



# Full wwPDB NMR Structure Validation Report ⓘ

Apr 26, 2016 – 09:01 PM BST

PDB ID : 2IL6  
Title : HUMAN INTERLEUKIN-6, NMR, 32 STRUCTURES  
Authors : Xu, G.Y.; Yu, H.A.; Hong, J.; Stahl, M.; Mcdonagh, T.; Kay, L.E.; Cumming, D.A.  
Deposited on : 1997-01-31

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/NMRValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

Cyrange : Kirchner and Güntert (2011)  
NmrClust : Kelley et al. (1996)  
MolProbity : 4.02b-467  
Mogul : unknown  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
RCI : v\_1n\_11\_5\_13\_A (Berjanski et al., 2005)  
PANAV : Wang et al. (2010)  
ShiftChecker : rb-20027457  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20027457

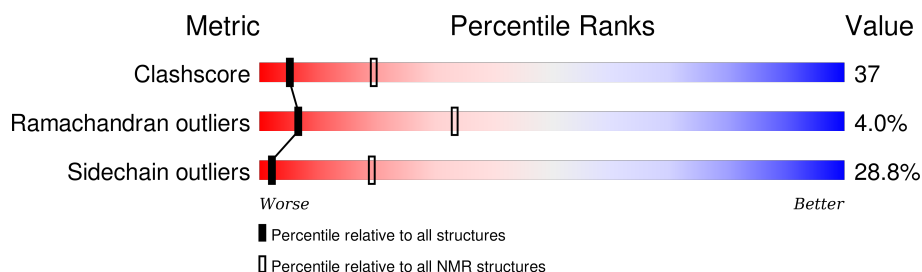
# 1 Overall quality at a glance

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            | 114402                      | 11133                     |
| Ramachandran outliers | 111179                      | 9975                      |
| Sidechain outliers    | 111093                      | 9958                      |

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     | 185    |                  |

## 2 Ensemble composition and analysis

This entry contains 32 models. Model 28 is the overall representative, medoid model (most similar to other models).

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

| Well-defined (core) protein residues |   |                   |              |
|--------------------------------------|---|-------------------|--------------|
| Well-defined core                    | Residue range (total)                       | Backbone RMSD (Å) | Medoid model |
| 1                                    | A:21-A:50, A:62-A:139,<br>A:143-A:185 (151) | 0.54              | 28           |

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

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

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

| Cluster number        | Models   |
|-----------------------|--|
| 1                     | 2, 4, 5, 9, 12, 13, 14, 16, 18, 19, 20, 21, 22, 25, 29 |
| 2                     | 3, 7, 23, 27, 28, 31                                   |
| 3                     | 26, 30   |
| 4                     | 1, 17  |
| 5                     | 11, 24   |
| Single-model clusters | 6; 8; 10; 15; 32                                       |

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

There is only 1 type of molecule in this entry. The entry contains 2680 atoms, of which 1349 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called INTERLEUKIN-6.

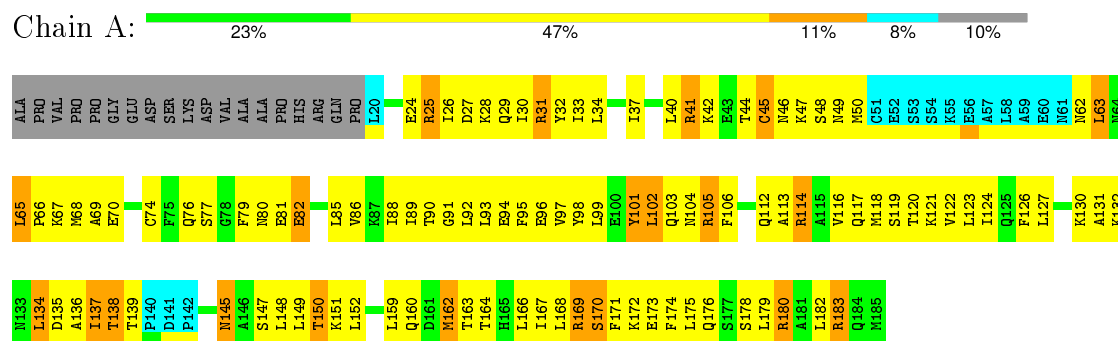
| Mol | Chain | Residues | Atoms |     |      |     |     |   | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|-------|
| 1   | A     | 166      | Total | C   | H    | N   | O   | S | 0     |
|     |       |          | 2680  | 832 | 1349 | 229 | 261 | 9 |       |

## 4 Residue-property plots

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

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

- Molecule 1: INTERLEUKIN-6

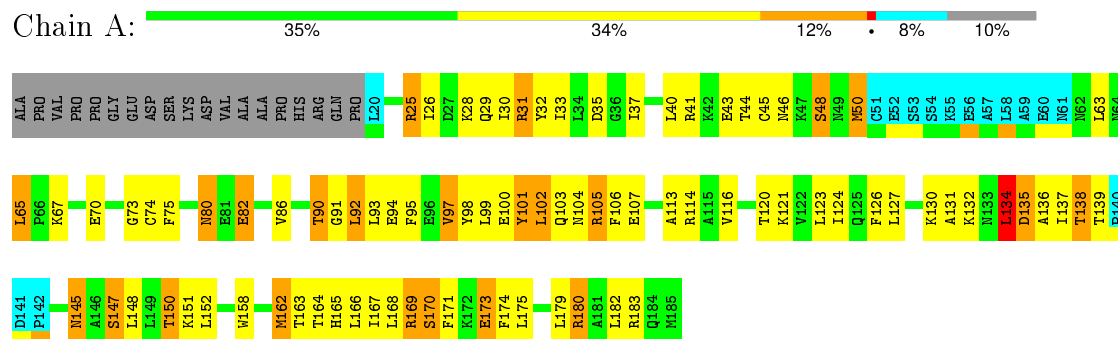


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

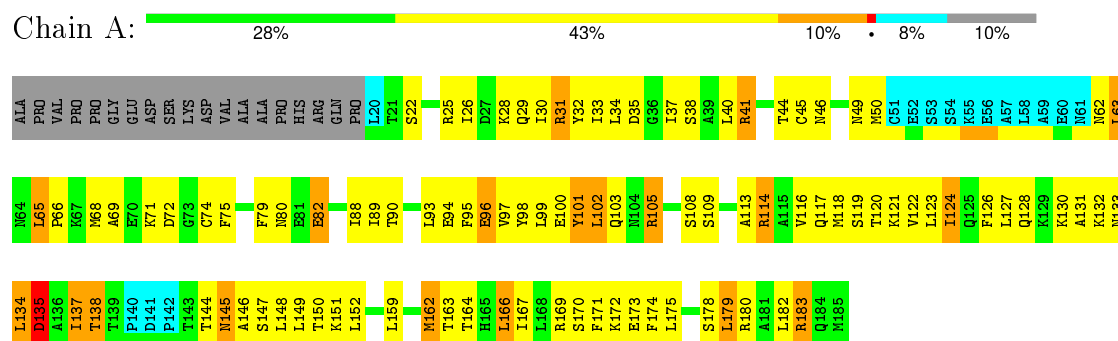
#### 4.2.1 Score per residue for model 1

- Molecule 1: INTERLEUKIN-6



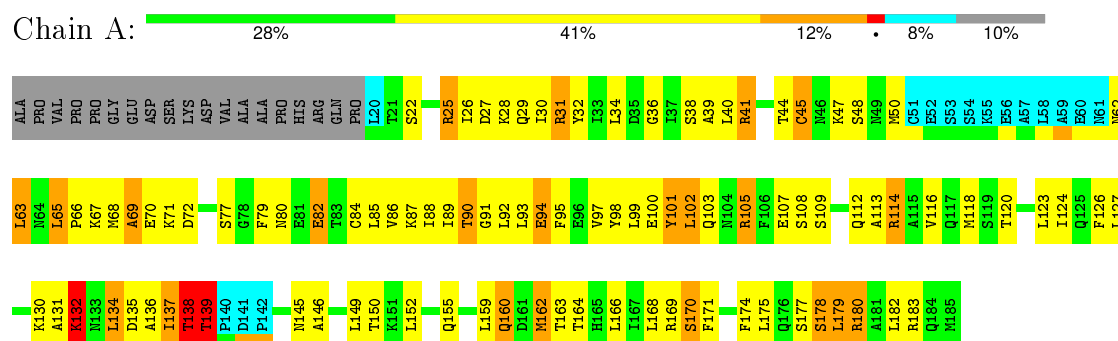
## 4.2.2 Score per residue for model 2

### • Molecule 1: INTERLEUKIN-6



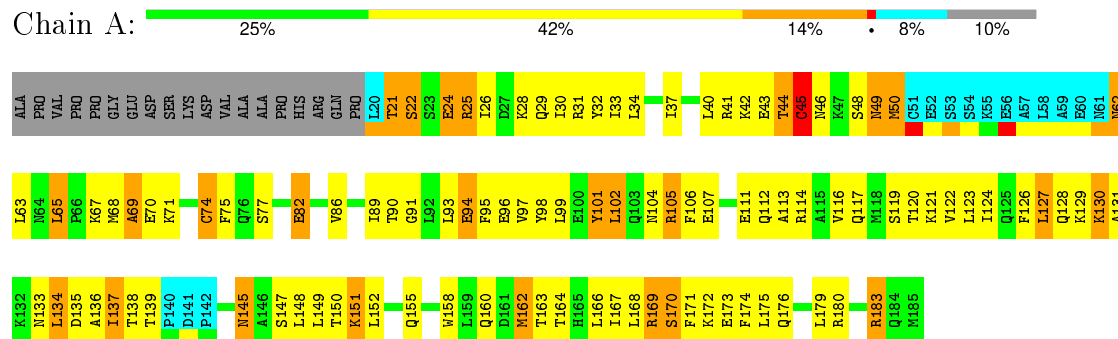
## 4.2.3 Score per residue for model 3

### • Molecule 1: INTERLEUKIN-6



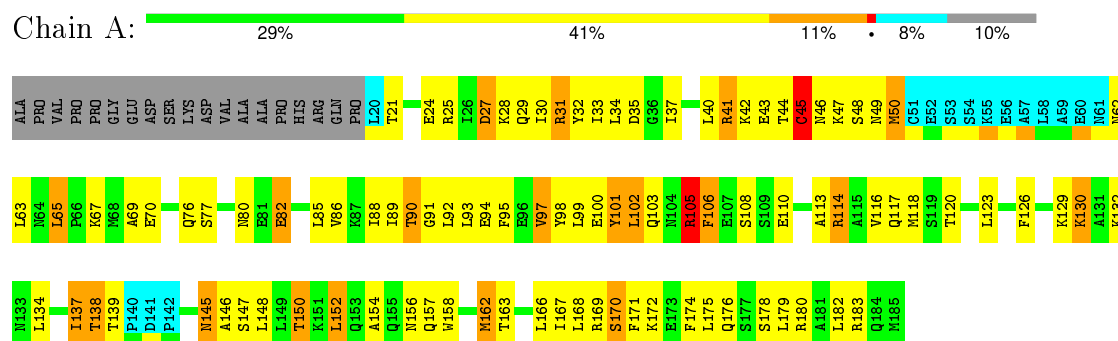
## 4.2.4 Score per residue for model 4

### • Molecule 1: INTERLEUKIN-6



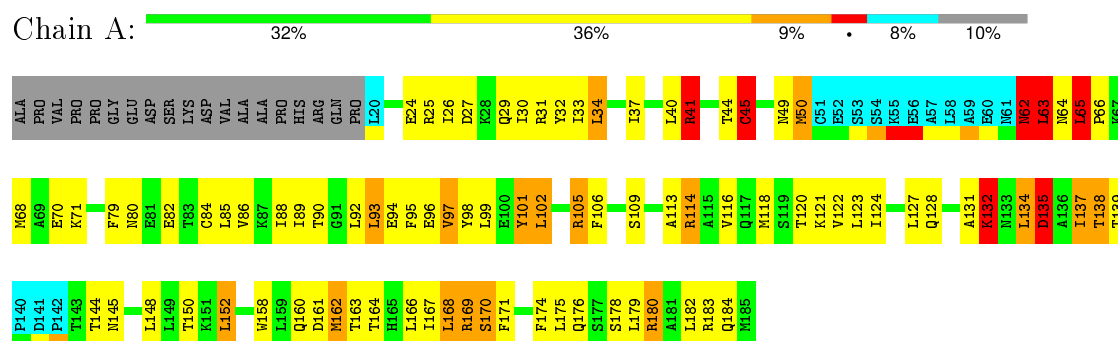
### 4.2.5 Score per residue for model 5

#### • Molecule 1: INTERLEUKIN-6



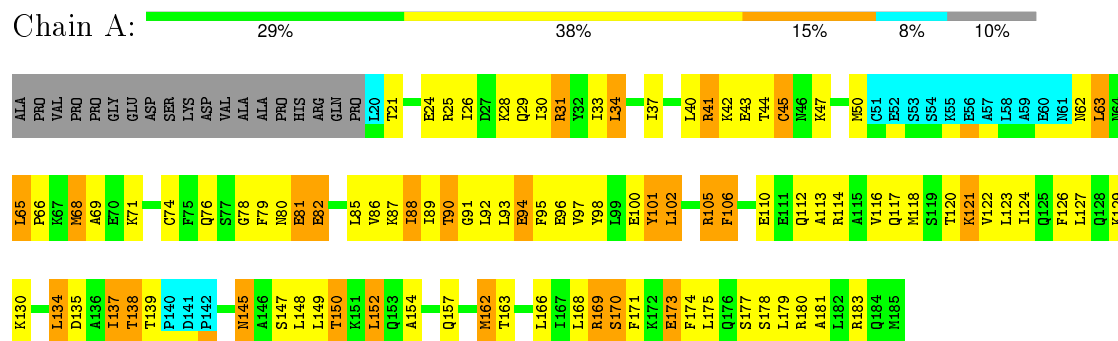
### 4.2.6 Score per residue for model 6

#### • Molecule 1: INTERLEUKIN-6



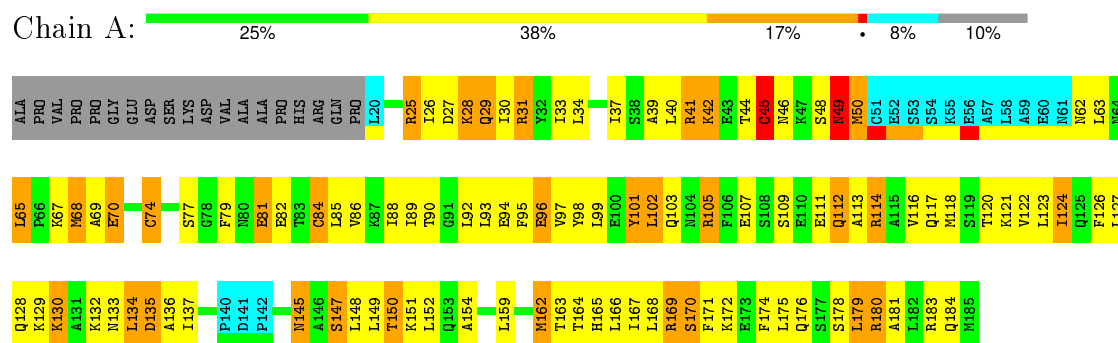
### 4.2.7 Score per residue for model 7

#### • Molecule 1: INTERLEUKIN-6



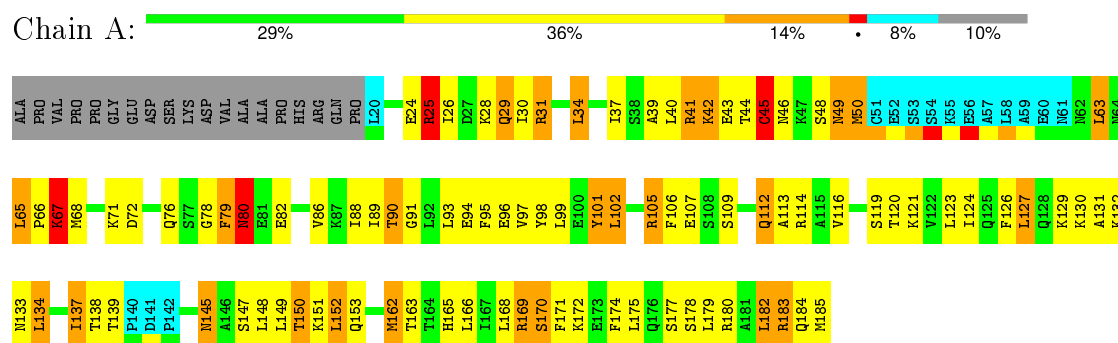
### 4.2.8 Score per residue for model 8

- Molecule 1: INTERLEUKIN-6



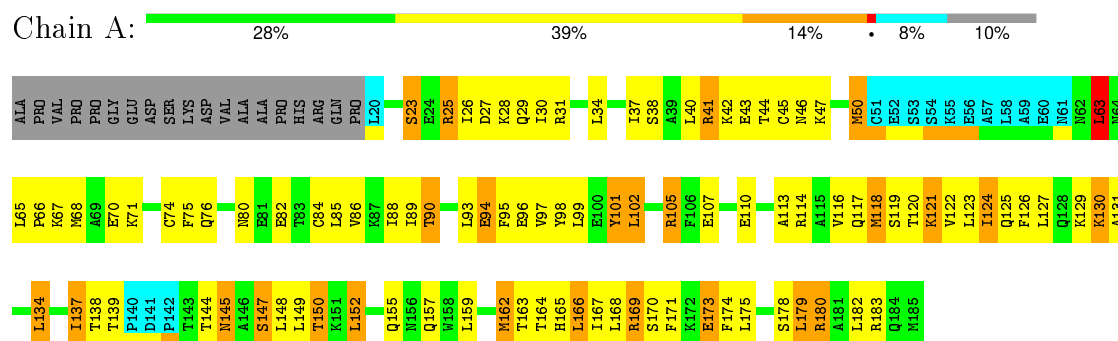
### 4.2.9 Score per residue for model 9

- Molecule 1: INTERLEUKIN-6



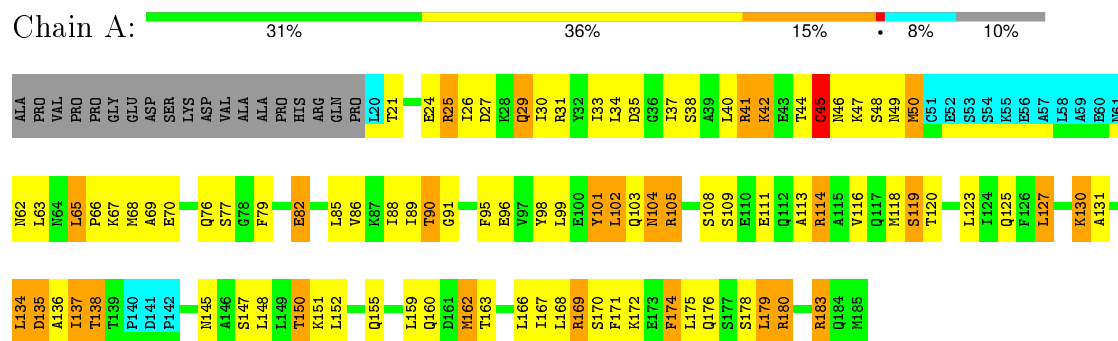
### 4.2.11 Score per residue for model 11

- Molecule 1: INTERLEUKIN-6



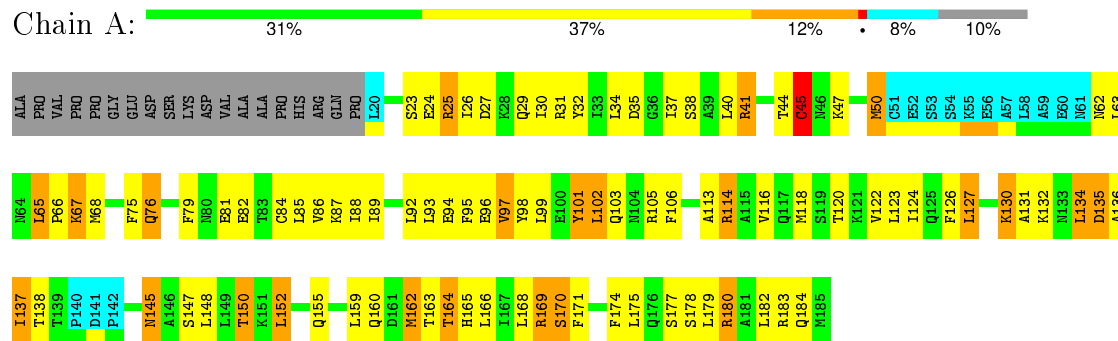
### 4.2.12 Score per residue for model 12

- Molecule 1: INTERLEUKIN-6



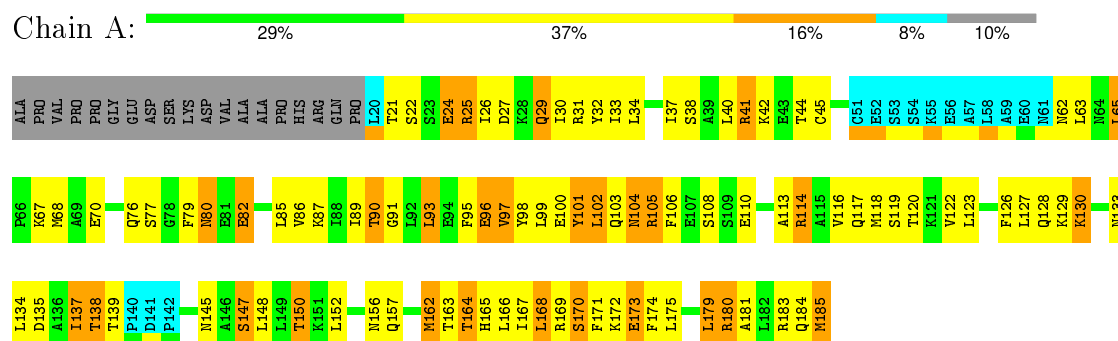
### 4.2.13 Score per residue for model 13

- Molecule 1: INTERLEUKIN-6



### 4.2.14 Score per residue for model 14

- Molecule 1: INTERLEUKIN-6



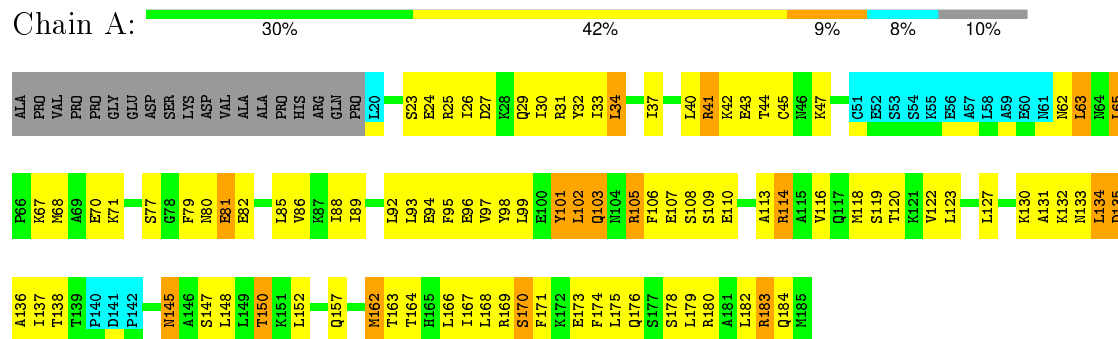
### 4.2.15 Score per residue for model 15

- Molecule 1: INTERLEUKIN-6



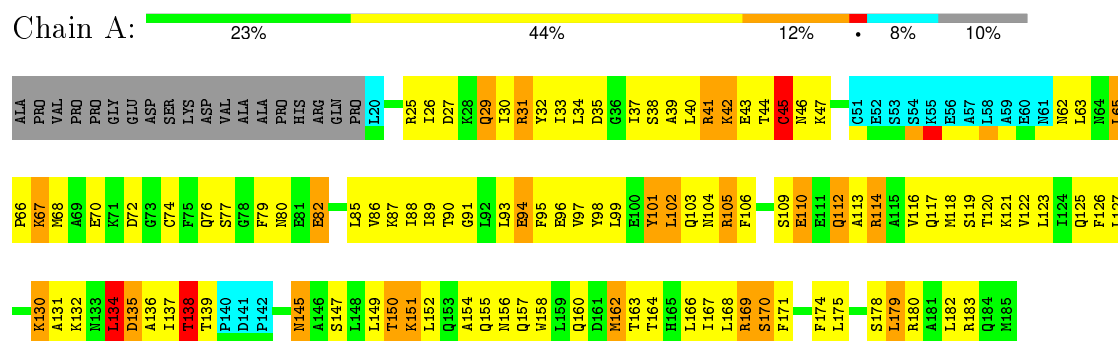
### 4.2.16 Score per residue for model 16

- Molecule 1: INTERLEUKIN-6



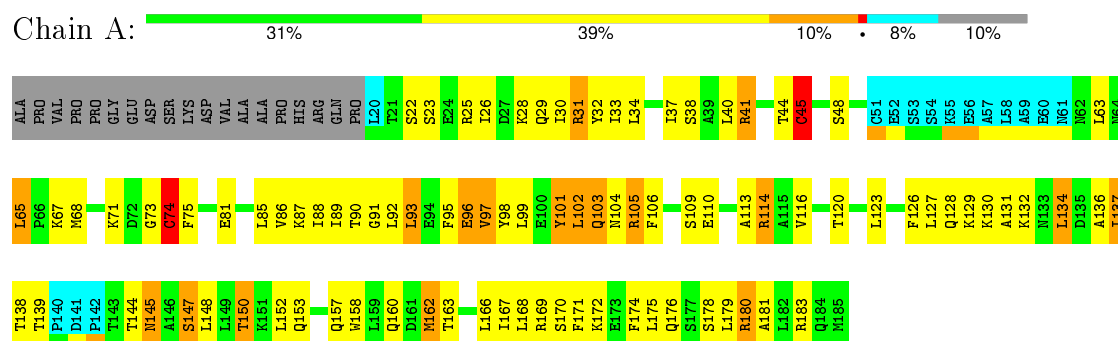
## 4.2.17 Score per residue for model 17

- Molecule 1: INTERLEUKIN-6



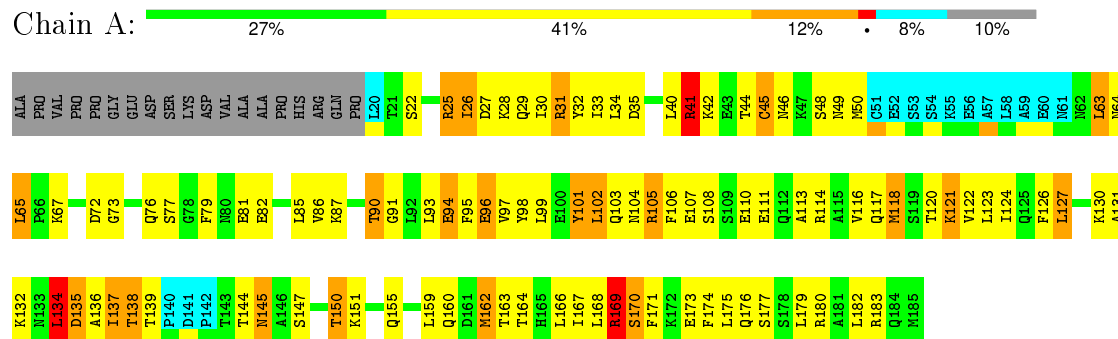
## 4.2.18 Score per residue for model 18

- Molecule 1: INTERLEUKIN-6



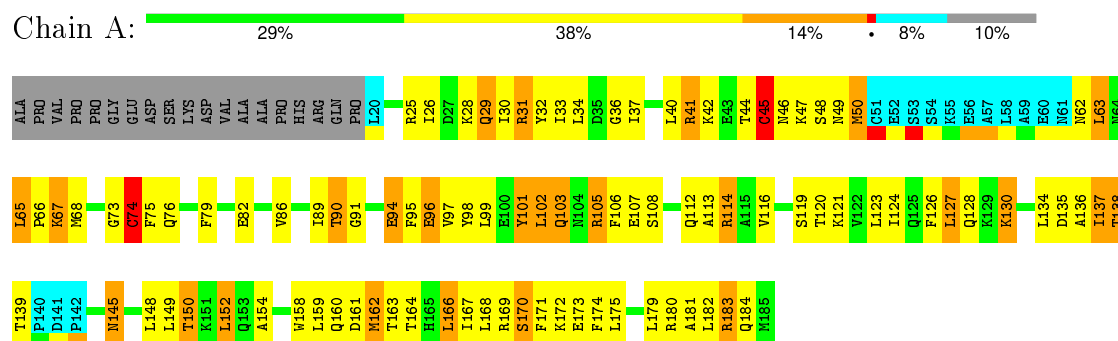
## 4.2.19 Score per residue for model 19

- Molecule 1: INTERLEUKIN-6



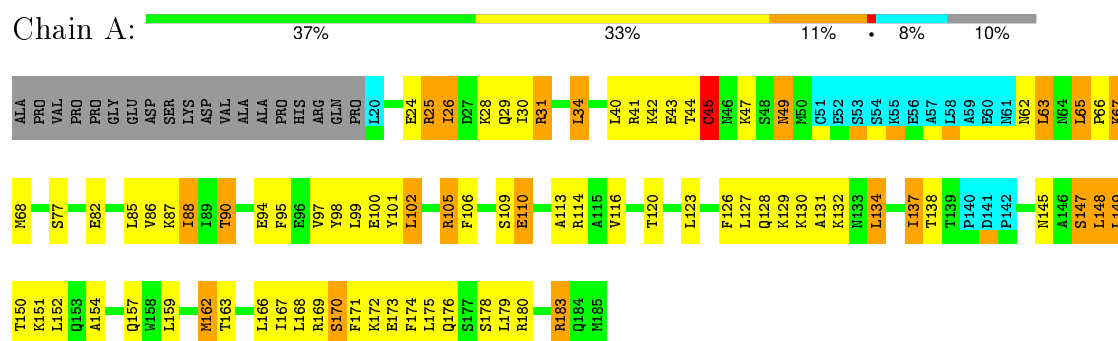
### 4.2.20 Score per residue for model 20

- Molecule 1: INTERLEUKIN-6



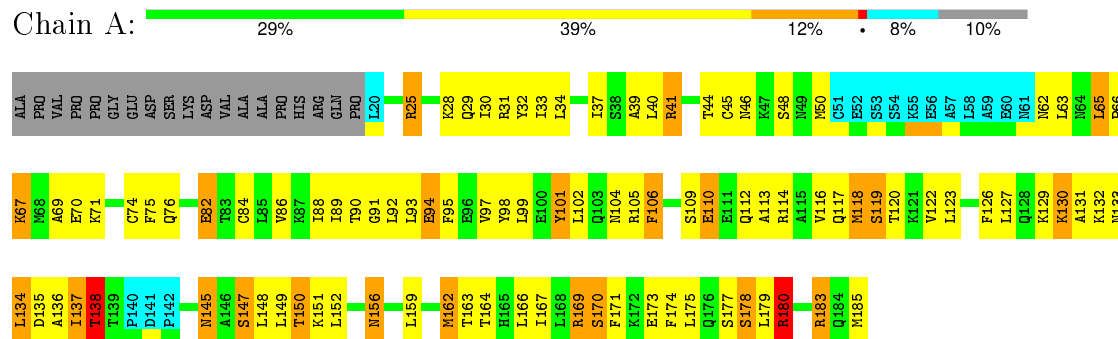
### 4.2.21 Score per residue for model 21

- Molecule 1: INTERLEUKIN-6



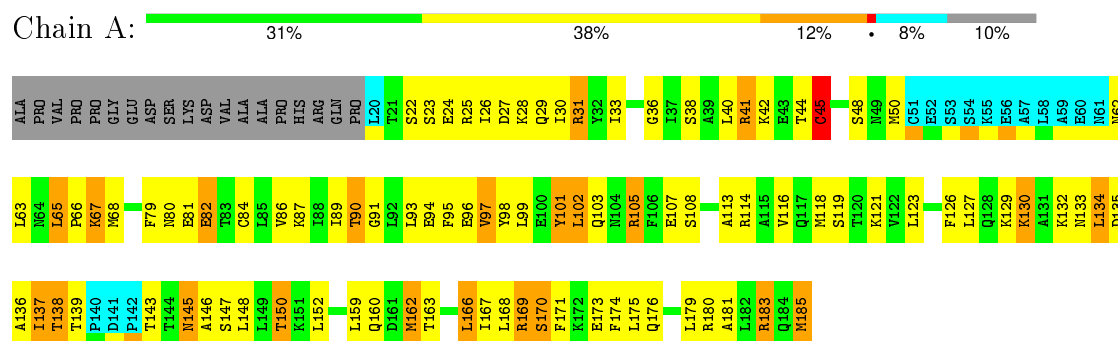
### 4.2.22 Score per residue for model 22

- Molecule 1: INTERLEUKIN-6



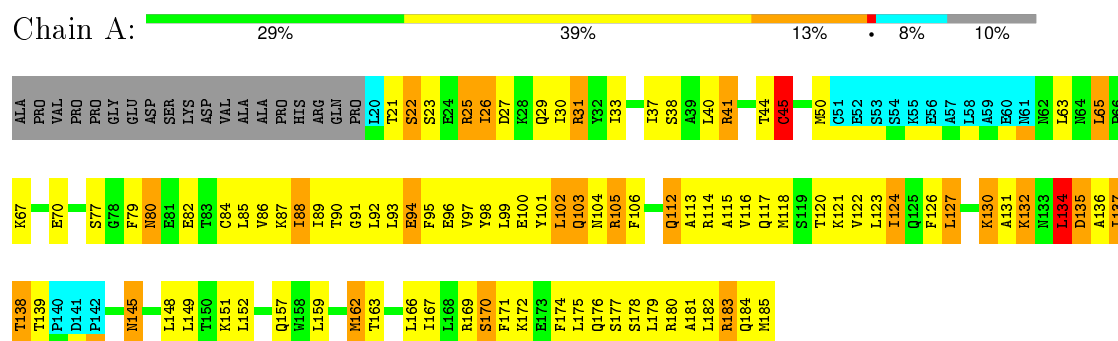
### 4.2.23 Score per residue for model 23

- Molecule 1: INTERLEUKIN-6



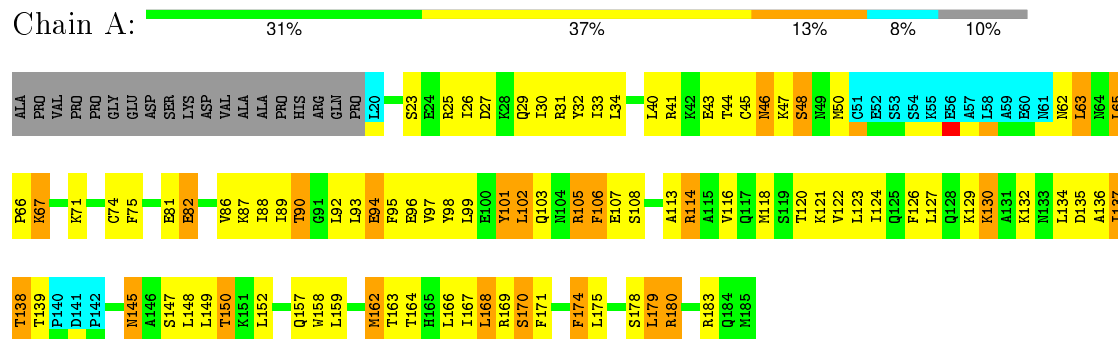
### 4.2.24 Score per residue for model 24

- Molecule 1: INTERLEUKIN-6



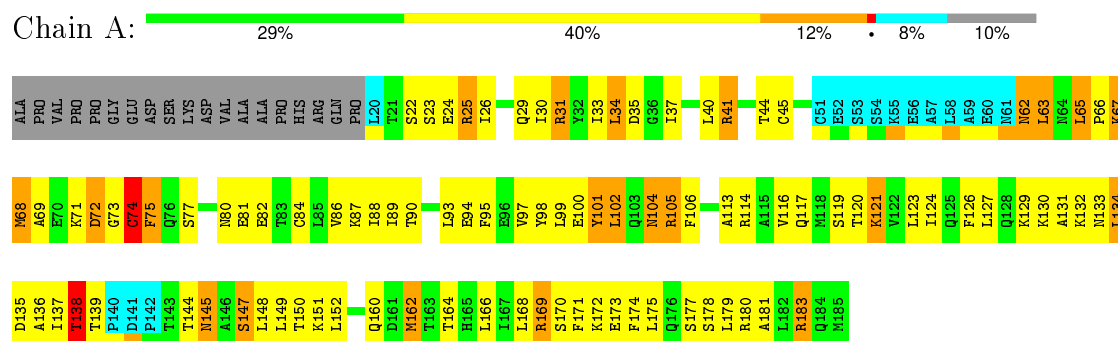
### 4.2.25 Score per residue for model 25

- Molecule 1: INTERLEUKIN-6



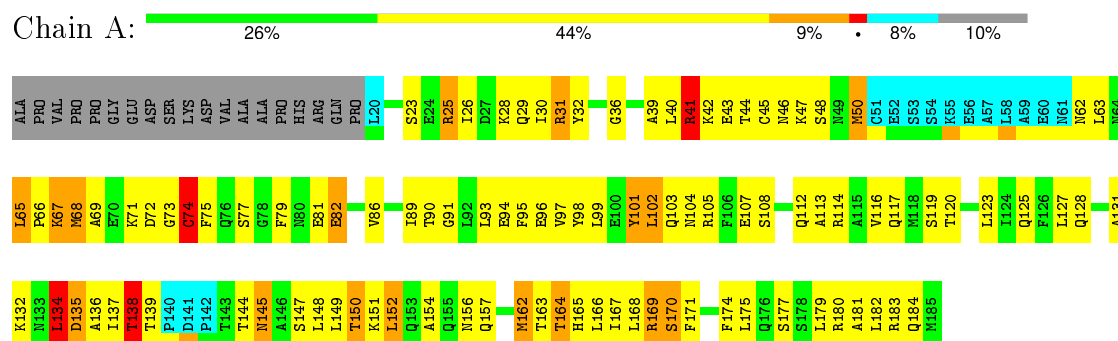
### 4.2.26 Score per residue for model 26

- Molecule 1: INTERLEUKIN-6



### 4.2.29 Score per residue for model 29

- Molecule 1: INTERLEUKIN-6



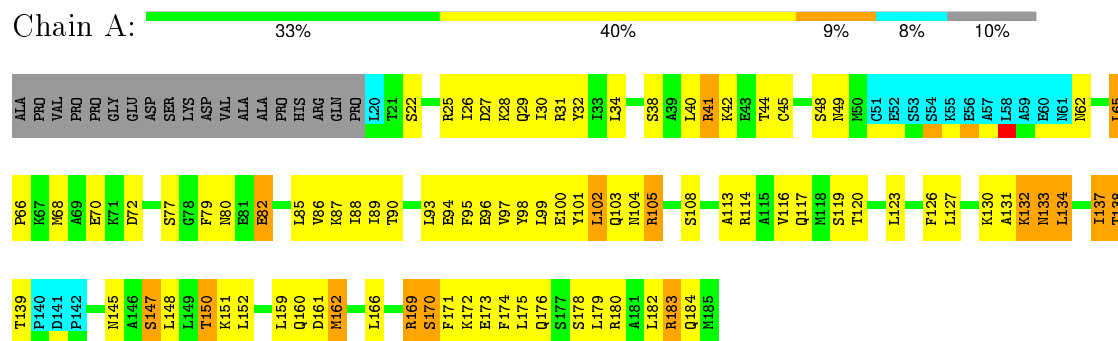
### 4.2.30 Score per residue for model 30

- Molecule 1: INTERLEUKIN-6



### 4.2.31 Score per residue for model 31

- Molecule 1: INTERLEUKIN-6



- Molecule 1: INTERLEUKIN-6

Chain A:

22% 46% 11% 8% 10%

ALA PRO VAL PRO PRO GLY GLU ASP SER LYS ASP VAL ALA PRO PRO ARG HIS GLN LYS PRO E24 R25 R28 Q29 I30 R31 Y32 I33 L34 I37 L40 R41 R42 E43 Y44 Q45 N46 K47 S48 N49 M50 Q51 E52 S53 S54 R55 E56 A57 L58 A59 E60 E61 M62 L63 N64 L65 P66 K67 M68 A69 E70 K71 D72 G73 C74 F75 G76 S77 F79 N80 E81 E82 L85 R86 K87 I88 R89 T90 G91 E92 E94 F95 E96 Y97 Y98 L99 E100 Y101 L102 R105 E106 F106 S109 E110 E111 Q112 A113 R114 A115 V116 Q117 M118 S119 T120 K121 V122 L123 I124 Q125 F126 L127 K130 A131 K132 M133 L134 D135 A136 I137 T138 T139 P140 D141 P142 N145 A146 S147 L148 L149 T150 K151 L152 Q153 A154 M158 L159 Q160 D161 M162 T163 T164 L165 L166 L167 L168 R169 S170 F171 K172 E173 F174 L175 S178 L179 R180 A181 L182 R183 Q184 M185

## 5 Refinement protocol and experimental data overview

The models were refined using the following method: *DISTANCE GEOMETRY AND SIMULATED ANNEALING..*

Of the 75 calculated structures, 32 were deposited, based on the following criterion: *LEAST RESTRAINT VIOLATION*.

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

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

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

## 6 Model quality

### 6.1 Standard geometry

There are no covalent bond-length or bond-angle outliers.

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

| Mol | Chain | Chirality | Planarity |
|-----|-------|-----------|-----------|
| 1   | A     | 0.0±0.0   | 8.0±0.2   |
| All | All   | 0         | 255       |

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

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

| Mol | Chain | Res | Type | Group     | Models (Total) |
|-----|-------|-----|------|-----------|----------------|
| 1   | A     | 183 | ARG  | Sidechain | 32             |
| 1   | A     | 180 | ARG  | Sidechain | 32             |
| 1   | A     | 41  | ARG  | Sidechain | 32             |
| 1   | A     | 105 | ARG  | Sidechain | 32             |
| 1   | A     | 114 | ARG  | Sidechain | 32             |
| 1   | A     | 169 | ARG  | Sidechain | 32             |
| 1   | A     | 31  | ARG  | Sidechain | 32             |
| 1   | A     | 25  | ARG  | Sidechain | 31             |

### 6.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes |
|-----|-------|-------|----------|----------|---------|
| 1   | A     | 1221  | 1248     | 1248     | 91±10   |
| All | All   | 39072 | 39936    | 39936    | 2915    |

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 37.

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

| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:26:ILE:HG23  | 1:A:123:LEU:HD12 | 1.08     | 1.22        | 14     | 16    |
| 1:A:63:LEU:HD11  | 1:A:65:LEU:HD23  | 1.07     | 1.25        | 11     | 2     |
| 1:A:63:LEU:HD21  | 1:A:163:THR:HG23 | 1.02     | 1.32        | 6      | 3     |
| 1:A:63:LEU:HD23  | 1:A:152:LEU:HD22 | 0.95     | 1.37        | 6      | 1     |
| 1:A:101:TYR:CE1  | 1:A:152:LEU:HD12 | 0.95     | 1.97        | 15     | 4     |
| 1:A:99:LEU:HD11  | 1:A:120:THR:HG21 | 0.94     | 1.38        | 16     | 12    |
| 1:A:40:LEU:HD11  | 1:A:116:VAL:HG11 | 0.93     | 1.41        | 8      | 3     |
| 1:A:89:ILE:HG21  | 1:A:137:ILE:HD12 | 0.92     | 1.37        | 6      | 6     |
| 1:A:97:VAL:HG11  | 1:A:145:ASN:ND2  | 0.91     | 1.80        | 24     | 18    |
| 1:A:90:THR:HG23  | 1:A:137:ILE:CG2  | 0.90     | 1.96        | 7      | 14    |
| 1:A:89:ILE:HD12  | 1:A:137:ILE:HD13 | 0.88     | 1.43        | 22     | 12    |
| 1:A:102:LEU:CD2  | 1:A:164:THR:HG23 | 0.88     | 1.98        | 32     | 11    |
| 1:A:63:LEU:HD11  | 1:A:163:THR:HG23 | 0.88     | 1.45        | 16     | 7     |
| 1:A:29:GLN:CB    | 1:A:123:LEU:HD21 | 0.87     | 1.98        | 8      | 15    |
| 1:A:30:ILE:HD13  | 1:A:123:LEU:HD23 | 0.87     | 1.46        | 2      | 1     |
| 1:A:63:LEU:CD1   | 1:A:166:LEU:HD22 | 0.86     | 2.00        | 32     | 1     |
| 1:A:102:LEU:O    | 1:A:113:ALA:HB1  | 0.86     | 1.70        | 8      | 32    |
| 1:A:30:ILE:HD13  | 1:A:123:LEU:HD13 | 0.86     | 1.46        | 32     | 2     |
| 1:A:94:GLU:O     | 1:A:97:VAL:HG12  | 0.86     | 1.71        | 2      | 21    |
| 1:A:40:LEU:CD1   | 1:A:116:VAL:HG11 | 0.85     | 2.01        | 2      | 17    |
| 1:A:39:ALA:HB1   | 1:A:112:GLN:OE1  | 0.85     | 1.71        | 15     | 3     |
| 1:A:74:CYS:SG    | 1:A:181:ALA:HB2  | 0.85     | 2.12        | 26     | 4     |
| 1:A:147:SER:O    | 1:A:150:THR:HG22 | 0.85     | 1.70        | 21     | 18    |
| 1:A:127:LEU:O    | 1:A:131:ALA:HB2  | 0.84     | 1.72        | 15     | 15    |
| 1:A:86:VAL:HG22  | 1:A:137:ILE:HD11 | 0.84     | 1.48        | 12     | 7     |
| 1:A:30:ILE:CD1   | 1:A:123:LEU:HD13 | 0.84     | 2.02        | 32     | 3     |
| 1:A:29:GLN:HB3   | 1:A:123:LEU:HD21 | 0.84     | 1.50        | 24     | 20    |
| 1:A:89:ILE:HG23  | 1:A:137:ILE:HG23 | 0.84     | 1.47        | 16     | 2     |
| 1:A:118:MET:O    | 1:A:122:VAL:HG23 | 0.83     | 1.74        | 27     | 16    |
| 1:A:65:LEU:HD21  | 1:A:166:LEU:CD2  | 0.83     | 2.02        | 8      | 5     |
| 1:A:63:LEU:CD1   | 1:A:65:LEU:HD23  | 0.83     | 2.03        | 11     | 2     |
| 1:A:63:LEU:CD2   | 1:A:163:THR:HG23 | 0.83     | 2.03        | 32     | 1     |
| 1:A:102:LEU:HD11 | 1:A:167:ILE:HG21 | 0.82     | 1.50        | 21     | 18    |
| 1:A:85:LEU:O     | 1:A:88:ILE:HG22  | 0.82     | 1.75        | 7      | 3     |
| 1:A:178:SER:O    | 1:A:182:LEU:HD12 | 0.82     | 1.74        | 15     | 2     |
| 1:A:116:VAL:O    | 1:A:120:THR:HG23 | 0.82     | 1.75        | 19     | 14    |
| 1:A:166:LEU:O    | 1:A:166:LEU:HD13 | 0.82     | 1.74        | 17     | 5     |
| 1:A:30:ILE:CD1   | 1:A:123:LEU:HD23 | 0.82     | 2.05        | 2      | 1     |
| 1:A:89:ILE:CG2   | 1:A:137:ILE:HG23 | 0.82     | 2.05        | 8      | 2     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:161:ASP:O    | 1:A:164:THR:HG22 | 0.82     | 1.75        | 20     | 3     |
| 1:A:89:ILE:HD13  | 1:A:137:ILE:HD13 | 0.81     | 1.50        | 31     | 3     |
| 1:A:30:ILE:HG23  | 1:A:175:LEU:HD22 | 0.81     | 1.51        | 3      | 23    |
| 1:A:86:VAL:HG13  | 1:A:137:ILE:HG13 | 0.81     | 1.51        | 5      | 14    |
| 1:A:86:VAL:HG13  | 1:A:137:ILE:CG1  | 0.81     | 2.04        | 3      | 14    |
| 1:A:99:LEU:HD11  | 1:A:120:THR:CG2  | 0.81     | 2.05        | 24     | 10    |
| 1:A:89:ILE:HD13  | 1:A:137:ILE:CD1  | 0.81     | 2.05        | 24     | 3     |
| 1:A:29:GLN:HB2   | 1:A:123:LEU:HD21 | 0.81     | 1.51        | 32     | 9     |
| 1:A:29:GLN:CB    | 1:A:123:LEU:HD11 | 0.81     | 2.05        | 4      | 12    |
| 1:A:98:TYR:OH    | 1:A:148:LEU:HD21 | 0.80     | 1.76        | 1      | 21    |
| 1:A:62:ASN:O     | 1:A:63:LEU:HD12  | 0.80     | 1.76        | 32     | 2     |
| 1:A:133:ASN:C    | 1:A:134:LEU:HD22 | 0.80     | 1.97        | 15     | 1     |
| 1:A:93:LEU:HD22  | 1:A:139:THR:OG1  | 0.79     | 1.77        | 14     | 7     |
| 1:A:33:ILE:HD11  | 1:A:123:LEU:HD12 | 0.79     | 1.55        | 8      | 3     |
| 1:A:40:LEU:CD1   | 1:A:116:VAL:HG21 | 0.79     | 2.07        | 29     | 7     |
| 1:A:162:MET:SD   | 1:A:166:LEU:HD23 | 0.78     | 2.18        | 6      | 2     |
| 1:A:96:GLU:HA    | 1:A:99:LEU:HD12  | 0.78     | 1.55        | 29     | 20    |
| 1:A:93:LEU:HD13  | 1:A:139:THR:OG1  | 0.78     | 1.77        | 32     | 6     |
| 1:A:82:GLU:O     | 1:A:86:VAL:HG23  | 0.78     | 1.78        | 19     | 28    |
| 1:A:127:LEU:O    | 1:A:127:LEU:HD13 | 0.77     | 1.79        | 6      | 3     |
| 1:A:166:LEU:HD13 | 1:A:166:LEU:O    | 0.77     | 1.79        | 30     | 5     |
| 1:A:179:LEU:HD12 | 1:A:180:ARG:N    | 0.77     | 1.93        | 18     | 3     |
| 1:A:164:THR:O    | 1:A:168:LEU:HD12 | 0.77     | 1.80        | 13     | 10    |
| 1:A:40:LEU:HD11  | 1:A:116:VAL:HG21 | 0.77     | 1.54        | 23     | 7     |
| 1:A:90:THR:HA    | 1:A:93:LEU:HD12  | 0.77     | 1.54        | 4      | 16    |
| 1:A:97:VAL:HG23  | 1:A:145:ASN:ND2  | 0.76     | 1.96        | 21     | 1     |
| 1:A:102:LEU:HD21 | 1:A:164:THR:HG23 | 0.76     | 1.55        | 3      | 10    |
| 1:A:89:ILE:HD12  | 1:A:137:ILE:CD1  | 0.76     | 2.10        | 15     | 10    |
| 1:A:89:ILE:HD11  | 1:A:127:LEU:HD12 | 0.76     | 1.58        | 24     | 2     |
| 1:A:63:LEU:HB2   | 1:A:166:LEU:HD22 | 0.75     | 1.57        | 5      | 3     |
| 1:A:90:THR:HG23  | 1:A:137:ILE:HG22 | 0.75     | 1.59        | 9      | 4     |
| 1:A:63:LEU:HD11  | 1:A:65:LEU:CD2   | 0.75     | 2.10        | 11     | 2     |
| 1:A:121:LYS:HA   | 1:A:124:ILE:HD12 | 0.75     | 1.57        | 26     | 8     |
| 1:A:65:LEU:HD21  | 1:A:166:LEU:HD22 | 0.75     | 1.58        | 24     | 1     |
| 1:A:85:LEU:HD21  | 1:A:127:LEU:HD21 | 0.74     | 1.54        | 6      | 2     |
| 1:A:63:LEU:HD11  | 1:A:163:THR:CG2  | 0.74     | 2.11        | 16     | 3     |
| 1:A:86:VAL:HG22  | 1:A:134:LEU:HD21 | 0.74     | 1.57        | 16     | 2     |
| 1:A:89:ILE:HD11  | 1:A:127:LEU:CG   | 0.74     | 2.12        | 13     | 2     |
| 1:A:148:LEU:CD1  | 1:A:152:LEU:HD21 | 0.74     | 2.12        | 21     | 11    |
| 1:A:137:ILE:HG22 | 1:A:137:ILE:O    | 0.74     | 1.82        | 32     | 11    |
| 1:A:162:MET:CE   | 1:A:166:LEU:HD23 | 0.74     | 2.11        | 6      | 6     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:37:ILE:CD1   | 1:A:116:VAL:HG21 | 0.74     | 2.13        | 8      | 16    |
| 1:A:26:ILE:CG2   | 1:A:123:LEU:HD12 | 0.74     | 2.10        | 27     | 4     |
| 1:A:89:ILE:HG21  | 1:A:137:ILE:CD1  | 0.73     | 2.13        | 6      | 6     |
| 1:A:89:ILE:CD1   | 1:A:137:ILE:HD13 | 0.73     | 2.13        | 11     | 12    |
| 1:A:149:LEU:HD12 | 1:A:152:LEU:HD12 | 0.73     | 1.57        | 21     | 9     |
| 1:A:92:LEU:HD22  | 1:A:120:THR:OG1  | 0.73     | 1.82        | 8      | 2     |
| 1:A:175:LEU:O    | 1:A:179:LEU:HD12 | 0.73     | 1.82        | 20     | 11    |
| 1:A:137:ILE:O    | 1:A:137:ILE:HG22 | 0.73     | 1.83        | 26     | 15    |
| 1:A:99:LEU:HD13  | 1:A:120:THR:OG1  | 0.73     | 1.83        | 29     | 13    |
| 1:A:37:ILE:HD11  | 1:A:116:VAL:HG21 | 0.73     | 1.59        | 17     | 6     |
| 1:A:98:TYR:CZ    | 1:A:148:LEU:HD21 | 0.72     | 2.19        | 29     | 21    |
| 1:A:26:ILE:HG23  | 1:A:123:LEU:CD1  | 0.72     | 2.12        | 27     | 6     |
| 1:A:148:LEU:HD13 | 1:A:152:LEU:HD21 | 0.72     | 1.58        | 30     | 1     |
| 1:A:88:ILE:HD12  | 1:A:178:SER:CB   | 0.72     | 2.14        | 22     | 8     |
| 1:A:29:GLN:HB3   | 1:A:123:LEU:HD11 | 0.72     | 1.58        | 23     | 13    |
| 1:A:93:LEU:HD13  | 1:A:139:THR:CB   | 0.72     | 2.14        | 19     | 6     |
| 1:A:30:ILE:HB    | 1:A:179:LEU:HD11 | 0.72     | 1.61        | 24     | 4     |
| 1:A:82:GLU:CG    | 1:A:134:LEU:HD11 | 0.72     | 2.15        | 1      | 4     |
| 1:A:89:ILE:HD13  | 1:A:137:ILE:HD11 | 0.71     | 1.61        | 24     | 1     |
| 1:A:145:ASN:ND2  | 1:A:148:LEU:HD23 | 0.71     | 2.01        | 1      | 5     |
| 1:A:65:LEU:HD21  | 1:A:166:LEU:HD23 | 0.71     | 1.61        | 8      | 3     |
| 1:A:29:GLN:HB2   | 1:A:123:LEU:HD11 | 0.71     | 1.63        | 11     | 11    |
| 1:A:137:ILE:N    | 1:A:137:ILE:HD12 | 0.70     | 2.01        | 4      | 13    |
| 1:A:88:ILE:HD12  | 1:A:178:SER:OG   | 0.70     | 1.86        | 9      | 7     |
| 1:A:99:LEU:HD13  | 1:A:117:GLN:HA   | 0.70     | 1.62        | 22     | 7     |
| 1:A:89:ILE:HG13  | 1:A:127:LEU:HD23 | 0.70     | 1.62        | 16     | 1     |
| 1:A:101:TYR:CE2  | 1:A:163:THR:HG21 | 0.70     | 2.21        | 19     | 19    |
| 1:A:88:ILE:HD13  | 1:A:178:SER:HB2  | 0.70     | 1.64        | 6      | 4     |
| 1:A:26:ILE:HG23  | 1:A:123:LEU:HD11 | 0.70     | 1.61        | 28     | 1     |
| 1:A:85:LEU:HD23  | 1:A:134:LEU:HD13 | 0.69     | 1.63        | 17     | 4     |
| 1:A:69:ALA:HB3   | 1:A:74:CYS:SG    | 0.69     | 2.27        | 32     | 1     |
| 1:A:44:THR:O     | 1:A:44:THR:HG23  | 0.69     | 1.88        | 8      | 8     |
| 1:A:63:LEU:HD12  | 1:A:166:LEU:HB3  | 0.69     | 1.64        | 23     | 6     |
| 1:A:44:THR:HG23  | 1:A:44:THR:O     | 0.69     | 1.86        | 4      | 9     |
| 1:A:88:ILE:HD11  | 1:A:178:SER:HB3  | 0.69     | 1.64        | 21     | 1     |
| 1:A:65:LEU:N     | 1:A:66:PRO:CD    | 0.69     | 2.55        | 9      | 20    |
| 1:A:113:ALA:O    | 1:A:116:VAL:HG12 | 0.69     | 1.87        | 9      | 4     |
| 1:A:99:LEU:CD1   | 1:A:120:THR:HG21 | 0.69     | 2.18        | 8      | 5     |
| 1:A:88:ILE:HD11  | 1:A:178:SER:CB   | 0.69     | 2.17        | 7      | 3     |
| 1:A:162:MET:HE3  | 1:A:166:LEU:HD23 | 0.69     | 1.63        | 3      | 4     |
| 1:A:63:LEU:HD22  | 1:A:152:LEU:CD2  | 0.69     | 2.18        | 27     | 2     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:23:SER:O     | 1:A:26:ILE:HG22  | 0.68     | 1.88        | 13     | 2     |
| 1:A:37:ILE:HG23  | 1:A:168:LEU:CD1  | 0.68     | 2.18        | 11     | 2     |
| 1:A:131:ALA:HB3  | 1:A:135:ASP:HB3  | 0.68     | 1.65        | 1      | 2     |
| 1:A:133:ASN:O    | 1:A:134:LEU:HD12 | 0.68     | 1.89        | 4      | 2     |
| 1:A:27:ASP:CG    | 1:A:179:LEU:HD23 | 0.68     | 2.08        | 28     | 4     |
| 1:A:40:LEU:HD11  | 1:A:116:VAL:CG1  | 0.68     | 2.17        | 9      | 5     |
| 1:A:85:LEU:O     | 1:A:89:ILE:HD12  | 0.68     | 1.87        | 24     | 1     |
| 1:A:128:GLN:CD   | 1:A:137:ILE:HG21 | 0.68     | 2.09        | 2      | 2     |
| 1:A:40:LEU:O     | 1:A:44:THR:HG22  | 0.68     | 1.89        | 4      | 18    |
| 1:A:97:VAL:HG11  | 1:A:145:ASN:HD21 | 0.67     | 1.48        | 26     | 15    |
| 1:A:65:LEU:HD21  | 1:A:166:LEU:HD12 | 0.67     | 1.64        | 30     | 3     |
| 1:A:27:ASP:OD1   | 1:A:179:LEU:HD23 | 0.67     | 1.88        | 17     | 7     |
| 1:A:26:ILE:HD11  | 1:A:126:PHE:C    | 0.67     | 2.09        | 7      | 3     |
| 1:A:148:LEU:HD11 | 1:A:152:LEU:HD21 | 0.67     | 1.66        | 8      | 12    |
| 1:A:30:ILE:CG2   | 1:A:179:LEU:HD11 | 0.67     | 2.19        | 1      | 9     |
| 1:A:137:ILE:HG22 | 1:A:138:THR:N    | 0.67     | 2.05        | 24     | 3     |
| 1:A:88:ILE:HD13  | 1:A:178:SER:CB   | 0.67     | 2.20        | 10     | 5     |
| 1:A:137:ILE:HD12 | 1:A:137:ILE:N    | 0.67     | 2.05        | 14     | 11    |
| 1:A:155:GLN:HB3  | 1:A:159:LEU:HD23 | 0.67     | 1.65        | 12     | 1     |
| 1:A:88:ILE:HD12  | 1:A:178:SER:HB3  | 0.66     | 1.67        | 31     | 6     |
| 1:A:85:LEU:HD13  | 1:A:182:LEU:HD11 | 0.66     | 1.65        | 3      | 2     |
| 1:A:89:ILE:HD11  | 1:A:127:LEU:HB3  | 0.66     | 1.67        | 13     | 3     |
| 1:A:101:TYR:CZ   | 1:A:152:LEU:HD12 | 0.65     | 2.25        | 9      | 3     |
| 1:A:86:VAL:CG1   | 1:A:136:ALA:HB3  | 0.65     | 2.20        | 13     | 2     |
| 1:A:89:ILE:HD11  | 1:A:127:LEU:CB   | 0.65     | 2.21        | 13     | 2     |
| 1:A:30:ILE:CB    | 1:A:179:LEU:HD11 | 0.65     | 2.21        | 24     | 2     |
| 1:A:26:ILE:HD13  | 1:A:127:LEU:HD13 | 0.65     | 1.68        | 16     | 1     |
| 1:A:127:LEU:HD22 | 1:A:130:LYS:HE3  | 0.65     | 1.69        | 4      | 1     |
| 1:A:163:THR:HG22 | 1:A:167:ILE:CD1  | 0.65     | 2.21        | 10     | 4     |
| 1:A:26:ILE:HD13  | 1:A:127:LEU:HG   | 0.65     | 1.67        | 7      | 6     |
| 1:A:106:PHE:CD2  | 1:A:113:ALA:HB2  | 0.65     | 2.27        | 9      | 2     |
| 1:A:131:ALA:HB1  | 1:A:134:LEU:HB2  | 0.65     | 1.68        | 15     | 2     |
| 1:A:40:LEU:HD11  | 1:A:116:VAL:CG2  | 0.65     | 2.22        | 23     | 7     |
| 1:A:62:ASN:HA    | 1:A:166:LEU:HD13 | 0.65     | 1.67        | 2      | 1     |
| 1:A:162:MET:HE2  | 1:A:166:LEU:HD23 | 0.65     | 1.65        | 9      | 2     |
| 1:A:139:THR:HG23 | 1:A:139:THR:O    | 0.64     | 1.92        | 11     | 5     |
| 1:A:88:ILE:HD13  | 1:A:178:SER:OG   | 0.64     | 1.93        | 10     | 2     |
| 1:A:93:LEU:HD13  | 1:A:138:THR:O    | 0.64     | 1.92        | 22     | 3     |
| 1:A:30:ILE:HD13  | 1:A:123:LEU:CD1  | 0.64     | 2.19        | 32     | 3     |
| 1:A:65:LEU:HD11  | 1:A:170:SER:CB   | 0.64     | 2.22        | 26     | 3     |
| 1:A:89:ILE:HG21  | 1:A:137:ILE:HD13 | 0.64     | 1.69        | 26     | 3     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:101:TYR:CD1  | 1:A:149:LEU:HD11 | 0.64     | 2.28        | 25     | 10    |
| 1:A:36:GLY:HA3   | 1:A:116:VAL:HG22 | 0.64     | 1.68        | 23     | 6     |
| 1:A:171:PHE:CD2  | 1:A:175:LEU:HD11 | 0.64     | 2.27        | 7      | 23    |
| 1:A:29:GLN:NE2   | 1:A:122:VAL:HG11 | 0.64     | 2.08        | 6      | 3     |
| 1:A:26:ILE:HD11  | 1:A:126:PHE:HB3  | 0.63     | 1.69        | 26     | 11    |
| 1:A:63:LEU:HD13  | 1:A:166:LEU:HD22 | 0.63     | 1.70        | 32     | 1     |
| 1:A:131:ALA:HB1  | 1:A:134:LEU:CB   | 0.63     | 2.23        | 31     | 3     |
| 1:A:90:THR:HG23  | 1:A:137:ILE:HG23 | 0.63     | 1.69        | 27     | 5     |
| 1:A:39:ALA:HB1   | 1:A:112:GLN:NE2  | 0.63     | 2.07        | 3      | 2     |
| 1:A:82:GLU:HG2   | 1:A:134:LEU:HD11 | 0.63     | 1.69        | 30     | 4     |
| 1:A:99:LEU:HD11  | 1:A:120:THR:OG1  | 0.63     | 1.94        | 27     | 2     |
| 1:A:139:THR:O    | 1:A:139:THR:HG23 | 0.63     | 1.94        | 24     | 3     |
| 1:A:86:VAL:HG13  | 1:A:137:ILE:HG12 | 0.62     | 1.70        | 7      | 5     |
| 1:A:63:LEU:HD12  | 1:A:166:LEU:CB   | 0.62     | 2.24        | 19     | 2     |
| 1:A:131:ALA:HB3  | 1:A:135:ASP:HB2  | 0.62     | 1.70        | 26     | 2     |
| 1:A:82:GLU:HG2   | 1:A:134:LEU:HD21 | 0.62     | 1.71        | 7      | 3     |
| 1:A:65:LEU:HD12  | 1:A:95:PHE:CE1   | 0.62     | 2.29        | 16     | 4     |
| 1:A:62:ASN:HA    | 1:A:166:LEU:HD22 | 0.62     | 1.69        | 26     | 2     |
| 1:A:34:LEU:HD11  | 1:A:175:LEU:HB2  | 0.62     | 1.71        | 10     | 7     |
| 1:A:171:PHE:O    | 1:A:175:LEU:HD12 | 0.62     | 1.93        | 2      | 5     |
| 1:A:39:ALA:HB1   | 1:A:112:GLN:CD   | 0.62     | 2.15        | 10     | 3     |
| 1:A:63:LEU:HB3   | 1:A:65:LEU:HD23  | 0.62     | 1.70        | 23     | 12    |
| 1:A:33:ILE:O     | 1:A:116:VAL:HG23 | 0.62     | 1.93        | 19     | 9     |
| 1:A:93:LEU:HD22  | 1:A:139:THR:HB   | 0.62     | 1.71        | 7      | 4     |
| 1:A:40:LEU:CB    | 1:A:168:LEU:HD21 | 0.62     | 2.25        | 32     | 2     |
| 1:A:63:LEU:HD13  | 1:A:65:LEU:CD2   | 0.61     | 2.25        | 6      | 1     |
| 1:A:37:ILE:HD13  | 1:A:40:LEU:HD12  | 0.61     | 1.71        | 9      | 2     |
| 1:A:150:THR:O    | 1:A:154:ALA:HB2  | 0.61     | 1.96        | 20     | 10    |
| 1:A:148:LEU:HD12 | 1:A:152:LEU:HD11 | 0.61     | 1.73        | 21     | 1     |
| 1:A:86:VAL:HG22  | 1:A:134:LEU:CD2  | 0.61     | 2.26        | 16     | 2     |
| 1:A:40:LEU:HD13  | 1:A:116:VAL:HG11 | 0.61     | 1.72        | 7      | 14    |
| 1:A:123:LEU:O    | 1:A:127:LEU:HD12 | 0.61     | 1.96        | 29     | 3     |
| 1:A:34:LEU:HD11  | 1:A:171:PHE:O    | 0.61     | 1.96        | 9      | 4     |
| 1:A:139:THR:O    | 1:A:139:THR:HG22 | 0.61     | 1.95        | 6      | 1     |
| 1:A:62:ASN:O     | 1:A:166:LEU:HD13 | 0.61     | 1.96        | 32     | 1     |
| 1:A:127:LEU:HD22 | 1:A:130:LYS:CE   | 0.61     | 2.26        | 4      | 1     |
| 1:A:37:ILE:HG23  | 1:A:168:LEU:HD23 | 0.60     | 1.74        | 16     | 2     |
| 1:A:41:ARG:HB2   | 1:A:168:LEU:HD23 | 0.60     | 1.72        | 18     | 1     |
| 1:A:137:ILE:N    | 1:A:137:ILE:CD1  | 0.60     | 2.63        | 22     | 9     |
| 1:A:26:ILE:CG2   | 1:A:182:LEU:HD11 | 0.60     | 2.27        | 29     | 1     |
| 1:A:72:ASP:O     | 1:A:83:THR:HG22  | 0.60     | 1.95        | 30     | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:50:MET:HE1   | 1:A:158:TRP:CE3  | 0.60     | 2.32        | 32     | 1     |
| 1:A:26:ILE:HG13  | 1:A:127:LEU:HD23 | 0.60     | 1.74        | 6      | 1     |
| 1:A:30:ILE:HB    | 1:A:179:LEU:HD21 | 0.60     | 1.72        | 6      | 3     |
| 1:A:163:THR:HG22 | 1:A:167:ILE:HD11 | 0.60     | 1.72        | 10     | 2     |
| 1:A:85:LEU:HD23  | 1:A:134:LEU:HD22 | 0.60     | 1.73        | 11     | 3     |
| 1:A:164:THR:HG22 | 1:A:168:LEU:HD11 | 0.59     | 1.73        | 25     | 4     |
| 1:A:95:PHE:CD2   | 1:A:171:PHE:CZ   | 0.59     | 2.90        | 9      | 10    |
| 1:A:95:PHE:CD2   | 1:A:171:PHE:CE1  | 0.59     | 2.91        | 12     | 20    |
| 1:A:27:ASP:CA    | 1:A:182:LEU:HD13 | 0.59     | 2.27        | 16     | 2     |
| 1:A:135:ASP:O    | 1:A:136:ALA:HB3  | 0.59     | 1.98        | 4      | 15    |
| 1:A:99:LEU:HD21  | 1:A:171:PHE:CE2  | 0.59     | 2.33        | 18     | 5     |
| 1:A:29:GLN:CG    | 1:A:123:LEU:HD11 | 0.59     | 2.28        | 2      | 1     |
| 1:A:89:ILE:HD11  | 1:A:127:LEU:HG   | 0.59     | 1.73        | 13     | 1     |
| 1:A:65:LEU:HD11  | 1:A:170:SER:OG   | 0.59     | 1.98        | 30     | 2     |
| 1:A:33:ILE:HD13  | 1:A:120:THR:HG22 | 0.59     | 1.74        | 14     | 3     |
| 1:A:137:ILE:N    | 1:A:137:ILE:HD13 | 0.59     | 2.13        | 6      | 4     |
| 1:A:137:ILE:CD1  | 1:A:137:ILE:N    | 0.59     | 2.66        | 2      | 19    |
| 1:A:26:ILE:HD12  | 1:A:127:LEU:HG   | 0.59     | 1.74        | 29     | 4     |
| 1:A:95:PHE:CD1   | 1:A:171:PHE:CZ   | 0.59     | 2.91        | 15     | 4     |
| 1:A:93:LEU:HD11  | 1:A:137:ILE:CG2  | 0.59     | 2.28        | 10     | 1     |
| 1:A:95:PHE:CZ    | 1:A:174:PHE:CD2  | 0.58     | 2.90        | 31     | 3     |
| 1:A:131:ALA:HB1  | 1:A:134:LEU:HB3  | 0.58     | 1.75        | 13     | 7     |
| 1:A:127:LEU:HD23 | 1:A:130:LYS:HE3  | 0.58     | 1.75        | 25     | 1     |
| 1:A:37:ILE:HG23  | 1:A:168:LEU:HD22 | 0.58     | 1.74        | 20     | 2     |
| 1:A:95:PHE:CG    | 1:A:171:PHE:CE1  | 0.58     | 2.92        | 15     | 3     |
| 1:A:63:LEU:HD11  | 1:A:163:THR:HA   | 0.58     | 1.75        | 21     | 3     |
| 1:A:26:ILE:HG12  | 1:A:123:LEU:HD13 | 0.58     | 1.76        | 16     | 3     |
| 1:A:89:ILE:CG2   | 1:A:137:ILE:HD12 | 0.58     | 2.28        | 16     | 2     |
| 1:A:86:VAL:CG2   | 1:A:134:LEU:HD13 | 0.58     | 2.29        | 24     | 1     |
| 1:A:26:ILE:HG13  | 1:A:123:LEU:HD13 | 0.58     | 1.74        | 13     | 1     |
| 1:A:179:LEU:C    | 1:A:179:LEU:HD12 | 0.57     | 2.19        | 22     | 2     |
| 1:A:149:LEU:HA   | 1:A:152:LEU:HD12 | 0.57     | 1.75        | 24     | 6     |
| 1:A:37:ILE:HD12  | 1:A:168:LEU:HD23 | 0.57     | 1.75        | 5      | 6     |
| 1:A:137:ILE:O    | 1:A:137:ILE:CG2  | 0.57     | 2.53        | 19     | 14    |
| 1:A:40:LEU:O     | 1:A:168:LEU:HD13 | 0.57     | 1.98        | 7      | 3     |
| 1:A:171:PHE:CD1  | 1:A:175:LEU:HD11 | 0.57     | 2.34        | 17     | 7     |
| 1:A:33:ILE:HG23  | 1:A:120:THR:OG1  | 0.57     | 2.00        | 26     | 6     |
| 1:A:50:MET:CE    | 1:A:158:TRP:CE3  | 0.57     | 2.88        | 32     | 1     |
| 1:A:166:LEU:C    | 1:A:166:LEU:HD23 | 0.57     | 2.18        | 24     | 1     |
| 1:A:63:LEU:CG    | 1:A:65:LEU:HD23  | 0.57     | 2.30        | 26     | 2     |
| 1:A:37:ILE:HG23  | 1:A:168:LEU:HD12 | 0.57     | 1.74        | 11     | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:37:ILE:HD13  | 1:A:116:VAL:HG21 | 0.56     | 1.77        | 8      | 1     |
| 1:A:99:LEU:HD22  | 1:A:117:GLN:HA   | 0.56     | 1.75        | 27     | 2     |
| 1:A:145:ASN:HD21 | 1:A:149:LEU:HD22 | 0.56     | 1.58        | 21     | 1     |
| 1:A:155:GLN:NE2  | 1:A:159:LEU:HD12 | 0.56     | 2.14        | 10     | 1     |
| 1:A:97:VAL:HG21  | 1:A:145:ASN:ND2  | 0.56     | 2.15        | 19     | 2     |
| 1:A:86:VAL:HG13  | 1:A:136:ALA:HB3  | 0.56     | 1.75        | 13     | 2     |
| 1:A:166:LEU:HD13 | 1:A:166:LEU:C    | 0.56     | 2.21        | 27     | 3     |
| 1:A:137:ILE:CG2  | 1:A:137:ILE:O    | 0.56     | 2.53        | 32     | 9     |
| 1:A:69:ALA:HB1   | 1:A:72:ASP:HB3   | 0.56     | 1.77        | 32     | 1     |
| 1:A:99:LEU:HD11  | 1:A:120:THR:HG22 | 0.56     | 1.74        | 24     | 1     |
| 1:A:101:TYR:CD1  | 1:A:152:LEU:HD12 | 0.56     | 2.36        | 9      | 4     |
| 1:A:155:GLN:OE1  | 1:A:159:LEU:HD13 | 0.56     | 2.01        | 27     | 3     |
| 1:A:123:LEU:N    | 1:A:123:LEU:HD22 | 0.56     | 2.16        | 9      | 3     |
| 1:A:93:LEU:HD13  | 1:A:139:THR:HB   | 0.56     | 1.78        | 17     | 3     |
| 1:A:34:LEU:HD23  | 1:A:172:LYS:CE   | 0.56     | 2.30        | 21     | 1     |
| 1:A:162:MET:HE3  | 1:A:162:MET:O    | 0.56     | 2.01        | 29     | 8     |
| 1:A:148:LEU:O    | 1:A:148:LEU:HD12 | 0.56     | 2.00        | 27     | 3     |
| 1:A:85:LEU:HD23  | 1:A:134:LEU:CD2  | 0.56     | 2.30        | 18     | 2     |
| 1:A:63:LEU:HB2   | 1:A:166:LEU:HD12 | 0.55     | 1.78        | 27     | 1     |
| 1:A:166:LEU:C    | 1:A:166:LEU:HD13 | 0.55     | 2.21        | 17     | 3     |
| 1:A:119:SER:O    | 1:A:123:LEU:HD22 | 0.55     | 2.02        | 12     | 2     |
| 1:A:96:GLU:OE1   | 1:A:124:ILE:HD11 | 0.55     | 2.01        | 4      | 1     |
| 1:A:89:ILE:HD11  | 1:A:127:LEU:CD1  | 0.55     | 2.30        | 24     | 2     |
| 1:A:139:THR:HG22 | 1:A:139:THR:O    | 0.55     | 2.00        | 3      | 2     |
| 1:A:88:ILE:HD12  | 1:A:178:SER:HB2  | 0.55     | 1.79        | 25     | 4     |
| 1:A:147:SER:HA   | 1:A:150:THR:HG22 | 0.55     | 1.77        | 1      | 4     |
| 1:A:26:ILE:CD1   | 1:A:127:LEU:HD13 | 0.55     | 2.31        | 16     | 1     |
| 1:A:131:ALA:HB3  | 1:A:135:ASP:CB   | 0.55     | 2.31        | 1      | 2     |
| 1:A:137:ILE:O    | 1:A:138:THR:HG23 | 0.55     | 2.02        | 24     | 1     |
| 1:A:65:LEU:CB    | 1:A:98:TYR:CE2   | 0.55     | 2.89        | 21     | 10    |
| 1:A:101:TYR:HD1  | 1:A:149:LEU:HD11 | 0.55     | 1.61        | 17     | 8     |
| 1:A:33:ILE:HG23  | 1:A:120:THR:CG2  | 0.55     | 2.31        | 7      | 2     |
| 1:A:63:LEU:CD1   | 1:A:163:THR:HG23 | 0.55     | 2.28        | 30     | 3     |
| 1:A:63:LEU:HD21  | 1:A:152:LEU:CD2  | 0.55     | 2.31        | 25     | 3     |
| 1:A:149:LEU:CD1  | 1:A:152:LEU:HD12 | 0.55     | 2.31        | 28     | 5     |
| 1:A:162:MET:HE1  | 1:A:163:THR:HA   | 0.55     | 1.78        | 11     | 1     |
| 1:A:26:ILE:HG22  | 1:A:182:LEU:HD11 | 0.55     | 1.79        | 29     | 1     |
| 1:A:21:THR:HG23  | 1:A:22:SER:N     | 0.55     | 2.15        | 4      | 2     |
| 1:A:63:LEU:CB    | 1:A:65:LEU:HD23  | 0.55     | 2.31        | 22     | 4     |
| 1:A:65:LEU:HD11  | 1:A:170:SER:HB2  | 0.55     | 1.77        | 26     | 3     |
| 1:A:85:LEU:HD11  | 1:A:127:LEU:HD11 | 0.54     | 1.77        | 19     | 2     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:123:LEU:HD22 | 1:A:123:LEU:N    | 0.54     | 2.17        | 22     | 12    |
| 1:A:44:THR:CG2   | 1:A:44:THR:O     | 0.54     | 2.56        | 4      | 3     |
| 1:A:148:LEU:HD12 | 1:A:148:LEU:O    | 0.54     | 2.03        | 1      | 3     |
| 1:A:68:MET:HE3   | 1:A:88:ILE:HD11  | 0.54     | 1.78        | 16     | 1     |
| 1:A:26:ILE:HD13  | 1:A:127:LEU:CD2  | 0.54     | 2.32        | 13     | 1     |
| 1:A:37:ILE:HG23  | 1:A:168:LEU:CD2  | 0.54     | 2.33        | 4      | 4     |
| 1:A:63:LEU:HD13  | 1:A:65:LEU:HD23  | 0.54     | 1.79        | 6      | 2     |
| 1:A:101:TYR:CE2  | 1:A:163:THR:CG2  | 0.54     | 2.91        | 3      | 17    |
| 1:A:26:ILE:HG21  | 1:A:127:LEU:HD21 | 0.54     | 1.80        | 17     | 2     |
| 1:A:26:ILE:HD12  | 1:A:130:LYS:CE   | 0.54     | 2.33        | 21     | 1     |
| 1:A:133:ASN:O    | 1:A:134:LEU:HD22 | 0.54     | 2.03        | 31     | 2     |
| 1:A:90:THR:HG23  | 1:A:137:ILE:HG21 | 0.53     | 1.80        | 1      | 2     |
| 1:A:102:LEU:HD23 | 1:A:106:PHE:CE1  | 0.53     | 2.39        | 10     | 4     |
| 1:A:88:ILE:HG22  | 1:A:92:LEU:HD11  | 0.53     | 1.80        | 18     | 1     |
| 1:A:98:TYR:CE1   | 1:A:148:LEU:HD21 | 0.53     | 2.38        | 10     | 2     |
| 1:A:89:ILE:HG13  | 1:A:137:ILE:HD13 | 0.53     | 1.78        | 29     | 2     |
| 1:A:96:GLU:CG    | 1:A:124:ILE:HD11 | 0.53     | 2.34        | 13     | 2     |
| 1:A:33:ILE:CG2   | 1:A:175:LEU:HD13 | 0.53     | 2.33        | 22     | 22    |
| 1:A:65:LEU:HD12  | 1:A:95:PHE:HE1   | 0.53     | 1.63        | 16     | 2     |
| 1:A:120:THR:HG21 | 1:A:171:PHE:HE2  | 0.53     | 1.64        | 18     | 2     |
| 1:A:26:ILE:HD13  | 1:A:127:LEU:HD23 | 0.53     | 1.81        | 13     | 1     |
| 1:A:30:ILE:HG21  | 1:A:179:LEU:HD11 | 0.53     | 1.80        | 1      | 1     |
| 1:A:30:ILE:HG22  | 1:A:179:LEU:HD11 | 0.53     | 1.80        | 16     | 2     |
| 1:A:163:THR:CG2  | 1:A:167:ILE:HD11 | 0.53     | 2.33        | 10     | 1     |
| 1:A:84:CYS:SG    | 1:A:181:ALA:HB1  | 0.53     | 2.44        | 8      | 1     |
| 1:A:134:LEU:O    | 1:A:135:ASP:CB   | 0.53     | 2.56        | 13     | 13    |
| 1:A:29:GLN:CD    | 1:A:122:VAL:HG11 | 0.53     | 2.25        | 10     | 1     |
| 1:A:85:LEU:HG    | 1:A:127:LEU:HD21 | 0.52     | 1.80        | 14     | 1     |
| 1:A:65:LEU:CD1   | 1:A:95:PHE:CE1   | 0.52     | 2.92        | 24     | 2     |
| 1:A:135:ASP:O    | 1:A:136:ALA:CB   | 0.52     | 2.57        | 27     | 11    |
| 1:A:27:ASP:HB2   | 1:A:182:LEU:HD13 | 0.52     | 1.80        | 13     | 1     |
| 1:A:97:VAL:HG11  | 1:A:148:LEU:HD23 | 0.52     | 1.81        | 5      | 4     |
| 1:A:26:ILE:HG23  | 1:A:123:LEU:HD22 | 0.52     | 1.81        | 17     | 2     |
| 1:A:63:LEU:HD21  | 1:A:152:LEU:HD22 | 0.52     | 1.79        | 18     | 3     |
| 1:A:102:LEU:HD11 | 1:A:167:ILE:CG2  | 0.52     | 2.30        | 21     | 4     |
| 1:A:37:ILE:HD12  | 1:A:168:LEU:HD13 | 0.52     | 1.81        | 11     | 1     |
| 1:A:31:ARG:N     | 1:A:179:LEU:HD21 | 0.52     | 2.19        | 23     | 1     |
| 1:A:90:THR:HB    | 1:A:137:ILE:HG22 | 0.52     | 1.81        | 4      | 4     |
| 1:A:27:ASP:OD2   | 1:A:179:LEU:HD23 | 0.52     | 2.04        | 28     | 3     |
| 1:A:88:ILE:HD11  | 1:A:178:SER:HB2  | 0.52     | 1.82        | 7      | 1     |
| 1:A:34:LEU:HD11  | 1:A:175:LEU:CB   | 0.52     | 2.34        | 31     | 5     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:131:ALA:O    | 1:A:132:LYS:O    | 0.52     | 2.28        | 3      | 4     |
| 1:A:40:LEU:CD1   | 1:A:116:VAL:CG1  | 0.52     | 2.88        | 11     | 4     |
| 1:A:97:VAL:CG2   | 1:A:145:ASN:ND2  | 0.52     | 2.72        | 21     | 1     |
| 1:A:97:VAL:HG23  | 1:A:145:ASN:CG   | 0.52     | 2.24        | 21     | 1     |
| 1:A:89:ILE:HD13  | 1:A:135:ASP:HA   | 0.52     | 1.81        | 17     | 1     |
| 1:A:62:ASN:CA    | 1:A:166:LEU:HD13 | 0.51     | 2.35        | 2      | 1     |
| 1:A:179:LEU:HD12 | 1:A:179:LEU:C    | 0.51     | 2.25        | 10     | 1     |
| 1:A:134:LEU:HD22 | 1:A:134:LEU:N    | 0.51     | 2.20        | 15     | 1     |
| 1:A:162:MET:O    | 1:A:162:MET:HE3  | 0.51     | 2.06        | 20     | 7     |
| 1:A:127:LEU:HD23 | 1:A:130:LYS:HE2  | 0.51     | 1.82        | 27     | 1     |
| 1:A:33:ILE:HG21  | 1:A:175:LEU:CD1  | 0.51     | 2.36        | 22     | 8     |
| 1:A:95:PHE:CD1   | 1:A:171:PHE:CE1  | 0.51     | 2.99        | 15     | 4     |
| 1:A:95:PHE:CE2   | 1:A:174:PHE:CD2  | 0.51     | 2.99        | 19     | 1     |
| 1:A:44:THR:O     | 1:A:48:SER:N     | 0.51     | 2.44        | 25     | 2     |
| 1:A:75:PHE:CD1   | 1:A:75:PHE:N     | 0.51     | 2.78        | 26     | 2     |
| 1:A:137:ILE:HD13 | 1:A:137:ILE:N    | 0.51     | 2.20        | 8      | 1     |
| 1:A:26:ILE:HD11  | 1:A:126:PHE:CB   | 0.51     | 2.36        | 26     | 2     |
| 1:A:74:CYS:O     | 1:A:75:PHE:CG    | 0.51     | 2.64        | 4      | 6     |
| 1:A:40:LEU:HB3   | 1:A:168:LEU:HD21 | 0.51     | 1.81        | 32     | 1     |
| 1:A:27:ASP:HB2   | 1:A:182:LEU:HD21 | 0.51     | 1.80        | 24     | 1     |
| 1:A:50:MET:CE    | 1:A:158:TRP:CZ3  | 0.51     | 2.94        | 32     | 1     |
| 1:A:30:ILE:CD1   | 1:A:123:LEU:CD1  | 0.51     | 2.89        | 17     | 1     |
| 1:A:63:LEU:HB2   | 1:A:166:LEU:HD23 | 0.51     | 1.82        | 25     | 1     |
| 1:A:40:LEU:HD21  | 1:A:113:ALA:HA   | 0.51     | 1.81        | 17     | 1     |
| 1:A:89:ILE:HG22  | 1:A:90:THR:N     | 0.50     | 2.20        | 8      | 3     |
| 1:A:41:ARG:CD    | 1:A:168:LEU:HD13 | 0.50     | 2.35        | 10     | 1     |
| 1:A:99:LEU:CD1   | 1:A:120:THR:CG2  | 0.50     | 2.88        | 8      | 7     |
| 1:A:99:LEU:HD13  | 1:A:117:GLN:HG3  | 0.50     | 1.84        | 17     | 1     |
| 1:A:65:LEU:N     | 1:A:66:PRO:HD3   | 0.50     | 2.21        | 29     | 9     |
| 1:A:63:LEU:CD2   | 1:A:152:LEU:CD2  | 0.50     | 2.90        | 20     | 3     |
| 1:A:65:LEU:HD22  | 1:A:98:TYR:CZ    | 0.50     | 2.41        | 17     | 1     |
| 1:A:90:THR:N     | 1:A:137:ILE:HG21 | 0.50     | 2.21        | 15     | 5     |
| 1:A:48:SER:O     | 1:A:50:MET:N     | 0.50     | 2.45        | 32     | 9     |
| 1:A:85:LEU:CD1   | 1:A:182:LEU:HD11 | 0.50     | 2.36        | 28     | 1     |
| 1:A:162:MET:HE3  | 1:A:166:LEU:CB   | 0.50     | 2.37        | 4      | 1     |
| 1:A:29:GLN:CG    | 1:A:123:LEU:HD21 | 0.50     | 2.36        | 30     | 2     |
| 1:A:106:PHE:HB2  | 1:A:113:ALA:HB2  | 0.50     | 1.83        | 20     | 5     |
| 1:A:30:ILE:CG2   | 1:A:175:LEU:HD22 | 0.50     | 2.32        | 3      | 2     |
| 1:A:30:ILE:HG12  | 1:A:33:ILE:HD12  | 0.50     | 1.82        | 19     | 2     |
| 1:A:88:ILE:HG22  | 1:A:92:LEU:CD1   | 0.50     | 2.37        | 18     | 2     |
| 1:A:37:ILE:HG23  | 1:A:168:LEU:HB2  | 0.50     | 1.84        | 10     | 1     |

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| Atom-1          | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|-----------------|------------------|----------|-------------|--------|-------|
|                 |                  |          |             | Worst  | Total |
| 1:A:27:ASP:CB   | 1:A:182:LEU:HD13 | 0.50     | 2.37        | 13     | 1     |
| 1:A:170:SER:O   | 1:A:174:PHE:CB   | 0.50     | 2.60        | 24     | 32    |
| 1:A:91:GLY:O    | 1:A:95:PHE:CD2   | 0.50     | 2.65        | 5      | 9     |
| 1:A:89:ILE:HD11 | 1:A:134:LEU:CD2  | 0.50     | 2.36        | 3      | 1     |
| 1:A:27:ASP:O    | 1:A:179:LEU:HD23 | 0.49     | 2.07        | 23     | 1     |
| 1:A:136:ALA:O   | 1:A:138:THR:N    | 0.49     | 2.46        | 24     | 2     |
| 1:A:65:LEU:CD2  | 1:A:65:LEU:N     | 0.49     | 2.75        | 6      | 1     |
| 1:A:42:LYS:O    | 1:A:46:ASN:CB    | 0.49     | 2.60        | 32     | 11    |
| 1:A:33:ILE:HD11 | 1:A:123:LEU:HD23 | 0.49     | 1.83        | 10     | 8     |
| 1:A:44:THR:O    | 1:A:44:THR:CG2   | 0.49     | 2.59        | 32     | 2     |
| 1:A:65:LEU:HB3  | 1:A:98:TYR:CZ    | 0.49     | 2.43        | 9      | 16    |
| 1:A:122:VAL:O   | 1:A:126:PHE:CD1  | 0.49     | 2.66        | 8      | 11    |
| 1:A:128:GLN:OE1 | 1:A:137:ILE:HG21 | 0.49     | 2.07        | 2      | 1     |
| 1:A:37:ILE:HG23 | 1:A:168:LEU:HG   | 0.49     | 1.83        | 18     | 2     |
| 1:A:26:ILE:CG1  | 1:A:123:LEU:HD13 | 0.49     | 2.37        | 13     | 1     |
| 1:A:50:MET:CE   | 1:A:158:TRP:NE1  | 0.49     | 2.76        | 1      | 1     |
| 1:A:45:CYS:N    | 1:A:48:SER:OG    | 0.49     | 2.46        | 9      | 2     |
| 1:A:65:LEU:H    | 1:A:65:LEU:HD23  | 0.49     | 1.67        | 15     | 1     |
| 1:A:101:TYR:CE1 | 1:A:152:LEU:HB2  | 0.49     | 2.42        | 24     | 14    |
| 1:A:86:VAL:HG23 | 1:A:134:LEU:HD21 | 0.49     | 1.83        | 21     | 1     |
| 1:A:88:ILE:HD11 | 1:A:178:SER:OG   | 0.49     | 2.07        | 7      | 1     |
| 1:A:27:ASP:HA   | 1:A:182:LEU:HD13 | 0.49     | 1.83        | 16     | 1     |
| 1:A:152:LEU:N   | 1:A:152:LEU:HD23 | 0.49     | 2.21        | 5      | 1     |
| 1:A:34:LEU:N    | 1:A:34:LEU:HD12  | 0.49     | 2.23        | 17     | 1     |
| 1:A:82:GLU:CG   | 1:A:134:LEU:HD21 | 0.48     | 2.38        | 2      | 3     |
| 1:A:30:ILE:HG21 | 1:A:179:LEU:CD1  | 0.48     | 2.38        | 24     | 1     |
| 1:A:85:LEU:CG   | 1:A:127:LEU:HD21 | 0.48     | 2.38        | 14     | 1     |
| 1:A:94:GLU:O    | 1:A:98:TYR:CD2   | 0.48     | 2.66        | 10     | 7     |
| 1:A:102:LEU:CD1 | 1:A:167:ILE:HG21 | 0.48     | 2.37        | 8      | 2     |
| 1:A:76:GLN:O    | 1:A:77:SER:CB    | 0.48     | 2.61        | 30     | 2     |
| 1:A:91:GLY:O    | 1:A:95:PHE:CG    | 0.48     | 2.66        | 14     | 4     |
| 1:A:91:GLY:O    | 1:A:95:PHE:CD1   | 0.48     | 2.66        | 18     | 8     |
| 1:A:33:ILE:CG2  | 1:A:175:LEU:CD1  | 0.48     | 2.92        | 17     | 13    |
| 1:A:48:SER:O    | 1:A:49:ASN:CB    | 0.48     | 2.61        | 28     | 1     |
| 1:A:33:ILE:HG21 | 1:A:175:LEU:HD13 | 0.48     | 1.84        | 22     | 2     |
| 1:A:112:GLN:O   | 1:A:115:ALA:HB3  | 0.48     | 2.08        | 24     | 1     |
| 1:A:92:LEU:HD22 | 1:A:124:ILE:CG1  | 0.48     | 2.39        | 1      | 1     |
| 1:A:29:GLN:CB   | 1:A:123:LEU:CD2  | 0.48     | 2.91        | 25     | 4     |
| 1:A:22:SER:CB   | 1:A:130:LYS:CD   | 0.48     | 2.92        | 24     | 1     |
| 1:A:34:LEU:HD23 | 1:A:172:LYS:HE2  | 0.48     | 1.84        | 21     | 1     |
| 1:A:40:LEU:O    | 1:A:168:LEU:HD22 | 0.48     | 2.09        | 16     | 1     |

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| Atom-1          | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|-----------------|------------------|----------|-------------|--------|-------|
|                 |                  |          |             | Worst  | Total |
| 1:A:171:PHE:CD2 | 1:A:175:LEU:CD1  | 0.48     | 2.95        | 23     | 3     |
| 1:A:30:ILE:HD13 | 1:A:33:ILE:HD12  | 0.48     | 1.86        | 14     | 3     |
| 1:A:65:LEU:HB2  | 1:A:98:TYR:CE2   | 0.48     | 2.44        | 11     | 7     |
| 1:A:155:GLN:CB  | 1:A:159:LEU:CB   | 0.48     | 2.92        | 10     | 1     |
| 1:A:63:LEU:HD12 | 1:A:166:LEU:HB2  | 0.48     | 1.84        | 19     | 1     |
| 1:A:86:VAL:HG23 | 1:A:134:LEU:HD13 | 0.48     | 1.85        | 24     | 1     |
| 1:A:26:ILE:CG1  | 1:A:123:LEU:CD1  | 0.48     | 2.92        | 13     | 1     |
| 1:A:146:ALA:O   | 1:A:150:THR:OG1  | 0.48     | 2.32        | 5      | 1     |
| 1:A:75:PHE:N    | 1:A:75:PHE:CD1   | 0.48     | 2.82        | 1      | 1     |
| 1:A:65:LEU:HD21 | 1:A:166:LEU:HD21 | 0.48     | 1.85        | 8      | 1     |
| 1:A:29:GLN:CG   | 1:A:123:LEU:CD2  | 0.48     | 2.92        | 18     | 3     |
| 1:A:30:ILE:CG2  | 1:A:179:LEU:CD1  | 0.48     | 2.92        | 24     | 2     |
| 1:A:90:THR:H    | 1:A:137:ILE:HG21 | 0.47     | 1.69        | 15     | 3     |
| 1:A:30:ILE:CG2  | 1:A:175:LEU:HB3  | 0.47     | 2.39        | 2      | 21    |
| 1:A:39:ALA:CB   | 1:A:112:GLN:NE2  | 0.47     | 2.77        | 8      | 2     |
| 1:A:156:ASN:O   | 1:A:157:GLN:CB   | 0.47     | 2.61        | 30     | 4     |
| 1:A:155:GLN:CB  | 1:A:159:LEU:HD23 | 0.47     | 2.38        | 12     | 1     |
| 1:A:30:ILE:HA   | 1:A:33:ILE:HD12  | 0.47     | 1.85        | 20     | 3     |
| 1:A:26:ILE:HD12 | 1:A:127:LEU:HD23 | 0.47     | 1.85        | 4      | 1     |
| 1:A:74:CYS:O    | 1:A:75:PHE:CD2   | 0.47     | 2.67        | 22     | 1     |
| 1:A:99:LEU:HD21 | 1:A:171:PHE:CZ   | 0.47     | 2.44        | 5      | 1     |
| 1:A:96:GLU:CG   | 1:A:124:ILE:CD1  | 0.47     | 2.92        | 13     | 1     |
| 1:A:89:ILE:CD1  | 1:A:137:ILE:CD1  | 0.47     | 2.92        | 31     | 1     |
| 1:A:117:GLN:O   | 1:A:120:THR:HG22 | 0.47     | 2.09        | 8      | 1     |
| 1:A:37:ILE:HD12 | 1:A:168:LEU:HG   | 0.47     | 1.86        | 32     | 1     |
| 1:A:99:LEU:CD1  | 1:A:120:THR:HG22 | 0.47     | 2.39        | 24     | 1     |
| 1:A:30:ILE:HD13 | 1:A:123:LEU:HG   | 0.47     | 1.86        | 21     | 4     |
| 1:A:79:PHE:CE2  | 1:A:80:ASN:O     | 0.47     | 2.68        | 6      | 7     |
| 1:A:66:PRO:O    | 1:A:174:PHE:CE1  | 0.47     | 2.68        | 6      | 1     |
| 1:A:89:ILE:HB   | 1:A:137:ILE:HG21 | 0.47     | 1.86        | 4      | 1     |
| 1:A:170:SER:O   | 1:A:174:PHE:N    | 0.47     | 2.48        | 5      | 31    |
| 1:A:93:LEU:HD21 | 1:A:124:ILE:HD11 | 0.47     | 1.85        | 27     | 1     |
| 1:A:162:MET:HE3 | 1:A:166:LEU:HB2  | 0.47     | 1.84        | 7      | 2     |
| 1:A:69:ALA:O    | 1:A:70:GLU:CB    | 0.47     | 2.62        | 3      | 3     |
| 1:A:97:VAL:CG1  | 1:A:98:TYR:N     | 0.47     | 2.77        | 10     | 9     |
| 1:A:101:TYR:CZ  | 1:A:152:LEU:HB2  | 0.47     | 2.45        | 29     | 5     |
| 1:A:26:ILE:HG13 | 1:A:127:LEU:HD21 | 0.47     | 1.87        | 10     | 1     |
| 1:A:40:LEU:O    | 1:A:44:THR:CG2   | 0.47     | 2.63        | 23     | 29    |
| 1:A:65:LEU:N    | 1:A:66:PRO:HD2   | 0.47     | 2.24        | 9      | 13    |
| 1:A:162:MET:CE  | 1:A:166:LEU:HB2  | 0.47     | 2.40        | 9      | 27    |
| 1:A:73:GLY:O    | 1:A:79:PHE:CD1   | 0.47     | 2.67        | 19     | 2     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:92:LEU:CD1   | 1:A:127:LEU:CD1  | 0.47     | 2.93        | 28     | 4     |
| 1:A:93:LEU:CD2   | 1:A:124:ILE:HD11 | 0.47     | 2.40        | 27     | 1     |
| 1:A:148:LEU:CD1  | 1:A:152:LEU:CD2  | 0.47     | 2.93        | 11     | 3     |
| 1:A:93:LEU:HD22  | 1:A:139:THR:CB   | 0.47     | 2.40        | 11     | 2     |
| 1:A:26:ILE:HA    | 1:A:123:LEU:HD21 | 0.47     | 1.87        | 3      | 1     |
| 1:A:92:LEU:HD22  | 1:A:120:THR:HG23 | 0.47     | 1.87        | 5      | 1     |
| 1:A:62:ASN:O     | 1:A:63:LEU:O     | 0.47     | 2.32        | 6      | 1     |
| 1:A:65:LEU:HB3   | 1:A:98:TYR:CE2   | 0.47     | 2.45        | 14     | 20    |
| 1:A:33:ILE:CG2   | 1:A:120:THR:HG22 | 0.47     | 2.38        | 27     | 2     |
| 1:A:63:LEU:CB    | 1:A:65:LEU:CD2   | 0.47     | 2.93        | 27     | 3     |
| 1:A:63:LEU:HD12  | 1:A:163:THR:HG23 | 0.47     | 1.86        | 15     | 1     |
| 1:A:62:ASN:ND2   | 1:A:162:MET:CG   | 0.47     | 2.78        | 6      | 1     |
| 1:A:168:LEU:N    | 1:A:168:LEU:HD12 | 0.47     | 2.23        | 23     | 1     |
| 1:A:27:ASP:O     | 1:A:179:LEU:HD21 | 0.47     | 2.09        | 8      | 2     |
| 1:A:65:LEU:HD22  | 1:A:167:ILE:HG12 | 0.47     | 1.86        | 11     | 1     |
| 1:A:158:TRP:CG   | 1:A:159:LEU:N    | 0.47     | 2.83        | 32     | 1     |
| 1:A:33:ILE:HG23  | 1:A:120:THR:HG23 | 0.47     | 1.86        | 10     | 1     |
| 1:A:102:LEU:HD23 | 1:A:106:PHE:HE1  | 0.47     | 1.70        | 10     | 2     |
| 1:A:86:VAL:CG2   | 1:A:134:LEU:CD1  | 0.47     | 2.92        | 24     | 1     |
| 1:A:162:MET:CE   | 1:A:166:LEU:CB   | 0.46     | 2.93        | 25     | 5     |
| 1:A:65:LEU:CB    | 1:A:98:TYR:CZ    | 0.46     | 2.98        | 11     | 2     |
| 1:A:179:LEU:HD12 | 1:A:179:LEU:H    | 0.46     | 1.70        | 16     | 2     |
| 1:A:89:ILE:O     | 1:A:93:LEU:HD12  | 0.46     | 2.10        | 14     | 2     |
| 1:A:93:LEU:CD1   | 1:A:138:THR:O    | 0.46     | 2.63        | 24     | 3     |
| 1:A:82:GLU:O     | 1:A:86:VAL:CG2   | 0.46     | 2.63        | 30     | 15    |
| 1:A:89:ILE:CD1   | 1:A:134:LEU:CD2  | 0.46     | 2.93        | 16     | 1     |
| 1:A:86:VAL:CG2   | 1:A:134:LEU:HD21 | 0.46     | 2.38        | 16     | 1     |
| 1:A:158:TRP:C    | 1:A:158:TRP:CD2  | 0.46     | 2.89        | 32     | 1     |
| 1:A:88:ILE:CD1   | 1:A:178:SER:CB   | 0.46     | 2.93        | 31     | 4     |
| 1:A:41:ARG:O     | 1:A:45:CYS:CB    | 0.46     | 2.63        | 17     | 16    |
| 1:A:63:LEU:HD11  | 1:A:166:LEU:HB3  | 0.46     | 1.87        | 32     | 1     |
| 1:A:158:TRP:CE3  | 1:A:158:TRP:O    | 0.46     | 2.69        | 32     | 1     |
| 1:A:94:GLU:O     | 1:A:97:VAL:CG1   | 0.46     | 2.63        | 32     | 3     |
| 1:A:92:LEU:HD22  | 1:A:124:ILE:HG12 | 0.46     | 1.87        | 1      | 1     |
| 1:A:131:ALA:O    | 1:A:132:LYS:CG   | 0.46     | 2.64        | 3      | 4     |
| 1:A:162:MET:O    | 1:A:162:MET:CE   | 0.46     | 2.64        | 9      | 11    |
| 1:A:126:PHE:O    | 1:A:130:LYS:CB   | 0.46     | 2.64        | 23     | 7     |
| 1:A:127:LEU:O    | 1:A:131:ALA:CB   | 0.46     | 2.64        | 30     | 6     |
| 1:A:119:SER:O    | 1:A:123:LEU:CD2  | 0.46     | 2.64        | 9      | 9     |
| 1:A:26:ILE:HG22  | 1:A:182:LEU:CD1  | 0.46     | 2.40        | 29     | 1     |
| 1:A:39:ALA:HB1   | 1:A:112:GLN:HE22 | 0.46     | 1.70        | 9      | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:134:LEU:O    | 1:A:135:ASP:HB2  | 0.46     | 2.10        | 8      | 1     |
| 1:A:44:THR:O     | 1:A:48:SER:CB    | 0.46     | 2.64        | 25     | 2     |
| 1:A:102:LEU:HD23 | 1:A:164:THR:HG23 | 0.46     | 1.88        | 27     | 3     |
| 1:A:65:LEU:HD23  | 1:A:65:LEU:H     | 0.46     | 1.71        | 14     | 4     |
| 1:A:122:VAL:O    | 1:A:126:PHE:CG   | 0.46     | 2.68        | 27     | 1     |
| 1:A:171:PHE:O    | 1:A:175:LEU:HB2  | 0.46     | 2.11        | 26     | 25    |
| 1:A:137:ILE:O    | 1:A:138:THR:O    | 0.46     | 2.33        | 17     | 5     |
| 1:A:37:ILE:HG23  | 1:A:168:LEU:HD13 | 0.46     | 1.88        | 11     | 2     |
| 1:A:139:THR:O    | 1:A:139:THR:CG2  | 0.46     | 2.63        | 11     | 4     |
| 1:A:148:LEU:O    | 1:A:152:LEU:CD2  | 0.46     | 2.64        | 32     | 3     |
| 1:A:124:ILE:O    | 1:A:128:GLN:CB   | 0.46     | 2.64        | 6      | 2     |
| 1:A:132:LYS:O    | 1:A:133:ASN:CB   | 0.46     | 2.64        | 15     | 1     |
| 1:A:159:LEU:HD23 | 1:A:162:MET:HG2  | 0.46     | 1.88        | 19     | 1     |
| 1:A:122:VAL:HG13 | 1:A:126:PHE:CE1  | 0.46     | 2.45        | 19     | 1     |
| 1:A:50:MET:CB    | 1:A:165:HIS:CE1  | 0.46     | 2.98        | 29     | 1     |
| 1:A:21:THR:HG1   | 1:A:23:SER:HG    | 0.46     | 1.54        | 24     | 1     |
| 1:A:150:THR:O    | 1:A:154:ALA:CB   | 0.45     | 2.64        | 32     | 6     |
| 1:A:74:CYS:C     | 1:A:75:PHE:CG    | 0.45     | 2.89        | 18     | 2     |
| 1:A:79:PHE:CE2   | 1:A:184:GLN:CB   | 0.45     | 2.99        | 29     | 2     |
| 1:A:86:VAL:O     | 1:A:90:THR:HG22  | 0.45     | 2.10        | 8      | 1     |
| 1:A:74:CYS:SG    | 1:A:181:ALA:CB   | 0.45     | 3.04        | 29     | 2     |
| 1:A:97:VAL:CB    | 1:A:145:ASN:ND2  | 0.45     | 2.80        | 5      | 1     |
| 1:A:26:ILE:HG22  | 1:A:182:LEU:HD13 | 0.45     | 1.89        | 17     | 1     |
| 1:A:156:ASN:N    | 1:A:156:ASN:OD1  | 0.45     | 2.49        | 22     | 1     |
| 1:A:127:LEU:C    | 1:A:127:LEU:HD13 | 0.45     | 2.29        | 6      | 1     |
| 1:A:99:LEU:O     | 1:A:103:GLN:N    | 0.45     | 2.50        | 3      | 20    |
| 1:A:26:ILE:HG22  | 1:A:182:LEU:CD2  | 0.45     | 2.42        | 19     | 1     |
| 1:A:93:LEU:HD13  | 1:A:139:THR:HA   | 0.45     | 1.88        | 25     | 2     |
| 1:A:164:THR:HA   | 1:A:167:ILE:HD12 | 0.45     | 1.87        | 11     | 2     |
| 1:A:63:LEU:HD21  | 1:A:163:THR:HA   | 0.45     | 1.88        | 32     | 1     |
| 1:A:131:ALA:O    | 1:A:132:LYS:C    | 0.45     | 2.55        | 24     | 1     |
| 1:A:127:LEU:O    | 1:A:131:ALA:N    | 0.45     | 2.50        | 4      | 5     |
| 1:A:80:ASN:O     | 1:A:81:GLU:CB    | 0.45     | 2.64        | 7      | 4     |
| 1:A:121:LYS:O    | 1:A:124:ILE:CG2  | 0.45     | 2.65        | 2      | 1     |
| 1:A:26:ILE:CD1   | 1:A:127:LEU:HD23 | 0.45     | 2.41        | 4      | 1     |
| 1:A:86:VAL:CG1   | 1:A:136:ALA:CB   | 0.45     | 2.94        | 13     | 1     |
| 1:A:178:SER:O    | 1:A:182:LEU:HD13 | 0.45     | 2.10        | 27     | 1     |
| 1:A:65:LEU:HD13  | 1:A:98:TYR:CE2   | 0.45     | 2.47        | 32     | 2     |
| 1:A:126:PHE:O    | 1:A:130:LYS:CG   | 0.45     | 2.65        | 27     | 7     |
| 1:A:85:LEU:HD13  | 1:A:182:LEU:HD21 | 0.45     | 1.89        | 31     | 1     |
| 1:A:68:MET:SD    | 1:A:174:PHE:CD2  | 0.45     | 3.10        | 8      | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:162:MET:CE   | 1:A:162:MET:O    | 0.44     | 2.65        | 28     | 5     |
| 1:A:65:LEU:HD21  | 1:A:166:LEU:CD1  | 0.44     | 2.37        | 30     | 1     |
| 1:A:127:LEU:HD22 | 1:A:130:LYS:HE2  | 0.44     | 1.88        | 12     | 1     |
| 1:A:88:ILE:HG22  | 1:A:92:LEU:HD12  | 0.44     | 1.90        | 25     | 1     |
| 1:A:101:TYR:CZ   | 1:A:152:LEU:HB3  | 0.44     | 2.47        | 17     | 1     |
| 1:A:41:ARG:O     | 1:A:45:CYS:HB2   | 0.44     | 2.12        | 24     | 8     |
| 1:A:98:TYR:HH    | 1:A:148:LEU:HD21 | 0.44     | 1.72        | 27     | 1     |
| 1:A:41:ARG:HG3   | 1:A:45:CYS:CB    | 0.44     | 2.42        | 32     | 3     |
| 1:A:139:THR:CG2  | 1:A:139:THR:O    | 0.44     | 2.66        | 18     | 4     |
| 1:A:102:LEU:O    | 1:A:113:ALA:CB   | 0.44     | 2.66        | 29     | 5     |
| 1:A:41:ARG:CB    | 1:A:168:LEU:HD23 | 0.44     | 2.41        | 18     | 1     |
| 1:A:34:LEU:HD21  | 1:A:176:GLN:HG3  | 0.44     | 1.90        | 15     | 1     |
| 1:A:86:VAL:O     | 1:A:137:ILE:HG21 | 0.44     | 2.12        | 17     | 1     |
| 1:A:99:LEU:CD1   | 1:A:120:THR:OG1  | 0.44     | 2.65        | 19     | 5     |
| 1:A:131:ALA:O    | 1:A:134:LEU:CB   | 0.44     | 2.65        | 13     | 3     |
| 1:A:106:PHE:O    | 1:A:110:GLU:CA   | 0.44     | 2.66        | 7      | 7     |
| 1:A:168:LEU:HD12 | 1:A:168:LEU:C    | 0.44     | 2.32        | 10     | 1     |
| 1:A:82:GLU:HG3   | 1:A:134:LEU:HD11 | 0.44     | 1.89        | 24     | 2     |
| 1:A:79:PHE:CZ    | 1:A:184:GLN:HB2  | 0.44     | 2.47        | 20     | 2     |
| 1:A:148:LEU:O    | 1:A:152:LEU:HG   | 0.44     | 2.13        | 20     | 2     |
| 1:A:85:LEU:HD11  | 1:A:127:LEU:HD21 | 0.44     | 1.89        | 12     | 1     |
| 1:A:98:TYR:OH    | 1:A:148:LEU:CD2  | 0.44     | 2.65        | 11     | 3     |
| 1:A:74:CYS:SG    | 1:A:79:PHE:CE1   | 0.44     | 3.10        | 20     | 1     |
| 1:A:181:ALA:O    | 1:A:185:MET:CG   | 0.44     | 2.65        | 15     | 5     |
| 1:A:73:GLY:O     | 1:A:79:PHE:CG    | 0.44     | 2.71        | 15     | 1     |
| 1:A:62:ASN:ND2   | 1:A:162:MET:HG2  | 0.44     | 2.28        | 6      | 1     |
| 1:A:62:ASN:O     | 1:A:63:LEU:CD1   | 0.44     | 2.62        | 6      | 1     |
| 1:A:79:PHE:CE2   | 1:A:184:GLN:CG   | 0.44     | 3.01        | 8      | 1     |
| 1:A:80:ASN:O     | 1:A:81:GLU:CG    | 0.44     | 2.65        | 15     | 3     |
| 1:A:123:LEU:N    | 1:A:123:LEU:CD2  | 0.44     | 2.81        | 21     | 1     |
| 1:A:34:LEU:HD21  | 1:A:172:LYS:HA   | 0.44     | 1.89        | 26     | 1     |
| 1:A:99:LEU:HD13  | 1:A:117:GLN:HG2  | 0.44     | 1.89        | 15     | 1     |
| 1:A:158:TRP:C    | 1:A:158:TRP:CE3  | 0.44     | 2.91        | 32     | 1     |
| 1:A:116:VAL:CG1  | 1:A:117:GLN:N    | 0.44     | 2.81        | 5      | 3     |
| 1:A:29:GLN:NE2   | 1:A:122:VAL:CG1  | 0.44     | 2.79        | 6      | 1     |
| 1:A:33:ILE:CG2   | 1:A:120:THR:CG2  | 0.44     | 2.96        | 7      | 1     |
| 1:A:68:MET:CE    | 1:A:88:ILE:HD11  | 0.44     | 2.42        | 16     | 1     |
| 1:A:79:PHE:CE2   | 1:A:81:GLU:CG    | 0.44     | 3.01        | 16     | 1     |
| 1:A:127:LEU:O    | 1:A:131:ALA:CA   | 0.44     | 2.65        | 6      | 2     |
| 1:A:50:MET:O     | 1:A:165:HIS:CG   | 0.44     | 2.71        | 9      | 1     |
| 1:A:102:LEU:CD2  | 1:A:164:THR:HG22 | 0.44     | 2.43        | 14     | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:164:THR:O    | 1:A:168:LEU:CD1  | 0.43     | 2.66        | 14     | 3     |
| 1:A:79:PHE:CD1   | 1:A:80:ASN:N     | 0.43     | 2.86        | 30     | 1     |
| 1:A:88:ILE:O     | 1:A:92:LEU:HD12  | 0.43     | 2.12        | 18     | 2     |
| 1:A:101:TYR:CZ   | 1:A:152:LEU:CB   | 0.43     | 3.01        | 29     | 1     |
| 1:A:27:ASP:OD1   | 1:A:179:LEU:CG   | 0.43     | 2.66        | 16     | 1     |
| 1:A:114:ARG:O    | 1:A:118:MET:CG   | 0.43     | 2.66        | 16     | 4     |
| 1:A:75:PHE:O     | 1:A:76:GLN:CB    | 0.43     | 2.66        | 13     | 1     |
| 1:A:121:LYS:HA   | 1:A:124:ILE:HG22 | 0.43     | 1.89        | 8      | 4     |
| 1:A:41:ARG:O     | 1:A:45:CYS:HB3   | 0.43     | 2.13        | 22     | 7     |
| 1:A:63:LEU:HB2   | 1:A:65:LEU:CD2   | 0.43     | 2.43        | 19     | 4     |
| 1:A:130:LYS:O    | 1:A:130:LYS:CD   | 0.43     | 2.67        | 13     | 2     |
| 1:A:162:MET:HG3  | 1:A:163:THR:N    | 0.43     | 2.29        | 13     | 3     |
| 1:A:68:MET:O     | 1:A:69:ALA:HB2   | 0.43     | 2.13        | 2      | 6     |
| 1:A:101:TYR:O    | 1:A:105:ARG:CG   | 0.43     | 2.67        | 7      | 3     |
| 1:A:130:LYS:CG   | 1:A:130:LYS:O    | 0.43     | 2.66        | 26     | 1     |
| 1:A:50:MET:CE    | 1:A:158:TRP:CD1  | 0.43     | 3.02        | 1      | 1     |
| 1:A:63:LEU:HD12  | 1:A:167:ILE:HG13 | 0.43     | 1.90        | 30     | 1     |
| 1:A:29:GLN:HB3   | 1:A:123:LEU:CD2  | 0.43     | 2.43        | 19     | 4     |
| 1:A:40:LEU:O     | 1:A:168:LEU:CD1  | 0.43     | 2.66        | 3      | 4     |
| 1:A:119:SER:O    | 1:A:123:LEU:HD13 | 0.43     | 2.13        | 2      | 1     |
| 1:A:89:ILE:CD1   | 1:A:134:LEU:HD22 | 0.43     | 2.42        | 16     | 1     |
| 1:A:164:THR:O    | 1:A:168:LEU:CD2  | 0.43     | 2.67        | 10     | 1     |
| 1:A:30:ILE:CG1   | 1:A:123:LEU:HD13 | 0.43     | 2.42        | 3      | 1     |
| 1:A:106:PHE:CB   | 1:A:113:ALA:HB2  | 0.43     | 2.44        | 24     | 2     |
| 1:A:166:LEU:O    | 1:A:166:LEU:HD23 | 0.43     | 2.12        | 24     | 1     |
| 1:A:27:ASP:CB    | 1:A:182:LEU:HD21 | 0.43     | 2.44        | 24     | 1     |
| 1:A:79:PHE:CZ    | 1:A:184:GLN:HB3  | 0.43     | 2.48        | 14     | 2     |
| 1:A:148:LEU:O    | 1:A:152:LEU:CD1  | 0.43     | 2.67        | 23     | 1     |
| 1:A:146:ALA:O    | 1:A:150:THR:CB   | 0.43     | 2.67        | 32     | 5     |
| 1:A:127:LEU:HD13 | 1:A:127:LEU:O    | 0.43     | 2.13        | 20     | 1     |
| 1:A:74:CYS:C     | 1:A:75:PHE:CD2   | 0.43     | 2.92        | 18     | 2     |
| 1:A:151:LYS:O    | 1:A:155:GLN:CG   | 0.43     | 2.67        | 19     | 4     |
| 1:A:179:LEU:CD1  | 1:A:180:ARG:N    | 0.43     | 2.77        | 22     | 1     |
| 1:A:86:VAL:HG22  | 1:A:134:LEU:HD22 | 0.43     | 1.90        | 24     | 1     |
| 1:A:41:ARG:CG    | 1:A:45:CYS:CB    | 0.43     | 2.97        | 20     | 4     |
| 1:A:158:TRP:C    | 1:A:158:TRP:CD1  | 0.43     | 2.91        | 25     | 1     |
| 1:A:92:LEU:CD1   | 1:A:127:LEU:HD11 | 0.43     | 2.43        | 28     | 1     |
| 1:A:106:PHE:O    | 1:A:110:GLU:N    | 0.43     | 2.51        | 22     | 5     |
| 1:A:30:ILE:HG13  | 1:A:123:LEU:HD11 | 0.43     | 1.91        | 16     | 1     |
| 1:A:176:GLN:HA   | 1:A:179:LEU:HD21 | 0.43     | 1.91        | 10     | 1     |
| 1:A:95:PHE:CZ    | 1:A:174:PHE:CG   | 0.43     | 3.07        | 18     | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:148:LEU:HD12 | 1:A:152:LEU:HD21 | 0.43     | 1.88        | 6      | 1     |
| 1:A:168:LEU:N    | 1:A:168:LEU:CD1  | 0.43     | 2.81        | 23     | 1     |
| 1:A:27:ASP:O     | 1:A:179:LEU:CD2  | 0.43     | 2.67        | 14     | 2     |
| 1:A:50:MET:HE1   | 1:A:158:TRP:NE1  | 0.43     | 2.28        | 20     | 1     |
| 1:A:130:LYS:CE   | 1:A:130:LYS:O    | 0.43     | 2.66        | 14     | 2     |
| 1:A:25:ARG:O     | 1:A:29:GLN:CG    | 0.43     | 2.67        | 15     | 2     |
| 1:A:88:ILE:CD1   | 1:A:178:SER:OG   | 0.43     | 2.67        | 24     | 3     |
| 1:A:50:MET:HE2   | 1:A:158:TRP:CD1  | 0.43     | 2.48        | 28     | 1     |
| 1:A:96:GLU:OE2   | 1:A:124:ILE:HD13 | 0.43     | 2.14        | 7      | 1     |
| 1:A:89:ILE:O     | 1:A:93:LEU:CD1   | 0.43     | 2.67        | 18     | 2     |
| 1:A:132:LYS:O    | 1:A:134:LEU:CD2  | 0.43     | 2.67        | 15     | 1     |
| 1:A:134:LEU:O    | 1:A:135:ASP:HB3  | 0.43     | 2.13        | 30     | 1     |
| 1:A:40:LEU:O     | 1:A:168:LEU:CD2  | 0.43     | 2.67        | 23     | 3     |
| 1:A:34:LEU:HD11  | 1:A:175:LEU:HB3  | 0.42     | 1.89        | 31     | 1     |
| 1:A:63:LEU:HD11  | 1:A:166:LEU:HD22 | 0.42     | 1.87        | 32     | 1     |
| 1:A:24:GLU:HG3   | 1:A:25:ARG:N     | 0.42     | 2.28        | 4      | 2     |
| 1:A:26:ILE:CG2   | 1:A:182:LEU:CD2  | 0.42     | 2.97        | 19     | 1     |
| 1:A:22:SER:CB    | 1:A:130:LYS:HD3  | 0.42     | 2.44        | 24     | 1     |
| 1:A:27:ASP:OD1   | 1:A:28:LYS:N     | 0.42     | 2.52        | 8      | 2     |
| 1:A:121:LYS:HA   | 1:A:124:ILE:CG2  | 0.42     | 2.44        | 8      | 3     |
| 1:A:93:LEU:HG    | 1:A:124:ILE:HD11 | 0.42     | 1.91        | 8      | 1     |
| 1:A:170:SER:O    | 1:A:174:PHE:HB2  | 0.42     | 2.14        | 25     | 2     |
| 1:A:66:PRO:O     | 1:A:67:LYS:CG    | 0.42     | 2.67        | 28     | 2     |
| 1:A:137:ILE:O    | 1:A:138:THR:C    | 0.42     | 2.57        | 27     | 2     |
| 1:A:26:ILE:HG13  | 1:A:123:LEU:CD1  | 0.42     | 2.44        | 13     | 2     |
| 1:A:166:LEU:O    | 1:A:166:LEU:CD1  | 0.42     | 2.66        | 11     | 1     |
| 1:A:63:LEU:HD22  | 1:A:152:LEU:HD23 | 0.42     | 1.90        | 7      | 1     |
| 1:A:96:GLU:HG3   | 1:A:124:ILE:CD1  | 0.42     | 2.44        | 9      | 2     |
| 1:A:109:SER:OG   | 1:A:112:GLN:CG   | 0.42     | 2.67        | 15     | 1     |
| 1:A:29:GLN:OE1   | 1:A:29:GLN:N     | 0.42     | 2.52        | 17     | 1     |
| 1:A:62:ASN:N     | 1:A:62:ASN:OD1   | 0.42     | 2.52        | 20     | 1     |
| 1:A:79:PHE:CE2   | 1:A:184:GLN:HB3  | 0.42     | 2.49        | 9      | 3     |
| 1:A:33:ILE:CD1   | 1:A:120:THR:N    | 0.42     | 2.82        | 2      | 1     |
| 1:A:74:CYS:O     | 1:A:75:PHE:CD1   | 0.42     | 2.72        | 2      | 1     |
| 1:A:49:ASN:OD1   | 1:A:49:ASN:N     | 0.42     | 2.52        | 2      | 1     |
| 1:A:93:LEU:O     | 1:A:96:GLU:CB    | 0.42     | 2.68        | 2      | 1     |
| 1:A:93:LEU:HD11  | 1:A:137:ILE:HG23 | 0.42     | 1.90        | 10     | 1     |
| 1:A:41:ARG:CG    | 1:A:168:LEU:HD13 | 0.42     | 2.44        | 10     | 1     |
| 1:A:137:ILE:O    | 1:A:138:THR:CB   | 0.42     | 2.67        | 3      | 2     |
| 1:A:138:THR:O    | 1:A:139:THR:CB   | 0.42     | 2.67        | 3      | 1     |
| 1:A:40:LEU:O     | 1:A:44:THR:HG21  | 0.42     | 2.14        | 1      | 2     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:26:ILE:CG2   | 1:A:182:LEU:HD21 | 0.42     | 2.43        | 28     | 1     |
| 1:A:26:ILE:HD12  | 1:A:127:LEU:CD2  | 0.42     | 2.45        | 20     | 1     |
| 1:A:155:GLN:CB   | 1:A:159:LEU:HB3  | 0.42     | 2.43        | 10     | 1     |
| 1:A:158:TRP:CD1  | 1:A:158:TRP:C    | 0.42     | 2.93        | 5      | 2     |
| 1:A:85:LEU:HD13  | 1:A:182:LEU:CD1  | 0.42     | 2.44        | 5      | 1     |
| 1:A:123:LEU:H    | 1:A:123:LEU:HD22 | 0.42     | 1.74        | 12     | 1     |
| 1:A:152:LEU:HD23 | 1:A:152:LEU:N    | 0.42     | 2.29        | 29     | 1     |
| 1:A:34:LEU:HD23  | 1:A:172:LYS:NZ   | 0.42     | 2.30        | 15     | 1     |
| 1:A:175:LEU:O    | 1:A:179:LEU:CD1  | 0.42     | 2.67        | 19     | 1     |
| 1:A:50:MET:SD    | 1:A:158:TRP:CZ2  | 0.42     | 3.12        | 6      | 1     |
| 1:A:40:LEU:CG    | 1:A:116:VAL:HG21 | 0.42     | 2.44        | 4      | 1     |
| 1:A:98:TYR:O     | 1:A:101:TYR:CB   | 0.42     | 2.67        | 8      | 1     |
| 1:A:63:LEU:HD21  | 1:A:152:LEU:HD23 | 0.42     | 1.91        | 25     | 1     |
| 1:A:116:VAL:O    | 1:A:120:THR:CB   | 0.42     | 2.68        | 26     | 3     |
| 1:A:95:PHE:CE1   | 1:A:170:SER:HB3  | 0.42     | 2.50        | 4      | 1     |
| 1:A:39:ALA:CB    | 1:A:112:GLN:OE1  | 0.42     | 2.68        | 30     | 2     |
| 1:A:123:LEU:O    | 1:A:127:LEU:CG   | 0.42     | 2.67        | 1      | 3     |
| 1:A:128:GLN:OE1  | 1:A:137:ILE:CB   | 0.42     | 2.67        | 2      | 1     |
| 1:A:63:LEU:HD21  | 1:A:163:THR:CG2  | 0.42     | 2.41        | 32     | 1     |
| 1:A:137:ILE:HD12 | 1:A:137:ILE:H    | 0.42     | 1.72        | 3      | 1     |
| 1:A:79:PHE:CG    | 1:A:80:ASN:N     | 0.42     | 2.87        | 3      | 3     |
| 1:A:49:ASN:N     | 1:A:49:ASN:OD1   | 0.42     | 2.53        | 31     | 1     |
| 1:A:44:THR:O     | 1:A:48:SER:CA    | 0.42     | 2.68        | 25     | 2     |
| 1:A:75:PHE:O     | 1:A:79:PHE:N     | 0.42     | 2.53        | 20     | 1     |
| 1:A:89:ILE:HD12  | 1:A:137:ILE:CG1  | 0.42     | 2.44        | 15     | 1     |
| 1:A:33:ILE:HG23  | 1:A:120:THR:HG1  | 0.42     | 1.74        | 17     | 1     |
| 1:A:160:GLN:HG3  | 1:A:161:ASP:N    | 0.42     | 2.30        | 31     | 1     |
| 1:A:50:MET:O     | 1:A:165:HIS:CE1  | 0.42     | 2.73        | 11     | 1     |
| 1:A:33:ILE:CG2   | 1:A:120:THR:OG1  | 0.42     | 2.67        | 26     | 3     |
| 1:A:69:ALA:CB    | 1:A:72:ASP:HB3   | 0.42     | 2.45        | 32     | 1     |
| 1:A:126:PHE:CD2  | 1:A:130:LYS:HE2  | 0.42     | 2.50        | 10     | 1     |
| 1:A:65:LEU:HD13  | 1:A:98:TYR:CD2   | 0.42     | 2.50        | 15     | 1     |
| 1:A:85:LEU:HD11  | 1:A:127:LEU:HD22 | 0.41     | 1.92        | 8      | 1     |
| 1:A:123:LEU:O    | 1:A:127:LEU:CD1  | 0.41     | 2.67        | 29     | 1     |
| 1:A:145:ASN:O    | 1:A:145:ASN:ND2  | 0.41     | 2.52        | 21     | 1     |
| 1:A:166:LEU:CD1  | 1:A:166:LEU:C    | 0.41     | 2.89        | 30     | 2     |
| 1:A:116:VAL:O    | 1:A:120:THR:CG2  | 0.41     | 2.68        | 30     | 1     |
| 1:A:50:MET:HB3   | 1:A:165:HIS:CE1  | 0.41     | 2.50        | 29     | 1     |
| 1:A:84:CYS:SG    | 1:A:181:ALA:HB2  | 0.41     | 2.54        | 26     | 1     |
| 1:A:63:LEU:CD2   | 1:A:163:THR:CG2  | 0.41     | 2.90        | 32     | 1     |
| 1:A:30:ILE:N     | 1:A:123:LEU:HD11 | 0.41     | 2.30        | 32     | 1     |

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| Atom-1          | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|-----------------|------------------|----------|-------------|--------|-------|
|                 |                  |          |             | Worst  | Total |
| 1:A:130:LYS:CD  | 1:A:130:LYS:O    | 0.41     | 2.68        | 1      | 3     |
| 1:A:160:GLN:CG  | 1:A:161:ASP:N    | 0.41     | 2.83        | 31     | 1     |
| 1:A:40:LEU:HB2  | 1:A:168:LEU:HD11 | 0.41     | 1.92        | 11     | 2     |
| 1:A:138:THR:O   | 1:A:139:THR:HB   | 0.41     | 2.15        | 17     | 2     |
| 1:A:156:ASN:O   | 1:A:157:GLN:HB3  | 0.41     | 2.15        | 29     | 1     |
| 1:A:101:TYR:CZ  | 1:A:163:THR:HG21 | 0.41     | 2.50        | 7      | 1     |
| 1:A:30:ILE:HG23 | 1:A:175:LEU:CD2  | 0.41     | 2.38        | 2      | 1     |
| 1:A:103:GLN:OE1 | 1:A:117:GLN:NE2  | 0.41     | 2.54        | 2      | 1     |
| 1:A:62:ASN:ND2  | 1:A:62:ASN:N     | 0.41     | 2.67        | 32     | 1     |
| 1:A:63:LEU:HD12 | 1:A:166:LEU:HD13 | 0.41     | 1.93        | 32     | 1     |
| 1:A:82:GLU:CG   | 1:A:133:ASN:O    | 0.41     | 2.68        | 4      | 1     |
| 1:A:173:GLU:O   | 1:A:174:PHE:C    | 0.41     | 2.59        | 32     | 9     |
| 1:A:136:ALA:O   | 1:A:137:ILE:HB   | 0.41     | 2.16        | 23     | 3     |
| 1:A:131:ALA:O   | 1:A:134:LEU:HB2  | 0.41     | 2.15        | 22     | 2     |
| 1:A:47:LYS:O    | 1:A:49:ASN:N     | 0.41     | 2.53        | 10     | 1     |
| 1:A:48:SER:O    | 1:A:49:ASN:C     | 0.41     | 2.59        | 8      | 2     |
| 1:A:78:GLY:O    | 1:A:80:ASN:N     | 0.41     | 2.54        | 9      | 2     |
| 1:A:89:ILE:HD13 | 1:A:137:ILE:HD12 | 0.41     | 1.93        | 16     | 1     |
| 1:A:34:LEU:N    | 1:A:34:LEU:CD1   | 0.41     | 2.83        | 17     | 1     |
| 1:A:79:PHE:CZ   | 1:A:184:GLN:HG3  | 0.41     | 2.51        | 8      | 1     |
| 1:A:66:PRO:O    | 1:A:67:LYS:CB    | 0.41     | 2.68        | 20     | 1     |
| 1:A:65:LEU:O    | 1:A:65:LEU:CG    | 0.41     | 2.68        | 2      | 1     |
| 1:A:170:SER:O   | 1:A:174:PHE:HB3  | 0.41     | 2.16        | 16     | 2     |
| 1:A:40:LEU:HD11 | 1:A:116:VAL:CB   | 0.41     | 2.45        | 4      | 2     |
| 1:A:126:PHE:O   | 1:A:130:LYS:HG3  | 0.41     | 2.16        | 15     | 1     |
| 1:A:62:ASN:C    | 1:A:63:LEU:HG    | 0.41     | 2.36        | 6      | 1     |
| 1:A:74:CYS:C    | 1:A:75:PHE:CD1   | 0.41     | 2.94        | 25     | 2     |
| 1:A:90:THR:CG2  | 1:A:137:ILE:CG2  | 0.41     | 2.91        | 28     | 2     |
| 1:A:137:ILE:H   | 1:A:137:ILE:HD12 | 0.41     | 1.74        | 22     | 1     |
| 1:A:126:PHE:O   | 1:A:130:LYS:HB3  | 0.41     | 2.15        | 22     | 1     |
| 1:A:95:PHE:CZ   | 1:A:170:SER:HB3  | 0.41     | 2.50        | 5      | 3     |
| 1:A:29:GLN:HB3  | 1:A:123:LEU:CD1  | 0.41     | 2.45        | 14     | 1     |
| 1:A:29:GLN:HG2  | 1:A:123:LEU:CD2  | 0.41     | 2.46        | 16     | 1     |
| 1:A:21:THR:O    | 1:A:24:GLU:HG3   | 0.41     | 2.16        | 4      | 1     |
| 1:A:130:LYS:O   | 1:A:130:LYS:CG   | 0.41     | 2.69        | 9      | 1     |
| 1:A:40:LEU:O    | 1:A:168:LEU:HD21 | 0.41     | 2.16        | 18     | 1     |
| 1:A:63:LEU:HD11 | 1:A:167:ILE:HG13 | 0.41     | 1.92        | 18     | 1     |
| 1:A:88:ILE:O    | 1:A:92:LEU:CG    | 0.41     | 2.69        | 18     | 1     |
| 1:A:89:ILE:CG1  | 1:A:137:ILE:HD13 | 0.41     | 2.45        | 24     | 1     |
| 1:A:97:VAL:CG1  | 1:A:145:ASN:ND2  | 0.41     | 2.81        | 30     | 1     |
| 1:A:105:ARG:O   | 1:A:107:GLU:N    | 0.41     | 2.54        | 25     | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:79:PHE:CD2   | 1:A:81:GLU:HG3   | 0.41     | 2.51        | 16     | 1     |
| 1:A:105:ARG:CZ   | 1:A:160:GLN:OE1  | 0.41     | 2.69        | 3      | 1     |
| 1:A:162:MET:HE1  | 1:A:166:LEU:HB2  | 0.41     | 1.93        | 15     | 1     |
| 1:A:106:PHE:O    | 1:A:110:GLU:CB   | 0.41     | 2.69        | 5      | 1     |
| 1:A:131:ALA:O    | 1:A:134:LEU:O    | 0.41     | 2.39        | 24     | 1     |
| 1:A:137:ILE:HG22 | 1:A:138:THR:H    | 0.41     | 1.74        | 24     | 1     |
| 1:A:22:SER:HB3   | 1:A:130:LYS:CD   | 0.41     | 2.46        | 24     | 1     |
| 1:A:45:CYS:SG    | 1:A:165:HIS:CD2  | 0.41     | 3.14        | 28     | 1     |
| 1:A:168:LEU:O    | 1:A:172:LYS:CG   | 0.41     | 2.69        | 26     | 1     |
| 1:A:67:LYS:CD    | 1:A:170:SER:OG   | 0.41     | 2.69        | 19     | 1     |
| 1:A:137:ILE:C    | 1:A:138:THR:OG1  | 0.41     | 2.59        | 22     | 1     |
| 1:A:68:MET:SD    | 1:A:174:PHE:CZ   | 0.40     | 3.14        | 27     | 1     |
| 1:A:97:VAL:HG13  | 1:A:98:TYR:CD1   | 0.40     | 2.51        | 32     | 1     |
| 1:A:29:GLN:C     | 1:A:123:LEU:HD11 | 0.40     | 2.36        | 32     | 1     |
| 1:A:26:ILE:HA    | 1:A:123:LEU:CD1  | 0.40     | 2.46        | 9      | 1     |
| 1:A:92:LEU:HB3   | 1:A:124:ILE:CG1  | 0.40     | 2.45        | 3      | 1     |
| 1:A:73:GLY:O     | 1:A:80:ASN:N     | 0.40     | 2.53        | 1      | 1     |
| 1:A:98:TYR:CD1   | 1:A:167:ILE:HG12 | 0.40     | 2.51        | 23     | 1     |
| 1:A:96:GLU:HG3   | 1:A:97:VAL:N     | 0.40     | 2.31        | 8      | 1     |
| 1:A:40:LEU:HB2   | 1:A:168:LEU:CD2  | 0.40     | 2.46        | 25     | 1     |
| 1:A:62:ASN:N     | 1:A:62:ASN:ND2   | 0.40     | 2.69        | 12     | 1     |
| 1:A:124:ILE:HG23 | 1:A:125:GLN:N    | 0.40     | 2.31        | 11     | 1     |
| 1:A:64:ASN:O     | 1:A:65:LEU:O     | 0.40     | 2.39        | 6      | 1     |
| 1:A:145:ASN:HD21 | 1:A:148:LEU:HD23 | 0.40     | 1.76        | 1      | 1     |
| 1:A:29:GLN:HG3   | 1:A:123:LEU:HD11 | 0.40     | 1.91        | 2      | 1     |
| 1:A:127:LEU:CD1  | 1:A:127:LEU:C    | 0.40     | 2.90        | 13     | 1     |
| 1:A:50:MET:O     | 1:A:165:HIS:ND1  | 0.40     | 2.55        | 13     | 1     |
| 1:A:86:VAL:HG13  | 1:A:136:ALA:O    | 0.40     | 2.17        | 16     | 2     |
| 1:A:88:ILE:CD1   | 1:A:178:SER:HA   | 0.40     | 2.47        | 8      | 1     |
| 1:A:124:ILE:HG22 | 1:A:128:GLN:OE1  | 0.40     | 2.17        | 30     | 1     |
| 1:A:44:THR:O     | 1:A:45:CYS:CB    | 0.40     | 2.70        | 20     | 1     |
| 1:A:173:GLU:CA   | 1:A:173:GLU:OE1  | 0.40     | 2.70        | 7      | 1     |
| 1:A:45:CYS:SG    | 1:A:50:MET:O     | 0.40     | 2.79        | 32     | 1     |
| 1:A:69:ALA:O     | 1:A:75:PHE:CD2   | 0.40     | 2.75        | 4      | 1     |
| 1:A:41:ARG:HG2   | 1:A:45:CYS:CB    | 0.40     | 2.47        | 18     | 1     |
| 1:A:27:ASP:OD1   | 1:A:179:LEU:CD2  | 0.40     | 2.67        | 19     | 1     |
| 1:A:143:THR:O    | 1:A:146:ALA:HB3  | 0.40     | 2.16        | 23     | 1     |
| 1:A:92:LEU:HD13  | 1:A:127:LEU:CD1  | 0.40     | 2.45        | 25     | 1     |
| 1:A:26:ILE:HA    | 1:A:123:LEU:HD12 | 0.40     | 1.92        | 12     | 1     |
| 1:A:74:CYS:SG    | 1:A:181:ALA:HB1  | 0.40     | 2.56        | 20     | 1     |
| 1:A:101:TYR:CE1  | 1:A:152:LEU:CB   | 0.40     | 3.05        | 21     | 1     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:27:ASP:HA   | 1:A:182:LEU:CD1 | 0.40     | 2.46        | 16     | 1     |
| 1:A:25:ARG:O    | 1:A:29:GLN:NE2  | 0.40     | 2.54        | 9      | 1     |
| 1:A:166:LEU:C   | 1:A:166:LEU:CD1 | 0.40     | 2.89        | 22     | 1     |
| 1:A:96:GLU:HG2  | 1:A:97:VAL:N    | 0.40     | 2.31        | 24     | 1     |
| 1:A:162:MET:HA  | 1:A:165:HIS:CE1 | 0.40     | 2.52        | 13     | 1     |
| 1:A:40:LEU:HD21 | 1:A:113:ALA:CA  | 0.40     | 2.47        | 17     | 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     | 150/185 (81%)   | 123±4 (82±2%) | 21±3 (14±2%) | 6±2 (4±1%) | 6           | 33 |
| All | All   | 4800/5920 (81%) | 3945 (82%)    | 663 (14%)    | 192 (4%)   | 6           | 33 |

All 31 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     | 137 | ILE  | 21             |
| 1   | A     | 45  | CYS  | 19             |
| 1   | A     | 138 | THR  | 19             |
| 1   | A     | 63  | LEU  | 17             |
| 1   | A     | 67  | LYS  | 14             |
| 1   | A     | 81  | GLU  | 9              |
| 1   | A     | 104 | ASN  | 8              |
| 1   | A     | 49  | ASN  | 8              |
| 1   | A     | 69  | ALA  | 7              |
| 1   | A     | 135 | ASP  | 7              |
| 1   | A     | 134 | LEU  | 7              |
| 1   | A     | 79  | PHE  | 7              |
| 1   | A     | 62  | ASN  | 7              |
| 1   | A     | 74  | CYS  | 6              |
| 1   | A     | 77  | SER  | 6              |
| 1   | A     | 73  | GLY  | 4              |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 132 | LYS  | 4              |
| 1   | A     | 76  | GLN  | 3              |
| 1   | A     | 70  | GLU  | 3              |
| 1   | A     | 156 | ASN  | 2              |
| 1   | A     | 72  | ASP  | 2              |
| 1   | A     | 46  | ASN  | 2              |
| 1   | A     | 165 | HIS  | 2              |
| 1   | A     | 155 | GLN  | 1              |
| 1   | A     | 80  | ASN  | 1              |
| 1   | A     | 65  | LEU  | 1              |
| 1   | A     | 139 | THR  | 1              |
| 1   | A     | 48  | SER  | 1              |
| 1   | A     | 21  | THR  | 1              |
| 1   | A     | 50  | MET  | 1              |
| 1   | A     | 106 | 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     | 138/166 (83%)   | 98±4 (71±3%) | 40±4 (29±3%) | 2           | 19 |
| All | All   | 4416/5312 (83%) | 3143 (71%)   | 1273 (29%)   | 2           | 19 |

All 113 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     | 162 | MET  | 32             |
| 1   | A     | 138 | THR  | 31             |
| 1   | A     | 134 | LEU  | 31             |
| 1   | A     | 145 | ASN  | 30             |
| 1   | A     | 101 | TYR  | 30             |
| 1   | A     | 102 | LEU  | 30             |
| 1   | A     | 65  | LEU  | 29             |
| 1   | A     | 132 | LYS  | 24             |
| 1   | A     | 130 | LYS  | 24             |
| 1   | A     | 150 | THR  | 23             |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 68  | MET  | 23             |
| 1   | A     | 170 | SER  | 22             |
| 1   | A     | 105 | ARG  | 22             |
| 1   | A     | 67  | LYS  | 21             |
| 1   | A     | 32  | TYR  | 21             |
| 1   | A     | 34  | LEU  | 21             |
| 1   | A     | 50  | MET  | 20             |
| 1   | A     | 169 | ARG  | 19             |
| 1   | A     | 31  | ARG  | 19             |
| 1   | A     | 82  | GLU  | 19             |
| 1   | A     | 28  | LYS  | 18             |
| 1   | A     | 45  | CYS  | 18             |
| 1   | A     | 47  | LYS  | 16             |
| 1   | A     | 147 | SER  | 16             |
| 1   | A     | 90  | THR  | 16             |
| 1   | A     | 151 | LYS  | 16             |
| 1   | A     | 183 | ARG  | 16             |
| 1   | A     | 76  | GLN  | 15             |
| 1   | A     | 160 | GLN  | 15             |
| 1   | A     | 94  | GLU  | 15             |
| 1   | A     | 108 | SER  | 15             |
| 1   | A     | 71  | LYS  | 15             |
| 1   | A     | 176 | GLN  | 15             |
| 1   | A     | 135 | ASP  | 14             |
| 1   | A     | 109 | SER  | 14             |
| 1   | A     | 107 | GLU  | 14             |
| 1   | A     | 42  | LYS  | 14             |
| 1   | A     | 87  | LYS  | 14             |
| 1   | A     | 180 | ARG  | 14             |
| 1   | A     | 114 | ARG  | 13             |
| 1   | A     | 119 | SER  | 13             |
| 1   | A     | 172 | LYS  | 13             |
| 1   | A     | 129 | LYS  | 13             |
| 1   | A     | 43  | GLU  | 13             |
| 1   | A     | 25  | ARG  | 13             |
| 1   | A     | 24  | GLU  | 13             |
| 1   | A     | 38  | SER  | 12             |
| 1   | A     | 179 | LEU  | 12             |
| 1   | A     | 77  | SER  | 12             |
| 1   | A     | 121 | LYS  | 12             |
| 1   | A     | 104 | ASN  | 11             |
| 1   | A     | 100 | GLU  | 11             |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 152 | LEU  | 11             |
| 1   | A     | 182 | LEU  | 10             |
| 1   | A     | 35  | ASP  | 10             |
| 1   | A     | 70  | GLU  | 10             |
| 1   | A     | 22  | SER  | 10             |
| 1   | A     | 23  | SER  | 10             |
| 1   | A     | 173 | GLU  | 10             |
| 1   | A     | 97  | VAL  | 9              |
| 1   | A     | 177 | SER  | 9              |
| 1   | A     | 157 | GLN  | 9              |
| 1   | A     | 133 | ASN  | 8              |
| 1   | A     | 80  | ASN  | 8              |
| 1   | A     | 118 | MET  | 8              |
| 1   | A     | 84  | CYS  | 8              |
| 1   | A     | 48  | SER  | 8              |
| 1   | A     | 96  | GLU  | 8              |
| 1   | A     | 72  | ASP  | 8              |
| 1   | A     | 127 | LEU  | 7              |
| 1   | A     | 74  | CYS  | 7              |
| 1   | A     | 112 | GLN  | 7              |
| 1   | A     | 159 | LEU  | 7              |
| 1   | A     | 128 | GLN  | 7              |
| 1   | A     | 184 | GLN  | 6              |
| 1   | A     | 29  | GLN  | 6              |
| 1   | A     | 111 | GLU  | 6              |
| 1   | A     | 46  | ASN  | 6              |
| 1   | A     | 93  | LEU  | 6              |
| 1   | A     | 117 | GLN  | 5              |
| 1   | A     | 92  | LEU  | 5              |
| 1   | A     | 106 | PHE  | 5              |
| 1   | A     | 185 | MET  | 5              |
| 1   | A     | 103 | GLN  | 5              |
| 1   | A     | 63  | LEU  | 5              |
| 1   | A     | 166 | LEU  | 5              |
| 1   | A     | 125 | GLN  | 5              |
| 1   | A     | 168 | LEU  | 5              |
| 1   | A     | 124 | ILE  | 5              |
| 1   | A     | 41  | ARG  | 5              |
| 1   | A     | 153 | GLN  | 4              |
| 1   | A     | 110 | GLU  | 4              |
| 1   | A     | 137 | ILE  | 4              |
| 1   | A     | 62  | ASN  | 4              |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 81  | GLU  | 4              |
| 1   | A     | 144 | THR  | 3              |
| 1   | A     | 164 | THR  | 3              |
| 1   | A     | 178 | SER  | 3              |
| 1   | A     | 49  | ASN  | 3              |
| 1   | A     | 88  | ILE  | 3              |
| 1   | A     | 26  | ILE  | 3              |
| 1   | A     | 21  | THR  | 3              |
| 1   | A     | 64  | ASN  | 2              |
| 1   | A     | 75  | PHE  | 2              |
| 1   | A     | 174 | PHE  | 2              |
| 1   | A     | 148 | LEU  | 2              |
| 1   | A     | 27  | ASP  | 2              |
| 1   | A     | 126 | PHE  | 1              |
| 1   | A     | 149 | LEU  | 1              |
| 1   | A     | 139 | THR  | 1              |
| 1   | A     | 158 | TRP  | 1              |
| 1   | A     | 44  | THR  | 1              |
| 1   | A     | 95  | PHE  | 1              |

### 6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 6.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.6 Ligand geometry [i](#)

There are no ligands in this entry.

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

There are no such molecules in this entry.

## 6.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 7 Chemical shift validation

No chemical shift data were provided