



# Full wwPDB NMR Structure Validation Report ⓘ

Mar 4, 2026 – 09:37 PM UTC

PDB ID : 1N6U / pdb\_00001n6u  
Title : NMR structure of the interferon-binding ectodomain of the human interferon receptor  
Authors : Chill, J.H.; Quadt, S.R.; Levy, R.; Schreiber, G.; Anglister, J.  
Deposited on : 2002-11-12

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                                                             |

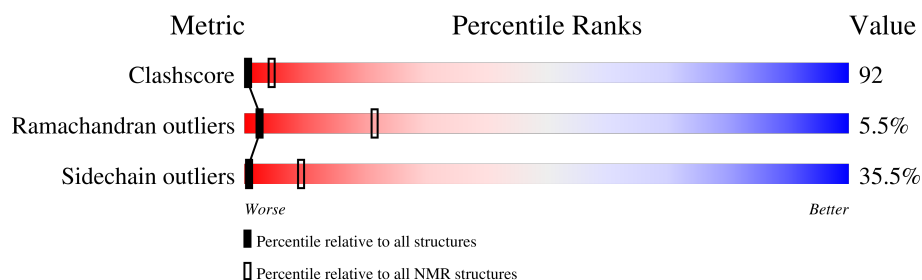
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment was not calculated.

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



| Metric                | Whole archive<br>(#Entries) | NMR archive<br>(#Entries) |
|-----------------------|-----------------------------|---------------------------|
| Clashscore            | 229148                      | 14424                     |
| Ramachandran outliers | 224038                      | 12848                     |
| Sidechain outliers    | 223484                      | 12823                     |

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

| Mol | Chain | Length | Quality of chain                                                                      |
|-----|-------|--------|---------------------------------------------------------------------------------------|
| 1   | A     | 212    | <div> <div></div> <div>12%</div> <div>58%</div> <div>21%</div> <div>• 8%</div> </div> |

## 2 Ensemble composition and analysis

This entry contains 22 models. Model 12 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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:11-A:205 (195)      | 0.81              | 12           |

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 4 clusters and 4 single-model clusters were found.

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

### 3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 3366 atoms, of which 1656 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Interferon-alpha/beta receptor beta chain.

| Mol | Chain | Residues | Atoms |      |      |     |     |    | Trace |
|-----|-------|----------|-------|------|------|-----|-----|----|-------|
| 1   | A     | 212      | Total | C    | H    | N   | O   | S  | 0     |
|     |       |          | 3366  | 1094 | 1656 | 270 | 336 | 10 |       |

There are 2 discrepancies between the modelled and reference sequences:

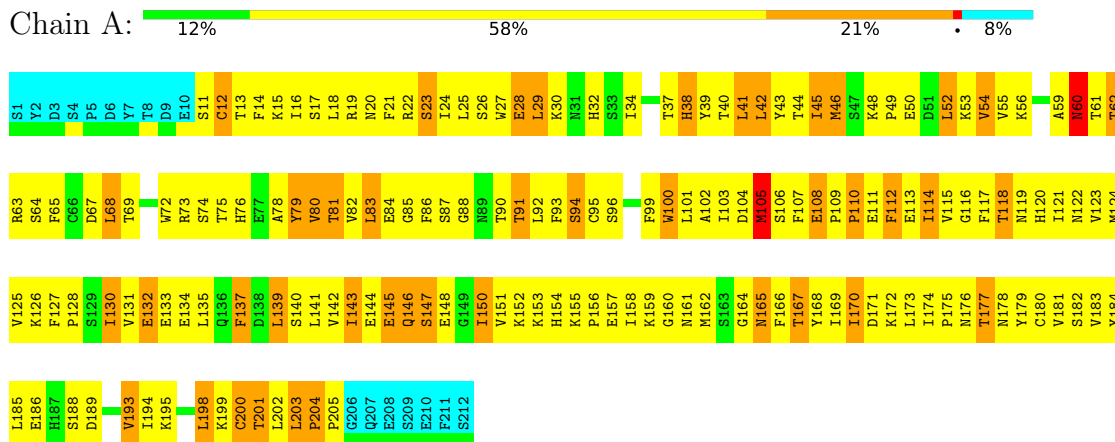
| Chain | Residue | Modelled | Actual | Comment          | Reference  |
|-------|---------|----------|--------|------------------|------------|
| A     | 211     | PHE      | -      | cloning artifact | UNP P48551 |
| A     | 212     | SER      | -      | cloning artifact | UNP P48551 |

## 4 Residue-property plots [i](#)

### 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: Interferon-alpha/beta receptor beta chain

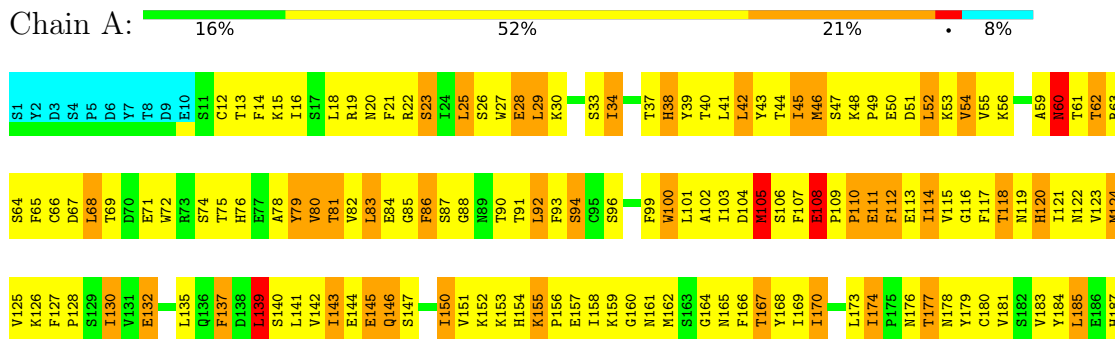


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

#### 4.2.1 Score per residue for model 1

- Molecule 1: Interferon-alpha/beta receptor beta chain

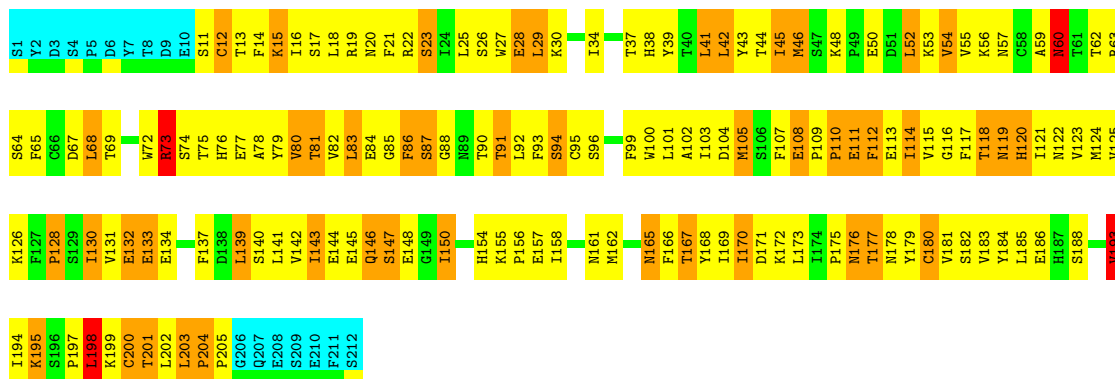




#### 4.2.2 Score per residue for model 2

- Molecule 1: Interferon-alpha/beta receptor beta chain

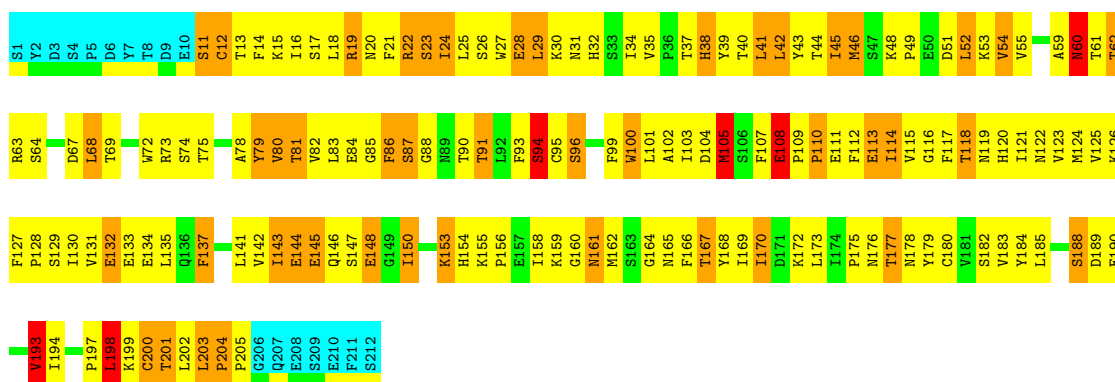
Chain A: 18% 49% 23% 8%



#### 4.2.3 Score per residue for model 3

- Molecule 1: Interferon-alpha/beta receptor beta chain

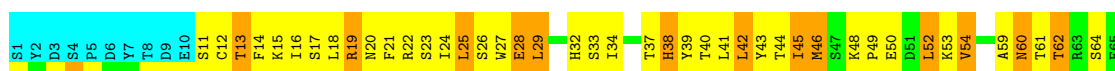
Chain A: 17% 50% 22% 8%

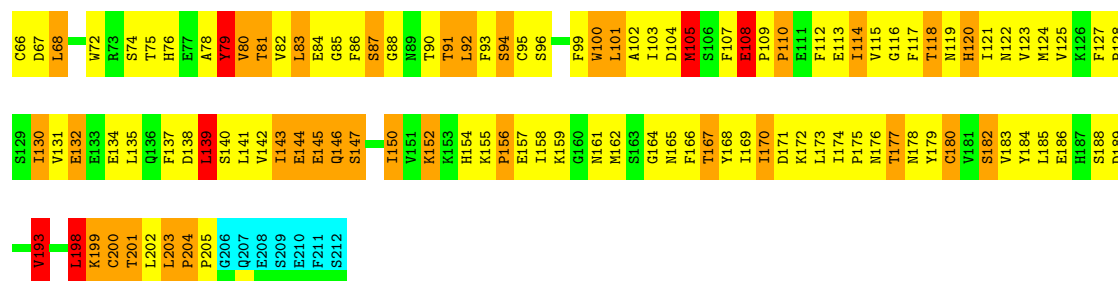


#### 4.2.4 Score per residue for model 4

- Molecule 1: Interferon-alpha/beta receptor beta chain

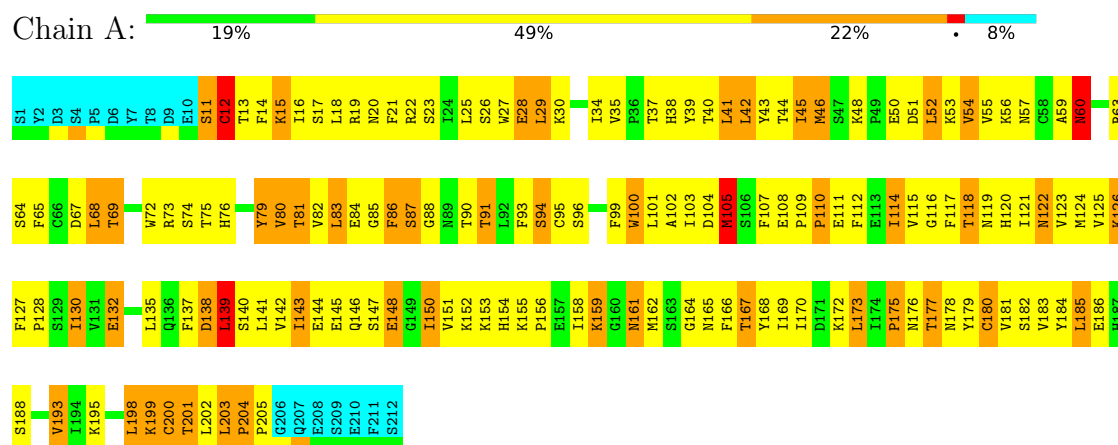
Chain A: 19% 48% 22% 8%





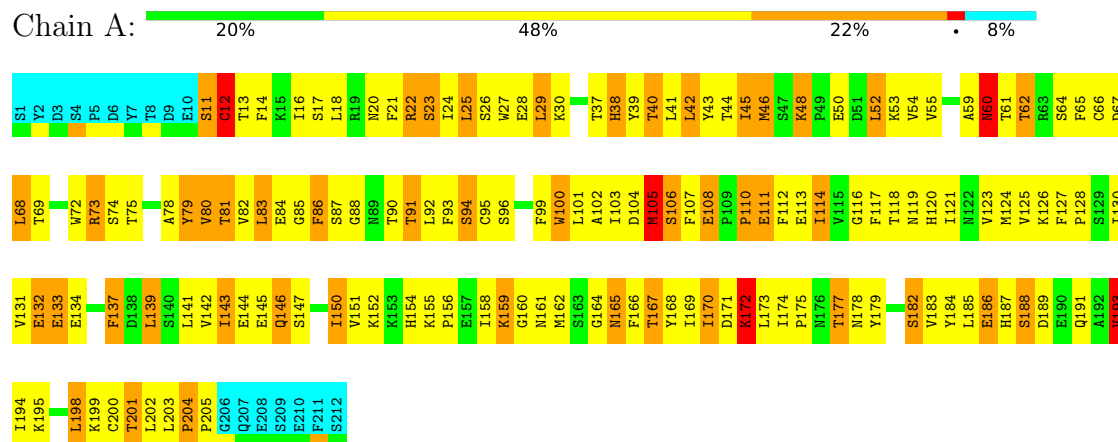
#### 4.2.5 Score per residue for model 5

- Molecule 1: Interferon-alpha/beta receptor beta chain



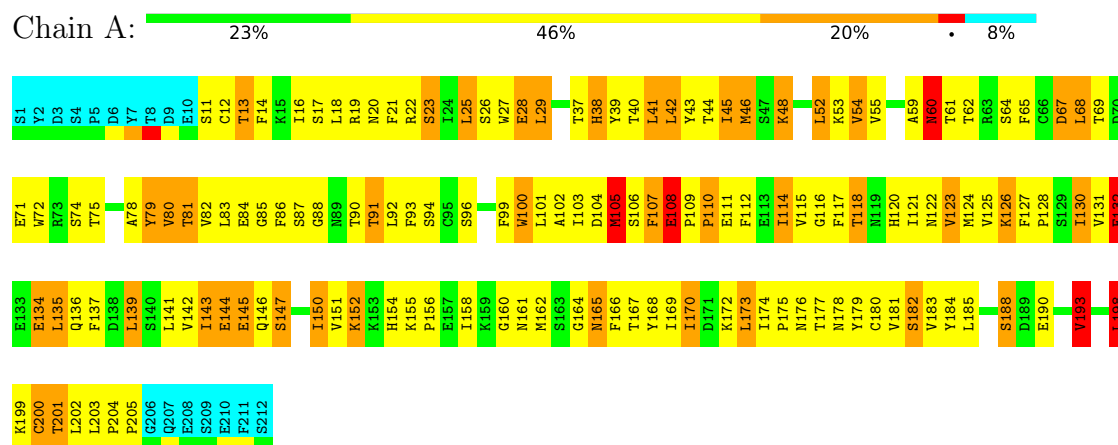
#### 4.2.6 Score per residue for model 6

- Molecule 1: Interferon-alpha/beta receptor beta chain



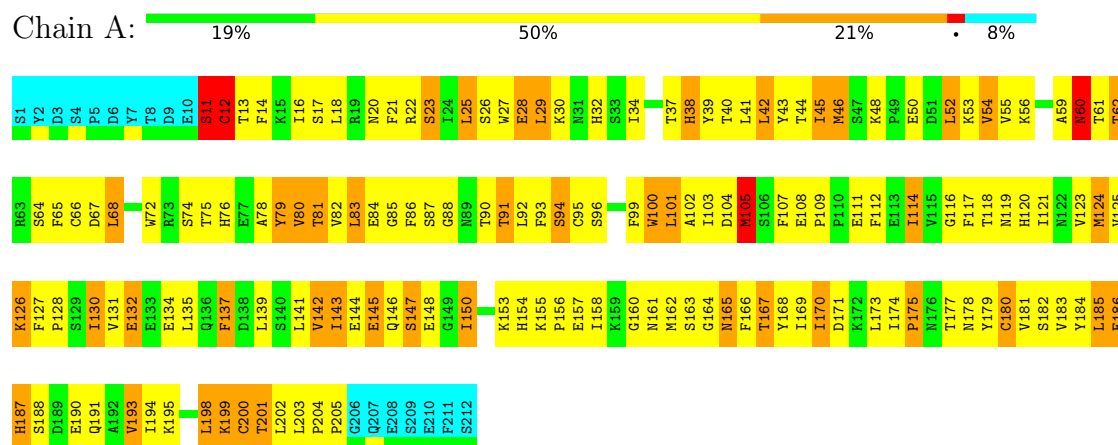
### 4.2.7 Score per residue for model 7

- Molecule 1: Interferon-alpha/beta receptor beta chain



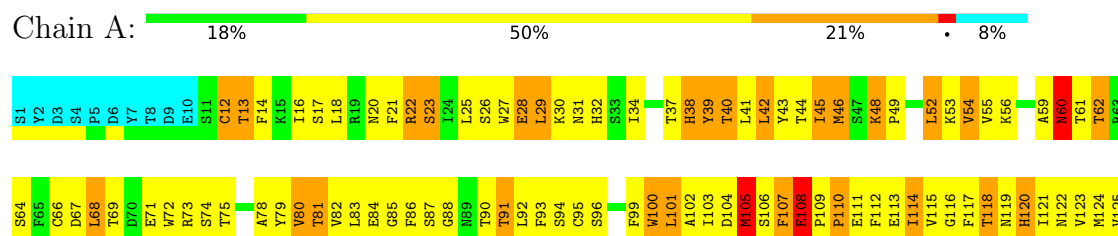
### 4.2.8 Score per residue for model 8

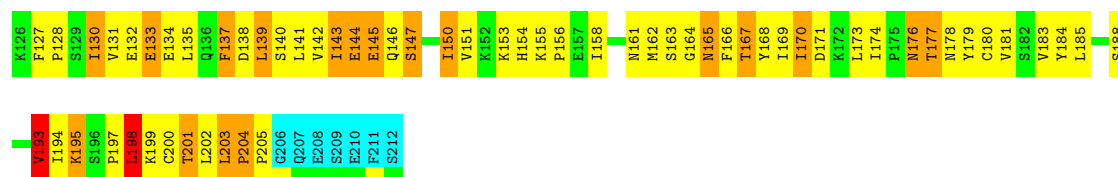
- Molecule 1: Interferon-alpha/beta receptor beta chain



### 4.2.9 Score per residue for model 9

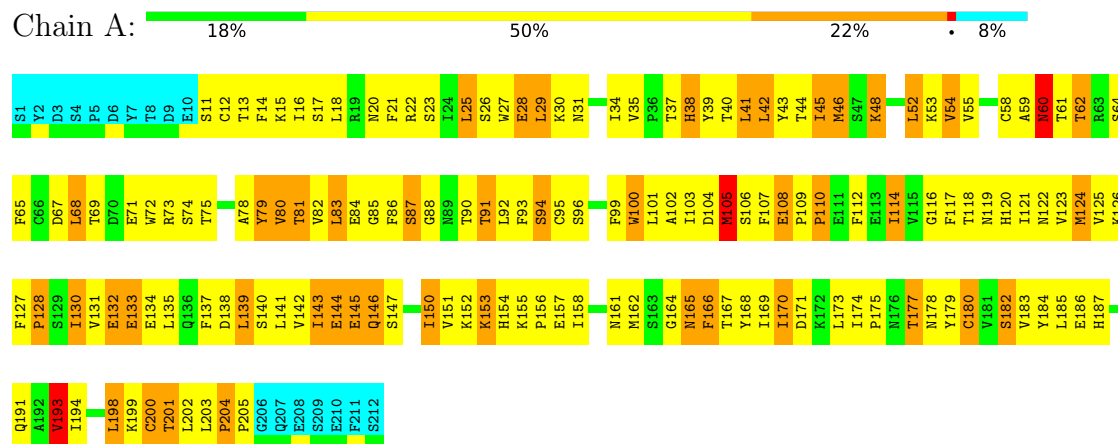
- Molecule 1: Interferon-alpha/beta receptor beta chain





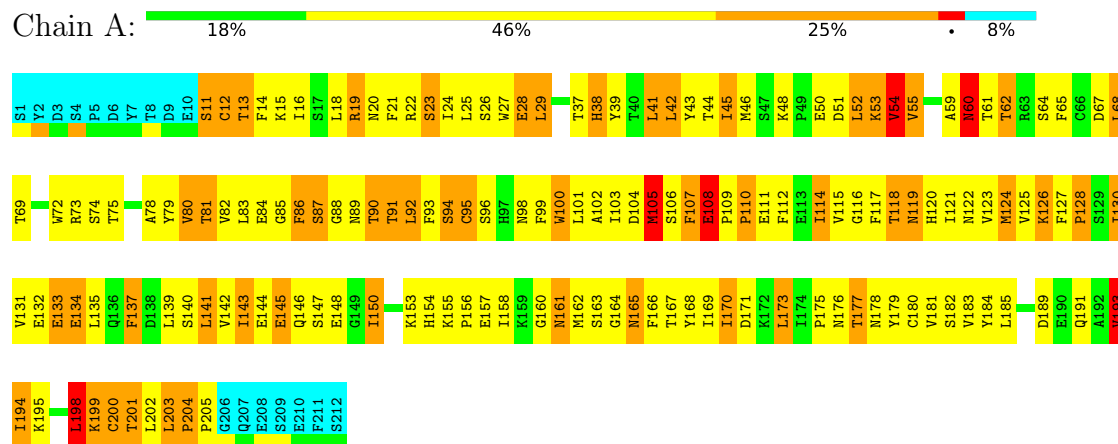
#### 4.2.10 Score per residue for model 10

- Molecule 1: Interferon-alpha/beta receptor beta chain



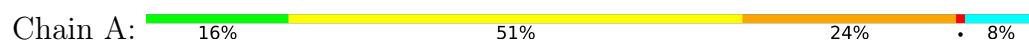
#### 4.2.11 Score per residue for model 11

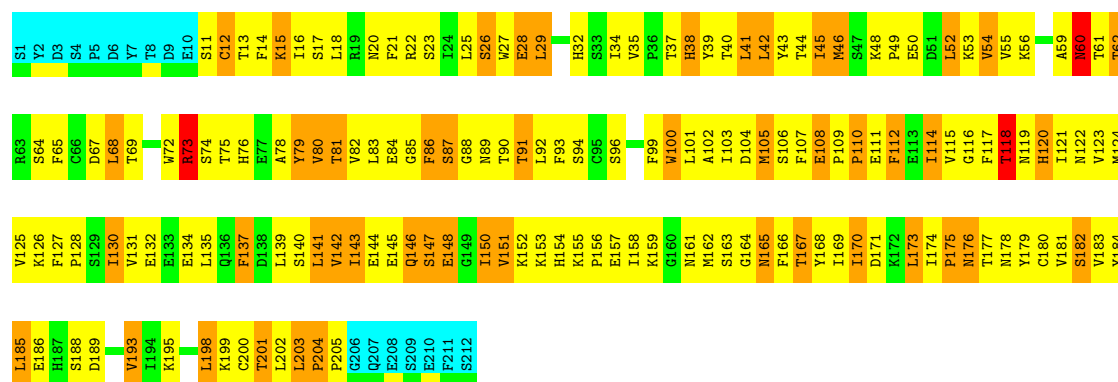
- Molecule 1: Interferon-alpha/beta receptor beta chain



#### 4.2.12 Score per residue for model 12 (medoid)

- Molecule 1: Interferon-alpha/beta receptor beta chain

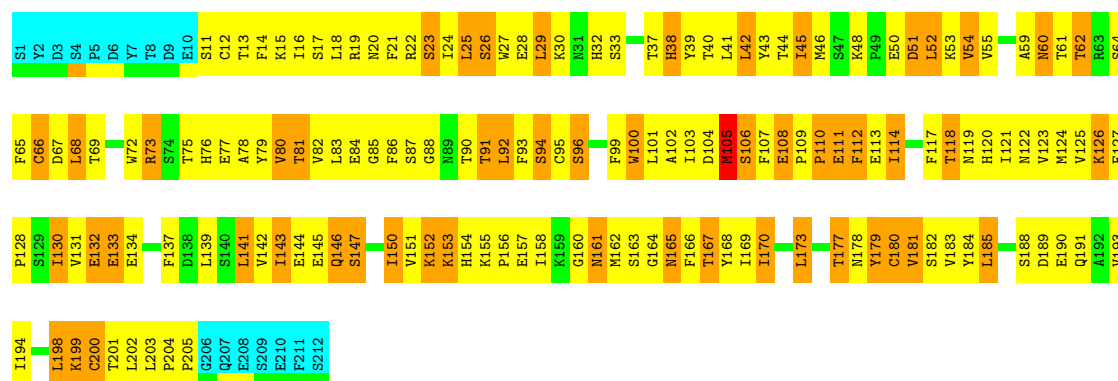




#### 4.2.13 Score per residue for model 13

- Molecule 1: Interferon-alpha/beta receptor beta chain

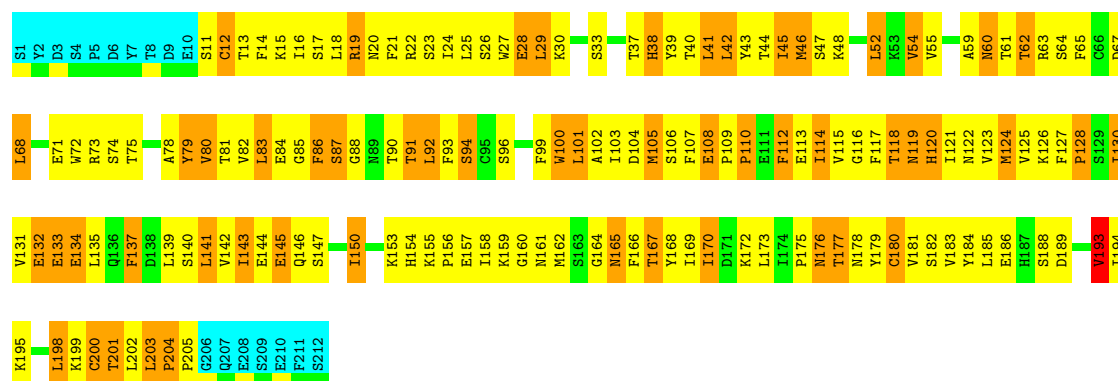
Chain A: 17% 49% 25% 8%



#### 4.2.14 Score per residue for model 14

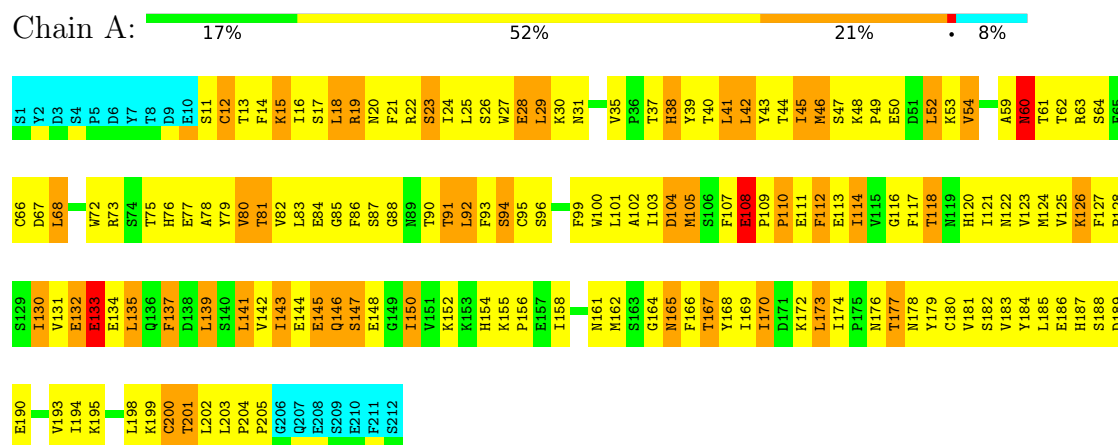
- Molecule 1: Interferon-alpha/beta receptor beta chain

Chain A: 18% 48% 25% 8%



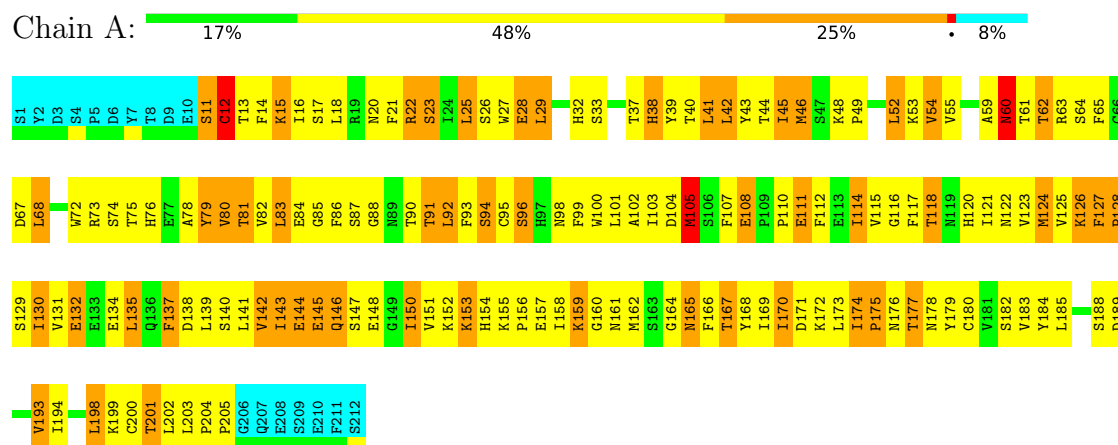
### 4.2.15 Score per residue for model 15

- Molecule 1: Interferon-alpha/beta receptor beta chain



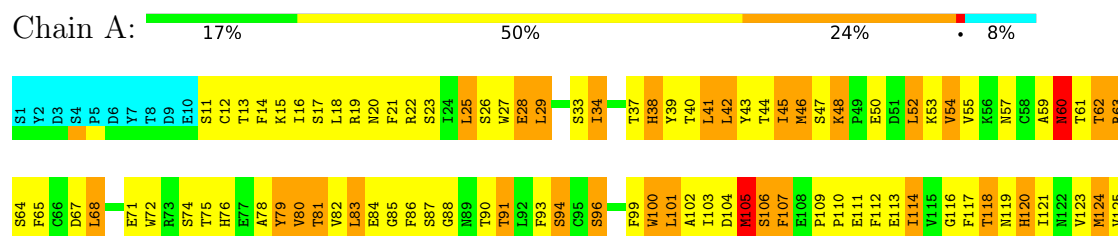
### 4.2.16 Score per residue for model 16

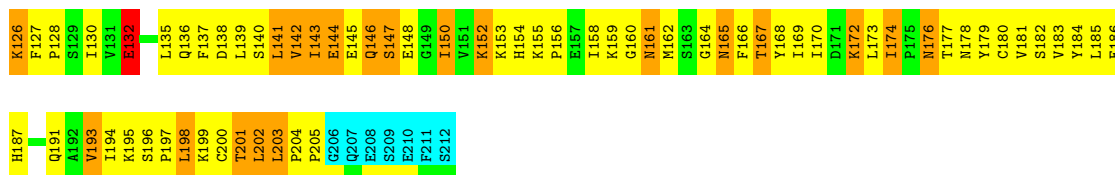
- Molecule 1: Interferon-alpha/beta receptor beta chain



### 4.2.17 Score per residue for model 17

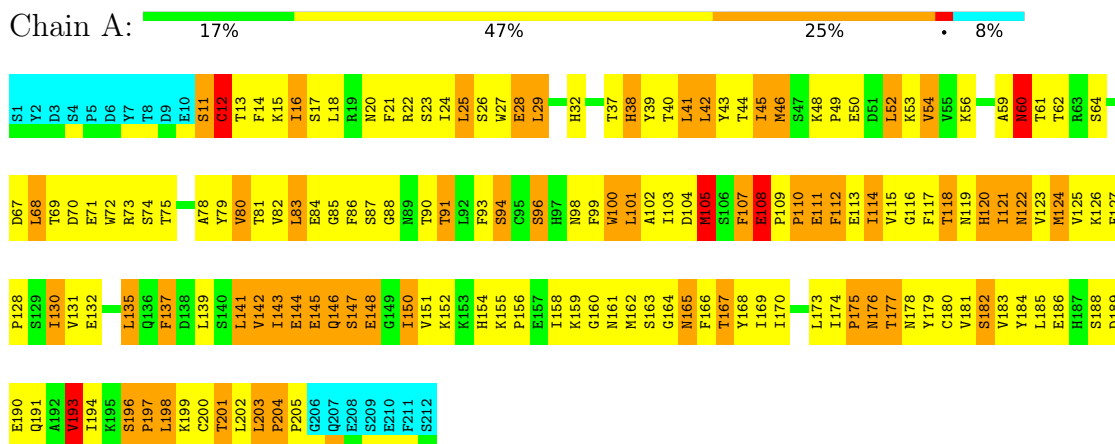
- Molecule 1: Interferon-alpha/beta receptor beta chain





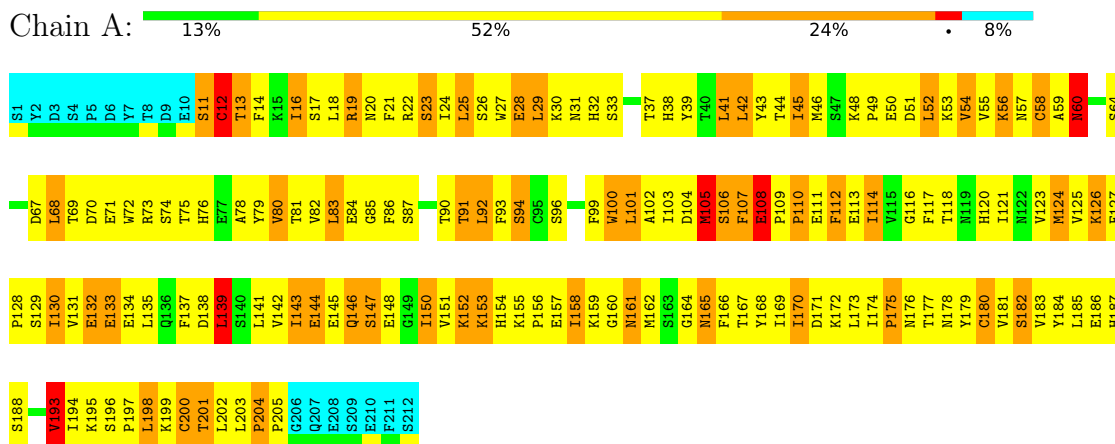
#### 4.2.18 Score per residue for model 18

- Molecule 1: Interferon-alpha/beta receptor beta chain



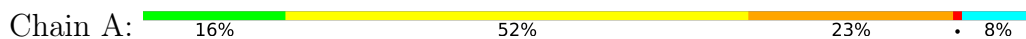
#### 4.2.19 Score per residue for model 19

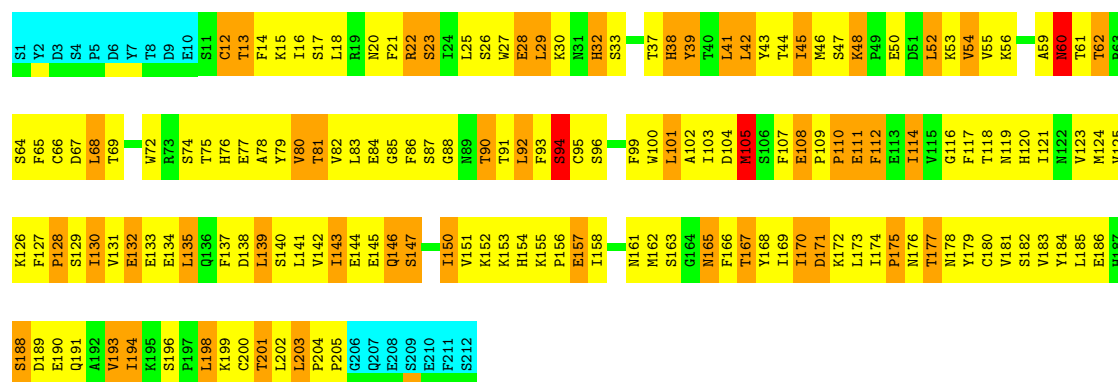
- Molecule 1: Interferon-alpha/beta receptor beta chain



#### 4.2.20 Score per residue for model 20

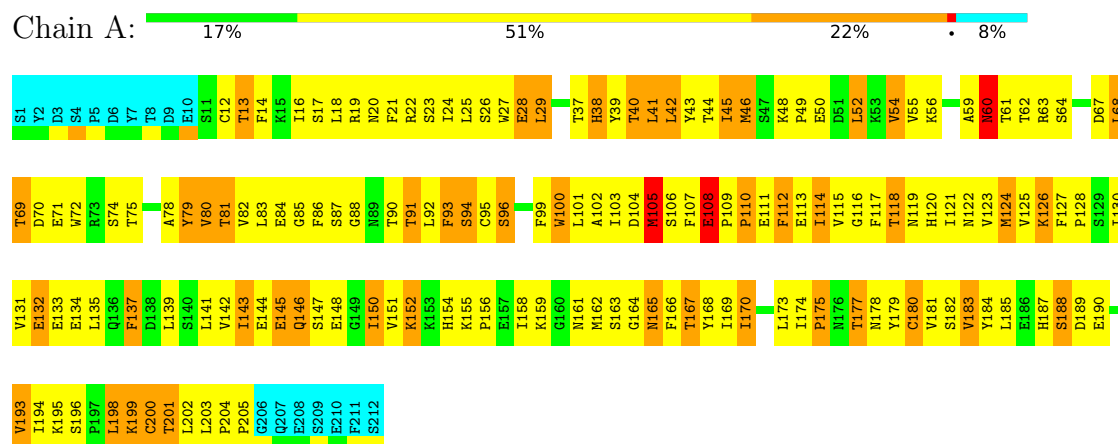
- Molecule 1: Interferon-alpha/beta receptor beta chain





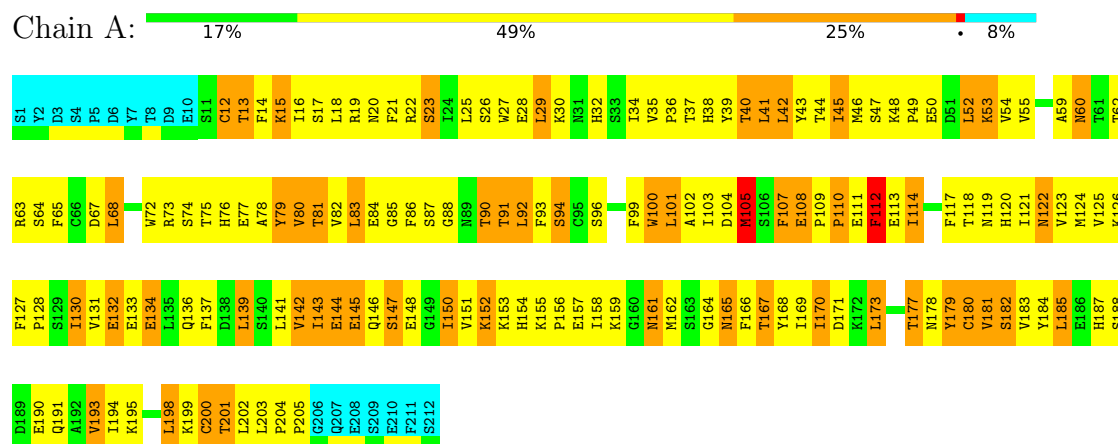
#### 4.2.21 Score per residue for model 21

- Molecule 1: Interferon-alpha/beta receptor beta chain



#### 4.2.22 Score per residue for model 22

- Molecule 1: Interferon-alpha/beta receptor beta chain



## 5 Refinement protocol and experimental data overview ⓘ

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

Of the 35 calculated structures, 22 were deposited, based on the following criterion: *structures with the lowest energy*.

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

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

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     | 0.44±0.01    | 0±0/1613 ( 0.0± 0.0%) | 0.78±0.01   | 1±1/2193 ( 0.0± 0.0%) |
| All | All   | 0.44         | 0/35486 ( 0.0%)       | 0.78        | 16/48246 ( 0.0%)      |

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     | 193 | VAL  | N-CA-C  | 6.67  | 113.34      | 106.21   | 7      | 13    |
| 1   | A     | 193 | VAL  | CB-CA-C | -5.10 | 107.51      | 113.22   | 19     | 3     |

There are no chirality outliers.

There are no planarity outliers.

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

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes averaged over the ensemble.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes |
|-----|-------|-------|----------|----------|---------|
| 1   | A     | 1572  | 1552     | 1545     | 288±12  |
| All | All   | 34584 | 34144    | 33990    | 6340    |

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 92.

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

| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:180:CYS:HB3  | 1:A:198:LEU:HG   | 1.06     | 1.26        | 9      | 6     |
| 1:A:34:ILE:HD11  | 1:A:92:LEU:HD13  | 1.05     | 1.21        | 12     | 3     |
| 1:A:114:ILE:HD12 | 1:A:201:THR:HG22 | 0.99     | 1.32        | 22     | 15    |
| 1:A:44:THR:HG23  | 1:A:80:VAL:HG23  | 0.99     | 1.34        | 11     | 22    |
| 1:A:158:ILE:HG21 | 1:A:162:MET:HE3  | 0.97     | 1.32        | 17     | 20    |
| 1:A:124:MET:SD   | 1:A:167:THR:HG23 | 0.95     | 2.01        | 9      | 18    |
| 1:A:86:PHE:CD2   | 1:A:91:THR:HG23  | 0.94     | 1.97        | 3      | 19    |
| 1:A:143:ILE:HD13 | 1:A:143:ILE:N    | 0.93     | 1.79        | 21     | 22    |
| 1:A:147:SER:O    | 1:A:150:ILE:HD12 | 0.93     | 1.63        | 13     | 14    |
| 1:A:18:LEU:HD22  | 1:A:105:MET:HE2  | 0.92     | 1.40        | 8      | 4     |
| 1:A:121:ILE:HG23 | 1:A:170:ILE:O    | 0.91     | 1.64        | 18     | 1     |
| 1:A:18:LEU:HD23  | 1:A:107:PHE:CE1  | 0.91     | 1.99        | 20     | 8     |
| 1:A:43:TYR:CB    | 1:A:81:THR:HG23  | 0.90     | 1.97        | 16     | 19    |
| 1:A:114:ILE:HD12 | 1:A:201:THR:CG2  | 0.90     | 1.96        | 22     | 19    |
| 1:A:25:LEU:HD11  | 1:A:41:LEU:HD11  | 0.89     | 1.45        | 14     | 22    |
| 1:A:184:TYR:CE2  | 1:A:193:VAL:HG12 | 0.88     | 2.02        | 6      | 5     |
| 1:A:114:ILE:HG22 | 1:A:123:VAL:HA   | 0.88     | 1.46        | 13     | 21    |
| 1:A:107:PHE:CE1  | 1:A:185:LEU:HD22 | 0.88     | 2.04        | 4      | 1     |
| 1:A:107:PHE:CE2  | 1:A:139:LEU:HD11 | 0.87     | 2.05        | 15     | 1     |
| 1:A:85:GLY:HA3   | 1:A:93:PHE:CZ    | 0.87     | 2.04        | 20     | 22    |
| 1:A:25:LEU:HD11  | 1:A:41:LEU:HD21  | 0.87     | 1.47        | 18     | 19    |
| 1:A:179:TYR:O    | 1:A:199:LYS:O    | 0.86     | 1.93        | 13     | 2     |
| 1:A:170:ILE:HD13 | 1:A:179:TYR:CE2  | 0.86     | 2.06        | 13     | 1     |
| 1:A:147:SER:HB2  | 1:A:177:THR:HG22 | 0.85     | 1.49        | 2      | 16    |
| 1:A:29:LEU:HD13  | 1:A:29:LEU:N     | 0.85     | 1.86        | 8      | 11    |
| 1:A:170:ILE:HG22 | 1:A:173:LEU:HD11 | 0.85     | 1.49        | 18     | 2     |
| 1:A:143:ILE:HD11 | 1:A:156:PRO:HD2  | 0.84     | 1.45        | 5      | 20    |
| 1:A:158:ILE:HD13 | 1:A:166:PHE:CZ   | 0.84     | 2.08        | 19     | 7     |
| 1:A:18:LEU:HD23  | 1:A:107:PHE:CZ   | 0.84     | 2.08        | 4      | 1     |
| 1:A:25:LEU:HD23  | 1:A:25:LEU:O     | 0.84     | 1.71        | 16     | 2     |
| 1:A:67:ASP:C     | 1:A:68:LEU:HD23  | 0.84     | 1.97        | 2      | 22    |
| 1:A:178:ASN:N    | 1:A:202:LEU:HD13 | 0.83     | 1.88        | 5      | 19    |
| 1:A:141:LEU:HD21 | 1:A:183:VAL:HG12 | 0.83     | 1.49        | 21     | 5     |
| 1:A:27:TRP:CE3   | 1:A:83:LEU:HD13  | 0.83     | 2.08        | 10     | 22    |
| 1:A:107:PHE:CZ   | 1:A:185:LEU:HD12 | 0.83     | 2.08        | 13     | 1     |
| 1:A:179:TYR:CE1  | 1:A:201:THR:HG22 | 0.82     | 2.08        | 7      | 13    |
| 1:A:25:LEU:HD21  | 1:A:41:LEU:HD21  | 0.82     | 1.51        | 17     | 1     |
| 1:A:86:PHE:CD1   | 1:A:91:THR:HG22  | 0.82     | 2.08        | 1      | 2     |
| 1:A:72:TRP:HA    | 1:A:79:TYR:CZ    | 0.82     | 2.09        | 5      | 22    |
| 1:A:25:LEU:CD1   | 1:A:41:LEU:HD11  | 0.82     | 2.05        | 17     | 12    |
| 1:A:59:ALA:O     | 1:A:60:ASN:C     | 0.81     | 2.24        | 7      | 22    |
| 1:A:143:ILE:HD11 | 1:A:156:PRO:CD   | 0.81     | 2.06        | 5      | 22    |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:25:LEU:CD1   | 1:A:41:LEU:HD21  | 0.80     | 2.06        | 18     | 19    |
| 1:A:107:PHE:CD2  | 1:A:185:LEU:HD23 | 0.80     | 2.10        | 2      | 1     |
| 1:A:29:LEU:HD22  | 1:A:93:PHE:CE2   | 0.80     | 2.11        | 3      | 11    |
| 1:A:141:LEU:HD13 | 1:A:142:VAL:N    | 0.80     | 1.92        | 10     | 12    |
| 1:A:34:ILE:CD1   | 1:A:92:LEU:HD13  | 0.80     | 2.06        | 12     | 3     |
| 1:A:114:ILE:HD11 | 1:A:199:LYS:O    | 0.80     | 1.77        | 22     | 21    |
| 1:A:105:MET:O    | 1:A:185:LEU:HD21 | 0.80     | 1.77        | 2      | 5     |
| 1:A:100:TRP:CD1  | 1:A:103:ILE:HD13 | 0.79     | 2.12        | 2      | 4     |
| 1:A:22:ARG:CD    | 1:A:24:ILE:HD11  | 0.79     | 2.07        | 21     | 2     |
| 1:A:107:PHE:CG   | 1:A:185:LEU:HD21 | 0.79     | 2.12        | 22     | 1     |
| 1:A:130:ILE:HD13 | 1:A:131:VAL:N    | 0.79     | 1.93        | 9      | 6     |
| 1:A:137:PHE:CD1  | 1:A:139:LEU:HD23 | 0.79     | 2.12        | 20     | 2     |
| 1:A:118:THR:HG23 | 1:A:204:PRO:HG2  | 0.79     | 1.55        | 15     | 14    |
| 1:A:25:LEU:H     | 1:A:68:LEU:HD21  | 0.78     | 1.36        | 2      | 22    |
| 1:A:141:LEU:HD11 | 1:A:183:VAL:CG1  | 0.78     | 2.09        | 7      | 4     |
| 1:A:139:LEU:HD23 | 1:A:139:LEU:O    | 0.78     | 1.77        | 2      | 2     |
| 1:A:142:VAL:HG22 | 1:A:184:TYR:O    | 0.78     | 1.78        | 18     | 6     |
| 1:A:37:THR:HG21  | 1:A:88:GLY:O     | 0.78     | 1.77        | 20     | 1     |
| 1:A:125:VAL:HG21 | 1:A:141:LEU:HD21 | 0.78     | 1.53        | 20     | 5     |
| 1:A:42:LEU:HD12  | 1:A:82:VAL:O     | 0.78     | 1.79        | 8      | 21    |
| 1:A:158:ILE:HG21 | 1:A:162:MET:CE   | 0.78     | 2.08        | 17     | 15    |
| 1:A:135:LEU:HD23 | 1:A:137:PHE:O    | 0.78     | 1.79        | 20     | 2     |
| 1:A:54:VAL:HG23  | 1:A:59:ALA:HB2   | 0.77     | 1.56        | 20     | 18    |
| 1:A:121:ILE:HG23 | 1:A:179:TYR:CZ   | 0.77     | 2.14        | 11     | 19    |
| 1:A:137:PHE:CE2  | 1:A:139:LEU:HD11 | 0.77     | 2.14        | 6      | 1     |
| 1:A:121:ILE:HD12 | 1:A:179:TYR:CD1  | 0.77     | 2.14        | 18     | 1     |
| 1:A:145:GLU:HG3  | 1:A:170:ILE:HG21 | 0.77     | 1.57        | 9      | 14    |
| 1:A:123:VAL:CG2  | 1:A:170:ILE:HD11 | 0.77     | 2.10        | 13     | 10    |
| 1:A:82:VAL:HG22  | 1:A:96:SER:HB3   | 0.77     | 1.55        | 8      | 13    |
| 1:A:142:VAL:HG11 | 1:A:184:TYR:CZ   | 0.77     | 2.15        | 4      | 9     |
| 1:A:38:HIS:CE1   | 1:A:86:PHE:HB2   | 0.77     | 2.14        | 1      | 8     |
| 1:A:184:TYR:CE1  | 1:A:193:VAL:HG12 | 0.77     | 2.15        | 21     | 16    |
| 1:A:29:LEU:HD21  | 1:A:83:LEU:HD21  | 0.77     | 1.55        | 3      | 10    |
| 1:A:112:PHE:CG   | 1:A:183:VAL:HG21 | 0.77     | 2.15        | 7      | 17    |
| 1:A:185:LEU:HD21 | 1:A:194:ILE:HD12 | 0.76     | 1.55        | 13     | 1     |
| 1:A:27:TRP:CZ3   | 1:A:83:LEU:HD13  | 0.76     | 2.15        | 20     | 19    |
| 1:A:18:LEU:HD12  | 1:A:22:ARG:O     | 0.76     | 1.80        | 13     | 22    |
| 1:A:121:ILE:O    | 1:A:169:ILE:HG23 | 0.76     | 1.80        | 15     | 20    |
| 1:A:121:ILE:HG21 | 1:A:170:ILE:HD12 | 0.76     | 1.58        | 10     | 12    |
| 1:A:86:PHE:CE2   | 1:A:91:THR:HG23  | 0.76     | 2.16        | 21     | 19    |
| 1:A:145:GLU:CG   | 1:A:170:ILE:HD13 | 0.76     | 2.09        | 8      | 9     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:100:TRP:CE2  | 1:A:103:ILE:HD12 | 0.76     | 2.16        | 11     | 8     |
| 1:A:179:TYR:CE2  | 1:A:201:THR:HG22 | 0.76     | 2.15        | 3      | 7     |
| 1:A:121:ILE:HD12 | 1:A:179:TYR:CE1  | 0.76     | 2.16        | 18     | 1     |
| 1:A:25:LEU:HD22  | 1:A:72:TRP:CZ2   | 0.75     | 2.17        | 18     | 20    |
| 1:A:202:LEU:HD23 | 1:A:203:LEU:N    | 0.75     | 1.97        | 7      | 3     |
| 1:A:139:LEU:CD1  | 1:A:162:MET:HE1  | 0.75     | 2.11        | 18     | 3     |
| 1:A:27:TRP:CE3   | 1:A:41:LEU:HD13  | 0.75     | 2.16        | 13     | 3     |
| 1:A:82:VAL:HG22  | 1:A:96:SER:HB2   | 0.75     | 1.59        | 1      | 6     |
| 1:A:25:LEU:HD11  | 1:A:41:LEU:CD1   | 0.75     | 2.12        | 21     | 17    |
| 1:A:75:THR:O     | 1:A:102:ALA:HB2  | 0.75     | 1.82        | 14     | 22    |
| 1:A:142:VAL:HG12 | 1:A:144:GLU:OE1  | 0.75     | 1.81        | 3      | 3     |
| 1:A:145:GLU:HG2  | 1:A:170:ILE:HD13 | 0.75     | 1.55        | 4      | 1     |
| 1:A:182:SER:OG   | 1:A:198:LEU:HD11 | 0.75     | 1.82        | 18     | 3     |
| 1:A:87:SER:OG    | 1:A:92:LEU:HD22  | 0.75     | 1.82        | 19     | 7     |
| 1:A:34:ILE:HD11  | 1:A:92:LEU:CD1   | 0.75     | 2.09        | 12     | 3     |
| 1:A:147:SER:OG   | 1:A:150:ILE:HD12 | 0.75     | 1.81        | 5      | 4     |
| 1:A:158:ILE:HG21 | 1:A:162:MET:SD   | 0.75     | 2.21        | 14     | 4     |
| 1:A:114:ILE:HG22 | 1:A:123:VAL:HB   | 0.75     | 1.59        | 7      | 1     |
| 1:A:82:VAL:HG22  | 1:A:96:SER:OG    | 0.74     | 1.80        | 13     | 3     |
| 1:A:185:LEU:HD13 | 1:A:185:LEU:N    | 0.74     | 1.96        | 1      | 2     |
| 1:A:146:GLN:HG2  | 1:A:151:VAL:HG22 | 0.74     | 1.59        | 21     | 8     |
| 1:A:25:LEU:HD11  | 1:A:41:LEU:CG    | 0.74     | 2.13        | 5      | 14    |
| 1:A:146:GLN:OE1  | 1:A:151:VAL:HG13 | 0.74     | 1.83        | 18     | 1     |
| 1:A:114:ILE:HG22 | 1:A:123:VAL:CB   | 0.74     | 2.13        | 7      | 3     |
| 1:A:135:LEU:O    | 1:A:135:LEU:HD23 | 0.74     | 1.83        | 18     | 3     |
| 1:A:19:ARG:HG3   | 1:A:24:ILE:HD13  | 0.74     | 1.57        | 15     | 3     |
| 1:A:170:ILE:HG21 | 1:A:179:TYR:OH   | 0.74     | 1.83        | 13     | 1     |
| 1:A:121:ILE:HB   | 1:A:179:TYR:CZ   | 0.74     | 2.18        | 18     | 1     |
| 1:A:202:LEU:HD23 | 1:A:203:LEU:H    | 0.74     | 1.42        | 17     | 3     |
| 1:A:121:ILE:HD11 | 1:A:173:LEU:HD22 | 0.74     | 1.58        | 13     | 1     |
| 1:A:127:PHE:CZ   | 1:A:141:LEU:HD23 | 0.73     | 2.17        | 13     | 1     |
| 1:A:170:ILE:O    | 1:A:173:LEU:HD21 | 0.73     | 1.82        | 17     | 1     |
| 1:A:121:ILE:HB   | 1:A:179:TYR:CE2  | 0.73     | 2.19        | 18     | 1     |
| 1:A:123:VAL:HG11 | 1:A:143:ILE:CG2  | 0.73     | 2.13        | 13     | 12    |
| 1:A:105:MET:HB3  | 1:A:185:LEU:HD11 | 0.73     | 1.57        | 20     | 3     |
| 1:A:145:GLU:HG3  | 1:A:170:ILE:HD13 | 0.73     | 1.57        | 8      | 10    |
| 1:A:180:CYS:HB3  | 1:A:198:LEU:CG   | 0.73     | 2.12        | 9      | 9     |
| 1:A:171:ASP:O    | 1:A:173:LEU:HD12 | 0.73     | 1.84        | 22     | 1     |
| 1:A:142:VAL:HG21 | 1:A:184:TYR:CZ   | 0.73     | 2.19        | 18     | 7     |
| 1:A:29:LEU:HD11  | 1:A:83:LEU:HD21  | 0.73     | 1.59        | 22     | 1     |
| 1:A:27:TRP:CE3   | 1:A:41:LEU:HD23  | 0.73     | 2.19        | 12     | 17    |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:139:LEU:HD13 | 1:A:185:LEU:HD23 | 0.73     | 1.60        | 4      | 2     |
| 1:A:146:GLN:HG3  | 1:A:151:VAL:HG22 | 0.73     | 1.60        | 6      | 2     |
| 1:A:137:PHE:CD2  | 1:A:139:LEU:HD23 | 0.72     | 2.19        | 5      | 3     |
| 1:A:184:TYR:CZ   | 1:A:193:VAL:HG12 | 0.72     | 2.19        | 1      | 16    |
| 1:A:146:GLN:O    | 1:A:179:TYR:HA   | 0.72     | 1.83        | 17     | 19    |
| 1:A:114:ILE:CG2  | 1:A:123:VAL:HG13 | 0.72     | 2.14        | 19     | 15    |
| 1:A:147:SER:OG   | 1:A:177:THR:HG23 | 0.72     | 1.84        | 12     | 3     |
| 1:A:198:LEU:N    | 1:A:198:LEU:HD22 | 0.72     | 1.99        | 9      | 1     |
| 1:A:143:ILE:HD11 | 1:A:156:PRO:CG   | 0.72     | 2.15        | 14     | 6     |
| 1:A:105:MET:O    | 1:A:185:LEU:HD11 | 0.72     | 1.84        | 12     | 3     |
| 1:A:27:TRP:CD1   | 1:A:29:LEU:HD11  | 0.72     | 2.19        | 6      | 18    |
| 1:A:174:ILE:HD12 | 1:A:175:PRO:O    | 0.72     | 1.85        | 8      | 1     |
| 1:A:118:THR:O    | 1:A:203:LEU:HD13 | 0.71     | 1.85        | 1      | 5     |
| 1:A:29:LEU:HD23  | 1:A:39:TYR:CE1   | 0.71     | 2.18        | 8      | 4     |
| 1:A:180:CYS:O    | 1:A:198:LEU:HD22 | 0.71     | 1.85        | 13     | 12    |
| 1:A:202:LEU:HD12 | 1:A:203:LEU:H    | 0.71     | 1.44        | 16     | 19    |
| 1:A:107:PHE:CD1  | 1:A:185:LEU:HD22 | 0.71     | 2.20        | 4      | 3     |
| 1:A:141:LEU:HB2  | 1:A:162:MET:HE2  | 0.71     | 1.63        | 19     | 6     |
| 1:A:147:SER:CB   | 1:A:177:THR:HG22 | 0.71     | 2.15        | 5      | 17    |
| 1:A:18:LEU:HD22  | 1:A:105:MET:HG3  | 0.71     | 1.62        | 22     | 3     |
| 1:A:138:ASP:O    | 1:A:139:LEU:HD12 | 0.71     | 1.86        | 5      | 2     |
| 1:A:44:THR:HG23  | 1:A:80:VAL:CG2   | 0.71     | 2.15        | 12     | 20    |
| 1:A:143:ILE:N    | 1:A:143:ILE:CD1  | 0.71     | 2.51        | 21     | 19    |
| 1:A:27:TRP:CD1   | 1:A:29:LEU:HD21  | 0.71     | 2.20        | 8      | 6     |
| 1:A:185:LEU:HD22 | 1:A:186:GLU:N    | 0.71     | 2.00        | 12     | 1     |
| 1:A:42:LEU:HD11  | 1:A:84:GLU:HB2   | 0.70     | 1.63        | 8      | 20    |
| 1:A:16:ILE:HB    | 1:A:99:PHE:CE1   | 0.70     | 2.21        | 19     | 2     |
| 1:A:81:THR:O     | 1:A:96:SER:HA    | 0.70     | 1.87        | 19     | 22    |
| 1:A:123:VAL:HG21 | 1:A:170:ILE:HD11 | 0.70     | 1.62        | 22     | 11    |
| 1:A:34:ILE:HG21  | 1:A:92:LEU:HD13  | 0.70     | 1.62        | 4      | 1     |
| 1:A:135:LEU:CD1  | 1:A:137:PHE:O    | 0.70     | 2.39        | 17     | 2     |
| 1:A:107:PHE:HB2  | 1:A:185:LEU:HD22 | 0.70     | 1.64        | 9      | 2     |
| 1:A:185:LEU:CD2  | 1:A:194:ILE:HD12 | 0.70     | 2.16        | 13     | 1     |
| 1:A:185:LEU:HD21 | 1:A:194:ILE:CD1  | 0.70     | 2.16        | 13     | 1     |
| 1:A:141:LEU:HD11 | 1:A:183:VAL:HG13 | 0.70     | 1.62        | 22     | 10    |
| 1:A:105:MET:HG2  | 1:A:139:LEU:HD22 | 0.70     | 1.63        | 6      | 1     |
| 1:A:118:THR:CB   | 1:A:204:PRO:HG2  | 0.69     | 2.17        | 17     | 22    |
| 1:A:27:TRP:CG    | 1:A:83:LEU:HD22  | 0.69     | 2.23        | 9      | 2     |
| 1:A:86:PHE:CE1   | 1:A:91:THR:HG22  | 0.69     | 2.23        | 1      | 1     |
| 1:A:139:LEU:HD12 | 1:A:162:MET:HE1  | 0.69     | 1.64        | 18     | 2     |
| 1:A:117:PHE:O    | 1:A:203:LEU:HD22 | 0.69     | 1.88        | 6      | 8     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:25:LEU:HD11  | 1:A:41:LEU:CD2   | 0.69     | 2.18        | 2      | 17    |
| 1:A:25:LEU:HD22  | 1:A:72:TRP:CH2   | 0.69     | 2.22        | 18     | 3     |
| 1:A:14:PHE:HA    | 1:A:26:SER:O     | 0.69     | 1.88        | 22     | 21    |
| 1:A:131:VAL:HG23 | 1:A:134:GLU:HG2  | 0.69     | 1.65        | 3      | 2     |
| 1:A:127:PHE:CZ   | 1:A:141:LEU:HD13 | 0.69     | 2.23        | 1      | 5     |
| 1:A:43:TYR:N     | 1:A:52:LEU:HD23  | 0.69     | 2.03        | 13     | 22    |
| 1:A:127:PHE:CE2  | 1:A:141:LEU:HD13 | 0.69     | 2.23        | 7      | 4     |
| 1:A:122:ASN:OD1  | 1:A:169:ILE:HD12 | 0.69     | 1.87        | 18     | 4     |
| 1:A:107:PHE:HB2  | 1:A:185:LEU:HD23 | 0.69     | 1.65        | 7      | 3     |
| 1:A:127:PHE:O    | 1:A:164:GLY:HA2  | 0.68     | 1.88        | 16     | 9     |
| 1:A:177:THR:HB   | 1:A:203:LEU:HD21 | 0.68     | 1.64        | 11     | 4     |
| 1:A:142:VAL:HG21 | 1:A:184:TYR:CE2  | 0.68     | 2.24        | 6      | 5     |
| 1:A:38:HIS:HA    | 1:A:61:THR:O     | 0.68     | 1.89        | 13     | 18    |
| 1:A:180:CYS:CB   | 1:A:198:LEU:HG   | 0.68     | 2.18        | 17     | 4     |
| 1:A:18:LEU:HD12  | 1:A:22:ARG:C     | 0.68     | 2.13        | 17     | 19    |
| 1:A:28:GLU:C     | 1:A:29:LEU:HD13  | 0.68     | 2.14        | 8      | 1     |
| 1:A:22:ARG:HD2   | 1:A:24:ILE:HD11  | 0.68     | 1.64        | 21     | 1     |
| 1:A:173:LEU:HD13 | 1:A:203:LEU:HD11 | 0.68     | 1.65        | 7      | 1     |
| 1:A:27:TRP:CZ2   | 1:A:64:SER:HA    | 0.68     | 2.24        | 17     | 22    |
| 1:A:27:TRP:HB2   | 1:A:29:LEU:HD11  | 0.68     | 1.64        | 8      | 3     |
| 1:A:25:LEU:HD11  | 1:A:81:THR:HG21  | 0.68     | 1.65        | 4      | 2     |
| 1:A:37:THR:HG23  | 1:A:38:HIS:H     | 0.67     | 1.48        | 20     | 2     |
| 1:A:132:GLU:HG3  | 1:A:135:LEU:HD22 | 0.67     | 1.64        | 20     | 1     |
| 1:A:37:THR:HG23  | 1:A:38:HIS:N     | 0.67     | 2.05        | 20     | 22    |
| 1:A:142:VAL:C    | 1:A:143:ILE:HD13 | 0.67     | 2.15        | 21     | 7     |
| 1:A:118:THR:CG2  | 1:A:204:PRO:HG2  | 0.67     | 2.18        | 15     | 14    |
| 1:A:118:THR:HG22 | 1:A:175:PRO:HG3  | 0.67     | 1.66        | 19     | 4     |
| 1:A:118:THR:OG1  | 1:A:204:PRO:CG   | 0.67     | 2.42        | 22     | 15    |
| 1:A:14:PHE:CE1   | 1:A:83:LEU:HD23  | 0.67     | 2.25        | 19     | 19    |
| 1:A:125:VAL:CG1  | 1:A:183:VAL:HG11 | 0.67     | 2.20        | 17     | 11    |
| 1:A:107:PHE:CE2  | 1:A:185:LEU:HD12 | 0.67     | 2.25        | 13     | 1     |
| 1:A:117:PHE:O    | 1:A:203:LEU:HD13 | 0.67     | 1.89        | 15     | 1     |
| 1:A:18:LEU:HD21  | 1:A:105:MET:HE3  | 0.66     | 1.66        | 2      | 3     |
| 1:A:27:TRP:CZ3   | 1:A:41:LEU:HD23  | 0.66     | 2.25        | 3      | 15    |
| 1:A:68:LEU:CD1   | 1:A:72:TRP:CD2   | 0.66     | 2.77        | 18     | 22    |
| 1:A:142:VAL:HG13 | 1:A:154:HIS:O    | 0.66     | 1.91        | 1      | 4     |
| 1:A:42:LEU:HD23  | 1:A:54:VAL:HG12  | 0.66     | 1.66        | 13     | 9     |
| 1:A:147:SER:OG   | 1:A:150:ILE:HD11 | 0.66     | 1.90        | 3      | 1     |
| 1:A:25:LEU:CD2   | 1:A:41:LEU:HD21  | 0.66     | 2.21        | 17     | 1     |
| 1:A:141:LEU:CD2  | 1:A:183:VAL:HG12 | 0.66     | 2.19        | 21     | 1     |
| 1:A:18:LEU:HA    | 1:A:22:ARG:O     | 0.66     | 1.90        | 18     | 20    |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:46:MET:N     | 1:A:80:VAL:HG22  | 0.66     | 2.04        | 11     | 21    |
| 1:A:82:VAL:HG22  | 1:A:96:SER:CB    | 0.66     | 2.19        | 4      | 20    |
| 1:A:121:ILE:CG2  | 1:A:170:ILE:HD12 | 0.66     | 2.19        | 15     | 3     |
| 1:A:27:TRP:CZ3   | 1:A:41:LEU:HD13  | 0.66     | 2.25        | 6      | 2     |
| 1:A:72:TRP:HA    | 1:A:79:TYR:CE2   | 0.66     | 2.25        | 16     | 16    |
| 1:A:118:THR:OG1  | 1:A:204:PRO:HG3  | 0.66     | 1.91        | 6      | 15    |
| 1:A:139:LEU:HD21 | 1:A:185:LEU:HD22 | 0.66     | 1.68        | 7      | 1     |
| 1:A:125:VAL:HG13 | 1:A:183:VAL:HG11 | 0.66     | 1.67        | 21     | 10    |
| 1:A:100:TRP:NE1  | 1:A:103:ILE:HD12 | 0.66     | 2.06        | 21     | 8     |
| 1:A:121:ILE:HG23 | 1:A:179:TYR:CE1  | 0.66     | 2.25        | 12     | 12    |
| 1:A:137:PHE:C    | 1:A:137:PHE:CD1  | 0.66     | 2.73        | 17     | 2     |
| 1:A:114:ILE:O    | 1:A:201:THR:HG21 | 0.66     | 1.90        | 7      | 9     |
| 1:A:143:ILE:HG12 | 1:A:154:HIS:O    | 0.65     | 1.90        | 16     | 1     |
| 1:A:43:TYR:HB2   | 1:A:81:THR:HG23  | 0.65     | 1.68        | 4      | 19    |
| 1:A:29:LEU:HD13  | 1:A:39:TYR:CE1   | 0.65     | 2.26        | 15     | 10    |
| 1:A:176:ASN:HA   | 1:A:202:LEU:HD21 | 0.65     | 1.68        | 7      | 3     |
| 1:A:121:ILE:HD11 | 1:A:170:ILE:HD13 | 0.65     | 1.68        | 18     | 1     |
| 1:A:25:LEU:HD21  | 1:A:41:LEU:CD1   | 0.65     | 2.22        | 16     | 1     |
| 1:A:114:ILE:HG22 | 1:A:123:VAL:CA   | 0.65     | 2.22        | 22     | 12    |
| 1:A:72:TRP:CD2   | 1:A:79:TYR:CD2   | 0.65     | 2.85        | 6      | 9     |
| 1:A:176:ASN:CG   | 1:A:176:ASN:O    | 0.65     | 2.39        | 18     | 6     |
| 1:A:18:LEU:CD2   | 1:A:105:MET:HE3  | 0.65     | 2.22        | 3      | 2     |
| 1:A:86:PHE:CD1   | 1:A:86:PHE:N     | 0.65     | 2.64        | 1      | 14    |
| 1:A:147:SER:HB3  | 1:A:177:THR:HG22 | 0.65     | 1.68        | 19     | 5     |
| 1:A:84:GLU:HG2   | 1:A:94:SER:CB    | 0.65     | 2.21        | 9      | 9     |
| 1:A:121:ILE:HG21 | 1:A:170:ILE:CD1  | 0.65     | 2.21        | 10     | 11    |
| 1:A:27:TRP:CD1   | 1:A:29:LEU:HD12  | 0.65     | 2.27        | 22     | 1     |
| 1:A:145:GLU:HG3  | 1:A:170:ILE:HD12 | 0.65     | 1.69        | 22     | 1     |
| 1:A:25:LEU:CG    | 1:A:41:LEU:HD21  | 0.64     | 2.22        | 13     | 5     |
| 1:A:54:VAL:CG2   | 1:A:59:ALA:HB2   | 0.64     | 2.22        | 10     | 13    |
| 1:A:27:TRP:CG    | 1:A:29:LEU:HD11  | 0.64     | 2.28        | 6      | 8     |
| 1:A:38:HIS:CE1   | 1:A:88:GLY:O     | 0.64     | 2.50        | 1      | 20    |
| 1:A:42:LEU:HD23  | 1:A:54:VAL:HB    | 0.64     | 1.67        | 6      | 20    |
| 1:A:144:GLU:HB2  | 1:A:182:SER:OG   | 0.64     | 1.92        | 3      | 2     |
| 1:A:107:PHE:CG   | 1:A:185:LEU:HD11 | 0.64     | 2.27        | 14     | 2     |
| 1:A:34:ILE:HG21  | 1:A:92:LEU:CD1   | 0.64     | 2.23        | 4      | 1     |
| 1:A:29:LEU:HD11  | 1:A:83:LEU:CD2   | 0.64     | 2.22        | 20     | 2     |
| 1:A:146:GLN:HG2  | 1:A:151:VAL:HG12 | 0.64     | 1.69        | 10     | 3     |
| 1:A:130:ILE:HD11 | 1:A:135:LEU:CD2  | 0.64     | 2.22        | 14     | 1     |
| 1:A:105:MET:HE3  | 1:A:105:MET:HA   | 0.64     | 1.69        | 11     | 4     |
| 1:A:14:PHE:HE1   | 1:A:83:LEU:HD23  | 0.64     | 1.53        | 21     | 22    |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:137:PHE:CD1  | 1:A:138:ASP:N    | 0.64     | 2.65        | 20     | 3     |
| 1:A:145:GLU:CD   | 1:A:170:ILE:HG21 | 0.64     | 2.18        | 19     | 2     |
| 1:A:143:ILE:O    | 1:A:154:HIS:HB2  | 0.64     | 1.92        | 12     | 22    |
| 1:A:23:SER:HB3   | 1:A:68:LEU:O     | 0.64     | 1.92        | 13     | 22    |
| 1:A:42:LEU:HB2   | 1:A:82:VAL:O     | 0.64     | 1.92        | 11     | 17    |
| 1:A:23:SER:C     | 1:A:24:ILE:HD12  | 0.64     | 2.18        | 15     | 3     |
| 1:A:107:PHE:O    | 1:A:194:ILE:HG21 | 0.63     | 1.93        | 17     | 5     |
| 1:A:25:LEU:N     | 1:A:68:LEU:HD21  | 0.63     | 2.08        | 6      | 20    |
| 1:A:147:SER:O    | 1:A:150:ILE:HD13 | 0.63     | 1.94        | 16     | 6     |
| 1:A:202:LEU:C    | 1:A:203:LEU:HD13 | 0.63     | 2.17        | 3      | 1     |
| 1:A:135:LEU:O    | 1:A:135:LEU:HD12 | 0.63     | 1.93        | 21     | 1     |
| 1:A:179:TYR:O    | 1:A:200:CYS:HA   | 0.63     | 1.93        | 9      | 22    |
| 1:A:92:LEU:HD23  | 1:A:93:PHE:CE1   | 0.63     | 2.29        | 20     | 12    |
| 1:A:37:THR:HG22  | 1:A:86:PHE:O     | 0.63     | 1.94        | 20     | 1     |
| 1:A:46:MET:HE3   | 1:A:78:ALA:HB3   | 0.63     | 1.70        | 17     | 11    |
| 1:A:141:LEU:HD21 | 1:A:183:VAL:CG1  | 0.63     | 2.23        | 8      | 4     |
| 1:A:142:VAL:HG21 | 1:A:184:TYR:CE1  | 0.62     | 2.28        | 15     | 8     |
| 1:A:54:VAL:HG13  | 1:A:54:VAL:O     | 0.62     | 1.94        | 6      | 2     |
| 1:A:158:ILE:HD13 | 1:A:166:PHE:HZ   | 0.62     | 1.54        | 19     | 6     |
| 1:A:121:ILE:HB   | 1:A:170:ILE:HD12 | 0.62     | 1.71        | 13     | 1     |
| 1:A:100:TRP:CD2  | 1:A:103:ILE:HD13 | 0.62     | 2.30        | 22     | 9     |
| 1:A:127:PHE:HE1  | 1:A:141:LEU:HD22 | 0.62     | 1.54        | 18     | 1     |
| 1:A:139:LEU:O    | 1:A:139:LEU:HD12 | 0.62     | 1.95        | 8      | 1     |
| 1:A:198:LEU:N    | 1:A:198:LEU:CD2  | 0.62     | 2.62        | 9      | 1     |
| 1:A:179:TYR:CE1  | 1:A:203:LEU:HD11 | 0.62     | 2.28        | 3      | 1     |
| 1:A:179:TYR:CD2  | 1:A:181:VAL:HG23 | 0.62     | 2.29        | 13     | 1     |
| 1:A:121:ILE:HG23 | 1:A:179:TYR:CE2  | 0.62     | 2.30        | 6      | 7     |
| 1:A:127:PHE:CZ   | 1:A:162:MET:HE2  | 0.62     | 2.29        | 21     | 6     |
| 1:A:50:GLU:O     | 1:A:52:LEU:N     | 0.62     | 2.33        | 13     | 1     |
| 1:A:127:PHE:CE1  | 1:A:141:LEU:HD22 | 0.62     | 2.29        | 18     | 1     |
| 1:A:78:ALA:HB1   | 1:A:100:TRP:CE3  | 0.62     | 2.30        | 20     | 4     |
| 1:A:25:LEU:HG    | 1:A:41:LEU:HD21  | 0.62     | 1.72        | 13     | 3     |
| 1:A:54:VAL:CG2   | 1:A:54:VAL:O     | 0.62     | 2.47        | 1      | 16    |
| 1:A:158:ILE:CG2  | 1:A:162:MET:HE3  | 0.62     | 2.21        | 1      | 4     |
| 1:A:139:LEU:HD12 | 1:A:185:LEU:HD22 | 0.62     | 1.72        | 15     | 2     |
| 1:A:19:ARG:O     | 1:A:22:ARG:HB3   | 0.62     | 1.94        | 21     | 2     |
| 1:A:148:GLU:HG2  | 1:A:177:THR:HG23 | 0.62     | 1.70        | 22     | 4     |
| 1:A:11:SER:N     | 1:A:28:GLU:O     | 0.62     | 2.32        | 8      | 1     |
| 1:A:141:LEU:HD12 | 1:A:143:ILE:CD1  | 0.62     | 2.25        | 13     | 5     |
| 1:A:27:TRP:CB    | 1:A:83:LEU:HD22  | 0.61     | 2.25        | 17     | 22    |
| 1:A:147:SER:O    | 1:A:150:ILE:CD1  | 0.61     | 2.48        | 16     | 17    |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:22:ARG:HD3   | 1:A:24:ILE:HD11  | 0.61     | 1.72        | 3      | 2     |
| 1:A:18:LEU:HD22  | 1:A:105:MET:SD   | 0.61     | 2.35        | 14     | 1     |
| 1:A:144:GLU:O    | 1:A:181:VAL:HA   | 0.61     | 1.96        | 20     | 12    |
| 1:A:104:ASP:O    | 1:A:105:MET:C    | 0.61     | 2.44        | 21     | 22    |
| 1:A:139:LEU:HD21 | 1:A:162:MET:SD   | 0.61     | 2.35        | 2      | 1     |
| 1:A:42:LEU:HD23  | 1:A:54:VAL:CB    | 0.61     | 2.25        | 4      | 18    |
| 1:A:177:THR:OG1  | 1:A:203:LEU:HD11 | 0.61     | 1.96        | 11     | 4     |
| 1:A:27:TRP:CZ2   | 1:A:64:SER:O     | 0.61     | 2.54        | 4      | 21    |
| 1:A:43:TYR:CE2   | 1:A:55:VAL:HG22  | 0.61     | 2.31        | 17     | 18    |
| 1:A:142:VAL:HB   | 1:A:155:LYS:CG   | 0.61     | 2.26        | 12     | 1     |
| 1:A:34:ILE:HG22  | 1:A:87:SER:OG    | 0.61     | 1.95        | 9      | 2     |
| 1:A:125:VAL:O    | 1:A:166:PHE:HB2  | 0.60     | 1.95        | 8      | 19    |
| 1:A:141:LEU:HD23 | 1:A:143:ILE:CD1  | 0.60     | 2.26        | 14     | 1     |
| 1:A:42:LEU:O     | 1:A:81:THR:HG22  | 0.60     | 1.95        | 10     | 19    |
| 1:A:12:CYS:HA    | 1:A:29:LEU:HD12  | 0.60     | 1.73        | 8      | 1     |
| 1:A:132:GLU:HA   | 1:A:135:LEU:HD22 | 0.60     | 1.73        | 16     | 1     |
| 1:A:27:TRP:CZ2   | 1:A:39:TYR:CD2   | 0.60     | 2.89        | 20     | 12    |
| 1:A:25:LEU:CD1   | 1:A:81:THR:HG21  | 0.60     | 2.26        | 4      | 2     |
| 1:A:142:VAL:HA   | 1:A:154:HIS:O    | 0.60     | 1.96        | 9      | 11    |
| 1:A:25:LEU:HD22  | 1:A:68:LEU:CD2   | 0.60     | 2.26        | 16     | 2     |
| 1:A:184:TYR:CD1  | 1:A:193:VAL:HG23 | 0.60     | 2.31        | 15     | 1     |
| 1:A:185:LEU:N    | 1:A:185:LEU:HD12 | 0.60     | 2.11        | 19     | 3     |
| 1:A:114:ILE:HG22 | 1:A:123:VAL:HG13 | 0.60     | 1.73        | 17     | 6     |
| 1:A:42:LEU:HD13  | 1:A:54:VAL:HA    | 0.60     | 1.70        | 11     | 1     |
| 1:A:146:GLN:HA   | 1:A:150:ILE:O    | 0.60     | 1.97        | 18     | 21    |
| 1:A:185:LEU:HD22 | 1:A:185:LEU:C    | 0.60     | 2.22        | 12     | 1     |
| 1:A:147:SER:CB   | 1:A:179:TYR:HB3  | 0.60     | 2.26        | 21     | 20    |
| 1:A:142:VAL:HG11 | 1:A:184:TYR:CE1  | 0.60     | 2.32        | 22     | 5     |
| 1:A:123:VAL:CG1  | 1:A:181:VAL:HG11 | 0.60     | 2.27        | 18     | 3     |
| 1:A:112:PHE:CE2  | 1:A:183:VAL:HG22 | 0.60     | 2.31        | 21     | 1     |
| 1:A:114:ILE:HG22 | 1:A:123:VAL:HG22 | 0.60     | 1.73        | 17     | 6     |
| 1:A:72:TRP:CD1   | 1:A:79:TYR:CE2   | 0.59     | 2.90        | 5      | 10    |
| 1:A:130:ILE:HD11 | 1:A:135:LEU:CB   | 0.59     | 2.27        | 16     | 3     |
| 1:A:144:GLU:O    | 1:A:181:VAL:HG13 | 0.59     | 1.97        | 21     | 1     |
| 1:A:79:TYR:HB2   | 1:A:101:LEU:HD11 | 0.59     | 1.74        | 20     | 19    |
| 1:A:111:GLU:O    | 1:A:126:LYS:CG   | 0.59     | 2.50        | 17     | 2     |
| 1:A:16:ILE:CD1   | 1:A:72:TRP:CZ3   | 0.59     | 2.85        | 4      | 19    |
| 1:A:46:MET:HG2   | 1:A:78:ALA:HB3   | 0.59     | 1.74        | 8      | 10    |
| 1:A:107:PHE:HB2  | 1:A:185:LEU:HD11 | 0.59     | 1.75        | 1      | 2     |
| 1:A:121:ILE:CD1  | 1:A:179:TYR:CE1  | 0.59     | 2.85        | 3      | 8     |
| 1:A:127:PHE:CZ   | 1:A:162:MET:HA   | 0.59     | 2.32        | 14     | 2     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:79:TYR:O     | 1:A:99:PHE:HB2   | 0.59     | 1.97        | 14     | 7     |
| 1:A:121:ILE:HG13 | 1:A:173:LEU:HD11 | 0.59     | 1.75        | 7      | 2     |
| 1:A:72:TRP:CH2   | 1:A:79:TYR:HB3   | 0.59     | 2.33        | 9      | 15    |
| 1:A:203:LEU:O    | 1:A:205:PRO:HD3  | 0.59     | 1.98        | 16     | 19    |
| 1:A:185:LEU:C    | 1:A:185:LEU:HD12 | 0.59     | 2.22        | 17     | 3     |
| 1:A:107:PHE:HB2  | 1:A:185:LEU:HD13 | 0.59     | 1.73        | 19     | 3     |
| 1:A:142:VAL:HG11 | 1:A:184:TYR:OH   | 0.59     | 1.96        | 4      | 4     |
| 1:A:18:LEU:HD21  | 1:A:105:MET:HE2  | 0.59     | 1.75        | 15     | 1     |
| 1:A:170:ILE:O    | 1:A:173:LEU:HD13 | 0.59     | 1.98        | 22     | 1     |
| 1:A:108:GLU:N    | 1:A:109:PRO:CD   | 0.59     | 2.66        | 5      | 8     |
| 1:A:121:ILE:HD12 | 1:A:170:ILE:HB   | 0.59     | 1.75        | 13     | 14    |
| 1:A:142:VAL:HG13 | 1:A:184:TYR:O    | 0.59     | 1.97        | 17     | 4     |
| 1:A:139:LEU:HD23 | 1:A:139:LEU:C    | 0.59     | 2.22        | 2      | 2     |
| 1:A:139:LEU:HD13 | 1:A:162:MET:HE1  | 0.59     | 1.73        | 8      | 1     |
| 1:A:182:SER:HB2  | 1:A:198:LEU:CD1  | 0.59     | 2.28        | 17     | 2     |
| 1:A:42:LEU:CD2   | 1:A:54:VAL:HG12  | 0.59     | 2.27        | 13     | 17    |
| 1:A:130:ILE:HD13 | 1:A:131:VAL:C    | 0.59     | 2.23        | 15     | 5     |
| 1:A:203:LEU:HD13 | 1:A:203:LEU:N    | 0.59     | 2.13        | 3      | 1     |
| 1:A:44:THR:CG2   | 1:A:80:VAL:HG23  | 0.59     | 2.24        | 8      | 3     |
| 1:A:121:ILE:CD1  | 1:A:179:TYR:CE2  | 0.59     | 2.86        | 8      | 12    |
| 1:A:34:ILE:CG2   | 1:A:92:LEU:HD13  | 0.59     | 2.28        | 8      | 1     |
| 1:A:46:MET:HE3   | 1:A:78:ALA:CB    | 0.58     | 2.28        | 17     | 10    |
| 1:A:22:ARG:HB3   | 1:A:69:THR:HG22  | 0.58     | 1.74        | 11     | 8     |
| 1:A:168:TYR:O    | 1:A:169:ILE:HD13 | 0.58     | 1.98        | 18     | 2     |
| 1:A:124:MET:HG3  | 1:A:166:PHE:O    | 0.58     | 1.97        | 13     | 18    |
| 1:A:41:LEU:HD22  | 1:A:83:LEU:HB2   | 0.58     | 1.75        | 5      | 8     |
| 1:A:114:ILE:HG13 | 1:A:199:LYS:HG2  | 0.58     | 1.74        | 22     | 3     |
| 1:A:175:PRO:HA   | 1:A:203:LEU:HD12 | 0.58     | 1.74        | 5      | 2     |
| 1:A:107:PHE:CE1  | 1:A:185:LEU:HD12 | 0.58     | 2.33        | 13     | 1     |
| 1:A:144:GLU:HG3  | 1:A:184:TYR:CE2  | 0.58     | 2.34        | 9      | 4     |
| 1:A:131:VAL:O    | 1:A:131:VAL:HG13 | 0.58     | 1.98        | 14     | 3     |
| 1:A:68:LEU:HD12  | 1:A:72:TRP:CG    | 0.58     | 2.33        | 21     | 21    |
| 1:A:182:SER:N    | 1:A:198:LEU:HD23 | 0.58     | 2.13        | 8      | 8     |
| 1:A:121:ILE:HD13 | 1:A:179:TYR:CZ   | 0.58     | 2.34        | 13     | 7     |
| 1:A:203:LEU:HD23 | 1:A:203:LEU:N    | 0.58     | 2.13        | 5      | 1     |
| 1:A:46:MET:HB3   | 1:A:78:ALA:HB3   | 0.58     | 1.75        | 20     | 2     |
| 1:A:141:LEU:HD23 | 1:A:185:LEU:HG   | 0.58     | 1.76        | 4      | 1     |
| 1:A:21:PHE:CD1   | 1:A:130:ILE:HG21 | 0.58     | 2.34        | 20     | 2     |
| 1:A:27:TRP:HB3   | 1:A:83:LEU:HD22  | 0.58     | 1.76        | 3      | 20    |
| 1:A:29:LEU:HD21  | 1:A:83:LEU:CD2   | 0.58     | 2.27        | 3      | 2     |
| 1:A:145:GLU:HB2  | 1:A:170:ILE:HD13 | 0.58     | 1.75        | 19     | 2     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:43:TYR:HB3   | 1:A:81:THR:HG23  | 0.58     | 1.76        | 4      | 2     |
| 1:A:144:GLU:HB3  | 1:A:182:SER:OG   | 0.58     | 1.98        | 12     | 7     |
| 1:A:202:LEU:C    | 1:A:203:LEU:HD12 | 0.58     | 2.24        | 13     | 1     |
| 1:A:54:VAL:O     | 1:A:54:VAL:HG22  | 0.58     | 1.99        | 4      | 19    |
| 1:A:185:LEU:HD22 | 1:A:185:LEU:H    | 0.58     | 1.59        | 1      | 1     |
| 1:A:101:LEU:HB3  | 1:A:105:MET:HE1  | 0.58     | 1.75        | 11     | 3     |
| 1:A:124:MET:HA   | 1:A:166:PHE:O    | 0.58     | 1.99        | 2      | 19    |
| 1:A:146:GLN:CG   | 1:A:151:VAL:HG22 | 0.58     | 2.26        | 21     | 9     |
| 1:A:118:THR:CA   | 1:A:204:PRO:HG2  | 0.57     | 2.29        | 12     | 16    |
| 1:A:54:VAL:O     | 1:A:54:VAL:CG2   | 0.57     | 2.51        | 20     | 3     |
| 1:A:139:LEU:HD12 | 1:A:162:MET:SD   | 0.57     | 2.39        | 4      | 2     |
| 1:A:176:ASN:HB2  | 1:A:205:PRO:CB   | 0.57     | 2.29        | 4      | 10    |
| 1:A:140:SER:HA   | 1:A:162:MET:HE1  | 0.57     | 1.74        | 14     | 2     |
| 1:A:84:GLU:CG    | 1:A:94:SER:HB3   | 0.57     | 2.30        | 4      | 17    |
| 1:A:118:THR:OG1  | 1:A:204:PRO:HB2  | 0.57     | 1.99        | 4      | 7     |
| 1:A:171:ASP:C    | 1:A:173:LEU:HD12 | 0.57     | 2.24        | 10     | 8     |
| 1:A:27:TRP:CE3   | 1:A:41:LEU:HD12  | 0.57     | 2.34        | 17     | 1     |
| 1:A:107:PHE:CB   | 1:A:185:LEU:HD21 | 0.57     | 2.30        | 22     | 1     |
| 1:A:178:ASN:CA   | 1:A:202:LEU:HD13 | 0.57     | 2.29        | 20     | 19    |
| 1:A:78:ALA:HB1   | 1:A:100:TRP:CZ3  | 0.57     | 2.35        | 2      | 4     |
| 1:A:135:LEU:HD21 | 1:A:137:PHE:CB   | 0.57     | 2.30        | 8      | 2     |
| 1:A:137:PHE:CZ   | 1:A:139:LEU:HD23 | 0.57     | 2.35        | 18     | 4     |
| 1:A:198:LEU:HD22 | 1:A:198:LEU:H    | 0.57     | 1.59        | 9      | 1     |
| 1:A:42:LEU:HD13  | 1:A:54:VAL:CA    | 0.57     | 2.29        | 11     | 1     |
| 1:A:194:ILE:HD12 | 1:A:194:ILE:N    | 0.57     | 2.13        | 20     | 1     |
| 1:A:40:THR:HG22  | 1:A:40:THR:O     | 0.57     | 1.99        | 6      | 7     |
| 1:A:105:MET:HA   | 1:A:105:MET:HE2  | 0.57     | 1.76        | 12     | 1     |
| 1:A:43:TYR:CD1   | 1:A:43:TYR:C     | 0.57     | 2.82        | 18     | 22    |
| 1:A:72:TRP:CG    | 1:A:79:TYR:CD2   | 0.57     | 2.92        | 12     | 13    |
| 1:A:107:PHE:CB   | 1:A:185:LEU:HD13 | 0.57     | 2.30        | 19     | 2     |
| 1:A:184:TYR:CG   | 1:A:193:VAL:HG23 | 0.57     | 2.35        | 15     | 1     |
| 1:A:121:ILE:HD12 | 1:A:179:TYR:CG   | 0.57     | 2.35        | 18     | 1     |
| 1:A:35:VAL:HG13  | 1:A:35:VAL:O     | 0.57     | 1.99        | 22     | 4     |
| 1:A:34:ILE:HD12  | 1:A:34:ILE:O     | 0.57     | 1.99        | 22     | 1     |
| 1:A:173:LEU:HD21 | 1:A:179:TYR:OH   | 0.57     | 2.00        | 22     | 1     |
| 1:A:121:ILE:HG23 | 1:A:179:TYR:OH   | 0.57     | 2.00        | 21     | 19    |
| 1:A:177:THR:C    | 1:A:202:LEU:CD1  | 0.57     | 2.77        | 13     | 16    |
| 1:A:135:LEU:HD12 | 1:A:135:LEU:C    | 0.56     | 2.25        | 21     | 1     |
| 1:A:161:ASN:HB3  | 1:A:166:PHE:CE2  | 0.56     | 2.35        | 13     | 19    |
| 1:A:75:THR:HG21  | 1:A:137:PHE:CZ   | 0.56     | 2.35        | 9      | 1     |
| 1:A:131:VAL:HG23 | 1:A:134:GLU:CG   | 0.56     | 2.30        | 16     | 3     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:184:TYR:CD2  | 1:A:193:VAL:HG12 | 0.56     | 2.35        | 12     | 1     |
| 1:A:178:ASN:N    | 1:A:202:LEU:CD1  | 0.56     | 2.68        | 20     | 15    |
| 1:A:121:ILE:CD1  | 1:A:170:ILE:HD13 | 0.56     | 2.30        | 18     | 1     |
| 1:A:72:TRP:CD2   | 1:A:79:TYR:CG    | 0.56     | 2.94        | 4      | 17    |
| 1:A:156:PRO:HG3  | 1:A:168:TYR:CD2  | 0.56     | 2.36        | 7      | 15    |
| 1:A:180:CYS:HA   | 1:A:199:LYS:O    | 0.56     | 2.01        | 20     | 9     |
| 1:A:108:GLU:H    | 1:A:109:PRO:CD   | 0.56     | 2.14        | 5      | 1     |
| 1:A:142:VAL:HB   | 1:A:154:HIS:O    | 0.56     | 2.01        | 21     | 5     |
| 1:A:45:ILE:HD13  | 1:A:45:ILE:N     | 0.56     | 2.15        | 19     | 2     |
| 1:A:72:TRP:HE3   | 1:A:101:LEU:HD21 | 0.56     | 1.60        | 15     | 16    |
| 1:A:86:PHE:HD2   | 1:A:91:THR:HG23  | 0.56     | 1.54        | 6      | 1     |
| 1:A:27:TRP:CD1   | 1:A:29:LEU:CD1   | 0.56     | 2.89        | 22     | 12    |
| 1:A:127:PHE:HZ   | 1:A:141:LEU:HD23 | 0.56     | 1.57        | 13     | 1     |
| 1:A:174:ILE:HD13 | 1:A:174:ILE:H    | 0.56     | 1.61        | 17     | 1     |
| 1:A:123:VAL:HG11 | 1:A:143:ILE:HG21 | 0.56     | 1.78        | 5      | 3     |
| 1:A:87:SER:HG    | 1:A:92:LEU:HD22  | 0.56     | 1.58        | 10     | 1     |
| 1:A:142:VAL:HG11 | 1:A:184:TYR:CE2  | 0.56     | 2.36        | 12     | 1     |
| 1:A:81:THR:OG1   | 1:A:99:PHE:CE1   | 0.56     | 2.54        | 20     | 12    |
| 1:A:141:LEU:HD21 | 1:A:183:VAL:HG13 | 0.56     | 1.77        | 15     | 1     |
| 1:A:131:VAL:HG23 | 1:A:134:GLU:HG3  | 0.56     | 1.77        | 16     | 1     |
| 1:A:25:LEU:HD21  | 1:A:41:LEU:HD11  | 0.56     | 1.76        | 2      | 4     |
| 1:A:144:GLU:CB   | 1:A:182:SER:OG   | 0.56     | 2.54        | 12     | 3     |
| 1:A:161:ASN:CB   | 1:A:166:PHE:CE2  | 0.56     | 2.89        | 4      | 7     |
| 1:A:29:LEU:CD2   | 1:A:39:TYR:CE1   | 0.56     | 2.89        | 8      | 5     |
| 1:A:45:ILE:HD12  | 1:A:48:LYS:HD3   | 0.56     | 1.78        | 6      | 1     |
| 1:A:168:TYR:CE1  | 1:A:170:ILE:HD13 | 0.56     | 2.36        | 22     | 1     |
| 1:A:29:LEU:CD2   | 1:A:83:LEU:HD21  | 0.55     | 2.31        | 15     | 8     |
| 1:A:112:PHE:CD2  | 1:A:125:VAL:HG22 | 0.55     | 2.36        | 21     | 1     |
| 1:A:21:PHE:CE2   | 1:A:130:ILE:HG21 | 0.55     | 2.36        | 2      | 1     |
| 1:A:92:LEU:HD23  | 1:A:93:PHE:CD1   | 0.55     | 2.37        | 22     | 4     |
| 1:A:125:VAL:O    | 1:A:165:ASN:HA   | 0.55     | 2.02        | 16     | 1     |
| 1:A:31:ASN:HB3   | 1:A:35:VAL:HG12  | 0.55     | 1.78        | 3      | 1     |
| 1:A:20:ASN:O     | 1:A:21:PHE:CD1   | 0.55     | 2.59        | 10     | 8     |
| 1:A:105:MET:HB3  | 1:A:185:LEU:HD21 | 0.55     | 1.78        | 6      | 2     |
| 1:A:185:LEU:CD2  | 1:A:194:ILE:HD13 | 0.55     | 2.31        | 8      | 1     |
| 1:A:141:LEU:HD13 | 1:A:141:LEU:C    | 0.55     | 2.25        | 3      | 6     |
| 1:A:146:GLN:CG   | 1:A:151:VAL:HG12 | 0.55     | 2.30        | 10     | 3     |
| 1:A:121:ILE:HD13 | 1:A:179:TYR:CE2  | 0.55     | 2.37        | 13     | 11    |
| 1:A:173:LEU:HD23 | 1:A:177:THR:HG21 | 0.55     | 1.77        | 16     | 4     |
| 1:A:121:ILE:CB   | 1:A:170:ILE:HD12 | 0.55     | 2.31        | 13     | 1     |
| 1:A:54:VAL:HG22  | 1:A:59:ALA:HB2   | 0.55     | 1.77        | 22     | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:114:ILE:CG1  | 1:A:199:LYS:HB3  | 0.55     | 2.32        | 1      | 4     |
| 1:A:147:SER:HB3  | 1:A:179:TYR:HB3  | 0.55     | 1.78        | 2      | 3     |
| 1:A:29:LEU:HD11  | 1:A:83:LEU:HD23  | 0.55     | 1.76        | 9      | 2     |
| 1:A:27:TRP:CE2   | 1:A:64:SER:HA    | 0.55     | 2.35        | 17     | 22    |
| 1:A:107:PHE:HB2  | 1:A:185:LEU:HD21 | 0.55     | 1.78        | 1      | 1     |
| 1:A:112:PHE:CD1  | 1:A:112:PHE:C    | 0.55     | 2.84        | 22     | 14    |
| 1:A:137:PHE:C    | 1:A:137:PHE:HD1  | 0.55     | 2.09        | 6      | 1     |
| 1:A:114:ILE:HD12 | 1:A:201:THR:HB   | 0.54     | 1.79        | 20     | 16    |
| 1:A:72:TRP:CD1   | 1:A:79:TYR:CE1   | 0.54     | 2.95        | 22     | 4     |
| 1:A:139:LEU:HD12 | 1:A:139:LEU:C    | 0.54     | 2.27        | 8      | 2     |
| 1:A:21:PHE:CE1   | 1:A:130:ILE:HG21 | 0.54     | 2.38        | 20     | 2     |
| 1:A:123:VAL:HG13 | 1:A:181:VAL:HG11 | 0.54     | 1.77        | 18     | 1     |
| 1:A:68:LEU:CD1   | 1:A:72:TRP:CG    | 0.54     | 2.91        | 13     | 22    |
| 1:A:25:LEU:HD23  | 1:A:25:LEU:C     | 0.54     | 2.27        | 4      | 2     |
| 1:A:135:LEU:HD12 | 1:A:138:ASP:N    | 0.54     | 2.18        | 4      | 3     |
| 1:A:29:LEU:N     | 1:A:29:LEU:CD1   | 0.54     | 2.60        | 8      | 8     |
| 1:A:100:TRP:CE3  | 1:A:103:ILE:HD13 | 0.54     | 2.38        | 5      | 10    |
| 1:A:100:TRP:CZ3  | 1:A:103:ILE:HD13 | 0.54     | 2.38        | 18     | 5     |
| 1:A:107:PHE:CZ   | 1:A:139:LEU:HD13 | 0.54     | 2.38        | 5      | 1     |
| 1:A:145:GLU:OE2  | 1:A:173:LEU:HD21 | 0.54     | 2.02        | 14     | 5     |
| 1:A:60:ASN:O     | 1:A:60:ASN:CG    | 0.54     | 2.51        | 15     | 7     |
| 1:A:42:LEU:CB    | 1:A:82:VAL:O     | 0.54     | 2.55        | 11     | 1     |
| 1:A:140:SER:CA   | 1:A:162:MET:HE1  | 0.54     | 2.31        | 14     | 2     |
| 1:A:141:LEU:HD22 | 1:A:142:VAL:H    | 0.54     | 1.63        | 21     | 2     |
| 1:A:34:ILE:HD12  | 1:A:34:ILE:C     | 0.54     | 2.27        | 22     | 1     |
| 1:A:25:LEU:CD2   | 1:A:72:TRP:CZ2   | 0.54     | 2.90        | 14     | 14    |
| 1:A:138:ASP:C    | 1:A:139:LEU:HG   | 0.54     | 2.26        | 4      | 2     |
| 1:A:18:LEU:O     | 1:A:107:PHE:HA   | 0.54     | 2.01        | 5      | 4     |
| 1:A:179:TYR:CE1  | 1:A:201:THR:CG2  | 0.54     | 2.88        | 21     | 4     |
| 1:A:29:LEU:HG    | 1:A:93:PHE:CE2   | 0.54     | 2.38        | 20     | 4     |
| 1:A:180:CYS:C    | 1:A:198:LEU:HG   | 0.54     | 2.27        | 20     | 5     |
| 1:A:121:ILE:HD12 | 1:A:179:TYR:CZ   | 0.54     | 2.37        | 18     | 1     |
| 1:A:107:PHE:CD2  | 1:A:185:LEU:HD21 | 0.54     | 2.37        | 22     | 1     |
| 1:A:45:ILE:O     | 1:A:48:LYS:N     | 0.54     | 2.41        | 22     | 22    |
| 1:A:168:TYR:CD1  | 1:A:169:ILE:N    | 0.54     | 2.76        | 13     | 14    |
| 1:A:131:VAL:HG22 | 1:A:133:GLU:HB2  | 0.54     | 1.79        | 2      | 2     |
| 1:A:182:SER:OG   | 1:A:198:LEU:CD2  | 0.54     | 2.55        | 6      | 3     |
| 1:A:85:GLY:O     | 1:A:93:PHE:CE1   | 0.54     | 2.61        | 9      | 2     |
| 1:A:135:LEU:HD11 | 1:A:137:PHE:O    | 0.54     | 2.02        | 17     | 1     |
| 1:A:125:VAL:O    | 1:A:166:PHE:N    | 0.54     | 2.40        | 16     | 21    |
| 1:A:27:TRP:CD2   | 1:A:83:LEU:HD22  | 0.54     | 2.37        | 9      | 2     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:101:LEU:HB3  | 1:A:105:MET:HE3  | 0.54     | 1.78        | 12     | 1     |
| 1:A:72:TRP:CE3   | 1:A:101:LEU:HD21 | 0.54     | 2.38        | 4      | 12    |
| 1:A:120:HIS:HA   | 1:A:173:LEU:HD23 | 0.54     | 1.80        | 17     | 1     |
| 1:A:135:LEU:HD11 | 1:A:138:ASP:HA   | 0.54     | 1.78        | 17     | 1     |
| 1:A:158:ILE:HG23 | 1:A:162:MET:HG3  | 0.54     | 1.77        | 20     | 1     |
| 1:A:27:TRP:CE3   | 1:A:83:LEU:CD1   | 0.54     | 2.89        | 4      | 15    |
| 1:A:108:GLU:C    | 1:A:110:PRO:HD2  | 0.54     | 2.28        | 21     | 6     |
| 1:A:35:VAL:HG23  | 1:A:35:VAL:O     | 0.54     | 2.02        | 12     | 1     |
| 1:A:196:SER:CB   | 1:A:197:PRO:CD   | 0.54     | 2.86        | 18     | 1     |
| 1:A:184:TYR:CD1  | 1:A:193:VAL:HG12 | 0.54     | 2.37        | 21     | 1     |
| 1:A:14:PHE:CE1   | 1:A:83:LEU:HB3   | 0.54     | 2.38        | 11     | 20    |
| 1:A:16:ILE:HD12  | 1:A:99:PHE:CD2   | 0.54     | 2.38        | 14     | 16    |
| 1:A:43:TYR:HE2   | 1:A:55:VAL:HG22  | 0.54     | 1.62        | 10     | 17    |
| 1:A:135:LEU:HD12 | 1:A:137:PHE:O    | 0.54     | 2.03        | 1      | 1     |
| 1:A:121:ILE:HG12 | 1:A:179:TYR:CE2  | 0.54     | 2.37        | 20     | 12    |
| 1:A:43:TYR:O     | 1:A:52:LEU:HA    | 0.53     | 2.03        | 10     | 13    |
| 1:A:85:GLY:HA3   | 1:A:93:PHE:CE1   | 0.53     | 2.39        | 1      | 14    |
| 1:A:72:TRP:CE2   | 1:A:79:TYR:CD2   | 0.53     | 2.96        | 5      | 10    |
| 1:A:185:LEU:N    | 1:A:185:LEU:CD1  | 0.53     | 2.69        | 1      | 3     |
| 1:A:21:PHE:CE2   | 1:A:128:PRO:HG2  | 0.53     | 2.38        | 4      | 8     |
| 1:A:121:ILE:CD1  | 1:A:173:LEU:HD22 | 0.53     | 2.30        | 13     | 1     |
| 1:A:146:GLN:CD   | 1:A:151:VAL:HG22 | 0.53     | 2.28        | 13     | 1     |
| 1:A:184:TYR:CE2  | 1:A:193:VAL:HG23 | 0.53     | 2.39        | 13     | 1     |
| 1:A:132:GLU:CA   | 1:A:135:LEU:HD22 | 0.53     | 2.34        | 16     | 1     |
| 1:A:132:GLU:CB   | 1:A:135:LEU:CD2  | 0.53     | 2.85        | 21     | 1     |
| 1:A:121:ILE:CD1  | 1:A:179:TYR:CD2  | 0.53     | 2.91        | 20     | 12    |
| 1:A:17:SER:OG    | 1:A:24:ILE:HB    | 0.53     | 2.04        | 6      | 2     |
| 1:A:139:LEU:HD12 | 1:A:162:MET:CE   | 0.53     | 2.33        | 16     | 4     |
| 1:A:145:GLU:HA   | 1:A:181:VAL:HG22 | 0.53     | 1.79        | 13     | 1     |
| 1:A:132:GLU:CG   | 1:A:135:LEU:HD22 | 0.53     | 2.34        | 20     | 1     |
| 1:A:116:GLY:CA   | 1:A:179:TYR:OH   | 0.53     | 2.57        | 12     | 20    |
| 1:A:180:CYS:O    | 1:A:198:LEU:CD2  | 0.53     | 2.56        | 13     | 10    |
| 1:A:193:VAL:HG13 | 1:A:193:VAL:O    | 0.53     | 2.04        | 13     | 2     |
| 1:A:158:ILE:HG22 | 1:A:158:ILE:O    | 0.53     | 2.02        | 16     | 3     |
| 1:A:143:ILE:N    | 1:A:154:HIS:O    | 0.53     | 2.41        | 15     | 15    |
| 1:A:43:TYR:CD1   | 1:A:79:TYR:CE1   | 0.53     | 2.96        | 14     | 7     |
| 1:A:180:CYS:CB   | 1:A:198:LEU:CG   | 0.53     | 2.87        | 17     | 4     |
| 1:A:27:TRP:CH2   | 1:A:64:SER:O     | 0.53     | 2.62        | 4      | 22    |
| 1:A:87:SER:N     | 1:A:90:THR:O     | 0.53     | 2.42        | 9      | 22    |
| 1:A:137:PHE:CG   | 1:A:139:LEU:HD22 | 0.53     | 2.39        | 12     | 2     |
| 1:A:127:PHE:CD1  | 1:A:162:MET:HG2  | 0.53     | 2.39        | 10     | 2     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:135:LEU:HD13 | 1:A:137:PHE:O    | 0.53     | 2.04        | 21     | 1     |
| 1:A:27:TRP:CG    | 1:A:83:LEU:CD2   | 0.53     | 2.91        | 9      | 2     |
| 1:A:25:LEU:HD21  | 1:A:41:LEU:CD2   | 0.53     | 2.32        | 17     | 1     |
| 1:A:140:SER:HA   | 1:A:158:ILE:HG13 | 0.53     | 1.79        | 1      | 9     |
| 1:A:104:ASP:O    | 1:A:105:MET:O    | 0.53     | 2.25        | 18     | 3     |
| 1:A:114:ILE:CD1  | 1:A:201:THR:HG22 | 0.53     | 2.22        | 22     | 1     |
| 1:A:72:TRP:CA    | 1:A:79:TYR:CE2   | 0.53     | 2.92        | 8      | 8     |
| 1:A:142:VAL:HG21 | 1:A:186:GLU:CG   | 0.53     | 2.33        | 14     | 3     |
| 1:A:106:SER:HA   | 1:A:194:ILE:HG21 | 0.53     | 1.80        | 11     | 1     |
| 1:A:130:ILE:HD13 | 1:A:130:ILE:C    | 0.52     | 2.29        | 16     | 14    |
| 1:A:72:TRP:CG    | 1:A:79:TYR:CE2   | 0.52     | 2.97        | 19     | 8     |
| 1:A:106:SER:CB   | 1:A:194:ILE:HD13 | 0.52     | 2.34        | 13     | 1     |
| 1:A:131:VAL:HG23 | 1:A:131:VAL:O    | 0.52     | 2.04        | 16     | 1     |
| 1:A:43:TYR:CE1   | 1:A:79:TYR:HE2   | 0.52     | 2.23        | 2      | 5     |
| 1:A:139:LEU:CD1  | 1:A:162:MET:CE   | 0.52     | 2.86        | 11     | 3     |
| 1:A:180:CYS:HB2  | 1:A:198:LEU:CD2  | 0.52     | 2.34        | 18     | 4     |
| 1:A:50:GLU:O     | 1:A:51:ASP:C     | 0.52     | 2.51        | 13     | 1     |
| 1:A:72:TRP:CZ2   | 1:A:81:THR:CG2   | 0.52     | 2.92        | 19     | 3     |
| 1:A:127:PHE:O    | 1:A:164:GLY:CA   | 0.52     | 2.58        | 16     | 16    |
| 1:A:107:PHE:CB   | 1:A:185:LEU:HD22 | 0.52     | 2.33        | 9      | 1     |
| 1:A:139:LEU:HD12 | 1:A:139:LEU:O    | 0.52     | 2.04        | 18     | 2     |
| 1:A:78:ALA:HA    | 1:A:99:PHE:O     | 0.52     | 2.04        | 7      | 17    |
| 1:A:118:THR:OG1  | 1:A:204:PRO:HG2  | 0.52     | 2.04        | 18     | 9     |
| 1:A:121:ILE:CG2  | 1:A:179:TYR:CE2  | 0.52     | 2.93        | 9      | 7     |
| 1:A:121:ILE:CD1  | 1:A:179:TYR:CD1  | 0.52     | 2.92        | 9      | 7     |
| 1:A:143:ILE:CD1  | 1:A:156:PRO:CD   | 0.52     | 2.87        | 12     | 17    |
| 1:A:21:PHE:CE1   | 1:A:130:ILE:CG2  | 0.52     | 2.93        | 10     | 2     |
| 1:A:105:MET:HG2  | 1:A:139:LEU:HD13 | 0.52     | 1.81        | 1      | 1     |
| 1:A:121:ILE:HG12 | 1:A:179:TYR:CE1  | 0.52     | 2.39        | 9      | 7     |
| 1:A:44:THR:HB    | 1:A:52:LEU:HA    | 0.52     | 1.81        | 11     | 11    |
| 1:A:21:PHE:CD2   | 1:A:21:PHE:O     | 0.52     | 2.62        | 8      | 5     |
| 1:A:25:LEU:HD12  | 1:A:41:LEU:HD11  | 0.52     | 1.78        | 17     | 2     |
| 1:A:180:CYS:HB2  | 1:A:198:LEU:HD23 | 0.52     | 1.82        | 12     | 4     |
| 1:A:121:ILE:CG2  | 1:A:170:ILE:O    | 0.52     | 2.51        | 18     | 1     |
| 1:A:132:GLU:HA   | 1:A:135:LEU:HD13 | 0.52     | 1.81        | 11     | 2     |
| 1:A:107:PHE:N    | 1:A:194:ILE:HG21 | 0.52     | 2.20        | 16     | 2     |
| 1:A:139:LEU:O    | 1:A:162:MET:HE1  | 0.52     | 2.05        | 16     | 2     |
| 1:A:111:GLU:HB3  | 1:A:126:LYS:HB2  | 0.52     | 1.81        | 21     | 10    |
| 1:A:145:GLU:HG3  | 1:A:170:ILE:CD1  | 0.52     | 2.34        | 10     | 7     |
| 1:A:179:TYR:HE1  | 1:A:203:LEU:HD11 | 0.52     | 1.65        | 3      | 1     |
| 1:A:27:TRP:HE3   | 1:A:41:LEU:HD12  | 0.52     | 1.64        | 17     | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:170:ILE:HG22 | 1:A:173:LEU:CD1  | 0.52     | 2.30        | 18     | 1     |
| 1:A:132:GLU:C    | 1:A:134:GLU:N    | 0.52     | 2.67        | 15     | 13    |
| 1:A:18:LEU:HD21  | 1:A:105:MET:SD   | 0.52     | 2.45        | 5      | 2     |
| 1:A:114:ILE:CG2  | 1:A:123:VAL:HG22 | 0.52     | 2.35        | 17     | 6     |
| 1:A:146:GLN:CG   | 1:A:151:VAL:HG13 | 0.52     | 2.35        | 13     | 1     |
| 1:A:142:VAL:CG1  | 1:A:184:TYR:CZ   | 0.51     | 2.90        | 4      | 6     |
| 1:A:141:LEU:HD11 | 1:A:183:VAL:HG12 | 0.51     | 1.82        | 7      | 1     |
| 1:A:107:PHE:CB   | 1:A:194:ILE:HD13 | 0.51     | 2.35        | 11     | 1     |
| 1:A:113:GLU:HA   | 1:A:199:LYS:CD   | 0.51     | 2.35        | 15     | 9     |
| 1:A:19:ARG:HG3   | 1:A:24:ILE:HD12  | 0.51     | 1.80        | 4      | 1     |
| 1:A:138:ASP:O    | 1:A:139:LEU:O    | 0.51     | 2.28        | 4      | 2     |
| 1:A:156:PRO:HG3  | 1:A:168:TYR:CD1  | 0.51     | 2.40        | 5      | 1     |
| 1:A:75:THR:HG21  | 1:A:137:PHE:HB3  | 0.51     | 1.83        | 6      | 2     |
| 1:A:179:TYR:HD1  | 1:A:181:VAL:HG23 | 0.51     | 1.65        | 21     | 7     |
| 1:A:201:THR:HG23 | 1:A:201:THR:O    | 0.51     | 2.05        | 13     | 1     |
| 1:A:39:TYR:O     | 1:A:60:ASN:N     | 0.51     | 2.44        | 1      | 18    |
| 1:A:137:PHE:O    | 1:A:137:PHE:CD1  | 0.51     | 2.63        | 1      | 6     |
| 1:A:137:PHE:CE2  | 1:A:139:LEU:CD1  | 0.51     | 2.92        | 6      | 1     |
| 1:A:112:PHE:CE1  | 1:A:199:LYS:HG3  | 0.51     | 2.40        | 8      | 1     |
| 1:A:13:THR:O     | 1:A:28:GLU:N     | 0.51     | 2.44        | 10     | 20    |
| 1:A:72:TRP:CE2   | 1:A:79:TYR:CD1   | 0.51     | 2.98        | 7      | 3     |
| 1:A:180:CYS:CB   | 1:A:198:LEU:HB3  | 0.51     | 2.36        | 19     | 4     |
| 1:A:34:ILE:HD13  | 1:A:34:ILE:N     | 0.51     | 2.20        | 17     | 1     |
| 1:A:107:PHE:CB   | 1:A:185:LEU:HD11 | 0.51     | 2.35        | 1      | 1     |
| 1:A:141:LEU:HB3  | 1:A:158:ILE:CD1  | 0.51     | 2.36        | 20     | 9     |
| 1:A:116:GLY:HA3  | 1:A:203:LEU:HD12 | 0.51     | 1.82        | 3      | 1     |
| 1:A:142:VAL:N    | 1:A:184:TYR:O    | 0.51     | 2.43        | 19     | 3     |
| 1:A:147:SER:OG   | 1:A:177:THR:HG22 | 0.51     | 2.06        | 16     | 5     |
| 1:A:27:TRP:CD1   | 1:A:29:LEU:CD2   | 0.51     | 2.91        | 8      | 1     |
| 1:A:111:GLU:O    | 1:A:126:LYS:CB   | 0.51     | 2.59        | 8      | 1     |
| 1:A:106:SER:HB3  | 1:A:194:ILE:HD13 | 0.51     | 1.82        | 13     | 1     |
| 1:A:137:PHE:CE2  | 1:A:139:LEU:CD2  | 0.51     | 2.94        | 16     | 1     |
| 1:A:57:ASN:O     | 1:A:58:CYS:SG    | 0.51     | 2.68        | 19     | 1     |
| 1:A:114:ILE:HG23 | 1:A:123:VAL:HG13 | 0.51     | 1.81        | 22     | 1     |
| 1:A:42:LEU:HD23  | 1:A:54:VAL:CG1   | 0.51     | 2.34        | 13     | 18    |
| 1:A:132:GLU:O    | 1:A:135:LEU:HD22 | 0.51     | 2.05        | 17     | 6     |
| 1:A:121:ILE:CG2  | 1:A:179:TYR:CE1  | 0.51     | 2.94        | 12     | 11    |
| 1:A:182:SER:OG   | 1:A:198:LEU:HD23 | 0.51     | 2.05        | 6      | 2     |
| 1:A:114:ILE:CG1  | 1:A:199:LYS:HG2  | 0.51     | 2.36        | 14     | 13    |
| 1:A:154:HIS:CD2  | 1:A:170:ILE:HG23 | 0.51     | 2.40        | 16     | 1     |
| 1:A:20:ASN:O     | 1:A:21:PHE:CG    | 0.51     | 2.64        | 4      | 13    |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:12:CYS:CB    | 1:A:14:PHE:CZ    | 0.51     | 2.94        | 9      | 2     |
| 1:A:135:LEU:HG   | 1:A:137:PHE:H    | 0.51     | 1.66        | 18     | 2     |
| 1:A:57:ASN:O     | 1:A:58:CYS:CB    | 0.51     | 2.59        | 19     | 1     |
| 1:A:93:PHE:N     | 1:A:93:PHE:CD1   | 0.51     | 2.78        | 21     | 1     |
| 1:A:100:TRP:O    | 1:A:104:ASP:N    | 0.50     | 2.44        | 22     | 22    |
| 1:A:141:LEU:HD23 | 1:A:143:ILE:HD12 | 0.50     | 1.82        | 14     | 1     |
| 1:A:81:THR:OG1   | 1:A:99:PHE:CE2   | 0.50     | 2.64        | 18     | 2     |
| 1:A:184:TYR:CD2  | 1:A:193:VAL:HG23 | 0.50     | 2.40        | 13     | 1     |
| 1:A:14:PHE:CA    | 1:A:26:SER:O     | 0.50     | 2.60        | 22     | 4     |
| 1:A:107:PHE:H    | 1:A:194:ILE:HG21 | 0.50     | 1.66        | 20     | 2     |
| 1:A:16:ILE:CG1   | 1:A:99:PHE:CE1   | 0.50     | 2.94        | 18     | 1     |
| 1:A:180:CYS:HB3  | 1:A:198:LEU:CB   | 0.50     | 2.37        | 14     | 11    |
| 1:A:154:HIS:NE2  | 1:A:170:ILE:HG23 | 0.50     | 2.21        | 5      | 1     |
| 1:A:132:GLU:O    | 1:A:134:GLU:N    | 0.50     | 2.44        | 15     | 4     |
| 1:A:147:SER:CB   | 1:A:179:TYR:CE1  | 0.50     | 2.93        | 13     | 2     |
| 1:A:201:THR:CG2  | 1:A:201:THR:O    | 0.50     | 2.59        | 13     | 2     |
| 1:A:62:THR:O     | 1:A:62:THR:OG1   | 0.50     | 2.29        | 1      | 14    |
| 1:A:72:TRP:CD1   | 1:A:79:TYR:CD2   | 0.50     | 3.00        | 5      | 6     |
| 1:A:161:ASN:CB   | 1:A:166:PHE:CZ   | 0.50     | 2.95        | 21     | 7     |
| 1:A:12:CYS:HA    | 1:A:29:LEU:HD23  | 0.50     | 1.83        | 22     | 1     |
| 1:A:127:PHE:CD2  | 1:A:162:MET:HG2  | 0.50     | 2.42        | 11     | 6     |
| 1:A:161:ASN:HB3  | 1:A:166:PHE:CZ   | 0.50     | 2.41        | 21     | 14    |
| 1:A:27:TRP:HE3   | 1:A:41:LEU:HD23  | 0.50     | 1.63        | 7      | 7     |
| 1:A:130:ILE:HD11 | 1:A:135:LEU:HB3  | 0.50     | 1.82        | 16     | 1     |
| 1:A:107:PHE:CD2  | 1:A:185:LEU:CD2  | 0.50     | 2.94        | 21     | 1     |
| 1:A:72:TRP:CH2   | 1:A:99:PHE:CD2   | 0.50     | 3.00        | 12     | 17    |
| 1:A:174:ILE:O    | 1:A:177:THR:OG1  | 0.50     | 2.30        | 7      | 11    |
| 1:A:139:LEU:CD1  | 1:A:185:LEU:HD22 | 0.50     | 2.37        | 2      | 2     |
| 1:A:141:LEU:HD23 | 1:A:142:VAL:N    | 0.50     | 2.22        | 11     | 1     |
| 1:A:139:LEU:HD13 | 1:A:185:LEU:HD13 | 0.50     | 1.82        | 14     | 1     |
| 1:A:123:VAL:CG2  | 1:A:170:ILE:HD12 | 0.50     | 2.37        | 18     | 2     |
| 1:A:27:TRP:HB2   | 1:A:29:LEU:CD1   | 0.50     | 2.37        | 6      | 10    |
| 1:A:27:TRP:NE1   | 1:A:29:LEU:HD11  | 0.50     | 2.21        | 12     | 10    |
| 1:A:29:LEU:CD1   | 1:A:39:TYR:CZ    | 0.50     | 2.94        | 12     | 8     |
| 1:A:125:VAL:HG21 | 1:A:141:LEU:HD11 | 0.50     | 1.84        | 15     | 1     |
| 1:A:115:VAL:O    | 1:A:122:ASN:HB2  | 0.50     | 2.06        | 5      | 8     |
| 1:A:72:TRP:CB    | 1:A:79:TYR:CE2   | 0.50     | 2.95        | 19     | 4     |
| 1:A:107:PHE:CD1  | 1:A:185:LEU:HD11 | 0.50     | 2.42        | 14     | 2     |
| 1:A:114:ILE:HD11 | 1:A:179:TYR:O    | 0.50     | 2.07        | 22     | 1     |
| 1:A:22:ARG:HG2   | 1:A:69:THR:HG23  | 0.50     | 1.83        | 19     | 3     |
| 1:A:158:ILE:O    | 1:A:160:GLY:N    | 0.50     | 2.45        | 16     | 12    |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:44:THR:HB    | 1:A:52:LEU:HG    | 0.50     | 1.84        | 8      | 17    |
| 1:A:144:GLU:CD   | 1:A:153:LYS:HA   | 0.50     | 2.31        | 3      | 4     |
| 1:A:81:THR:OG1   | 1:A:99:PHE:CD1   | 0.49     | 2.65        | 12     | 10    |
| 1:A:39:TYR:CD1   | 1:A:39:TYR:N     | 0.49     | 2.80        | 9      | 2     |
| 1:A:125:VAL:H    | 1:A:166:PHE:HB3  | 0.49     | 1.67        | 11     | 2     |
| 1:A:137:PHE:CD2  | 1:A:139:LEU:HD22 | 0.49     | 2.41        | 12     | 1     |
| 1:A:107:PHE:CB   | 1:A:185:LEU:HD23 | 0.49     | 2.36        | 17     | 1     |
| 1:A:123:VAL:HG11 | 1:A:181:VAL:HG11 | 0.49     | 1.83        | 19     | 1     |
| 1:A:29:LEU:HD22  | 1:A:93:PHE:CZ    | 0.49     | 2.42        | 12     | 8     |
| 1:A:182:SER:HB3  | 1:A:195:LYS:HG3  | 0.49     | 1.83        | 22     | 1     |
| 1:A:121:ILE:HB   | 1:A:170:ILE:HB   | 0.49     | 1.84        | 15     | 7     |
| 1:A:46:MET:CG    | 1:A:78:ALA:HB3   | 0.49     | 2.37        | 8      | 10    |
| 1:A:42:LEU:CD1   | 1:A:84:GLU:HG3   | 0.49     | 2.36        | 20     | 4     |
| 1:A:203:LEU:HD12 | 1:A:203:LEU:N    | 0.49     | 2.22        | 13     | 1     |
| 1:A:147:SER:CA   | 1:A:179:TYR:HB3  | 0.49     | 2.37        | 21     | 18    |
| 1:A:78:ALA:CB    | 1:A:100:TRP:CZ3  | 0.49     | 2.96        | 20     | 3     |
| 1:A:42:LEU:HD13  | 1:A:84:GLU:OE2   | 0.49     | 2.08        | 7      | 1     |
| 1:A:178:ASN:HB3  | 1:A:202:LEU:HD12 | 0.49     | 1.85        | 17     | 3     |
| 1:A:72:TRP:CD1   | 1:A:79:TYR:CZ    | 0.49     | 3.00        | 18     | 1     |
| 1:A:55:VAL:O     | 1:A:56:LYS:C     | 0.49     | 2.56        | 19     | 1     |
| 1:A:26:SER:HB2   | 1:A:65:PHE:HB3   | 0.49     | 1.85        | 17     | 12    |
| 1:A:143:ILE:HG12 | 1:A:156:PRO:HD3  | 0.49     | 1.84        | 14     | 11    |
| 1:A:38:HIS:C     | 1:A:39:TYR:HD1   | 0.49     | 2.15        | 20     | 2     |
| 1:A:179:TYR:HE2  | 1:A:203:LEU:HD21 | 0.49     | 1.67        | 10     | 3     |
| 1:A:42:LEU:HD21  | 1:A:54:VAL:HB    | 0.49     | 1.83        | 11     | 1     |
| 1:A:107:PHE:CD2  | 1:A:110:PRO:HG2  | 0.49     | 2.43        | 11     | 3     |
| 1:A:112:PHE:CD2  | 1:A:183:VAL:CG2  | 0.49     | 2.96        | 21     | 1     |
| 1:A:20:ASN:O     | 1:A:21:PHE:CD2   | 0.49     | 2.65        | 13     | 13    |
| 1:A:130:ILE:HD11 | 1:A:135:LEU:HD21 | 0.49     | 1.84        | 14     | 1     |
| 1:A:72:TRP:HH2   | 1:A:99:PHE:CD2   | 0.49     | 2.26        | 19     | 2     |
| 1:A:25:LEU:HD22  | 1:A:68:LEU:HD22  | 0.49     | 1.85        | 16     | 2     |
| 1:A:141:LEU:CB   | 1:A:158:ILE:CD1  | 0.49     | 2.90        | 15     | 5     |
| 1:A:137:PHE:CD1  | 1:A:139:LEU:HG   | 0.49     | 2.42        | 6      | 1     |
| 1:A:114:ILE:HG21 | 1:A:181:VAL:CB   | 0.49     | 2.38        | 7      | 3     |
| 1:A:123:VAL:HG21 | 1:A:170:ILE:CD1  | 0.49     | 2.37        | 17     | 2     |
| 1:A:21:PHE:O     | 1:A:21:PHE:CD1   | 0.49     | 2.65        | 13     | 12    |
| 1:A:76:HIS:HA    | 1:A:102:ALA:HB2  | 0.49     | 1.85        | 12     | 5     |
| 1:A:165:ASN:O    | 1:A:166:PHE:C    | 0.49     | 2.55        | 10     | 16    |
| 1:A:27:TRP:CE2   | 1:A:64:SER:O     | 0.49     | 2.65        | 4      | 5     |
| 1:A:18:LEU:CD2   | 1:A:105:MET:HE2  | 0.49     | 2.35        | 16     | 4     |
| 1:A:185:LEU:HG   | 1:A:194:ILE:HD13 | 0.49     | 1.85        | 17     | 2     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:42:LEU:CD1   | 1:A:54:VAL:CA    | 0.49     | 2.91        | 11     | 1     |
| 1:A:18:LEU:CD2   | 1:A:107:PHE:CE1  | 0.48     | 2.95        | 3      | 2     |
| 1:A:72:TRP:HA    | 1:A:79:TYR:CE1   | 0.48     | 2.42        | 21     | 5     |
| 1:A:25:LEU:HD23  | 1:A:68:LEU:CD2   | 0.48     | 2.38        | 17     | 5     |
| 1:A:142:VAL:HG21 | 1:A:186:GLU:HG2  | 0.48     | 1.84        | 15     | 1     |
| 1:A:126:LYS:HA   | 1:A:164:GLY:O    | 0.48     | 2.08        | 8      | 4     |
| 1:A:135:LEU:HD23 | 1:A:135:LEU:C    | 0.48     | 2.32        | 18     | 1     |
| 1:A:179:TYR:CZ   | 1:A:201:THR:CG2  | 0.48     | 2.96        | 21     | 1     |
| 1:A:132:GLU:CB   | 1:A:135:LEU:HG   | 0.48     | 2.38        | 15     | 1     |
| 1:A:135:LEU:HD13 | 1:A:137:PHE:HB2  | 0.48     | 1.85        | 15     | 1     |
| 1:A:146:GLN:HG3  | 1:A:151:VAL:HG12 | 0.48     | 1.83        | 5      | 1     |
| 1:A:11:SER:O     | 1:A:12:CYS:CB    | 0.48     | 2.60        | 8      | 1     |
| 1:A:27:TRP:CZ3   | 1:A:83:LEU:CD1   | 0.48     | 2.95        | 20     | 1     |
| 1:A:179:TYR:HE1  | 1:A:203:LEU:HD23 | 0.48     | 1.68        | 2      | 2     |
| 1:A:72:TRP:CZ3   | 1:A:79:TYR:CB    | 0.48     | 2.96        | 9      | 13    |
| 1:A:132:GLU:C    | 1:A:134:GLU:H    | 0.48     | 2.16        | 15     | 5     |
| 1:A:145:GLU:CG   | 1:A:170:ILE:HG21 | 0.48     | 2.37        | 4      | 3     |
| 1:A:16:ILE:HD12  | 1:A:72:TRP:CZ3   | 0.48     | 2.44        | 20     | 18    |
| 1:A:114:ILE:HG12 | 1:A:199:LYS:CB   | 0.48     | 2.39        | 1      | 4     |
| 1:A:142:VAL:CG1  | 1:A:154:HIS:O    | 0.48     | 2.61        | 1      | 1     |
| 1:A:168:TYR:CD1  | 1:A:168:TYR:C    | 0.48     | 2.91        | 19     | 11    |
| 1:A:143:ILE:CD1  | 1:A:156:PRO:HD2  | 0.48     | 2.38        | 4      | 8     |
| 1:A:114:ILE:CD1  | 1:A:199:LYS:O    | 0.48     | 2.60        | 21     | 8     |
| 1:A:144:GLU:HA   | 1:A:152:LYS:O    | 0.48     | 2.08        | 22     | 3     |
| 1:A:31:ASN:ND2   | 1:A:35:VAL:HG23  | 0.48     | 2.23        | 10     | 1     |
| 1:A:145:GLU:HB2  | 1:A:179:TYR:CZ   | 0.48     | 2.43        | 13     | 1     |
| 1:A:43:TYR:CE1   | 1:A:79:TYR:CE1   | 0.48     | 3.01        | 14     | 5     |
| 1:A:131:VAL:HG12 | 1:A:133:GLU:HB2  | 0.48     | 1.85        | 15     | 4     |
| 1:A:146:GLN:HG2  | 1:A:151:VAL:HG13 | 0.48     | 1.85        | 13     | 1     |
| 1:A:68:LEU:HD13  | 1:A:72:TRP:CD2   | 0.48     | 2.43        | 2      | 4     |
| 1:A:85:GLY:O     | 1:A:93:PHE:CD1   | 0.48     | 2.67        | 8      | 14    |
| 1:A:100:TRP:CZ3  | 1:A:102:ALA:HB3  | 0.48     | 2.43        | 21     | 6     |
| 1:A:18:LEU:HD23  | 1:A:107:PHE:HD1  | 0.48     | 1.67        | 5      | 1     |
| 1:A:25:LEU:HD11  | 1:A:41:LEU:HG    | 0.48     | 1.84        | 11     | 2     |
| 1:A:107:PHE:CD1  | 1:A:185:LEU:CD2  | 0.48     | 2.97        | 6      | 3     |
| 1:A:142:VAL:HG23 | 1:A:154:HIS:O    | 0.48     | 2.09        | 22     | 2     |
| 1:A:127:PHE:CE2  | 1:A:141:LEU:HD23 | 0.48     | 2.44        | 13     | 1     |
| 1:A:29:LEU:HG    | 1:A:93:PHE:CZ    | 0.48     | 2.43        | 1      | 7     |
| 1:A:117:PHE:CD2  | 1:A:120:HIS:NE2  | 0.48     | 2.82        | 4      | 11    |
| 1:A:114:ILE:CD1  | 1:A:201:THR:HB   | 0.48     | 2.38        | 18     | 11    |
| 1:A:142:VAL:CG2  | 1:A:184:TYR:CE2  | 0.48     | 2.97        | 18     | 3     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:130:ILE:HD11 | 1:A:135:LEU:CD1  | 0.48     | 2.38        | 9      | 2     |
| 1:A:46:MET:O     | 1:A:49:PRO:HD3   | 0.48     | 2.08        | 9      | 11    |
| 1:A:127:PHE:CG   | 1:A:162:MET:HG2  | 0.48     | 2.44        | 1      | 7     |
| 1:A:179:TYR:HD2  | 1:A:181:VAL:HG23 | 0.48     | 1.69        | 2      | 3     |
| 1:A:145:GLU:HG3  | 1:A:152:LYS:CB   | 0.48     | 2.38        | 13     | 1     |
| 1:A:178:ASN:HA   | 1:A:202:LEU:HA   | 0.48     | 1.86        | 22     | 2     |
| 1:A:161:ASN:CG   | 1:A:166:PHE:CZ   | 0.47     | 2.91        | 10     | 14    |
| 1:A:112:PHE:CG   | 1:A:183:VAL:CG2  | 0.47     | 2.95        | 22     | 7     |
| 1:A:18:LEU:N     | 1:A:106:SER:O    | 0.47     | 2.44        | 17     | 4     |
| 1:A:139:LEU:HD21 | 1:A:185:LEU:HD13 | 0.47     | 1.84        | 22     | 1     |
| 1:A:18:LEU:CD2   | 1:A:105:MET:HG3  | 0.47     | 2.38        | 6      | 3     |
| 1:A:23:SER:O     | 1:A:68:LEU:N     | 0.47     | 2.46        | 21     | 22    |
| 1:A:114:ILE:HG21 | 1:A:181:VAL:HG11 | 0.47     | 1.85        | 12     | 2     |
| 1:A:27:TRP:CE2   | 1:A:39:TYR:CD2   | 0.47     | 3.01        | 20     | 2     |
| 1:A:121:ILE:CD1  | 1:A:179:TYR:CZ   | 0.47     | 2.97        | 13     | 1     |
| 1:A:41:LEU:HD12  | 1:A:83:LEU:HB2   | 0.47     | 1.85        | 6      | 3     |
| 1:A:121:ILE:HD13 | 1:A:179:TYR:CD2  | 0.47     | 2.44        | 11     | 7     |
| 1:A:81:THR:O     | 1:A:96:SER:CA    | 0.47     | 2.62        | 12     | 9     |
| 1:A:137:PHE:CE1  | 1:A:139:LEU:HD23 | 0.47     | 2.45        | 11     | 2     |
| 1:A:38:HIS:CD2   | 1:A:60:ASN:ND2   | 0.47     | 2.82        | 14     | 1     |
| 1:A:18:LEU:O     | 1:A:107:PHE:CD1  | 0.47     | 2.67        | 18     | 1     |
| 1:A:23:SER:CB    | 1:A:68:LEU:O     | 0.47     | 2.62        | 15     | 20    |
| 1:A:100:TRP:O    | 1:A:104:ASP:CB   | 0.47     | 2.62        | 12     | 19    |
| 1:A:112:PHE:CD2  | 1:A:183:VAL:HG21 | 0.47     | 2.43        | 19     | 6     |
| 1:A:171:ASP:O    | 1:A:172:LYS:CB   | 0.47     | 2.62        | 6      | 1     |
| 1:A:12:CYS:HB3   | 1:A:14:PHE:CZ    | 0.47     | 2.44        | 20     | 2     |
| 1:A:112:PHE:CD2  | 1:A:183:VAL:HG22 | 0.47     | 2.44        | 21     | 1     |
| 1:A:44:THR:OG1   | 1:A:48:LYS:O     | 0.47     | 2.32        | 7      | 10    |
| 1:A:117:PHE:CB   | 1:A:120:HIS:CE1  | 0.47     | 2.97        | 10     | 8     |
| 1:A:34:ILE:HD11  | 1:A:87:SER:HB3   | 0.47     | 1.87        | 4      | 1     |
| 1:A:107:PHE:C    | 1:A:108:GLU:CG   | 0.47     | 2.87        | 11     | 1     |
| 1:A:145:GLU:CG   | 1:A:152:LYS:HB3  | 0.47     | 2.39        | 13     | 1     |
| 1:A:141:LEU:HB3  | 1:A:158:ILE:HD12 | 0.47     | 1.86        | 18     | 1     |
| 1:A:34:ILE:HD12  | 1:A:36:PRO:HD3   | 0.47     | 1.86        | 22     | 1     |
| 1:A:201:THR:O    | 1:A:201:THR:HG23 | 0.47     | 2.09        | 22     | 1     |
| 1:A:45:ILE:HG22  | 1:A:77:GLU:HB3   | 0.47     | 1.86        | 13     | 5     |
| 1:A:113:GLU:HA   | 1:A:199:LYS:HD3  | 0.47     | 1.86        | 2      | 7     |
| 1:A:135:LEU:CD1  | 1:A:138:ASP:N    | 0.47     | 2.77        | 19     | 3     |
| 1:A:125:VAL:O    | 1:A:166:PHE:CB   | 0.47     | 2.62        | 5      | 9     |
| 1:A:135:LEU:HD21 | 1:A:137:PHE:HB3  | 0.47     | 1.85        | 8      | 1     |
| 1:A:114:ILE:HA   | 1:A:122:ASN:O    | 0.47     | 2.09        | 10     | 2     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:141:LEU:HB3  | 1:A:158:ILE:HD11 | 0.47     | 1.87        | 1      | 2     |
| 1:A:68:LEU:HD13  | 1:A:72:TRP:CE2   | 0.47     | 2.45        | 12     | 6     |
| 1:A:40:THR:O     | 1:A:40:THR:CG2   | 0.47     | 2.62        | 6      | 2     |
| 1:A:108:GLU:H    | 1:A:109:PRO:HD2  | 0.47     | 1.69        | 21     | 4     |
| 1:A:42:LEU:C     | 1:A:52:LEU:HD23  | 0.47     | 2.35        | 13     | 1     |
| 1:A:179:TYR:CD1  | 1:A:181:VAL:HG23 | 0.47     | 2.44        | 18     | 2     |
| 1:A:145:GLU:HG2  | 1:A:154:HIS:CD2  | 0.47     | 2.44        | 22     | 1     |
| 1:A:161:ASN:HB2  | 1:A:166:PHE:CE2  | 0.47     | 2.45        | 12     | 3     |
| 1:A:107:PHE:CZ   | 1:A:185:LEU:HB3  | 0.47     | 2.44        | 13     | 2     |
| 1:A:142:VAL:CG2  | 1:A:184:TYR:CD2  | 0.47     | 2.98        | 21     | 3     |
| 1:A:34:ILE:HG23  | 1:A:87:SER:OG    | 0.47     | 2.09        | 8      | 1     |
| 1:A:160:GLY:O    | 1:A:162:MET:N    | 0.47     | 2.48        | 13     | 1     |
| 1:A:142:VAL:CG1  | 1:A:184:TYR:CE1  | 0.47     | 2.98        | 14     | 3     |
| 1:A:112:PHE:HD2  | 1:A:125:VAL:HG22 | 0.47     | 1.70        | 21     | 1     |
| 1:A:72:TRP:CE3   | 1:A:79:TYR:CB    | 0.47     | 2.98        | 10     | 12    |
| 1:A:115:VAL:O    | 1:A:122:ASN:N    | 0.47     | 2.48        | 1      | 10    |
| 1:A:84:GLU:HG2   | 1:A:94:SER:HB3   | 0.47     | 1.86        | 20     | 8     |
| 1:A:13:THR:O     | 1:A:27:TRP:HA    | 0.47     | 2.10        | 20     | 5     |
| 1:A:18:LEU:CB    | 1:A:106:SER:O    | 0.47     | 2.63        | 12     | 6     |
| 1:A:177:THR:C    | 1:A:202:LEU:HD12 | 0.47     | 2.35        | 13     | 2     |
| 1:A:117:PHE:HB2  | 1:A:120:HIS:CD2  | 0.47     | 2.45        | 18     | 6     |
| 1:A:158:ILE:HG22 | 1:A:162:MET:HB2  | 0.47     | 1.86        | 15     | 3     |
| 1:A:118:THR:HA   | 1:A:204:PRO:HG2  | 0.47     | 1.87        | 17     | 5     |
| 1:A:107:PHE:CE2  | 1:A:185:LEU:CD1  | 0.47     | 2.98        | 13     | 1     |
| 1:A:143:ILE:HD11 | 1:A:156:PRO:HG3  | 0.47     | 1.87        | 14     | 1     |
| 1:A:150:ILE:HG12 | 1:A:150:ILE:O    | 0.47     | 2.10        | 19     | 1     |
| 1:A:121:ILE:HD13 | 1:A:179:TYR:CE1  | 0.46     | 2.45        | 7      | 2     |
| 1:A:182:SER:OG   | 1:A:198:LEU:CD1  | 0.46     | 2.62        | 12     | 1     |
| 1:A:72:TRP:CZ3   | 1:A:99:PHE:CD2   | 0.46     | 3.03        | 12     | 14    |
| 1:A:18:LEU:HD21  | 1:A:105:MET:CE   | 0.46     | 2.39        | 3      | 1     |
| 1:A:179:TYR:CZ   | 1:A:201:THR:HG22 | 0.46     | 2.45        | 15     | 5     |
| 1:A:132:GLU:O    | 1:A:135:LEU:N    | 0.46     | 2.48        | 15     | 3     |
| 1:A:185:LEU:HD13 | 1:A:185:LEU:H    | 0.46     | 1.67        | 13     | 1     |
| 1:A:146:GLN:CD   | 1:A:151:VAL:HG13 | 0.46     | 2.34        | 18     | 1     |
| 1:A:145:GLU:CG   | 1:A:170:ILE:HD12 | 0.46     | 2.39        | 22     | 1     |
| 1:A:20:ASN:CA    | 1:A:128:PRO:HG3  | 0.46     | 2.40        | 15     | 11    |
| 1:A:46:MET:CE    | 1:A:78:ALA:HB3   | 0.46     | 2.41        | 17     | 6     |
| 1:A:109:PRO:N    | 1:A:110:PRO:HD2  | 0.46     | 2.25        | 20     | 10    |
| 1:A:147:SER:OG   | 1:A:150:ILE:CD1  | 0.46     | 2.62        | 3      | 1     |
| 1:A:189:ASP:C    | 1:A:191:GLN:H    | 0.46     | 2.17        | 13     | 1     |
| 1:A:114:ILE:HG22 | 1:A:123:VAL:CG2  | 0.46     | 2.41        | 17     | 2     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:123:VAL:HG23 | 1:A:170:ILE:HD12 | 0.46     | 1.87        | 18     | 1     |
| 1:A:54:VAL:HG23  | 1:A:59:ALA:CB    | 0.46     | 2.36        | 20     | 1     |
| 1:A:141:LEU:HD22 | 1:A:142:VAL:N    | 0.46     | 2.24        | 21     | 1     |
| 1:A:112:PHE:HE1  | 1:A:181:VAL:HG13 | 0.46     | 1.70        | 22     | 1     |
| 1:A:114:ILE:HD12 | 1:A:201:THR:CB   | 0.46     | 2.41        | 18     | 17    |
| 1:A:84:GLU:HG2   | 1:A:94:SER:HB2   | 0.46     | 1.87        | 9      | 1     |
| 1:A:137:PHE:CD1  | 1:A:139:LEU:HB3  | 0.46     | 2.46        | 17     | 1     |
| 1:A:177:THR:O    | 1:A:177:THR:HG22 | 0.46     | 2.09        | 17     | 1     |
| 1:A:100:TRP:CD1  | 1:A:103:ILE:HD12 | 0.46     | 2.46        | 21     | 1     |
| 1:A:106:SER:CB   | 1:A:194:ILE:HD12 | 0.46     | 2.40        | 21     | 1     |
| 1:A:184:TYR:CE1  | 1:A:193:VAL:CG1  | 0.46     | 2.95        | 21     | 1     |
| 1:A:21:PHE:CD2   | 1:A:128:PRO:HG2  | 0.46     | 2.46        | 5      | 12    |
| 1:A:148:GLU:HB2  | 1:A:177:THR:HG23 | 0.46     | 1.86        | 3      | 1     |
| 1:A:184:TYR:CD1  | 1:A:184:TYR:C    | 0.46     | 2.93        | 15     | 10    |
| 1:A:38:HIS:CD2   | 1:A:60:ASN:HA    | 0.46     | 2.46        | 19     | 3     |
| 1:A:142:VAL:HG11 | 1:A:186:GLU:CG   | 0.46     | 2.41        | 6      | 2     |
| 1:A:142:VAL:CG2  | 1:A:144:GLU:OE1  | 0.46     | 2.64        | 22     | 2     |
| 1:A:121:ILE:CG2  | 1:A:179:TYR:CZ   | 0.46     | 2.99        | 9      | 13    |
| 1:A:131:VAL:O    | 1:A:133:GLU:N    | 0.46     | 2.49        | 21     | 5     |
| 1:A:114:ILE:HG22 | 1:A:123:VAL:CG1  | 0.46     | 2.41        | 17     | 3     |
| 1:A:84:GLU:O     | 1:A:86:PHE:CE1   | 0.46     | 2.69        | 1      | 1     |
| 1:A:158:ILE:O    | 1:A:158:ILE:HG22 | 0.46     | 2.11        | 19     | 3     |
| 1:A:107:PHE:CZ   | 1:A:185:LEU:CB   | 0.46     | 2.99        | 5      | 1     |
| 1:A:142:VAL:CG2  | 1:A:184:TYR:CZ   | 0.46     | 2.99        | 12     | 2     |
| 1:A:72:TRP:CH2   | 1:A:81:THR:CG2   | 0.46     | 2.99        | 14     | 3     |
| 1:A:107:PHE:CG   | 1:A:185:LEU:CD1  | 0.46     | 2.98        | 14     | 1     |
| 1:A:202:LEU:CD1  | 1:A:203:LEU:H    | 0.46     | 2.23        | 15     | 2     |
| 1:A:135:LEU:HD12 | 1:A:137:PHE:C    | 0.46     | 2.36        | 19     | 1     |
| 1:A:38:HIS:NE2   | 1:A:86:PHE:HB2   | 0.46     | 2.26        | 5      | 4     |
| 1:A:43:TYR:CE1   | 1:A:79:TYR:CE2   | 0.46     | 3.04        | 13     | 2     |
| 1:A:142:VAL:CG1  | 1:A:184:TYR:O    | 0.46     | 2.64        | 12     | 1     |
| 1:A:34:ILE:HG13  | 1:A:92:LEU:HD13  | 0.46     | 1.88        | 1      | 1     |
| 1:A:161:ASN:ND2  | 1:A:166:PHE:CZ   | 0.46     | 2.84        | 19     | 2     |
| 1:A:107:PHE:CD1  | 1:A:185:LEU:HD23 | 0.46     | 2.46        | 10     | 1     |
| 1:A:137:PHE:CD1  | 1:A:139:LEU:CD2  | 0.46     | 2.94        | 20     | 2     |
| 1:A:142:VAL:CG1  | 1:A:184:TYR:CD2  | 0.46     | 2.99        | 12     | 1     |
| 1:A:34:ILE:HD13  | 1:A:87:SER:HB2   | 0.46     | 1.88        | 22     | 1     |
| 1:A:40:THR:HA    | 1:A:59:ALA:HA    | 0.45     | 1.88        | 3      | 16    |
| 1:A:127:PHE:N    | 1:A:164:GLY:O    | 0.45     | 2.49        | 7      | 12    |
| 1:A:135:LEU:HD12 | 1:A:138:ASP:CA   | 0.45     | 2.41        | 5      | 2     |
| 1:A:142:VAL:CG1  | 1:A:184:TYR:CE2  | 0.45     | 2.99        | 12     | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:180:CYS:HB3  | 1:A:198:LEU:HB3  | 0.45     | 1.88        | 18     | 4     |
| 1:A:107:PHE:O    | 1:A:107:PHE:CD1  | 0.45     | 2.69        | 13     | 1     |
| 1:A:203:LEU:N    | 1:A:203:LEU:CD1  | 0.45     | 2.78        | 13     | 1     |
| 1:A:29:LEU:CD1   | 1:A:39:TYR:CE1   | 0.45     | 2.98        | 15     | 1     |
| 1:A:148:GLU:CG   | 1:A:177:THR:HG23 | 0.45     | 2.41        | 22     | 1     |
| 1:A:180:CYS:HB3  | 1:A:198:LEU:HD23 | 0.45     | 1.86        | 22     | 1     |
| 1:A:121:ILE:O    | 1:A:169:ILE:CG2  | 0.45     | 2.62        | 11     | 13    |
| 1:A:124:MET:SD   | 1:A:167:THR:CG2  | 0.45     | 3.04        | 16     | 7     |
| 1:A:156:PRO:HG3  | 1:A:168:TYR:CE2  | 0.45     | 2.46        | 15     | 6     |
| 1:A:121:ILE:HG13 | 1:A:170:ILE:O    | 0.45     | 2.10        | 17     | 2     |
| 1:A:21:PHE:CZ    | 1:A:130:ILE:HB   | 0.45     | 2.46        | 14     | 1     |
| 1:A:175:PRO:O    | 1:A:176:ASN:HB3  | 0.45     | 2.11        | 20     | 1     |
| 1:A:194:ILE:O    | 1:A:194:ILE:HG22 | 0.45     | 2.10        | 20     | 1     |
| 1:A:135:LEU:C    | 1:A:135:LEU:CD1  | 0.45     | 2.89        | 21     | 1     |
| 1:A:100:TRP:CE3  | 1:A:100:TRP:HA   | 0.45     | 2.46        | 5      | 14    |
| 1:A:107:PHE:CE1  | 1:A:185:LEU:HD13 | 0.45     | 2.47        | 5      | 1     |
| 1:A:126:LYS:HD2  | 1:A:165:ASN:HA   | 0.45     | 1.88        | 6      | 1     |
| 1:A:55:VAL:O     | 1:A:59:ALA:N     | 0.45     | 2.49        | 8      | 1     |
| 1:A:141:LEU:HD12 | 1:A:143:ILE:HD12 | 0.45     | 1.88        | 13     | 2     |
| 1:A:145:GLU:CD   | 1:A:147:SER:HG   | 0.45     | 2.19        | 18     | 1     |
| 1:A:21:PHE:CD2   | 1:A:128:PRO:CG   | 0.45     | 2.99        | 22     | 10    |
| 1:A:19:ARG:O     | 1:A:22:ARG:CB    | 0.45     | 2.64        | 3      | 1     |
| 1:A:117:PHE:CG   | 1:A:120:HIS:NE2  | 0.45     | 2.84        | 3      | 5     |
| 1:A:18:LEU:HD23  | 1:A:107:PHE:HE1  | 0.45     | 1.71        | 22     | 3     |
| 1:A:42:LEU:CD1   | 1:A:54:VAL:HA    | 0.45     | 2.38        | 11     | 1     |
| 1:A:121:ILE:HG22 | 1:A:122:ASN:N    | 0.45     | 2.26        | 13     | 1     |
| 1:A:147:SER:HB3  | 1:A:179:TYR:CE1  | 0.45     | 2.47        | 22     | 2     |
| 1:A:21:PHE:CE2   | 1:A:128:PRO:HB2  | 0.45     | 2.45        | 21     | 2     |
| 1:A:142:VAL:CG2  | 1:A:184:TYR:CE1  | 0.45     | 2.99        | 15     | 1     |
| 1:A:142:VAL:HG23 | 1:A:186:GLU:OE1  | 0.45     | 2.10        | 20     | 1     |
| 1:A:124:MET:HE2  | 1:A:167:THR:HA   | 0.45     | 1.89        | 18     | 3     |
| 1:A:156:PRO:CG   | 1:A:168:TYR:CD2  | 0.45     | 2.99        | 21     | 5     |
| 1:A:37:THR:O     | 1:A:62:THR:HA    | 0.45     | 2.11        | 2      | 2     |
| 1:A:116:GLY:HA3  | 1:A:203:LEU:CD1  | 0.45     | 2.41        | 3      | 1     |
| 1:A:11:SER:O     | 1:A:28:GLU:O     | 0.45     | 2.35        | 7      | 2     |
| 1:A:161:ASN:ND2  | 1:A:166:PHE:CG   | 0.45     | 2.85        | 17     | 2     |
| 1:A:178:ASN:HB3  | 1:A:202:LEU:CD1  | 0.45     | 2.42        | 17     | 2     |
| 1:A:127:PHE:O    | 1:A:128:PRO:C    | 0.45     | 2.60        | 16     | 2     |
| 1:A:139:LEU:HD23 | 1:A:139:LEU:H    | 0.45     | 1.71        | 17     | 1     |
| 1:A:170:ILE:O    | 1:A:173:LEU:CD1  | 0.45     | 2.64        | 18     | 1     |
| 1:A:176:ASN:O    | 1:A:176:ASN:CG   | 0.45     | 2.58        | 2      | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:109:PRO:O    | 1:A:110:PRO:C    | 0.45     | 2.58        | 21     | 7     |
| 1:A:161:ASN:ND2  | 1:A:166:PHE:CD1  | 0.45     | 2.85        | 22     | 3     |
| 1:A:137:PHE:CD2  | 1:A:139:LEU:HD11 | 0.45     | 2.46        | 6      | 1     |
| 1:A:147:SER:CB   | 1:A:177:THR:CG2  | 0.45     | 2.95        | 19     | 2     |
| 1:A:83:LEU:N     | 1:A:95:CYS:O     | 0.45     | 2.50        | 11     | 1     |
| 1:A:117:PHE:O    | 1:A:203:LEU:HD23 | 0.45     | 2.11        | 13     | 1     |
| 1:A:131:VAL:HG13 | 1:A:134:GLU:HG2  | 0.45     | 1.88        | 14     | 1     |
| 1:A:119:ASN:ND2  | 1:A:173:LEU:O    | 0.45     | 2.49        | 18     | 8     |
| 1:A:137:PHE:CD2  | 1:A:139:LEU:CD2  | 0.45     | 3.00        | 16     | 2     |
| 1:A:121:ILE:HB   | 1:A:170:ILE:CB   | 0.45     | 2.41        | 20     | 5     |
| 1:A:40:THR:CG2   | 1:A:54:VAL:HB    | 0.45     | 2.42        | 8      | 1     |
| 1:A:114:ILE:HD11 | 1:A:199:LYS:HG2  | 0.45     | 1.87        | 17     | 2     |
| 1:A:125:VAL:HG11 | 1:A:183:VAL:CG1  | 0.45     | 2.42        | 17     | 1     |
| 1:A:121:ILE:HD13 | 1:A:179:TYR:CD1  | 0.45     | 2.47        | 7      | 4     |
| 1:A:141:LEU:CD1  | 1:A:183:VAL:HG13 | 0.45     | 2.40        | 18     | 1     |
| 1:A:16:ILE:HB    | 1:A:99:PHE:CD1   | 0.45     | 2.46        | 19     | 1     |
| 1:A:111:GLU:HG3  | 1:A:112:PHE:N    | 0.45     | 2.27        | 21     | 1     |
| 1:A:27:TRP:CB    | 1:A:83:LEU:CD2   | 0.45     | 2.95        | 1      | 10    |
| 1:A:86:PHE:HA    | 1:A:91:THR:HA    | 0.45     | 1.88        | 1      | 1     |
| 1:A:158:ILE:CD1  | 1:A:166:PHE:CZ   | 0.45     | 2.97        | 3      | 2     |
| 1:A:105:MET:SD   | 1:A:139:LEU:HD13 | 0.45     | 2.51        | 7      | 1     |
| 1:A:179:TYR:CE2  | 1:A:203:LEU:HD21 | 0.45     | 2.47        | 10     | 2     |
| 1:A:107:PHE:CE2  | 1:A:185:LEU:HB3  | 0.45     | 2.47        | 21     | 2     |
| 1:A:144:GLU:OE2  | 1:A:184:TYR:CE2  | 0.45     | 2.70        | 16     | 1     |
| 1:A:180:CYS:C    | 1:A:198:LEU:HD22 | 0.45     | 2.37        | 16     | 1     |
| 1:A:196:SER:HB2  | 1:A:197:PRO:CD   | 0.45     | 2.41        | 18     | 1     |
| 1:A:117:PHE:O    | 1:A:118:THR:C    | 0.45     | 2.61        | 1      | 7     |
| 1:A:184:TYR:CB   | 1:A:194:ILE:C    | 0.45     | 2.89        | 20     | 10    |
| 1:A:43:TYR:CD2   | 1:A:55:VAL:CG2   | 0.45     | 3.00        | 6      | 10    |
| 1:A:43:TYR:CE1   | 1:A:79:TYR:HE1   | 0.45     | 2.29        | 20     | 4     |
| 1:A:111:GLU:O    | 1:A:126:LYS:N    | 0.45     | 2.49        | 11     | 5     |
| 1:A:177:THR:HG22 | 1:A:179:TYR:HD2  | 0.45     | 1.72        | 7      | 3     |
| 1:A:202:LEU:CD2  | 1:A:203:LEU:O    | 0.45     | 2.65        | 7      | 3     |
| 1:A:21:PHE:CD1   | 1:A:128:PRO:HG2  | 0.45     | 2.47        | 8      | 2     |
| 1:A:39:TYR:N     | 1:A:39:TYR:HD1   | 0.45     | 2.10        | 9      | 1     |
| 1:A:137:PHE:CG   | 1:A:138:ASP:N    | 0.45     | 2.85        | 10     | 2     |
| 1:A:179:TYR:HB2  | 1:A:201:THR:O    | 0.45     | 2.11        | 13     | 1     |
| 1:A:121:ILE:CB   | 1:A:179:TYR:CZ   | 0.45     | 2.96        | 18     | 1     |
| 1:A:121:ILE:CG1  | 1:A:179:TYR:CZ   | 0.45     | 2.99        | 18     | 1     |
| 1:A:186:GLU:C    | 1:A:187:HIS:CG   | 0.45     | 2.95        | 19     | 1     |
| 1:A:100:TRP:CE2  | 1:A:103:ILE:HD13 | 0.44     | 2.46        | 22     | 4     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:118:THR:CB   | 1:A:204:PRO:CG   | 0.44     | 2.94        | 7      | 5     |
| 1:A:126:LYS:CD   | 1:A:165:ASN:HB3  | 0.44     | 2.43        | 8      | 2     |
| 1:A:42:LEU:CD2   | 1:A:54:VAL:CG1   | 0.44     | 2.96        | 18     | 4     |
| 1:A:137:PHE:CE1  | 1:A:138:ASP:C    | 0.44     | 2.95        | 20     | 3     |
| 1:A:184:TYR:CZ   | 1:A:193:VAL:HG23 | 0.44     | 2.47        | 13     | 1     |
| 1:A:15:LYS:O     | 1:A:26:SER:N     | 0.44     | 2.48        | 2      | 10    |
| 1:A:122:ASN:ND2  | 1:A:169:ILE:HD12 | 0.44     | 2.27        | 1      | 2     |
| 1:A:31:ASN:CB    | 1:A:35:VAL:HG12  | 0.44     | 2.42        | 3      | 1     |
| 1:A:141:LEU:H    | 1:A:158:ILE:CD1  | 0.44     | 2.26        | 14     | 2     |
| 1:A:182:SER:HB2  | 1:A:198:LEU:HD11 | 0.44     | 1.88        | 14     | 1     |
| 1:A:137:PHE:CE2  | 1:A:139:LEU:HD23 | 0.44     | 2.48        | 16     | 1     |
| 1:A:37:THR:CG2   | 1:A:38:HIS:H     | 0.44     | 2.17        | 20     | 1     |
| 1:A:19:ARG:HB3   | 1:A:109:PRO:HG2  | 0.44     | 1.89        | 1      | 2     |
| 1:A:137:PHE:CD2  | 1:A:139:LEU:HB2  | 0.44     | 2.47        | 1      | 1     |
| 1:A:68:LEU:HD13  | 1:A:72:TRP:CG    | 0.44     | 2.47        | 2      | 1     |
| 1:A:117:PHE:CB   | 1:A:120:HIS:CD2  | 0.44     | 3.00        | 9      | 4     |
| 1:A:135:LEU:HD11 | 1:A:137:PHE:HE1  | 0.44     | 1.73        | 3      | 1     |
| 1:A:21:PHE:HD1   | 1:A:21:PHE:O     | 0.44     | 1.94        | 4      | 1     |
| 1:A:179:TYR:HE1  | 1:A:203:LEU:HD21 | 0.44     | 1.72        | 19     | 2     |
| 1:A:117:PHE:N    | 1:A:203:LEU:HD22 | 0.44     | 2.27        | 16     | 3     |
| 1:A:177:THR:HG22 | 1:A:177:THR:O    | 0.44     | 2.10        | 7      | 1     |
| 1:A:85:GLY:CA    | 1:A:93:PHE:CZ    | 0.44     | 2.97        | 9      | 1     |
| 1:A:42:LEU:HD12  | 1:A:52:LEU:CD2   | 0.44     | 2.42        | 11     | 1     |
| 1:A:107:PHE:CD1  | 1:A:185:LEU:CD1  | 0.44     | 3.00        | 11     | 1     |
| 1:A:158:ILE:HG23 | 1:A:166:PHE:HE2  | 0.44     | 1.72        | 15     | 1     |
| 1:A:122:ASN:CG   | 1:A:169:ILE:HD12 | 0.44     | 2.38        | 3      | 6     |
| 1:A:203:LEU:O    | 1:A:205:PRO:CD   | 0.44     | 2.65        | 3      | 15    |
| 1:A:29:LEU:HD13  | 1:A:39:TYR:CZ    | 0.44     | 2.47        | 2      | 2     |
| 1:A:184:TYR:HB3  | 1:A:195:LYS:HA   | 0.44     | 1.90        | 9      | 11    |
| 1:A:23:SER:O     | 1:A:68:LEU:HG    | 0.44     | 2.12        | 21     | 2     |
| 1:A:56:LYS:O     | 1:A:57:ASN:CB    | 0.44     | 2.65        | 5      | 1     |
| 1:A:145:GLU:OE2  | 1:A:173:LEU:CD2  | 0.44     | 2.65        | 14     | 2     |
| 1:A:142:VAL:CA   | 1:A:154:HIS:O    | 0.44     | 2.66        | 9      | 1     |
| 1:A:127:PHE:O    | 1:A:128:PRO:O    | 0.44     | 2.36        | 14     | 2     |
| 1:A:21:PHE:CZ    | 1:A:128:PRO:HB2  | 0.44     | 2.48        | 16     | 1     |
| 1:A:12:CYS:CA    | 1:A:29:LEU:HD23  | 0.44     | 2.43        | 22     | 1     |
| 1:A:144:GLU:CD   | 1:A:152:LYS:O    | 0.44     | 2.60        | 4      | 1     |
| 1:A:78:ALA:CB    | 1:A:100:TRP:CE3  | 0.44     | 3.00        | 20     | 4     |
| 1:A:38:HIS:CE1   | 1:A:86:PHE:O     | 0.44     | 2.70        | 12     | 10    |
| 1:A:100:TRP:CE2  | 1:A:103:ILE:CD1  | 0.44     | 2.98        | 8      | 5     |
| 1:A:43:TYR:N     | 1:A:52:LEU:CD2   | 0.44     | 2.81        | 14     | 8     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:125:VAL:HG11 | 1:A:183:VAL:HG11 | 0.44     | 1.89        | 16     | 2     |
| 1:A:85:GLY:C     | 1:A:86:PHE:CD1   | 0.44     | 2.96        | 11     | 1     |
| 1:A:18:LEU:HD23  | 1:A:107:PHE:CD1  | 0.44     | 2.47        | 6      | 2     |
| 1:A:131:VAL:C    | 1:A:133:GLU:N    | 0.44     | 2.76        | 21     | 6     |
| 1:A:150:ILE:O    | 1:A:150:ILE:HG12 | 0.44     | 2.12        | 3      | 4     |
| 1:A:132:GLU:HA   | 1:A:135:LEU:HB3  | 0.44     | 1.88        | 16     | 3     |
| 1:A:135:LEU:CD1  | 1:A:138:ASP:HB3  | 0.44     | 2.43        | 19     | 2     |
| 1:A:114:ILE:HG21 | 1:A:181:VAL:CG1  | 0.44     | 2.43        | 7      | 2     |
| 1:A:130:ILE:O    | 1:A:163:SER:CB   | 0.44     | 2.65        | 13     | 6     |
| 1:A:141:LEU:CD2  | 1:A:142:VAL:N    | 0.44     | 2.80        | 11     | 2     |
| 1:A:25:LEU:HD21  | 1:A:41:LEU:CG    | 0.44     | 2.42        | 16     | 1     |
| 1:A:146:GLN:HB2  | 1:A:180:CYS:O    | 0.44     | 2.13        | 17     | 3     |
| 1:A:117:PHE:HB3  | 1:A:120:HIS:CE1  | 0.44     | 2.48        | 19     | 10    |
| 1:A:54:VAL:O     | 1:A:54:VAL:CG1   | 0.44     | 2.65        | 6      | 2     |
| 1:A:38:HIS:CD2   | 1:A:38:HIS:C     | 0.44     | 2.96        | 19     | 3     |
| 1:A:27:TRP:CD2   | 1:A:83:LEU:CD2   | 0.44     | 3.00        | 9      | 2     |
| 1:A:141:LEU:N    | 1:A:162:MET:CE   | 0.44     | 2.81        | 16     | 2     |
| 1:A:84:GLU:HG3   | 1:A:94:SER:HB3   | 0.43     | 1.89        | 12     | 6     |
| 1:A:38:HIS:CD2   | 1:A:60:ASN:CG    | 0.43     | 2.95        | 13     | 2     |
| 1:A:114:ILE:HG12 | 1:A:199:LYS:HB3  | 0.43     | 1.90        | 4      | 4     |
| 1:A:177:THR:O    | 1:A:179:TYR:CD2  | 0.43     | 2.71        | 17     | 4     |
| 1:A:27:TRP:CZ2   | 1:A:39:TYR:HB2   | 0.43     | 2.48        | 7      | 3     |
| 1:A:185:LEU:HD23 | 1:A:185:LEU:H    | 0.43     | 1.73        | 9      | 1     |
| 1:A:107:PHE:CE2  | 1:A:127:PHE:CE2  | 0.43     | 3.05        | 11     | 1     |
| 1:A:39:TYR:HD1   | 1:A:39:TYR:N     | 0.43     | 2.11        | 20     | 1     |
| 1:A:194:ILE:N    | 1:A:194:ILE:CD1  | 0.43     | 2.81        | 20     | 1     |
| 1:A:82:VAL:HA    | 1:A:95:CYS:O     | 0.43     | 2.13        | 21     | 1     |
| 1:A:38:HIS:CG    | 1:A:60:ASN:CG    | 0.43     | 2.97        | 22     | 1     |
| 1:A:37:THR:CG2   | 1:A:38:HIS:N     | 0.43     | 2.81        | 19     | 21    |
| 1:A:103:ILE:N    | 1:A:103:ILE:HD12 | 0.43     | 2.28        | 15     | 6     |
| 1:A:143:ILE:O    | 1:A:154:HIS:N    | 0.43     | 2.52        | 22     | 7     |
| 1:A:102:ALA:O    | 1:A:187:HIS:CG   | 0.43     | 2.71        | 8      | 4     |
| 1:A:170:ILE:HD13 | 1:A:179:TYR:CD2  | 0.43     | 2.47        | 13     | 1     |
| 1:A:16:ILE:HD13  | 1:A:24:ILE:C     | 0.43     | 2.38        | 19     | 1     |
| 1:A:118:THR:N    | 1:A:204:PRO:HD2  | 0.43     | 2.27        | 22     | 1     |
| 1:A:202:LEU:HD12 | 1:A:203:LEU:N    | 0.43     | 2.23        | 16     | 5     |
| 1:A:142:VAL:HB   | 1:A:184:TYR:O    | 0.43     | 2.13        | 11     | 2     |
| 1:A:18:LEU:HD22  | 1:A:105:MET:HE3  | 0.43     | 1.89        | 19     | 2     |
| 1:A:135:LEU:CD1  | 1:A:137:PHE:HB2  | 0.43     | 2.43        | 16     | 1     |
| 1:A:144:GLU:HG3  | 1:A:152:LYS:O    | 0.43     | 2.12        | 17     | 1     |
| 1:A:72:TRP:CZ3   | 1:A:79:TYR:HB3   | 0.43     | 2.47        | 16     | 14    |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:84:GLU:CG    | 1:A:94:SER:CB    | 0.43     | 2.96        | 19     | 7     |
| 1:A:25:LEU:HD23  | 1:A:68:LEU:HD22  | 0.43     | 1.91        | 6      | 2     |
| 1:A:27:TRP:CZ3   | 1:A:64:SER:O     | 0.43     | 2.71        | 9      | 1     |
| 1:A:182:SER:CB   | 1:A:198:LEU:HD11 | 0.43     | 2.44        | 10     | 1     |
| 1:A:42:LEU:CD2   | 1:A:54:VAL:HG23  | 0.43     | 2.44        | 11     | 1     |
| 1:A:84:GLU:HA    | 1:A:94:SER:HA    | 0.43     | 1.90        | 11     | 2     |
| 1:A:105:MET:HB2  | 1:A:185:LEU:HD21 | 0.43     | 1.90        | 12     | 1     |
| 1:A:185:LEU:HD13 | 1:A:185:LEU:O    | 0.43     | 2.14        | 12     | 1     |
| 1:A:157:GLU:O    | 1:A:161:ASN:ND2  | 0.43     | 2.51        | 13     | 1     |
| 1:A:108:GLU:CB   | 1:A:109:PRO:HD3  | 0.43     | 2.43        | 15     | 1     |
| 1:A:142:VAL:CB   | 1:A:184:TYR:CE1  | 0.43     | 3.02        | 15     | 2     |
| 1:A:16:ILE:HB    | 1:A:99:PHE:HE1   | 0.43     | 1.72        | 18     | 1     |
| 1:A:29:LEU:HD22  | 1:A:29:LEU:H     | 0.43     | 1.73        | 20     | 1     |
| 1:A:145:GLU:OE1  | 1:A:147:SER:OG   | 0.43     | 2.36        | 2      | 1     |
| 1:A:11:SER:O     | 1:A:12:CYS:C     | 0.43     | 2.62        | 19     | 7     |
| 1:A:125:VAL:CG1  | 1:A:183:VAL:CG1  | 0.43     | 2.95        | 17     | 3     |
| 1:A:43:TYR:O     | 1:A:53:LYS:N     | 0.43     | 2.51        | 22     | 1     |
| 1:A:65:PHE:CD2   | 1:A:65:PHE:O     | 0.43     | 2.72        | 6      | 6     |
| 1:A:142:VAL:CG1  | 1:A:186:GLU:CG   | 0.43     | 2.96        | 6      | 2     |
| 1:A:142:VAL:HB   | 1:A:155:LYS:HG3  | 0.43     | 1.91        | 12     | 1     |
| 1:A:100:TRP:O    | 1:A:101:LEU:C    | 0.43     | 2.62        | 22     | 2     |
| 1:A:44:THR:O     | 1:A:80:VAL:O     | 0.43     | 2.36        | 22     | 2     |
| 1:A:108:GLU:O    | 1:A:110:PRO:HD3  | 0.43     | 2.14        | 16     | 1     |
| 1:A:154:HIS:CD2  | 1:A:170:ILE:CG2  | 0.43     | 3.02        | 16     | 1     |
| 1:A:127:PHE:HZ   | 1:A:141:LEU:HD13 | 0.43     | 1.72        | 18     | 1     |
| 1:A:141:LEU:CG   | 1:A:183:VAL:HG12 | 0.43     | 2.43        | 21     | 1     |
| 1:A:21:PHE:CE2   | 1:A:128:PRO:CG   | 0.43     | 3.01        | 3      | 11    |
| 1:A:145:GLU:OE1  | 1:A:147:SER:N    | 0.43     | 2.52        | 7      | 1     |
| 1:A:117:PHE:N    | 1:A:120:HIS:O    | 0.43     | 2.48        | 13     | 2     |
| 1:A:116:GLY:C    | 1:A:203:LEU:HD22 | 0.43     | 2.39        | 15     | 1     |
| 1:A:107:PHE:CG   | 1:A:185:LEU:HD23 | 0.43     | 2.49        | 17     | 1     |
| 1:A:87:SER:HB2   | 1:A:92:LEU:HD22  | 0.43     | 1.91        | 6      | 2     |
| 1:A:177:THR:C    | 1:A:202:LEU:HD13 | 0.43     | 2.38        | 4      | 2     |
| 1:A:100:TRP:HA   | 1:A:100:TRP:CE3  | 0.43     | 2.49        | 9      | 4     |
| 1:A:121:ILE:N    | 1:A:170:ILE:O    | 0.43     | 2.52        | 12     | 1     |
| 1:A:137:PHE:CE1  | 1:A:138:ASP:O    | 0.43     | 2.72        | 17     | 1     |
| 1:A:106:SER:HB3  | 1:A:194:ILE:HD12 | 0.43     | 1.90        | 21     | 1     |
| 1:A:114:ILE:CG1  | 1:A:199:LYS:CB   | 0.43     | 2.97        | 1      | 2     |
| 1:A:145:GLU:OE1  | 1:A:179:TYR:HB2  | 0.43     | 2.13        | 4      | 1     |
| 1:A:22:ARG:HB2   | 1:A:69:THR:HG23  | 0.43     | 1.91        | 6      | 1     |
| 1:A:102:ALA:O    | 1:A:187:HIS:CD2  | 0.43     | 2.72        | 15     | 2     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:144:GLU:CD   | 1:A:153:LYS:CB   | 0.43     | 2.92        | 17     | 2     |
| 1:A:173:LEU:HD21 | 1:A:179:TYR:HE1  | 0.43     | 1.73        | 13     | 1     |
| 1:A:126:LYS:N    | 1:A:126:LYS:CD   | 0.43     | 2.82        | 16     | 1     |
| 1:A:173:LEU:N    | 1:A:173:LEU:HD22 | 0.43     | 2.28        | 17     | 1     |
| 1:A:84:GLU:CD    | 1:A:94:SER:HB3   | 0.43     | 2.38        | 18     | 1     |
| 1:A:113:GLU:HB2  | 1:A:199:LYS:HE3  | 0.43     | 1.90        | 1      | 1     |
| 1:A:44:THR:N     | 1:A:80:VAL:O     | 0.43     | 2.49        | 3      | 2     |
| 1:A:127:PHE:CE2  | 1:A:162:MET:HG2  | 0.43     | 2.49        | 5      | 4     |
| 1:A:18:LEU:HB2   | 1:A:106:SER:O    | 0.43     | 2.14        | 9      | 1     |
| 1:A:143:ILE:O    | 1:A:154:HIS:CD2  | 0.43     | 2.71        | 13     | 1     |
| 1:A:125:VAL:HG11 | 1:A:141:LEU:HD11 | 0.43     | 1.90        | 14     | 1     |
| 1:A:127:PHE:CZ   | 1:A:162:MET:HG2  | 0.43     | 2.49        | 16     | 2     |
| 1:A:14:PHE:HA    | 1:A:27:TRP:HA    | 0.42     | 1.90        | 1      | 7     |
| 1:A:113:GLU:CB   | 1:A:199:LYS:CE   | 0.42     | 2.96        | 19     | 2     |
| 1:A:121:ILE:HG13 | 1:A:173:LEU:CD1  | 0.42     | 2.44        | 7      | 1     |
| 1:A:108:GLU:CB   | 1:A:109:PRO:CD   | 0.42     | 2.97        | 14     | 1     |
| 1:A:130:ILE:HD11 | 1:A:135:LEU:HB2  | 0.42     | 1.90        | 16     | 1     |
| 1:A:116:GLY:HA2  | 1:A:179:TYR:OH   | 0.42     | 2.14        | 20     | 2     |
| 1:A:123:VAL:CG2  | 1:A:181:VAL:HG11 | 0.42     | 2.44        | 7      | 1     |
| 1:A:176:ASN:N    | 1:A:205:PRO:HA   | 0.42     | 2.29        | 7      | 4     |
| 1:A:184:TYR:HB2  | 1:A:194:ILE:C    | 0.42     | 2.39        | 8      | 4     |
| 1:A:117:PHE:O    | 1:A:203:LEU:CB   | 0.42     | 2.67        | 12     | 2     |
| 1:A:112:PHE:CE1  | 1:A:199:LYS:HB2  | 0.42     | 2.49        | 16     | 1     |
| 1:A:121:ILE:CG1  | 1:A:179:TYR:CE2  | 0.42     | 3.03        | 20     | 1     |
| 1:A:42:LEU:C     | 1:A:52:LEU:CD2   | 0.42     | 2.93        | 22     | 4     |
| 1:A:25:LEU:HD21  | 1:A:41:LEU:HG    | 0.42     | 1.90        | 16     | 2     |
| 1:A:42:LEU:HD13  | 1:A:54:VAL:N     | 0.42     | 2.29        | 11     | 1     |
| 1:A:23:SER:C     | 1:A:68:LEU:HG    | 0.42     | 2.38        | 13     | 1     |
| 1:A:175:PRO:HA   | 1:A:203:LEU:CD1  | 0.42     | 2.45        | 20     | 1     |
| 1:A:107:PHE:CD1  | 1:A:107:PHE:C    | 0.42     | 2.97        | 21     | 1     |
| 1:A:113:GLU:O    | 1:A:114:ILE:HG23 | 0.42     | 2.14        | 13     | 3     |
| 1:A:120:HIS:ND1  | 1:A:120:HIS:N    | 0.42     | 2.68        | 14     | 5     |
| 1:A:158:ILE:CG2  | 1:A:162:MET:HG3  | 0.42     | 2.45        | 11     | 1     |
| 1:A:145:GLU:N    | 1:A:152:LYS:O    | 0.42     | 2.51        | 12     | 1     |
| 1:A:144:GLU:HG2  | 1:A:152:LYS:O    | 0.42     | 2.15        | 20     | 2     |
| 1:A:157:GLU:O    | 1:A:158:ILE:HD13 | 0.42     | 2.15        | 20     | 1     |
| 1:A:168:TYR:CE1  | 1:A:170:ILE:HG12 | 0.42     | 2.49        | 19     | 2     |
| 1:A:68:LEU:HD23  | 1:A:68:LEU:N     | 0.42     | 2.29        | 12     | 5     |
| 1:A:161:ASN:CG   | 1:A:166:PHE:CE1  | 0.42     | 2.98        | 22     | 7     |
| 1:A:43:TYR:CZ    | 1:A:53:LYS:HD3   | 0.42     | 2.50        | 8      | 1     |
| 1:A:80:VAL:HG13  | 1:A:98:ASN:OD1   | 0.42     | 2.15        | 11     | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:147:SER:HB2  | 1:A:179:TYR:CE1  | 0.42     | 2.50        | 13     | 1     |
| 1:A:127:PHE:CE2  | 1:A:162:MET:SD   | 0.42     | 3.12        | 18     | 1     |
| 1:A:34:ILE:HG23  | 1:A:34:ILE:O     | 0.42     | 2.14        | 5      | 1     |
| 1:A:147:SER:HA   | 1:A:179:TYR:HA   | 0.42     | 1.92        | 6      | 2     |
| 1:A:65:PHE:O     | 1:A:65:PHE:CD1   | 0.42     | 2.73        | 8      | 3     |
| 1:A:141:LEU:N    | 1:A:158:ILE:HG13 | 0.42     | 2.30        | 17     | 4     |
| 1:A:109:PRO:HB2  | 1:A:110:PRO:HD3  | 0.42     | 1.92        | 22     | 3     |
| 1:A:44:THR:CB    | 1:A:50:GLU:O     | 0.42     | 2.67        | 13     | 1     |
| 1:A:34:ILE:HD13  | 1:A:34:ILE:H     | 0.42     | 1.75        | 17     | 1     |
| 1:A:19:ARG:HB2   | 1:A:109:PRO:HG2  | 0.42     | 1.92        | 19     | 1     |
| 1:A:101:LEU:O    | 1:A:102:ALA:C    | 0.42     | 2.63        | 20     | 2     |
| 1:A:20:ASN:HB3   | 1:A:128:PRO:CG   | 0.42     | 2.45        | 21     | 1     |
| 1:A:154:HIS:CE1  | 1:A:168:TYR:OH   | 0.42     | 2.72        | 22     | 1     |
| 1:A:109:PRO:N    | 1:A:110:PRO:CD   | 0.42     | 2.83        | 2      | 9     |
| 1:A:22:ARG:HG3   | 1:A:69:THR:HG23  | 0.42     | 1.92        | 3      | 2     |
| 1:A:161:ASN:O    | 1:A:166:PHE:CD2  | 0.42     | 2.72        | 12     | 2     |
| 1:A:179:TYR:CE1  | 1:A:203:LEU:HD21 | 0.42     | 2.50        | 6      | 2     |
| 1:A:29:LEU:HD22  | 1:A:93:PHE:HE2   | 0.42     | 1.71        | 10     | 1     |
| 1:A:140:SER:CA   | 1:A:158:ILE:HG13 | 0.42     | 2.45        | 10     | 1     |
| 1:A:147:SER:HB2  | 1:A:179:TYR:HB3  | 0.42     | 1.90        | 12     | 1     |
| 1:A:173:LEU:HD22 | 1:A:177:THR:HG21 | 0.42     | 1.92        | 12     | 1     |
| 1:A:24:ILE:HG23  | 1:A:66:CYS:O     | 0.42     | 2.14        | 13     | 1     |
| 1:A:107:PHE:CE2  | 1:A:185:LEU:CG   | 0.42     | 3.03        | 13     | 1     |
| 1:A:18:LEU:HD21  | 1:A:137:PHE:HZ   | 0.42     | 1.74        | 16     | 1     |
| 1:A:42:LEU:CD1   | 1:A:84:GLU:CG    | 0.42     | 2.98        | 7      | 1     |
| 1:A:174:ILE:O    | 1:A:175:PRO:C    | 0.42     | 2.62        | 20     | 2     |
| 1:A:111:GLU:CB   | 1:A:126:LYS:HB2  | 0.42     | 2.45        | 16     | 1     |
| 1:A:180:CYS:CB   | 1:A:198:LEU:HD23 | 0.42     | 2.45        | 18     | 1     |
| 1:A:45:ILE:N     | 1:A:45:ILE:CD1   | 0.42     | 2.81        | 19     | 1     |
| 1:A:186:GLU:OE1  | 1:A:186:GLU:N    | 0.42     | 2.53        | 20     | 1     |
| 1:A:107:PHE:CD2  | 1:A:185:LEU:HD22 | 0.42     | 2.50        | 21     | 1     |
| 1:A:174:ILE:CG2  | 1:A:175:PRO:HD2  | 0.42     | 2.45        | 18     | 3     |
| 1:A:121:ILE:O    | 1:A:169:ILE:HA   | 0.42     | 2.15        | 5      | 1     |
| 1:A:118:THR:CA   | 1:A:204:PRO:CG   | 0.42     | 2.98        | 7      | 1     |
| 1:A:42:LEU:HD12  | 1:A:52:LEU:HD22  | 0.42     | 1.90        | 11     | 1     |
| 1:A:20:ASN:HB3   | 1:A:128:PRO:HG2  | 0.42     | 1.92        | 16     | 1     |
| 1:A:121:ILE:CG1  | 1:A:170:ILE:HB   | 0.42     | 2.45        | 18     | 1     |
| 1:A:132:GLU:HA   | 1:A:135:LEU:CG   | 0.42     | 2.44        | 21     | 1     |
| 1:A:22:ARG:CG    | 1:A:69:THR:HG23  | 0.42     | 2.45        | 1      | 2     |
| 1:A:116:GLY:CA   | 1:A:203:LEU:HD12 | 0.42     | 2.45        | 3      | 1     |
| 1:A:121:ILE:CD1  | 1:A:145:GLU:OE2  | 0.42     | 2.68        | 9      | 4     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:145:GLU:OE1  | 1:A:145:GLU:HA   | 0.42     | 2.15        | 4      | 1     |
| 1:A:124:MET:CB   | 1:A:166:PHE:O    | 0.42     | 2.68        | 11     | 1     |
| 1:A:143:ILE:CG1  | 1:A:156:PRO:HD3  | 0.42     | 2.44        | 12     | 1     |
| 1:A:18:LEU:HD22  | 1:A:105:MET:CE   | 0.42     | 2.40        | 16     | 1     |
| 1:A:156:PRO:HG3  | 1:A:168:TYR:CE1  | 0.41     | 2.49        | 5      | 1     |
| 1:A:141:LEU:HD22 | 1:A:184:TYR:O    | 0.41     | 2.14        | 6      | 1     |
| 1:A:141:LEU:HD23 | 1:A:142:VAL:H    | 0.41     | 1.75        | 11     | 1     |
| 1:A:130:ILE:CD1  | 1:A:135:LEU:CD2  | 0.41     | 2.98        | 14     | 1     |
| 1:A:44:THR:CG2   | 1:A:52:LEU:HG    | 0.41     | 2.45        | 19     | 3     |
| 1:A:114:ILE:HG21 | 1:A:181:VAL:HG21 | 0.41     | 1.91        | 18     | 1     |
| 1:A:176:ASN:HB2  | 1:A:205:PRO:HB3  | 0.41     | 1.91        | 18     | 1     |
| 1:A:83:LEU:O     | 1:A:83:LEU:HG    | 0.41     | 2.15        | 1      | 1     |
| 1:A:19:ARG:CG    | 1:A:24:ILE:HD12  | 0.41     | 2.45        | 4      | 1     |
| 1:A:86:PHE:HD1   | 1:A:91:THR:HG22  | 0.41     | 1.74        | 11     | 1     |
| 1:A:145:GLU:HG3  | 1:A:145:GLU:O    | 0.41     | 2.15        | 13     | 1     |
| 1:A:20:ASN:C     | 1:A:21:PHE:CG    | 0.41     | 2.97        | 14     | 1     |
| 1:A:141:LEU:CD1  | 1:A:183:VAL:CG1  | 0.41     | 2.98        | 18     | 1     |
| 1:A:141:LEU:O    | 1:A:155:LYS:HA   | 0.41     | 2.15        | 1      | 1     |
| 1:A:145:GLU:OE2  | 1:A:179:TYR:CB   | 0.41     | 2.68        | 8      | 2     |
| 1:A:121:ILE:CD1  | 1:A:170:ILE:HD12 | 0.41     | 2.46        | 10     | 1     |
| 1:A:107:PHE:CE1  | 1:A:127:PHE:CZ   | 0.41     | 3.08        | 13     | 1     |
| 1:A:173:LEU:HD21 | 1:A:179:TYR:CE1  | 0.41     | 2.50        | 13     | 1     |
| 1:A:34:ILE:HD13  | 1:A:87:SER:CB    | 0.41     | 2.45        | 22     | 1     |
| 1:A:137:PHE:CZ   | 1:A:162:MET:SD   | 0.41     | 3.14        | 1      | 1     |
| 1:A:147:SER:O    | 1:A:150:ILE:HG12 | 0.41     | 2.15        | 3      | 2     |
| 1:A:142:VAL:CB   | 1:A:154:HIS:O    | 0.41     | 2.69        | 6      | 1     |
| 1:A:93:PHE:C     | 1:A:94:SER:HG    | 0.41     | 2.23        | 8      | 1     |
| 1:A:180:CYS:HB3  | 1:A:198:LEU:HD22 | 0.41     | 1.92        | 8      | 2     |
| 1:A:203:LEU:O    | 1:A:203:LEU:HD12 | 0.41     | 2.15        | 9      | 1     |
| 1:A:16:ILE:HD13  | 1:A:101:LEU:CD2  | 0.41     | 2.45        | 14     | 1     |
| 1:A:114:ILE:HG12 | 1:A:181:VAL:CG1  | 0.41     | 2.46        | 22     | 1     |
| 1:A:73:ARG:O     | 1:A:74:SER:C     | 0.41     | 2.62        | 6      | 3     |
| 1:A:127:PHE:CE1  | 1:A:162:MET:SD   | 0.41     | 3.14        | 3      | 2     |
| 1:A:103:ILE:HD12 | 1:A:103:ILE:N    | 0.41     | 2.31        | 6      | 3     |
| 1:A:121:ILE:HD13 | 1:A:179:TYR:CG   | 0.41     | 2.49        | 17     | 2     |
| 1:A:16:ILE:CB    | 1:A:99:PHE:CE1   | 0.41     | 3.03        | 18     | 1     |
| 1:A:121:ILE:HG12 | 1:A:170:ILE:HB   | 0.41     | 1.93        | 18     | 1     |
| 1:A:22:ARG:HG3   | 1:A:69:THR:OG1   | 0.41     | 2.15        | 21     | 1     |
| 1:A:147:SER:HB2  | 1:A:177:THR:CG2  | 0.41     | 2.44        | 9      | 3     |
| 1:A:111:GLU:CG   | 1:A:126:LYS:HB2  | 0.41     | 2.45        | 6      | 1     |
| 1:A:145:GLU:OE1  | 1:A:154:HIS:NE2  | 0.41     | 2.54        | 13     | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:107:PHE:CD2  | 1:A:185:LEU:HD11 | 0.41     | 2.50        | 14     | 1     |
| 1:A:130:ILE:O    | 1:A:162:MET:O    | 0.41     | 2.38        | 16     | 1     |
| 1:A:22:ARG:CB    | 1:A:69:THR:OG1   | 0.41     | 2.68        | 21     | 1     |
| 1:A:154:HIS:NE2  | 1:A:170:ILE:CG2  | 0.41     | 2.84        | 5      | 1     |
| 1:A:38:HIS:CD2   | 1:A:60:ASN:HB3   | 0.41     | 2.50        | 17     | 3     |
| 1:A:107:PHE:O    | 1:A:194:ILE:CG2  | 0.41     | 2.68        | 9      | 3     |
| 1:A:114:ILE:HG21 | 1:A:181:VAL:HB   | 0.41     | 1.92        | 7      | 2     |
| 1:A:12:CYS:HB2   | 1:A:14:PHE:CZ    | 0.41     | 2.50        | 9      | 1     |
| 1:A:67:ASP:C     | 1:A:68:LEU:CD2   | 0.41     | 2.87        | 15     | 1     |
| 1:A:107:PHE:CE1  | 1:A:110:PRO:CG   | 0.41     | 3.04        | 18     | 1     |
| 1:A:12:CYS:HA    | 1:A:29:LEU:CD2   | 0.41     | 2.46        | 22     | 1     |
| 1:A:65:PHE:O     | 1:A:65:PHE:CD2   | 0.41     | 2.74        | 16     | 4     |
| 1:A:154:HIS:CG   | 1:A:168:TYR:OH   | 0.41     | 2.73        | 3      | 1     |
| 1:A:170:ILE:O    | 1:A:173:LEU:HD11 | 0.41     | 2.16        | 4      | 2     |
| 1:A:72:TRP:CD1   | 1:A:79:TYR:CD1   | 0.41     | 3.09        | 22     | 2     |
| 1:A:124:MET:CA   | 1:A:166:PHE:O    | 0.41     | 2.68        | 11     | 1     |
| 1:A:160:GLY:O    | 1:A:161:ASN:C    | 0.41     | 2.64        | 13     | 1     |
| 1:A:179:TYR:C    | 1:A:200:CYS:HA   | 0.41     | 2.40        | 13     | 1     |
| 1:A:145:GLU:CD   | 1:A:147:SER:HB3  | 0.41     | 2.41        | 14     | 1     |
| 1:A:123:VAL:CG2  | 1:A:170:ILE:CD1  | 0.41     | 2.99        | 18     | 2     |
| 1:A:14:PHE:CE1   | 1:A:83:LEU:CD2   | 0.41     | 3.01        | 19     | 2     |
| 1:A:20:ASN:CB    | 1:A:128:PRO:HG3  | 0.41     | 2.45        | 21     | 1     |
| 1:A:22:ARG:HG3   | 1:A:69:THR:CG2   | 0.41     | 2.44        | 3      | 1     |
| 1:A:72:TRP:CA    | 1:A:79:TYR:CZ    | 0.41     | 3.02        | 12     | 2     |
| 1:A:147:SER:OG   | 1:A:177:THR:CG2  | 0.41     | 2.69        | 6      | 1     |
| 1:A:128:PRO:O    | 1:A:164:GLY:N    | 0.41     | 2.54        | 10     | 1     |
| 1:A:123:VAL:N    | 1:A:168:TYR:O    | 0.41     | 2.52        | 11     | 1     |
| 1:A:20:ASN:CG    | 1:A:128:PRO:CG   | 0.41     | 2.94        | 16     | 1     |
| 1:A:98:ASN:OD1   | 1:A:100:TRP:CE3  | 0.41     | 2.74        | 16     | 1     |
| 1:A:21:PHE:CE1   | 1:A:128:PRO:HG2  | 0.41     | 2.51        | 17     | 1     |
| 1:A:27:TRP:HZ2   | 1:A:63:ARG:O     | 0.41     | 1.99        | 17     | 1     |
| 1:A:75:THR:HG21  | 1:A:136:GLN:HG3  | 0.41     | 1.93        | 17     | 1     |
| 1:A:194:ILE:HG22 | 1:A:194:ILE:O    | 0.41     | 2.16        | 17     | 1     |
| 1:A:105:MET:O    | 1:A:194:ILE:HG13 | 0.41     | 2.16        | 18     | 1     |
| 1:A:145:GLU:CD   | 1:A:147:SER:OG   | 0.41     | 2.64        | 18     | 1     |
| 1:A:174:ILE:HG23 | 1:A:175:PRO:HD2  | 0.41     | 1.92        | 18     | 1     |
| 1:A:14:PHE:HZ    | 1:A:95:CYS:HB2   | 0.41     | 1.76        | 21     | 1     |
| 1:A:113:GLU:HA   | 1:A:199:LYS:CE   | 0.41     | 2.46        | 21     | 1     |
| 1:A:145:GLU:CG   | 1:A:170:ILE:CD1  | 0.41     | 2.93        | 8      | 2     |
| 1:A:120:HIS:CA   | 1:A:173:LEU:HD12 | 0.41     | 2.45        | 7      | 1     |
| 1:A:42:LEU:CD1   | 1:A:82:VAL:O     | 0.41     | 2.60        | 8      | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:40:THR:HA    | 1:A:58:CYS:O     | 0.41     | 2.15        | 10     | 1     |
| 1:A:13:THR:O     | 1:A:14:PHE:CD1   | 0.41     | 2.74        | 13     | 1     |
| 1:A:45:ILE:HD12  | 1:A:48:LYS:HB2   | 0.41     | 1.93        | 13     | 1     |
| 1:A:132:GLU:O    | 1:A:135:LEU:HB2  | 0.41     | 2.15        | 15     | 1     |
| 1:A:42:LEU:HB3   | 1:A:52:LEU:HD22  | 0.41     | 1.92        | 18     | 1     |
| 1:A:107:PHE:CD1  | 1:A:110:PRO:HG2  | 0.41     | 2.51        | 18     | 1     |
| 1:A:177:THR:N    | 1:A:202:LEU:CD1  | 0.41     | 2.84        | 19     | 1     |
| 1:A:107:PHE:CE2  | 1:A:185:LEU:CD2  | 0.41     | 3.03        | 21     | 1     |
| 1:A:108:GLU:HB3  | 1:A:109:PRO:HD3  | 0.40     | 1.92        | 1      | 1     |
| 1:A:18:LEU:HD12  | 1:A:23:SER:HA    | 0.40     | 1.92        | 4      | 1     |
| 1:A:137:PHE:CE1  | 1:A:139:LEU:HB3  | 0.40     | 2.51        | 10     | 1     |
| 1:A:147:SER:C    | 1:A:148:GLU:HG3  | 0.40     | 2.41        | 12     | 1     |
| 1:A:144:GLU:HG2  | 1:A:153:LYS:HA   | 0.40     | 1.93        | 13     | 1     |
| 1:A:161:ASN:HB3  | 1:A:166:PHE:CD2  | 0.40     | 2.51        | 13     | 1     |
| 1:A:184:TYR:CE1  | 1:A:193:VAL:HG23 | 0.40     | 2.51        | 15     | 1     |
| 1:A:115:VAL:N    | 1:A:122:ASN:O    | 0.40     | 2.53        | 16     | 1     |
| 1:A:85:GLY:O     | 1:A:86:PHE:CD1   | 0.40     | 2.74        | 20     | 1     |
| 1:A:29:LEU:H     | 1:A:29:LEU:HD22  | 0.40     | 1.76        | 21     | 1     |
| 1:A:114:ILE:HD11 | 1:A:199:LYS:C    | 0.40     | 2.40        | 21     | 1     |
| 1:A:132:GLU:CB   | 1:A:135:LEU:HD23 | 0.40     | 2.46        | 21     | 1     |
| 1:A:121:ILE:HG12 | 1:A:179:TYR:CZ   | 0.40     | 2.51        | 1      | 1     |
| 1:A:141:LEU:N    | 1:A:162:MET:HE3  | 0.40     | 2.31        | 6      | 1     |
| 1:A:53:LYS:O     | 1:A:55:VAL:N     | 0.40     | 2.54        | 11     | 1     |
| 1:A:108:GLU:O    | 1:A:109:PRO:C    | 0.40     | 2.63        | 14     | 1     |
| 1:A:141:LEU:HD12 | 1:A:166:PHE:CD2  | 0.40     | 2.51        | 15     | 1     |
| 1:A:114:ILE:HG13 | 1:A:199:LYS:HE3  | 0.40     | 1.91        | 21     | 1     |
| 1:A:138:ASP:O    | 1:A:139:LEU:CD1  | 0.40     | 2.69        | 4      | 1     |
| 1:A:145:GLU:O    | 1:A:152:LYS:N    | 0.40     | 2.54        | 10     | 1     |
| 1:A:117:PHE:O    | 1:A:119:ASN:N    | 0.40     | 2.55        | 17     | 2     |
| 1:A:105:MET:SD   | 1:A:137:PHE:CE1  | 0.40     | 3.14        | 15     | 1     |
| 1:A:114:ILE:N    | 1:A:199:LYS:HD3  | 0.40     | 2.31        | 15     | 1     |
| 1:A:132:GLU:CB   | 1:A:135:LEU:HD22 | 0.40     | 2.46        | 16     | 1     |
| 1:A:29:LEU:CD2   | 1:A:39:TYR:CZ    | 0.40     | 3.04        | 19     | 2     |
| 1:A:25:LEU:HD13  | 1:A:72:TRP:CZ2   | 0.40     | 2.52        | 4      | 1     |
| 1:A:112:PHE:CE1  | 1:A:181:VAL:O    | 0.40     | 2.74        | 9      | 1     |
| 1:A:43:TYR:CB    | 1:A:81:THR:CG2   | 0.40     | 2.99        | 12     | 1     |
| 1:A:131:VAL:O    | 1:A:131:VAL:HG23 | 0.40     | 2.17        | 12     | 1     |
| 1:A:189:ASP:C    | 1:A:191:GLN:N    | 0.40     | 2.80        | 13     | 1     |
| 1:A:44:THR:OG1   | 1:A:45:ILE:N     | 0.40     | 2.54        | 21     | 1     |
| 1:A:38:HIS:CE1   | 1:A:60:ASN:ND2   | 0.40     | 2.90        | 22     | 1     |
| 1:A:140:SER:HA   | 1:A:158:ILE:CG1  | 0.40     | 2.45        | 4      | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:111:GLU:HB2  | 1:A:126:LYS:HB2  | 0.40     | 1.94        | 5      | 1     |
| 1:A:185:LEU:HD12 | 1:A:186:GLU:N    | 0.40     | 2.31        | 6      | 1     |
| 1:A:132:GLU:HA   | 1:A:135:LEU:CB   | 0.40     | 2.47        | 8      | 1     |
| 1:A:182:SER:CB   | 1:A:198:LEU:CD1  | 0.40     | 2.99        | 12     | 1     |
| 1:A:185:LEU:C    | 1:A:185:LEU:HD13 | 0.40     | 2.42        | 12     | 1     |
| 1:A:131:VAL:O    | 1:A:131:VAL:CG1  | 0.40     | 2.69        | 14     | 1     |
| 1:A:93:PHE:O     | 1:A:94:SER:CB    | 0.40     | 2.70        | 21     | 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     | 195/212 (92%)   | 148±3 (76±2%) | 37±3 (19±2%) | 11±2 (6±1%) | 2           | 21 |
| All | All   | 4290/4664 (92%) | 3245 (76%)    | 807 (19%)    | 238 (6%)    | 2           | 21 |

All 36 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     | 60  | ASN  | 22             |
| 1   | A     | 105 | MET  | 22             |
| 1   | A     | 110 | PRO  | 20             |
| 1   | A     | 108 | GLU  | 17             |
| 1   | A     | 132 | GLU  | 17             |
| 1   | A     | 175 | PRO  | 15             |
| 1   | A     | 79  | TYR  | 13             |
| 1   | A     | 204 | PRO  | 13             |
| 1   | A     | 198 | LEU  | 12             |
| 1   | A     | 188 | SER  | 12             |
| 1   | A     | 12  | CYS  | 11             |
| 1   | A     | 197 | PRO  | 7              |
| 1   | A     | 128 | PRO  | 6              |
| 1   | A     | 159 | LYS  | 6              |
| 1   | A     | 73  | ARG  | 5              |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 118 | THR  | 5              |
| 1   | A     | 139 | LEU  | 4              |
| 1   | A     | 133 | GLU  | 4              |
| 1   | A     | 187 | HIS  | 3              |
| 1   | A     | 94  | SER  | 3              |
| 1   | A     | 172 | LYS  | 3              |
| 1   | A     | 148 | GLU  | 3              |
| 1   | A     | 109 | PRO  | 2              |
| 1   | A     | 156 | PRO  | 1              |
| 1   | A     | 11  | SER  | 1              |
| 1   | A     | 166 | PHE  | 1              |
| 1   | A     | 54  | VAL  | 1              |
| 1   | A     | 55  | VAL  | 1              |
| 1   | A     | 51  | ASP  | 1              |
| 1   | A     | 161 | ASN  | 1              |
| 1   | A     | 190 | GLU  | 1              |
| 1   | A     | 98  | ASN  | 1              |
| 1   | A     | 196 | SER  | 1              |
| 1   | A     | 58  | CYS  | 1              |
| 1   | A     | 32  | HIS  | 1              |
| 1   | A     | 112 | PHE  | 1              |

### 6.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the sidechain conformation was analysed and the total number of residues.

| Mol | Chain | Analysed        | Rotameric     | Outliers     | Percentiles |   |
|-----|-------|-----------------|---------------|--------------|-------------|---|
| 1   | A     | 185/201 (92%)   | 119±5 (64±3%) | 66±5 (35±2%) | 1           | 9 |
| All | All   | 4060/4422 (92%) | 2619 (65%)    | 1441 (35%)   | 1           | 9 |

All 142 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     | 29  | LEU  | 22             |
| 1   | A     | 42  | LEU  | 22             |
| 1   | A     | 45  | ILE  | 22             |
| 1   | A     | 52  | LEU  | 22             |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 68  | LEU  | 22             |
| 1   | A     | 80  | VAL  | 22             |
| 1   | A     | 114 | ILE  | 22             |
| 1   | A     | 130 | ILE  | 22             |
| 1   | A     | 143 | ILE  | 22             |
| 1   | A     | 150 | ILE  | 22             |
| 1   | A     | 165 | ASN  | 22             |
| 1   | A     | 167 | THR  | 22             |
| 1   | A     | 28  | GLU  | 21             |
| 1   | A     | 155 | LYS  | 21             |
| 1   | A     | 201 | THR  | 21             |
| 1   | A     | 12  | CYS  | 21             |
| 1   | A     | 91  | THR  | 21             |
| 1   | A     | 54  | VAL  | 20             |
| 1   | A     | 193 | VAL  | 20             |
| 1   | A     | 53  | LYS  | 19             |
| 1   | A     | 81  | THR  | 19             |
| 1   | A     | 170 | ILE  | 19             |
| 1   | A     | 38  | HIS  | 18             |
| 1   | A     | 60  | ASN  | 18             |
| 1   | A     | 62  | THR  | 18             |
| 1   | A     | 94  | SER  | 18             |
| 1   | A     | 100 | TRP  | 18             |
| 1   | A     | 105 | MET  | 18             |
| 1   | A     | 17  | SER  | 18             |
| 1   | A     | 46  | MET  | 17             |
| 1   | A     | 74  | SER  | 17             |
| 1   | A     | 177 | THR  | 17             |
| 1   | A     | 108 | GLU  | 16             |
| 1   | A     | 198 | LEU  | 16             |
| 1   | A     | 41  | LEU  | 16             |
| 1   | A     | 50  | GLU  | 15             |
| 1   | A     | 145 | GLU  | 15             |
| 1   | A     | 11  | SER  | 15             |
| 1   | A     | 23  | SER  | 14             |
| 1   | A     | 30  | LYS  | 14             |
| 1   | A     | 139 | LEU  | 14             |
| 1   | A     | 146 | GLN  | 14             |
| 1   | A     | 200 | CYS  | 14             |
| 1   | A     | 126 | LYS  | 14             |
| 1   | A     | 83  | LEU  | 13             |
| 1   | A     | 137 | PHE  | 13             |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 152 | LYS  | 13             |
| 1   | A     | 153 | LYS  | 13             |
| 1   | A     | 73  | ARG  | 13             |
| 1   | A     | 95  | CYS  | 13             |
| 1   | A     | 147 | SER  | 13             |
| 1   | A     | 118 | THR  | 12             |
| 1   | A     | 119 | ASN  | 12             |
| 1   | A     | 157 | GLU  | 12             |
| 1   | A     | 188 | SER  | 12             |
| 1   | A     | 189 | ASP  | 12             |
| 1   | A     | 203 | LEU  | 12             |
| 1   | A     | 15  | LYS  | 12             |
| 1   | A     | 25  | LEU  | 11             |
| 1   | A     | 111 | GLU  | 11             |
| 1   | A     | 112 | PHE  | 11             |
| 1   | A     | 124 | MET  | 11             |
| 1   | A     | 172 | LYS  | 11             |
| 1   | A     | 32  | HIS  | 11             |
| 1   | A     | 63  | ARG  | 10             |
| 1   | A     | 92  | LEU  | 10             |
| 1   | A     | 159 | LYS  | 10             |
| 1   | A     | 173 | LEU  | 10             |
| 1   | A     | 19  | ARG  | 10             |
| 1   | A     | 180 | CYS  | 10             |
| 1   | A     | 144 | GLU  | 10             |
| 1   | A     | 56  | LYS  | 9              |
| 1   | A     | 71  | GLU  | 9              |
| 1   | A     | 190 | GLU  | 9              |
| 1   | A     | 133 | GLU  | 9              |
| 1   | A     | 101 | LEU  | 9              |
| 1   | A     | 33  | SER  | 8              |
| 1   | A     | 66  | CYS  | 8              |
| 1   | A     | 76  | HIS  | 8              |
| 1   | A     | 86  | PHE  | 8              |
| 1   | A     | 120 | HIS  | 8              |
| 1   | A     | 87  | SER  | 8              |
| 1   | A     | 148 | GLU  | 8              |
| 1   | A     | 13  | THR  | 8              |
| 1   | A     | 182 | SER  | 8              |
| 1   | A     | 191 | GLN  | 8              |
| 1   | A     | 107 | PHE  | 8              |
| 1   | A     | 199 | LYS  | 7              |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 186 | GLU  | 7              |
| 1   | A     | 134 | GLU  | 7              |
| 1   | A     | 141 | LEU  | 7              |
| 1   | A     | 47  | SER  | 6              |
| 1   | A     | 106 | SER  | 6              |
| 1   | A     | 185 | LEU  | 6              |
| 1   | A     | 176 | ASN  | 6              |
| 1   | A     | 96  | SER  | 6              |
| 1   | A     | 161 | ASN  | 6              |
| 1   | A     | 48  | LYS  | 6              |
| 1   | A     | 142 | VAL  | 6              |
| 1   | A     | 51  | ASP  | 5              |
| 1   | A     | 22  | ARG  | 5              |
| 1   | A     | 135 | LEU  | 5              |
| 1   | A     | 174 | ILE  | 4              |
| 1   | A     | 129 | SER  | 4              |
| 1   | A     | 40  | THR  | 4              |
| 1   | A     | 132 | GLU  | 4              |
| 1   | A     | 196 | SER  | 4              |
| 1   | A     | 34  | ILE  | 3              |
| 1   | A     | 195 | LYS  | 3              |
| 1   | A     | 113 | GLU  | 3              |
| 1   | A     | 122 | ASN  | 3              |
| 1   | A     | 138 | ASP  | 3              |
| 1   | A     | 31  | ASN  | 3              |
| 1   | A     | 90  | THR  | 3              |
| 1   | A     | 171 | ASP  | 3              |
| 1   | A     | 70  | ASP  | 3              |
| 1   | A     | 57  | ASN  | 2              |
| 1   | A     | 79  | TYR  | 2              |
| 1   | A     | 69  | THR  | 2              |
| 1   | A     | 136 | GLN  | 2              |
| 1   | A     | 187 | HIS  | 2              |
| 1   | A     | 39  | TYR  | 2              |
| 1   | A     | 89  | ASN  | 2              |
| 1   | A     | 194 | ILE  | 2              |
| 1   | A     | 26  | SER  | 2              |
| 1   | A     | 179 | TYR  | 2              |
| 1   | A     | 181 | VAL  | 2              |
| 1   | A     | 16  | ILE  | 2              |
| 1   | A     | 163 | SER  | 2              |
| 1   | A     | 24  | ILE  | 1              |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 67  | ASP  | 1              |
| 1   | A     | 123 | VAL  | 1              |
| 1   | A     | 140 | SER  | 1              |
| 1   | A     | 151 | VAL  | 1              |
| 1   | A     | 18  | LEU  | 1              |
| 1   | A     | 104 | ASP  | 1              |
| 1   | A     | 127 | PHE  | 1              |
| 1   | A     | 202 | LEU  | 1              |
| 1   | A     | 121 | ILE  | 1              |
| 1   | A     | 158 | ILE  | 1              |
| 1   | A     | 93  | PHE  | 1              |
| 1   | A     | 183 | VAL  | 1              |

### 6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 6.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 6.6 Ligand geometry ⓘ

There are no ligands in this entry.

## 6.7 Other polymers ⓘ

There are no such molecules in this entry.

## 6.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 7 Chemical shift validation

No chemical shift data were provided