



# Full wwPDB NMR Structure Validation Report ⓘ

Feb 12, 2017 – 05:53 pm GMT

PDB ID : 1DS9  
Title : SOLUTION STRUCTURE OF CHLAMYDOMONAS OUTER ARM  
DYNEIN LIGHT CHAIN 1  
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Deposited on : 2000-01-07

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

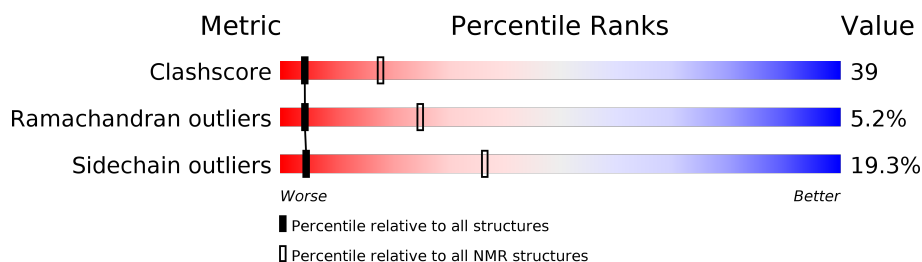
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 75%.

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



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

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

| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 1   | A     | 198    |  |

## 2 Ensemble composition and analysis

This entry contains 17 models. Model 1 is the overall representative, medoid model (most similar to other models). The authors have identified model 8 as representative, based on the following criterion: *lowest energy*.

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

| Well-defined (core) protein residues |                       |                   |              |
|--------------------------------------|-----------------------|-------------------|--------------|
| Well-defined core                    | Residue range (total) | Backbone RMSD (Å) | Medoid model |
| 1                                    | A:2-A:195 (194)       | 0.46              | 1            |

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

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

The models can be grouped into 2 clusters. No single-model clusters were found.

| Cluster number | Models                                       |
|----------------|----------------------------------------------|
| 1              | 1, 4, 5, 6, 7, 8, 10, 11, 12, 14, 15, 16, 17 |
| 2              | 2, 3, 9, 13                                  |

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

There is only 1 type of molecule in this entry. The entry contains 3161 atoms, of which 1610 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called OUTER ARM DYNEIN.

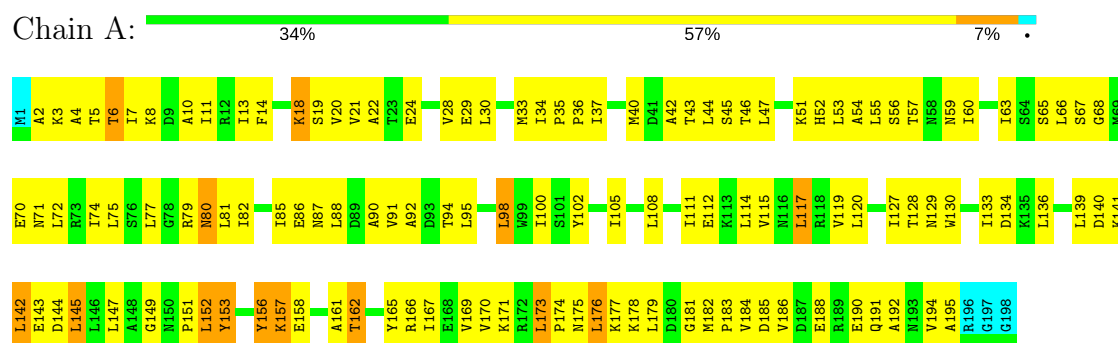
| Mol | Chain | Residues | Atoms |     |      |     |     |   | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|-------|
| 1   | A     | 198      | Total | C   | H    | N   | O   | S | 0     |
|     |       |          | 3161  | 975 | 1610 | 267 | 302 | 7 |       |

## 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: OUTER ARM DYNEIN



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

Colouring as in section 4.1 above.

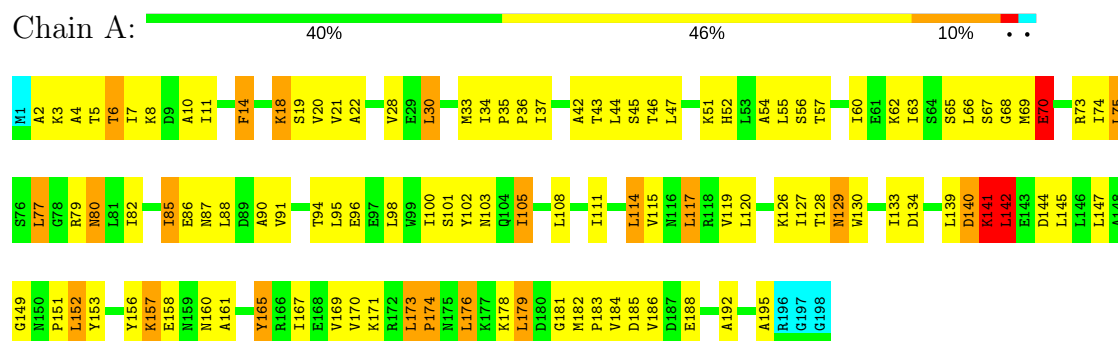
#### 4.2.1 Score per residue for model 1 (medoid)

#### • Molecule 1: OUTER ARM DYNEIN



### 4.2.2 Score per residue for model 2

- Molecule 1: OUTER ARM DYNEIN



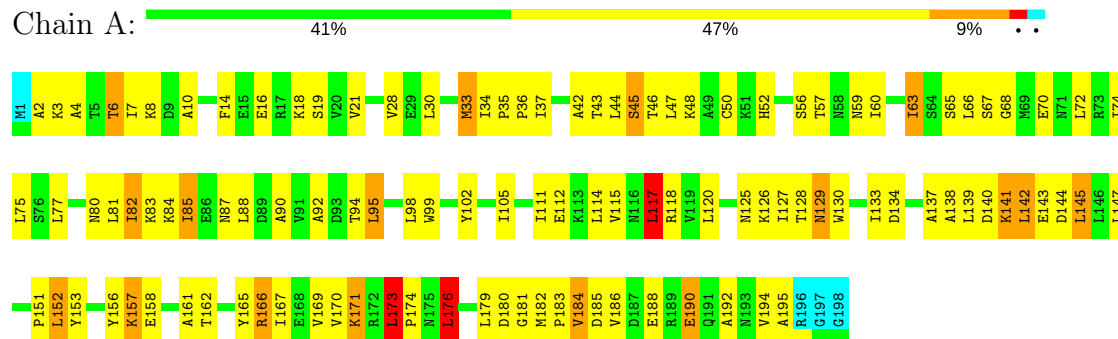
### 4.2.3 Score per residue for model 3

- Molecule 1: OUTER ARM DYNEIN



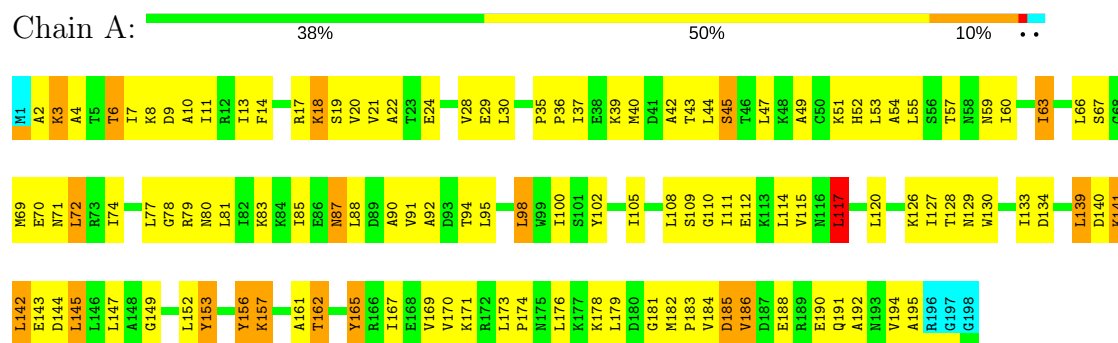
#### 4.2.4 Score per residue for model 4

- Molecule 1: OUTER ARM DYNEIN



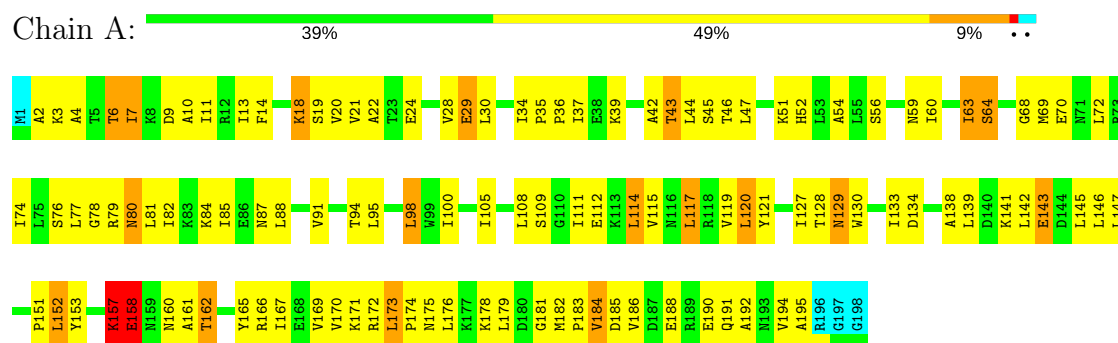
### 4.2.5 Score per residue for model 5

#### • Molecule 1: OUTER ARM DYNEIN



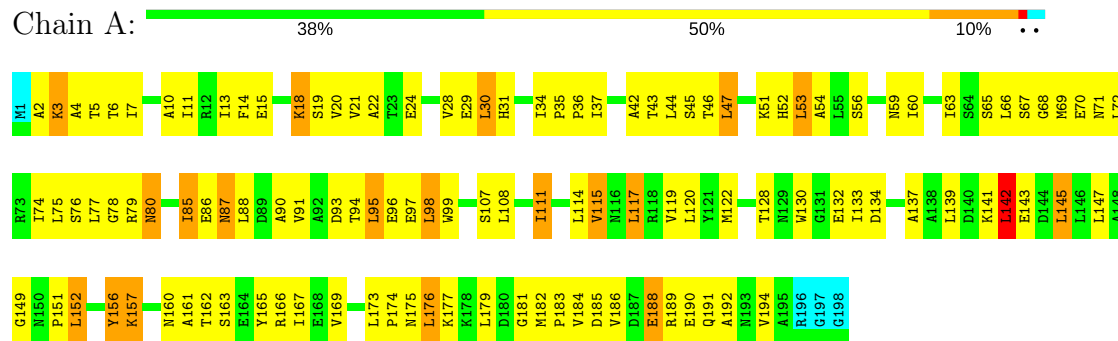
### 4.2.6 Score per residue for model 6

#### • Molecule 1: OUTER ARM DYNEIN



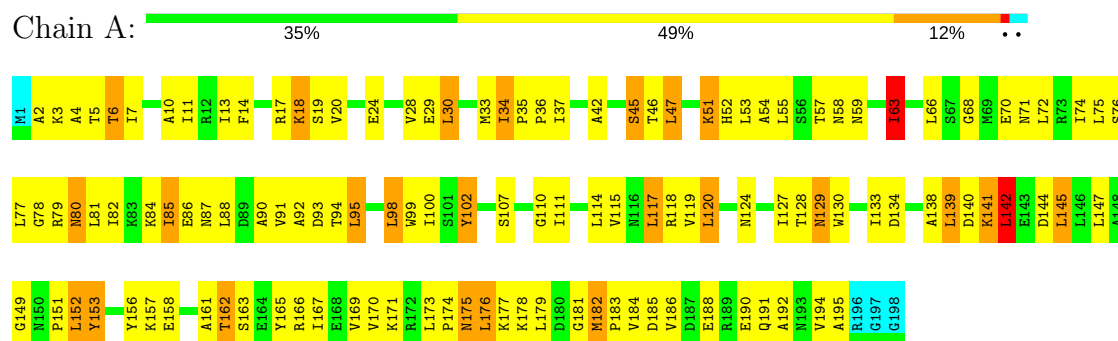
### 4.2.7 Score per residue for model 7

#### • Molecule 1: OUTER ARM DYNEIN



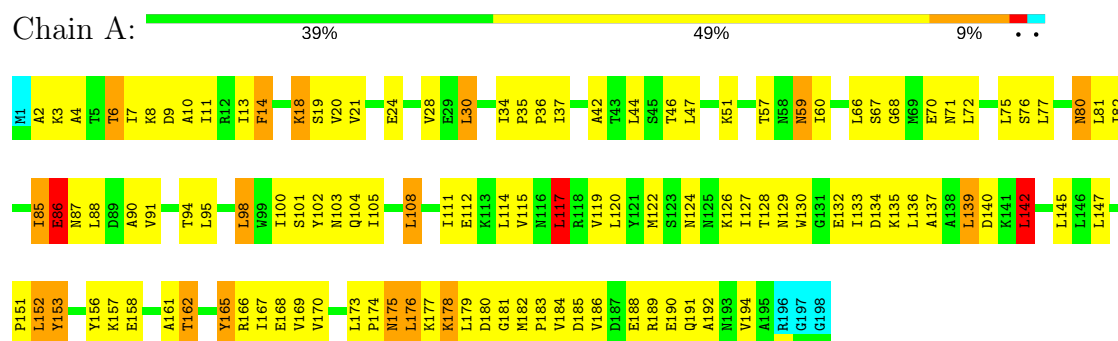
#### 4.2.8 Score per residue for model 8

- Molecule 1: OUTER ARM DYNEIN



#### 4.2.9 Score per residue for model 9

- Molecule 1: OUTER ARM DYNEIN



#### 4.2.10 Score per residue for model 10

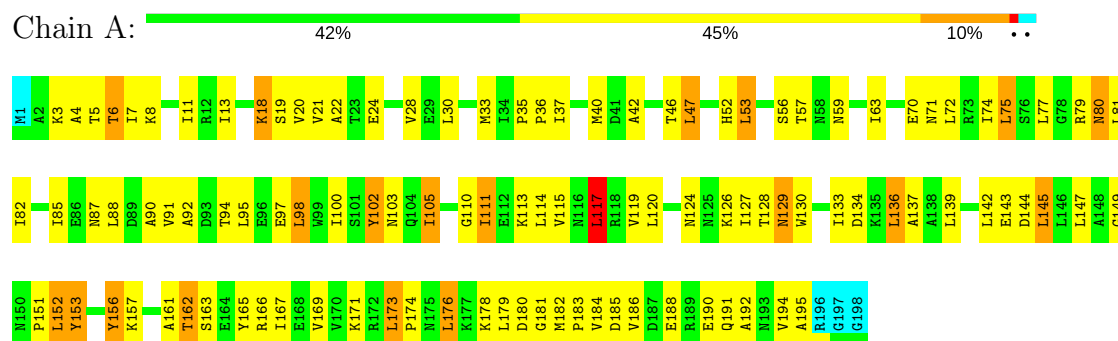
- Molecule 1: OUTER ARM DYNEIN





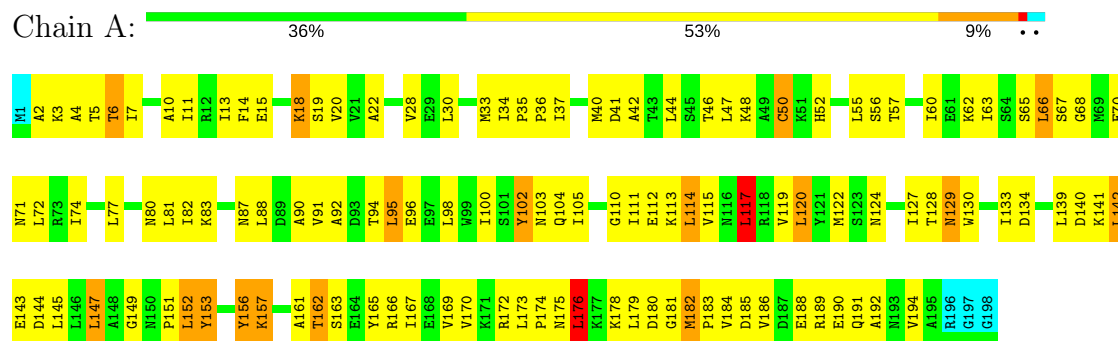
### 4.2.11 Score per residue for model 11

#### • Molecule 1: OUTER ARM DYNEIN



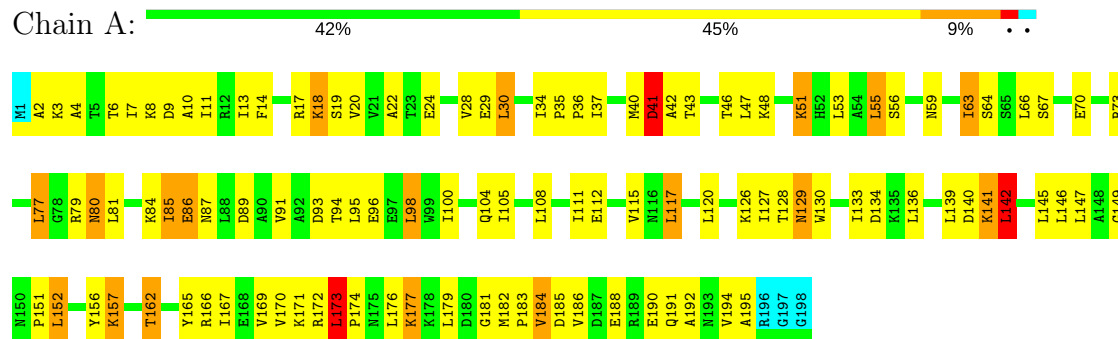
### 4.2.12 Score per residue for model 12

#### • Molecule 1: OUTER ARM DYNEIN



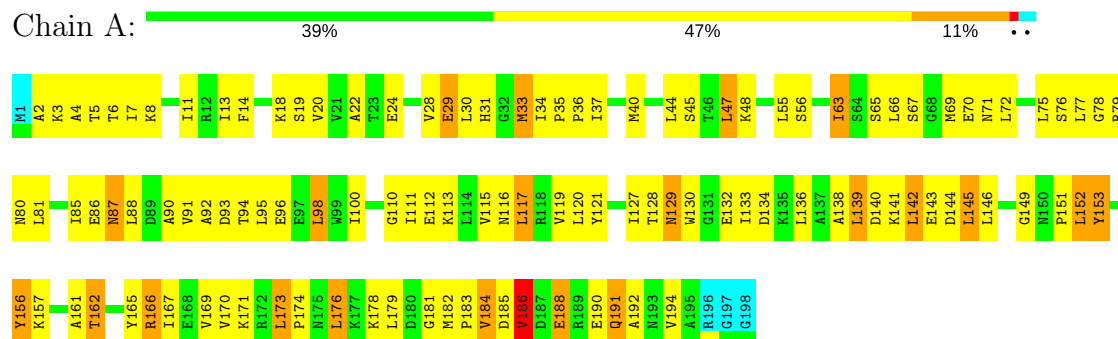
### 4.2.13 Score per residue for model 13

#### • Molecule 1: OUTER ARM DYNEIN



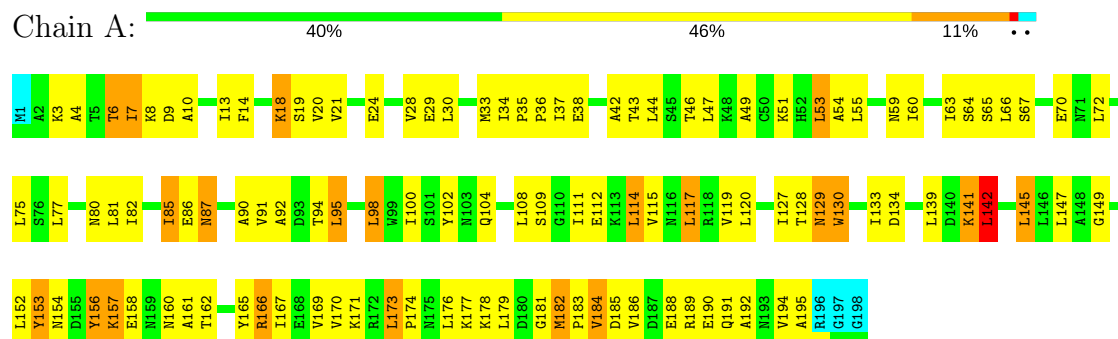
#### 4.2.14 Score per residue for model 14

- Molecule 1: OUTER ARM DYNEIN



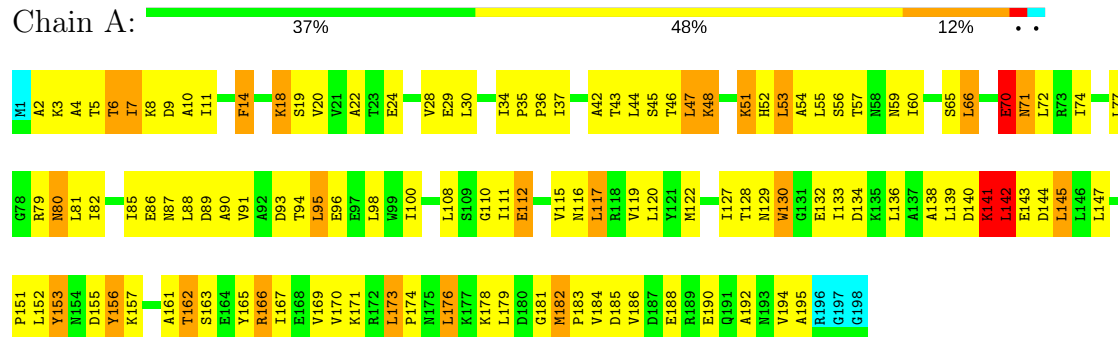
#### 4.2.15 Score per residue for model 15

- Molecule 1: OUTER ARM DYNEIN



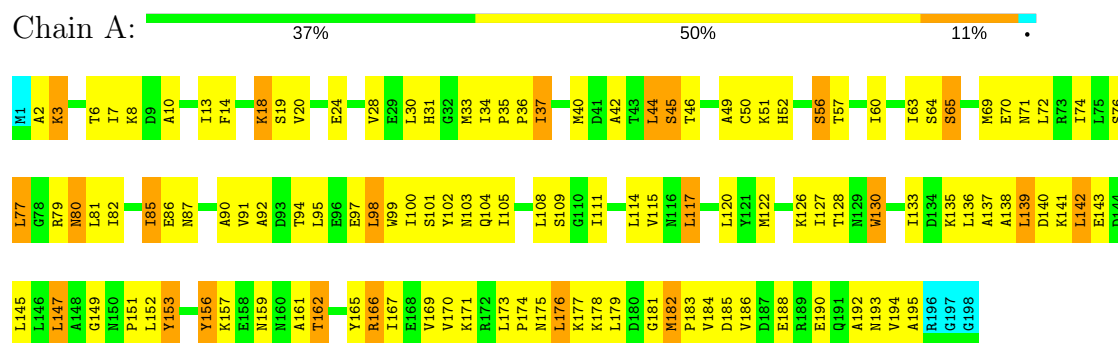
#### 4.2.16 Score per residue for model 16

- Molecule 1: OUTER ARM DYNEIN



## 4.2.17 Score per residue for model 17

### • Molecule 1: OUTER ARM DYNEIN



## 5 Refinement protocol and experimental data overview

The models were refined using the following method: *simulated annealing, torsion angle dynamics*.

Of the 150 calculated structures, 17 were deposited, based on the following criterion: *structures with the least restraint violations, structures with the lowest energy, target function*.

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

| Software name | Classification     | Version |
|---------------|--------------------|---------|
| X-PLOR        | refinement         | 4.0     |
| DYANA         | structure solution | 1.5     |

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

|                                              |                 |
|----------------------------------------------|-----------------|
| Chemical shift file(s)                       | BMRB entry 4265 |
| Number of chemical shift lists               | 1               |
| Total number of shifts                       | 2006            |
| Number of shifts mapped to atoms             | 2006            |
| Number of unparsed shifts                    | 0               |
| Number of shifts with mapping errors         | 0               |
| Number of shifts with mapping warnings       | 0               |
| Assignment completeness (well-defined parts) | 75%             |

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.

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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     | 1524  | 1582     | 1582     | 121±6   |
| All | All   | 25908 | 26894    | 26894    | 2059    |

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 39.

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

| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:115:VAL:HG22 | 1:A:142:LEU:HD21 | 1.07     | 1.25        | 17     | 2     |
| 1:A:145:LEU:HD12 | 1:A:147:LEU:HD11 | 1.06     | 1.27        | 4      | 11    |
| 1:A:60:ILE:HD11  | 1:A:82:ILE:HG23  | 1.01     | 1.27        | 9      | 3     |
| 1:A:142:LEU:HD13 | 1:A:145:LEU:HD13 | 1.00     | 1.31        | 7      | 5     |
| 1:A:173:LEU:HD23 | 1:A:176:LEU:HD21 | 1.00     | 1.25        | 10     | 1     |
| 1:A:142:LEU:HD13 | 1:A:145:LEU:HD21 | 0.99     | 1.28        | 4      | 1     |
| 1:A:145:LEU:HD11 | 1:A:179:LEU:HD12 | 0.99     | 1.31        | 7      | 4     |
| 1:A:170:VAL:HG11 | 1:A:192:ALA:HB1  | 0.98     | 1.31        | 15     | 12    |
| 1:A:115:VAL:HG22 | 1:A:142:LEU:HD11 | 0.97     | 1.31        | 7      | 3     |
| 1:A:77:LEU:HD22  | 1:A:100:ILE:HG23 | 0.97     | 1.34        | 6      | 3     |
| 1:A:105:ILE:HD12 | 1:A:111:ILE:HG22 | 0.95     | 1.34        | 6      | 3     |
| 1:A:169:VAL:HG13 | 1:A:176:LEU:HD12 | 0.95     | 1.32        | 17     | 4     |
| 1:A:82:ILE:HG21  | 1:A:88:LEU:HD12  | 0.93     | 1.36        | 11     | 1     |
| 1:A:85:ILE:HG21  | 1:A:88:LEU:HD12  | 0.91     | 1.43        | 6      | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:37:ILE:HG21  | 1:A:60:ILE:HG22  | 0.88     | 1.42        | 4      | 8     |
| 1:A:55:LEU:HD11  | 1:A:77:LEU:HD13  | 0.88     | 1.44        | 14     | 1     |
| 1:A:98:LEU:HD12  | 1:A:117:LEU:HD13 | 0.87     | 1.46        | 4      | 2     |
| 1:A:114:LEU:HD13 | 1:A:115:VAL:N    | 0.85     | 1.87        | 6      | 1     |
| 1:A:115:VAL:HG22 | 1:A:142:LEU:CD1  | 0.84     | 2.02        | 12     | 3     |
| 1:A:47:LEU:HD13  | 1:A:48:LYS:N     | 0.84     | 1.87        | 16     | 1     |
| 1:A:115:VAL:HG22 | 1:A:142:LEU:CD2  | 0.84     | 2.02        | 17     | 2     |
| 1:A:169:VAL:HG13 | 1:A:176:LEU:HD11 | 0.83     | 1.47        | 14     | 3     |
| 1:A:169:VAL:HG13 | 1:A:176:LEU:CD1  | 0.83     | 2.03        | 6      | 7     |
| 1:A:82:ILE:CG2   | 1:A:105:ILE:HG22 | 0.83     | 2.04        | 1      | 3     |
| 1:A:145:LEU:HD11 | 1:A:179:LEU:CD1  | 0.82     | 2.03        | 7      | 9     |
| 1:A:28:VAL:HG12  | 1:A:30:LEU:HD11  | 0.81     | 1.51        | 7      | 4     |
| 1:A:165:TYR:O    | 1:A:169:VAL:HG23 | 0.80     | 1.76        | 7      | 17    |
| 1:A:169:VAL:HG21 | 1:A:179:LEU:HB3  | 0.80     | 1.52        | 5      | 14    |
| 1:A:144:ASP:O    | 1:A:145:LEU:HD13 | 0.80     | 1.75        | 14     | 1     |
| 1:A:128:THR:HG22 | 1:A:151:PRO:CG   | 0.80     | 2.07        | 1      | 14    |
| 1:A:70:GLU:O     | 1:A:94:THR:HG21  | 0.80     | 1.76        | 16     | 14    |
| 1:A:107:SER:O    | 1:A:111:ILE:HG22 | 0.79     | 1.77        | 1      | 2     |
| 1:A:4:ALA:HB2    | 1:A:34:ILE:HG21  | 0.79     | 1.54        | 14     | 2     |
| 1:A:115:VAL:CG1  | 1:A:142:LEU:HD11 | 0.78     | 2.08        | 13     | 2     |
| 1:A:173:LEU:HD23 | 1:A:176:LEU:CD2  | 0.78     | 2.07        | 10     | 1     |
| 1:A:188:GLU:O    | 1:A:192:ALA:HB3  | 0.78     | 1.79        | 12     | 17    |
| 1:A:20:VAL:HG21  | 1:A:30:LEU:HD23  | 0.78     | 1.56        | 3      | 1     |
| 1:A:114:LEU:HD23 | 1:A:115:VAL:N    | 0.78     | 1.94        | 12     | 3     |
| 1:A:115:VAL:O    | 1:A:142:LEU:HD11 | 0.78     | 1.79        | 6      | 5     |
| 1:A:28:VAL:HG12  | 1:A:30:LEU:HD13  | 0.78     | 1.56        | 14     | 2     |
| 1:A:42:ALA:O     | 1:A:46:THR:HG23  | 0.77     | 1.79        | 17     | 2     |
| 1:A:169:VAL:HG22 | 1:A:173:LEU:HD12 | 0.77     | 1.53        | 5      | 3     |
| 1:A:95:LEU:O     | 1:A:117:LEU:HD11 | 0.77     | 1.79        | 16     | 5     |
| 1:A:47:LEU:HD23  | 1:A:68:GLY:O     | 0.77     | 1.79        | 7      | 3     |
| 1:A:66:LEU:CD2   | 1:A:90:ALA:HB2   | 0.77     | 2.08        | 8      | 1     |
| 1:A:2:ALA:CB     | 1:A:13:ILE:HG22  | 0.77     | 2.09        | 5      | 3     |
| 1:A:190:GLU:O    | 1:A:194:VAL:HG23 | 0.77     | 1.80        | 14     | 15    |
| 1:A:111:ILE:HD11 | 1:A:137:ALA:HB2  | 0.77     | 1.57        | 1      | 3     |
| 1:A:138:ALA:CB   | 1:A:142:LEU:HD23 | 0.77     | 2.08        | 14     | 1     |
| 1:A:145:LEU:CD1  | 1:A:147:LEU:HD11 | 0.76     | 2.09        | 4      | 3     |
| 1:A:170:VAL:HG21 | 1:A:192:ALA:HB1  | 0.76     | 1.57        | 14     | 2     |
| 1:A:42:ALA:O     | 1:A:46:THR:HG22  | 0.76     | 1.81        | 8      | 12    |
| 1:A:173:LEU:HD13 | 1:A:176:LEU:HD12 | 0.75     | 1.57        | 8      | 1     |
| 1:A:98:LEU:HD13  | 1:A:117:LEU:HD13 | 0.75     | 1.57        | 13     | 1     |
| 1:A:163:SER:O    | 1:A:167:ILE:HD12 | 0.75     | 1.81        | 12     | 4     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:129:ASN:HB2  | 1:A:133:ILE:HD12 | 0.75     | 1.59        | 8      | 7     |
| 1:A:129:ASN:CB   | 1:A:133:ILE:HD12 | 0.75     | 2.10        | 2      | 9     |
| 1:A:130:TRP:N    | 1:A:152:LEU:HD11 | 0.74     | 1.97        | 11     | 9     |
| 1:A:44:LEU:O     | 1:A:47:LEU:HD12  | 0.74     | 1.82        | 16     | 1     |
| 1:A:95:LEU:HD22  | 1:A:98:LEU:HD12  | 0.74     | 1.60        | 9      | 2     |
| 1:A:2:ALA:O      | 1:A:34:ILE:HD13  | 0.74     | 1.81        | 4      | 1     |
| 1:A:20:VAL:HG21  | 1:A:30:LEU:HD12  | 0.74     | 1.57        | 13     | 6     |
| 1:A:47:LEU:HD21  | 1:A:71:ASN:CB    | 0.74     | 2.11        | 3      | 3     |
| 1:A:128:THR:HG22 | 1:A:151:PRO:HG2  | 0.74     | 1.57        | 2      | 14    |
| 1:A:2:ALA:HB1    | 1:A:14:PHE:CD1   | 0.74     | 2.18        | 6      | 2     |
| 1:A:7:ILE:HD12   | 1:A:45:SER:HB2   | 0.74     | 1.60        | 10     | 5     |
| 1:A:80:ASN:C     | 1:A:81:LEU:HD12  | 0.74     | 2.04        | 5      | 5     |
| 1:A:181:GLY:O    | 1:A:184:VAL:HG23 | 0.73     | 1.82        | 7      | 12    |
| 1:A:98:LEU:HD12  | 1:A:117:LEU:CD1  | 0.73     | 2.13        | 14     | 2     |
| 1:A:77:LEU:HD21  | 1:A:80:ASN:CG    | 0.73     | 2.04        | 5      | 7     |
| 1:A:77:LEU:HD23  | 1:A:100:ILE:HG22 | 0.73     | 1.58        | 15     | 4     |
| 1:A:69:MET:HB3   | 1:A:91:VAL:HG22  | 0.73     | 1.59        | 10     | 2     |
| 1:A:69:MET:CB    | 1:A:91:VAL:HG22  | 0.73     | 2.13        | 6      | 2     |
| 1:A:176:LEU:HD11 | 1:A:179:LEU:HD23 | 0.72     | 1.58        | 2      | 1     |
| 1:A:142:LEU:HD23 | 1:A:145:LEU:HD22 | 0.72     | 1.60        | 11     | 2     |
| 1:A:4:ALA:HB2    | 1:A:37:ILE:HD12  | 0.72     | 1.60        | 7      | 10    |
| 1:A:85:ILE:HD13  | 1:A:86:GLU:N     | 0.72     | 2.00        | 2      | 8     |
| 1:A:82:ILE:HG23  | 1:A:105:ILE:HG22 | 0.72     | 1.61        | 12     | 1     |
| 1:A:28:VAL:CG1   | 1:A:30:LEU:HD11  | 0.72     | 2.14        | 7      | 7     |
| 1:A:111:ILE:HG21 | 1:A:133:ILE:CD1  | 0.72     | 2.13        | 1      | 2     |
| 1:A:100:ILE:HD12 | 1:A:103:ASN:CG   | 0.72     | 2.05        | 9      | 4     |
| 1:A:60:ILE:HD12  | 1:A:82:ILE:CD1   | 0.72     | 2.14        | 17     | 1     |
| 1:A:95:LEU:HD13  | 1:A:98:LEU:HD21  | 0.72     | 1.61        | 2      | 1     |
| 1:A:169:VAL:CG1  | 1:A:176:LEU:HD22 | 0.72     | 2.15        | 13     | 1     |
| 1:A:141:LYS:O    | 1:A:142:LEU:O    | 0.71     | 2.07        | 13     | 9     |
| 1:A:178:LYS:HE2  | 1:A:184:VAL:HG21 | 0.71     | 1.60        | 9      | 1     |
| 1:A:95:LEU:HD23  | 1:A:96:GLU:N     | 0.71     | 2.01        | 14     | 1     |
| 1:A:120:LEU:HD21 | 1:A:122:MET:CE   | 0.71     | 2.16        | 10     | 1     |
| 1:A:60:ILE:HD11  | 1:A:82:ILE:HG12  | 0.71     | 1.62        | 10     | 3     |
| 1:A:28:VAL:CG1   | 1:A:30:LEU:HD21  | 0.71     | 2.15        | 13     | 9     |
| 1:A:77:LEU:HD11  | 1:A:80:ASN:HB3   | 0.71     | 1.61        | 17     | 13    |
| 1:A:145:LEU:HD23 | 1:A:146:LEU:N    | 0.71     | 2.00        | 13     | 3     |
| 1:A:81:LEU:HD13  | 1:A:104:GLN:HB2  | 0.71     | 1.62        | 17     | 1     |
| 1:A:142:LEU:HD13 | 1:A:145:LEU:CD2  | 0.70     | 2.14        | 4      | 1     |
| 1:A:34:ILE:O     | 1:A:34:ILE:HD12  | 0.70     | 1.86        | 6      | 1     |
| 1:A:77:LEU:CD2   | 1:A:100:ILE:HG23 | 0.70     | 2.16        | 6      | 4     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:111:ILE:HD11 | 1:A:137:ALA:CB   | 0.70     | 2.17        | 1      | 3     |
| 1:A:95:LEU:HB3   | 1:A:117:LEU:HD21 | 0.70     | 1.64        | 6      | 2     |
| 1:A:63:ILE:HD13  | 1:A:64:SER:N     | 0.70     | 2.01        | 6      | 1     |
| 1:A:171:LYS:NZ   | 1:A:195:ALA:HB1  | 0.70     | 2.01        | 15     | 7     |
| 1:A:20:VAL:HG21  | 1:A:30:LEU:HD22  | 0.70     | 1.62        | 5      | 2     |
| 1:A:92:ALA:HA    | 1:A:117:LEU:HD12 | 0.70     | 1.64        | 4      | 2     |
| 1:A:181:GLY:O    | 1:A:184:VAL:HG13 | 0.69     | 1.86        | 17     | 4     |
| 1:A:142:LEU:O    | 1:A:176:LEU:HD22 | 0.69     | 1.87        | 9      | 2     |
| 1:A:70:GLU:CB    | 1:A:90:ALA:HB1   | 0.69     | 2.17        | 4      | 10    |
| 1:A:169:VAL:HG13 | 1:A:176:LEU:HD22 | 0.69     | 1.62        | 13     | 1     |
| 1:A:114:LEU:O    | 1:A:117:LEU:HD22 | 0.69     | 1.86        | 3      | 1     |
| 1:A:153:TYR:CZ   | 1:A:162:THR:HG23 | 0.69     | 2.22        | 8      | 4     |
| 1:A:66:LEU:HD22  | 1:A:67:SER:N     | 0.69     | 2.03        | 12     | 1     |
| 1:A:70:GLU:C     | 1:A:94:THR:HG21  | 0.69     | 2.08        | 10     | 10    |
| 1:A:28:VAL:HG12  | 1:A:30:LEU:CD1   | 0.69     | 2.17        | 7      | 5     |
| 1:A:37:ILE:CG2   | 1:A:60:ILE:HG23  | 0.69     | 2.18        | 2      | 1     |
| 1:A:70:GLU:CG    | 1:A:90:ALA:HB1   | 0.69     | 2.17        | 7      | 8     |
| 1:A:134:ASP:O    | 1:A:139:LEU:HD22 | 0.69     | 1.88        | 11     | 14    |
| 1:A:29:GLU:HA    | 1:A:54:ALA:HB3   | 0.69     | 1.65        | 8      | 8     |
| 1:A:173:LEU:CD1  | 1:A:176:LEU:HD11 | 0.69     | 2.18        | 7      | 1     |
| 1:A:3:LYS:HB2    | 1:A:13:ILE:HG21  | 0.68     | 1.64        | 12     | 2     |
| 1:A:47:LEU:HD21  | 1:A:71:ASN:HB2   | 0.68     | 1.65        | 8      | 4     |
| 1:A:167:ILE:HG22 | 1:A:171:LYS:HE2  | 0.68     | 1.64        | 1      | 3     |
| 1:A:14:PHE:CD1   | 1:A:30:LEU:HD22  | 0.68     | 2.22        | 3      | 2     |
| 1:A:111:ILE:O    | 1:A:115:VAL:HG22 | 0.68     | 1.88        | 1      | 3     |
| 1:A:3:LYS:HB3    | 1:A:13:ILE:HD13  | 0.68     | 1.64        | 7      | 4     |
| 1:A:162:THR:HG22 | 1:A:183:PRO:HG3  | 0.68     | 1.66        | 9      | 6     |
| 1:A:69:MET:HB2   | 1:A:91:VAL:HG22  | 0.68     | 1.64        | 6      | 1     |
| 1:A:81:LEU:HD22  | 1:A:104:GLN:NE2  | 0.68     | 2.03        | 9      | 1     |
| 1:A:4:ALA:CB     | 1:A:34:ILE:HG21  | 0.68     | 2.18        | 14     | 2     |
| 1:A:138:ALA:HB1  | 1:A:142:LEU:HD23 | 0.68     | 1.65        | 14     | 1     |
| 1:A:173:LEU:HD13 | 1:A:174:PRO:HD2  | 0.68     | 1.65        | 2      | 1     |
| 1:A:44:LEU:HD12  | 1:A:45:SER:N     | 0.67     | 2.04        | 6      | 2     |
| 1:A:92:ALA:O     | 1:A:117:LEU:HD12 | 0.67     | 1.88        | 11     | 2     |
| 1:A:115:VAL:HG12 | 1:A:142:LEU:HD11 | 0.67     | 1.64        | 15     | 1     |
| 1:A:145:LEU:N    | 1:A:145:LEU:HD22 | 0.67     | 2.03        | 14     | 1     |
| 1:A:11:ILE:HG23  | 1:A:22:ALA:HB3   | 0.67     | 1.65        | 14     | 12    |
| 1:A:90:ALA:O     | 1:A:94:THR:HG22  | 0.67     | 1.89        | 8      | 4     |
| 1:A:142:LEU:CD1  | 1:A:145:LEU:HD13 | 0.67     | 2.18        | 5      | 2     |
| 1:A:44:LEU:HD12  | 1:A:65:SER:OG    | 0.67     | 1.89        | 2      | 1     |
| 1:A:53:LEU:HD22  | 1:A:72:LEU:HD21  | 0.67     | 1.66        | 10     | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:66:LEU:HD21  | 1:A:90:ALA:HB2   | 0.67     | 1.65        | 8      | 1     |
| 1:A:7:ILE:HD12   | 1:A:45:SER:CB    | 0.67     | 2.20        | 10     | 5     |
| 1:A:63:ILE:HD11  | 1:A:87:ASN:HB2   | 0.67     | 1.66        | 10     | 1     |
| 1:A:140:ASP:HA   | 1:A:173:LEU:HD11 | 0.67     | 1.65        | 12     | 1     |
| 1:A:77:LEU:HG    | 1:A:100:ILE:HG22 | 0.66     | 1.65        | 11     | 1     |
| 1:A:91:VAL:HG22  | 1:A:95:LEU:CD1   | 0.66     | 2.20        | 2      | 1     |
| 1:A:77:LEU:HB3   | 1:A:100:ILE:HG22 | 0.66     | 1.67        | 2      | 5     |
| 1:A:134:ASP:O    | 1:A:139:LEU:HD13 | 0.66     | 1.90        | 16     | 11    |
| 1:A:91:VAL:HG12  | 1:A:95:LEU:HD12  | 0.66     | 1.66        | 6      | 1     |
| 1:A:98:LEU:HD22  | 1:A:100:ILE:HD11 | 0.66     | 1.68        | 10     | 2     |
| 1:A:144:ASP:C    | 1:A:145:LEU:HD13 | 0.66     | 2.09        | 14     | 1     |
| 1:A:52:HIS:CE1   | 1:A:74:ILE:HG21  | 0.66     | 2.24        | 8      | 5     |
| 1:A:176:LEU:HD22 | 1:A:179:LEU:HB2  | 0.66     | 1.67        | 8      | 2     |
| 1:A:72:LEU:HB3   | 1:A:95:LEU:HD12  | 0.66     | 1.64        | 14     | 3     |
| 1:A:140:ASP:HA   | 1:A:173:LEU:HD21 | 0.66     | 1.66        | 5      | 2     |
| 1:A:111:ILE:HD12 | 1:A:112:GLU:N    | 0.66     | 2.06        | 4      | 11    |
| 1:A:169:VAL:CG2  | 1:A:179:LEU:HD23 | 0.66     | 2.20        | 10     | 10    |
| 1:A:167:ILE:HG23 | 1:A:192:ALA:HA   | 0.66     | 1.66        | 12     | 13    |
| 1:A:14:PHE:O     | 1:A:20:VAL:HG22  | 0.66     | 1.91        | 6      | 14    |
| 1:A:53:LEU:HD12  | 1:A:55:LEU:HD11  | 0.66     | 1.67        | 16     | 1     |
| 1:A:34:ILE:HD13  | 1:A:36:PRO:HG2   | 0.66     | 1.67        | 6      | 1     |
| 1:A:116:ASN:HA   | 1:A:142:LEU:HD21 | 0.66     | 1.67        | 14     | 2     |
| 1:A:91:VAL:HG12  | 1:A:95:LEU:CD1   | 0.66     | 2.20        | 6      | 1     |
| 1:A:115:VAL:HG12 | 1:A:142:LEU:HD21 | 0.66     | 1.65        | 8      | 1     |
| 1:A:127:ILE:HG22 | 1:A:152:LEU:HD13 | 0.65     | 1.65        | 8      | 6     |
| 1:A:171:LYS:HD3  | 1:A:195:ALA:HB1  | 0.65     | 1.67        | 5      | 2     |
| 1:A:114:LEU:HD23 | 1:A:115:VAL:HG23 | 0.65     | 1.66        | 15     | 1     |
| 1:A:53:LEU:HD22  | 1:A:55:LEU:HD23  | 0.65     | 1.69        | 15     | 1     |
| 1:A:145:LEU:HD21 | 1:A:176:LEU:HD21 | 0.65     | 1.66        | 16     | 4     |
| 1:A:114:LEU:O    | 1:A:120:LEU:HD13 | 0.65     | 1.91        | 9      | 2     |
| 1:A:170:VAL:HG11 | 1:A:192:ALA:HB2  | 0.65     | 1.67        | 1      | 1     |
| 1:A:10:ALA:CB    | 1:A:42:ALA:HB2   | 0.65     | 2.22        | 8      | 4     |
| 1:A:173:LEU:HD22 | 1:A:176:LEU:HB2  | 0.65     | 1.69        | 5      | 1     |
| 1:A:117:LEU:HB2  | 1:A:120:LEU:HD21 | 0.65     | 1.66        | 14     | 1     |
| 1:A:91:VAL:HG13  | 1:A:95:LEU:HD13  | 0.65     | 1.68        | 8      | 2     |
| 1:A:173:LEU:HD21 | 1:A:176:LEU:O    | 0.65     | 1.92        | 11     | 1     |
| 1:A:59:ASN:OD1   | 1:A:81:LEU:HD13  | 0.65     | 1.91        | 1      | 3     |
| 1:A:95:LEU:HB3   | 1:A:117:LEU:HD11 | 0.65     | 1.68        | 4      | 2     |
| 1:A:142:LEU:CD1  | 1:A:145:LEU:HD21 | 0.64     | 2.15        | 4      | 1     |
| 1:A:77:LEU:HD23  | 1:A:100:ILE:CG2  | 0.64     | 2.22        | 3      | 2     |
| 1:A:142:LEU:O    | 1:A:142:LEU:HD13 | 0.64     | 1.91        | 1      | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:4:ALA:HB2    | 1:A:34:ILE:CG2   | 0.64     | 2.22        | 14     | 2     |
| 1:A:69:MET:O     | 1:A:91:VAL:HG12  | 0.64     | 1.92        | 14     | 1     |
| 1:A:66:LEU:HD12  | 1:A:67:SER:N     | 0.64     | 2.07        | 7      | 11    |
| 1:A:2:ALA:HB3    | 1:A:13:ILE:HG22  | 0.64     | 1.69        | 5      | 1     |
| 1:A:92:ALA:HA    | 1:A:117:LEU:HD13 | 0.64     | 1.70        | 17     | 3     |
| 1:A:111:ILE:CD1  | 1:A:133:ILE:HD13 | 0.64     | 2.23        | 2      | 2     |
| 1:A:75:LEU:HD23  | 1:A:98:LEU:HD21  | 0.64     | 1.68        | 8      | 2     |
| 1:A:169:VAL:HG13 | 1:A:176:LEU:HB3  | 0.64     | 1.70        | 2      | 3     |
| 1:A:63:ILE:HD12  | 1:A:87:ASN:CB    | 0.64     | 2.22        | 6      | 1     |
| 1:A:111:ILE:HD12 | 1:A:133:ILE:HD13 | 0.64     | 1.70        | 2      | 2     |
| 1:A:55:LEU:HD22  | 1:A:55:LEU:N     | 0.64     | 2.07        | 13     | 1     |
| 1:A:82:ILE:HG22  | 1:A:105:ILE:HG13 | 0.64     | 1.70        | 4      | 1     |
| 1:A:69:MET:CG    | 1:A:72:LEU:HD12  | 0.64     | 2.23        | 17     | 1     |
| 1:A:130:TRP:N    | 1:A:152:LEU:HD21 | 0.63     | 2.08        | 2      | 8     |
| 1:A:47:LEU:HD12  | 1:A:68:GLY:O     | 0.63     | 1.93        | 6      | 2     |
| 1:A:170:VAL:HG11 | 1:A:192:ALA:CB   | 0.63     | 2.23        | 13     | 6     |
| 1:A:142:LEU:HB2  | 1:A:176:LEU:HD12 | 0.63     | 1.69        | 13     | 1     |
| 1:A:37:ILE:HG21  | 1:A:60:ILE:CG2   | 0.63     | 2.21        | 12     | 1     |
| 1:A:167:ILE:HG13 | 1:A:192:ALA:HB2  | 0.63     | 1.68        | 16     | 2     |
| 1:A:63:ILE:HG21  | 1:A:87:ASN:OD1   | 0.63     | 1.93        | 12     | 1     |
| 1:A:72:LEU:O     | 1:A:95:LEU:HD12  | 0.63     | 1.94        | 8      | 3     |
| 1:A:75:LEU:HD23  | 1:A:98:LEU:CD2   | 0.63     | 2.23        | 8      | 1     |
| 1:A:170:VAL:O    | 1:A:173:LEU:HD23 | 0.63     | 1.93        | 1      | 1     |
| 1:A:70:GLU:HG3   | 1:A:90:ALA:HB1   | 0.63     | 1.69        | 7      | 6     |
| 1:A:47:LEU:HD11  | 1:A:71:ASN:CB    | 0.63     | 2.24        | 3      | 2     |
| 1:A:145:LEU:N    | 1:A:145:LEU:HD23 | 0.63     | 2.09        | 17     | 5     |
| 1:A:59:ASN:ND2   | 1:A:81:LEU:HD12  | 0.63     | 2.08        | 9      | 2     |
| 1:A:34:ILE:HG23  | 1:A:37:ILE:HB    | 0.63     | 1.70        | 14     | 2     |
| 1:A:47:LEU:HD12  | 1:A:48:LYS:N     | 0.62     | 2.09        | 12     | 2     |
| 1:A:145:LEU:HD23 | 1:A:145:LEU:N    | 0.62     | 2.09        | 15     | 5     |
| 1:A:2:ALA:HB1    | 1:A:14:PHE:CE1   | 0.62     | 2.28        | 14     | 6     |
| 1:A:20:VAL:HG11  | 1:A:30:LEU:HD23  | 0.62     | 1.70        | 6      | 2     |
| 1:A:119:VAL:HG23 | 1:A:144:ASP:HB3  | 0.62     | 1.69        | 10     | 6     |
| 1:A:115:VAL:HG12 | 1:A:142:LEU:CD2  | 0.62     | 2.24        | 8      | 1     |
| 1:A:171:LYS:CE   | 1:A:195:ALA:HB1  | 0.62     | 2.24        | 8      | 6     |
| 1:A:117:LEU:CB   | 1:A:120:LEU:HD11 | 0.62     | 2.24        | 1      | 1     |
| 1:A:127:ILE:CG2  | 1:A:133:ILE:HD13 | 0.62     | 2.24        | 11     | 11    |
| 1:A:54:ALA:O     | 1:A:55:LEU:HD22  | 0.62     | 1.93        | 5      | 2     |
| 1:A:82:ILE:CG2   | 1:A:88:LEU:HD12  | 0.62     | 2.17        | 11     | 1     |
| 1:A:88:LEU:HD12  | 1:A:114:LEU:HB3  | 0.62     | 1.70        | 7      | 2     |
| 1:A:120:LEU:N    | 1:A:120:LEU:HD22 | 0.62     | 2.09        | 15     | 2     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:98:LEU:HD23  | 1:A:117:LEU:HD13 | 0.62     | 1.71        | 2      | 1     |
| 1:A:111:ILE:O    | 1:A:115:VAL:HG12 | 0.62     | 1.94        | 6      | 5     |
| 1:A:87:ASN:O     | 1:A:91:VAL:HG23  | 0.62     | 1.93        | 1      | 8     |
| 1:A:43:THR:HG21  | 1:A:69:MET:HG3   | 0.62     | 1.72        | 7      | 1     |
| 1:A:100:ILE:HD13 | 1:A:120:LEU:HD11 | 0.62     | 1.70        | 3      | 1     |
| 1:A:2:ALA:HB3    | 1:A:14:PHE:CE2   | 0.62     | 2.28        | 10     | 2     |
| 1:A:115:VAL:O    | 1:A:142:LEU:HD23 | 0.62     | 1.95        | 1      | 1     |
| 1:A:119:VAL:C    | 1:A:120:LEU:HD22 | 0.62     | 2.16        | 14     | 2     |
| 1:A:82:ILE:HD13  | 1:A:83:LYS:N     | 0.61     | 2.09        | 4      | 1     |
| 1:A:60:ILE:HD11  | 1:A:82:ILE:CG2   | 0.61     | 2.15        | 9      | 1     |
| 1:A:18:LYS:HE3   | 1:A:20:VAL:HG13  | 0.61     | 1.70        | 6      | 15    |
| 1:A:171:LYS:NZ   | 1:A:195:ALA:HB3  | 0.61     | 2.11        | 4      | 1     |
| 1:A:169:VAL:HG21 | 1:A:179:LEU:CB   | 0.61     | 2.25        | 5      | 6     |
| 1:A:28:VAL:HG12  | 1:A:30:LEU:HG    | 0.61     | 1.71        | 5      | 3     |
| 1:A:88:LEU:HD22  | 1:A:114:LEU:HB3  | 0.61     | 1.70        | 8      | 1     |
| 1:A:77:LEU:HD21  | 1:A:80:ASN:ND2   | 0.61     | 2.10        | 17     | 5     |
| 1:A:115:VAL:HG11 | 1:A:137:ALA:O    | 0.61     | 1.95        | 4      | 1     |
| 1:A:77:LEU:CG    | 1:A:100:ILE:HG22 | 0.61     | 2.25        | 11     | 1     |
| 1:A:132:GLU:HB2  | 1:A:136:LEU:HD12 | 0.61     | 1.72        | 9      | 1     |
| 1:A:70:GLU:HB2   | 1:A:90:ALA:HB1   | 0.61     | 1.73        | 17     | 7     |
| 1:A:140:ASP:HA   | 1:A:173:LEU:HD22 | 0.61     | 1.73        | 9      | 1     |
| 1:A:3:LYS:CB     | 1:A:13:ILE:HG21  | 0.61     | 2.25        | 12     | 1     |
| 1:A:111:ILE:HA   | 1:A:114:LEU:HD22 | 0.61     | 1.73        | 15     | 3     |
| 1:A:169:VAL:HG22 | 1:A:173:LEU:CD1  | 0.61     | 2.25        | 5      | 1     |
| 1:A:87:ASN:O     | 1:A:91:VAL:HG22  | 0.60     | 1.96        | 16     | 5     |
| 1:A:105:ILE:CD1  | 1:A:111:ILE:HG22 | 0.60     | 2.26        | 17     | 2     |
| 1:A:115:VAL:HG22 | 1:A:142:LEU:HD22 | 0.60     | 1.71        | 11     | 1     |
| 1:A:28:VAL:CG1   | 1:A:30:LEU:HD13  | 0.60     | 2.26        | 14     | 2     |
| 1:A:169:VAL:HG22 | 1:A:179:LEU:HD23 | 0.60     | 1.73        | 11     | 2     |
| 1:A:169:VAL:HG21 | 1:A:179:LEU:HB2  | 0.60     | 1.73        | 2      | 1     |
| 1:A:34:ILE:HD12  | 1:A:36:PRO:HG2   | 0.60     | 1.72        | 12     | 2     |
| 1:A:30:LEU:N     | 1:A:30:LEU:HD22  | 0.60     | 2.11        | 13     | 6     |
| 1:A:63:ILE:HG21  | 1:A:87:ASN:HB2   | 0.60     | 1.72        | 15     | 1     |
| 1:A:88:LEU:HD13  | 1:A:114:LEU:HD23 | 0.60     | 1.74        | 8      | 1     |
| 1:A:63:ILE:HD11  | 1:A:87:ASN:CB    | 0.60     | 2.26        | 10     | 1     |
| 1:A:169:VAL:CG1  | 1:A:176:LEU:HD12 | 0.60     | 2.27        | 7      | 1     |
| 1:A:3:LYS:HA     | 1:A:34:ILE:HD13  | 0.60     | 1.73        | 17     | 3     |
| 1:A:80:ASN:C     | 1:A:81:LEU:HD22  | 0.60     | 2.17        | 12     | 2     |
| 1:A:95:LEU:HG    | 1:A:98:LEU:HD11  | 0.60     | 1.72        | 13     | 1     |
| 1:A:138:ALA:HB3  | 1:A:142:LEU:CD2  | 0.60     | 2.26        | 16     | 2     |
| 1:A:2:ALA:O      | 1:A:34:ILE:HG23  | 0.60     | 1.96        | 16     | 2     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:77:LEU:HD11  | 1:A:80:ASN:CG    | 0.60     | 2.16        | 6      | 1     |
| 1:A:145:LEU:CD2  | 1:A:147:LEU:HD11 | 0.60     | 2.26        | 12     | 1     |
| 1:A:114:LEU:CD2  | 1:A:115:VAL:HG23 | 0.60     | 2.26        | 15     | 1     |
| 1:A:156:TYR:CD1  | 1:A:161:ALA:HB2  | 0.59     | 2.32        | 16     | 5     |
| 1:A:104:GLN:O    | 1:A:105:ILE:HD13 | 0.59     | 1.96        | 13     | 1     |
| 1:A:165:TYR:HB3  | 1:A:179:LEU:HD23 | 0.59     | 1.72        | 9      | 1     |
| 1:A:81:LEU:N     | 1:A:81:LEU:HD22  | 0.59     | 2.12        | 12     | 2     |
| 1:A:141:LYS:HA   | 1:A:176:LEU:HD23 | 0.59     | 1.74        | 6      | 1     |
| 1:A:111:ILE:O    | 1:A:115:VAL:HG13 | 0.59     | 1.97        | 9      | 2     |
| 1:A:96:GLU:CA    | 1:A:117:LEU:HD21 | 0.59     | 2.27        | 12     | 1     |
| 1:A:11:ILE:HD13  | 1:A:24:GLU:N     | 0.59     | 2.12        | 8      | 8     |
| 1:A:171:LYS:CD   | 1:A:195:ALA:HB1  | 0.59     | 2.27        | 5      | 1     |
| 1:A:105:ILE:HD13 | 1:A:105:ILE:N    | 0.59     | 2.12        | 11     | 1     |
| 1:A:142:LEU:HD13 | 1:A:145:LEU:HD22 | 0.59     | 1.74        | 12     | 2     |
| 1:A:47:LEU:HD13  | 1:A:48:LYS:H     | 0.59     | 1.54        | 16     | 1     |
| 1:A:75:LEU:HB2   | 1:A:95:LEU:HD11  | 0.59     | 1.75        | 10     | 1     |
| 1:A:173:LEU:HD13 | 1:A:176:LEU:CD1  | 0.59     | 2.28        | 8      | 1     |
| 1:A:47:LEU:C     | 1:A:47:LEU:HD22  | 0.59     | 2.18        | 16     | 1     |
| 1:A:137:ALA:O    | 1:A:142:LEU:HD11 | 0.59     | 1.98        | 17     | 1     |
| 1:A:127:ILE:HG21 | 1:A:133:ILE:HG21 | 0.59     | 1.75        | 1      | 3     |
| 1:A:85:ILE:HD12  | 1:A:110:GLY:N    | 0.59     | 2.13        | 16     | 1     |
| 1:A:111:ILE:HD12 | 1:A:133:ILE:CD1  | 0.59     | 2.27        | 2      | 1     |
| 1:A:14:PHE:CE1   | 1:A:30:LEU:HD22  | 0.58     | 2.32        | 3      | 1     |
| 1:A:63:ILE:HD12  | 1:A:63:ILE:O     | 0.58     | 1.98        | 2      | 1     |
| 1:A:37:ILE:HD11  | 1:A:40:MET:SD    | 0.58     | 2.37        | 17     | 4     |
| 1:A:142:LEU:HD22 | 1:A:145:LEU:HB3  | 0.58     | 1.75        | 9      | 1     |
| 1:A:142:LEU:CD2  | 1:A:145:LEU:HD22 | 0.58     | 2.28        | 11     | 2     |
| 1:A:30:LEU:HD22  | 1:A:30:LEU:N     | 0.58     | 2.13        | 11     | 3     |
| 1:A:95:LEU:C     | 1:A:117:LEU:HD11 | 0.58     | 2.18        | 8      | 2     |
| 1:A:80:ASN:O     | 1:A:81:LEU:HD23  | 0.58     | 1.98        | 9      | 2     |
| 1:A:115:VAL:HG13 | 1:A:145:LEU:CD1  | 0.58     | 2.28        | 10     | 1     |
| 1:A:173:LEU:HD12 | 1:A:173:LEU:N    | 0.58     | 2.13        | 10     | 1     |
| 1:A:88:LEU:HD22  | 1:A:110:GLY:HA2  | 0.58     | 1.75        | 12     | 1     |
| 1:A:77:LEU:HD11  | 1:A:80:ASN:CB    | 0.58     | 2.29        | 9      | 6     |
| 1:A:72:LEU:HD22  | 1:A:75:LEU:CD2   | 0.58     | 2.28        | 11     | 1     |
| 1:A:7:ILE:HG21   | 1:A:45:SER:CB    | 0.58     | 2.29        | 8      | 2     |
| 1:A:142:LEU:HD23 | 1:A:143:GLU:N    | 0.58     | 2.13        | 6      | 1     |
| 1:A:115:VAL:CG2  | 1:A:142:LEU:HD21 | 0.58     | 2.17        | 17     | 1     |
| 1:A:77:LEU:HD23  | 1:A:100:ILE:HG23 | 0.58     | 1.74        | 3      | 1     |
| 1:A:115:VAL:HG22 | 1:A:142:LEU:HD12 | 0.58     | 1.74        | 12     | 2     |
| 1:A:3:LYS:CB     | 1:A:13:ILE:HD13  | 0.58     | 2.29        | 7      | 3     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:115:VAL:O    | 1:A:142:LEU:HD21 | 0.58     | 1.99        | 15     | 7     |
| 1:A:4:ALA:HB1    | 1:A:37:ILE:HD13  | 0.58     | 1.76        | 1      | 1     |
| 1:A:145:LEU:HD21 | 1:A:147:LEU:HD21 | 0.58     | 1.76        | 2      | 2     |
| 1:A:117:LEU:HB2  | 1:A:120:LEU:HD11 | 0.58     | 1.74        | 2      | 2     |
| 1:A:47:LEU:HD11  | 1:A:71:ASN:HB2   | 0.58     | 1.74        | 3      | 2     |
| 1:A:95:LEU:HD23  | 1:A:117:LEU:HD21 | 0.58     | 1.75        | 15     | 2     |
| 1:A:126:LYS:O    | 1:A:127:ILE:HD13 | 0.57     | 1.99        | 4      | 1     |
| 1:A:60:ILE:CD1   | 1:A:82:ILE:HG23  | 0.57     | 2.18        | 9      | 1     |
| 1:A:66:LEU:HD23  | 1:A:90:ALA:HB2   | 0.57     | 1.74        | 12     | 2     |
| 1:A:47:LEU:HD22  | 1:A:47:LEU:O     | 0.57     | 1.99        | 8      | 2     |
| 1:A:60:ILE:HD12  | 1:A:82:ILE:HD12  | 0.57     | 1.75        | 17     | 1     |
| 1:A:66:LEU:C     | 1:A:66:LEU:HD22  | 0.57     | 2.20        | 12     | 1     |
| 1:A:173:LEU:HD13 | 1:A:176:LEU:HD13 | 0.57     | 1.76        | 5      | 1     |
| 1:A:140:ASP:CA   | 1:A:173:LEU:HD21 | 0.57     | 2.29        | 2      | 2     |
| 1:A:95:LEU:CD2   | 1:A:117:LEU:HD21 | 0.57     | 2.29        | 15     | 1     |
| 1:A:184:VAL:HG13 | 1:A:188:GLU:HG2  | 0.57     | 1.75        | 7      | 3     |
| 1:A:43:THR:HG22  | 1:A:68:GLY:HA3   | 0.57     | 1.75        | 1      | 4     |
| 1:A:7:ILE:HG23   | 1:A:42:ALA:HA    | 0.57     | 1.76        | 8      | 3     |
| 1:A:176:LEU:HD23 | 1:A:177:LYS:N    | 0.57     | 2.15        | 13     | 3     |
| 1:A:37:ILE:HD11  | 1:A:40:MET:HG2   | 0.57     | 1.76        | 1      | 1     |
| 1:A:2:ALA:HB1    | 1:A:13:ILE:HG22  | 0.57     | 1.77        | 10     | 3     |
| 1:A:169:VAL:HG12 | 1:A:173:LEU:CD1  | 0.57     | 2.29        | 16     | 1     |
| 1:A:111:ILE:HD13 | 1:A:111:ILE:C    | 0.56     | 2.19        | 7      | 1     |
| 1:A:105:ILE:HD12 | 1:A:111:ILE:CG2  | 0.56     | 2.20        | 6      | 2     |
| 1:A:63:ILE:HD12  | 1:A:87:ASN:HB2   | 0.56     | 1.77        | 13     | 2     |
| 1:A:53:LEU:HD23  | 1:A:55:LEU:HD21  | 0.56     | 1.77        | 13     | 1     |
| 1:A:142:LEU:HD12 | 1:A:145:LEU:HD22 | 0.56     | 1.76        | 8      | 1     |
| 1:A:115:VAL:HB   | 1:A:142:LEU:HD11 | 0.56     | 1.77        | 9      | 1     |
| 1:A:75:LEU:HB3   | 1:A:98:LEU:HD13  | 0.56     | 1.76        | 2      | 1     |
| 1:A:53:LEU:CD2   | 1:A:55:LEU:HD23  | 0.56     | 2.30        | 15     | 1     |
| 1:A:2:ALA:O      | 1:A:34:ILE:HG21  | 0.56     | 2.01        | 12     | 1     |
| 1:A:60:ILE:HG13  | 1:A:82:ILE:HD13  | 0.56     | 1.77        | 12     | 1     |
| 1:A:20:VAL:HG11  | 1:A:30:LEU:HA    | 0.56     | 1.76        | 7      | 4     |
| 1:A:47:LEU:O     | 1:A:47:LEU:HD13  | 0.56     | 2.01        | 3      | 2     |
| 1:A:80:ASN:O     | 1:A:81:LEU:HD12  | 0.56     | 2.01        | 4      | 5     |
| 1:A:3:LYS:HB2    | 1:A:13:ILE:HD13  | 0.56     | 1.77        | 13     | 3     |
| 1:A:142:LEU:O    | 1:A:176:LEU:HA   | 0.56     | 2.01        | 8      | 3     |
| 1:A:85:ILE:O     | 1:A:85:ILE:HG23  | 0.56     | 2.00        | 5      | 2     |
| 1:A:111:ILE:C    | 1:A:111:ILE:HD13 | 0.56     | 2.21        | 1      | 2     |
| 1:A:142:LEU:HB3  | 1:A:145:LEU:HD22 | 0.55     | 1.78        | 9      | 4     |
| 1:A:157:LYS:HB3  | 1:A:161:ALA:HB3  | 0.55     | 1.79        | 6      | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:100:ILE:HD12 | 1:A:122:MET:HE2  | 0.55     | 1.77        | 10     | 1     |
| 1:A:47:LEU:HD13  | 1:A:71:ASN:ND2   | 0.55     | 2.16        | 12     | 1     |
| 1:A:28:VAL:HG12  | 1:A:30:LEU:HD21  | 0.55     | 1.76        | 13     | 2     |
| 1:A:24:GLU:O     | 1:A:49:ALA:HB1   | 0.55     | 2.02        | 15     | 2     |
| 1:A:167:ILE:HG23 | 1:A:192:ALA:CA   | 0.55     | 2.31        | 7      | 3     |
| 1:A:153:TYR:CE1  | 1:A:162:THR:HG23 | 0.55     | 2.36        | 8      | 9     |
| 1:A:117:LEU:HB3  | 1:A:120:LEU:HD21 | 0.55     | 1.78        | 15     | 1     |
| 1:A:185:ASP:O    | 1:A:186:VAL:HG12 | 0.55     | 2.01        | 14     | 11    |
| 1:A:105:ILE:N    | 1:A:105:ILE:HD13 | 0.55     | 2.16        | 2      | 1     |
| 1:A:95:LEU:C     | 1:A:117:LEU:HD21 | 0.55     | 2.22        | 9      | 2     |
| 1:A:111:ILE:HD13 | 1:A:133:ILE:HG23 | 0.55     | 1.78        | 13     | 10    |
| 1:A:70:GLU:HB3   | 1:A:90:ALA:HB1   | 0.54     | 1.79        | 12     | 1     |
| 1:A:77:LEU:HD21  | 1:A:80:ASN:CB    | 0.54     | 2.32        | 14     | 6     |
| 1:A:145:LEU:CD1  | 1:A:179:LEU:HD12 | 0.54     | 2.20        | 7      | 2     |
| 1:A:140:ASP:CA   | 1:A:173:LEU:HD11 | 0.54     | 2.31        | 12     | 1     |
| 1:A:145:LEU:HD22 | 1:A:147:LEU:CD1  | 0.54     | 2.32        | 10     | 2     |
| 1:A:166:ARG:HG3  | 1:A:184:VAL:HG22 | 0.54     | 1.78        | 16     | 1     |
| 1:A:138:ALA:HB3  | 1:A:142:LEU:HD12 | 0.54     | 1.79        | 6      | 1     |
| 1:A:20:VAL:HG21  | 1:A:30:LEU:CD2   | 0.54     | 2.33        | 6      | 4     |
| 1:A:173:LEU:HD22 | 1:A:176:LEU:CB   | 0.54     | 2.32        | 5      | 1     |
| 1:A:77:LEU:HD22  | 1:A:80:ASN:ND2   | 0.54     | 2.16        | 1      | 1     |
| 1:A:20:VAL:HG11  | 1:A:30:LEU:CD2   | 0.54     | 2.33        | 5      | 2     |
| 1:A:170:VAL:CG1  | 1:A:192:ALA:HB1  | 0.54     | 2.32        | 3      | 8     |
| 1:A:114:LEU:O    | 1:A:117:LEU:HD13 | 0.54     | 2.02        | 6      | 1     |
| 1:A:29:GLU:C     | 1:A:30:LEU:HD12  | 0.54     | 2.23        | 14     | 2     |
| 1:A:173:LEU:CD2  | 1:A:176:LEU:HD21 | 0.54     | 2.15        | 10     | 1     |
| 1:A:85:ILE:HG23  | 1:A:85:ILE:O     | 0.54     | 2.03        | 3      | 9     |
| 1:A:47:LEU:HD21  | 1:A:71:ASN:ND2   | 0.54     | 2.17        | 9      | 2     |
| 1:A:135:LYS:HG3  | 1:A:136:LEU:HD12 | 0.54     | 1.78        | 17     | 1     |
| 1:A:72:LEU:CB    | 1:A:95:LEU:HD21  | 0.54     | 2.32        | 7      | 1     |
| 1:A:11:ILE:HD13  | 1:A:24:GLU:H     | 0.54     | 1.63        | 3      | 5     |
| 1:A:145:LEU:HD11 | 1:A:179:LEU:HD13 | 0.54     | 1.78        | 11     | 2     |
| 1:A:95:LEU:O     | 1:A:117:LEU:HD21 | 0.54     | 2.03        | 5      | 2     |
| 1:A:82:ILE:HD13  | 1:A:88:LEU:HD21  | 0.54     | 1.79        | 3      | 2     |
| 1:A:186:VAL:O    | 1:A:186:VAL:HG22 | 0.54     | 2.03        | 13     | 6     |
| 1:A:115:VAL:HG12 | 1:A:142:LEU:CG   | 0.54     | 2.33        | 8      | 1     |
| 1:A:20:VAL:HG21  | 1:A:30:LEU:HG    | 0.54     | 1.80        | 14     | 1     |
| 1:A:181:GLY:CA   | 1:A:184:VAL:HG23 | 0.54     | 2.33        | 2      | 5     |
| 1:A:47:LEU:C     | 1:A:47:LEU:HD13  | 0.54     | 2.23        | 3      | 3     |
| 1:A:66:LEU:HD11  | 1:A:86:GLU:O     | 0.54     | 2.02        | 16     | 1     |
| 1:A:120:LEU:HD21 | 1:A:122:MET:SD   | 0.54     | 2.43        | 10     | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:169:VAL:HA   | 1:A:173:LEU:HD12 | 0.54     | 1.79        | 9      | 2     |
| 1:A:82:ILE:HG21  | 1:A:88:LEU:HD11  | 0.54     | 1.79        | 2      | 3     |
| 1:A:34:ILE:HG23  | 1:A:34:ILE:O     | 0.54     | 2.03        | 14     | 1     |
| 1:A:10:ALA:HB3   | 1:A:42:ALA:HB2   | 0.54     | 1.78        | 17     | 4     |
| 1:A:100:ILE:HD12 | 1:A:103:ASN:ND2  | 0.54     | 2.18        | 17     | 2     |
| 1:A:34:ILE:O     | 1:A:34:ILE:HG23  | 0.53     | 2.02        | 13     | 2     |
| 1:A:111:ILE:HD13 | 1:A:137:ALA:HB2  | 0.53     | 1.79        | 4      | 1     |
| 1:A:178:LYS:CE   | 1:A:184:VAL:HG21 | 0.53     | 2.34        | 9      | 1     |
| 1:A:88:LEU:O     | 1:A:92:ALA:HB2   | 0.53     | 2.03        | 3      | 2     |
| 1:A:43:THR:HG22  | 1:A:68:GLY:CA    | 0.53     | 2.32        | 1      | 4     |
| 1:A:82:ILE:HG21  | 1:A:105:ILE:HG22 | 0.53     | 1.80        | 1      | 1     |
| 1:A:7:ILE:C      | 1:A:7:ILE:HD13   | 0.53     | 2.24        | 16     | 1     |
| 1:A:138:ALA:O    | 1:A:142:LEU:HD23 | 0.53     | 2.03        | 4      | 1     |
| 1:A:153:TYR:OH   | 1:A:162:THR:HG23 | 0.53     | 2.02        | 9      | 1     |
| 1:A:114:LEU:HD12 | 1:A:115:VAL:N    | 0.53     | 2.17        | 17     | 2     |
| 1:A:63:ILE:O     | 1:A:63:ILE:HD12  | 0.53     | 2.04        | 7      | 1     |
| 1:A:4:ALA:HB1    | 1:A:37:ILE:HG13  | 0.53     | 1.81        | 15     | 2     |
| 1:A:98:LEU:HD13  | 1:A:117:LEU:HD22 | 0.53     | 1.78        | 12     | 1     |
| 1:A:88:LEU:HD22  | 1:A:110:GLY:CA   | 0.53     | 2.34        | 12     | 1     |
| 1:A:95:LEU:HD12  | 1:A:98:LEU:CD2   | 0.53     | 2.33        | 7      | 1     |
| 1:A:157:LYS:HB2  | 1:A:161:ALA:HB2  | 0.53     | 1.81        | 4      | 2     |
| 1:A:169:VAL:CG2  | 1:A:179:LEU:HD22 | 0.53     | 2.34        | 9      | 1     |
| 1:A:4:ALA:HB3    | 1:A:34:ILE:HD11  | 0.53     | 1.79        | 2      | 2     |
| 1:A:185:ASP:O    | 1:A:186:VAL:HG22 | 0.53     | 2.04        | 7      | 6     |
| 1:A:111:ILE:O    | 1:A:115:VAL:HG23 | 0.53     | 2.04        | 8      | 6     |
| 1:A:63:ILE:C     | 1:A:63:ILE:HD13  | 0.53     | 2.23        | 14     | 5     |
| 1:A:105:ILE:HD13 | 1:A:105:ILE:H    | 0.53     | 1.63        | 2      | 2     |
| 1:A:82:ILE:HG22  | 1:A:105:ILE:HG22 | 0.53     | 1.81        | 2      | 1     |
| 1:A:98:LEU:CB    | 1:A:120:LEU:HD23 | 0.53     | 2.34        | 2      | 1     |
| 1:A:24:GLU:HG3   | 1:A:49:ALA:HB3   | 0.53     | 1.80        | 17     | 1     |
| 1:A:70:GLU:HA    | 1:A:91:VAL:HG22  | 0.53     | 1.81        | 15     | 1     |
| 1:A:57:THR:HG23  | 1:A:57:THR:O     | 0.53     | 2.04        | 5      | 5     |
| 1:A:96:GLU:HA    | 1:A:117:LEU:HD21 | 0.52     | 1.81        | 12     | 1     |
| 1:A:28:VAL:HG12  | 1:A:30:LEU:CD2   | 0.52     | 2.33        | 12     | 8     |
| 1:A:145:LEU:HD12 | 1:A:147:LEU:CD1  | 0.52     | 2.18        | 4      | 1     |
| 1:A:21:VAL:O     | 1:A:21:VAL:HG13  | 0.52     | 2.04        | 4      | 4     |
| 1:A:4:ALA:CB     | 1:A:37:ILE:HD12  | 0.52     | 2.33        | 11     | 8     |
| 1:A:50:CYS:SG    | 1:A:72:LEU:HD21  | 0.52     | 2.44        | 12     | 2     |
| 1:A:72:LEU:HD12  | 1:A:95:LEU:HD21  | 0.52     | 1.82        | 5      | 1     |
| 1:A:79:ARG:NH1   | 1:A:81:LEU:HD11  | 0.52     | 2.19        | 1      | 1     |
| 1:A:180:ASP:O    | 1:A:182:MET:N    | 0.52     | 2.42        | 9      | 2     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:55:LEU:HD12  | 1:A:56:SER:N     | 0.52     | 2.20        | 14     | 1     |
| 1:A:6:THR:O      | 1:A:10:ALA:HB2   | 0.52     | 2.05        | 8      | 11    |
| 1:A:186:VAL:HG22 | 1:A:186:VAL:O    | 0.52     | 2.05        | 4      | 4     |
| 1:A:2:ALA:HB1    | 1:A:14:PHE:HE1   | 0.52     | 1.64        | 7      | 3     |
| 1:A:114:LEU:C    | 1:A:114:LEU:HD22 | 0.52     | 2.25        | 6      | 1     |
| 1:A:119:VAL:HG22 | 1:A:121:TYR:CE1  | 0.52     | 2.40        | 3      | 1     |
| 1:A:122:MET:CE   | 1:A:145:LEU:HD11 | 0.52     | 2.35        | 12     | 1     |
| 1:A:63:ILE:HG23  | 1:A:63:ILE:O     | 0.52     | 2.05        | 8      | 3     |
| 1:A:105:ILE:HD11 | 1:A:127:ILE:CG1  | 0.52     | 2.35        | 11     | 2     |
| 1:A:44:LEU:HD11  | 1:A:65:SER:HB2   | 0.52     | 1.81        | 12     | 1     |
| 1:A:50:CYS:SG    | 1:A:72:LEU:HD11  | 0.52     | 2.45        | 12     | 1     |
| 1:A:105:ILE:HD13 | 1:A:114:LEU:CD2  | 0.52     | 2.34        | 5      | 1     |
| 1:A:153:TYR:HH   | 1:A:165:TYR:CB   | 0.52     | 2.18        | 10     | 2     |
| 1:A:43:THR:HA    | 1:A:46:THR:HG22  | 0.52     | 1.81        | 6      | 5     |
| 1:A:135:LYS:HA   | 1:A:139:LEU:HD13 | 0.52     | 1.82        | 17     | 1     |
| 1:A:120:LEU:HD22 | 1:A:122:MET:CE   | 0.52     | 2.35        | 7      | 1     |
| 1:A:117:LEU:HD12 | 1:A:118:ARG:N    | 0.52     | 2.20        | 10     | 1     |
| 1:A:108:LEU:HD11 | 1:A:136:LEU:CD2  | 0.52     | 2.34        | 1      | 1     |
| 1:A:145:LEU:HD21 | 1:A:179:LEU:HD12 | 0.52     | 1.81        | 9      | 2     |
| 1:A:173:LEU:HD12 | 1:A:176:LEU:HB2  | 0.51     | 1.81        | 12     | 1     |
| 1:A:181:GLY:O    | 1:A:184:VAL:HG22 | 0.51     | 2.05        | 5      | 3     |
| 1:A:96:GLU:N     | 1:A:117:LEU:HD21 | 0.51     | 2.20        | 16     | 1     |
| 1:A:40:MET:HB3   | 1:A:43:THR:HG22  | 0.51     | 1.82        | 5      | 1     |
| 1:A:3:LYS:HG3    | 1:A:34:ILE:HD13  | 0.51     | 1.81        | 12     | 1     |
| 1:A:80:ASN:OD1   | 1:A:82:ILE:HD11  | 0.51     | 2.05        | 6      | 4     |
| 1:A:127:ILE:HB   | 1:A:152:LEU:HD12 | 0.51     | 1.81        | 17     | 1     |
| 1:A:98:LEU:CB    | 1:A:120:LEU:HD22 | 0.51     | 2.36        | 3      | 1     |
| 1:A:47:LEU:HD22  | 1:A:50:CYS:HB2   | 0.51     | 1.81        | 3      | 1     |
| 1:A:92:ALA:HB3   | 1:A:113:LYS:HB3  | 0.51     | 1.81        | 10     | 2     |
| 1:A:87:ASN:O     | 1:A:91:VAL:HG12  | 0.51     | 2.04        | 2      | 1     |
| 1:A:24:GLU:CG    | 1:A:49:ALA:HB3   | 0.51     | 2.35        | 17     | 1     |
| 1:A:82:ILE:HD12  | 1:A:84:LYS:O     | 0.51     | 2.05        | 4      | 1     |
| 1:A:176:LEU:HD11 | 1:A:179:LEU:HD13 | 0.51     | 1.82        | 5      | 2     |
| 1:A:37:ILE:HG23  | 1:A:60:ILE:HG23  | 0.51     | 1.82        | 2      | 1     |
| 1:A:167:ILE:HD11 | 1:A:191:GLN:HB3  | 0.51     | 1.82        | 13     | 3     |
| 1:A:108:LEU:HD21 | 1:A:136:LEU:HD23 | 0.51     | 1.82        | 16     | 1     |
| 1:A:173:LEU:HB3  | 1:A:176:LEU:HD21 | 0.51     | 1.83        | 7      | 1     |
| 1:A:142:LEU:HD13 | 1:A:145:LEU:CD1  | 0.51     | 2.31        | 5      | 2     |
| 1:A:167:ILE:HG22 | 1:A:171:LYS:HE3  | 0.51     | 1.82        | 15     | 2     |
| 1:A:91:VAL:HG22  | 1:A:95:LEU:HD11  | 0.51     | 1.81        | 2      | 1     |
| 1:A:100:ILE:HG21 | 1:A:103:ASN:HB3  | 0.51     | 1.82        | 3      | 2     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:138:ALA:HB3  | 1:A:142:LEU:HD23 | 0.51     | 1.82        | 16     | 3     |
| 1:A:72:LEU:HB3   | 1:A:95:LEU:HD21  | 0.51     | 1.82        | 7      | 2     |
| 1:A:77:LEU:HD12  | 1:A:78:GLY:N     | 0.51     | 2.21        | 14     | 3     |
| 1:A:47:LEU:HD21  | 1:A:71:ASN:HB3   | 0.51     | 1.83        | 3      | 1     |
| 1:A:117:LEU:C    | 1:A:117:LEU:HD12 | 0.51     | 2.25        | 10     | 1     |
| 1:A:91:VAL:O     | 1:A:95:LEU:HD23  | 0.51     | 2.05        | 13     | 1     |
| 1:A:142:LEU:HD22 | 1:A:143:GLU:N    | 0.51     | 2.21        | 1      | 1     |
| 1:A:2:ALA:HB2    | 1:A:14:PHE:CE1   | 0.51     | 2.40        | 9      | 2     |
| 1:A:139:LEU:HD21 | 1:A:165:TYR:CE2  | 0.51     | 2.40        | 11     | 1     |
| 1:A:173:LEU:O    | 1:A:173:LEU:HD12 | 0.51     | 2.06        | 1      | 1     |
| 1:A:88:LEU:HD12  | 1:A:113:LYS:HD2  | 0.50     | 1.83        | 12     | 1     |
| 1:A:35:PRO:N     | 1:A:36:PRO:CD    | 0.50     | 2.74        | 5      | 17    |
| 1:A:63:ILE:O     | 1:A:63:ILE:HG23  | 0.50     | 2.06        | 1      | 4     |
| 1:A:4:ALA:CB     | 1:A:37:ILE:HD13  | 0.50     | 2.36        | 1      | 1     |
| 1:A:21:VAL:HG13  | 1:A:21:VAL:O     | 0.50     | 2.06        | 11     | 2     |
| 1:A:115:VAL:HA   | 1:A:120:LEU:HD22 | 0.50     | 1.82        | 8      | 2     |
| 1:A:63:ILE:HD13  | 1:A:63:ILE:C     | 0.50     | 2.27        | 4      | 2     |
| 1:A:82:ILE:HD13  | 1:A:83:LYS:H     | 0.50     | 1.65        | 4      | 1     |
| 1:A:77:LEU:HD12  | 1:A:78:GLY:H     | 0.50     | 1.66        | 14     | 3     |
| 1:A:35:PRO:N     | 1:A:36:PRO:HD2   | 0.50     | 2.22        | 6      | 6     |
| 1:A:142:LEU:HD22 | 1:A:145:LEU:HD13 | 0.50     | 1.82        | 17     | 1     |
| 1:A:91:VAL:CG1   | 1:A:95:LEU:HD13  | 0.50     | 2.35        | 17     | 1     |
| 1:A:139:LEU:HD23 | 1:A:165:TYR:CE1  | 0.50     | 2.41        | 14     | 1     |
| 1:A:85:ILE:C     | 1:A:85:ILE:HD13  | 0.50     | 2.27        | 1      | 3     |
| 1:A:156:TYR:CD2  | 1:A:165:TYR:CE2  | 0.50     | 2.99        | 2      | 5     |
| 1:A:135:LYS:HA   | 1:A:139:LEU:HD22 | 0.50     | 1.83        | 17     | 1     |
| 1:A:18:LYS:CE    | 1:A:20:VAL:HG13  | 0.50     | 2.36        | 5      | 2     |
| 1:A:139:LEU:O    | 1:A:176:LEU:HD12 | 0.50     | 2.07        | 2      | 1     |
| 1:A:100:ILE:HD12 | 1:A:120:LEU:HD21 | 0.50     | 1.83        | 12     | 1     |
| 1:A:129:ASN:C    | 1:A:152:LEU:HD11 | 0.50     | 2.27        | 6      | 6     |
| 1:A:72:LEU:CB    | 1:A:95:LEU:HD23  | 0.50     | 2.36        | 4      | 2     |
| 1:A:81:LEU:HD22  | 1:A:104:GLN:OE1  | 0.50     | 2.07        | 15     | 1     |
| 1:A:30:LEU:HD22  | 1:A:30:LEU:H     | 0.50     | 1.67        | 2      | 5     |
| 1:A:85:ILE:HD13  | 1:A:85:ILE:C     | 0.50     | 2.26        | 4      | 6     |
| 1:A:69:MET:HG3   | 1:A:72:LEU:HD12  | 0.50     | 1.82        | 17     | 1     |
| 1:A:98:LEU:CD2   | 1:A:117:LEU:HD13 | 0.50     | 2.37        | 2      | 1     |
| 1:A:133:ILE:HG21 | 1:A:152:LEU:CD1  | 0.50     | 2.36        | 17     | 1     |
| 1:A:173:LEU:HD12 | 1:A:176:LEU:HD11 | 0.50     | 1.83        | 7      | 1     |
| 1:A:91:VAL:CG1   | 1:A:95:LEU:HD23  | 0.50     | 2.37        | 7      | 1     |
| 1:A:47:LEU:HD22  | 1:A:68:GLY:HA2   | 0.50     | 1.84        | 12     | 1     |
| 1:A:37:ILE:HD13  | 1:A:37:ILE:C     | 0.50     | 2.28        | 17     | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:171:LYS:HE2  | 1:A:195:ALA:HB1  | 0.49     | 1.83        | 2      | 1     |
| 1:A:44:LEU:HD12  | 1:A:65:SER:HB2   | 0.49     | 1.84        | 1      | 2     |
| 1:A:44:LEU:C     | 1:A:44:LEU:HD12  | 0.49     | 2.28        | 6      | 2     |
| 1:A:105:ILE:HB   | 1:A:127:ILE:HD11 | 0.49     | 1.83        | 4      | 1     |
| 1:A:103:ASN:HB2  | 1:A:105:ILE:HD11 | 0.49     | 1.83        | 9      | 1     |
| 1:A:60:ILE:N     | 1:A:60:ILE:HD12  | 0.49     | 2.22        | 5      | 1     |
| 1:A:85:ILE:HD13  | 1:A:110:GLY:CA   | 0.49     | 2.37        | 5      | 3     |
| 1:A:30:LEU:H     | 1:A:30:LEU:HD22  | 0.49     | 1.66        | 9      | 3     |
| 1:A:44:LEU:HD12  | 1:A:65:SER:HB3   | 0.49     | 1.84        | 17     | 2     |
| 1:A:7:ILE:HD13   | 1:A:7:ILE:O      | 0.49     | 2.06        | 15     | 1     |
| 1:A:119:VAL:HG13 | 1:A:119:VAL:O    | 0.49     | 2.06        | 6      | 5     |
| 1:A:57:THR:O     | 1:A:57:THR:HG23  | 0.49     | 2.07        | 1      | 5     |
| 1:A:140:ASP:CA   | 1:A:173:LEU:HD22 | 0.49     | 2.37        | 9      | 2     |
| 1:A:37:ILE:HG23  | 1:A:37:ILE:O     | 0.49     | 2.08        | 12     | 2     |
| 1:A:70:GLU:O     | 1:A:94:THR:HG23  | 0.49     | 2.08        | 12     | 1     |
| 1:A:105:ILE:O    | 1:A:127:ILE:HD13 | 0.49     | 2.07        | 4      | 1     |
| 1:A:108:LEU:HD13 | 1:A:108:LEU:O    | 0.49     | 2.08        | 9      | 1     |
| 1:A:53:LEU:HD23  | 1:A:55:LEU:HD11  | 0.49     | 1.83        | 3      | 1     |
| 1:A:4:ALA:CB     | 1:A:34:ILE:HD11  | 0.49     | 2.38        | 2      | 1     |
| 1:A:147:LEU:HD12 | 1:A:180:ASP:HB2  | 0.49     | 1.83        | 12     | 2     |
| 1:A:59:ASN:OD1   | 1:A:81:LEU:HD23  | 0.49     | 2.05        | 8      | 2     |
| 1:A:170:VAL:HA   | 1:A:173:LEU:HD12 | 0.49     | 1.85        | 4      | 1     |
| 1:A:7:ILE:HD13   | 1:A:7:ILE:C      | 0.49     | 2.27        | 6      | 2     |
| 1:A:81:LEU:HD22  | 1:A:104:GLN:HE21 | 0.49     | 1.62        | 9      | 1     |
| 1:A:115:VAL:HG23 | 1:A:142:LEU:HD11 | 0.49     | 1.85        | 3      | 1     |
| 1:A:2:ALA:HB3    | 1:A:14:PHE:CE1   | 0.49     | 2.43        | 3      | 2     |
| 1:A:156:TYR:CE2  | 1:A:161:ALA:HB1  | 0.49     | 2.43        | 2      | 3     |
| 1:A:75:LEU:HD23  | 1:A:95:LEU:CD1   | 0.49     | 2.37        | 11     | 1     |
| 1:A:47:LEU:HD11  | 1:A:71:ASN:ND2   | 0.49     | 2.22        | 11     | 1     |
| 1:A:145:LEU:HD23 | 1:A:147:LEU:HD11 | 0.49     | 1.85        | 12     | 1     |
| 1:A:145:LEU:HD22 | 1:A:147:LEU:HG   | 0.49     | 1.84        | 1      | 3     |
| 1:A:139:LEU:HD23 | 1:A:140:ASP:N    | 0.49     | 2.23        | 17     | 1     |
| 1:A:69:MET:HG2   | 1:A:72:LEU:HD12  | 0.49     | 1.84        | 17     | 1     |
| 1:A:142:LEU:HB3  | 1:A:145:LEU:HD21 | 0.49     | 1.84        | 14     | 1     |
| 1:A:5:THR:HG22   | 1:A:6:THR:N      | 0.49     | 2.22        | 11     | 2     |
| 1:A:142:LEU:C    | 1:A:142:LEU:HD13 | 0.49     | 2.28        | 1      | 1     |
| 1:A:182:MET:N    | 1:A:183:PRO:CD   | 0.48     | 2.76        | 12     | 15    |
| 1:A:142:LEU:HD11 | 1:A:145:LEU:HB2  | 0.48     | 1.84        | 1      | 1     |
| 1:A:59:ASN:ND2   | 1:A:81:LEU:HD13  | 0.48     | 2.22        | 11     | 1     |
| 1:A:14:PHE:CD2   | 1:A:30:LEU:HD21  | 0.48     | 2.42        | 15     | 1     |
| 1:A:63:ILE:HD12  | 1:A:87:ASN:HB3   | 0.48     | 1.85        | 1      | 3     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:95:LEU:HD13  | 1:A:98:LEU:CD1   | 0.48     | 2.38        | 5      | 1     |
| 1:A:119:VAL:HG23 | 1:A:144:ASP:CB   | 0.48     | 2.38        | 16     | 4     |
| 1:A:115:VAL:HG21 | 1:A:137:ALA:O    | 0.48     | 2.08        | 11     | 1     |
| 1:A:69:MET:HA    | 1:A:72:LEU:HD23  | 0.48     | 1.84        | 14     | 1     |
| 1:A:114:LEU:O    | 1:A:120:LEU:HD22 | 0.48     | 2.08        | 4      | 2     |
| 1:A:98:LEU:HD12  | 1:A:117:LEU:HD22 | 0.48     | 1.86        | 15     | 2     |
| 1:A:136:LEU:HD13 | 1:A:136:LEU:O    | 0.48     | 2.08        | 11     | 1     |
| 1:A:66:LEU:N     | 1:A:66:LEU:HD13  | 0.48     | 2.24        | 12     | 1     |
| 1:A:77:LEU:HD23  | 1:A:78:GLY:N     | 0.48     | 2.23        | 6      | 2     |
| 1:A:46:THR:HG23  | 1:A:50:CYS:SG    | 0.48     | 2.49        | 4      | 1     |
| 1:A:21:VAL:HG22  | 1:A:21:VAL:O     | 0.48     | 2.08        | 3      | 2     |
| 1:A:169:VAL:HG13 | 1:A:176:LEU:HD13 | 0.48     | 1.85        | 11     | 1     |
| 1:A:130:TRP:HA   | 1:A:152:LEU:HD21 | 0.48     | 1.84        | 8      | 2     |
| 1:A:37:ILE:CG2   | 1:A:60:ILE:HG22  | 0.48     | 2.28        | 4      | 1     |
| 1:A:37:ILE:O     | 1:A:37:ILE:HG23  | 0.48     | 2.08        | 6      | 3     |
| 1:A:108:LEU:HD22 | 1:A:108:LEU:N    | 0.48     | 2.24        | 7      | 1     |
| 1:A:77:LEU:HD21  | 1:A:80:ASN:HB3   | 0.48     | 1.86        | 3      | 3     |
| 1:A:139:LEU:HD21 | 1:A:165:TYR:CZ   | 0.48     | 2.43        | 11     | 1     |
| 1:A:136:LEU:O    | 1:A:136:LEU:HD23 | 0.48     | 2.09        | 14     | 1     |
| 1:A:145:LEU:HD22 | 1:A:147:LEU:CG   | 0.48     | 2.39        | 13     | 3     |
| 1:A:136:LEU:HD23 | 1:A:136:LEU:O    | 0.48     | 2.09        | 3      | 2     |
| 1:A:108:LEU:HD21 | 1:A:136:LEU:HD22 | 0.48     | 1.86        | 1      | 1     |
| 1:A:139:LEU:HD23 | 1:A:140:ASP:H    | 0.48     | 1.68        | 17     | 1     |
| 1:A:130:TRP:HA   | 1:A:152:LEU:HD11 | 0.48     | 1.83        | 7      | 3     |
| 1:A:88:LEU:HD22  | 1:A:114:LEU:HD23 | 0.48     | 1.86        | 5      | 1     |
| 1:A:47:LEU:HD13  | 1:A:47:LEU:O     | 0.48     | 2.09        | 11     | 1     |
| 1:A:81:LEU:HD12  | 1:A:104:GLN:NE2  | 0.48     | 2.24        | 12     | 1     |
| 1:A:47:LEU:HD12  | 1:A:47:LEU:C     | 0.48     | 2.29        | 13     | 2     |
| 1:A:134:ASP:O    | 1:A:139:LEU:HD23 | 0.48     | 2.09        | 9      | 1     |
| 1:A:91:VAL:HG13  | 1:A:95:LEU:HD23  | 0.48     | 1.85        | 7      | 1     |
| 1:A:91:VAL:HG13  | 1:A:95:LEU:CD2   | 0.48     | 2.39        | 7      | 1     |
| 1:A:100:ILE:CD1  | 1:A:120:LEU:HD11 | 0.48     | 2.39        | 3      | 1     |
| 1:A:2:ALA:HB3    | 1:A:14:PHE:CD2   | 0.48     | 2.43        | 10     | 1     |
| 1:A:63:ILE:HG21  | 1:A:87:ASN:ND2   | 0.48     | 2.24        | 14     | 1     |
| 1:A:145:LEU:HD22 | 1:A:147:LEU:HD11 | 0.47     | 1.86        | 10     | 2     |
| 1:A:127:ILE:CG2  | 1:A:152:LEU:HD12 | 0.47     | 2.38        | 16     | 1     |
| 1:A:7:ILE:HD13   | 1:A:45:SER:CB    | 0.47     | 2.39        | 5      | 1     |
| 1:A:95:LEU:HB2   | 1:A:117:LEU:HD11 | 0.47     | 1.86        | 5      | 1     |
| 1:A:63:ILE:HG21  | 1:A:87:ASN:CG    | 0.47     | 2.29        | 11     | 1     |
| 1:A:37:ILE:HG21  | 1:A:60:ILE:HG23  | 0.47     | 1.85        | 2      | 1     |
| 1:A:20:VAL:HG21  | 1:A:30:LEU:CD1   | 0.47     | 2.39        | 12     | 2     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:156:TYR:CD1  | 1:A:161:ALA:CB   | 0.47     | 2.96        | 15     | 9     |
| 1:A:108:LEU:HD11 | 1:A:136:LEU:HD22 | 0.47     | 1.84        | 1      | 1     |
| 1:A:52:HIS:NE2   | 1:A:74:ILE:HG22  | 0.47     | 2.25        | 1      | 1     |
| 1:A:72:LEU:HB2   | 1:A:95:LEU:HD21  | 0.47     | 1.85        | 16     | 1     |
| 1:A:10:ALA:HB1   | 1:A:14:PHE:CZ    | 0.47     | 2.44        | 5      | 2     |
| 1:A:166:ARG:NH1  | 1:A:169:VAL:HG11 | 0.47     | 2.24        | 15     | 1     |
| 1:A:167:ILE:HD11 | 1:A:191:GLN:CG   | 0.47     | 2.40        | 13     | 1     |
| 1:A:114:LEU:CD1  | 1:A:115:VAL:N    | 0.47     | 2.72        | 6      | 1     |
| 1:A:60:ILE:HD12  | 1:A:82:ILE:HD11  | 0.47     | 1.85        | 17     | 1     |
| 1:A:111:ILE:HG21 | 1:A:127:ILE:HD13 | 0.47     | 1.86        | 14     | 1     |
| 1:A:72:LEU:HD13  | 1:A:75:LEU:HD21  | 0.47     | 1.86        | 11     | 1     |
| 1:A:81:LEU:HD23  | 1:A:104:GLN:CD   | 0.47     | 2.29        | 1      | 1     |
| 1:A:77:LEU:HD22  | 1:A:80:ASN:HD22  | 0.47     | 1.69        | 1      | 1     |
| 1:A:166:ARG:O    | 1:A:170:VAL:HG23 | 0.47     | 2.10        | 14     | 1     |
| 1:A:156:TYR:CG   | 1:A:161:ALA:CB   | 0.47     | 2.98        | 12     | 4     |
| 1:A:72:LEU:HB2   | 1:A:95:LEU:HD23  | 0.47     | 1.87        | 4      | 1     |
| 1:A:142:LEU:HB3  | 1:A:176:LEU:HD21 | 0.47     | 1.86        | 8      | 1     |
| 1:A:95:LEU:HD22  | 1:A:98:LEU:HG    | 0.47     | 1.86        | 17     | 2     |
| 1:A:35:PRO:HG2   | 1:A:36:PRO:HD3   | 0.47     | 1.87        | 9      | 4     |
| 1:A:108:LEU:HD23 | 1:A:108:LEU:C    | 0.47     | 2.30        | 16     | 1     |
| 1:A:21:VAL:O     | 1:A:21:VAL:HG22  | 0.47     | 2.10        | 9      | 3     |
| 1:A:72:LEU:O     | 1:A:95:LEU:HD22  | 0.46     | 2.09        | 12     | 1     |
| 1:A:33:MET:HG3   | 1:A:55:LEU:HD13  | 0.46     | 1.87        | 8      | 1     |
| 1:A:111:ILE:HG21 | 1:A:133:ILE:HD11 | 0.46     | 1.85        | 1      | 1     |
| 1:A:54:ALA:C     | 1:A:55:LEU:HD12  | 0.46     | 2.30        | 3      | 4     |
| 1:A:166:ARG:NH1  | 1:A:184:VAL:HG13 | 0.46     | 2.24        | 4      | 1     |
| 1:A:169:VAL:HG21 | 1:A:179:LEU:HD22 | 0.46     | 1.87        | 9      | 1     |
| 1:A:33:MET:HE2   | 1:A:55:LEU:HD22  | 0.46     | 1.85        | 12     | 1     |
| 1:A:95:LEU:CG    | 1:A:98:LEU:HD11  | 0.46     | 2.41        | 13     | 1     |
| 1:A:60:ILE:HD12  | 1:A:81:LEU:O     | 0.46     | 2.09        | 1      | 1     |
| 1:A:173:LEU:HD13 | 1:A:176:LEU:HD11 | 0.46     | 1.88        | 7      | 1     |
| 1:A:114:LEU:C    | 1:A:114:LEU:HD12 | 0.46     | 2.30        | 11     | 2     |
| 1:A:142:LEU:HD23 | 1:A:145:LEU:HD13 | 0.46     | 1.86        | 11     | 1     |
| 1:A:142:LEU:HB3  | 1:A:145:LEU:HD11 | 0.46     | 1.87        | 14     | 1     |
| 1:A:69:MET:HA    | 1:A:72:LEU:HD13  | 0.46     | 1.86        | 10     | 1     |
| 1:A:142:LEU:O    | 1:A:176:LEU:CA   | 0.46     | 2.63        | 4      | 1     |
| 1:A:120:LEU:HD23 | 1:A:120:LEU:C    | 0.46     | 2.31        | 7      | 1     |
| 1:A:47:LEU:C     | 1:A:47:LEU:HD23  | 0.46     | 2.31        | 4      | 2     |
| 1:A:77:LEU:HD22  | 1:A:100:ILE:HG22 | 0.46     | 1.88        | 9      | 2     |
| 1:A:98:LEU:HD12  | 1:A:117:LEU:CD2  | 0.46     | 2.41        | 17     | 1     |
| 1:A:52:HIS:CD2   | 1:A:74:ILE:HG21  | 0.46     | 2.45        | 2      | 2     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:120:LEU:HD12 | 1:A:122:MET:CG   | 0.46     | 2.40        | 3      | 1     |
| 1:A:59:ASN:CG    | 1:A:81:LEU:HD12  | 0.46     | 2.30        | 3      | 1     |
| 1:A:153:TYR:CD1  | 1:A:154:ASN:N    | 0.46     | 2.84        | 15     | 1     |
| 1:A:167:ILE:HG22 | 1:A:171:LYS:CE   | 0.46     | 2.39        | 15     | 1     |
| 1:A:173:LEU:N    | 1:A:173:LEU:CD2  | 0.46     | 2.79        | 13     | 1     |
| 1:A:82:ILE:HB    | 1:A:105:ILE:HG22 | 0.46     | 1.86        | 6      | 1     |
| 1:A:173:LEU:CD1  | 1:A:176:LEU:HD13 | 0.46     | 2.40        | 5      | 1     |
| 1:A:58:ASN:OD1   | 1:A:77:LEU:HD11  | 0.46     | 2.10        | 3      | 1     |
| 1:A:82:ILE:O     | 1:A:82:ILE:HG23  | 0.46     | 2.11        | 2      | 1     |
| 1:A:43:THR:HG22  | 1:A:68:GLY:C     | 0.46     | 2.31        | 2      | 4     |
| 1:A:108:LEU:HD12 | 1:A:108:LEU:N    | 0.46     | 2.26        | 10     | 1     |
| 1:A:88:LEU:HD23  | 1:A:114:LEU:CD2  | 0.46     | 2.41        | 10     | 1     |
| 1:A:95:LEU:HD22  | 1:A:98:LEU:CG    | 0.46     | 2.40        | 10     | 1     |
| 1:A:139:LEU:HD21 | 1:A:165:TYR:HE1  | 0.46     | 1.70        | 13     | 2     |
| 1:A:171:LYS:HZ1  | 1:A:195:ALA:HB1  | 0.46     | 1.70        | 15     | 2     |
| 1:A:95:LEU:CB    | 1:A:117:LEU:HD21 | 0.46     | 2.39        | 6      | 1     |
| 1:A:88:LEU:HD22  | 1:A:114:LEU:CD2  | 0.46     | 2.41        | 5      | 1     |
| 1:A:9:ASP:O      | 1:A:13:ILE:HD12  | 0.46     | 2.11        | 15     | 3     |
| 1:A:142:LEU:HD21 | 1:A:179:LEU:HD13 | 0.46     | 1.86        | 4      | 1     |
| 1:A:145:LEU:N    | 1:A:145:LEU:CD2  | 0.46     | 2.76        | 14     | 3     |
| 1:A:108:LEU:HD12 | 1:A:132:GLU:HB3  | 0.46     | 1.88        | 7      | 1     |
| 1:A:69:MET:CB    | 1:A:91:VAL:HG12  | 0.46     | 2.41        | 5      | 1     |
| 1:A:95:LEU:HD13  | 1:A:98:LEU:HD11  | 0.46     | 1.88        | 5      | 1     |
| 1:A:52:HIS:CE1   | 1:A:74:ILE:HG22  | 0.46     | 2.46        | 10     | 1     |
| 1:A:145:LEU:HD23 | 1:A:146:LEU:H    | 0.46     | 1.67        | 13     | 1     |
| 1:A:28:VAL:HG12  | 1:A:30:LEU:CG    | 0.46     | 2.40        | 5      | 4     |
| 1:A:81:LEU:HD23  | 1:A:104:GLN:NE2  | 0.46     | 2.26        | 1      | 1     |
| 1:A:108:LEU:HD12 | 1:A:109:SER:N    | 0.46     | 2.26        | 6      | 3     |
| 1:A:92:ALA:HB1   | 1:A:113:LYS:C    | 0.46     | 2.32        | 3      | 1     |
| 1:A:153:TYR:CE1  | 1:A:162:THR:CG2  | 0.45     | 3.00        | 12     | 1     |
| 1:A:33:MET:CE    | 1:A:55:LEU:HD22  | 0.45     | 2.41        | 12     | 1     |
| 1:A:4:ALA:HB1    | 1:A:37:ILE:CG1   | 0.45     | 2.41        | 15     | 1     |
| 1:A:52:HIS:CD2   | 1:A:74:ILE:CG2   | 0.45     | 2.99        | 17     | 5     |
| 1:A:95:LEU:HD21  | 1:A:97:GLU:C     | 0.45     | 2.32        | 11     | 2     |
| 1:A:21:VAL:HG12  | 1:A:21:VAL:O     | 0.45     | 2.12        | 15     | 1     |
| 1:A:55:LEU:N     | 1:A:55:LEU:CD2   | 0.45     | 2.80        | 13     | 1     |
| 1:A:2:ALA:CB     | 1:A:14:PHE:CZ    | 0.45     | 2.99        | 9      | 2     |
| 1:A:28:VAL:HB    | 1:A:53:LEU:HD23  | 0.45     | 1.88        | 11     | 1     |
| 1:A:52:HIS:CE1   | 1:A:74:ILE:CG2   | 0.45     | 3.00        | 12     | 6     |
| 1:A:108:LEU:N    | 1:A:108:LEU:HD22 | 0.45     | 2.27        | 13     | 1     |
| 1:A:104:GLN:C    | 1:A:105:ILE:HD12 | 0.45     | 2.32        | 9      | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:117:LEU:HD11 | 1:A:120:LEU:HD23 | 0.45     | 1.89        | 3      | 1     |
| 1:A:53:LEU:HD12  | 1:A:72:LEU:HD21  | 0.45     | 1.89        | 11     | 1     |
| 1:A:47:LEU:HD11  | 1:A:71:ASN:CG    | 0.45     | 2.32        | 11     | 1     |
| 1:A:2:ALA:HB3    | 1:A:33:MET:HA    | 0.45     | 1.88        | 14     | 1     |
| 1:A:173:LEU:HD13 | 1:A:174:PRO:CD   | 0.45     | 2.38        | 2      | 1     |
| 1:A:135:LYS:CA   | 1:A:139:LEU:HD22 | 0.45     | 2.42        | 17     | 1     |
| 1:A:99:TRP:CD1   | 1:A:99:TRP:N     | 0.45     | 2.84        | 7      | 2     |
| 1:A:63:ILE:HG21  | 1:A:87:ASN:CB    | 0.45     | 2.42        | 11     | 1     |
| 1:A:167:ILE:HD12 | 1:A:191:GLN:HB3  | 0.45     | 1.87        | 1      | 1     |
| 1:A:7:ILE:O      | 1:A:7:ILE:HD13   | 0.45     | 2.11        | 16     | 1     |
| 1:A:181:GLY:C    | 1:A:184:VAL:HG23 | 0.45     | 2.32        | 2      | 3     |
| 1:A:170:VAL:O    | 1:A:173:LEU:HD13 | 0.45     | 2.12        | 13     | 1     |
| 1:A:142:LEU:CB   | 1:A:176:LEU:HD12 | 0.45     | 2.40        | 13     | 1     |
| 1:A:2:ALA:CB     | 1:A:14:PHE:CE1   | 0.45     | 3.00        | 13     | 2     |
| 1:A:156:TYR:CD2  | 1:A:161:ALA:CB   | 0.45     | 3.00        | 8      | 1     |
| 1:A:31:HIS:CE1   | 1:A:56:SER:CB    | 0.45     | 3.00        | 7      | 2     |
| 1:A:14:PHE:CD1   | 1:A:30:LEU:CD2   | 0.45     | 3.00        | 3      | 1     |
| 1:A:7:ILE:HG23   | 1:A:8:LYS:N      | 0.44     | 2.28        | 10     | 12    |
| 1:A:144:ASP:C    | 1:A:145:LEU:HD23 | 0.44     | 2.33        | 4      | 3     |
| 1:A:54:ALA:C     | 1:A:55:LEU:HD22  | 0.44     | 2.32        | 5      | 1     |
| 1:A:117:LEU:HD23 | 1:A:117:LEU:C    | 0.44     | 2.31        | 3      | 1     |
| 1:A:139:LEU:HD21 | 1:A:165:TYR:OH   | 0.44     | 2.12        | 11     | 1     |
| 1:A:2:ALA:CB     | 1:A:14:PHE:CD2   | 0.44     | 3.00        | 10     | 1     |
| 1:A:120:LEU:CD2  | 1:A:120:LEU:N    | 0.44     | 2.80        | 15     | 1     |
| 1:A:44:LEU:HD21  | 1:A:65:SER:HA    | 0.44     | 1.89        | 10     | 1     |
| 1:A:142:LEU:C    | 1:A:142:LEU:HD23 | 0.44     | 2.33        | 12     | 1     |
| 1:A:115:VAL:HG21 | 1:A:137:ALA:CA   | 0.44     | 2.42        | 9      | 1     |
| 1:A:139:LEU:CD2  | 1:A:165:TYR:CE1  | 0.44     | 3.00        | 16     | 1     |
| 1:A:105:ILE:HD12 | 1:A:105:ILE:N    | 0.44     | 2.26        | 9      | 1     |
| 1:A:121:TYR:CD1  | 1:A:121:TYR:N    | 0.44     | 2.85        | 3      | 1     |
| 1:A:94:THR:HG23  | 1:A:95:LEU:N     | 0.44     | 2.27        | 15     | 1     |
| 1:A:130:TRP:CD1  | 1:A:152:LEU:HD13 | 0.44     | 2.47        | 2      | 1     |
| 1:A:142:LEU:O    | 1:A:176:LEU:CB   | 0.44     | 2.66        | 1      | 5     |
| 1:A:44:LEU:HD13  | 1:A:65:SER:OG    | 0.44     | 2.13        | 7      | 1     |
| 1:A:10:ALA:O     | 1:A:14:PHE:CG    | 0.44     | 2.70        | 5      | 1     |
| 1:A:133:ILE:HG21 | 1:A:152:LEU:HD11 | 0.44     | 1.90        | 10     | 1     |
| 1:A:82:ILE:HG21  | 1:A:88:LEU:CD1   | 0.44     | 2.26        | 11     | 1     |
| 1:A:73:ARG:HB3   | 1:A:74:ILE:HD12  | 0.44     | 1.89        | 2      | 1     |
| 1:A:6:THR:HG23   | 1:A:9:ASP:H      | 0.44     | 1.73        | 13     | 1     |
| 1:A:69:MET:HG2   | 1:A:72:LEU:HD11  | 0.44     | 1.90        | 3      | 1     |
| 1:A:105:ILE:CD1  | 1:A:105:ILE:N    | 0.44     | 2.80        | 11     | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:142:LEU:O    | 1:A:176:LEU:HD23 | 0.44     | 2.13        | 11     | 1     |
| 1:A:139:LEU:HD23 | 1:A:140:ASP:OD1  | 0.44     | 2.13        | 17     | 1     |
| 1:A:75:LEU:CD1   | 1:A:98:LEU:HD21  | 0.44     | 2.43        | 15     | 1     |
| 1:A:120:LEU:HD11 | 1:A:122:MET:HE3  | 0.44     | 1.90        | 10     | 1     |
| 1:A:75:LEU:HD13  | 1:A:98:LEU:HD21  | 0.43     | 1.89        | 15     | 2     |
| 1:A:99:TRP:N     | 1:A:99:TRP:CD1   | 0.43     | 2.84        | 4      | 1     |
| 1:A:3:LYS:HE3    | 1:A:13:ILE:HD13  | 0.43     | 1.90        | 1      | 1     |
| 1:A:171:LYS:HZ3  | 1:A:195:ALA:HB3  | 0.43     | 1.71        | 4      | 1     |
| 1:A:115:VAL:HG21 | 1:A:137:ALA:HA   | 0.43     | 1.90        | 9      | 1     |
| 1:A:137:ALA:O    | 1:A:142:LEU:HD12 | 0.43     | 2.14        | 9      | 1     |
| 1:A:63:ILE:HG21  | 1:A:87:ASN:HB3   | 0.43     | 1.89        | 11     | 1     |
| 1:A:142:LEU:HD22 | 1:A:145:LEU:HD22 | 0.43     | 1.89        | 15     | 1     |
| 1:A:91:VAL:HG22  | 1:A:95:LEU:HD12  | 0.43     | 1.88        | 2      | 1     |
| 1:A:66:LEU:N     | 1:A:66:LEU:CD1   | 0.43     | 2.82        | 12     | 1     |
| 1:A:91:VAL:HA    | 1:A:95:LEU:HD23  | 0.43     | 1.91        | 16     | 1     |
| 1:A:14:PHE:CZ    | 1:A:33:MET:CE    | 0.43     | 3.01        | 4      | 1     |
| 1:A:70:GLU:HG2   | 1:A:94:THR:HG22  | 0.43     | 1.90        | 17     | 1     |
| 1:A:95:LEU:HD21  | 1:A:97:GLU:O     | 0.43     | 2.13        | 17     | 1     |
| 1:A:99:TRP:CD1   | 1:A:121:TYR:CD2  | 0.43     | 3.07        | 10     | 1     |
| 1:A:44:LEU:HD11  | 1:A:65:SER:CB    | 0.43     | 2.43        | 12     | 1     |
| 1:A:81:LEU:HD12  | 1:A:81:LEU:N     | 0.43     | 2.27        | 5      | 2     |
| 1:A:43:THR:HG21  | 1:A:69:MET:HG2   | 0.43     | 1.90        | 2      | 2     |
| 1:A:37:ILE:HG12  | 1:A:63:ILE:HG22  | 0.43     | 1.91        | 10     | 1     |
| 1:A:185:ASP:O    | 1:A:186:VAL:CG1  | 0.43     | 2.67        | 8      | 10    |
| 1:A:7:ILE:HA     | 1:A:42:ALA:HB2   | 0.43     | 1.90        | 6      | 2     |
| 1:A:105:ILE:CG2  | 1:A:111:ILE:HG23 | 0.43     | 2.43        | 3      | 1     |
| 1:A:120:LEU:N    | 1:A:120:LEU:CD2  | 0.43     | 2.81        | 14     | 1     |
| 1:A:138:ALA:O    | 1:A:142:LEU:HD12 | 0.43     | 2.13        | 10     | 1     |
| 1:A:185:ASP:O    | 1:A:186:VAL:CG2  | 0.43     | 2.67        | 9      | 6     |
| 1:A:10:ALA:O     | 1:A:14:PHE:CD2   | 0.43     | 2.72        | 4      | 7     |
| 1:A:108:LEU:N    | 1:A:108:LEU:HD12 | 0.43     | 2.28        | 3      | 1     |
| 1:A:115:VAL:HG13 | 1:A:145:LEU:HD11 | 0.43     | 1.89        | 10     | 1     |
| 1:A:115:VAL:HG13 | 1:A:145:LEU:HD12 | 0.43     | 1.89        | 10     | 1     |
| 1:A:47:LEU:HD23  | 1:A:71:ASN:CB    | 0.43     | 2.44        | 16     | 1     |
| 1:A:63:ILE:HD13  | 1:A:87:ASN:HB2   | 0.43     | 1.90        | 15     | 1     |
| 1:A:105:ILE:N    | 1:A:105:ILE:CD1  | 0.43     | 2.81        | 2      | 1     |
| 1:A:140:ASP:C    | 1:A:173:LEU:HD11 | 0.43     | 2.33        | 2      | 1     |
| 1:A:173:LEU:CG   | 1:A:173:LEU:O    | 0.43     | 2.67        | 13     | 1     |
| 1:A:142:LEU:HD22 | 1:A:142:LEU:C    | 0.43     | 2.34        | 1      | 1     |
| 1:A:121:TYR:CD2  | 1:A:146:LEU:HD23 | 0.43     | 2.49        | 14     | 1     |
| 1:A:35:PRO:HA    | 1:A:59:ASN:O     | 0.43     | 2.14        | 13     | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:129:ASN:HB3  | 1:A:133:ILE:HD12 | 0.43     | 1.90        | 2      | 2     |
| 1:A:43:THR:HG23  | 1:A:44:LEU:N     | 0.43     | 2.29        | 15     | 1     |
| 1:A:120:LEU:O    | 1:A:145:LEU:HD12 | 0.42     | 2.14        | 12     | 1     |
| 1:A:81:LEU:HD23  | 1:A:104:GLN:OE1  | 0.42     | 2.14        | 13     | 1     |
| 1:A:59:ASN:HD22  | 1:A:81:LEU:HD12  | 0.42     | 1.69        | 9      | 1     |
| 1:A:34:ILE:C     | 1:A:34:ILE:HD12  | 0.42     | 2.34        | 6      | 1     |
| 1:A:59:ASN:ND2   | 1:A:81:LEU:HD22  | 0.42     | 2.29        | 5      | 1     |
| 1:A:30:LEU:N     | 1:A:30:LEU:CD2   | 0.42     | 2.82        | 13     | 2     |
| 1:A:73:ARG:C     | 1:A:95:LEU:HD13  | 0.42     | 2.34        | 13     | 1     |
| 1:A:52:HIS:CD2   | 1:A:74:ILE:HG22  | 0.42     | 2.50        | 4      | 2     |
| 1:A:95:LEU:HD12  | 1:A:98:LEU:HD23  | 0.42     | 1.90        | 7      | 1     |
| 1:A:138:ALA:HB3  | 1:A:142:LEU:CD1  | 0.42     | 2.44        | 3      | 1     |
| 1:A:178:LYS:NZ   | 1:A:184:VAL:HG21 | 0.42     | 2.28        | 3      | 1     |
| 1:A:119:VAL:O    | 1:A:120:LEU:HD13 | 0.42     | 2.14        | 15     | 1     |
| 1:A:81:LEU:N     | 1:A:81:LEU:HD12  | 0.42     | 2.29        | 14     | 1     |
| 1:A:167:ILE:HD11 | 1:A:191:GLN:CD   | 0.42     | 2.35        | 8      | 1     |
| 1:A:63:ILE:C     | 1:A:63:ILE:HD12  | 0.42     | 2.35        | 7      | 1     |
| 1:A:175:ASN:O    | 1:A:176:LEU:C    | 0.42     | 2.57        | 8      | 3     |
| 1:A:72:LEU:C     | 1:A:95:LEU:HD22  | 0.42     | 2.35        | 4      | 1     |
| 1:A:77:LEU:HD21  | 1:A:80:ASN:HD22  | 0.42     | 1.73        | 6      | 1     |
| 1:A:77:LEU:HD12  | 1:A:77:LEU:C     | 0.42     | 2.35        | 11     | 1     |
| 1:A:130:TRP:N    | 1:A:152:LEU:CD2  | 0.42     | 2.81        | 2      | 1     |
| 1:A:167:ILE:HD11 | 1:A:191:GLN:CB   | 0.42     | 2.45        | 13     | 1     |
| 1:A:110:GLY:O    | 1:A:114:LEU:HD23 | 0.42     | 2.14        | 8      | 1     |
| 1:A:140:ASP:C    | 1:A:176:LEU:HD23 | 0.42     | 2.35        | 14     | 1     |
| 1:A:81:LEU:N     | 1:A:81:LEU:CD2   | 0.42     | 2.81        | 12     | 1     |
| 1:A:119:VAL:HG23 | 1:A:144:ASP:CG   | 0.42     | 2.34        | 1      | 1     |
| 1:A:117:LEU:HB3  | 1:A:120:LEU:HD11 | 0.42     | 1.91        | 1      | 2     |
| 1:A:59:ASN:HD21  | 1:A:81:LEU:HD22  | 0.42     | 1.75        | 1      | 1     |
| 1:A:153:TYR:OH   | 1:A:165:TYR:CD2  | 0.42     | 2.72        | 17     | 1     |
| 1:A:182:MET:N    | 1:A:183:PRO:HD2  | 0.42     | 2.29        | 9      | 4     |
| 1:A:138:ALA:HB3  | 1:A:142:LEU:HG   | 0.42     | 1.91        | 17     | 1     |
| 1:A:153:TYR:CZ   | 1:A:165:TYR:CD2  | 0.42     | 3.08        | 10     | 2     |
| 1:A:31:HIS:CD2   | 1:A:56:SER:HG    | 0.42     | 2.32        | 7      | 1     |
| 1:A:173:LEU:CD1  | 1:A:173:LEU:N    | 0.42     | 2.83        | 10     | 1     |
| 1:A:30:LEU:HD13  | 1:A:30:LEU:N     | 0.42     | 2.30        | 9      | 1     |
| 1:A:142:LEU:HD12 | 1:A:145:LEU:HD11 | 0.42     | 1.92        | 14     | 1     |
| 1:A:132:GLU:O    | 1:A:136:LEU:CB   | 0.42     | 2.68        | 3      | 3     |
| 1:A:85:ILE:HD12  | 1:A:85:ILE:N     | 0.42     | 2.30        | 6      | 1     |
| 1:A:140:ASP:CB   | 1:A:173:LEU:HD22 | 0.42     | 2.44        | 9      | 1     |
| 1:A:140:ASP:C    | 1:A:173:LEU:HD21 | 0.42     | 2.35        | 5      | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:102:TYR:CD1  | 1:A:124:ASN:O    | 0.41     | 2.73        | 12     | 6     |
| 1:A:117:LEU:HD23 | 1:A:118:ARG:N    | 0.41     | 2.30        | 4      | 1     |
| 1:A:127:ILE:CG2  | 1:A:133:ILE:CD1  | 0.41     | 2.98        | 5      | 4     |
| 1:A:130:TRP:CH2  | 1:A:134:ASP:OD2  | 0.41     | 2.74        | 16     | 3     |
| 1:A:20:VAL:CG2   | 1:A:30:LEU:HD12  | 0.41     | 2.39        | 13     | 2     |
| 1:A:121:TYR:CE2  | 1:A:146:LEU:HD22 | 0.41     | 2.49        | 6      | 1     |
| 1:A:88:LEU:HD12  | 1:A:114:LEU:CB   | 0.41     | 2.43        | 7      | 1     |
| 1:A:7:ILE:HD13   | 1:A:45:SER:HB2   | 0.41     | 1.91        | 5      | 1     |
| 1:A:127:ILE:HG23 | 1:A:133:ILE:HD13 | 0.41     | 1.89        | 11     | 1     |
| 1:A:77:LEU:HD13  | 1:A:80:ASN:HB3   | 0.41     | 1.92        | 11     | 1     |
| 1:A:120:LEU:HD21 | 1:A:122:MET:HE3  | 0.41     | 1.92        | 10     | 1     |
| 1:A:173:LEU:HG   | 1:A:173:LEU:O    | 0.41     | 2.16        | 13     | 1     |
| 1:A:82:ILE:HD13  | 1:A:88:LEU:HD11  | 0.41     | 1.92        | 16     | 1     |
| 1:A:53:LEU:HD12  | 1:A:72:LEU:HD11  | 0.41     | 1.92        | 7      | 1     |
| 1:A:30:LEU:CD1   | 1:A:30:LEU:N     | 0.41     | 2.83        | 15     | 2     |
| 1:A:3:LYS:HA     | 1:A:34:ILE:HG21  | 0.41     | 1.90        | 2      | 1     |
| 1:A:114:LEU:HD12 | 1:A:114:LEU:C    | 0.41     | 2.36        | 17     | 1     |
| 1:A:74:ILE:CG2   | 1:A:99:TRP:CH2   | 0.41     | 3.04        | 17     | 1     |
| 1:A:184:VAL:HG13 | 1:A:188:GLU:CG   | 0.41     | 2.46        | 15     | 1     |
| 1:A:3:LYS:N      | 1:A:13:ILE:HG21  | 0.41     | 2.31        | 13     | 1     |
| 1:A:111:ILE:HD13 | 1:A:127:ILE:HD13 | 0.41     | 1.92        | 8      | 1     |
| 1:A:47:LEU:CD2   | 1:A:71:ASN:CB    | 0.41     | 2.99        | 8      | 1     |
| 1:A:88:LEU:HD12  | 1:A:88:LEU:N     | 0.41     | 2.30        | 16     | 1     |
| 1:A:127:ILE:HG21 | 1:A:133:ILE:HD13 | 0.41     | 1.91        | 14     | 1     |
| 1:A:133:ILE:HG23 | 1:A:137:ALA:HB2  | 0.41     | 1.91        | 4      | 1     |
| 1:A:3:LYS:HA     | 1:A:34:ILE:HD12  | 0.41     | 1.92        | 9      | 1     |
| 1:A:176:LEU:H    | 1:A:176:LEU:HD23 | 0.41     | 1.76        | 7      | 1     |
| 1:A:69:MET:CB    | 1:A:91:VAL:CG1   | 0.41     | 2.99        | 5      | 1     |
| 1:A:40:MET:O     | 1:A:41:ASP:C     | 0.41     | 2.59        | 13     | 1     |
| 1:A:44:LEU:HD23  | 1:A:65:SER:OG    | 0.41     | 2.14        | 16     | 1     |
| 1:A:133:ILE:HG21 | 1:A:152:LEU:HG   | 0.41     | 1.92        | 7      | 1     |
| 1:A:2:ALA:HB3    | 1:A:14:PHE:CZ    | 0.41     | 2.51        | 3      | 1     |
| 1:A:44:LEU:CD1   | 1:A:65:SER:CB    | 0.41     | 2.98        | 12     | 1     |
| 1:A:77:LEU:CD2   | 1:A:80:ASN:ND2   | 0.41     | 2.84        | 13     | 2     |
| 1:A:130:TRP:CZ2  | 1:A:134:ASP:OD1  | 0.41     | 2.73        | 16     | 4     |
| 1:A:21:VAL:O     | 1:A:21:VAL:HG12  | 0.41     | 2.15        | 6      | 2     |
| 1:A:2:ALA:CB     | 1:A:14:PHE:CD1   | 0.41     | 3.04        | 3      | 1     |
| 1:A:99:TRP:CD1   | 1:A:121:TYR:CE2  | 0.41     | 3.09        | 10     | 1     |
| 1:A:6:THR:O      | 1:A:10:ALA:CB    | 0.41     | 2.69        | 12     | 1     |
| 1:A:129:ASN:CB   | 1:A:133:ILE:CD1  | 0.41     | 2.99        | 13     | 3     |
| 1:A:4:ALA:N      | 1:A:34:ILE:HG21  | 0.41     | 2.30        | 13     | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:128:THR:HG22 | 1:A:151:PRO:HG3  | 0.41     | 1.83        | 1      | 2     |
| 1:A:4:ALA:HB1    | 1:A:37:ILE:CD1   | 0.41     | 2.44        | 1      | 1     |
| 1:A:70:GLU:O     | 1:A:94:THR:CG2   | 0.41     | 2.69        | 9      | 2     |
| 1:A:7:ILE:CG2    | 1:A:8:LYS:N      | 0.41     | 2.84        | 15     | 1     |
| 1:A:88:LEU:HA    | 1:A:91:VAL:HG12  | 0.41     | 1.92        | 2      | 1     |
| 1:A:156:TYR:CD2  | 1:A:161:ALA:HB1  | 0.41     | 2.51        | 8      | 1     |
| 1:A:24:GLU:HG2   | 1:A:49:ALA:HB3   | 0.41     | 1.93        | 1      | 1     |
| 1:A:47:LEU:HD12  | 1:A:68:GLY:HA2   | 0.41     | 1.93        | 1      | 1     |
| 1:A:43:THR:CG2   | 1:A:44:LEU:N     | 0.41     | 2.84        | 6      | 1     |
| 1:A:108:LEU:CD2  | 1:A:108:LEU:N    | 0.41     | 2.84        | 7      | 1     |
| 1:A:169:VAL:CG2  | 1:A:179:LEU:CD2  | 0.41     | 2.99        | 7      | 2     |
| 1:A:98:LEU:HB3   | 1:A:120:LEU:HD22 | 0.41     | 1.92        | 3      | 1     |
| 1:A:77:LEU:CD2   | 1:A:100:ILE:HG22 | 0.41     | 2.38        | 15     | 1     |
| 1:A:153:TYR:CZ   | 1:A:158:GLU:O    | 0.41     | 2.74        | 15     | 1     |
| 1:A:47:LEU:HD23  | 1:A:47:LEU:C     | 0.41     | 2.35        | 2      | 1     |
| 1:A:47:LEU:CD1   | 1:A:48:LYS:N     | 0.40     | 2.84        | 13     | 1     |
| 1:A:76:SER:OG    | 1:A:99:TRP:CZ3   | 0.40     | 2.75        | 8      | 1     |
| 1:A:22:ALA:O     | 1:A:25:ALA:HB2   | 0.40     | 2.16        | 1      | 1     |
| 1:A:145:LEU:HD21 | 1:A:176:LEU:CD2  | 0.40     | 2.40        | 16     | 1     |
| 1:A:166:ARG:NH1  | 1:A:167:ILE:CG1  | 0.40     | 2.84        | 9      | 1     |
| 1:A:114:LEU:O    | 1:A:120:LEU:HD21 | 0.40     | 2.16        | 17     | 1     |
| 1:A:153:TYR:CE2  | 1:A:158:GLU:O    | 0.40     | 2.74        | 15     | 1     |
| 1:A:55:LEU:HD12  | 1:A:55:LEU:N     | 0.40     | 2.31        | 12     | 2     |
| 1:A:100:ILE:HD11 | 1:A:122:MET:CG   | 0.40     | 2.46        | 16     | 1     |
| 1:A:142:LEU:HD22 | 1:A:145:LEU:HD11 | 0.40     | 1.93        | 4      | 1     |
| 1:A:120:LEU:CD2  | 1:A:122:MET:CG   | 0.40     | 3.00        | 9      | 1     |
| 1:A:31:HIS:CG    | 1:A:56:SER:OG    | 0.40     | 2.74        | 17     | 1     |
| 1:A:111:ILE:CD1  | 1:A:133:ILE:CD1  | 0.40     | 2.99        | 3      | 1     |
| 1:A:146:LEU:HD12 | 1:A:180:ASP:O    | 0.40     | 2.16        | 3      | 1     |
| 1:A:167:ILE:CG2  | 1:A:195:ALA:CB   | 0.40     | 2.99        | 15     | 1     |
| 1:A:166:ARG:HH12 | 1:A:169:VAL:HG11 | 0.40     | 1.75        | 15     | 1     |
| 1:A:47:LEU:CD1   | 1:A:71:ASN:CB    | 0.40     | 2.99        | 14     | 1     |
| 1:A:184:VAL:HG13 | 1:A:188:GLU:HB2  | 0.40     | 1.93        | 2      | 1     |
| 1:A:154:ASN:ND2  | 1:A:158:GLU:CG   | 0.40     | 2.84        | 10     | 1     |
| 1:A:142:LEU:HD22 | 1:A:145:LEU:HB2  | 0.40     | 1.92        | 12     | 1     |
| 1:A:4:ALA:CB     | 1:A:37:ILE:CD1   | 0.40     | 2.99        | 4      | 4     |
| 1:A:184:VAL:HG23 | 1:A:185:ASP:N    | 0.40     | 2.32        | 5      | 1     |
| 1:A:117:LEU:CD1  | 1:A:120:LEU:HD23 | 0.40     | 2.46        | 3      | 1     |
| 1:A:129:ASN:C    | 1:A:152:LEU:HD21 | 0.40     | 2.37        | 3      | 1     |
| 1:A:59:ASN:ND2   | 1:A:81:LEU:CD1   | 0.40     | 2.85        | 11     | 1     |
| 1:A:145:LEU:CD2  | 1:A:145:LEU:N    | 0.40     | 2.81        | 15     | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:37:ILE:CD1   | 1:A:63:ILE:HG22  | 0.40     | 2.46        | 10     | 1     |
| 1:A:96:GLU:C     | 1:A:117:LEU:HD21 | 0.40     | 2.37        | 12     | 1     |
| 1:A:111:ILE:HD13 | 1:A:137:ALA:CB   | 0.40     | 2.46        | 4      | 1     |
| 1:A:157:LYS:O    | 1:A:158:GLU:C    | 0.40     | 2.60        | 6      | 2     |
| 1:A:166:ARG:CZ   | 1:A:188:GLU:CB   | 0.40     | 3.00        | 17     | 1     |
| 1:A:18:LYS:CE    | 1:A:20:VAL:CG1   | 0.40     | 2.99        | 5      | 1     |
| 1:A:69:MET:HB3   | 1:A:91:VAL:HG12  | 0.40     | 1.93        | 5      | 1     |
| 1:A:81:LEU:CD2   | 1:A:81:LEU:N     | 0.40     | 2.85        | 8      | 1     |
| 1:A:111:ILE:HG13 | 1:A:133:ILE:HD12 | 0.40     | 1.92        | 1      | 1     |
| 1:A:173:LEU:O    | 1:A:173:LEU:CG   | 0.40     | 2.69        | 1      | 1     |
| 1:A:141:LYS:N    | 1:A:176:LEU:CD2  | 0.40     | 2.85        | 4      | 1     |
| 1:A:28:VAL:CG1   | 1:A:30:LEU:CD2   | 0.40     | 2.99        | 4      | 1     |
| 1:A:98:LEU:HB3   | 1:A:120:LEU:HD23 | 0.40     | 1.93        | 17     | 1     |
| 1:A:75:LEU:HB3   | 1:A:98:LEU:HD23  | 0.40     | 1.93        | 3      | 1     |
| 1:A:108:LEU:HD12 | 1:A:108:LEU:H    | 0.40     | 1.77        | 2      | 1     |
| 1:A:63:ILE:CD1   | 1:A:87:ASN:CB    | 0.40     | 2.98        | 10     | 1     |

## 6.3 Torsion angles ⓘ

### 6.3.1 Protein backbone ⓘ

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

| Mol | Chain | Analysed        | Favoured      | Allowed      | Outliers    | Percentiles |    |
|-----|-------|-----------------|---------------|--------------|-------------|-------------|----|
| 1   | A     | 194/198 (98%)   | 144±4 (74±2%) | 40±4 (20±2%) | 10±2 (5±1%) | 4           | 25 |
| All | All   | 3298/3366 (98%) | 2456 (74%)    | 672 (20%)    | 170 (5%)    | 4           | 25 |

All 26 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     | 174 | PRO  | 17             |
| 1   | A     | 117 | LEU  | 17             |
| 1   | A     | 157 | LYS  | 17             |
| 1   | A     | 142 | LEU  | 14             |
| 1   | A     | 141 | LYS  | 13             |
| 1   | A     | 51  | LYS  | 13             |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 149 | GLY  | 13             |
| 1   | A     | 173 | LEU  | 9              |
| 1   | A     | 143 | GLU  | 8              |
| 1   | A     | 87  | ASN  | 7              |
| 1   | A     | 158 | GLU  | 6              |
| 1   | A     | 176 | LEU  | 6              |
| 1   | A     | 184 | VAL  | 5              |
| 1   | A     | 175 | ASN  | 5              |
| 1   | A     | 96  | GLU  | 3              |
| 1   | A     | 95  | LEU  | 2              |
| 1   | A     | 186 | VAL  | 2              |
| 1   | A     | 86  | GLU  | 2              |
| 1   | A     | 70  | GLU  | 2              |
| 1   | A     | 181 | GLY  | 2              |
| 1   | A     | 63  | ILE  | 2              |
| 1   | A     | 42  | ALA  | 1              |
| 1   | A     | 41  | ASP  | 1              |
| 1   | A     | 22  | ALA  | 1              |
| 1   | A     | 64  | SER  | 1              |
| 1   | A     | 56  | SER  | 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     | 170/172 (99%)   | 137±3 (81±2%) | 33±3 (19±2%) | 4           | 36 |
| All | All   | 2890/2924 (99%) | 2333 (81%)    | 557 (19%)    | 4           | 36 |

All 119 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     | 18  | LYS  | 17             |
| 1   | A     | 19  | SER  | 17             |
| 1   | A     | 162 | THR  | 16             |
| 1   | A     | 6   | THR  | 15             |
| 1   | A     | 153 | TYR  | 14             |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 166 | ARG  | 14             |
| 1   | A     | 98  | LEU  | 14             |
| 1   | A     | 178 | LYS  | 12             |
| 1   | A     | 152 | LEU  | 12             |
| 1   | A     | 102 | TYR  | 12             |
| 1   | A     | 156 | TYR  | 12             |
| 1   | A     | 129 | ASN  | 11             |
| 1   | A     | 80  | ASN  | 11             |
| 1   | A     | 79  | ARG  | 11             |
| 1   | A     | 157 | LYS  | 10             |
| 1   | A     | 142 | LEU  | 10             |
| 1   | A     | 191 | GLN  | 9              |
| 1   | A     | 85  | ILE  | 9              |
| 1   | A     | 145 | LEU  | 9              |
| 1   | A     | 56  | SER  | 8              |
| 1   | A     | 120 | LEU  | 8              |
| 1   | A     | 176 | LEU  | 8              |
| 1   | A     | 33  | MET  | 8              |
| 1   | A     | 63  | ILE  | 8              |
| 1   | A     | 53  | LEU  | 7              |
| 1   | A     | 3   | LYS  | 7              |
| 1   | A     | 173 | LEU  | 7              |
| 1   | A     | 139 | LEU  | 7              |
| 1   | A     | 75  | LEU  | 7              |
| 1   | A     | 30  | LEU  | 7              |
| 1   | A     | 5   | THR  | 7              |
| 1   | A     | 117 | LEU  | 6              |
| 1   | A     | 177 | LYS  | 6              |
| 1   | A     | 182 | MET  | 6              |
| 1   | A     | 93  | ASP  | 6              |
| 1   | A     | 45  | SER  | 6              |
| 1   | A     | 76  | SER  | 6              |
| 1   | A     | 140 | ASP  | 6              |
| 1   | A     | 126 | LYS  | 6              |
| 1   | A     | 59  | ASN  | 5              |
| 1   | A     | 160 | ASN  | 5              |
| 1   | A     | 14  | PHE  | 5              |
| 1   | A     | 95  | LEU  | 5              |
| 1   | A     | 47  | LEU  | 5              |
| 1   | A     | 189 | ARG  | 4              |
| 1   | A     | 40  | MET  | 4              |
| 1   | A     | 9   | ASP  | 4              |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 89  | ASP  | 4              |
| 1   | A     | 130 | TRP  | 4              |
| 1   | A     | 48  | LYS  | 4              |
| 1   | A     | 114 | LEU  | 4              |
| 1   | A     | 51  | LYS  | 4              |
| 1   | A     | 165 | TYR  | 4              |
| 1   | A     | 44  | LEU  | 4              |
| 1   | A     | 17  | ARG  | 3              |
| 1   | A     | 143 | GLU  | 3              |
| 1   | A     | 34  | ILE  | 3              |
| 1   | A     | 65  | SER  | 3              |
| 1   | A     | 172 | ARG  | 3              |
| 1   | A     | 71  | ASN  | 3              |
| 1   | A     | 158 | GLU  | 3              |
| 1   | A     | 70  | GLU  | 3              |
| 1   | A     | 43  | THR  | 3              |
| 1   | A     | 128 | THR  | 3              |
| 1   | A     | 29  | GLU  | 3              |
| 1   | A     | 175 | ASN  | 3              |
| 1   | A     | 86  | GLU  | 3              |
| 1   | A     | 77  | LEU  | 3              |
| 1   | A     | 101 | SER  | 3              |
| 1   | A     | 84  | LYS  | 3              |
| 1   | A     | 64  | SER  | 3              |
| 1   | A     | 111 | ILE  | 3              |
| 1   | A     | 7   | ILE  | 3              |
| 1   | A     | 83  | LYS  | 2              |
| 1   | A     | 15  | GLU  | 2              |
| 1   | A     | 141 | LYS  | 2              |
| 1   | A     | 62  | LYS  | 2              |
| 1   | A     | 185 | ASP  | 2              |
| 1   | A     | 73  | ARG  | 2              |
| 1   | A     | 39  | LYS  | 2              |
| 1   | A     | 41  | ASP  | 2              |
| 1   | A     | 188 | GLU  | 2              |
| 1   | A     | 171 | LYS  | 2              |
| 1   | A     | 58  | ASN  | 2              |
| 1   | A     | 105 | ILE  | 2              |
| 1   | A     | 147 | LEU  | 2              |
| 1   | A     | 57  | THR  | 2              |
| 1   | A     | 108 | LEU  | 2              |
| 1   | A     | 66  | LEU  | 2              |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 179 | LEU  | 2              |
| 1   | A     | 38  | GLU  | 1              |
| 1   | A     | 112 | GLU  | 1              |
| 1   | A     | 155 | ASP  | 1              |
| 1   | A     | 82  | ILE  | 1              |
| 1   | A     | 190 | GLU  | 1              |
| 1   | A     | 118 | ARG  | 1              |
| 1   | A     | 144 | ASP  | 1              |
| 1   | A     | 180 | ASP  | 1              |
| 1   | A     | 115 | VAL  | 1              |
| 1   | A     | 55  | LEU  | 1              |
| 1   | A     | 135 | LYS  | 1              |
| 1   | A     | 24  | GLU  | 1              |
| 1   | A     | 124 | ASN  | 1              |
| 1   | A     | 37  | ILE  | 1              |
| 1   | A     | 168 | GLU  | 1              |
| 1   | A     | 193 | ASN  | 1              |
| 1   | A     | 122 | MET  | 1              |
| 1   | A     | 186 | VAL  | 1              |
| 1   | A     | 72  | LEU  | 1              |
| 1   | A     | 50  | CYS  | 1              |
| 1   | A     | 125 | ASN  | 1              |
| 1   | A     | 113 | LYS  | 1              |
| 1   | A     | 163 | SER  | 1              |
| 1   | A     | 136 | LEU  | 1              |
| 1   | A     | 97  | GLU  | 1              |
| 1   | A     | 16  | GLU  | 1              |
| 1   | A     | 107 | SER  | 1              |
| 1   | A     | 159 | ASN  | 1              |
| 1   | A     | 109 | SER  | 1              |

### 6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 6.5 Carbohydrates [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 [i](#)

There are no chain breaks in this entry.



## 7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 75% for the well-defined parts and 75% for the entire structure.

### 7.1 Chemical shift list 1

File name: BMRB entry 4265

Chemical shift list name: *assigned\_chem\_shift\_list\_1*

#### 7.1.1 Bookkeeping

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

|                                         |      |
|-----------------------------------------|------|
| Total number of shifts                  | 2006 |
| Number of shifts mapped to atoms        | 2006 |
| Number of unparsed shifts               | 0    |
| Number of shifts with mapping errors    | 0    |
| Number of shifts with mapping warnings  | 0    |
| Number of shift outliers (ShiftChecker) | 5    |

#### 7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

| Nucleus                | # values | Correction $\pm$ precision, ppm | Suggested action           |
|------------------------|----------|---------------------------------|----------------------------|
| $^{13}\text{C}_\alpha$ | 197      | $-0.87 \pm 0.10$                | Should be applied          |
| $^{13}\text{C}_\beta$  | 188      | $-0.34 \pm 0.15$                | None needed ( $< 0.5$ ppm) |
| $^{13}\text{C}'$       | 191      | $-0.08 \pm 0.09$                | None needed ( $< 0.5$ ppm) |
| $^{15}\text{N}$        | 191      | $-0.07 \pm 0.25$                | None needed ( $< 0.5$ ppm) |

#### 7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 75%, i.e. 1806 atoms were assigned a chemical shift out of a possible 2411. 0 out of 38 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | Total          | $^1\text{H}$  | $^{13}\text{C}$ | $^{15}\text{N}$ |
|-----------|----------------|---------------|-----------------|-----------------|
| Backbone  | 948/960 (99%)  | 379/383 (99%) | 381/388 (98%)   | 188/189 (99%)   |
| Sidechain | 852/1364 (62%) | 518/790 (66%) | 319/514 (62%)   | 15/60 (25%)     |

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|          | <b>Total</b>    | <b><sup>1</sup>H</b> | <b><sup>13</sup>C</b> | <b><sup>15</sup>N</b> |
|----------|-----------------|----------------------|-----------------------|-----------------------|
| Aromatic | 6/87 (7%)       | 4/45 (9%)            | 0/38 (0%)             | 2/4 (50%)             |
| Overall  | 1806/2411 (75%) | 901/1218 (74%)       | 700/940 (74%)         | 205/253 (81%)         |

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 75%, i.e. 1840 atoms were assigned a chemical shift out of a possible 2457. 0 out of 38 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | <b>Total</b>    | <b><sup>1</sup>H</b> | <b><sup>13</sup>C</b> | <b><sup>15</sup>N</b> |
|-----------|-----------------|----------------------|-----------------------|-----------------------|
| Backbone  | 965/980 (98%)   | 386/391 (99%)        | 388/396 (98%)         | 191/193 (99%)         |
| Sidechain | 869/1390 (63%)  | 529/806 (66%)        | 324/521 (62%)         | 16/63 (25%)           |
| Aromatic  | 6/87 (7%)       | 4/45 (9%)            | 0/38 (0%)             | 2/4 (50%)             |
| Overall   | 1840/2457 (75%) | 919/1242 (74%)       | 712/955 (75%)         | 209/260 (80%)         |

#### 7.1.4 Statistically unusual chemical shifts [i](#)

The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

| Mol | Chain | Res | Type | Atom | Shift, ppm | Expected range, ppm | Z-score |
|-----|-------|-----|------|------|------------|---------------------|---------|
| 1   | A     | 24  | GLU  | CG   | 51.92      | 42.24 – 29.94       | 12.9    |
| 1   | A     | 169 | VAL  | HG21 | 3.32       | 2.20 – -0.60        | 9.0     |
| 1   | A     | 169 | VAL  | HG23 | 3.32       | 2.20 – -0.60        | 9.0     |
| 1   | A     | 169 | VAL  | HG22 | 3.32       | 2.20 – -0.60        | 9.0     |
| 1   | A     | 22  | ALA  | H    | 11.58      | 11.19 – 5.19        | 5.7     |

#### 7.1.5 Random Coil Index (RCI) plots [i](#)

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition.

Random coil index (RCI) for chain A:

