | 1:A:109:SER:N    | 0.53     | 2.42        | 23     | 8     |
| 1:A:77:LEU:C    | 1:A:77:LEU:CD1   | 0.53     | 2.80        | 1      | 6     |
| 1:A:80:GLN:NE2  | 1:A:81:ASN:C     | 0.53     | 2.67        | 22     | 3     |
| 1:A:81:ASN:ND2  | 1:A:124:GLN:CD   | 0.53     | 2.67        | 1      | 1     |
| 1:A:89:LEU:CD1  | 1:A:106:PHE:CE1  | 0.53     | 2.89        | 2      | 4     |
| 1:A:36:VAL:CG1  | 1:A:40:SER:OG    | 0.53     | 2.56        | 21     | 3     |
| 1:A:52:VAL:HG23 | 1:A:123:GLY:O    | 0.53     | 2.04        | 8      | 2     |
| 1:A:89:LEU:CD1  | 1:A:106:PHE:CZ   | 0.53     | 2.86        | 14     | 2     |
| 1:A:126:ALA:O   | 1:A:127:PHE:CD1  | 0.53     | 2.61        | 24     | 1     |
| 1:A:41:ALA:O    | 1:A:42:GLN:HG2   | 0.53     | 2.03        | 16     | 10    |
| 1:A:133:SER:CB  | 1:A:137:TRP:CE3  | 0.53     | 2.92        | 22     | 8     |
| 1:A:143:ASP:C   | 1:A:144:VAL:CG2  | 0.53     | 2.81        | 10     | 3     |
| 1:A:13:PRO:O    | 1:A:14:GLU:C     | 0.53     | 2.50        | 22     | 9     |
| 1:A:77:LEU:CD1  | 1:A:77:LEU:C     | 0.53     | 2.81        | 16     | 6     |
| 1:A:9:PHE:CD2   | 1:A:142:ASP:CA   | 0.53     | 2.91        | 20     | 2     |
| 1:A:40:SER:HB3  | 1:A:137:TRP:CH2  | 0.53     | 2.38        | 12     | 4     |
| 1:A:80:GLN:CD   | 1:A:81:ASN:N     | 0.53     | 2.66        | 1      | 3     |
| 1:A:45:VAL:N    | 1:A:130:GLY:HA3  | 0.53     | 2.18        | 10     | 1     |
| 1:A:58:THR:CG2  | 1:A:60:TYR:CE1   | 0.53     | 2.84        | 12     | 1     |
| 1:A:20:GLY:O    | 1:A:21:THR:OG1   | 0.53     | 2.23        | 15     | 1     |
| 1:A:55:GLU:O    | 1:A:56:GLU:CG    | 0.53     | 2.57        | 15     | 17    |
| 1:A:43:TYR:O    | 1:A:45:VAL:N     | 0.53     | 2.42        | 16     | 2     |
| 1:A:6:GLU:CG    | 1:A:145:ALA:CB   | 0.53     | 2.87        | 24     | 2     |
| 1:A:7:GLY:O     | 1:A:8:THR:CG2    | 0.53     | 2.57        | 17     | 1     |
| 1:A:9:PHE:CE1   | 1:A:144:VAL:CG2  | 0.53     | 2.91        | 22     | 1     |
| 1:A:40:SER:OG   | 1:A:45:VAL:CG2   | 0.53     | 2.56        | 12     | 5     |
| 1:A:68:ALA:CB   | 1:A:138:THR:O    | 0.53     | 2.57        | 25     | 14    |
| 1:A:8:THR:CB    | 1:A:142:ASP:O    | 0.53     | 2.57        | 4      | 3     |
| 1:A:74:VAL:O    | 1:A:92:SER:CB    | 0.53     | 2.57        | 23     | 3     |
| 1:A:80:GLN:CG   | 1:A:122:GLU:O    | 0.53     | 2.57        | 25     | 2     |
| 1:A:22:ASP:O    | 1:A:23:GLY:C     | 0.53     | 2.52        | 25     | 9     |
| 1:A:130:GLY:O   | 1:A:132:PHE:N    | 0.53     | 2.42        | 23     | 2     |
| 1:A:24:PRO:O    | 1:A:26:ASP:N     | 0.53     | 2.42        | 5      | 2     |

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| Atom-1          | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|-----------------|------------------|----------|-------------|--------|-------|
|                 |                  |          |             | Worst  | Total |
| 1:A:9:PHE:CG    | 1:A:142:ASP:HA   | 0.53     | 2.39        | 10     | 2     |
| 1:A:29:THR:HG23 | 1:A:31:ALA:HB3   | 0.53     | 1.81        | 19     | 2     |
| 1:A:42:GLN:O    | 1:A:44:GLY:N     | 0.53     | 2.42        | 22     | 10    |
| 1:A:22:ASP:HB3  | 1:A:35:ALA:CB    | 0.53     | 2.34        | 17     | 3     |
| 1:A:142:ASP:O   | 1:A:144:VAL:CG2  | 0.53     | 2.57        | 10     | 1     |
| 1:A:72:VAL:CG2  | 1:A:133:SER:HB2  | 0.53     | 2.34        | 22     | 21    |
| 1:A:64:TYR:CE1  | 1:A:102:VAL:HG21 | 0.53     | 2.37        | 2      | 8     |
| 1:A:103:THR:O   | 1:A:104:GLU:CG   | 0.53     | 2.57        | 22     | 6     |
| 1:A:52:VAL:CG1  | 1:A:53:ALA:N     | 0.53     | 2.71        | 11     | 10    |
| 1:A:5:GLY:O     | 1:A:6:GLU:CG     | 0.53     | 2.56        | 12     | 1     |
| 1:A:22:ASP:HB2  | 1:A:35:ALA:HB1   | 0.53     | 1.81        | 17     | 1     |
| 1:A:38:ALA:O    | 1:A:39:GLY:C     | 0.53     | 2.49        | 23     | 19    |
| 1:A:4:ILE:CG2   | 1:A:51:GLY:O     | 0.53     | 2.57        | 11     | 6     |
| 1:A:54:ILE:HG22 | 1:A:55:GLU:N     | 0.53     | 2.19        | 9      | 5     |
| 1:A:4:ILE:CG2   | 1:A:49:LEU:HD21  | 0.53     | 2.34        | 6      | 1     |
| 1:A:133:SER:O   | 1:A:134:ALA:C    | 0.53     | 2.51        | 7      | 1     |
| 1:A:64:TYR:CZ   | 1:A:102:VAL:CG2  | 0.53     | 2.85        | 8      | 1     |
| 1:A:47:VAL:C    | 1:A:48:VAL:HG13  | 0.53     | 2.29        | 9      | 1     |
| 1:A:70:THR:CG2  | 1:A:133:SER:OG   | 0.53     | 2.57        | 10     | 2     |
| 1:A:16:TRP:O    | 1:A:25:LEU:CD1   | 0.52     | 2.57        | 25     | 11    |
| 1:A:133:SER:HB3 | 1:A:137:TRP:CD2  | 0.52     | 2.39        | 12     | 13    |
| 1:A:39:GLY:N    | 1:A:134:ALA:O    | 0.52     | 2.42        | 14     | 9     |
| 1:A:4:ILE:CD1   | 1:A:144:VAL:HG12 | 0.52     | 2.34        | 5      | 4     |
| 1:A:37:PRO:CG   | 1:A:43:TYR:OH    | 0.52     | 2.57        | 8      | 1     |
| 1:A:46:GLY:CA   | 1:A:127:PHE:O    | 0.52     | 2.57        | 10     | 8     |
| 1:A:19:TYR:CE1  | 1:A:46:GLY:N     | 0.52     | 2.77        | 7      | 8     |
| 1:A:141:LEU:O   | 1:A:142:ASP:CB   | 0.52     | 2.56        | 5      | 21    |
| 1:A:47:VAL:O    | 1:A:48:VAL:CG1   | 0.52     | 2.57        | 9      | 1     |
| 1:A:9:PHE:O     | 1:A:10:ASP:C     | 0.52     | 2.51        | 4      | 5     |
| 1:A:65:THR:N    | 1:A:143:ASP:OD2  | 0.52     | 2.43        | 6      | 1     |
| 1:A:21:THR:CG2  | 1:A:43:TYR:OH    | 0.52     | 2.57        | 6      | 1     |
| 1:A:37:PRO:O    | 1:A:137:TRP:CZ3  | 0.52     | 2.62        | 7      | 1     |
| 1:A:64:TYR:CB   | 1:A:144:VAL:HG22 | 0.52     | 2.32        | 11     | 2     |
| 1:A:74:VAL:HA   | 1:A:132:PHE:CE2  | 0.52     | 2.40        | 15     | 7     |
| 1:A:106:PHE:C   | 1:A:106:PHE:CD1  | 0.52     | 2.87        | 23     | 1     |
| 1:A:46:GLY:C    | 1:A:47:VAL:HG23  | 0.52     | 2.29        | 10     | 8     |
| 1:A:43:TYR:O    | 1:A:45:VAL:CG2   | 0.52     | 2.58        | 16     | 2     |
| 1:A:5:GLY:N     | 1:A:14:GLU:CG    | 0.52     | 2.73        | 21     | 1     |
| 1:A:40:SER:CB   | 1:A:129:LEU:O    | 0.52     | 2.58        | 24     | 1     |
| 1:A:28:SER:O    | 1:A:29:THR:CB    | 0.52     | 2.57        | 5      | 4     |
| 1:A:122:GLU:N   | 1:A:122:GLU:OE1  | 0.52     | 2.43        | 21     | 6     |

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| Atom-1          | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|-----------------|------------------|----------|-------------|--------|-------|
|                 |                  |          |             | Worst  | Total |
| 1:A:70:THR:CG2  | 1:A:137:TRP:HB2  | 0.52     | 2.35        | 12     | 23    |
| 1:A:9:PHE:O     | 1:A:11:ASP:N     | 0.52     | 2.43        | 16     | 3     |
| 1:A:19:TYR:CD1  | 1:A:19:TYR:C     | 0.52     | 2.88        | 9      | 5     |
| 1:A:80:GLN:CG   | 1:A:86:GLY:N     | 0.52     | 2.72        | 5      | 4     |
| 1:A:50:ASN:O    | 1:A:50:ASN:ND2   | 0.52     | 2.43        | 15     | 2     |
| 1:A:81:ASN:OD1  | 1:A:124:GLN:NE2  | 0.52     | 2.43        | 15     | 1     |
| 1:A:40:SER:HB2  | 1:A:137:TRP:CZ3  | 0.52     | 2.40        | 1      | 1     |
| 1:A:38:ALA:O    | 1:A:40:SER:N     | 0.52     | 2.43        | 14     | 8     |
| 1:A:16:TRP:NE1  | 1:A:49:LEU:CD2   | 0.52     | 2.72        | 18     | 6     |
| 1:A:55:GLU:O    | 1:A:56:GLU:HB3   | 0.52     | 2.05        | 12     | 3     |
| 1:A:90:ASP:O    | 1:A:91:THR:CG2   | 0.52     | 2.58        | 23     | 6     |
| 1:A:42:GLN:HG2  | 1:A:43:TYR:CE1   | 0.52     | 2.40        | 8      | 1     |
| 1:A:9:PHE:CG    | 1:A:32:LEU:HB2   | 0.52     | 2.40        | 25     | 2     |
| 1:A:122:GLU:CD  | 1:A:122:GLU:N    | 0.52     | 2.67        | 16     | 2     |
| 1:A:5:GLY:O     | 1:A:7:GLY:N      | 0.52     | 2.43        | 21     | 8     |
| 1:A:6:GLU:CG    | 1:A:6:GLU:O      | 0.52     | 2.57        | 19     | 1     |
| 1:A:83:ALA:HB2  | 1:A:85:TYR:CZ    | 0.52     | 2.40        | 15     | 4     |
| 1:A:43:TYR:CE2  | 1:A:44:GLY:O     | 0.52     | 2.63        | 18     | 3     |
| 1:A:74:VAL:HA   | 1:A:132:PHE:CE1  | 0.52     | 2.41        | 12     | 11    |
| 1:A:36:VAL:HG11 | 1:A:137:TRP:CH2  | 0.52     | 2.38        | 24     | 4     |
| 1:A:16:TRP:HB3  | 1:A:32:LEU:HD13  | 0.52     | 1.81        | 16     | 1     |
| 1:A:20:GLY:N    | 1:A:43:TYR:OH    | 0.52     | 2.43        | 17     | 2     |
| 1:A:113:PRO:O   | 1:A:114:ALA:C    | 0.51     | 2.51        | 25     | 2     |
| 1:A:54:ILE:CD1  | 1:A:60:TYR:CD2   | 0.51     | 2.93        | 12     | 1     |
| 1:A:80:GLN:OE1  | 1:A:82:GLY:N     | 0.51     | 2.43        | 15     | 1     |
| 1:A:81:ASN:OD1  | 1:A:124:GLN:CG   | 0.51     | 2.57        | 15     | 1     |
| 1:A:9:PHE:CD1   | 1:A:13:PRO:HB3   | 0.51     | 2.40        | 8      | 2     |
| 1:A:96:THR:HG22 | 1:A:100:ARG:HG3  | 0.51     | 1.80        | 14     | 1     |
| 1:A:20:GLY:O    | 1:A:45:VAL:CG1   | 0.51     | 2.57        | 21     | 3     |
| 1:A:9:PHE:CE2   | 1:A:144:VAL:HG23 | 0.51     | 2.41        | 2      | 1     |
| 1:A:142:ASP:OD1 | 1:A:142:ASP:N    | 0.51     | 2.44        | 9      | 4     |
| 1:A:112:TYR:CD2 | 1:A:123:GLY:HA3  | 0.51     | 2.41        | 13     | 1     |
| 1:A:9:PHE:CZ    | 1:A:16:TRP:CD1   | 0.51     | 2.98        | 1      | 4     |
| 1:A:21:THR:CG2  | 1:A:37:PRO:HD3   | 0.51     | 2.36        | 5      | 1     |
| 1:A:18:ALA:HB3  | 1:A:25:LEU:HB3   | 0.51     | 1.81        | 6      | 1     |
| 1:A:142:ASP:N   | 1:A:142:ASP:OD1  | 0.51     | 2.43        | 15     | 4     |
| 1:A:42:GLN:CG   | 1:A:43:TYR:CZ    | 0.51     | 2.94        | 8      | 1     |
| 1:A:74:VAL:CG2  | 1:A:129:LEU:HD22 | 0.51     | 2.32        | 10     | 1     |
| 1:A:103:THR:C   | 1:A:104:GLU:CG   | 0.51     | 2.83        | 10     | 2     |
| 1:A:94:ALA:O    | 1:A:100:ARG:NE   | 0.51     | 2.43        | 16     | 1     |
| 1:A:19:TYR:CE1  | 1:A:46:GLY:C     | 0.51     | 2.88        | 17     | 1     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:16:TRP:N    | 1:A:49:LEU:CD1  | 0.51     | 2.74        | 6      | 3     |
| 1:A:58:THR:HG21 | 1:A:148:SER:HB2 | 0.51     | 1.80        | 12     | 1     |
| 1:A:63:ARG:NH2  | 1:A:143:ASP:OD2 | 0.51     | 2.43        | 19     | 1     |
| 1:A:42:GLN:HG2  | 1:A:43:TYR:N    | 0.51     | 2.21        | 22     | 3     |
| 1:A:130:GLY:O   | 1:A:131:GLY:C   | 0.51     | 2.54        | 20     | 13    |
| 1:A:55:GLU:O    | 1:A:56:GLU:C    | 0.51     | 2.54        | 24     | 19    |
| 1:A:80:GLN:O    | 1:A:81:ASN:ND2  | 0.51     | 2.43        | 2      | 1     |
| 1:A:22:ASP:OD2  | 1:A:37:PRO:N    | 0.51     | 2.43        | 4      | 1     |
| 1:A:17:VAL:CG2  | 1:A:48:VAL:HG23 | 0.51     | 2.36        | 5      | 18    |
| 1:A:6:GLU:HA    | 1:A:145:ALA:HB2 | 0.51     | 1.83        | 15     | 1     |
| 1:A:36:VAL:HG13 | 1:A:40:SER:OG   | 0.51     | 2.06        | 21     | 2     |
| 1:A:64:TYR:OH   | 1:A:93:PRO:CB   | 0.51     | 2.57        | 21     | 1     |
| 1:A:20:GLY:C    | 1:A:43:TYR:HH   | 0.51     | 2.13        | 5      | 2     |
| 1:A:72:VAL:HG11 | 1:A:137:TRP:NE1 | 0.51     | 2.20        | 7      | 1     |
| 1:A:17:VAL:CG2  | 1:A:17:VAL:O    | 0.51     | 2.59        | 9      | 1     |
| 1:A:6:GLU:HG3   | 1:A:145:ALA:HB2 | 0.51     | 1.81        | 25     | 2     |
| 1:A:129:LEU:O   | 1:A:130:GLY:O   | 0.51     | 2.29        | 10     | 2     |
| 1:A:33:CYS:SG   | 1:A:138:THR:CG2 | 0.51     | 2.99        | 7      | 5     |
| 1:A:52:VAL:CG2  | 1:A:124:GLN:HA  | 0.51     | 2.36        | 6      | 15    |
| 1:A:37:PRO:CD   | 1:A:45:VAL:HG21 | 0.51     | 2.35        | 7      | 1     |
| 1:A:40:SER:HB3  | 1:A:137:TRP:CZ3 | 0.51     | 2.41        | 12     | 1     |
| 1:A:128:GLN:C   | 1:A:129:LEU:CD2 | 0.50     | 2.84        | 14     | 2     |
| 1:A:7:GLY:O     | 1:A:144:VAL:N   | 0.50     | 2.44        | 22     | 3     |
| 1:A:45:VAL:O    | 1:A:129:LEU:C   | 0.50     | 2.54        | 25     | 6     |
| 1:A:82:GLY:CA   | 1:A:85:TYR:CE1  | 0.50     | 2.93        | 25     | 4     |
| 1:A:19:TYR:N    | 1:A:22:ASP:OD2  | 0.50     | 2.44        | 20     | 1     |
| 1:A:40:SER:CB   | 1:A:137:TRP:CH2 | 0.50     | 2.95        | 1      | 3     |
| 1:A:40:SER:HB2  | 1:A:45:VAL:CG2  | 0.50     | 2.36        | 4      | 3     |
| 1:A:42:GLN:HG3  | 1:A:43:TYR:CD2  | 0.50     | 2.41        | 11     | 6     |
| 1:A:8:THR:HG21  | 1:A:144:VAL:HB  | 0.50     | 1.82        | 9      | 1     |
| 1:A:16:TRP:CD2  | 1:A:49:LEU:HD22 | 0.50     | 2.41        | 10     | 2     |
| 1:A:6:GLU:HG2   | 1:A:145:ALA:CB  | 0.50     | 2.36        | 24     | 2     |
| 1:A:5:GLY:N     | 1:A:14:GLU:HG3  | 0.50     | 2.21        | 21     | 1     |
| 1:A:74:VAL:HA   | 1:A:132:PHE:CD2 | 0.50     | 2.41        | 3      | 11    |
| 1:A:24:PRO:O    | 1:A:25:LEU:C    | 0.50     | 2.54        | 20     | 10    |
| 1:A:45:VAL:O    | 1:A:129:LEU:N   | 0.50     | 2.44        | 23     | 8     |
| 1:A:20:GLY:HA3  | 1:A:45:VAL:CG1  | 0.50     | 2.36        | 4      | 1     |
| 1:A:40:SER:OG   | 1:A:131:GLY:CA  | 0.50     | 2.59        | 5      | 1     |
| 1:A:81:ASN:CB   | 1:A:122:GLU:OE2 | 0.50     | 2.59        | 4      | 4     |
| 1:A:40:SER:CB   | 1:A:45:VAL:CG2  | 0.50     | 2.89        | 4      | 1     |
| 1:A:111:THR:C   | 1:A:112:TYR:CD1 | 0.50     | 2.90        | 25     | 9     |

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| Atom-1          | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|-----------------|------------------|----------|-------------|--------|-------|
|                 |                  |          |             | Worst  | Total |
| 1:A:66:ALA:CB   | 1:A:95:LEU:CD2   | 0.50     | 2.89        | 8      | 3     |
| 1:A:59:THR:CG2  | 1:A:105:THR:HG22 | 0.50     | 2.37        | 12     | 2     |
| 1:A:80:GLN:NE2  | 1:A:82:GLY:O     | 0.50     | 2.45        | 7      | 1     |
| 1:A:25:LEU:HB2  | 1:A:34:VAL:HG12  | 0.50     | 1.81        | 16     | 1     |
| 1:A:74:VAL:CG2  | 1:A:93:PRO:HG2   | 0.50     | 2.37        | 17     | 17    |
| 1:A:38:ALA:O    | 1:A:39:GLY:O     | 0.50     | 2.29        | 2      | 3     |
| 1:A:71:ASP:OD1  | 1:A:96:THR:CB    | 0.50     | 2.60        | 2      | 1     |
| 1:A:61:THR:OG1  | 1:A:105:THR:CG2  | 0.50     | 2.58        | 10     | 3     |
| 1:A:68:ALA:HB3  | 1:A:95:LEU:HB3   | 0.50     | 1.82        | 16     | 1     |
| 1:A:36:VAL:CG1  | 1:A:137:TRP:CE2  | 0.50     | 2.91        | 2      | 14    |
| 1:A:8:THR:HG22  | 1:A:143:ASP:N    | 0.50     | 2.20        | 3      | 1     |
| 1:A:20:GLY:HA2  | 1:A:43:TYR:CE1   | 0.50     | 2.42        | 14     | 7     |
| 1:A:60:TYR:HB3  | 1:A:106:PHE:CZ   | 0.50     | 2.42        | 21     | 3     |
| 1:A:43:TYR:CZ   | 1:A:44:GLY:O     | 0.50     | 2.65        | 9      | 2     |
| 1:A:55:GLU:O    | 1:A:56:GLU:CB    | 0.50     | 2.57        | 12     | 1     |
| 1:A:68:ALA:O    | 1:A:69:SER:C     | 0.50     | 2.55        | 17     | 16    |
| 1:A:74:VAL:HA   | 1:A:132:PHE:CD1  | 0.50     | 2.42        | 5      | 23    |
| 1:A:64:TYR:O    | 1:A:102:VAL:HG23 | 0.50     | 2.07        | 15     | 2     |
| 1:A:130:GLY:O   | 1:A:132:PHE:CD1  | 0.50     | 2.65        | 3      | 2     |
| 1:A:94:ALA:CB   | 1:A:100:ARG:NH1  | 0.50     | 2.75        | 15     | 1     |
| 1:A:36:VAL:CG1  | 1:A:137:TRP:CH2  | 0.50     | 2.95        | 14     | 10    |
| 1:A:32:LEU:O    | 1:A:139:LEU:O    | 0.50     | 2.30        | 18     | 8     |
| 1:A:129:LEU:N   | 1:A:129:LEU:CD2  | 0.50     | 2.67        | 4      | 3     |
| 1:A:32:LEU:HD23 | 1:A:32:LEU:O     | 0.50     | 2.06        | 5      | 1     |
| 1:A:79:GLY:CA   | 1:A:86:GLY:O     | 0.50     | 2.60        | 13     | 1     |
| 1:A:138:THR:O   | 1:A:139:LEU:HD12 | 0.50     | 2.07        | 18     | 1     |
| 1:A:25:LEU:HD13 | 1:A:32:LEU:CD1   | 0.49     | 2.37        | 6      | 2     |
| 1:A:20:GLY:HA2  | 1:A:43:TYR:CD1   | 0.49     | 2.42        | 25     | 3     |
| 1:A:8:THR:O     | 1:A:9:PHE:C      | 0.49     | 2.53        | 25     | 8     |
| 1:A:5:GLY:O     | 1:A:6:GLU:C      | 0.49     | 2.55        | 12     | 13    |
| 1:A:46:GLY:HA2  | 1:A:127:PHE:O    | 0.49     | 2.06        | 10     | 9     |
| 1:A:45:VAL:HG12 | 1:A:46:GLY:N     | 0.49     | 2.22        | 10     | 3     |
| 1:A:41:ALA:C    | 1:A:42:GLN:CD    | 0.49     | 2.80        | 12     | 3     |
| 1:A:17:VAL:O    | 1:A:47:VAL:HA    | 0.49     | 2.07        | 3      | 9     |
| 1:A:20:GLY:O    | 1:A:43:TYR:CZ    | 0.49     | 2.66        | 3      | 2     |
| 1:A:70:THR:HG21 | 1:A:137:TRP:HB3  | 0.49     | 1.84        | 14     | 4     |
| 1:A:16:TRP:HH2  | 1:A:125:ILE:HD13 | 0.49     | 1.66        | 6      | 1     |
| 1:A:25:LEU:HD23 | 1:A:34:VAL:CG1   | 0.49     | 2.37        | 22     | 1     |
| 1:A:84:PRO:O    | 1:A:85:TYR:CB    | 0.49     | 2.60        | 20     | 8     |
| 1:A:88:VAL:HG11 | 1:A:110:ALA:HB3  | 0.49     | 1.84        | 2      | 1     |
| 1:A:98:GLU:CB   | 1:A:99:PRO:HD2   | 0.49     | 2.37        | 24     | 9     |

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| Atom-1          | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|-----------------|------------------|----------|-------------|--------|-------|
|                 |                  |          |             | Worst  | Total |
| 1:A:22:ASP:C    | 1:A:24:PRO:HD3   | 0.49     | 2.33        | 12     | 3     |
| 1:A:64:TYR:CE2  | 1:A:102:VAL:HB   | 0.49     | 2.42        | 10     | 5     |
| 1:A:4:ILE:CG1   | 1:A:5:GLY:N      | 0.49     | 2.75        | 19     | 3     |
| 1:A:27:THR:O    | 1:A:28:SER:C     | 0.49     | 2.54        | 1      | 13    |
| 1:A:52:VAL:HG12 | 1:A:53:ALA:H     | 0.49     | 1.66        | 10     | 2     |
| 1:A:143:ASP:CG  | 1:A:143:ASP:O    | 0.49     | 2.55        | 21     | 5     |
| 1:A:72:VAL:HG21 | 1:A:133:SER:HB2  | 0.49     | 1.84        | 21     | 1     |
| 1:A:81:ASN:HB2  | 1:A:122:GLU:O    | 0.49     | 2.08        | 22     | 5     |
| 1:A:10:ASP:O    | 1:A:10:ASP:CG    | 0.49     | 2.56        | 22     | 8     |
| 1:A:80:GLN:CD   | 1:A:85:TYR:C     | 0.49     | 2.81        | 5      | 5     |
| 1:A:20:GLY:C    | 1:A:43:TYR:OH    | 0.49     | 2.55        | 6      | 1     |
| 1:A:10:ASP:C    | 1:A:11:ASP:CG    | 0.49     | 2.80        | 17     | 1     |
| 1:A:82:GLY:O    | 1:A:83:ALA:HB3   | 0.49     | 2.08        | 1      | 6     |
| 1:A:13:PRO:HB3  | 1:A:32:LEU:CD1   | 0.49     | 2.36        | 16     | 8     |
| 1:A:125:ILE:CG2 | 1:A:127:PHE:CE1  | 0.49     | 2.96        | 18     | 16    |
| 1:A:19:TYR:C    | 1:A:22:ASP:OD2   | 0.49     | 2.56        | 20     | 2     |
| 1:A:40:SER:OG   | 1:A:129:LEU:O    | 0.49     | 2.31        | 15     | 3     |
| 1:A:9:PHE:CG    | 1:A:13:PRO:HB3   | 0.49     | 2.43        | 20     | 1     |
| 1:A:27:THR:HG22 | 1:A:32:LEU:N     | 0.49     | 2.21        | 20     | 1     |
| 1:A:4:ILE:CD1   | 1:A:144:VAL:CG1  | 0.49     | 2.91        | 5      | 1     |
| 1:A:133:SER:HB3 | 1:A:137:TRP:CZ3  | 0.49     | 2.43        | 5      | 1     |
| 1:A:125:ILE:CG2 | 1:A:127:PHE:CE2  | 0.49     | 2.95        | 13     | 2     |
| 1:A:25:LEU:HB3  | 1:A:32:LEU:CD1   | 0.49     | 2.38        | 7      | 2     |
| 1:A:90:ASP:C    | 1:A:91:THR:HG23  | 0.49     | 2.32        | 18     | 4     |
| 1:A:6:GLU:HG3   | 1:A:145:ALA:CB   | 0.49     | 2.38        | 25     | 2     |
| 1:A:15:GLY:O    | 1:A:16:TRP:C     | 0.49     | 2.56        | 21     | 3     |
| 1:A:76:ALA:N    | 1:A:93:PRO:HD3   | 0.49     | 2.23        | 14     | 13    |
| 1:A:94:ALA:HB3  | 1:A:100:ARG:HE   | 0.49     | 1.60        | 2      | 1     |
| 1:A:17:VAL:CG2  | 1:A:48:VAL:HG22  | 0.48     | 2.38        | 6      | 13    |
| 1:A:56:GLU:O    | 1:A:108:ALA:O    | 0.48     | 2.31        | 23     | 24    |
| 1:A:135:ASP:O   | 1:A:136:ALA:C    | 0.48     | 2.56        | 5      | 4     |
| 1:A:70:THR:O    | 1:A:71:ASP:C     | 0.48     | 2.56        | 7      | 6     |
| 1:A:84:PRO:C    | 1:A:85:TYR:CG    | 0.48     | 2.89        | 15     | 5     |
| 1:A:52:VAL:HG13 | 1:A:146:LEU:HD23 | 0.48     | 1.85        | 6      | 1     |
| 1:A:122:GLU:HG2 | 1:A:123:GLY:N    | 0.48     | 2.23        | 25     | 3     |
| 1:A:9:PHE:O     | 1:A:30:GLY:C     | 0.48     | 2.56        | 1      | 3     |
| 1:A:41:ALA:C    | 1:A:42:GLN:OE1   | 0.48     | 2.56        | 1      | 1     |
| 1:A:4:ILE:HD11  | 1:A:144:VAL:HG12 | 0.48     | 1.84        | 21     | 2     |
| 1:A:9:PHE:O     | 1:A:10:ASP:CG    | 0.48     | 2.56        | 15     | 2     |
| 1:A:41:ALA:O    | 1:A:42:GLN:CD    | 0.48     | 2.56        | 22     | 2     |
| 1:A:74:VAL:HA   | 1:A:132:PHE:CG   | 0.48     | 2.44        | 11     | 19    |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:19:TYR:CD2  | 1:A:19:TYR:O    | 0.48     | 2.67        | 4      | 1     |
| 1:A:82:GLY:O    | 1:A:83:ALA:C    | 0.48     | 2.57        | 25     | 8     |
| 1:A:70:THR:HG23 | 1:A:133:SER:OG  | 0.48     | 2.08        | 21     | 1     |
| 1:A:17:VAL:CA   | 1:A:25:LEU:HD11 | 0.48     | 2.34        | 25     | 1     |
| 1:A:113:PRO:O   | 1:A:122:GLU:CB  | 0.48     | 2.61        | 2      | 4     |
| 1:A:141:LEU:C   | 1:A:142:ASP:OD1 | 0.48     | 2.57        | 3      | 4     |
| 1:A:42:GLN:HG3  | 1:A:43:TYR:CE2  | 0.48     | 2.44        | 8      | 2     |
| 1:A:17:VAL:O    | 1:A:17:VAL:HG23 | 0.48     | 2.07        | 9      | 1     |
| 1:A:7:GLY:C     | 1:A:8:THR:CG2   | 0.48     | 2.86        | 17     | 1     |
| 1:A:37:PRO:O    | 1:A:38:ALA:C    | 0.48     | 2.56        | 15     | 12    |
| 1:A:81:ASN:N    | 1:A:122:GLU:O   | 0.48     | 2.46        | 3      | 11    |
| 1:A:98:GLU:CG   | 1:A:99:PRO:HD2  | 0.48     | 2.39        | 24     | 6     |
| 1:A:112:TYR:CD1 | 1:A:112:TYR:N   | 0.48     | 2.76        | 25     | 4     |
| 1:A:80:GLN:OE1  | 1:A:85:TYR:CA   | 0.48     | 2.62        | 25     | 1     |
| 1:A:11:ASP:O    | 1:A:11:ASP:CG   | 0.48     | 2.57        | 18     | 4     |
| 1:A:124:GLN:NE2 | 1:A:125:ILE:O   | 0.48     | 2.46        | 3      | 2     |
| 1:A:142:ASP:O   | 1:A:143:ASP:C   | 0.48     | 2.55        | 10     | 5     |
| 1:A:43:TYR:O    | 1:A:44:GLY:C    | 0.48     | 2.57        | 7      | 6     |
| 1:A:15:GLY:O    | 1:A:17:VAL:N    | 0.48     | 2.46        | 17     | 2     |
| 1:A:63:ARG:O    | 1:A:143:ASP:O   | 0.48     | 2.32        | 9      | 20    |
| 1:A:112:TYR:CG  | 1:A:123:GLY:HA3 | 0.48     | 2.43        | 5      | 12    |
| 1:A:4:ILE:O     | 1:A:14:GLU:CD   | 0.48     | 2.57        | 19     | 5     |
| 1:A:41:ALA:O    | 1:A:42:GLN:HB3  | 0.48     | 2.08        | 24     | 5     |
| 1:A:50:ASN:OD1  | 1:A:122:GLU:CD  | 0.48     | 2.57        | 5      | 1     |
| 1:A:3:PRO:C     | 1:A:4:ILE:CG2   | 0.48     | 2.87        | 25     | 2     |
| 1:A:25:LEU:N    | 1:A:25:LEU:HD23 | 0.48     | 2.24        | 23     | 1     |
| 1:A:10:ASP:C    | 1:A:10:ASP:OD1  | 0.48     | 2.57        | 6      | 2     |
| 1:A:7:GLY:C     | 1:A:143:ASP:CG  | 0.48     | 2.81        | 10     | 1     |
| 1:A:7:GLY:C     | 1:A:8:THR:OG1   | 0.48     | 2.56        | 11     | 1     |
| 1:A:80:GLN:OE1  | 1:A:122:GLU:C   | 0.48     | 2.57        | 13     | 1     |
| 1:A:81:ASN:OD1  | 1:A:123:GLY:C   | 0.48     | 2.57        | 21     | 1     |
| 1:A:72:VAL:HG11 | 1:A:137:TRP:CD1 | 0.48     | 2.43        | 25     | 1     |
| 1:A:33:CYS:HA   | 1:A:139:LEU:O   | 0.48     | 2.09        | 17     | 19    |
| 1:A:74:VAL:HG23 | 1:A:93:PRO:HG2  | 0.48     | 1.86        | 1      | 6     |
| 1:A:81:ASN:O    | 1:A:122:GLU:N   | 0.48     | 2.47        | 23     | 3     |
| 1:A:46:GLY:C    | 1:A:47:VAL:CG2  | 0.48     | 2.86        | 24     | 8     |
| 1:A:73:THR:HG22 | 1:A:73:THR:O    | 0.48     | 2.09        | 22     | 2     |
| 1:A:4:ILE:HG13  | 1:A:5:GLY:N     | 0.48     | 2.24        | 16     | 3     |
| 1:A:22:ASP:OD1  | 1:A:22:ASP:O    | 0.48     | 2.32        | 20     | 1     |
| 1:A:63:ARG:CG   | 1:A:143:ASP:OD2 | 0.48     | 2.62        | 21     | 1     |
| 1:A:42:GLN:HG2  | 1:A:43:TYR:CD2  | 0.47     | 2.44        | 22     | 2     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:28:SER:O     | 1:A:29:THR:C     | 0.47     | 2.56        | 14     | 4     |
| 1:A:55:GLU:CG    | 1:A:111:THR:HG23 | 0.47     | 2.39        | 8      | 2     |
| 1:A:78:VAL:HG12  | 1:A:79:GLY:H     | 0.47     | 1.68        | 9      | 1     |
| 1:A:16:TRP:CA    | 1:A:49:LEU:HD13  | 0.47     | 2.38        | 21     | 1     |
| 1:A:71:ASP:O     | 1:A:71:ASP:CG    | 0.47     | 2.57        | 8      | 3     |
| 1:A:141:LEU:C    | 1:A:142:ASP:OD2  | 0.47     | 2.57        | 14     | 5     |
| 1:A:19:TYR:CE1   | 1:A:46:GLY:CA    | 0.47     | 2.97        | 8      | 4     |
| 1:A:131:GLY:O    | 1:A:132:PHE:CD2  | 0.47     | 2.67        | 13     | 1     |
| 1:A:142:ASP:CG   | 1:A:143:ASP:OD1  | 0.47     | 2.57        | 19     | 1     |
| 1:A:8:THR:C      | 1:A:142:ASP:O    | 0.47     | 2.57        | 20     | 1     |
| 1:A:74:VAL:CG2   | 1:A:75:ARG:N     | 0.47     | 2.70        | 25     | 2     |
| 1:A:28:SER:C     | 1:A:29:THR:OG1   | 0.47     | 2.57        | 23     | 1     |
| 1:A:3:PRO:CG     | 1:A:52:VAL:HA    | 0.47     | 2.39        | 25     | 1     |
| 1:A:79:GLY:HA2   | 1:A:112:TYR:OH   | 0.47     | 2.09        | 5      | 22    |
| 1:A:80:GLN:O     | 1:A:81:ASN:CG    | 0.47     | 2.57        | 10     | 7     |
| 1:A:107:THR:HG22 | 1:A:107:THR:O    | 0.47     | 2.09        | 2      | 2     |
| 1:A:94:ALA:O     | 1:A:100:ARG:HD3  | 0.47     | 2.09        | 7      | 11    |
| 1:A:67:THR:CG2   | 1:A:98:GLU:O     | 0.47     | 2.60        | 12     | 3     |
| 1:A:41:ALA:O     | 1:A:42:GLN:OE1   | 0.47     | 2.33        | 12     | 3     |
| 1:A:70:THR:CG2   | 1:A:137:TRP:HB3  | 0.47     | 2.38        | 7      | 2     |
| 1:A:43:TYR:O     | 1:A:44:GLY:O     | 0.47     | 2.32        | 15     | 3     |
| 1:A:78:VAL:O     | 1:A:87:THR:HG22  | 0.47     | 2.10        | 6      | 2     |
| 1:A:77:LEU:O     | 1:A:78:VAL:CG2   | 0.47     | 2.63        | 3      | 1     |
| 1:A:7:GLY:O      | 1:A:143:ASP:C    | 0.47     | 2.57        | 4      | 1     |
| 1:A:81:ASN:OD1   | 1:A:124:GLN:CD   | 0.47     | 2.57        | 9      | 3     |
| 1:A:68:ALA:O     | 1:A:96:THR:O     | 0.47     | 2.32        | 15     | 7     |
| 1:A:7:GLY:O      | 1:A:142:ASP:O    | 0.47     | 2.32        | 17     | 1     |
| 1:A:41:ALA:O     | 1:A:42:GLN:C     | 0.47     | 2.56        | 1      | 5     |
| 1:A:43:TYR:CE1   | 1:A:44:GLY:C     | 0.47     | 2.92        | 1      | 2     |
| 1:A:72:VAL:HG12  | 1:A:95:LEU:HB2   | 0.47     | 1.86        | 2      | 6     |
| 1:A:95:LEU:O     | 1:A:96:THR:CB    | 0.47     | 2.62        | 5      | 2     |
| 1:A:16:TRP:HB2   | 1:A:32:LEU:HD13  | 0.47     | 1.84        | 16     | 3     |
| 1:A:21:THR:HG23  | 1:A:43:TYR:OH    | 0.47     | 2.09        | 6      | 2     |
| 1:A:54:ILE:HB    | 1:A:112:TYR:CG   | 0.47     | 2.44        | 12     | 2     |
| 1:A:142:ASP:C    | 1:A:143:ASP:OD1  | 0.47     | 2.57        | 6      | 1     |
| 1:A:40:SER:O     | 1:A:130:GLY:C    | 0.47     | 2.58        | 10     | 1     |
| 1:A:10:ASP:HA    | 1:A:30:GLY:CA    | 0.47     | 2.39        | 16     | 2     |
| 1:A:90:ASP:CG    | 1:A:90:ASP:O     | 0.47     | 2.57        | 11     | 1     |
| 1:A:36:VAL:CG1   | 1:A:40:SER:HB3   | 0.47     | 2.39        | 15     | 1     |
| 1:A:10:ASP:O     | 1:A:11:ASP:CG    | 0.47     | 2.58        | 19     | 6     |
| 1:A:13:PRO:O     | 1:A:14:GLU:CB    | 0.47     | 2.63        | 24     | 8     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:80:GLN:HA   | 1:A:122:GLU:O   | 0.47     | 2.09        | 2      | 9     |
| 1:A:26:ASP:O    | 1:A:31:ALA:O    | 0.47     | 2.33        | 5      | 4     |
| 1:A:21:THR:CG2  | 1:A:43:TYR:HH   | 0.47     | 2.22        | 6      | 1     |
| 1:A:25:LEU:O    | 1:A:26:ASP:C    | 0.47     | 2.57        | 7      | 1     |
| 1:A:142:ASP:O   | 1:A:143:ASP:CG  | 0.47     | 2.58        | 23     | 7     |
| 1:A:40:SER:O    | 1:A:40:SER:OG   | 0.47     | 2.29        | 22     | 3     |
| 1:A:64:TYR:CZ   | 1:A:102:VAL:HB  | 0.47     | 2.45        | 10     | 2     |
| 1:A:54:ILE:HG23 | 1:A:108:ALA:CB  | 0.47     | 2.39        | 12     | 1     |
| 1:A:42:GLN:O    | 1:A:42:GLN:HG3  | 0.47     | 2.08        | 15     | 1     |
| 1:A:34:VAL:HG11 | 1:A:47:VAL:CG2  | 0.47     | 2.39        | 17     | 1     |
| 1:A:9:PHE:CE2   | 1:A:142:ASP:O   | 0.47     | 2.68        | 19     | 1     |
| 1:A:13:PRO:CG   | 1:A:32:LEU:HD12 | 0.47     | 2.38        | 20     | 1     |
| 1:A:82:GLY:O    | 1:A:83:ALA:O    | 0.47     | 2.33        | 8      | 6     |
| 1:A:106:PHE:CD1 | 1:A:106:PHE:C   | 0.47     | 2.93        | 1      | 7     |
| 1:A:9:PHE:O     | 1:A:10:ASP:OD2  | 0.47     | 2.33        | 6      | 1     |
| 1:A:43:TYR:O    | 1:A:43:TYR:CD1  | 0.47     | 2.67        | 10     | 1     |
| 1:A:16:TRP:CE2  | 1:A:49:LEU:HD23 | 0.47     | 2.44        | 15     | 1     |
| 1:A:80:GLN:CD   | 1:A:86:GLY:N    | 0.47     | 2.73        | 24     | 2     |
| 1:A:11:ASP:O    | 1:A:12:GLY:C    | 0.47     | 2.58        | 22     | 1     |
| 1:A:72:VAL:CB   | 1:A:133:SER:HB2 | 0.47     | 2.40        | 6      | 2     |
| 1:A:93:PRO:O    | 1:A:94:ALA:C    | 0.47     | 2.57        | 18     | 3     |
| 1:A:36:VAL:O    | 1:A:137:TRP:O   | 0.47     | 2.33        | 23     | 2     |
| 1:A:22:ASP:O    | 1:A:23:GLY:O    | 0.47     | 2.33        | 7      | 10    |
| 1:A:37:PRO:O    | 1:A:38:ALA:O    | 0.47     | 2.32        | 23     | 3     |
| 1:A:42:GLN:C    | 1:A:44:GLY:N    | 0.47     | 2.73        | 11     | 8     |
| 1:A:124:GLN:N   | 1:A:124:GLN:CD  | 0.47     | 2.72        | 2      | 1     |
| 1:A:10:ASP:O    | 1:A:10:ASP:OD2  | 0.47     | 2.33        | 5      | 3     |
| 1:A:103:THR:O   | 1:A:104:GLU:CD  | 0.47     | 2.58        | 7      | 1     |
| 1:A:133:SER:O   | 1:A:135:ASP:O   | 0.47     | 2.33        | 7      | 1     |
| 1:A:71:ASP:OD1  | 1:A:95:LEU:O    | 0.47     | 2.33        | 9      | 3     |
| 1:A:27:THR:C    | 1:A:28:SER:OG   | 0.47     | 2.58        | 9      | 2     |
| 1:A:71:ASP:CG   | 1:A:71:ASP:O    | 0.47     | 2.57        | 9      | 4     |
| 1:A:34:VAL:O    | 1:A:138:THR:OG1 | 0.47     | 2.32        | 13     | 12    |
| 1:A:24:PRO:O    | 1:A:25:LEU:O    | 0.47     | 2.33        | 16     | 5     |
| 1:A:67:THR:CA   | 1:A:95:LEU:HD22 | 0.47     | 2.40        | 6      | 1     |
| 1:A:71:ASP:O    | 1:A:71:ASP:OD1  | 0.47     | 2.33        | 9      | 1     |
| 1:A:50:ASN:OD1  | 1:A:50:ASN:O    | 0.47     | 2.33        | 19     | 7     |
| 1:A:54:ILE:CG2  | 1:A:108:ALA:CB  | 0.47     | 2.92        | 24     | 3     |
| 1:A:21:THR:HG21 | 1:A:37:PRO:HB3  | 0.47     | 1.85        | 20     | 1     |
| 1:A:70:THR:O    | 1:A:71:ASP:O    | 0.47     | 2.33        | 21     | 1     |
| 1:A:55:GLU:O    | 1:A:56:GLU:HG2  | 0.46     | 2.10        | 3      | 18    |

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| Atom-1          | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|-----------------|------------------|----------|-------------|--------|-------|
|                 |                  |          |             | Worst  | Total |
| 1:A:56:GLU:N    | 1:A:110:ALA:O    | 0.46     | 2.48        | 7      | 15    |
| 1:A:80:GLN:HG3  | 1:A:122:GLU:O    | 0.46     | 2.11        | 25     | 6     |
| 1:A:133:SER:OG  | 1:A:134:ALA:N    | 0.46     | 2.48        | 20     | 10    |
| 1:A:142:ASP:O   | 1:A:143:ASP:HB2  | 0.46     | 2.09        | 21     | 8     |
| 1:A:81:ASN:O    | 1:A:122:GLU:OE2  | 0.46     | 2.33        | 4      | 1     |
| 1:A:9:PHE:CD2   | 1:A:32:LEU:HB3   | 0.46     | 2.45        | 8      | 1     |
| 1:A:55:GLU:O    | 1:A:56:GLU:O     | 0.46     | 2.34        | 24     | 6     |
| 1:A:52:VAL:O    | 1:A:112:TYR:O    | 0.46     | 2.33        | 21     | 8     |
| 1:A:9:PHE:CD1   | 1:A:13:PRO:HA    | 0.46     | 2.44        | 15     | 1     |
| 1:A:20:GLY:O    | 1:A:21:THR:CB    | 0.46     | 2.62        | 15     | 1     |
| 1:A:34:VAL:HG11 | 1:A:47:VAL:HG21  | 0.46     | 1.86        | 17     | 1     |
| 1:A:65:THR:O    | 1:A:142:ASP:OD2  | 0.46     | 2.34        | 1      | 1     |
| 1:A:94:ALA:O    | 1:A:100:ARG:HD2  | 0.46     | 2.11        | 24     | 17    |
| 1:A:95:LEU:CD1  | 1:A:139:LEU:HG   | 0.46     | 2.41        | 4      | 10    |
| 1:A:42:GLN:HG3  | 1:A:43:TYR:CG    | 0.46     | 2.45        | 21     | 2     |
| 1:A:124:GLN:OE1 | 1:A:125:ILE:O    | 0.46     | 2.33        | 6      | 1     |
| 1:A:81:ASN:OD1  | 1:A:122:GLU:O    | 0.46     | 2.33        | 7      | 1     |
| 1:A:107:THR:O   | 1:A:108:ALA:C    | 0.46     | 2.57        | 9      | 5     |
| 1:A:81:ASN:CB   | 1:A:122:GLU:CD   | 0.46     | 2.88        | 12     | 2     |
| 1:A:54:ILE:HB   | 1:A:112:TYR:CD1  | 0.46     | 2.44        | 13     | 1     |
| 1:A:11:ASP:O    | 1:A:12:GLY:O     | 0.46     | 2.32        | 22     | 2     |
| 1:A:22:ASP:HB2  | 1:A:35:ALA:CB    | 0.46     | 2.38        | 17     | 1     |
| 1:A:40:SER:HB3  | 1:A:45:VAL:CG2   | 0.46     | 2.40        | 21     | 2     |
| 1:A:81:ASN:O    | 1:A:122:GLU:O    | 0.46     | 2.33        | 22     | 3     |
| 1:A:4:ILE:O     | 1:A:5:GLY:O      | 0.46     | 2.33        | 25     | 1     |
| 1:A:9:PHE:CD2   | 1:A:32:LEU:CB    | 0.46     | 2.98        | 3      | 3     |
| 1:A:9:PHE:CZ    | 1:A:144:VAL:HG23 | 0.46     | 2.45        | 10     | 1     |
| 1:A:83:ALA:HA   | 1:A:85:TYR:CD2   | 0.46     | 2.45        | 1      | 17    |
| 1:A:38:ALA:HA   | 1:A:136:ALA:N    | 0.46     | 2.26        | 23     | 12    |
| 1:A:32:LEU:O    | 1:A:32:LEU:HD23  | 0.46     | 2.10        | 17     | 3     |
| 1:A:65:THR:O    | 1:A:142:ASP:OD1  | 0.46     | 2.34        | 15     | 5     |
| 1:A:84:PRO:O    | 1:A:85:TYR:O     | 0.46     | 2.33        | 3      | 4     |
| 1:A:58:THR:CG2  | 1:A:148:SER:HB2  | 0.46     | 2.40        | 5      | 1     |
| 1:A:7:GLY:O     | 1:A:8:THR:O      | 0.46     | 2.33        | 11     | 2     |
| 1:A:4:ILE:O     | 1:A:14:GLU:OE1   | 0.46     | 2.34        | 3      | 2     |
| 1:A:40:SER:OG   | 1:A:43:TYR:O     | 0.46     | 2.34        | 16     | 2     |
| 1:A:42:GLN:O    | 1:A:43:TYR:HB3   | 0.46     | 2.10        | 9      | 3     |
| 1:A:9:PHE:O     | 1:A:10:ASP:OD1   | 0.46     | 2.33        | 5      | 1     |
| 1:A:11:ASP:OD1  | 1:A:11:ASP:C     | 0.46     | 2.57        | 7      | 2     |
| 1:A:130:GLY:O   | 1:A:131:GLY:O    | 0.46     | 2.33        | 17     | 5     |
| 1:A:80:GLN:O    | 1:A:81:ASN:OD1   | 0.46     | 2.34        | 6      | 2     |

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| Atom-1          | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|-----------------|------------------|----------|-------------|--------|-------|
|                 |                  |          |             | Worst  | Total |
| 1:A:71:ASP:O    | 1:A:71:ASP:OD2   | 0.46     | 2.34        | 7      | 2     |
| 1:A:20:GLY:HA3  | 1:A:43:TYR:OH    | 0.46     | 2.11        | 9      | 1     |
| 1:A:80:GLN:OE1  | 1:A:82:GLY:O     | 0.46     | 2.33        | 15     | 1     |
| 1:A:75:ARG:CA   | 1:A:93:PRO:HD2   | 0.46     | 2.41        | 5      | 4     |
| 1:A:25:LEU:CB   | 1:A:32:LEU:HD11  | 0.46     | 2.41        | 7      | 1     |
| 1:A:112:TYR:HB3 | 1:A:123:GLY:CA   | 0.46     | 2.41        | 9      | 1     |
| 1:A:39:GLY:O    | 1:A:42:GLN:OE1   | 0.46     | 2.33        | 13     | 1     |
| 1:A:80:GLN:C    | 1:A:80:GLN:CD    | 0.46     | 2.80        | 17     | 2     |
| 1:A:10:ASP:O    | 1:A:10:ASP:OD1   | 0.46     | 2.34        | 15     | 4     |
| 1:A:38:ALA:C    | 1:A:40:SER:N     | 0.46     | 2.74        | 3      | 8     |
| 1:A:8:THR:O     | 1:A:10:ASP:OD1   | 0.46     | 2.33        | 5      | 1     |
| 1:A:143:ASP:C   | 1:A:144:VAL:HG23 | 0.46     | 2.35        | 10     | 2     |
| 1:A:89:LEU:CD1  | 1:A:106:PHE:CE2  | 0.46     | 2.98        | 19     | 2     |
| 1:A:8:THR:O     | 1:A:30:GLY:O     | 0.46     | 2.33        | 24     | 1     |
| 1:A:28:SER:O    | 1:A:29:THR:HB    | 0.46     | 2.11        | 5      | 7     |
| 1:A:27:THR:C    | 1:A:29:THR:N     | 0.46     | 2.73        | 12     | 5     |
| 1:A:22:ASP:CB   | 1:A:24:PRO:HD3   | 0.46     | 2.41        | 5      | 1     |
| 1:A:40:SER:CB   | 1:A:45:VAL:HG23  | 0.46     | 2.41        | 7      | 1     |
| 1:A:13:PRO:HB3  | 1:A:25:LEU:HD11  | 0.46     | 1.88        | 9      | 1     |
| 1:A:80:GLN:HB3  | 1:A:112:TYR:CD1  | 0.46     | 2.45        | 9      | 1     |
| 1:A:45:VAL:HB   | 1:A:130:GLY:N    | 0.46     | 2.26        | 10     | 1     |
| 1:A:17:VAL:HG13 | 1:A:48:VAL:O     | 0.46     | 2.11        | 12     | 2     |
| 1:A:73:THR:O    | 1:A:73:THR:HG22  | 0.46     | 2.11        | 23     | 2     |
| 1:A:81:ASN:OD1  | 1:A:124:GLN:OE1  | 0.46     | 2.33        | 2      | 2     |
| 1:A:7:GLY:O     | 1:A:143:ASP:HA   | 0.46     | 2.10        | 4      | 5     |
| 1:A:111:THR:C   | 1:A:113:PRO:HD3  | 0.46     | 2.36        | 20     | 6     |
| 1:A:31:ALA:CB   | 1:A:142:ASP:HB3  | 0.46     | 2.41        | 12     | 2     |
| 1:A:68:ALA:O    | 1:A:96:THR:C     | 0.46     | 2.59        | 13     | 1     |
| 1:A:80:GLN:C    | 1:A:122:GLU:O    | 0.46     | 2.59        | 14     | 1     |
| 1:A:80:GLN:OE1  | 1:A:113:PRO:HD2  | 0.46     | 2.11        | 17     | 1     |
| 1:A:15:GLY:CA   | 1:A:49:LEU:HD13  | 0.46     | 2.40        | 23     | 1     |
| 1:A:40:SER:HB3  | 1:A:130:GLY:C    | 0.46     | 2.36        | 23     | 1     |
| 1:A:24:PRO:O    | 1:A:26:ASP:OD1   | 0.46     | 2.34        | 3      | 1     |
| 1:A:9:PHE:CE2   | 1:A:32:LEU:CB    | 0.46     | 2.99        | 16     | 3     |
| 1:A:141:LEU:C   | 1:A:142:ASP:CG   | 0.46     | 2.84        | 17     | 8     |
| 1:A:40:SER:OG   | 1:A:40:SER:O     | 0.46     | 2.32        | 12     | 2     |
| 1:A:37:PRO:O    | 1:A:40:SER:OG    | 0.45     | 2.33        | 10     | 2     |
| 1:A:6:GLU:HA    | 1:A:145:ALA:CB   | 0.45     | 2.41        | 7      | 1     |
| 1:A:63:ARG:HG2  | 1:A:103:THR:HG22 | 0.45     | 1.86        | 12     | 1     |
| 1:A:18:ALA:HB1  | 1:A:34:VAL:HG11  | 0.45     | 1.87        | 13     | 1     |
| 1:A:79:GLY:HA3  | 1:A:86:GLY:O     | 0.45     | 2.11        | 13     | 1     |

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| Atom-1           | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|------------------|-----------------|----------|-------------|--------|-------|
|                  |                 |          |             | Worst  | Total |
| 1:A:111:THR:O    | 1:A:113:PRO:HD3 | 0.45     | 2.11        | 18     | 2     |
| 1:A:22:ASP:O     | 1:A:35:ALA:CB   | 0.45     | 2.57        | 15     | 1     |
| 1:A:9:PHE:CD2    | 1:A:141:LEU:O   | 0.45     | 2.69        | 18     | 1     |
| 1:A:29:THR:CG2   | 1:A:30:GLY:N    | 0.45     | 2.80        | 2      | 3     |
| 1:A:52:VAL:HG11  | 1:A:112:TYR:HD2 | 0.45     | 1.70        | 7      | 5     |
| 1:A:22:ASP:O     | 1:A:22:ASP:OD1  | 0.45     | 2.34        | 7      | 3     |
| 1:A:58:THR:O     | 1:A:108:ALA:N   | 0.45     | 2.50        | 13     | 3     |
| 1:A:8:THR:O      | 1:A:9:PHE:HB2   | 0.45     | 2.11        | 15     | 3     |
| 1:A:112:TYR:CD1  | 1:A:123:GLY:HA3 | 0.45     | 2.46        | 10     | 1     |
| 1:A:10:ASP:OD1   | 1:A:29:THR:O    | 0.45     | 2.34        | 23     | 2     |
| 1:A:5:GLY:O      | 1:A:6:GLU:HG2   | 0.45     | 2.11        | 12     | 1     |
| 1:A:58:THR:HG23  | 1:A:59:THR:H    | 0.45     | 1.69        | 12     | 1     |
| 1:A:134:ALA:O    | 1:A:135:ASP:C   | 0.45     | 2.60        | 13     | 3     |
| 1:A:80:GLN:O     | 1:A:80:GLN:CG   | 0.45     | 2.63        | 17     | 2     |
| 1:A:40:SER:HB3   | 1:A:129:LEU:O   | 0.45     | 2.11        | 24     | 1     |
| 1:A:58:THR:HG22  | 1:A:59:THR:N    | 0.45     | 2.27        | 7      | 15    |
| 1:A:138:THR:HG23 | 1:A:139:LEU:N   | 0.45     | 2.26        | 12     | 6     |
| 1:A:37:PRO:HG3   | 1:A:43:TYR:OH   | 0.45     | 2.10        | 8      | 1     |
| 1:A:54:ILE:HG13  | 1:A:112:TYR:CE2 | 0.45     | 2.47        | 9      | 1     |
| 1:A:40:SER:CB    | 1:A:130:GLY:HA2 | 0.45     | 2.41        | 10     | 1     |
| 1:A:24:PRO:O     | 1:A:33:CYS:O    | 0.45     | 2.33        | 12     | 1     |
| 1:A:39:GLY:HA2   | 1:A:137:TRP:CZ3 | 0.45     | 2.47        | 23     | 1     |
| 1:A:13:PRO:CB    | 1:A:32:LEU:CD1  | 0.45     | 2.93        | 16     | 2     |
| 1:A:13:PRO:O     | 1:A:14:GLU:HB3  | 0.45     | 2.11        | 11     | 5     |
| 1:A:65:THR:O     | 1:A:65:THR:HG22 | 0.45     | 2.11        | 13     | 2     |
| 1:A:21:THR:HG23  | 1:A:42:GLN:NE2  | 0.45     | 2.27        | 17     | 1     |
| 1:A:143:ASP:OD1  | 1:A:143:ASP:O   | 0.45     | 2.33        | 19     | 1     |
| 1:A:20:GLY:HA2   | 1:A:43:TYR:OH   | 0.45     | 2.11        | 17     | 5     |
| 1:A:39:GLY:HA2   | 1:A:133:SER:O   | 0.45     | 2.11        | 7      | 8     |
| 1:A:124:GLN:N    | 1:A:124:GLN:OE1 | 0.45     | 2.49        | 2      | 1     |
| 1:A:38:ALA:HA    | 1:A:136:ALA:CA  | 0.45     | 2.42        | 7      | 15    |
| 1:A:52:VAL:HG13  | 1:A:146:LEU:CD2 | 0.45     | 2.40        | 6      | 1     |
| 1:A:8:THR:O      | 1:A:9:PHE:CB    | 0.45     | 2.64        | 15     | 2     |
| 1:A:142:ASP:OD1  | 1:A:142:ASP:C   | 0.45     | 2.57        | 10     | 2     |
| 1:A:81:ASN:HB3   | 1:A:122:GLU:CD  | 0.45     | 2.36        | 12     | 1     |
| 1:A:8:THR:HA     | 1:A:142:ASP:CA  | 0.45     | 2.41        | 21     | 2     |
| 1:A:113:PRO:O    | 1:A:122:GLU:HB2 | 0.45     | 2.12        | 17     | 7     |
| 1:A:21:THR:HG22  | 1:A:43:TYR:HH   | 0.45     | 1.72        | 6      | 1     |
| 1:A:7:GLY:O      | 1:A:9:PHE:CE1   | 0.45     | 2.69        | 8      | 1     |
| 1:A:70:THR:HG21  | 1:A:133:SER:OG  | 0.45     | 2.12        | 13     | 2     |
| 1:A:80:GLN:NE2   | 1:A:82:GLY:N    | 0.45     | 2.65        | 13     | 1     |

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| Atom-1          | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|-----------------|------------------|----------|-------------|--------|-------|
|                 |                  |          |             | Worst  | Total |
| 1:A:16:TRP:HB3  | 1:A:32:LEU:CD1   | 0.45     | 2.42        | 16     | 1     |
| 1:A:134:ALA:O   | 1:A:135:ASP:O    | 0.45     | 2.35        | 24     | 2     |
| 1:A:141:LEU:O   | 1:A:142:ASP:HB3  | 0.45     | 2.12        | 5      | 22    |
| 1:A:78:VAL:HG23 | 1:A:89:LEU:CD2   | 0.45     | 2.40        | 18     | 6     |
| 1:A:45:VAL:O    | 1:A:129:LEU:CG   | 0.45     | 2.65        | 3      | 1     |
| 1:A:10:ASP:OD1  | 1:A:10:ASP:C     | 0.45     | 2.59        | 7      | 1     |
| 1:A:28:SER:O    | 1:A:28:SER:OG    | 0.45     | 2.35        | 11     | 1     |
| 1:A:103:THR:O   | 1:A:104:GLU:HG3  | 0.45     | 2.12        | 25     | 1     |
| 1:A:42:GLN:CG   | 1:A:43:TYR:N     | 0.45     | 2.79        | 1      | 3     |
| 1:A:17:VAL:HA   | 1:A:25:LEU:CD2   | 0.45     | 2.42        | 6      | 1     |
| 1:A:81:ASN:ND2  | 1:A:124:GLN:HG2  | 0.45     | 2.27        | 8      | 1     |
| 1:A:90:ASP:OD1  | 1:A:90:ASP:N     | 0.45     | 2.49        | 9      | 2     |
| 1:A:19:TYR:O    | 1:A:45:VAL:CG1   | 0.45     | 2.63        | 20     | 1     |
| 1:A:65:THR:CG2  | 1:A:101:GLN:HG2  | 0.45     | 2.42        | 22     | 2     |
| 1:A:84:PRO:O    | 1:A:85:TYR:HB2   | 0.45     | 2.12        | 15     | 22    |
| 1:A:52:VAL:CG1  | 1:A:146:LEU:HD23 | 0.45     | 2.42        | 5      | 1     |
| 1:A:42:GLN:HG3  | 1:A:43:TYR:N     | 0.45     | 2.27        | 11     | 1     |
| 1:A:28:SER:O    | 1:A:30:GLY:N     | 0.45     | 2.49        | 14     | 1     |
| 1:A:27:THR:O    | 1:A:28:SER:OG    | 0.45     | 2.35        | 22     | 1     |
| 1:A:80:GLN:OE1  | 1:A:85:TYR:N     | 0.45     | 2.50        | 25     | 1     |
| 1:A:68:ALA:C    | 1:A:70:THR:N     | 0.45     | 2.74        | 6      | 17    |
| 1:A:64:TYR:OH   | 1:A:93:PRO:HB3   | 0.45     | 2.12        | 15     | 6     |
| 1:A:54:ILE:HD12 | 1:A:60:TYR:CE2   | 0.45     | 2.46        | 16     | 3     |
| 1:A:137:TRP:N   | 1:A:137:TRP:CE3  | 0.45     | 2.85        | 7      | 1     |
| 1:A:31:ALA:CB   | 1:A:140:CYS:HB3  | 0.45     | 2.42        | 15     | 1     |
| 1:A:10:ASP:O    | 1:A:11:ASP:HB3   | 0.45     | 2.11        | 17     | 1     |
| 1:A:39:GLY:HA3  | 1:A:133:SER:O    | 0.45     | 2.11        | 23     | 1     |
| 1:A:16:TRP:C    | 1:A:17:VAL:CG1   | 0.45     | 2.89        | 25     | 1     |
| 1:A:82:GLY:O    | 1:A:83:ALA:CB    | 0.44     | 2.64        | 4      | 3     |
| 1:A:44:GLY:HA2  | 1:A:130:GLY:CA   | 0.44     | 2.42        | 14     | 4     |
| 1:A:45:VAL:O    | 1:A:129:LEU:HB2  | 0.44     | 2.11        | 3      | 5     |
| 1:A:28:SER:O    | 1:A:29:THR:OG1   | 0.44     | 2.34        | 8      | 2     |
| 1:A:70:THR:HG21 | 1:A:137:TRP:CG   | 0.44     | 2.47        | 7      | 2     |
| 1:A:45:VAL:HG12 | 1:A:46:GLY:H     | 0.44     | 1.72        | 10     | 2     |
| 1:A:7:GLY:O     | 1:A:8:THR:OG1    | 0.44     | 2.33        | 11     | 1     |
| 1:A:41:ALA:HB2  | 1:A:131:GLY:CA   | 0.44     | 2.42        | 11     | 1     |
| 1:A:19:TYR:OH   | 1:A:48:VAL:HG13  | 0.44     | 2.11        | 20     | 1     |
| 1:A:56:GLU:HG3  | 1:A:57:GLY:N     | 0.44     | 2.26        | 5      | 5     |
| 1:A:34:VAL:CG2  | 1:A:139:LEU:HB2  | 0.44     | 2.42        | 6      | 3     |
| 1:A:52:VAL:CG1  | 1:A:54:ILE:HG12  | 0.44     | 2.42        | 7      | 4     |
| 1:A:59:THR:CG2  | 1:A:105:THR:CG2  | 0.44     | 2.94        | 12     | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:83:ALA:HA    | 1:A:85:TYR:CD1   | 0.44     | 2.47        | 18     | 1     |
| 1:A:9:PHE:CE2    | 1:A:142:ASP:CA   | 0.44     | 3.00        | 19     | 1     |
| 1:A:17:VAL:HA    | 1:A:25:LEU:HD21  | 0.44     | 1.89        | 21     | 1     |
| 1:A:35:ALA:HA    | 1:A:138:THR:HG1  | 0.44     | 1.72        | 2      | 2     |
| 1:A:75:ARG:HA    | 1:A:93:PRO:HD2   | 0.44     | 1.90        | 5      | 8     |
| 1:A:112:TYR:CB   | 1:A:123:GLY:HA3  | 0.44     | 2.42        | 18     | 13    |
| 1:A:84:PRO:O     | 1:A:85:TYR:CD2   | 0.44     | 2.70        | 9      | 4     |
| 1:A:16:TRP:CH2   | 1:A:125:ILE:CD1  | 0.44     | 2.99        | 6      | 1     |
| 1:A:60:TYR:CB    | 1:A:106:PHE:CE1  | 0.44     | 3.00        | 15     | 2     |
| 1:A:13:PRO:O     | 1:A:14:GLU:HB2   | 0.44     | 2.13        | 2      | 10    |
| 1:A:124:GLN:HG2  | 1:A:125:ILE:N    | 0.44     | 2.27        | 2      | 1     |
| 1:A:21:THR:CG2   | 1:A:37:PRO:HG3   | 0.44     | 2.43        | 6      | 3     |
| 1:A:58:THR:O     | 1:A:107:THR:HA   | 0.44     | 2.13        | 17     | 6     |
| 1:A:9:PHE:HB3    | 1:A:32:LEU:N     | 0.44     | 2.27        | 9      | 1     |
| 1:A:80:GLN:NE2   | 1:A:85:TYR:C     | 0.44     | 2.75        | 9      | 1     |
| 1:A:146:LEU:HG   | 1:A:147:ASP:N    | 0.44     | 2.27        | 12     | 1     |
| 1:A:143:ASP:O    | 1:A:143:ASP:CG   | 0.44     | 2.61        | 19     | 1     |
| 1:A:44:GLY:CA    | 1:A:130:GLY:HA3  | 0.44     | 2.43        | 1      | 1     |
| 1:A:50:ASN:HA    | 1:A:124:GLN:CB   | 0.44     | 2.42        | 6      | 18    |
| 1:A:70:THR:O     | 1:A:96:THR:HA    | 0.44     | 2.13        | 4      | 3     |
| 1:A:29:THR:HG23  | 1:A:30:GLY:H     | 0.44     | 1.73        | 21     | 1     |
| 1:A:76:ALA:O     | 1:A:77:LEU:HB3   | 0.44     | 2.12        | 18     | 24    |
| 1:A:107:THR:O    | 1:A:107:THR:HG22 | 0.44     | 2.11        | 8      | 3     |
| 1:A:83:ALA:HA    | 1:A:84:PRO:C     | 0.44     | 2.38        | 15     | 6     |
| 1:A:10:ASP:CA    | 1:A:30:GLY:HA2   | 0.44     | 2.42        | 16     | 2     |
| 1:A:125:ILE:HG21 | 1:A:127:PHE:HE2  | 0.44     | 1.72        | 13     | 2     |
| 1:A:88:VAL:HG23  | 1:A:89:LEU:HD13  | 0.44     | 1.82        | 13     | 1     |
| 1:A:130:GLY:O    | 1:A:132:PHE:CE2  | 0.44     | 2.71        | 15     | 1     |
| 1:A:63:ARG:HG2   | 1:A:143:ASP:OD2  | 0.44     | 2.12        | 21     | 1     |
| 1:A:63:ARG:HB2   | 1:A:103:THR:HG23 | 0.44     | 1.88        | 3      | 1     |
| 1:A:72:VAL:HG11  | 1:A:137:TRP:HE1  | 0.44     | 1.72        | 7      | 1     |
| 1:A:135:ASP:O    | 1:A:137:TRP:CE3  | 0.44     | 2.71        | 7      | 1     |
| 1:A:9:PHE:O      | 1:A:30:GLY:O     | 0.44     | 2.36        | 9      | 1     |
| 1:A:18:ALA:HB1   | 1:A:34:VAL:CG1   | 0.44     | 2.43        | 13     | 1     |
| 1:A:125:ILE:HG21 | 1:A:127:PHE:CE2  | 0.44     | 2.47        | 13     | 1     |
| 1:A:25:LEU:N     | 1:A:25:LEU:CD2   | 0.44     | 2.78        | 21     | 1     |
| 1:A:37:PRO:HG3   | 1:A:42:GLN:OE1   | 0.44     | 2.13        | 19     | 2     |
| 1:A:55:GLU:HA    | 1:A:111:THR:CB   | 0.44     | 2.42        | 8      | 1     |
| 1:A:90:ASP:O     | 1:A:90:ASP:OD1   | 0.44     | 2.36        | 18     | 2     |
| 1:A:31:ALA:CB    | 1:A:141:LEU:O    | 0.44     | 2.66        | 15     | 1     |
| 1:A:61:THR:O     | 1:A:146:LEU:HD12 | 0.44     | 2.12        | 19     | 2     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:14:GLU:HG3  | 1:A:15:GLY:N    | 0.43     | 2.28        | 20     | 3     |
| 1:A:7:GLY:O     | 1:A:8:THR:HG23  | 0.43     | 2.12        | 17     | 1     |
| 1:A:148:SER:O   | 1:A:148:SER:OG  | 0.43     | 2.33        | 18     | 1     |
| 1:A:19:TYR:CD2  | 1:A:19:TYR:N    | 0.43     | 2.86        | 24     | 1     |
| 1:A:95:LEU:O    | 1:A:96:THR:HB   | 0.43     | 2.12        | 5      | 2     |
| 1:A:68:ALA:O    | 1:A:70:THR:N    | 0.43     | 2.51        | 17     | 9     |
| 1:A:63:ARG:O    | 1:A:144:VAL:HA  | 0.43     | 2.13        | 22     | 11    |
| 1:A:55:GLU:HG3  | 1:A:60:TYR:OH   | 0.43     | 2.14        | 6      | 1     |
| 1:A:80:GLN:CA   | 1:A:112:TYR:CE1 | 0.43     | 3.01        | 11     | 1     |
| 1:A:8:THR:HA    | 1:A:142:ASP:C   | 0.43     | 2.39        | 12     | 1     |
| 1:A:54:ILE:HD13 | 1:A:60:TYR:CZ   | 0.43     | 2.48        | 3      | 1     |
| 1:A:142:ASP:O   | 1:A:143:ASP:OD1 | 0.43     | 2.35        | 14     | 1     |
| 1:A:9:PHE:C     | 1:A:11:ASP:N    | 0.43     | 2.76        | 15     | 2     |
| 1:A:31:ALA:HB3  | 1:A:140:CYS:CB  | 0.43     | 2.42        | 15     | 1     |
| 1:A:80:GLN:O    | 1:A:80:GLN:HG3  | 0.43     | 2.13        | 17     | 2     |
| 1:A:16:TRP:O    | 1:A:25:LEU:HD12 | 0.43     | 2.12        | 1      | 2     |
| 1:A:77:LEU:HB2  | 1:A:89:LEU:O    | 0.43     | 2.13        | 21     | 23    |
| 1:A:4:ILE:CD1   | 1:A:144:VAL:HB  | 0.43     | 2.44        | 10     | 2     |
| 1:A:8:THR:C     | 1:A:10:ASP:N    | 0.43     | 2.75        | 6      | 2     |
| 1:A:55:GLU:O    | 1:A:56:GLU:HB2  | 0.43     | 2.13        | 23     | 2     |
| 1:A:143:ASP:O   | 1:A:143:ASP:OD1 | 0.43     | 2.35        | 8      | 1     |
| 1:A:81:ASN:HB2  | 1:A:122:GLU:CD  | 0.43     | 2.38        | 2      | 4     |
| 1:A:15:GLY:CA   | 1:A:49:LEU:CD1  | 0.43     | 2.96        | 16     | 2     |
| 1:A:46:GLY:HA2  | 1:A:128:GLN:HA  | 0.43     | 1.91        | 2      | 2     |
| 1:A:3:PRO:N     | 1:A:53:ALA:HB2  | 0.43     | 2.29        | 8      | 1     |
| 1:A:142:ASP:O   | 1:A:143:ASP:OD2 | 0.43     | 2.36        | 11     | 2     |
| 1:A:74:VAL:O    | 1:A:93:PRO:HD2  | 0.43     | 2.13        | 18     | 1     |
| 1:A:43:TYR:HH   | 1:A:45:VAL:HG22 | 0.43     | 1.71        | 22     | 1     |
| 1:A:37:PRO:HD2  | 1:A:45:VAL:CG2  | 0.43     | 2.43        | 3      | 1     |
| 1:A:78:VAL:HG12 | 1:A:79:GLY:N    | 0.43     | 2.28        | 9      | 2     |
| 1:A:31:ALA:HA   | 1:A:141:LEU:O   | 0.43     | 2.14        | 20     | 3     |
| 1:A:54:ILE:CG2  | 1:A:55:GLU:N    | 0.43     | 2.82        | 6      | 3     |
| 1:A:103:THR:C   | 1:A:104:GLU:HG3 | 0.43     | 2.38        | 10     | 2     |
| 1:A:57:GLY:HA2  | 1:A:108:ALA:O   | 0.43     | 2.13        | 12     | 1     |
| 1:A:71:ASP:N    | 1:A:71:ASP:OD1  | 0.43     | 2.51        | 12     | 1     |
| 1:A:96:THR:HG23 | 1:A:97:SER:H    | 0.43     | 1.73        | 24     | 1     |
| 1:A:40:SER:O    | 1:A:130:GLY:HA2 | 0.43     | 2.13        | 10     | 2     |
| 1:A:55:GLU:C    | 1:A:56:GLU:HG2  | 0.43     | 2.39        | 11     | 13    |
| 1:A:103:THR:C   | 1:A:104:GLU:OE1 | 0.43     | 2.61        | 7      | 1     |
| 1:A:60:TYR:O    | 1:A:105:THR:HA  | 0.43     | 2.14        | 3      | 4     |
| 1:A:90:ASP:O    | 1:A:90:ASP:CG   | 0.43     | 2.61        | 20     | 4     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:78:VAL:CG1   | 1:A:112:TYR:CE2  | 0.43     | 3.02        | 14     | 3     |
| 1:A:39:GLY:C     | 1:A:41:ALA:N     | 0.43     | 2.74        | 10     | 1     |
| 1:A:41:ALA:HB2   | 1:A:131:GLY:HA2  | 0.43     | 1.91        | 11     | 1     |
| 1:A:45:VAL:HB    | 1:A:129:LEU:O    | 0.43     | 2.14        | 11     | 3     |
| 1:A:45:VAL:O     | 1:A:129:LEU:CA   | 0.43     | 2.67        | 16     | 1     |
| 1:A:76:ALA:HB1   | 1:A:127:PHE:CE1  | 0.43     | 2.49        | 25     | 1     |
| 1:A:8:THR:OG1    | 1:A:144:VAL:HG23 | 0.43     | 2.14        | 9      | 1     |
| 1:A:19:TYR:CD2   | 1:A:46:GLY:O     | 0.43     | 2.72        | 21     | 2     |
| 1:A:112:TYR:HB3  | 1:A:123:GLY:HA3  | 0.43     | 1.90        | 9      | 1     |
| 1:A:9:PHE:CE1    | 1:A:144:VAL:HG23 | 0.43     | 2.49        | 10     | 1     |
| 1:A:79:GLY:C     | 1:A:112:TYR:CE2  | 0.43     | 2.97        | 13     | 1     |
| 1:A:20:GLY:HA2   | 1:A:43:TYR:CE2   | 0.43     | 2.48        | 16     | 1     |
| 1:A:54:ILE:HG23  | 1:A:60:TYR:CZ    | 0.43     | 2.47        | 24     | 1     |
| 1:A:81:ASN:OD1   | 1:A:122:GLU:HG2  | 0.43     | 2.13        | 24     | 1     |
| 1:A:54:ILE:O     | 1:A:111:THR:HA   | 0.42     | 2.13        | 12     | 2     |
| 1:A:98:GLU:CB    | 1:A:99:PRO:CD    | 0.42     | 2.97        | 24     | 4     |
| 1:A:13:PRO:HG3   | 1:A:27:THR:CG2   | 0.42     | 2.43        | 8      | 1     |
| 1:A:88:VAL:HG12  | 1:A:109:SER:H    | 0.42     | 1.73        | 9      | 2     |
| 1:A:22:ASP:HB3   | 1:A:35:ALA:O     | 0.42     | 2.14        | 13     | 3     |
| 1:A:88:VAL:C     | 1:A:89:LEU:HD12  | 0.42     | 2.38        | 13     | 2     |
| 1:A:49:LEU:C     | 1:A:49:LEU:HD12  | 0.42     | 2.39        | 15     | 1     |
| 1:A:65:THR:OG1   | 1:A:101:GLN:HG2  | 0.42     | 2.14        | 16     | 1     |
| 1:A:19:TYR:CD1   | 1:A:19:TYR:O     | 0.42     | 2.72        | 18     | 1     |
| 1:A:58:THR:CG2   | 1:A:60:TYR:CZ    | 0.42     | 3.02        | 18     | 2     |
| 1:A:64:TYR:CE2   | 1:A:102:VAL:CG1  | 0.42     | 3.00        | 21     | 1     |
| 1:A:71:ASP:HA    | 1:A:95:LEU:O     | 0.42     | 2.14        | 7      | 9     |
| 1:A:32:LEU:O     | 1:A:140:CYS:HA   | 0.42     | 2.14        | 25     | 3     |
| 1:A:8:THR:HB     | 1:A:142:ASP:O    | 0.42     | 2.14        | 24     | 3     |
| 1:A:28:SER:C     | 1:A:30:GLY:N     | 0.42     | 2.77        | 14     | 1     |
| 1:A:6:GLU:O      | 1:A:6:GLU:HG3    | 0.42     | 2.12        | 19     | 1     |
| 1:A:76:ALA:CB    | 1:A:93:PRO:HD3   | 0.42     | 2.44        | 23     | 1     |
| 1:A:65:THR:OG1   | 1:A:142:ASP:OD1  | 0.42     | 2.37        | 1      | 1     |
| 1:A:7:GLY:C      | 1:A:143:ASP:HA   | 0.42     | 2.39        | 4      | 3     |
| 1:A:29:THR:HG23  | 1:A:31:ALA:H     | 0.42     | 1.74        | 6      | 1     |
| 1:A:25:LEU:CB    | 1:A:32:LEU:CD1   | 0.42     | 2.97        | 7      | 1     |
| 1:A:64:TYR:CE2   | 1:A:102:VAL:CB   | 0.42     | 3.03        | 21     | 2     |
| 1:A:9:PHE:CE2    | 1:A:16:TRP:CD1   | 0.42     | 3.07        | 11     | 1     |
| 1:A:63:ARG:HD3   | 1:A:103:THR:HG23 | 0.42     | 1.91        | 18     | 1     |
| 1:A:65:THR:HB    | 1:A:142:ASP:OD2  | 0.42     | 2.14        | 18     | 1     |
| 1:A:129:LEU:HD21 | 1:A:139:LEU:CD2  | 0.42     | 2.45        | 1      | 1     |
| 1:A:35:ALA:HA    | 1:A:138:THR:OG1  | 0.42     | 2.15        | 2      | 4     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:49:LEU:O    | 1:A:124:GLN:HB2 | 0.42     | 2.15        | 25     | 4     |
| 1:A:65:THR:HG23 | 1:A:101:GLN:N   | 0.42     | 2.29        | 7      | 1     |
| 1:A:71:ASP:C    | 1:A:71:ASP:OD1  | 0.42     | 2.60        | 9      | 1     |
| 1:A:19:TYR:CA   | 1:A:22:ASP:OD2  | 0.42     | 2.68        | 20     | 1     |
| 1:A:68:ALA:CB   | 1:A:95:LEU:HB3  | 0.42     | 2.45        | 1      | 3     |
| 1:A:105:THR:O   | 1:A:105:THR:CG2 | 0.42     | 2.66        | 1      | 1     |
| 1:A:16:TRP:CB   | 1:A:32:LEU:CD1  | 0.42     | 2.98        | 10     | 2     |
| 1:A:70:THR:HG22 | 1:A:137:TRP:CB  | 0.42     | 2.44        | 17     | 1     |
| 1:A:50:ASN:ND2  | 1:A:122:GLU:HG2 | 0.42     | 2.30        | 1      | 1     |
| 1:A:81:ASN:HB3  | 1:A:122:GLU:OE2 | 0.42     | 2.15        | 21     | 3     |
| 1:A:28:SER:C    | 1:A:29:THR:CG2  | 0.42     | 2.81        | 5      | 2     |
| 1:A:124:GLN:CD  | 1:A:125:ILE:O   | 0.42     | 2.63        | 6      | 1     |
| 1:A:52:VAL:HG11 | 1:A:112:TYR:CD2 | 0.42     | 2.50        | 7      | 1     |
| 1:A:65:THR:O    | 1:A:141:LEU:HA  | 0.42     | 2.15        | 14     | 9     |
| 1:A:76:ALA:C    | 1:A:77:LEU:HG   | 0.42     | 2.40        | 7      | 5     |
| 1:A:68:ALA:N    | 1:A:95:LEU:HB3  | 0.42     | 2.29        | 11     | 2     |
| 1:A:22:ASP:HB3  | 1:A:35:ALA:C    | 0.42     | 2.38        | 12     | 1     |
| 1:A:135:ASP:N   | 1:A:135:ASP:OD1 | 0.42     | 2.48        | 17     | 1     |
| 1:A:83:ALA:HA   | 1:A:85:TYR:N    | 0.42     | 2.30        | 18     | 1     |
| 1:A:78:VAL:HG21 | 1:A:89:LEU:HD22 | 0.42     | 1.87        | 18     | 2     |
| 1:A:42:GLN:CG   | 1:A:43:TYR:CD2  | 0.42     | 3.02        | 22     | 2     |
| 1:A:54:ILE:CG2  | 1:A:54:ILE:O    | 0.42     | 2.68        | 12     | 1     |
| 1:A:42:GLN:HG2  | 1:A:42:GLN:O    | 0.42     | 2.14        | 14     | 1     |
| 1:A:20:GLY:O    | 1:A:21:THR:HG23 | 0.42     | 2.13        | 15     | 1     |
| 1:A:78:VAL:HB   | 1:A:88:VAL:CG2  | 0.42     | 2.44        | 19     | 2     |
| 1:A:65:THR:HG23 | 1:A:101:GLN:CB  | 0.42     | 2.44        | 1      | 1     |
| 1:A:45:VAL:O    | 1:A:129:LEU:HG  | 0.42     | 2.14        | 3      | 1     |
| 1:A:74:VAL:HG12 | 1:A:132:PHE:HB3 | 0.42     | 1.92        | 3      | 2     |
| 1:A:22:ASP:HB2  | 1:A:35:ALA:O    | 0.42     | 2.15        | 4      | 1     |
| 1:A:53:ALA:C    | 1:A:54:ILE:HD13 | 0.42     | 2.38        | 5      | 1     |
| 1:A:19:TYR:O    | 1:A:21:THR:HG23 | 0.42     | 2.14        | 21     | 1     |
| 1:A:80:GLN:HA   | 1:A:123:GLY:HA2 | 0.42     | 1.91        | 21     | 1     |
| 1:A:59:THR:C    | 1:A:60:TYR:CG   | 0.42     | 2.98        | 2      | 11    |
| 1:A:60:TYR:O    | 1:A:105:THR:CG2 | 0.42     | 2.62        | 2      | 1     |
| 1:A:55:GLU:HA   | 1:A:111:THR:CG2 | 0.42     | 2.44        | 23     | 2     |
| 1:A:42:GLN:N    | 1:A:42:GLN:OE1  | 0.42     | 2.53        | 10     | 1     |
| 1:A:42:GLN:HG3  | 1:A:43:TYR:CD1  | 0.42     | 2.50        | 17     | 1     |
| 1:A:53:ALA:HA   | 1:A:112:TYR:O   | 0.42     | 2.15        | 18     | 1     |
| 1:A:8:THR:HA    | 1:A:142:ASP:O   | 0.41     | 2.15        | 2      | 1     |
| 1:A:4:ILE:O     | 1:A:14:GLU:CG   | 0.41     | 2.68        | 8      | 1     |
| 1:A:80:GLN:CA   | 1:A:122:GLU:O   | 0.41     | 2.68        | 14     | 2     |

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| Atom-1          | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|-----------------|------------------|----------|-------------|--------|-------|
|                 |                  |          |             | Worst  | Total |
| 1:A:44:GLY:HA2  | 1:A:130:GLY:HA2  | 0.41     | 1.92        | 15     | 1     |
| 1:A:80:GLN:HA   | 1:A:80:GLN:OE1   | 0.41     | 2.15        | 16     | 1     |
| 1:A:63:ARG:HG2  | 1:A:103:THR:CG2  | 0.41     | 2.45        | 20     | 1     |
| 1:A:94:ALA:C    | 1:A:95:LEU:HG    | 0.41     | 2.40        | 3      | 4     |
| 1:A:60:TYR:CE2  | 1:A:108:ALA:CB   | 0.41     | 3.00        | 19     | 2     |
| 1:A:8:THR:HG22  | 1:A:143:ASP:CB   | 0.41     | 2.45        | 3      | 1     |
| 1:A:21:THR:HG23 | 1:A:45:VAL:CG1   | 0.41     | 2.43        | 5      | 1     |
| 1:A:41:ALA:C    | 1:A:42:GLN:HG2   | 0.41     | 2.39        | 5      | 1     |
| 1:A:94:ALA:C    | 1:A:100:ARG:HD2  | 0.41     | 2.39        | 5      | 1     |
| 1:A:20:GLY:O    | 1:A:37:PRO:HD3   | 0.41     | 2.16        | 20     | 2     |
| 1:A:137:TRP:CD1 | 1:A:137:TRP:C    | 0.41     | 2.96        | 9      | 1     |
| 1:A:9:PHE:CD1   | 1:A:142:ASP:HA   | 0.41     | 2.50        | 18     | 1     |
| 1:A:9:PHE:CE2   | 1:A:142:ASP:N    | 0.41     | 2.88        | 19     | 1     |
| 1:A:96:THR:HG23 | 1:A:98:GLU:N     | 0.41     | 2.30        | 20     | 1     |
| 1:A:65:THR:CB   | 1:A:142:ASP:OD1  | 0.41     | 2.68        | 1      | 1     |
| 1:A:54:ILE:HA   | 1:A:60:TYR:OH    | 0.41     | 2.16        | 10     | 3     |
| 1:A:63:ARG:O    | 1:A:64:TYR:HB3   | 0.41     | 2.15        | 14     | 4     |
| 1:A:40:SER:HA   | 1:A:42:GLN:NE2   | 0.41     | 2.30        | 13     | 1     |
| 1:A:78:VAL:HG12 | 1:A:112:TYR:HE2  | 0.41     | 1.72        | 13     | 1     |
| 1:A:5:GLY:O     | 1:A:144:VAL:O    | 0.41     | 2.37        | 22     | 1     |
| 1:A:74:VAL:HG23 | 1:A:75:ARG:H     | 0.41     | 1.73        | 25     | 1     |
| 1:A:16:TRP:CH2  | 1:A:125:ILE:CG2  | 0.41     | 3.00        | 4      | 2     |
| 1:A:142:ASP:O   | 1:A:143:ASP:HB3  | 0.41     | 2.15        | 6      | 1     |
| 1:A:76:ALA:O    | 1:A:77:LEU:CB    | 0.41     | 2.67        | 7      | 3     |
| 1:A:59:THR:HG22 | 1:A:105:THR:HG22 | 0.41     | 1.92        | 8      | 1     |
| 1:A:8:THR:C     | 1:A:9:PHE:CG     | 0.41     | 2.96        | 9      | 1     |
| 1:A:15:GLY:O    | 1:A:49:LEU:HD12  | 0.41     | 2.14        | 12     | 1     |
| 1:A:9:PHE:HB3   | 1:A:31:ALA:HA    | 0.41     | 1.91        | 13     | 1     |
| 1:A:77:LEU:C    | 1:A:77:LEU:HD12  | 0.41     | 2.40        | 13     | 1     |
| 1:A:113:PRO:O   | 1:A:122:GLU:HA   | 0.41     | 2.15        | 13     | 1     |
| 1:A:109:SER:O   | 1:A:109:SER:OG   | 0.41     | 2.35        | 19     | 1     |
| 1:A:81:ASN:CB   | 1:A:122:GLU:O    | 0.41     | 2.69        | 1      | 1     |
| 1:A:9:PHE:HB2   | 1:A:30:GLY:O     | 0.41     | 2.16        | 2      | 1     |
| 1:A:66:ALA:HA   | 1:A:140:CYS:O    | 0.41     | 2.14        | 13     | 3     |
| 1:A:74:VAL:CG1  | 1:A:132:PHE:CD2  | 0.41     | 3.00        | 15     | 1     |
| 1:A:68:ALA:N    | 1:A:95:LEU:HD23  | 0.41     | 2.31        | 16     | 1     |
| 1:A:65:THR:HA   | 1:A:100:ARG:O    | 0.41     | 2.16        | 25     | 1     |
| 1:A:43:TYR:CE1  | 1:A:45:VAL:HG22  | 0.41     | 2.51        | 4      | 1     |
| 1:A:47:VAL:O    | 1:A:127:PHE:HB2  | 0.41     | 2.16        | 5      | 2     |
| 1:A:53:ALA:C    | 1:A:54:ILE:HG12  | 0.41     | 2.40        | 8      | 1     |
| 1:A:27:THR:CG2  | 1:A:32:LEU:HA    | 0.41     | 2.46        | 21     | 2     |

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| Atom-1          | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|-----------------|------------------|----------|-------------|--------|-------|
|                 |                  |          |             | Worst  | Total |
| 1:A:65:THR:CB   | 1:A:142:ASP:OD2  | 0.41     | 2.69        | 18     | 1     |
| 1:A:4:ILE:C     | 1:A:14:GLU:HG3   | 0.41     | 2.39        | 21     | 1     |
| 1:A:4:ILE:HD12  | 1:A:144:VAL:CG1  | 0.41     | 2.46        | 22     | 1     |
| 1:A:64:TYR:O    | 1:A:102:VAL:HB   | 0.41     | 2.15        | 5      | 1     |
| 1:A:9:PHE:HZ    | 1:A:144:VAL:HG21 | 0.41     | 1.76        | 17     | 1     |
| 1:A:65:THR:HB   | 1:A:142:ASP:OD1  | 0.41     | 2.15        | 1      | 1     |
| 1:A:47:VAL:HB   | 1:A:127:PHE:HB2  | 0.41     | 1.93        | 2      | 1     |
| 1:A:27:THR:O    | 1:A:28:SER:HB2   | 0.41     | 2.14        | 6      | 1     |
| 1:A:66:ALA:O    | 1:A:100:ARG:HB2  | 0.41     | 2.15        | 10     | 1     |
| 1:A:42:GLN:NE2  | 1:A:43:TYR:CE2   | 0.41     | 2.88        | 11     | 1     |
| 1:A:79:GLY:HA2  | 1:A:112:TYR:HH   | 0.41     | 1.75        | 13     | 1     |
| 1:A:110:ALA:HB3 | 1:A:112:TYR:HE1  | 0.41     | 1.76        | 13     | 1     |
| 1:A:84:PRO:C    | 1:A:85:TYR:CD1   | 0.41     | 2.98        | 18     | 1     |
| 1:A:38:ALA:N    | 1:A:136:ALA:HA   | 0.41     | 2.30        | 2      | 1     |
| 1:A:111:THR:O   | 1:A:113:PRO:CD   | 0.41     | 2.69        | 5      | 2     |
| 1:A:64:TYR:C    | 1:A:143:ASP:OD2  | 0.41     | 2.63        | 6      | 1     |
| 1:A:10:ASP:O    | 1:A:11:ASP:OD1   | 0.41     | 2.38        | 8      | 1     |
| 1:A:10:ASP:HA   | 1:A:30:GLY:N     | 0.41     | 2.30        | 8      | 1     |
| 1:A:53:ALA:C    | 1:A:54:ILE:CG1   | 0.41     | 2.94        | 8      | 1     |
| 1:A:9:PHE:CE1   | 1:A:142:ASP:O    | 0.41     | 2.74        | 10     | 1     |
| 1:A:68:ALA:HA   | 1:A:138:THR:O    | 0.41     | 2.15        | 10     | 4     |
| 1:A:10:ASP:CB   | 1:A:30:GLY:HA2   | 0.41     | 2.45        | 13     | 1     |
| 1:A:61:THR:HA   | 1:A:104:GLU:O    | 0.41     | 2.15        | 19     | 2     |
| 1:A:79:GLY:O    | 1:A:112:TYR:CZ   | 0.41     | 2.74        | 15     | 1     |
| 1:A:72:VAL:O    | 1:A:72:VAL:HG13  | 0.41     | 2.15        | 18     | 1     |
| 1:A:77:LEU:HA   | 1:A:89:LEU:HB3   | 0.41     | 1.93        | 18     | 1     |
| 1:A:8:THR:CG2   | 1:A:143:ASP:HB3  | 0.41     | 2.45        | 19     | 1     |
| 1:A:39:GLY:O    | 1:A:131:GLY:HA2  | 0.41     | 2.16        | 19     | 1     |
| 1:A:9:PHE:N     | 1:A:142:ASP:O    | 0.41     | 2.54        | 20     | 1     |
| 1:A:63:ARG:HG2  | 1:A:143:ASP:CG   | 0.41     | 2.41        | 21     | 1     |
| 1:A:40:SER:CB   | 1:A:131:GLY:N    | 0.41     | 2.84        | 23     | 1     |
| 1:A:122:GLU:OE1 | 1:A:122:GLU:N    | 0.41     | 2.53        | 25     | 1     |
| 1:A:4:ILE:HD11  | 1:A:144:VAL:HB   | 0.41     | 1.93        | 2      | 1     |
| 1:A:42:GLN:NE2  | 1:A:43:TYR:CZ    | 0.41     | 2.89        | 5      | 1     |
| 1:A:8:THR:O     | 1:A:10:ASP:N     | 0.41     | 2.54        | 6      | 1     |
| 1:A:42:GLN:CG   | 1:A:43:TYR:CE1   | 0.41     | 3.04        | 8      | 1     |
| 1:A:8:THR:HB    | 1:A:142:ASP:C    | 0.41     | 2.41        | 15     | 1     |
| 1:A:8:THR:HA    | 1:A:143:ASP:N    | 0.41     | 2.31        | 19     | 1     |
| 1:A:64:TYR:HA   | 1:A:143:ASP:O    | 0.41     | 2.16        | 20     | 1     |
| 1:A:41:ALA:C    | 1:A:43:TYR:N     | 0.40     | 2.77        | 3      | 1     |
| 1:A:122:GLU:N   | 1:A:122:GLU:CD   | 0.40     | 2.79        | 4      | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:14:GLU:OE1   | 1:A:14:GLU:HA    | 0.40     | 2.16        | 17     | 1     |
| 1:A:13:PRO:CG    | 1:A:32:LEU:CD1   | 0.40     | 2.99        | 20     | 1     |
| 1:A:40:SER:O     | 1:A:131:GLY:HA3  | 0.40     | 2.14        | 23     | 1     |
| 1:A:77:LEU:CG    | 1:A:126:ALA:HB3  | 0.40     | 2.46        | 5      | 1     |
| 1:A:39:GLY:CA    | 1:A:133:SER:O    | 0.40     | 2.69        | 7      | 1     |
| 1:A:74:VAL:O     | 1:A:92:SER:HB3   | 0.40     | 2.16        | 7      | 1     |
| 1:A:74:VAL:CG2   | 1:A:93:PRO:CG    | 0.40     | 2.99        | 10     | 1     |
| 1:A:54:ILE:HD13  | 1:A:60:TYR:CD2   | 0.40     | 2.50        | 12     | 1     |
| 1:A:54:ILE:HG23  | 1:A:108:ALA:HB1  | 0.40     | 1.88        | 12     | 1     |
| 1:A:130:GLY:N    | 1:A:132:PHE:CD1  | 0.40     | 2.90        | 14     | 1     |
| 1:A:76:ALA:HA    | 1:A:126:ALA:O    | 0.40     | 2.16        | 24     | 1     |
| 1:A:74:VAL:CB    | 1:A:129:LEU:HD22 | 0.40     | 2.46        | 10     | 1     |
| 1:A:55:GLU:HG2   | 1:A:111:THR:HG23 | 0.40     | 1.93        | 12     | 1     |
| 1:A:54:ILE:O     | 1:A:55:GLU:HB3   | 0.40     | 2.17        | 13     | 1     |
| 1:A:50:ASN:OD1   | 1:A:122:GLU:HG3  | 0.40     | 2.16        | 5      | 1     |
| 1:A:81:ASN:OD1   | 1:A:124:GLN:HG2  | 0.40     | 2.16        | 6      | 1     |
| 1:A:80:GLN:C     | 1:A:81:ASN:CG    | 0.40     | 2.89        | 10     | 1     |
| 1:A:27:THR:HA    | 1:A:31:ALA:O     | 0.40     | 2.16        | 18     | 1     |
| 1:A:6:GLU:HB3    | 1:A:145:ALA:CB   | 0.40     | 2.46        | 19     | 1     |
| 1:A:129:LEU:HD21 | 1:A:139:LEU:HD22 | 0.40     | 1.93        | 1      | 1     |
| 1:A:13:PRO:HD3   | 1:A:27:THR:CG2   | 0.40     | 2.44        | 5      | 1     |
| 1:A:26:ASP:O     | 1:A:32:LEU:HA    | 0.40     | 2.15        | 7      | 1     |
| 1:A:27:THR:C     | 1:A:29:THR:HG22  | 0.40     | 2.42        | 13     | 1     |
| 1:A:21:THR:OG1   | 1:A:22:ASP:N     | 0.40     | 2.51        | 15     | 1     |
| 1:A:64:TYR:HE2   | 1:A:102:VAL:HG11 | 0.40     | 1.72        | 15     | 1     |
| 1:A:72:VAL:HG21  | 1:A:137:TRP:CZ2  | 0.40     | 2.49        | 19     | 1     |
| 1:A:40:SER:HG    | 1:A:131:GLY:N    | 0.40     | 2.14        | 23     | 1     |
| 1:A:55:GLU:HA    | 1:A:111:THR:HA   | 0.40     | 1.92        | 23     | 1     |

## 6.3 Torsion angles [i](#)

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

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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     | 139/152 (91%) | 92±4 (66±3%) | 32±4 (23±3%) | 16±2 (11±2%) | <b>1</b> <b>8</b> |

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| Mol | Chain | Analysed        | Favoured   | Allowed   | Outliers  | Percentiles |
|-----|-------|-----------------|------------|-----------|-----------|-------------|
| All | All   | 3475/3800 (91%) | 2290 (66%) | 797 (23%) | 388 (11%) | 1 8         |

All 47 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     | 11  | ASP  | 25             |
| 1   | A     | 74  | VAL  | 25             |
| 1   | A     | 77  | LEU  | 25             |
| 1   | A     | 14  | GLU  | 22             |
| 1   | A     | 56  | GLU  | 21             |
| 1   | A     | 142 | ASP  | 21             |
| 1   | A     | 143 | ASP  | 19             |
| 1   | A     | 51  | GLY  | 17             |
| 1   | A     | 3   | PRO  | 16             |
| 1   | A     | 39  | GLY  | 14             |
| 1   | A     | 108 | ALA  | 12             |
| 1   | A     | 6   | GLU  | 11             |
| 1   | A     | 23  | GLY  | 11             |
| 1   | A     | 28  | SER  | 11             |
| 1   | A     | 131 | GLY  | 11             |
| 1   | A     | 85  | TYR  | 10             |
| 1   | A     | 43  | TYR  | 9              |
| 1   | A     | 25  | LEU  | 9              |
| 1   | A     | 29  | THR  | 8              |
| 1   | A     | 44  | GLY  | 8              |
| 1   | A     | 24  | PRO  | 7              |
| 1   | A     | 42  | GLN  | 7              |
| 1   | A     | 83  | ALA  | 6              |
| 1   | A     | 40  | SER  | 6              |
| 1   | A     | 122 | GLU  | 4              |
| 1   | A     | 30  | GLY  | 4              |
| 1   | A     | 113 | PRO  | 4              |
| 1   | A     | 12  | GLY  | 4              |
| 1   | A     | 38  | ALA  | 3              |
| 1   | A     | 135 | ASP  | 3              |
| 1   | A     | 82  | GLY  | 3              |
| 1   | A     | 4   | ILE  | 3              |
| 1   | A     | 10  | ASP  | 3              |
| 1   | A     | 55  | GLU  | 3              |
| 1   | A     | 132 | PHE  | 3              |
| 1   | A     | 16  | TRP  | 3              |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 96  | THR  | 2              |
| 1   | A     | 130 | GLY  | 2              |
| 1   | A     | 8   | THR  | 2              |
| 1   | A     | 9   | PHE  | 2              |
| 1   | A     | 5   | GLY  | 2              |
| 1   | A     | 134 | ALA  | 2              |
| 1   | A     | 80  | GLN  | 1              |
| 1   | A     | 114 | ALA  | 1              |
| 1   | A     | 20  | GLY  | 1              |
| 1   | A     | 21  | THR  | 1              |
| 1   | A     | 71  | ASP  | 1              |

### 6.3.2 Protein sidechains [i](#)

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     | 103/113 (91%)   | 82±3 (80±3%) | 21±3 (20±3%) | 3           | 32 |
| All | All   | 2575/2825 (91%) | 2054 (80%)   | 521 (20%)    | 3           | 32 |

All 57 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     | 17  | VAL  | 25             |
| 1   | A     | 58  | THR  | 25             |
| 1   | A     | 138 | THR  | 25             |
| 1   | A     | 103 | THR  | 21             |
| 1   | A     | 96  | THR  | 20             |
| 1   | A     | 32  | LEU  | 19             |
| 1   | A     | 97  | SER  | 19             |
| 1   | A     | 59  | THR  | 18             |
| 1   | A     | 100 | ARG  | 17             |
| 1   | A     | 27  | THR  | 17             |
| 1   | A     | 87  | THR  | 14             |
| 1   | A     | 98  | GLU  | 14             |
| 1   | A     | 144 | VAL  | 14             |
| 1   | A     | 14  | GLU  | 13             |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 55  | GLU  | 12             |
| 1   | A     | 42  | GLN  | 12             |
| 1   | A     | 141 | LEU  | 11             |
| 1   | A     | 122 | GLU  | 11             |
| 1   | A     | 147 | ASP  | 11             |
| 1   | A     | 143 | ASP  | 10             |
| 1   | A     | 26  | ASP  | 10             |
| 1   | A     | 101 | GLN  | 10             |
| 1   | A     | 40  | SER  | 9              |
| 1   | A     | 43  | TYR  | 9              |
| 1   | A     | 75  | ARG  | 9              |
| 1   | A     | 139 | LEU  | 9              |
| 1   | A     | 92  | SER  | 9              |
| 1   | A     | 33  | CYS  | 8              |
| 1   | A     | 140 | CYS  | 8              |
| 1   | A     | 148 | SER  | 8              |
| 1   | A     | 105 | THR  | 8              |
| 1   | A     | 69  | SER  | 7              |
| 1   | A     | 28  | SER  | 7              |
| 1   | A     | 129 | LEU  | 7              |
| 1   | A     | 11  | ASP  | 7              |
| 1   | A     | 25  | LEU  | 6              |
| 1   | A     | 142 | ASP  | 6              |
| 1   | A     | 22  | ASP  | 5              |
| 1   | A     | 29  | THR  | 5              |
| 1   | A     | 45  | VAL  | 4              |
| 1   | A     | 50  | ASN  | 4              |
| 1   | A     | 124 | GLN  | 4              |
| 1   | A     | 128 | GLN  | 4              |
| 1   | A     | 6   | GLU  | 4              |
| 1   | A     | 65  | THR  | 3              |
| 1   | A     | 8   | THR  | 3              |
| 1   | A     | 91  | THR  | 3              |
| 1   | A     | 90  | ASP  | 3              |
| 1   | A     | 135 | ASP  | 2              |
| 1   | A     | 80  | GLN  | 2              |
| 1   | A     | 71  | ASP  | 2              |
| 1   | A     | 104 | GLU  | 2              |
| 1   | A     | 56  | GLU  | 2              |
| 1   | A     | 10  | ASP  | 1              |
| 1   | A     | 19  | TYR  | 1              |
| 1   | A     | 74  | VAL  | 1              |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 63  | ARG  | 1              |

### 6.3.3 RNA [i](#)

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](#)

There are no ligands in this entry.

### 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