



# Full wwPDB NMR Structure Validation Report ⓘ

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PDB ID : 1R4T  
Title : Solution structure of exoenzyme S  
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Deposited on : 2003-10-08

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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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 : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
RCI : v\_1n\_11\_5\_13\_A (Berjanski et al., 2005)  
PANAV : Wang et al. (2010)  
ShiftChecker : trunk30686  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk30686

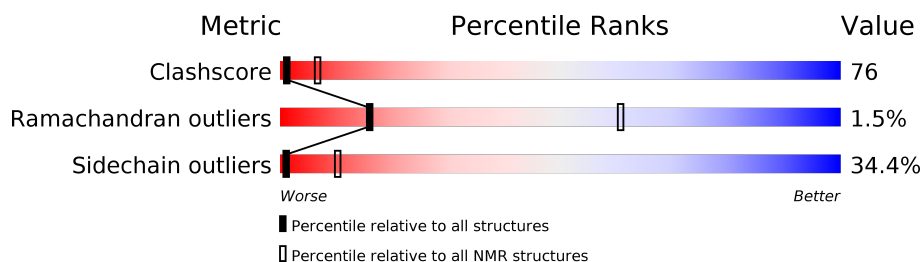
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment was not calculated.

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



| Metric                | Whole archive<br>(#Entries) | NMR archive<br>(#Entries) |
|-----------------------|-----------------------------|---------------------------|
| Clashscore            | 136279                      | 12091                     |
| Ramachandran outliers | 132675                      | 10835                     |
| Sidechain outliers    | 132484                      | 10811                     |

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     | 153    | <div> <span>24%</span> <span>44%</span> <span>9%</span> <span>••</span> <span>20%</span> </div> |

## 2 Ensemble composition and analysis

This entry contains 23 models. Model 23 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *fewest violations, 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:111-A:229 (119)     | 0.29              | 23           |

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

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

The models can be grouped into 4 clusters and 5 single-model clusters were found.

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

### 3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1826 atoms, of which 924 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called exoenzyme S.

| Mol | Chain | Residues | Atoms |     |     |     |     |   | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|-------|
| 1   | A     | 122      | Total | C   | H   | N   | O   | S | 0     |
|     |       |          | 1826  | 549 | 924 | 170 | 181 | 2 |       |

There are 14 discrepancies between the modelled and reference sequences:

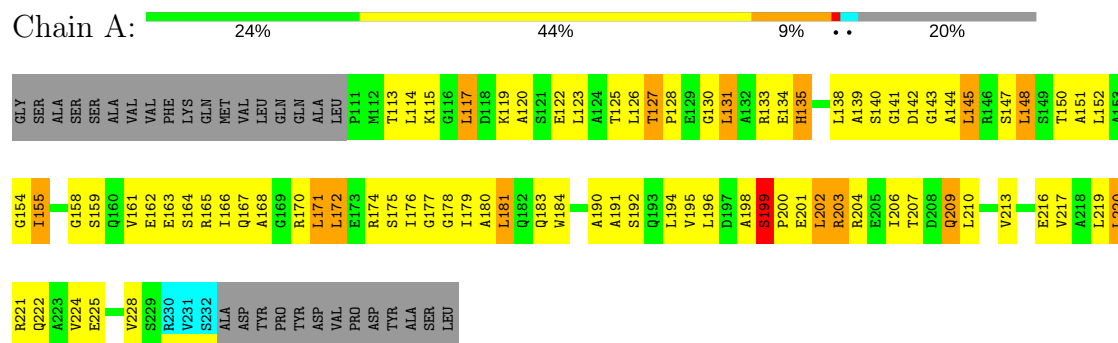
| Chain | Residue | Modelled | Actual | Comment          | Reference  |
|-------|---------|----------|--------|------------------|------------|
| A     | 93      | GLY      | -      | CLONING ARTIFACT | UNP Q93SQ1 |
| A     | 94      | SER      | -      | CLONING ARTIFACT | UNP Q93SQ1 |
| A     | 95      | ALA      | -      | CLONING ARTIFACT | UNP Q93SQ1 |
| A     | 235     | TYR      | -      | CLONING ARTIFACT | UNP Q93SQ1 |
| A     | 236     | PRO      | -      | CLONING ARTIFACT | UNP Q93SQ1 |
| A     | 237     | TYR      | -      | CLONING ARTIFACT | UNP Q93SQ1 |
| A     | 238     | ASP      | -      | CLONING ARTIFACT | UNP Q93SQ1 |
| A     | 239     | VAL      | -      | CLONING ARTIFACT | UNP Q93SQ1 |
| A     | 240     | PRO      | -      | CLONING ARTIFACT | UNP Q93SQ1 |
| A     | 241     | ASP      | -      | CLONING ARTIFACT | UNP Q93SQ1 |
| A     | 242     | TYR      | -      | CLONING ARTIFACT | UNP Q93SQ1 |
| A     | 243     | ALA      | -      | CLONING ARTIFACT | UNP Q93SQ1 |
| A     | 244     | SER      | -      | CLONING ARTIFACT | UNP Q93SQ1 |
| A     | 245     | LEU      | -      | CLONING ARTIFACT | UNP Q93SQ1 |

## 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: exoenzyme S

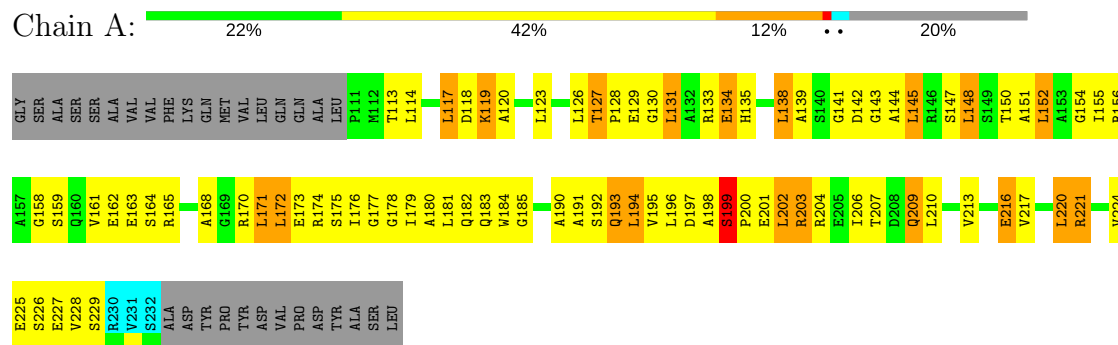


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

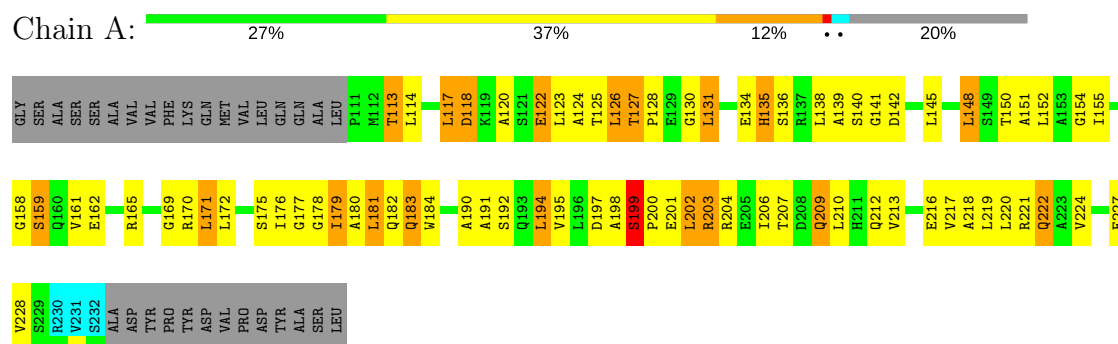
#### 4.2.1 Score per residue for model 1

- Molecule 1: exoenzyme S



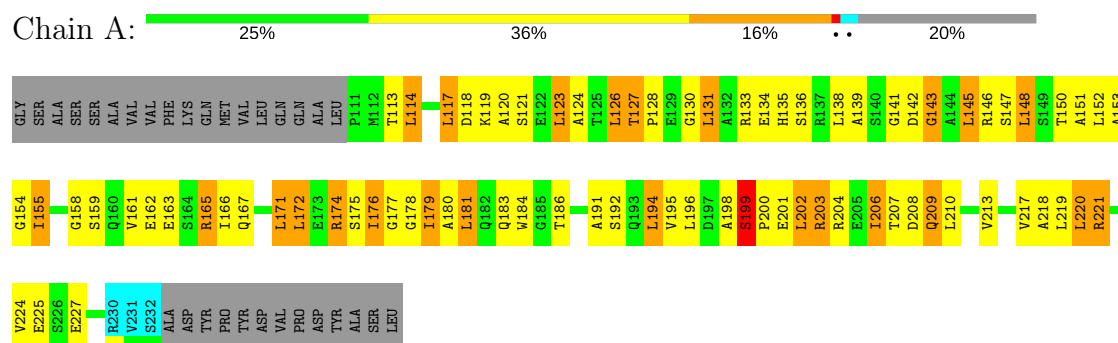
## 4.2.2 Score per residue for model 2

### • Molecule 1: exoenzyme S



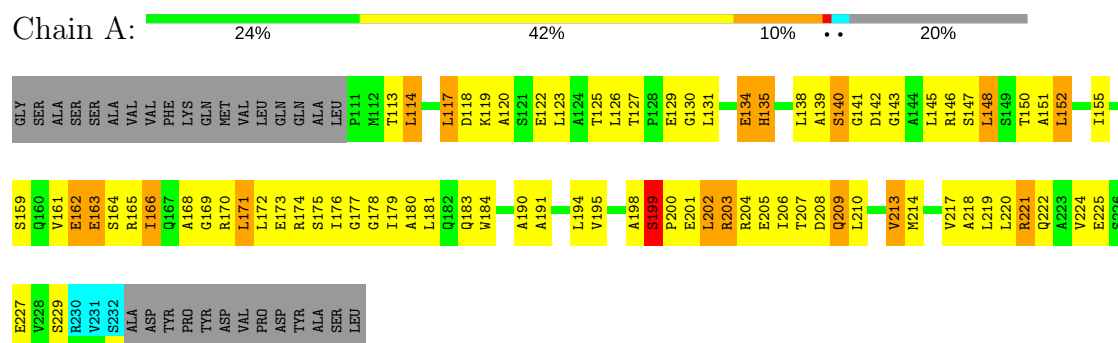
## 4.2.3 Score per residue for model 3

### • Molecule 1: exoenzyme S



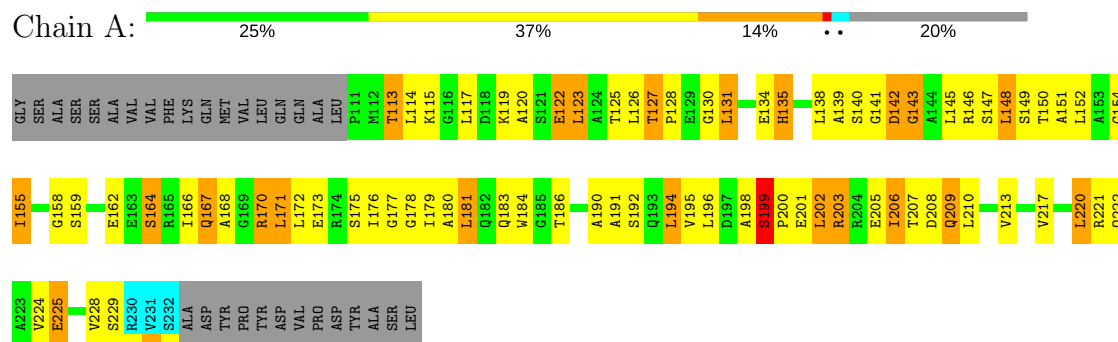
## 4.2.4 Score per residue for model 4

### • Molecule 1: exoenzyme S



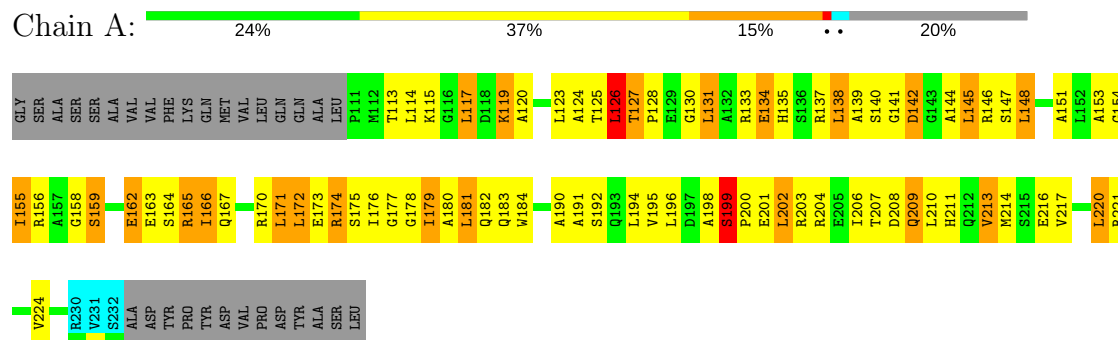
### 4.2.5 Score per residue for model 5

- Molecule 1: exoenzyme S



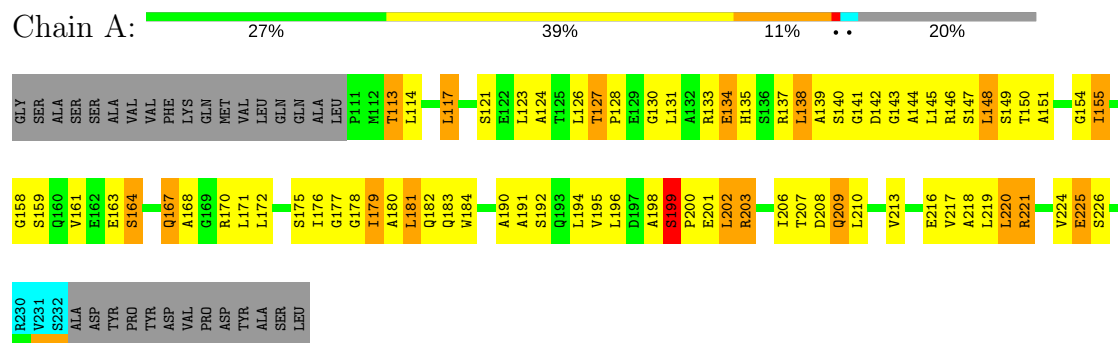
### 4.2.6 Score per residue for model 6

- Molecule 1: exoenzyme S



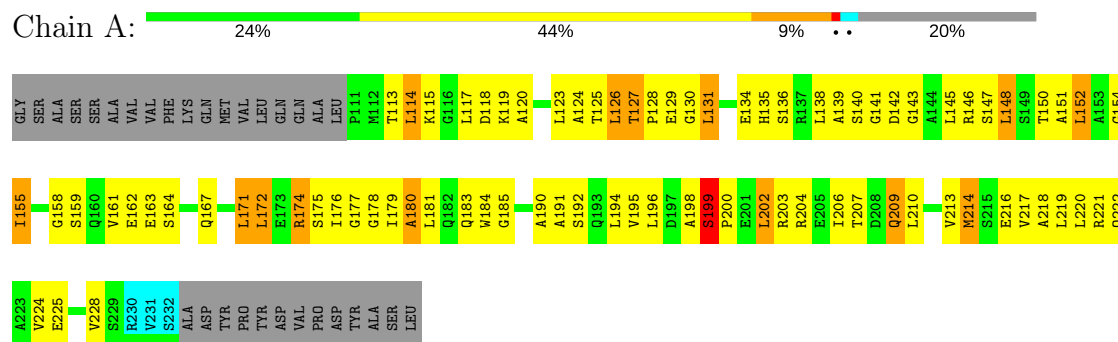
### 4.2.7 Score per residue for model 7

- Molecule 1: exoenzyme S



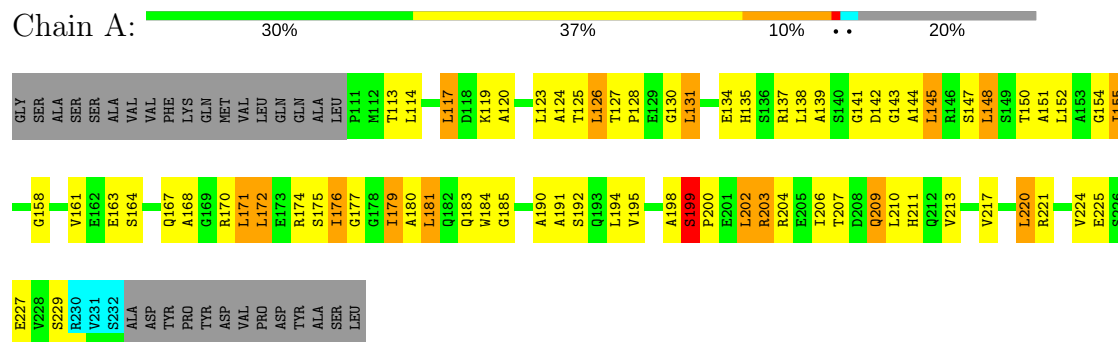
## 4.2.8 Score per residue for model 8

- Molecule 1: exoenzyme S



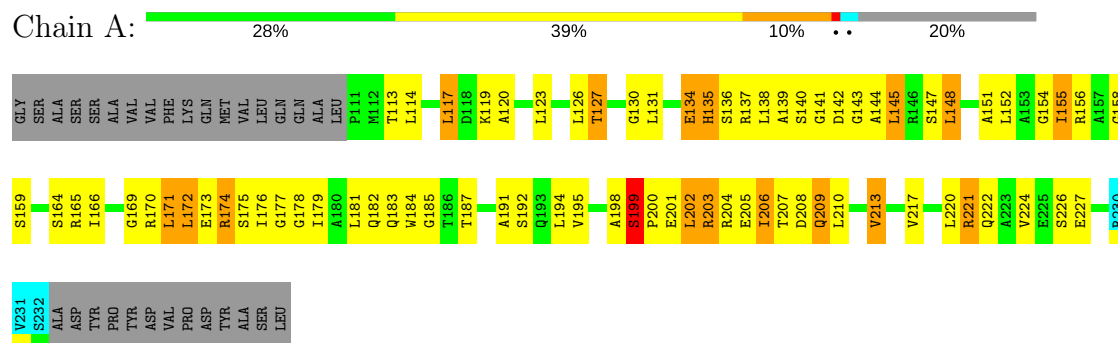
## 4.2.9 Score per residue for model 9

- Molecule 1: exoenzyme S



## 4.2.10 Score per residue for model 10

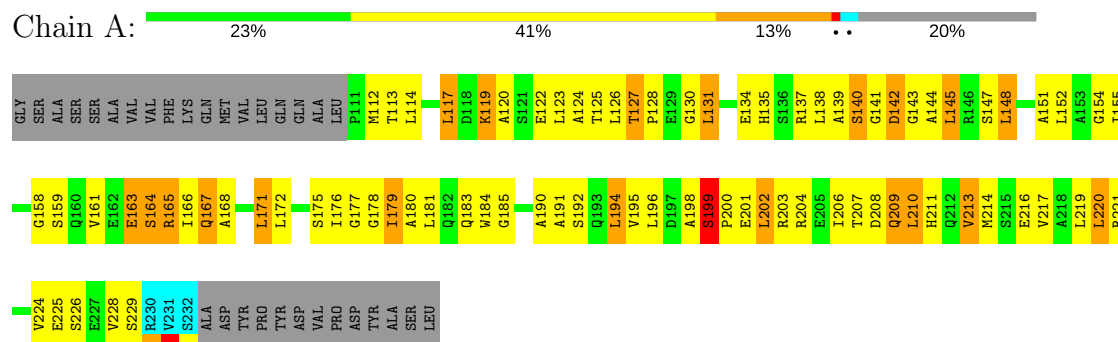
- Molecule 1: exoenzyme S





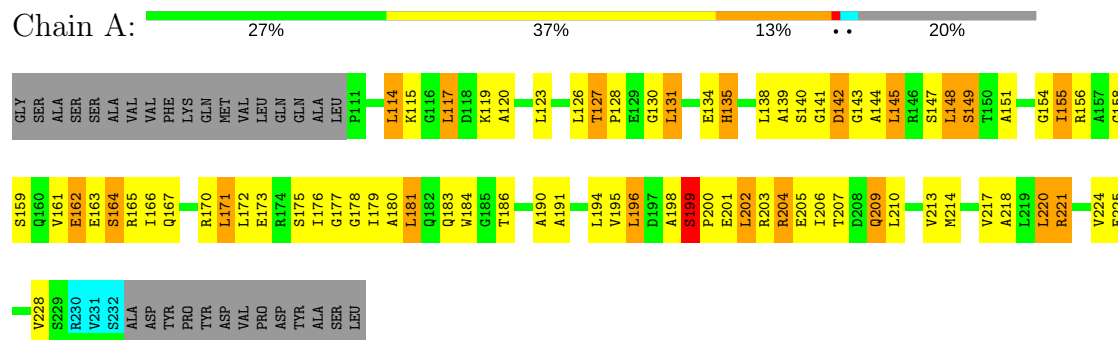
### 4.2.11 Score per residue for model 11

- Molecule 1: exoenzyme S



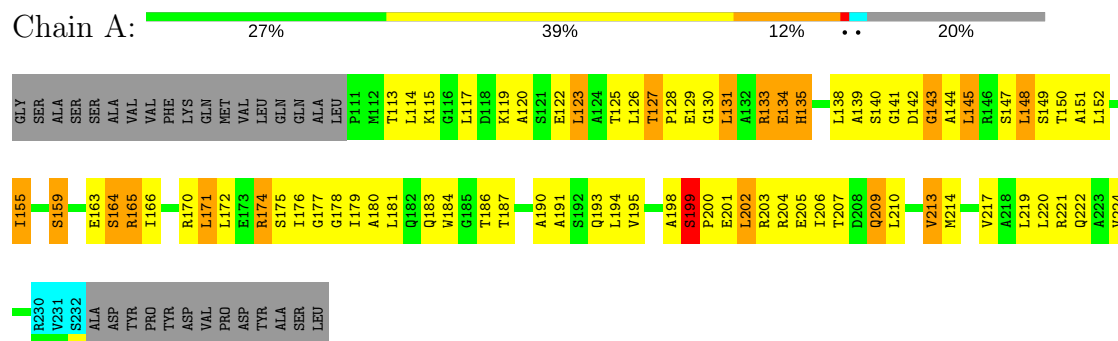
### 4.2.12 Score per residue for model 12

- Molecule 1: exoenzyme S



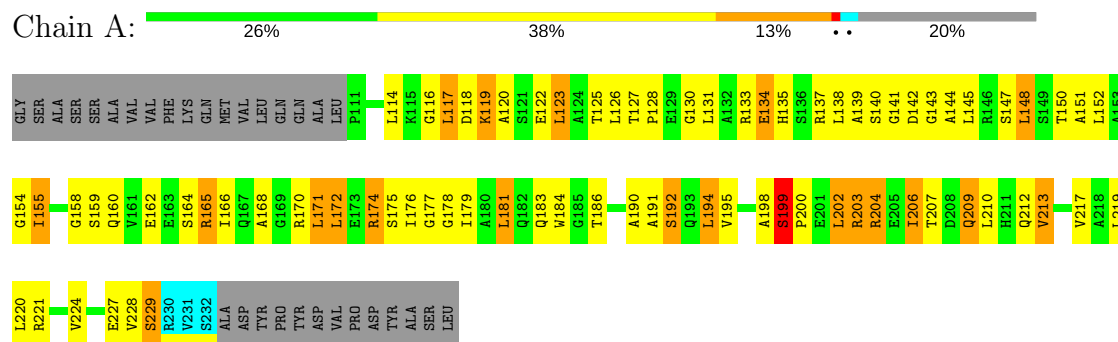
### 4.2.13 Score per residue for model 13

- Molecule 1: exoenzyme S



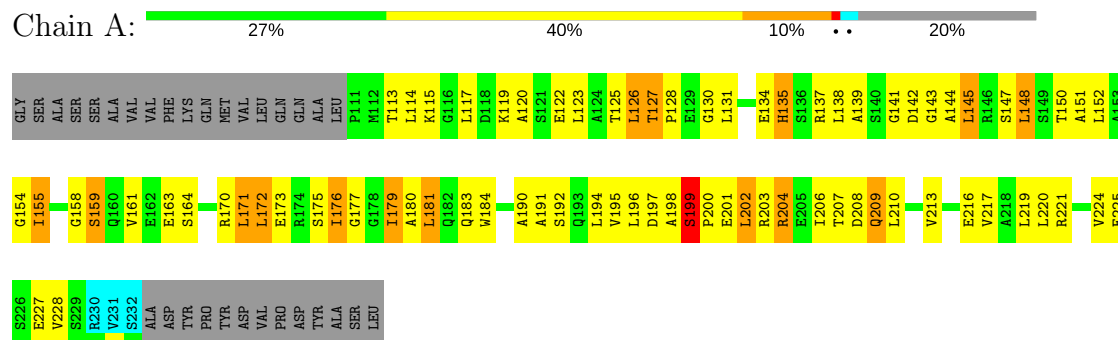
#### 4.2.14 Score per residue for model 14

- Molecule 1: exoenzyme S



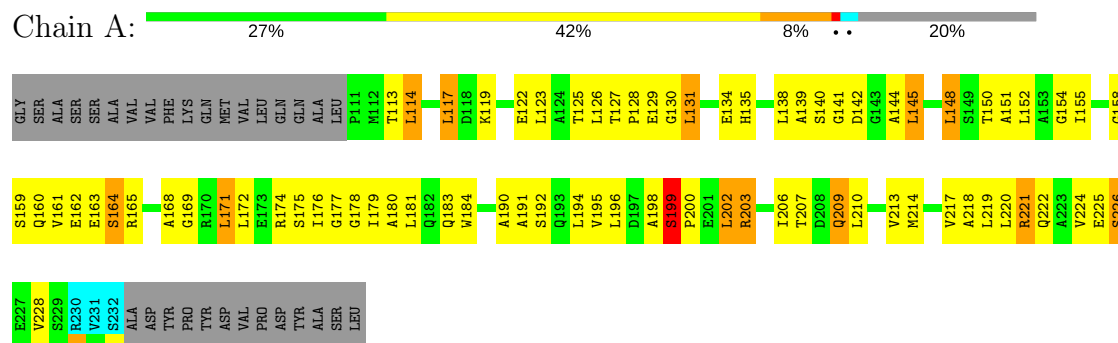
#### 4.2.15 Score per residue for model 15

- Molecule 1: exoenzyme S



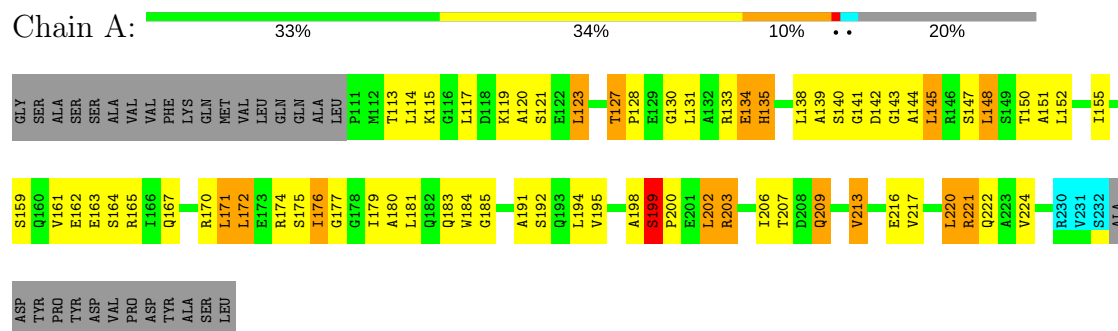
#### 4.2.16 Score per residue for model 16

- Molecule 1: exoenzyme S



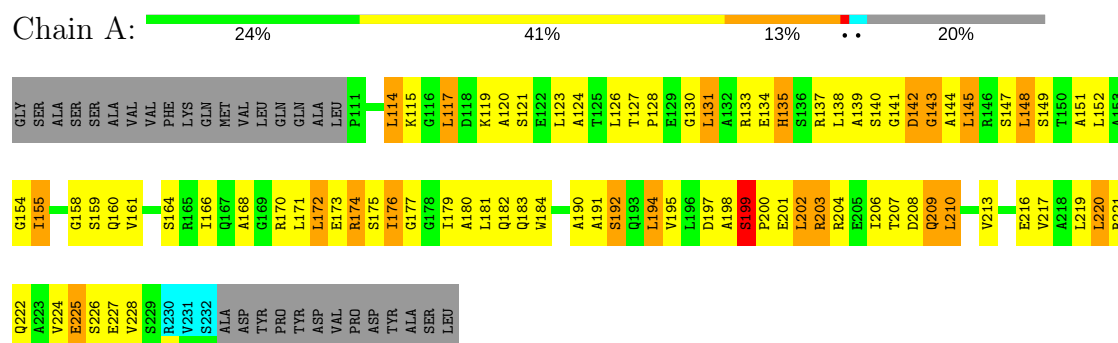
## 4.2.17 Score per residue for model 17

- Molecule 1: exoenzyme S



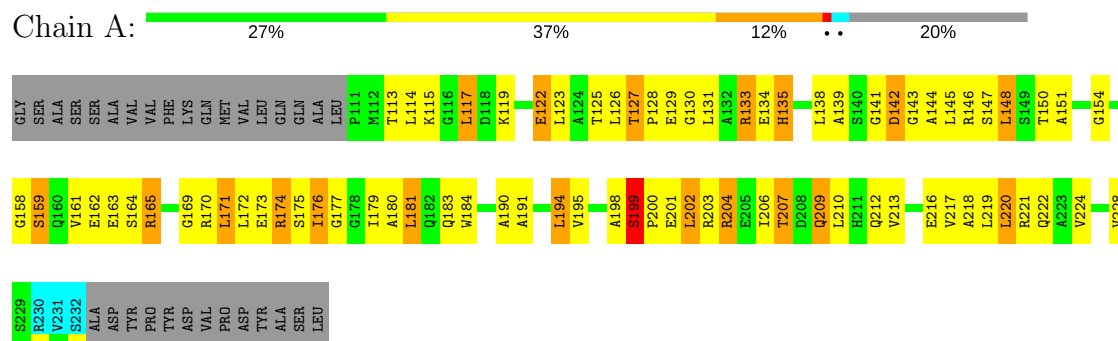
## 4.2.18 Score per residue for model 18

- Molecule 1: exoenzyme S



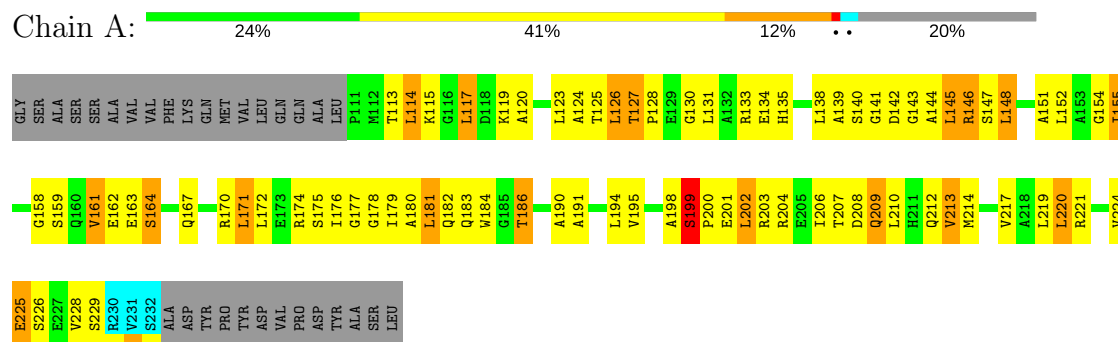
## 4.2.19 Score per residue for model 19

- Molecule 1: exoenzyme S



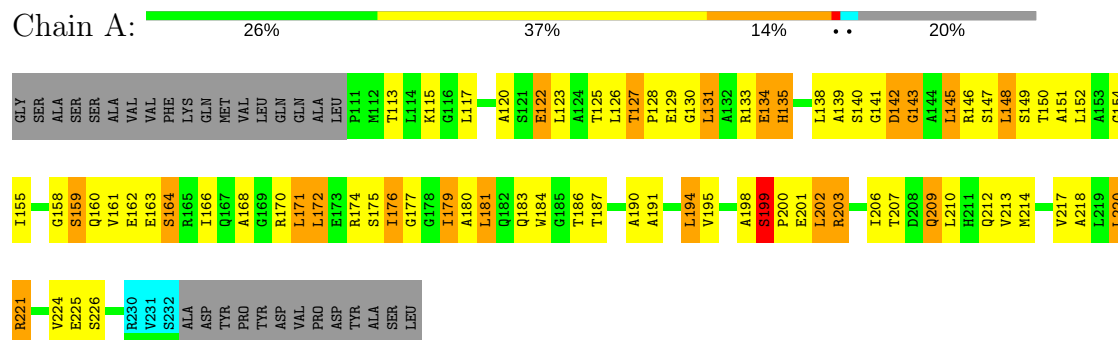
### 4.2.20 Score per residue for model 20

- Molecule 1: exoenzyme S



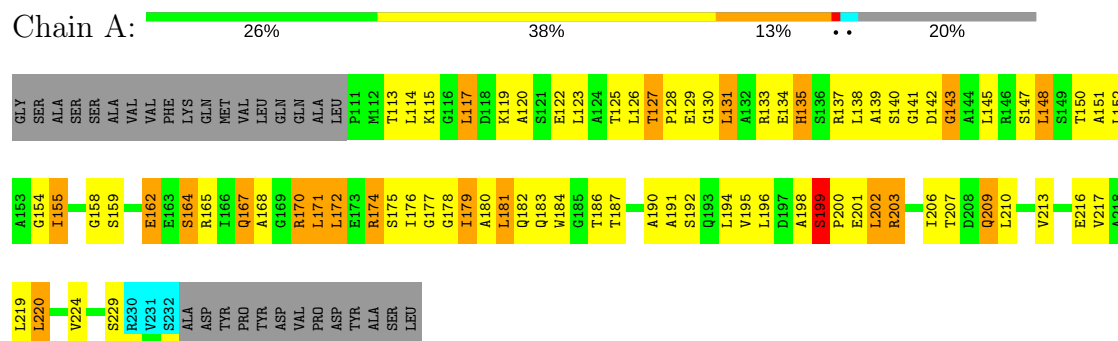
### 4.2.21 Score per residue for model 21

- Molecule 1: exoenzyme S



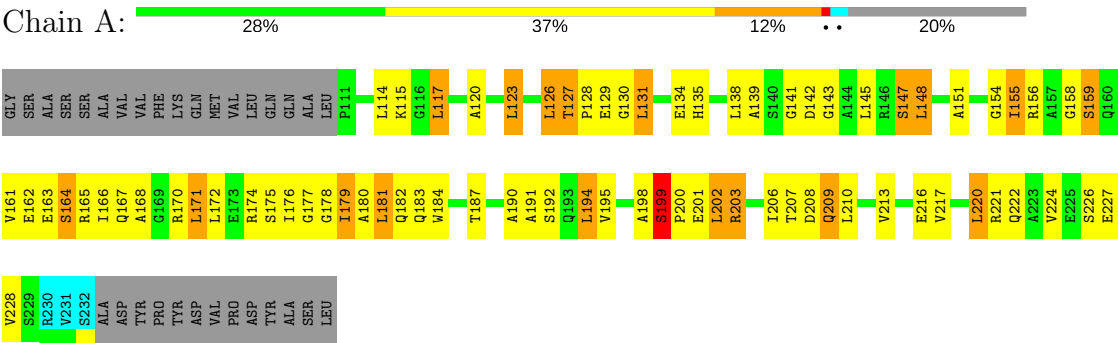
### 4.2.22 Score per residue for model 22

- Molecule 1: exoenzyme S



4.2.23 Score per residue for model 23 (medoid)

● Molecule 1: exoenzyme S



## 5 Refinement protocol and experimental data overview

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

Of the 71 calculated structures, 23 were deposited, based on the following criterion: *structures with acceptable covalent geometry, structures with favorable non-bond energy*.

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

| Software name | Classification     | Version |
|---------------|--------------------|---------|
| DYANA         | structure solution | 1.6     |
| AMBER         | refinement         | 7       |

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

## 6 Model quality

### 6.1 Standard geometry

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

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     | 878   | 897      | 897      | 134±9   |
| All | All   | 20194 | 20631    | 20631    | 3087    |

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 76.

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

| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:171:LEU:HD11 | 1:A:181:LEU:HD13 | 1.10     | 1.17        | 7      | 10    |
| 1:A:202:LEU:HD13 | 1:A:206:ILE:CG1  | 1.02     | 1.84        | 2      | 11    |
| 1:A:117:LEU:HD21 | 1:A:152:LEU:HD22 | 1.02     | 1.22        | 1      | 1     |
| 1:A:171:LEU:HD11 | 1:A:213:VAL:HG22 | 1.01     | 1.29        | 14     | 9     |
| 1:A:126:LEU:HD23 | 1:A:131:LEU:HD12 | 1.00     | 1.28        | 2      | 4     |
| 1:A:123:LEU:HD22 | 1:A:145:LEU:HD12 | 1.00     | 1.29        | 9      | 1     |
| 1:A:131:LEU:HD22 | 1:A:195:VAL:HG21 | 1.00     | 1.28        | 20     | 5     |
| 1:A:117:LEU:HD11 | 1:A:152:LEU:HD22 | 0.98     | 1.35        | 21     | 1     |
| 1:A:171:LEU:HD12 | 1:A:181:LEU:HD13 | 0.97     | 1.34        | 19     | 16    |
| 1:A:176:ILE:HG23 | 1:A:209:GLN:NE2  | 0.97     | 1.75        | 3      | 18    |
| 1:A:171:LEU:CD1  | 1:A:181:LEU:HD13 | 0.96     | 1.90        | 22     | 21    |
| 1:A:179:ILE:HG22 | 1:A:184:TRP:NE1  | 0.96     | 1.75        | 3      | 4     |
| 1:A:220:LEU:O    | 1:A:224:VAL:HG23 | 0.95     | 1.61        | 22     | 22    |
| 1:A:130:GLY:O    | 1:A:134:GLU:N    | 0.94     | 2.01        | 23     | 23    |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:198:ALA:HB3  | 1:A:202:LEU:HD22 | 0.93     | 1.39        | 22     | 6     |
| 1:A:117:LEU:HD21 | 1:A:152:LEU:CD2  | 0.93     | 1.92        | 21     | 1     |
| 1:A:131:LEU:HD22 | 1:A:202:LEU:HD21 | 0.93     | 1.37        | 15     | 1     |
| 1:A:123:LEU:CD1  | 1:A:145:LEU:HD12 | 0.93     | 1.93        | 17     | 4     |
| 1:A:179:ILE:HG21 | 1:A:191:ALA:N    | 0.92     | 1.80        | 12     | 11    |
| 1:A:131:LEU:HD23 | 1:A:195:VAL:HG21 | 0.92     | 1.37        | 5      | 4     |
| 1:A:126:LEU:CD2  | 1:A:131:LEU:HD12 | 0.92     | 1.94        | 2      | 4     |
| 1:A:213:VAL:O    | 1:A:217:VAL:HG23 | 0.91     | 1.66        | 22     | 12    |
| 1:A:155:ILE:CD1  | 1:A:224:VAL:HG21 | 0.91     | 1.95        | 5      | 2     |
| 1:A:179:ILE:HG21 | 1:A:191:ALA:HB2  | 0.91     | 1.42        | 6      | 14    |
| 1:A:171:LEU:HD11 | 1:A:213:VAL:HG13 | 0.91     | 1.36        | 1      | 3     |
| 1:A:171:LEU:HD11 | 1:A:213:VAL:CG2  | 0.90     | 1.96        | 10     | 7     |
| 1:A:171:LEU:HD12 | 1:A:181:LEU:HD22 | 0.90     | 1.41        | 10     | 14    |
| 1:A:171:LEU:HD22 | 1:A:216:GLU:OE1  | 0.88     | 1.68        | 7      | 1     |
| 1:A:117:LEU:HD22 | 1:A:151:ALA:HB1  | 0.88     | 1.45        | 16     | 15    |
| 1:A:123:LEU:HD12 | 1:A:210:LEU:CD1  | 0.88     | 1.97        | 10     | 5     |
| 1:A:113:THR:HG23 | 1:A:151:ALA:HA   | 0.88     | 1.45        | 17     | 1     |
| 1:A:224:VAL:O    | 1:A:228:VAL:HG23 | 0.87     | 1.69        | 12     | 10    |
| 1:A:138:LEU:HD13 | 1:A:144:ALA:HB3  | 0.87     | 1.45        | 6      | 3     |
| 1:A:202:LEU:HD13 | 1:A:206:ILE:HG13 | 0.87     | 1.45        | 4      | 9     |
| 1:A:198:ALA:O    | 1:A:202:LEU:HD22 | 0.87     | 1.69        | 14     | 5     |
| 1:A:176:ILE:HG23 | 1:A:209:GLN:CD   | 0.87     | 1.90        | 2      | 10    |
| 1:A:145:LEU:HD23 | 1:A:148:LEU:HD23 | 0.86     | 1.45        | 22     | 16    |
| 1:A:171:LEU:HD22 | 1:A:213:VAL:HG13 | 0.86     | 1.46        | 18     | 1     |
| 1:A:117:LEU:HD21 | 1:A:152:LEU:HD23 | 0.86     | 1.47        | 21     | 2     |
| 1:A:184:TRP:CH2  | 1:A:206:ILE:CD1  | 0.85     | 2.58        | 3      | 4     |
| 1:A:202:LEU:HD13 | 1:A:206:ILE:HG12 | 0.85     | 1.48        | 23     | 3     |
| 1:A:159:SER:OG   | 1:A:224:VAL:HG13 | 0.84     | 1.70        | 6      | 8     |
| 1:A:145:LEU:HD13 | 1:A:184:TRP:O    | 0.84     | 1.72        | 23     | 17    |
| 1:A:176:ILE:HB   | 1:A:184:TRP:CD1  | 0.84     | 2.06        | 8      | 23    |
| 1:A:131:LEU:HD23 | 1:A:195:VAL:CG2  | 0.84     | 2.01        | 5      | 4     |
| 1:A:117:LEU:HD22 | 1:A:217:VAL:HG11 | 0.83     | 1.49        | 5      | 2     |
| 1:A:134:GLU:O    | 1:A:138:LEU:N    | 0.83     | 2.10        | 10     | 23    |
| 1:A:117:LEU:HG   | 1:A:151:ALA:HB3  | 0.83     | 1.45        | 17     | 6     |
| 1:A:220:LEU:HD12 | 1:A:221:ARG:N    | 0.83     | 1.88        | 16     | 3     |
| 1:A:131:LEU:HD13 | 1:A:195:VAL:CG2  | 0.83     | 2.03        | 16     | 5     |
| 1:A:184:TRP:CH2  | 1:A:206:ILE:HD12 | 0.82     | 2.09        | 6      | 14    |
| 1:A:179:ILE:HD11 | 1:A:194:LEU:HD13 | 0.82     | 1.52        | 19     | 4     |
| 1:A:203:ARG:O    | 1:A:207:THR:OG1  | 0.82     | 1.98        | 1      | 23    |
| 1:A:206:ILE:HG23 | 1:A:209:GLN:NE2  | 0.82     | 1.90        | 21     | 4     |
| 1:A:120:ALA:HB1  | 1:A:214:MET:HE1  | 0.81     | 1.52        | 12     | 2     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:195:VAL:HA   | 1:A:202:LEU:HD23 | 0.81     | 1.52        | 11     | 5     |
| 1:A:123:LEU:CD2  | 1:A:145:LEU:HD12 | 0.81     | 2.04        | 9      | 2     |
| 1:A:123:LEU:CD1  | 1:A:138:LEU:HD23 | 0.81     | 2.04        | 11     | 1     |
| 1:A:179:ILE:HD13 | 1:A:194:LEU:HD13 | 0.81     | 1.50        | 5      | 9     |
| 1:A:120:ALA:HB1  | 1:A:214:MET:CE   | 0.81     | 2.05        | 12     | 2     |
| 1:A:117:LEU:HD22 | 1:A:151:ALA:CB   | 0.81     | 2.05        | 14     | 17    |
| 1:A:198:ALA:HB3  | 1:A:202:LEU:HD23 | 0.81     | 1.50        | 10     | 5     |
| 1:A:167:GLN:HB3  | 1:A:220:LEU:HD22 | 0.80     | 1.54        | 3      | 4     |
| 1:A:123:LEU:HD21 | 1:A:148:LEU:HD22 | 0.80     | 1.53        | 2      | 2     |
| 1:A:131:LEU:HD22 | 1:A:195:VAL:CG2  | 0.79     | 2.07        | 20     | 3     |
| 1:A:131:LEU:CD2  | 1:A:195:VAL:HG21 | 0.79     | 2.07        | 19     | 4     |
| 1:A:195:VAL:HG23 | 1:A:202:LEU:HD21 | 0.78     | 1.53        | 14     | 1     |
| 1:A:127:THR:HG23 | 1:A:128:PRO:HD2  | 0.78     | 1.56        | 8      | 5     |
| 1:A:155:ILE:HD13 | 1:A:224:VAL:HG21 | 0.78     | 1.54        | 5      | 2     |
| 1:A:123:LEU:CD1  | 1:A:148:LEU:HD22 | 0.78     | 2.09        | 9      | 3     |
| 1:A:171:LEU:HD11 | 1:A:181:LEU:CD1  | 0.77     | 2.06        | 7      | 1     |
| 1:A:184:TRP:CZ2  | 1:A:206:ILE:HD12 | 0.77     | 2.14        | 20     | 12    |
| 1:A:131:LEU:HD21 | 1:A:195:VAL:HG23 | 0.77     | 1.56        | 11     | 2     |
| 1:A:195:VAL:HA   | 1:A:202:LEU:HD13 | 0.77     | 1.56        | 1      | 5     |
| 1:A:194:LEU:HD23 | 1:A:202:LEU:HD11 | 0.77     | 1.55        | 23     | 5     |
| 1:A:123:LEU:HD12 | 1:A:124:ALA:N    | 0.77     | 1.95        | 2      | 1     |
| 1:A:176:ILE:O    | 1:A:184:TRP:NE1  | 0.77     | 2.18        | 1      | 23    |
| 1:A:179:ILE:HD13 | 1:A:194:LEU:HD22 | 0.76     | 1.56        | 22     | 5     |
| 1:A:203:ARG:O    | 1:A:207:THR:CB   | 0.76     | 2.34        | 1      | 22    |
| 1:A:131:LEU:HD13 | 1:A:195:VAL:HG23 | 0.76     | 1.56        | 16     | 5     |
| 1:A:203:ARG:O    | 1:A:207:THR:HG23 | 0.76     | 1.80        | 19     | 1     |
| 1:A:184:TRP:CZ3  | 1:A:206:ILE:HG21 | 0.76     | 2.16        | 10     | 11    |
| 1:A:171:LEU:HD13 | 1:A:217:VAL:HG23 | 0.76     | 1.56        | 18     | 1     |
| 1:A:202:LEU:O    | 1:A:206:ILE:CG1  | 0.76     | 2.33        | 17     | 23    |
| 1:A:131:LEU:O    | 1:A:135:HIS:HB2  | 0.76     | 1.80        | 18     | 22    |
| 1:A:179:ILE:CD1  | 1:A:194:LEU:HD13 | 0.76     | 2.10        | 18     | 9     |
| 1:A:177:GLY:HA3  | 1:A:206:ILE:HD13 | 0.75     | 1.55        | 17     | 9     |
| 1:A:130:GLY:O    | 1:A:134:GLU:CB   | 0.75     | 2.35        | 13     | 19    |
| 1:A:180:ALA:HB3  | 1:A:183:GLN:HG2  | 0.75     | 1.59        | 19     | 14    |
| 1:A:176:ILE:HD11 | 1:A:213:VAL:CG2  | 0.75     | 2.12        | 22     | 4     |
| 1:A:179:ILE:HG12 | 1:A:194:LEU:HD22 | 0.75     | 1.57        | 13     | 5     |
| 1:A:155:ILE:HG21 | 1:A:220:LEU:HD12 | 0.75     | 1.58        | 22     | 3     |
| 1:A:179:ILE:HG22 | 1:A:183:GLN:HB2  | 0.74     | 1.57        | 1      | 11    |
| 1:A:184:TRP:CZ2  | 1:A:206:ILE:CD1  | 0.74     | 2.70        | 14     | 3     |
| 1:A:179:ILE:CG2  | 1:A:191:ALA:HB2  | 0.74     | 2.12        | 18     | 13    |
| 1:A:179:ILE:HG21 | 1:A:191:ALA:CB   | 0.74     | 2.13        | 6      | 12    |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:152:LEU:HD21 | 1:A:220:LEU:HD12 | 0.74     | 1.60        | 9      | 1     |
| 1:A:176:ILE:HG12 | 1:A:181:LEU:HD12 | 0.73     | 1.57        | 3      | 10    |
| 1:A:123:LEU:HB3  | 1:A:210:LEU:HD13 | 0.73     | 1.60        | 5      | 14    |
| 1:A:138:LEU:HG   | 1:A:144:ALA:HB3  | 0.73     | 1.59        | 13     | 9     |
| 1:A:145:LEU:HD23 | 1:A:148:LEU:CD2  | 0.73     | 2.12        | 22     | 12    |
| 1:A:126:LEU:HD21 | 1:A:131:LEU:HD12 | 0.73     | 1.60        | 11     | 1     |
| 1:A:134:GLU:O    | 1:A:138:LEU:HB2  | 0.72     | 1.84        | 19     | 23    |
| 1:A:123:LEU:CD2  | 1:A:148:LEU:HD22 | 0.72     | 2.14        | 2      | 2     |
| 1:A:127:THR:HG22 | 1:A:130:GLY:H    | 0.72     | 1.45        | 6      | 5     |
| 1:A:126:LEU:HD11 | 1:A:131:LEU:HA   | 0.72     | 1.60        | 11     | 4     |
| 1:A:145:LEU:HD22 | 1:A:184:TRP:O    | 0.72     | 1.85        | 4      | 16    |
| 1:A:206:ILE:N    | 1:A:206:ILE:HD13 | 0.72     | 2.00        | 10     | 2     |
| 1:A:180:ALA:HB3  | 1:A:183:GLN:CG   | 0.72     | 2.14        | 7      | 17    |
| 1:A:131:LEU:HD23 | 1:A:203:ARG:HB2  | 0.72     | 1.61        | 10     | 1     |
| 1:A:123:LEU:HD11 | 1:A:145:LEU:HD12 | 0.71     | 1.61        | 10     | 4     |
| 1:A:126:LEU:HD21 | 1:A:131:LEU:HD23 | 0.71     | 1.61        | 16     | 1     |
| 1:A:117:LEU:CD2  | 1:A:152:LEU:HD22 | 0.71     | 2.11        | 1      | 1     |
| 1:A:155:ILE:HG21 | 1:A:220:LEU:CD1  | 0.71     | 2.15        | 7      | 6     |
| 1:A:130:GLY:O    | 1:A:134:GLU:HB2  | 0.71     | 1.86        | 22     | 15    |
| 1:A:155:ILE:HG12 | 1:A:224:VAL:HG11 | 0.71     | 1.63        | 17     | 18    |
| 1:A:202:LEU:O    | 1:A:206:ILE:N    | 0.70     | 2.22        | 5      | 22    |
| 1:A:161:VAL:HG23 | 1:A:227:GLU:OE2  | 0.70     | 1.86        | 18     | 2     |
| 1:A:123:LEU:HD12 | 1:A:210:LEU:HD13 | 0.70     | 1.64        | 20     | 5     |
| 1:A:164:SER:OG   | 1:A:224:VAL:HG22 | 0.70     | 1.87        | 20     | 11    |
| 1:A:134:GLU:HG3  | 1:A:138:LEU:HD13 | 0.70     | 1.63        | 13     | 1     |
| 1:A:155:ILE:HG13 | 1:A:224:VAL:HG11 | 0.70     | 1.61        | 9      | 1     |
| 1:A:176:ILE:CG2  | 1:A:209:GLN:NE2  | 0.69     | 2.55        | 23     | 14    |
| 1:A:206:ILE:HG23 | 1:A:209:GLN:HE22 | 0.69     | 1.46        | 9      | 8     |
| 1:A:180:ALA:HB3  | 1:A:183:GLN:HG3  | 0.69     | 1.64        | 13     | 8     |
| 1:A:148:LEU:HD12 | 1:A:152:LEU:HD12 | 0.69     | 1.63        | 4      | 5     |
| 1:A:209:GLN:CD   | 1:A:209:GLN:C    | 0.69     | 2.51        | 16     | 8     |
| 1:A:202:LEU:O    | 1:A:206:ILE:HG12 | 0.69     | 1.88        | 16     | 17    |
| 1:A:114:LEU:HD21 | 1:A:225:GLU:HB2  | 0.69     | 1.65        | 12     | 4     |
| 1:A:113:THR:HG23 | 1:A:151:ALA:CA   | 0.69     | 2.17        | 17     | 1     |
| 1:A:123:LEU:HD21 | 1:A:145:LEU:HA   | 0.69     | 1.64        | 11     | 1     |
| 1:A:217:VAL:HG12 | 1:A:221:ARG:HD2  | 0.69     | 1.65        | 20     | 3     |
| 1:A:117:LEU:CD1  | 1:A:152:LEU:HD22 | 0.69     | 2.16        | 21     | 1     |
| 1:A:127:THR:HG23 | 1:A:128:PRO:CD   | 0.68     | 2.17        | 8      | 5     |
| 1:A:176:ILE:HD11 | 1:A:213:VAL:HG21 | 0.68     | 1.63        | 12     | 3     |
| 1:A:155:ILE:HG12 | 1:A:224:VAL:HG21 | 0.68     | 1.63        | 9      | 18    |
| 1:A:217:VAL:HG12 | 1:A:221:ARG:CD   | 0.68     | 2.19        | 8      | 5     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:123:LEU:HD13 | 1:A:145:LEU:HD12 | 0.68     | 1.65        | 17     | 1     |
| 1:A:113:THR:O    | 1:A:151:ALA:HB1  | 0.68     | 1.88        | 15     | 4     |
| 1:A:171:LEU:O    | 1:A:181:LEU:HD22 | 0.68     | 1.89        | 23     | 6     |
| 1:A:171:LEU:HD12 | 1:A:181:LEU:CD1  | 0.68     | 2.18        | 19     | 9     |
| 1:A:159:SER:OG   | 1:A:224:VAL:HG22 | 0.68     | 1.89        | 2      | 5     |
| 1:A:123:LEU:HD21 | 1:A:145:LEU:HG   | 0.68     | 1.65        | 19     | 2     |
| 1:A:209:GLN:HG2  | 1:A:210:LEU:N    | 0.67     | 2.04        | 9      | 6     |
| 1:A:131:LEU:O    | 1:A:131:LEU:HD22 | 0.67     | 1.89        | 12     | 1     |
| 1:A:198:ALA:CB   | 1:A:202:LEU:HD23 | 0.67     | 2.20        | 9      | 4     |
| 1:A:177:GLY:HA3  | 1:A:206:ILE:CD1  | 0.67     | 2.19        | 13     | 15    |
| 1:A:172:LEU:CD1  | 1:A:181:LEU:HD23 | 0.67     | 2.20        | 10     | 3     |
| 1:A:123:LEU:HD11 | 1:A:138:LEU:HD23 | 0.67     | 1.66        | 11     | 1     |
| 1:A:161:VAL:HG23 | 1:A:227:GLU:CD   | 0.67     | 2.10        | 18     | 3     |
| 1:A:117:LEU:HD11 | 1:A:152:LEU:HG   | 0.67     | 1.66        | 13     | 5     |
| 1:A:179:ILE:HG23 | 1:A:183:GLN:HB2  | 0.67     | 1.66        | 9      | 12    |
| 1:A:131:LEU:HD21 | 1:A:195:VAL:CG2  | 0.67     | 2.19        | 11     | 2     |
| 1:A:161:VAL:HG23 | 1:A:227:GLU:OE1  | 0.67     | 1.89        | 15     | 5     |
| 1:A:117:LEU:O    | 1:A:120:ALA:HB3  | 0.67     | 1.89        | 8      | 14    |
| 1:A:199:SER:CB   | 1:A:200:PRO:HD3  | 0.67     | 2.20        | 6      | 23    |
| 1:A:206:ILE:HD13 | 1:A:206:ILE:N    | 0.67     | 2.05        | 5      | 5     |
| 1:A:202:LEU:CD1  | 1:A:206:ILE:HD11 | 0.66     | 2.21        | 16     | 3     |
| 1:A:203:ARG:O    | 1:A:207:THR:CG2  | 0.66     | 2.42        | 19     | 1     |
| 1:A:131:LEU:HD12 | 1:A:203:ARG:HA   | 0.66     | 1.65        | 8      | 7     |
| 1:A:171:LEU:HD12 | 1:A:181:LEU:CD2  | 0.66     | 2.19        | 10     | 6     |
| 1:A:145:LEU:HD22 | 1:A:184:TRP:C    | 0.66     | 2.11        | 21     | 11    |
| 1:A:195:VAL:HA   | 1:A:202:LEU:HD12 | 0.65     | 1.67        | 4      | 3     |
| 1:A:113:THR:HG23 | 1:A:151:ALA:O    | 0.65     | 1.91        | 19     | 14    |
| 1:A:152:LEU:HD22 | 1:A:168:ALA:CB   | 0.65     | 2.21        | 22     | 1     |
| 1:A:117:LEU:HD23 | 1:A:148:LEU:HB2  | 0.65     | 1.68        | 5      | 3     |
| 1:A:203:ARG:O    | 1:A:207:THR:N    | 0.65     | 2.27        | 10     | 12    |
| 1:A:184:TRP:CD2  | 1:A:191:ALA:HB1  | 0.65     | 2.25        | 16     | 11    |
| 1:A:135:HIS:O    | 1:A:139:ALA:HB3  | 0.65     | 1.91        | 4      | 11    |
| 1:A:171:LEU:HD22 | 1:A:174:ARG:NH1  | 0.65     | 2.07        | 10     | 1     |
| 1:A:126:LEU:O    | 1:A:207:THR:HG21 | 0.65     | 1.92        | 22     | 1     |
| 1:A:120:ALA:HA   | 1:A:123:LEU:HD22 | 0.65     | 1.67        | 5      | 1     |
| 1:A:177:GLY:CA   | 1:A:206:ILE:HD12 | 0.65     | 2.22        | 2      | 7     |
| 1:A:126:LEU:HD21 | 1:A:131:LEU:HG   | 0.65     | 1.69        | 21     | 9     |
| 1:A:123:LEU:HD12 | 1:A:126:LEU:HD22 | 0.65     | 1.69        | 3      | 4     |
| 1:A:218:ALA:HA   | 1:A:221:ARG:CG   | 0.65     | 2.22        | 4      | 5     |
| 1:A:120:ALA:HA   | 1:A:123:LEU:HD23 | 0.64     | 1.70        | 1      | 1     |
| 1:A:209:GLN:O    | 1:A:213:VAL:HG23 | 0.64     | 1.91        | 18     | 2     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:199:SER:O    | 1:A:203:ARG:CG   | 0.64     | 2.45        | 8      | 6     |
| 1:A:177:GLY:O    | 1:A:194:LEU:HD21 | 0.64     | 1.92        | 5      | 13    |
| 1:A:134:GLU:OE1  | 1:A:138:LEU:HD11 | 0.64     | 1.92        | 21     | 2     |
| 1:A:191:ALA:O    | 1:A:195:VAL:HG12 | 0.64     | 1.92        | 10     | 1     |
| 1:A:199:SER:O    | 1:A:203:ARG:CB   | 0.64     | 2.46        | 10     | 16    |
| 1:A:127:THR:HG22 | 1:A:128:PRO:CD   | 0.64     | 2.23        | 12     | 8     |
| 1:A:168:ALA:O    | 1:A:172:LEU:HD22 | 0.64     | 1.91        | 9      | 1     |
| 1:A:206:ILE:CD1  | 1:A:206:ILE:N    | 0.64     | 2.60        | 10     | 2     |
| 1:A:123:LEU:CD1  | 1:A:126:LEU:HD22 | 0.64     | 2.23        | 13     | 3     |
| 1:A:177:GLY:O    | 1:A:194:LEU:HD23 | 0.63     | 1.93        | 22     | 4     |
| 1:A:131:LEU:O    | 1:A:135:HIS:CD2  | 0.63     | 2.51        | 5      | 8     |
| 1:A:171:LEU:HD11 | 1:A:216:GLU:HB3  | 0.63     | 1.71        | 18     | 1     |
| 1:A:179:ILE:HD12 | 1:A:190:ALA:CB   | 0.63     | 2.24        | 8      | 4     |
| 1:A:202:LEU:O    | 1:A:206:ILE:CB   | 0.63     | 2.46        | 1      | 21    |
| 1:A:152:LEU:HD11 | 1:A:220:LEU:HD21 | 0.63     | 1.70        | 21     | 1     |
| 1:A:145:LEU:HD23 | 1:A:184:TRP:C    | 0.63     | 2.14        | 11     | 2     |
| 1:A:134:GLU:HB3  | 1:A:138:LEU:HD22 | 0.63     | 1.70        | 22     | 9     |
| 1:A:145:LEU:HG   | 1:A:184:TRP:O    | 0.63     | 1.94        | 8      | 6     |
| 1:A:198:ALA:HB3  | 1:A:202:LEU:CD2  | 0.63     | 2.20        | 22     | 7     |
| 1:A:155:ILE:CG1  | 1:A:224:VAL:HG11 | 0.62     | 2.24        | 9      | 8     |
| 1:A:117:LEU:HD23 | 1:A:155:ILE:HD12 | 0.62     | 1.71        | 2      | 2     |
| 1:A:195:VAL:HG23 | 1:A:202:LEU:CD2  | 0.62     | 2.23        | 14     | 1     |
| 1:A:123:LEU:CD2  | 1:A:138:LEU:HD13 | 0.62     | 2.25        | 4      | 1     |
| 1:A:172:LEU:HD12 | 1:A:181:LEU:HD23 | 0.62     | 1.70        | 1      | 5     |
| 1:A:145:LEU:HD23 | 1:A:184:TRP:O    | 0.62     | 1.93        | 9      | 2     |
| 1:A:220:LEU:C    | 1:A:220:LEU:HD12 | 0.62     | 2.14        | 21     | 1     |
| 1:A:176:ILE:HD13 | 1:A:181:LEU:HB2  | 0.62     | 1.71        | 10     | 5     |
| 1:A:119:LYS:HG2  | 1:A:144:ALA:HB2  | 0.62     | 1.69        | 17     | 9     |
| 1:A:131:LEU:CD1  | 1:A:195:VAL:HG23 | 0.62     | 2.23        | 16     | 1     |
| 1:A:198:ALA:HB3  | 1:A:202:LEU:CG   | 0.62     | 2.23        | 9      | 5     |
| 1:A:152:LEU:HD21 | 1:A:220:LEU:HD11 | 0.62     | 1.72        | 5      | 3     |
| 1:A:123:LEU:HD12 | 1:A:123:LEU:C    | 0.62     | 2.15        | 2      | 1     |
| 1:A:179:ILE:HG22 | 1:A:183:GLN:CB   | 0.62     | 2.25        | 1      | 8     |
| 1:A:123:LEU:CD1  | 1:A:210:LEU:HD22 | 0.62     | 2.25        | 14     | 1     |
| 1:A:171:LEU:CD2  | 1:A:213:VAL:HG13 | 0.62     | 2.21        | 18     | 1     |
| 1:A:126:LEU:HD21 | 1:A:131:LEU:CD1  | 0.61     | 2.25        | 11     | 1     |
| 1:A:176:ILE:N    | 1:A:176:ILE:CD1  | 0.61     | 2.62        | 21     | 7     |
| 1:A:123:LEU:HD13 | 1:A:210:LEU:HD22 | 0.61     | 1.72        | 14     | 1     |
| 1:A:117:LEU:HD12 | 1:A:217:VAL:HG11 | 0.61     | 1.71        | 7      | 3     |
| 1:A:131:LEU:O    | 1:A:135:HIS:CB   | 0.61     | 2.47        | 20     | 23    |
| 1:A:176:ILE:CG1  | 1:A:181:LEU:HD12 | 0.61     | 2.26        | 6      | 6     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:159:SER:CB   | 1:A:164:SER:CB   | 0.61     | 2.77        | 20     | 14    |
| 1:A:152:LEU:HD22 | 1:A:168:ALA:HB1  | 0.61     | 1.71        | 22     | 1     |
| 1:A:131:LEU:CD2  | 1:A:195:VAL:HG23 | 0.61     | 2.26        | 2      | 2     |
| 1:A:202:LEU:HD12 | 1:A:206:ILE:HG13 | 0.61     | 1.71        | 18     | 4     |
| 1:A:130:GLY:CA   | 1:A:134:GLU:HB2  | 0.61     | 2.25        | 9      | 10    |
| 1:A:152:LEU:HD11 | 1:A:220:LEU:CD2  | 0.61     | 2.26        | 21     | 1     |
| 1:A:117:LEU:HD22 | 1:A:151:ALA:HB3  | 0.61     | 1.71        | 9      | 6     |
| 1:A:179:ILE:HG22 | 1:A:184:TRP:CD1  | 0.61     | 2.30        | 3      | 4     |
| 1:A:123:LEU:HD22 | 1:A:145:LEU:HG   | 0.61     | 1.71        | 15     | 3     |
| 1:A:176:ILE:HG13 | 1:A:213:VAL:HG21 | 0.60     | 1.71        | 1      | 5     |
| 1:A:176:ILE:O    | 1:A:179:ILE:N    | 0.60     | 2.27        | 14     | 23    |
| 1:A:143:GLY:O    | 1:A:147:SER:N    | 0.60     | 2.30        | 10     | 19    |
| 1:A:131:LEU:O    | 1:A:135:HIS:CG   | 0.60     | 2.54        | 4      | 6     |
| 1:A:117:LEU:HD22 | 1:A:151:ALA:C    | 0.60     | 2.16        | 11     | 7     |
| 1:A:148:LEU:HD11 | 1:A:181:LEU:HD21 | 0.60     | 1.71        | 12     | 3     |
| 1:A:117:LEU:CD2  | 1:A:152:LEU:CD2  | 0.60     | 2.76        | 21     | 1     |
| 1:A:126:LEU:HD11 | 1:A:131:LEU:CA   | 0.60     | 2.27        | 11     | 3     |
| 1:A:176:ILE:HG13 | 1:A:209:GLN:NE2  | 0.60     | 2.11        | 4      | 7     |
| 1:A:155:ILE:O    | 1:A:159:SER:N    | 0.59     | 2.35        | 17     | 13    |
| 1:A:202:LEU:O    | 1:A:206:ILE:HB   | 0.59     | 1.97        | 15     | 13    |
| 1:A:220:LEU:HD13 | 1:A:224:VAL:CG2  | 0.59     | 2.27        | 22     | 2     |
| 1:A:131:LEU:HD13 | 1:A:202:LEU:HD21 | 0.59     | 1.73        | 18     | 3     |
| 1:A:171:LEU:CD1  | 1:A:217:VAL:HG23 | 0.59     | 2.27        | 18     | 1     |
| 1:A:199:SER:O    | 1:A:203:ARG:HB3  | 0.59     | 1.96        | 22     | 13    |
| 1:A:179:ILE:HG12 | 1:A:190:ALA:HB3  | 0.59     | 1.74        | 9      | 7     |
| 1:A:135:HIS:O    | 1:A:139:ALA:HB2  | 0.59     | 1.98        | 10     | 1     |
| 1:A:179:ILE:CG1  | 1:A:194:LEU:HD22 | 0.59     | 2.26        | 17     | 3     |
| 1:A:196:LEU:O    | 1:A:196:LEU:HD13 | 0.59     | 1.97        | 22     | 2     |
| 1:A:176:ILE:HG13 | 1:A:181:LEU:HD12 | 0.59     | 1.75        | 5      | 5     |
| 1:A:127:THR:CG2  | 1:A:128:PRO:HD2  | 0.59     | 2.28        | 8      | 6     |
| 1:A:209:GLN:C    | 1:A:209:GLN:CD   | 0.59     | 2.61        | 6      | 3     |
| 1:A:165:ARG:CD   | 1:A:165:ARG:C    | 0.59     | 2.71        | 11     | 2     |
| 1:A:162:GLU:O    | 1:A:165:ARG:HG3  | 0.59     | 1.98        | 6      | 1     |
| 1:A:131:LEU:O    | 1:A:131:LEU:HD23 | 0.59     | 1.98        | 14     | 1     |
| 1:A:135:HIS:O    | 1:A:139:ALA:CB   | 0.59     | 2.51        | 17     | 23    |
| 1:A:123:LEU:HD13 | 1:A:148:LEU:HD22 | 0.59     | 1.75        | 9      | 1     |
| 1:A:131:LEU:HD23 | 1:A:131:LEU:O    | 0.58     | 1.98        | 15     | 2     |
| 1:A:176:ILE:CG1  | 1:A:209:GLN:NE2  | 0.58     | 2.66        | 14     | 5     |
| 1:A:127:THR:O    | 1:A:131:LEU:HB2  | 0.58     | 1.98        | 6      | 20    |
| 1:A:152:LEU:HD22 | 1:A:168:ALA:HA   | 0.58     | 1.76        | 14     | 4     |
| 1:A:127:THR:OG1  | 1:A:128:PRO:CD   | 0.58     | 2.51        | 20     | 4     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:184:TRP:CE3  | 1:A:191:ALA:HB1  | 0.58     | 2.33        | 14     | 7     |
| 1:A:131:LEU:CD2  | 1:A:195:VAL:CG2  | 0.58     | 2.82        | 19     | 6     |
| 1:A:117:LEU:HD21 | 1:A:152:LEU:HG   | 0.58     | 1.74        | 15     | 3     |
| 1:A:217:VAL:HA   | 1:A:220:LEU:HD21 | 0.58     | 1.76        | 4      | 4     |
| 1:A:177:GLY:O    | 1:A:194:LEU:CD2  | 0.58     | 2.52        | 15     | 21    |
| 1:A:199:SER:HB3  | 1:A:200:PRO:HD3  | 0.58     | 1.75        | 18     | 3     |
| 1:A:203:ARG:O    | 1:A:207:THR:HB   | 0.58     | 1.99        | 15     | 14    |
| 1:A:134:GLU:CD   | 1:A:138:LEU:HD11 | 0.58     | 2.19        | 17     | 2     |
| 1:A:130:GLY:O    | 1:A:134:GLU:CG   | 0.58     | 2.51        | 10     | 1     |
| 1:A:120:ALA:CB   | 1:A:214:MET:HE1  | 0.58     | 2.26        | 12     | 1     |
| 1:A:159:SER:HG   | 1:A:224:VAL:HG22 | 0.57     | 1.59        | 21     | 1     |
| 1:A:176:ILE:N    | 1:A:179:ILE:O    | 0.57     | 2.34        | 22     | 22    |
| 1:A:117:LEU:CD1  | 1:A:217:VAL:HG11 | 0.57     | 2.29        | 23     | 1     |
| 1:A:145:LEU:CD1  | 1:A:184:TRP:O    | 0.57     | 2.48        | 12     | 16    |
| 1:A:148:LEU:HD12 | 1:A:152:LEU:CD1  | 0.57     | 2.29        | 4      | 4     |
| 1:A:184:TRP:CH2  | 1:A:206:ILE:HG21 | 0.57     | 2.34        | 5      | 3     |
| 1:A:123:LEU:HD22 | 1:A:145:LEU:CD1  | 0.57     | 2.20        | 9      | 1     |
| 1:A:123:LEU:HD21 | 1:A:145:LEU:CG   | 0.57     | 2.28        | 19     | 1     |
| 1:A:127:THR:CB   | 1:A:128:PRO:CD   | 0.57     | 2.82        | 19     | 15    |
| 1:A:139:ALA:O    | 1:A:140:SER:CB   | 0.57     | 2.52        | 4      | 2     |
| 1:A:124:ALA:HB1  | 1:A:211:HIS:CD2  | 0.57     | 2.35        | 9      | 3     |
| 1:A:122:GLU:HA   | 1:A:125:THR:HG22 | 0.57     | 1.75        | 16     | 1     |
| 1:A:123:LEU:CG   | 1:A:145:LEU:HD12 | 0.57     | 2.29        | 11     | 1     |
| 1:A:202:LEU:O    | 1:A:206:ILE:HG13 | 0.57     | 2.00        | 3      | 2     |
| 1:A:198:ALA:HB3  | 1:A:202:LEU:HB2  | 0.57     | 1.75        | 4      | 14    |
| 1:A:199:SER:CB   | 1:A:200:PRO:CD   | 0.57     | 2.83        | 6      | 23    |
| 1:A:145:LEU:CD2  | 1:A:184:TRP:O    | 0.56     | 2.52        | 9      | 11    |
| 1:A:134:GLU:O    | 1:A:138:LEU:CB   | 0.56     | 2.53        | 1      | 13    |
| 1:A:131:LEU:HD13 | 1:A:203:ARG:HA   | 0.56     | 1.75        | 19     | 4     |
| 1:A:152:LEU:HD13 | 1:A:172:LEU:HD13 | 0.56     | 1.76        | 17     | 2     |
| 1:A:217:VAL:HA   | 1:A:220:LEU:CD2  | 0.56     | 2.30        | 4      | 7     |
| 1:A:199:SER:O    | 1:A:202:LEU:HD23 | 0.56     | 2.00        | 18     | 4     |
| 1:A:177:GLY:CA   | 1:A:206:ILE:HD13 | 0.56     | 2.30        | 11     | 2     |
| 1:A:131:LEU:HD22 | 1:A:131:LEU:C    | 0.56     | 2.20        | 12     | 1     |
| 1:A:134:GLU:HG2  | 1:A:138:LEU:HD13 | 0.56     | 1.77        | 18     | 4     |
| 1:A:165:ARG:C    | 1:A:165:ARG:CD   | 0.56     | 2.73        | 14     | 1     |
| 1:A:120:ALA:HB2  | 1:A:148:LEU:HB2  | 0.56     | 1.78        | 15     | 12    |
| 1:A:167:GLN:HB3  | 1:A:220:LEU:HD23 | 0.56     | 1.77        | 22     | 2     |
| 1:A:164:SER:HA   | 1:A:220:LEU:HD21 | 0.56     | 1.77        | 22     | 5     |
| 1:A:179:ILE:HD13 | 1:A:194:LEU:CD1  | 0.56     | 2.29        | 18     | 3     |
| 1:A:217:VAL:O    | 1:A:221:ARG:CG   | 0.56     | 2.54        | 4      | 4     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:181:LEU:O    | 1:A:181:LEU:HD12 | 0.56     | 1.99        | 18     | 1     |
| 1:A:179:ILE:HG21 | 1:A:191:ALA:CA   | 0.56     | 2.29        | 12     | 18    |
| 1:A:184:TRP:CH2  | 1:A:206:ILE:HG13 | 0.56     | 2.36        | 10     | 6     |
| 1:A:127:THR:O    | 1:A:131:LEU:CB   | 0.56     | 2.53        | 17     | 6     |
| 1:A:204:ARG:O    | 1:A:207:THR:OG1  | 0.56     | 2.24        | 19     | 1     |
| 1:A:134:GLU:HB3  | 1:A:138:LEU:HD13 | 0.56     | 1.78        | 12     | 2     |
| 1:A:217:VAL:HG13 | 1:A:221:ARG:NH1  | 0.56     | 2.16        | 9      | 1     |
| 1:A:154:GLY:O    | 1:A:158:GLY:N    | 0.56     | 2.39        | 11     | 20    |
| 1:A:220:LEU:HD23 | 1:A:220:LEU:N    | 0.56     | 2.15        | 20     | 1     |
| 1:A:123:LEU:HB2  | 1:A:210:LEU:HD13 | 0.56     | 1.76        | 2      | 1     |
| 1:A:127:THR:OG1  | 1:A:128:PRO:HD2  | 0.56     | 2.00        | 20     | 4     |
| 1:A:123:LEU:HD21 | 1:A:145:LEU:CD2  | 0.56     | 2.31        | 19     | 1     |
| 1:A:198:ALA:CB   | 1:A:202:LEU:HB2  | 0.55     | 2.32        | 8      | 15    |
| 1:A:130:GLY:O    | 1:A:134:GLU:CA   | 0.55     | 2.55        | 6      | 18    |
| 1:A:177:GLY:CA   | 1:A:209:GLN:OE1  | 0.55     | 2.54        | 19     | 6     |
| 1:A:120:ALA:CB   | 1:A:214:MET:CE   | 0.55     | 2.83        | 12     | 1     |
| 1:A:123:LEU:CD1  | 1:A:123:LEU:N    | 0.55     | 2.68        | 5      | 1     |
| 1:A:123:LEU:HD11 | 1:A:148:LEU:HD22 | 0.55     | 1.78        | 6      | 1     |
| 1:A:141:GLY:O    | 1:A:142:ASP:CB   | 0.55     | 2.53        | 1      | 21    |
| 1:A:127:THR:HG22 | 1:A:128:PRO:HD3  | 0.55     | 1.78        | 12     | 5     |
| 1:A:134:GLU:CG   | 1:A:138:LEU:HG   | 0.55     | 2.32        | 4      | 6     |
| 1:A:225:GLU:HA   | 1:A:228:VAL:HG22 | 0.55     | 1.77        | 1      | 2     |
| 1:A:199:SER:HA   | 1:A:202:LEU:HD22 | 0.55     | 1.79        | 18     | 3     |
| 1:A:152:LEU:HD11 | 1:A:217:VAL:HG22 | 0.55     | 1.77        | 3      | 1     |
| 1:A:176:ILE:HG22 | 1:A:184:TRP:CD1  | 0.55     | 2.37        | 3      | 3     |
| 1:A:127:THR:HG22 | 1:A:130:GLY:N    | 0.55     | 2.16        | 8      | 2     |
| 1:A:202:LEU:CG   | 1:A:206:ILE:HG13 | 0.55     | 2.32        | 18     | 3     |
| 1:A:161:VAL:HG12 | 1:A:163:GLU:H    | 0.54     | 1.62        | 17     | 10    |
| 1:A:194:LEU:O    | 1:A:202:LEU:CD2  | 0.54     | 2.54        | 11     | 5     |
| 1:A:195:VAL:O    | 1:A:198:ALA:O    | 0.54     | 2.25        | 20     | 22    |
| 1:A:179:ILE:CG2  | 1:A:183:GLN:HB2  | 0.54     | 2.32        | 11     | 12    |
| 1:A:117:LEU:HD23 | 1:A:148:LEU:CB   | 0.54     | 2.32        | 15     | 2     |
| 1:A:176:ILE:CD1  | 1:A:213:VAL:CG2  | 0.54     | 2.86        | 7      | 5     |
| 1:A:152:LEU:CD2  | 1:A:220:LEU:CD1  | 0.54     | 2.86        | 18     | 3     |
| 1:A:203:ARG:CD   | 1:A:203:ARG:C    | 0.54     | 2.76        | 22     | 1     |
| 1:A:123:LEU:HG   | 1:A:145:LEU:HD12 | 0.54     | 1.78        | 11     | 1     |
| 1:A:176:ILE:N    | 1:A:176:ILE:HD12 | 0.54     | 2.18        | 14     | 3     |
| 1:A:148:LEU:O    | 1:A:152:LEU:HD23 | 0.54     | 2.01        | 21     | 1     |
| 1:A:179:ILE:HD12 | 1:A:190:ALA:HB3  | 0.54     | 1.80        | 14     | 3     |
| 1:A:126:LEU:HD13 | 1:A:134:GLU:OE2  | 0.54     | 2.03        | 10     | 1     |
| 1:A:126:LEU:HD21 | 1:A:131:LEU:CG   | 0.54     | 2.32        | 12     | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:202:LEU:CD1  | 1:A:206:ILE:HG13 | 0.54     | 2.33        | 18     | 3     |
| 1:A:177:GLY:N    | 1:A:209:GLN:OE1  | 0.53     | 2.40        | 1      | 10    |
| 1:A:123:LEU:CD1  | 1:A:148:LEU:CD2  | 0.53     | 2.83        | 9      | 2     |
| 1:A:131:LEU:HD21 | 1:A:202:LEU:HD11 | 0.53     | 1.79        | 15     | 1     |
| 1:A:200:PRO:O    | 1:A:204:ARG:CG   | 0.53     | 2.57        | 2      | 5     |
| 1:A:117:LEU:HD11 | 1:A:152:LEU:CD2  | 0.53     | 2.34        | 1      | 1     |
| 1:A:126:LEU:HD23 | 1:A:210:LEU:CD1  | 0.53     | 2.34        | 6      | 1     |
| 1:A:123:LEU:HD23 | 1:A:138:LEU:HD13 | 0.53     | 1.79        | 4      | 1     |
| 1:A:131:LEU:O    | 1:A:131:LEU:CD2  | 0.53     | 2.56        | 12     | 1     |
| 1:A:192:SER:O    | 1:A:195:VAL:CG1  | 0.53     | 2.57        | 18     | 11    |
| 1:A:126:LEU:HD23 | 1:A:210:LEU:HD12 | 0.53     | 1.80        | 6      | 1     |
| 1:A:174:ARG:HD2  | 1:A:176:ILE:HD11 | 0.53     | 1.79        | 16     | 1     |
| 1:A:152:LEU:CD1  | 1:A:220:LEU:HD21 | 0.53     | 2.32        | 21     | 1     |
| 1:A:113:THR:CG2  | 1:A:151:ALA:O    | 0.53     | 2.56        | 13     | 12    |
| 1:A:168:ALA:HB2  | 1:A:220:LEU:HD11 | 0.53     | 1.80        | 7      | 1     |
| 1:A:138:LEU:CG   | 1:A:144:ALA:HB3  | 0.53     | 2.33        | 10     | 1     |
| 1:A:168:ALA:HA   | 1:A:220:LEU:HD22 | 0.53     | 1.79        | 18     | 1     |
| 1:A:130:GLY:C    | 1:A:134:GLU:HB2  | 0.53     | 2.24        | 20     | 5     |
| 1:A:176:ILE:CD1  | 1:A:213:VAL:HG21 | 0.53     | 2.33        | 7      | 4     |
| 1:A:202:LEU:HD12 | 1:A:206:ILE:HG12 | 0.53     | 1.79        | 10     | 1     |
| 1:A:155:ILE:CG1  | 1:A:224:VAL:HG21 | 0.53     | 2.34        | 4      | 5     |
| 1:A:165:ARG:HG3  | 1:A:166:ILE:N    | 0.53     | 2.18        | 11     | 4     |
| 1:A:161:VAL:CG2  | 1:A:227:GLU:OE1  | 0.53     | 2.57        | 15     | 1     |
| 1:A:126:LEU:HD12 | 1:A:127:THR:H    | 0.53     | 1.64        | 10     | 3     |
| 1:A:177:GLY:CA   | 1:A:206:ILE:CD1  | 0.53     | 2.87        | 10     | 5     |
| 1:A:122:GLU:O    | 1:A:125:THR:HG22 | 0.53     | 2.04        | 19     | 10    |
| 1:A:127:THR:HG22 | 1:A:128:PRO:HD2  | 0.53     | 1.80        | 23     | 4     |
| 1:A:159:SER:HG   | 1:A:224:VAL:HG13 | 0.52     | 1.62        | 1      | 2     |
| 1:A:171:LEU:HD22 | 1:A:216:GLU:CD   | 0.52     | 2.25        | 7      | 1     |
| 1:A:195:VAL:CA   | 1:A:202:LEU:HD12 | 0.52     | 2.35        | 4      | 3     |
| 1:A:167:GLN:CB   | 1:A:220:LEU:HD23 | 0.52     | 2.33        | 7      | 2     |
| 1:A:206:ILE:O    | 1:A:209:GLN:NE2  | 0.52     | 2.41        | 3      | 4     |
| 1:A:123:LEU:HD21 | 1:A:144:ALA:C    | 0.52     | 2.25        | 1      | 1     |
| 1:A:179:ILE:HG23 | 1:A:190:ALA:HB3  | 0.52     | 1.81        | 12     | 3     |
| 1:A:119:LYS:CG   | 1:A:144:ALA:HB2  | 0.52     | 2.35        | 6      | 2     |
| 1:A:164:SER:OG   | 1:A:224:VAL:CG2  | 0.52     | 2.57        | 12     | 3     |
| 1:A:183:GLN:C    | 1:A:185:GLY:H    | 0.52     | 2.08        | 11     | 6     |
| 1:A:147:SER:O    | 1:A:151:ALA:CB   | 0.52     | 2.57        | 10     | 7     |
| 1:A:192:SER:O    | 1:A:195:VAL:HG12 | 0.52     | 2.04        | 14     | 11    |
| 1:A:209:GLN:CD   | 1:A:209:GLN:O    | 0.52     | 2.48        | 10     | 2     |
| 1:A:145:LEU:CD2  | 1:A:184:TRP:C    | 0.52     | 2.78        | 1      | 3     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:145:LEU:CG   | 1:A:184:TRP:O    | 0.52     | 2.58        | 9      | 6     |
| 1:A:123:LEU:CD2  | 1:A:148:LEU:CD2  | 0.52     | 2.87        | 2      | 1     |
| 1:A:143:GLY:O    | 1:A:147:SER:CB   | 0.52     | 2.58        | 21     | 6     |
| 1:A:177:GLY:HA3  | 1:A:206:ILE:HD12 | 0.52     | 1.82        | 2      | 5     |
| 1:A:225:GLU:O    | 1:A:229:SER:CB   | 0.52     | 2.58        | 1      | 3     |
| 1:A:152:LEU:CD2  | 1:A:220:LEU:HD11 | 0.52     | 2.35        | 18     | 2     |
| 1:A:155:ILE:O    | 1:A:159:SER:CB   | 0.52     | 2.58        | 22     | 6     |
| 1:A:176:ILE:CG2  | 1:A:184:TRP:CD1  | 0.52     | 2.93        | 3      | 8     |
| 1:A:198:ALA:CB   | 1:A:202:LEU:HB3  | 0.52     | 2.34        | 18     | 5     |
| 1:A:218:ALA:HB1  | 1:A:222:GLN:NE2  | 0.51     | 2.21        | 8      | 1     |
| 1:A:117:LEU:HD12 | 1:A:217:VAL:CG1  | 0.51     | 2.35        | 3      | 2     |
| 1:A:159:SER:OG   | 1:A:224:VAL:CG1  | 0.51     | 2.56        | 2      | 7     |
| 1:A:195:VAL:HG23 | 1:A:202:LEU:HD11 | 0.51     | 1.82        | 18     | 1     |
| 1:A:202:LEU:HD13 | 1:A:206:ILE:HD11 | 0.51     | 1.82        | 10     | 4     |
| 1:A:209:GLN:O    | 1:A:209:GLN:CD   | 0.51     | 2.48        | 4      | 1     |
| 1:A:126:LEU:HD23 | 1:A:131:LEU:CD1  | 0.51     | 2.29        | 5      | 1     |
| 1:A:179:ILE:HD12 | 1:A:190:ALA:HB1  | 0.51     | 1.83        | 13     | 4     |
| 1:A:216:GLU:O    | 1:A:220:LEU:CD2  | 0.51     | 2.58        | 1      | 1     |
| 1:A:176:ILE:CG2  | 1:A:209:GLN:CD   | 0.51     | 2.77        | 23     | 3     |
| 1:A:131:LEU:O    | 1:A:135:HIS:HB3  | 0.51     | 2.06        | 15     | 13    |
| 1:A:117:LEU:CG   | 1:A:151:ALA:HB3  | 0.51     | 2.27        | 17     | 1     |
| 1:A:131:LEU:HD12 | 1:A:203:ARG:CA   | 0.51     | 2.33        | 8      | 2     |
| 1:A:131:LEU:CD2  | 1:A:131:LEU:C    | 0.51     | 2.78        | 12     | 1     |
| 1:A:126:LEU:O    | 1:A:207:THR:CG2  | 0.51     | 2.59        | 22     | 1     |
| 1:A:162:GLU:O    | 1:A:165:ARG:CG   | 0.51     | 2.59        | 22     | 5     |
| 1:A:148:LEU:C    | 1:A:148:LEU:HD12 | 0.51     | 2.26        | 3      | 1     |
| 1:A:127:THR:HG23 | 1:A:128:PRO:N    | 0.51     | 2.21        | 8      | 5     |
| 1:A:123:LEU:HD12 | 1:A:138:LEU:HD23 | 0.50     | 1.79        | 11     | 1     |
| 1:A:131:LEU:HD13 | 1:A:195:VAL:HG21 | 0.50     | 1.81        | 9      | 2     |
| 1:A:119:LYS:HG3  | 1:A:144:ALA:HB2  | 0.50     | 1.84        | 19     | 1     |
| 1:A:129:GLU:O    | 1:A:133:ARG:CD   | 0.50     | 2.59        | 19     | 1     |
| 1:A:123:LEU:CD2  | 1:A:138:LEU:HD23 | 0.50     | 2.36        | 22     | 1     |
| 1:A:122:GLU:O    | 1:A:125:THR:CG2  | 0.50     | 2.59        | 11     | 1     |
| 1:A:177:GLY:HA2  | 1:A:206:ILE:HD12 | 0.50     | 1.84        | 10     | 5     |
| 1:A:126:LEU:HD11 | 1:A:131:LEU:HB2  | 0.50     | 1.83        | 10     | 1     |
| 1:A:176:ILE:HG22 | 1:A:184:TRP:NE1  | 0.50     | 2.22        | 22     | 7     |
| 1:A:117:LEU:HD23 | 1:A:155:ILE:CD1  | 0.50     | 2.36        | 2      | 3     |
| 1:A:113:THR:HG21 | 1:A:155:ILE:HG13 | 0.50     | 1.82        | 7      | 3     |
| 1:A:171:LEU:CD1  | 1:A:181:LEU:CD1  | 0.50     | 2.89        | 8      | 2     |
| 1:A:179:ILE:HD13 | 1:A:194:LEU:CD2  | 0.50     | 2.33        | 22     | 1     |
| 1:A:123:LEU:HD11 | 1:A:145:LEU:HA   | 0.50     | 1.82        | 17     | 2     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:176:ILE:CD1  | 1:A:176:ILE:N    | 0.50     | 2.75        | 4      | 2     |
| 1:A:171:LEU:O    | 1:A:181:LEU:HD23 | 0.50     | 2.07        | 18     | 1     |
| 1:A:152:LEU:HD23 | 1:A:168:ALA:CB   | 0.50     | 2.36        | 4      | 1     |
| 1:A:152:LEU:HD11 | 1:A:220:LEU:CD1  | 0.50     | 2.36        | 1      | 1     |
| 1:A:123:LEU:CD1  | 1:A:145:LEU:CD1  | 0.50     | 2.82        | 17     | 1     |
| 1:A:126:LEU:HD21 | 1:A:131:LEU:CD2  | 0.50     | 2.35        | 16     | 1     |
| 1:A:152:LEU:CD2  | 1:A:168:ALA:HA   | 0.50     | 2.37        | 4      | 1     |
| 1:A:179:ILE:CG2  | 1:A:183:GLN:CB   | 0.49     | 2.90        | 1      | 3     |
| 1:A:179:ILE:HG12 | 1:A:190:ALA:CB   | 0.49     | 2.37        | 6      | 10    |
| 1:A:179:ILE:CG1  | 1:A:194:LEU:HD13 | 0.49     | 2.37        | 19     | 1     |
| 1:A:203:ARG:O    | 1:A:203:ARG:CD   | 0.49     | 2.60        | 22     | 1     |
| 1:A:179:ILE:HG21 | 1:A:191:ALA:H    | 0.49     | 1.66        | 12     | 2     |
| 1:A:123:LEU:N    | 1:A:123:LEU:CD2  | 0.49     | 2.75        | 17     | 1     |
| 1:A:202:LEU:HG   | 1:A:206:ILE:HD11 | 0.49     | 1.85        | 11     | 1     |
| 1:A:209:GLN:NE2  | 1:A:210:LEU:HD23 | 0.49     | 2.21        | 14     | 3     |
| 1:A:176:ILE:HD12 | 1:A:209:GLN:NE2  | 0.49     | 2.23        | 17     | 6     |
| 1:A:128:PRO:HA   | 1:A:203:ARG:CG   | 0.49     | 2.37        | 12     | 2     |
| 1:A:202:LEU:CD1  | 1:A:206:ILE:CD1  | 0.49     | 2.91        | 16     | 1     |
| 1:A:117:LEU:O    | 1:A:120:ALA:CB   | 0.49     | 2.60        | 8      | 3     |
| 1:A:124:ALA:HB1  | 1:A:211:HIS:HD2  | 0.49     | 1.66        | 6      | 1     |
| 1:A:203:ARG:HG3  | 1:A:204:ARG:N    | 0.49     | 2.23        | 18     | 5     |
| 1:A:206:ILE:HA   | 1:A:209:GLN:OE1  | 0.49     | 2.08        | 3      | 2     |
| 1:A:202:LEU:CD1  | 1:A:206:ILE:CG1  | 0.49     | 2.90        | 16     | 2     |
| 1:A:206:ILE:HA   | 1:A:209:GLN:CD   | 0.49     | 2.28        | 18     | 3     |
| 1:A:213:VAL:O    | 1:A:216:GLU:CG   | 0.49     | 2.60        | 7      | 1     |
| 1:A:218:ALA:O    | 1:A:222:GLN:CG   | 0.49     | 2.61        | 19     | 2     |
| 1:A:145:LEU:HA   | 1:A:148:LEU:HD23 | 0.49     | 1.85        | 21     | 2     |
| 1:A:203:ARG:CZ   | 1:A:204:ARG:CG   | 0.49     | 2.91        | 8      | 1     |
| 1:A:155:ILE:CG2  | 1:A:224:VAL:HG21 | 0.49     | 2.38        | 4      | 3     |
| 1:A:120:ALA:O    | 1:A:123:LEU:HG   | 0.49     | 2.06        | 2      | 1     |
| 1:A:179:ILE:O    | 1:A:180:ALA:C    | 0.48     | 2.49        | 8      | 13    |
| 1:A:202:LEU:HD13 | 1:A:206:ILE:CD1  | 0.48     | 2.38        | 10     | 4     |
| 1:A:176:ILE:HG23 | 1:A:209:GLN:HE21 | 0.48     | 1.68        | 4      | 2     |
| 1:A:167:GLN:HG2  | 1:A:220:LEU:HD23 | 0.48     | 1.85        | 11     | 1     |
| 1:A:216:GLU:O    | 1:A:220:LEU:HD23 | 0.48     | 2.08        | 1      | 1     |
| 1:A:217:VAL:O    | 1:A:221:ARG:N    | 0.48     | 2.44        | 17     | 1     |
| 1:A:127:THR:CB   | 1:A:128:PRO:HD2  | 0.48     | 2.38        | 19     | 5     |
| 1:A:193:GLN:CD   | 1:A:193:GLN:C    | 0.48     | 2.72        | 1      | 1     |
| 1:A:145:LEU:O    | 1:A:148:LEU:HD23 | 0.48     | 2.07        | 15     | 1     |
| 1:A:117:LEU:N    | 1:A:151:ALA:CB   | 0.48     | 2.76        | 11     | 4     |
| 1:A:165:ARG:CG   | 1:A:166:ILE:N    | 0.48     | 2.75        | 3      | 3     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:184:TRP:CZ2  | 1:A:206:ILE:HD11 | 0.48     | 2.40        | 14     | 1     |
| 1:A:171:LEU:HD12 | 1:A:220:LEU:HD21 | 0.48     | 1.84        | 18     | 1     |
| 1:A:131:LEU:HD13 | 1:A:202:LEU:CD2  | 0.48     | 2.38        | 18     | 3     |
| 1:A:165:ARG:O    | 1:A:169:GLY:N    | 0.48     | 2.40        | 16     | 5     |
| 1:A:134:GLU:HG2  | 1:A:138:LEU:HD22 | 0.48     | 1.86        | 2      | 1     |
| 1:A:214:MET:O    | 1:A:218:ALA:N    | 0.48     | 2.47        | 4      | 2     |
| 1:A:203:ARG:CZ   | 1:A:204:ARG:HG2  | 0.48     | 2.38        | 8      | 3     |
| 1:A:176:ILE:CB   | 1:A:184:TRP:CD1  | 0.48     | 2.95        | 17     | 4     |
| 1:A:179:ILE:CG1  | 1:A:190:ALA:HB3  | 0.48     | 2.39        | 6      | 2     |
| 1:A:134:GLU:O    | 1:A:138:LEU:HD13 | 0.47     | 2.09        | 3      | 7     |
| 1:A:130:GLY:HA2  | 1:A:134:GLU:CG   | 0.47     | 2.39        | 20     | 1     |
| 1:A:123:LEU:N    | 1:A:123:LEU:CD1  | 0.47     | 2.77        | 12     | 1     |
| 1:A:217:VAL:O    | 1:A:221:ARG:HB2  | 0.47     | 2.09        | 17     | 2     |
| 1:A:156:ARG:NH1  | 1:A:165:ARG:O    | 0.47     | 2.47        | 1      | 1     |
| 1:A:123:LEU:CB   | 1:A:210:LEU:HD13 | 0.47     | 2.37        | 3      | 1     |
| 1:A:152:LEU:HD21 | 1:A:220:LEU:CD1  | 0.47     | 2.38        | 5      | 2     |
| 1:A:178:GLY:O    | 1:A:179:ILE:HD13 | 0.47     | 2.10        | 1      | 2     |
| 1:A:152:LEU:HD12 | 1:A:168:ALA:HA   | 0.47     | 1.86        | 21     | 1     |
| 1:A:147:SER:O    | 1:A:151:ALA:N    | 0.47     | 2.40        | 22     | 6     |
| 1:A:210:LEU:O    | 1:A:214:MET:CG   | 0.47     | 2.62        | 8      | 1     |
| 1:A:127:THR:CG2  | 1:A:128:PRO:CD   | 0.47     | 2.92        | 12     | 4     |
| 1:A:167:GLN:HB3  | 1:A:220:LEU:CD2  | 0.47     | 2.39        | 22     | 3     |
| 1:A:176:ILE:HD12 | 1:A:209:GLN:HG3  | 0.47     | 1.86        | 22     | 1     |
| 1:A:203:ARG:HD2  | 1:A:203:ARG:C    | 0.47     | 2.29        | 9      | 1     |
| 1:A:206:ILE:O    | 1:A:210:LEU:N    | 0.47     | 2.45        | 14     | 1     |
| 1:A:184:TRP:CZ2  | 1:A:206:ILE:HD13 | 0.47     | 2.44        | 3      | 1     |
| 1:A:152:LEU:CD1  | 1:A:168:ALA:HA   | 0.47     | 2.39        | 21     | 1     |
| 1:A:142:ASP:O    | 1:A:143:GLY:C    | 0.47     | 2.53        | 21     | 16    |
| 1:A:155:ILE:HD11 | 1:A:221:ARG:HE   | 0.47     | 1.69        | 17     | 1     |
| 1:A:165:ARG:HG2  | 1:A:166:ILE:N    | 0.47     | 2.25        | 3      | 1     |
| 1:A:131:LEU:HD12 | 1:A:135:HIS:HB2  | 0.47     | 1.86        | 10     | 1     |
| 1:A:134:GLU:OE1  | 1:A:138:LEU:CD1  | 0.47     | 2.62        | 17     | 2     |
| 1:A:155:ILE:HG21 | 1:A:220:LEU:HD11 | 0.47     | 1.83        | 7      | 1     |
| 1:A:171:LEU:CD1  | 1:A:181:LEU:HD22 | 0.46     | 2.37        | 1      | 2     |
| 1:A:128:PRO:N    | 1:A:203:ARG:HG3  | 0.46     | 2.26        | 9      | 3     |
| 1:A:131:LEU:HD12 | 1:A:131:LEU:O    | 0.46     | 2.10        | 10     | 1     |
| 1:A:174:ARG:O    | 1:A:181:LEU:N    | 0.46     | 2.47        | 8      | 10    |
| 1:A:120:ALA:O    | 1:A:214:MET:SD   | 0.46     | 2.72        | 8      | 1     |
| 1:A:200:PRO:HA   | 1:A:203:ARG:CG   | 0.46     | 2.41        | 20     | 5     |
| 1:A:184:TRP:CZ2  | 1:A:206:ILE:HG13 | 0.46     | 2.45        | 10     | 1     |
| 1:A:194:LEU:HG   | 1:A:202:LEU:HD21 | 0.46     | 1.87        | 11     | 2     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:131:LEU:HD12 | 1:A:203:ARG:HB2  | 0.46     | 1.86        | 16     | 1     |
| 1:A:160:GLN:CB   | 1:A:227:GLU:OE1  | 0.46     | 2.63        | 18     | 1     |
| 1:A:170:ARG:NH1  | 1:A:174:ARG:NH1  | 0.46     | 2.64        | 4      | 1     |
| 1:A:155:ILE:HD13 | 1:A:220:LEU:HD11 | 0.46     | 1.88        | 21     | 1     |
| 1:A:225:GLU:O    | 1:A:229:SER:N    | 0.46     | 2.48        | 9      | 2     |
| 1:A:113:THR:HG21 | 1:A:154:GLY:HA3  | 0.46     | 1.88        | 6      | 1     |
| 1:A:160:GLN:CA   | 1:A:227:GLU:OE1  | 0.46     | 2.64        | 18     | 1     |
| 1:A:161:VAL:CG1  | 1:A:161:VAL:O    | 0.46     | 2.63        | 20     | 1     |
| 1:A:146:ARG:NH1  | 1:A:186:THR:OG1  | 0.46     | 2.50        | 5      | 3     |
| 1:A:148:LEU:HD21 | 1:A:181:LEU:HD11 | 0.46     | 1.86        | 18     | 1     |
| 1:A:217:VAL:CG1  | 1:A:221:ARG:HD3  | 0.45     | 2.41        | 18     | 4     |
| 1:A:126:LEU:CD1  | 1:A:134:GLU:OE1  | 0.45     | 2.64        | 15     | 2     |
| 1:A:202:LEU:CD1  | 1:A:206:ILE:HG12 | 0.45     | 2.41        | 10     | 1     |
| 1:A:167:GLN:CB   | 1:A:220:LEU:HD22 | 0.45     | 2.41        | 20     | 1     |
| 1:A:123:LEU:HD13 | 1:A:123:LEU:N    | 0.45     | 2.26        | 5      | 1     |
| 1:A:120:ALA:CB   | 1:A:148:LEU:CB   | 0.45     | 2.94        | 21     | 1     |
| 1:A:176:ILE:CD1  | 1:A:209:GLN:NE2  | 0.45     | 2.79        | 17     | 4     |
| 1:A:152:LEU:HB3  | 1:A:172:LEU:HD21 | 0.45     | 1.89        | 9      | 1     |
| 1:A:190:ALA:O    | 1:A:194:LEU:N    | 0.45     | 2.45        | 5      | 2     |
| 1:A:155:ILE:HD11 | 1:A:221:ARG:HH21 | 0.45     | 1.71        | 17     | 1     |
| 1:A:131:LEU:HD23 | 1:A:195:VAL:HG23 | 0.45     | 1.81        | 2      | 1     |
| 1:A:167:GLN:CD   | 1:A:220:LEU:HD23 | 0.45     | 2.32        | 23     | 2     |
| 1:A:218:ALA:O    | 1:A:222:GLN:CB   | 0.45     | 2.64        | 16     | 1     |
| 1:A:114:LEU:HD21 | 1:A:225:GLU:HG3  | 0.45     | 1.88        | 18     | 1     |
| 1:A:117:LEU:HD11 | 1:A:152:LEU:CG   | 0.45     | 2.41        | 5      | 2     |
| 1:A:119:LYS:CG   | 1:A:144:ALA:CB   | 0.45     | 2.95        | 6      | 1     |
| 1:A:171:LEU:O    | 1:A:171:LEU:HD12 | 0.45     | 2.11        | 23     | 2     |
| 1:A:126:LEU:O    | 1:A:203:ARG:NH2  | 0.45     | 2.48        | 10     | 1     |
| 1:A:152:LEU:CD1  | 1:A:181:LEU:HD21 | 0.45     | 2.41        | 10     | 2     |
| 1:A:124:ALA:HB2  | 1:A:214:MET:HG2  | 0.45     | 1.88        | 20     | 1     |
| 1:A:217:VAL:O    | 1:A:221:ARG:HG2  | 0.45     | 2.10        | 12     | 2     |
| 1:A:225:GLU:C    | 1:A:225:GLU:CD   | 0.45     | 2.75        | 7      | 1     |
| 1:A:121:SER:O    | 1:A:124:ALA:HB3  | 0.45     | 2.12        | 3      | 3     |
| 1:A:128:PRO:HB3  | 1:A:203:ARG:NE   | 0.45     | 2.27        | 19     | 1     |
| 1:A:176:ILE:C    | 1:A:178:GLY:N    | 0.45     | 2.71        | 10     | 16    |
| 1:A:203:ARG:HG2  | 1:A:207:THR:OG1  | 0.45     | 2.12        | 10     | 1     |
| 1:A:209:GLN:OE1  | 1:A:209:GLN:O    | 0.45     | 2.34        | 10     | 1     |
| 1:A:159:SER:CB   | 1:A:164:SER:HB3  | 0.45     | 2.41        | 20     | 2     |
| 1:A:123:LEU:HD21 | 1:A:138:LEU:HD23 | 0.45     | 1.87        | 22     | 1     |
| 1:A:134:GLU:CG   | 1:A:138:LEU:HD13 | 0.45     | 2.38        | 13     | 1     |
| 1:A:179:ILE:HG12 | 1:A:194:LEU:HD23 | 0.45     | 1.89        | 1      | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:217:VAL:O    | 1:A:220:LEU:HG   | 0.45     | 2.11        | 15     | 5     |
| 1:A:225:GLU:HG3  | 1:A:226:SER:N    | 0.45     | 2.26        | 7      | 1     |
| 1:A:179:ILE:O    | 1:A:184:TRP:CD1  | 0.45     | 2.70        | 8      | 1     |
| 1:A:178:GLY:O    | 1:A:179:ILE:HD12 | 0.45     | 2.12        | 5      | 1     |
| 1:A:203:ARG:NE   | 1:A:204:ARG:CG   | 0.45     | 2.80        | 8      | 2     |
| 1:A:170:ARG:O    | 1:A:174:ARG:N    | 0.45     | 2.50        | 23     | 2     |
| 1:A:117:LEU:CD2  | 1:A:151:ALA:C    | 0.45     | 2.84        | 11     | 1     |
| 1:A:127:THR:O    | 1:A:203:ARG:HG3  | 0.45     | 2.12        | 16     | 1     |
| 1:A:171:LEU:HD11 | 1:A:213:VAL:CG1  | 0.44     | 2.25        | 1      | 1     |
| 1:A:161:VAL:N    | 1:A:227:GLU:OE1  | 0.44     | 2.50        | 9      | 1     |
| 1:A:168:ALA:CA   | 1:A:220:LEU:HD22 | 0.44     | 2.42        | 18     | 1     |
| 1:A:145:LEU:HD21 | 1:A:184:TRP:C    | 0.44     | 2.32        | 17     | 4     |
| 1:A:128:PRO:HB3  | 1:A:203:ARG:CD   | 0.44     | 2.42        | 20     | 4     |
| 1:A:123:LEU:C    | 1:A:123:LEU:CD1  | 0.44     | 2.86        | 2      | 1     |
| 1:A:177:GLY:HA2  | 1:A:209:GLN:OE1  | 0.44     | 2.12        | 9      | 2     |
| 1:A:155:ILE:HG21 | 1:A:220:LEU:HD13 | 0.44     | 1.86        | 7      | 1     |
| 1:A:152:LEU:HD23 | 1:A:168:ALA:HB1  | 0.44     | 1.87        | 4      | 1     |
| 1:A:198:ALA:HB3  | 1:A:202:LEU:CB   | 0.44     | 2.43        | 4      | 3     |
| 1:A:152:LEU:CD1  | 1:A:172:LEU:HD13 | 0.44     | 2.42        | 22     | 1     |
| 1:A:203:ARG:NE   | 1:A:203:ARG:O    | 0.44     | 2.50        | 22     | 1     |
| 1:A:131:LEU:HD13 | 1:A:203:ARG:CA   | 0.44     | 2.40        | 13     | 1     |
| 1:A:123:LEU:HD12 | 1:A:210:LEU:HD12 | 0.44     | 1.86        | 10     | 1     |
| 1:A:186:THR:HG22 | 1:A:187:THR:N    | 0.44     | 2.27        | 21     | 2     |
| 1:A:140:SER:OG   | 1:A:141:GLY:N    | 0.44     | 2.50        | 14     | 2     |
| 1:A:156:ARG:HD3  | 1:A:172:LEU:HD23 | 0.44     | 1.89        | 10     | 1     |
| 1:A:176:ILE:O    | 1:A:179:ILE:O    | 0.44     | 2.35        | 2      | 5     |
| 1:A:176:ILE:HD13 | 1:A:176:ILE:N    | 0.44     | 2.28        | 8      | 2     |
| 1:A:134:GLU:HG3  | 1:A:135:HIS:N    | 0.44     | 2.28        | 10     | 1     |
| 1:A:176:ILE:HG13 | 1:A:209:GLN:CD   | 0.44     | 2.33        | 10     | 2     |
| 1:A:176:ILE:HG12 | 1:A:181:LEU:CD1  | 0.44     | 2.43        | 11     | 1     |
| 1:A:123:LEU:CD1  | 1:A:210:LEU:HD13 | 0.44     | 2.38        | 23     | 2     |
| 1:A:120:ALA:HB2  | 1:A:148:LEU:CB   | 0.44     | 2.43        | 21     | 2     |
| 1:A:152:LEU:HD12 | 1:A:168:ALA:CA   | 0.44     | 2.43        | 21     | 1     |
| 1:A:119:LYS:NZ   | 1:A:142:ASP:O    | 0.44     | 2.51        | 11     | 1     |
| 1:A:176:ILE:HD12 | 1:A:176:ILE:N    | 0.44     | 2.28        | 16     | 2     |
| 1:A:171:LEU:O    | 1:A:171:LEU:CD1  | 0.44     | 2.65        | 3      | 1     |
| 1:A:209:GLN:O    | 1:A:209:GLN:OE1  | 0.44     | 2.35        | 4      | 1     |
| 1:A:203:ARG:HH21 | 1:A:207:THR:HG21 | 0.44     | 1.73        | 10     | 1     |
| 1:A:206:ILE:O    | 1:A:209:GLN:HG3  | 0.44     | 2.12        | 14     | 2     |
| 1:A:131:LEU:CD2  | 1:A:202:LEU:HD21 | 0.44     | 2.26        | 15     | 1     |
| 1:A:131:LEU:CD1  | 1:A:203:ARG:HA   | 0.44     | 2.42        | 13     | 2     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:128:PRO:HA   | 1:A:203:ARG:CB   | 0.44     | 2.43        | 12     | 1     |
| 1:A:217:VAL:O    | 1:A:221:ARG:HG3  | 0.43     | 2.13        | 15     | 10    |
| 1:A:176:ILE:CG1  | 1:A:213:VAL:HG21 | 0.43     | 2.43        | 1      | 1     |
| 1:A:159:SER:HB2  | 1:A:164:SER:CB   | 0.43     | 2.43        | 8      | 5     |
| 1:A:148:LEU:HG   | 1:A:149:SER:N    | 0.43     | 2.27        | 13     | 5     |
| 1:A:201:GLU:O    | 1:A:205:GLU:CG   | 0.43     | 2.67        | 12     | 1     |
| 1:A:179:ILE:HG22 | 1:A:184:TRP:CE2  | 0.43     | 2.45        | 3      | 1     |
| 1:A:199:SER:HA   | 1:A:202:LEU:CD2  | 0.43     | 2.44        | 18     | 1     |
| 1:A:181:LEU:C    | 1:A:183:GLN:N    | 0.43     | 2.72        | 4      | 7     |
| 1:A:167:GLN:CB   | 1:A:220:LEU:CD2  | 0.43     | 2.97        | 7      | 2     |
| 1:A:134:GLU:HG2  | 1:A:138:LEU:CD2  | 0.43     | 2.43        | 17     | 2     |
| 1:A:218:ALA:HA   | 1:A:221:ARG:CD   | 0.43     | 2.43        | 3      | 2     |
| 1:A:148:LEU:CD1  | 1:A:152:LEU:HD12 | 0.43     | 2.41        | 4      | 2     |
| 1:A:203:ARG:HD2  | 1:A:204:ARG:N    | 0.43     | 2.29        | 8      | 2     |
| 1:A:119:LYS:CD   | 1:A:144:ALA:HB2  | 0.43     | 2.44        | 10     | 1     |
| 1:A:193:GLN:HG3  | 1:A:194:LEU:N    | 0.43     | 2.28        | 1      | 1     |
| 1:A:179:ILE:CG1  | 1:A:190:ALA:CB   | 0.43     | 2.96        | 6      | 1     |
| 1:A:117:LEU:HB2  | 1:A:221:ARG:CD   | 0.43     | 2.44        | 10     | 1     |
| 1:A:134:GLU:HG2  | 1:A:138:LEU:CD1  | 0.43     | 2.44        | 5      | 2     |
| 1:A:194:LEU:CD2  | 1:A:202:LEU:HD11 | 0.43     | 2.43        | 12     | 1     |
| 1:A:118:ASP:OD1  | 1:A:221:ARG:NH1  | 0.43     | 2.51        | 2      | 1     |
| 1:A:131:LEU:CD1  | 1:A:195:VAL:CG2  | 0.43     | 2.87        | 16     | 1     |
| 1:A:225:GLU:CG   | 1:A:226:SER:N    | 0.43     | 2.82        | 16     | 1     |
| 1:A:128:PRO:HB3  | 1:A:203:ARG:CG   | 0.43     | 2.44        | 18     | 1     |
| 1:A:155:ILE:HG23 | 1:A:224:VAL:HG21 | 0.43     | 1.90        | 16     | 1     |
| 1:A:210:LEU:HD23 | 1:A:210:LEU:HA   | 0.43     | 1.77        | 16     | 2     |
| 1:A:162:GLU:O    | 1:A:165:ARG:HG2  | 0.43     | 2.13        | 22     | 4     |
| 1:A:123:LEU:CD2  | 1:A:145:LEU:HG   | 0.43     | 2.40        | 19     | 3     |
| 1:A:177:GLY:HA2  | 1:A:206:ILE:CD1  | 0.43     | 2.44        | 5      | 2     |
| 1:A:202:LEU:HG   | 1:A:206:ILE:CD1  | 0.43     | 2.43        | 11     | 2     |
| 1:A:159:SER:CB   | 1:A:164:SER:OG   | 0.43     | 2.67        | 6      | 1     |
| 1:A:130:GLY:HA3  | 1:A:134:GLU:CG   | 0.43     | 2.44        | 3      | 1     |
| 1:A:159:SER:CB   | 1:A:164:SER:HB2  | 0.42     | 2.45        | 18     | 4     |
| 1:A:176:ILE:N    | 1:A:176:ILE:HD13 | 0.42     | 2.28        | 17     | 1     |
| 1:A:203:ARG:HD3  | 1:A:204:ARG:N    | 0.42     | 2.29        | 14     | 1     |
| 1:A:114:LEU:CD2  | 1:A:225:GLU:HB3  | 0.42     | 2.44        | 7      | 1     |
| 1:A:117:LEU:CD2  | 1:A:151:ALA:HB1  | 0.42     | 2.34        | 7      | 1     |
| 1:A:123:LEU:CD1  | 1:A:145:LEU:HG   | 0.42     | 2.44        | 21     | 1     |
| 1:A:179:ILE:CD1  | 1:A:194:LEU:CD1  | 0.42     | 2.93        | 18     | 1     |
| 1:A:159:SER:OG   | 1:A:224:VAL:CG2  | 0.42     | 2.63        | 2      | 1     |
| 1:A:162:GLU:O    | 1:A:166:ILE:HB   | 0.42     | 2.13        | 6      | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:146:ARG:HA   | 1:A:185:GLY:O    | 0.42     | 2.14        | 8      | 1     |
| 1:A:199:SER:O    | 1:A:203:ARG:HB2  | 0.42     | 2.15        | 10     | 2     |
| 1:A:138:LEU:N    | 1:A:138:LEU:HD23 | 0.42     | 2.28        | 1      | 1     |
| 1:A:134:GLU:OE2  | 1:A:138:LEU:CD2  | 0.42     | 2.68        | 10     | 1     |
| 1:A:130:GLY:O    | 1:A:134:GLU:HB3  | 0.42     | 2.14        | 10     | 1     |
| 1:A:117:LEU:HG   | 1:A:217:VAL:CG1  | 0.42     | 2.45        | 10     | 2     |
| 1:A:164:SER:OG   | 1:A:220:LEU:HD13 | 0.42     | 2.15        | 12     | 1     |
| 1:A:176:ILE:HD12 | 1:A:209:GLN:CD   | 0.42     | 2.35        | 6      | 1     |
| 1:A:141:GLY:C    | 1:A:143:GLY:N    | 0.42     | 2.71        | 11     | 2     |
| 1:A:114:LEU:HD21 | 1:A:225:GLU:CB   | 0.42     | 2.44        | 16     | 1     |
| 1:A:160:GLN:N    | 1:A:227:GLU:OE1  | 0.42     | 2.49        | 14     | 1     |
| 1:A:148:LEU:CD1  | 1:A:152:LEU:CD1  | 0.42     | 2.98        | 4      | 2     |
| 1:A:120:ALA:CB   | 1:A:148:LEU:HB2  | 0.42     | 2.45        | 21     | 1     |
| 1:A:218:ALA:O    | 1:A:222:GLN:CD   | 0.42     | 2.58        | 2      | 2     |
| 1:A:155:ILE:HD13 | 1:A:220:LEU:HD12 | 0.42     | 1.92        | 11     | 1     |
| 1:A:126:LEU:HD23 | 1:A:207:THR:OG1  | 0.42     | 2.14        | 9      | 1     |
| 1:A:119:LYS:O    | 1:A:144:ALA:HB1  | 0.42     | 2.14        | 14     | 1     |
| 1:A:156:ARG:HG2  | 1:A:168:ALA:HB3  | 0.42     | 1.91        | 23     | 1     |
| 1:A:218:ALA:HA   | 1:A:221:ARG:HG2  | 0.42     | 1.90        | 4      | 1     |
| 1:A:126:LEU:HD11 | 1:A:131:LEU:CB   | 0.42     | 2.44        | 10     | 1     |
| 1:A:137:ARG:C    | 1:A:139:ALA:H    | 0.42     | 2.17        | 10     | 1     |
| 1:A:129:GLU:O    | 1:A:133:ARG:HB2  | 0.42     | 2.15        | 13     | 1     |
| 1:A:220:LEU:C    | 1:A:220:LEU:CD1  | 0.42     | 2.85        | 21     | 1     |
| 1:A:206:ILE:HG23 | 1:A:209:GLN:OE1  | 0.42     | 2.15        | 19     | 1     |
| 1:A:127:THR:CG2  | 1:A:130:GLY:H    | 0.42     | 2.22        | 20     | 2     |
| 1:A:125:THR:O    | 1:A:126:LEU:O    | 0.42     | 2.37        | 20     | 5     |
| 1:A:131:LEU:HA   | 1:A:134:GLU:CG   | 0.42     | 2.44        | 10     | 1     |
| 1:A:181:LEU:HD11 | 1:A:213:VAL:HG11 | 0.42     | 1.91        | 5      | 1     |
| 1:A:131:LEU:CG   | 1:A:195:VAL:HG21 | 0.42     | 2.45        | 17     | 1     |
| 1:A:218:ALA:O    | 1:A:222:GLN:OE1  | 0.42     | 2.38        | 2      | 1     |
| 1:A:126:LEU:HD11 | 1:A:131:LEU:HG   | 0.42     | 1.91        | 9      | 1     |
| 1:A:123:LEU:HD12 | 1:A:148:LEU:HD22 | 0.42     | 1.91        | 16     | 1     |
| 1:A:127:THR:C    | 1:A:203:ARG:HG3  | 0.42     | 2.35        | 23     | 2     |
| 1:A:134:GLU:CD   | 1:A:138:LEU:CD2  | 0.42     | 2.89        | 15     | 1     |
| 1:A:166:ILE:O    | 1:A:170:ARG:CG   | 0.42     | 2.68        | 5      | 1     |
| 1:A:201:GLU:O    | 1:A:205:GLU:CD   | 0.42     | 2.58        | 12     | 1     |
| 1:A:171:LEU:O    | 1:A:181:LEU:HB3  | 0.42     | 2.15        | 16     | 1     |
| 1:A:145:LEU:O    | 1:A:148:LEU:CD2  | 0.42     | 2.67        | 15     | 1     |
| 1:A:224:VAL:O    | 1:A:228:VAL:HG13 | 0.41     | 2.15        | 5      | 1     |
| 1:A:214:MET:O    | 1:A:214:MET:SD   | 0.41     | 2.78        | 13     | 3     |
| 1:A:200:PRO:HA   | 1:A:203:ARG:HG2  | 0.41     | 1.91        | 11     | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:128:PRO:HB3  | 1:A:203:ARG:CB   | 0.41     | 2.45        | 18     | 2     |
| 1:A:117:LEU:CD1  | 1:A:217:VAL:CG1  | 0.41     | 2.98        | 23     | 1     |
| 1:A:130:GLY:CA   | 1:A:134:GLU:HG2  | 0.41     | 2.45        | 3      | 1     |
| 1:A:203:ARG:C    | 1:A:203:ARG:CD   | 0.41     | 2.88        | 3      | 1     |
| 1:A:128:PRO:HG3  | 1:A:203:ARG:CZ   | 0.41     | 2.44        | 8      | 1     |
| 1:A:201:GLU:O    | 1:A:205:GLU:OE1  | 0.41     | 2.38        | 10     | 3     |
| 1:A:154:GLY:O    | 1:A:158:GLY:HA3  | 0.41     | 2.15        | 1      | 2     |
| 1:A:220:LEU:HD13 | 1:A:224:VAL:HG23 | 0.41     | 1.92        | 22     | 1     |
| 1:A:160:GLN:C    | 1:A:227:GLU:OE1  | 0.41     | 2.59        | 18     | 1     |
| 1:A:120:ALA:C    | 1:A:214:MET:SD   | 0.41     | 2.99        | 4      | 1     |
| 1:A:156:ARG:O    | 1:A:165:ARG:NE   | 0.41     | 2.54        | 10     | 1     |
| 1:A:172:LEU:HD13 | 1:A:181:LEU:HD23 | 0.41     | 1.91        | 10     | 1     |
| 1:A:128:PRO:CA   | 1:A:203:ARG:HD3  | 0.41     | 2.45        | 12     | 2     |
| 1:A:200:PRO:O    | 1:A:203:ARG:HG3  | 0.41     | 2.16        | 6      | 1     |
| 1:A:128:PRO:HA   | 1:A:203:ARG:HG3  | 0.41     | 1.92        | 16     | 1     |
| 1:A:123:LEU:C    | 1:A:123:LEU:HD12 | 0.41     | 2.35        | 14     | 1     |
| 1:A:176:ILE:O    | 1:A:178:GLY:N    | 0.41     | 2.53        | 14     | 1     |
| 1:A:134:GLU:HA   | 1:A:137:ARG:CG   | 0.41     | 2.45        | 7      | 1     |
| 1:A:152:LEU:HD21 | 1:A:217:VAL:HG22 | 0.41     | 1.92        | 18     | 1     |
| 1:A:156:ARG:O    | 1:A:165:ARG:CZ   | 0.41     | 2.68        | 10     | 1     |
| 1:A:152:LEU:HD12 | 1:A:168:ALA:CB   | 0.41     | 2.46        | 1      | 1     |
| 1:A:152:LEU:CD1  | 1:A:220:LEU:CD2  | 0.41     | 2.97        | 21     | 1     |
| 1:A:214:MET:SD   | 1:A:214:MET:O    | 0.41     | 2.78        | 11     | 1     |
| 1:A:181:LEU:CD1  | 1:A:213:VAL:HG11 | 0.41     | 2.46        | 1      | 2     |
| 1:A:195:VAL:HA   | 1:A:202:LEU:CD1  | 0.41     | 2.45        | 14     | 1     |
| 1:A:145:LEU:HB3  | 1:A:184:TRP:O    | 0.41     | 2.15        | 3      | 2     |
| 1:A:184:TRP:CH2  | 1:A:206:ILE:HD13 | 0.41     | 2.49        | 3      | 1     |
| 1:A:206:ILE:CG2  | 1:A:209:GLN:NE2  | 0.41     | 2.77        | 21     | 1     |
| 1:A:160:GLN:CB   | 1:A:227:GLU:CD   | 0.41     | 2.89        | 18     | 1     |
| 1:A:210:LEU:HA   | 1:A:210:LEU:HD23 | 0.41     | 1.78        | 8      | 1     |
| 1:A:117:LEU:HD13 | 1:A:117:LEU:HA   | 0.41     | 1.74        | 1      | 1     |
| 1:A:176:ILE:HG23 | 1:A:209:GLN:CG   | 0.41     | 2.45        | 7      | 2     |
| 1:A:135:HIS:O    | 1:A:139:ALA:N    | 0.41     | 2.53        | 7      | 1     |
| 1:A:159:SER:OG   | 1:A:164:SER:CB   | 0.41     | 2.68        | 20     | 1     |
| 1:A:225:GLU:O    | 1:A:229:SER:OG   | 0.41     | 2.38        | 1      | 1     |
| 1:A:153:ALA:N    | 1:A:172:LEU:HD21 | 0.41     | 2.30        | 6      | 2     |
| 1:A:154:GLY:O    | 1:A:158:GLY:CA   | 0.41     | 2.69        | 21     | 2     |
| 1:A:146:ARG:CG   | 1:A:185:GLY:O    | 0.41     | 2.68        | 8      | 1     |
| 1:A:199:SER:HB2  | 1:A:200:PRO:HD3  | 0.41     | 1.90        | 6      | 3     |
| 1:A:203:ARG:O    | 1:A:203:ARG:HD2  | 0.41     | 2.16        | 22     | 1     |
| 1:A:128:PRO:CA   | 1:A:203:ARG:HD2  | 0.41     | 2.46        | 16     | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:161:VAL:CG1  | 1:A:163:GLU:HB2  | 0.41     | 2.46        | 7      | 1     |
| 1:A:152:LEU:HB3  | 1:A:172:LEU:CD2  | 0.41     | 2.46        | 21     | 1     |
| 1:A:201:GLU:O    | 1:A:205:GLU:OE2  | 0.41     | 2.38        | 4      | 1     |
| 1:A:198:ALA:CB   | 1:A:202:LEU:HD22 | 0.41     | 2.28        | 22     | 1     |
| 1:A:152:LEU:HD12 | 1:A:168:ALA:HB1  | 0.41     | 1.92        | 1      | 1     |
| 1:A:117:LEU:HB3  | 1:A:221:ARG:CD   | 0.41     | 2.46        | 12     | 1     |
| 1:A:123:LEU:HD22 | 1:A:148:LEU:HD22 | 0.41     | 1.89        | 14     | 1     |
| 1:A:114:LEU:CD2  | 1:A:225:GLU:HG3  | 0.41     | 2.45        | 3      | 1     |
| 1:A:149:SER:HA   | 1:A:172:LEU:HD11 | 0.41     | 1.93        | 18     | 1     |
| 1:A:165:ARG:HD2  | 1:A:166:ILE:N    | 0.40     | 2.31        | 6      | 1     |
| 1:A:131:LEU:HD23 | 1:A:135:HIS:HB2  | 0.40     | 1.93        | 9      | 1     |
| 1:A:183:GLN:C    | 1:A:185:GLY:N    | 0.40     | 2.75        | 9      | 1     |
| 1:A:116:GLY:C    | 1:A:151:ALA:HB2  | 0.40     | 2.36        | 14     | 1     |
| 1:A:117:LEU:HA   | 1:A:117:LEU:HD13 | 0.40     | 1.72        | 23     | 1     |
| 1:A:120:ALA:HA   | 1:A:123:LEU:CD2  | 0.40     | 2.45        | 3      | 1     |
| 1:A:202:LEU:HA   | 1:A:202:LEU:HD22 | 0.40     | 1.76        | 20     | 2     |
| 1:A:156:ARG:O    | 1:A:165:ARG:NH2  | 0.40     | 2.54        | 10     | 1     |
| 1:A:171:LEU:CD1  | 1:A:213:VAL:HG22 | 0.40     | 2.37        | 10     | 1     |
| 1:A:138:LEU:N    | 1:A:138:LEU:CD1  | 0.40     | 2.85        | 22     | 1     |
| 1:A:181:LEU:CD1  | 1:A:213:VAL:HG21 | 0.40     | 2.46        | 11     | 1     |
| 1:A:165:ARG:CD   | 1:A:166:ILE:N    | 0.40     | 2.84        | 6      | 1     |
| 1:A:126:LEU:HG   | 1:A:127:THR:N    | 0.40     | 2.31        | 9      | 1     |
| 1:A:179:ILE:HB   | 1:A:184:TRP:NE1  | 0.40     | 2.31        | 14     | 1     |
| 1:A:221:ARG:CB   | 1:A:221:ARG:CZ   | 0.40     | 3.00        | 23     | 1     |
| 1:A:140:SER:O    | 1:A:146:ARG:CD   | 0.40     | 2.69        | 7      | 1     |
| 1:A:128:PRO:N    | 1:A:203:ARG:HD3  | 0.40     | 2.31        | 19     | 1     |
| 1:A:114:LEU:O    | 1:A:118:ASP:OD2  | 0.40     | 2.40        | 8      | 1     |
| 1:A:179:ILE:CD1  | 1:A:194:LEU:HD22 | 0.40     | 2.37        | 22     | 1     |
| 1:A:126:LEU:CD2  | 1:A:131:LEU:HG   | 0.40     | 2.47        | 12     | 2     |
| 1:A:162:GLU:O    | 1:A:166:ILE:HD12 | 0.40     | 2.15        | 12     | 1     |
| 1:A:186:THR:CG2  | 1:A:187:THR:N    | 0.40     | 2.85        | 21     | 1     |
| 1:A:209:GLN:NE2  | 1:A:210:LEU:HG   | 0.40     | 2.31        | 19     | 1     |
| 1:A:124:ALA:HB2  | 1:A:214:MET:SD   | 0.40     | 2.57        | 8      | 1     |
| 1:A:217:VAL:CG1  | 1:A:221:ARG:HD2  | 0.40     | 2.43        | 8      | 1     |
| 1:A:203:ARG:NE   | 1:A:204:ARG:HG2  | 0.40     | 2.32        | 20     | 1     |
| 1:A:134:GLU:HB3  | 1:A:138:LEU:CD2  | 0.40     | 2.47        | 12     | 1     |
| 1:A:156:ARG:CG   | 1:A:165:ARG:HG3  | 0.40     | 2.47        | 12     | 1     |
| 1:A:161:VAL:CG1  | 1:A:163:GLU:HG3  | 0.40     | 2.47        | 12     | 1     |
| 1:A:179:ILE:HG23 | 1:A:183:GLN:CB   | 0.40     | 2.44        | 9      | 1     |

## 6.3 Torsion angles [i](#)

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

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

| Mol | Chain | Analysed        | Favoured      | Allowed     | Outliers   | Percentiles |    |
|-----|-------|-----------------|---------------|-------------|------------|-------------|----|
| 1   | A     | 118/153 (77%)   | 106±1 (90±1%) | 10±2 (8±1%) | 2±1 (1±1%) | 16          | 61 |
| All | All   | 2714/3519 (77%) | 2448 (90%)    | 226 (8%)    | 40 (1%)    | 16          | 61 |

All 5 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     | 199 | SER  | 23             |
| 1   | A     | 126 | LEU  | 8              |
| 1   | A     | 143 | GLY  | 6              |
| 1   | A     | 140 | SER  | 2              |
| 1   | A     | 180 | ALA  | 1              |

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

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

| Mol | Chain | Analysed        | Rotameric    | Outliers     | Percentiles |    |
|-----|-------|-----------------|--------------|--------------|-------------|----|
| 1   | A     | 92/120 (77%)    | 60±4 (66±4%) | 32±4 (34±4%) | 1           | 10 |
| All | All   | 2116/2760 (77%) | 1389 (66%)   | 727 (34%)    | 1           | 10 |

All 79 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     | 172 | LEU  | 23             |
| 1   | A     | 202 | LEU  | 23             |
| 1   | A     | 199 | SER  | 23             |
| 1   | A     | 209 | GLN  | 23             |
| 1   | A     | 148 | LEU  | 23             |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 175 | SER  | 23             |
| 1   | A     | 171 | LEU  | 21             |
| 1   | A     | 114 | LEU  | 21             |
| 1   | A     | 127 | THR  | 18             |
| 1   | A     | 170 | ARG  | 17             |
| 1   | A     | 117 | LEU  | 17             |
| 1   | A     | 150 | THR  | 16             |
| 1   | A     | 203 | ARG  | 15             |
| 1   | A     | 155 | ILE  | 15             |
| 1   | A     | 131 | LEU  | 15             |
| 1   | A     | 220 | LEU  | 15             |
| 1   | A     | 145 | LEU  | 14             |
| 1   | A     | 219 | LEU  | 14             |
| 1   | A     | 181 | LEU  | 14             |
| 1   | A     | 115 | LYS  | 13             |
| 1   | A     | 164 | SER  | 13             |
| 1   | A     | 162 | GLU  | 13             |
| 1   | A     | 201 | GLU  | 13             |
| 1   | A     | 140 | SER  | 12             |
| 1   | A     | 135 | HIS  | 12             |
| 1   | A     | 133 | ARG  | 12             |
| 1   | A     | 174 | ARG  | 11             |
| 1   | A     | 208 | ASP  | 11             |
| 1   | A     | 216 | GLU  | 10             |
| 1   | A     | 194 | LEU  | 10             |
| 1   | A     | 179 | ILE  | 10             |
| 1   | A     | 119 | LYS  | 10             |
| 1   | A     | 196 | LEU  | 10             |
| 1   | A     | 134 | GLU  | 9              |
| 1   | A     | 173 | GLU  | 9              |
| 1   | A     | 213 | VAL  | 9              |
| 1   | A     | 182 | GLN  | 9              |
| 1   | A     | 221 | ARG  | 9              |
| 1   | A     | 142 | ASP  | 8              |
| 1   | A     | 225 | GLU  | 8              |
| 1   | A     | 159 | SER  | 7              |
| 1   | A     | 226 | SER  | 7              |
| 1   | A     | 167 | GLN  | 7              |
| 1   | A     | 222 | GLN  | 7              |
| 1   | A     | 137 | ARG  | 7              |
| 1   | A     | 176 | ILE  | 7              |
| 1   | A     | 129 | GLU  | 7              |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 163 | GLU  | 7              |
| 1   | A     | 192 | SER  | 7              |
| 1   | A     | 165 | ARG  | 6              |
| 1   | A     | 204 | ARG  | 6              |
| 1   | A     | 123 | LEU  | 6              |
| 1   | A     | 166 | ILE  | 6              |
| 1   | A     | 118 | ASP  | 5              |
| 1   | A     | 229 | SER  | 5              |
| 1   | A     | 146 | ARG  | 5              |
| 1   | A     | 212 | GLN  | 5              |
| 1   | A     | 122 | GLU  | 4              |
| 1   | A     | 206 | ILE  | 4              |
| 1   | A     | 186 | THR  | 4              |
| 1   | A     | 197 | ASP  | 4              |
| 1   | A     | 113 | THR  | 4              |
| 1   | A     | 136 | SER  | 4              |
| 1   | A     | 187 | THR  | 3              |
| 1   | A     | 152 | LEU  | 3              |
| 1   | A     | 138 | LEU  | 3              |
| 1   | A     | 160 | GLN  | 2              |
| 1   | A     | 210 | LEU  | 2              |
| 1   | A     | 193 | GLN  | 2              |
| 1   | A     | 161 | VAL  | 1              |
| 1   | A     | 147 | SER  | 1              |
| 1   | A     | 214 | MET  | 1              |
| 1   | A     | 126 | LEU  | 1              |
| 1   | A     | 149 | SER  | 1              |
| 1   | A     | 183 | GLN  | 1              |
| 1   | A     | 121 | SER  | 1              |
| 1   | A     | 207 | THR  | 1              |
| 1   | A     | 112 | MET  | 1              |
| 1   | A     | 156 | ARG  | 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

No chemical shift data were provided