



# Full wwPDB NMR Structure Validation Report ⓘ

Mar 18, 2026 – 10:18 AM UTC

PDB ID : 1DV9 / pdb\_00001dv9  
Title : STRUCTURAL CHANGES ACCOMPANYING PH-INDUCED DISSOCIATION OF THE B-LACTOGLOBULIN DIMER  
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Deposited on : 2000-01-20

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

|                                |   |                                                                  |
|--------------------------------|---|------------------------------------------------------------------|
| MolProbity                     | : | 4-5-2 with Phenix2.0                                             |
| Percentile statistics          | : | 20250101.v01 (using entries in the PDB archive January 1st 2025) |
| wwPDB-RCI                      | : | v_1n_11_5_13_A (Berjanski et al., 2005)                          |
| PANAV                          | : | Wang et al. (2010)                                               |
| wwPDB-ShiftChecker             | : | v1.2                                                             |
| Ideal geometry (proteins)      | : | Engh & Huber (2001)                                              |
| Ideal geometry (DNA, RNA)      | : | Parkinson et al. (1996)                                          |
| Validation Pipeline (wwPDB-VP) | : | 2.49                                                             |

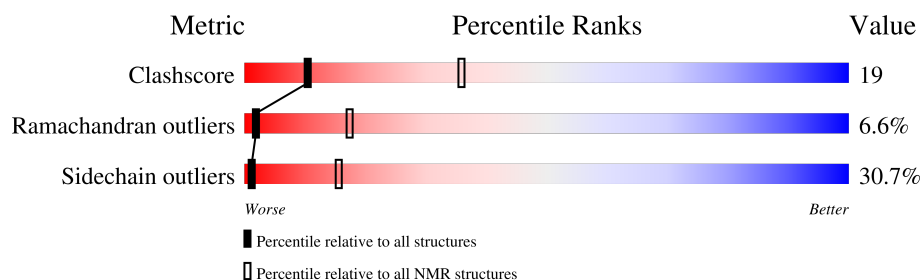
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment was not calculated.

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



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

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

| Mol | Chain | Length | Quality of chain                                                                   |
|-----|-------|--------|------------------------------------------------------------------------------------|
| 1   | A     | 162    | <div> <div></div> <div>31%</div> <div>54%</div> <div>•</div> <div>12%</div> </div> |

## 2 Ensemble composition and analysis

This entry contains 21 models. Model 5 is the overall representative, medoid model (most similar to other models). The authors have identified model 14 as representative, based on the following criterion: *closest to the average*.

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:6-A:33, A:37-A:60, A:66-A:156 (143) | 0.93              | 5            |

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 and 2 single-model clusters were found.

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

### 3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2590 atoms, of which 1303 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called BETA-LACTOGLOBULIN.

| Mol | Chain | Residues | Atoms |     |      |     |     |   | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|-------|
| 1   | A     | 162      | Total | C   | H    | N   | O   | S | 0     |
|     |       |          | 2590  | 821 | 1303 | 206 | 251 | 9 |       |

There are 3 discrepancies between the modelled and reference sequences:

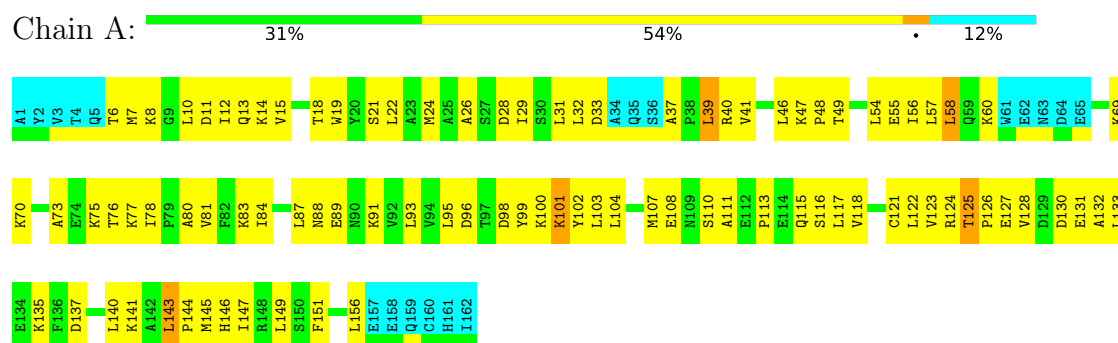
| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| A     | 1       | ALA      | LEU    | see remark 999 | UNP P02754 |
| A     | 2       | TYR      | ILE    | see remark 999 | UNP P02754 |
| A     | 105     | PHE      | VAL    | see remark 999 | UNP P02754 |

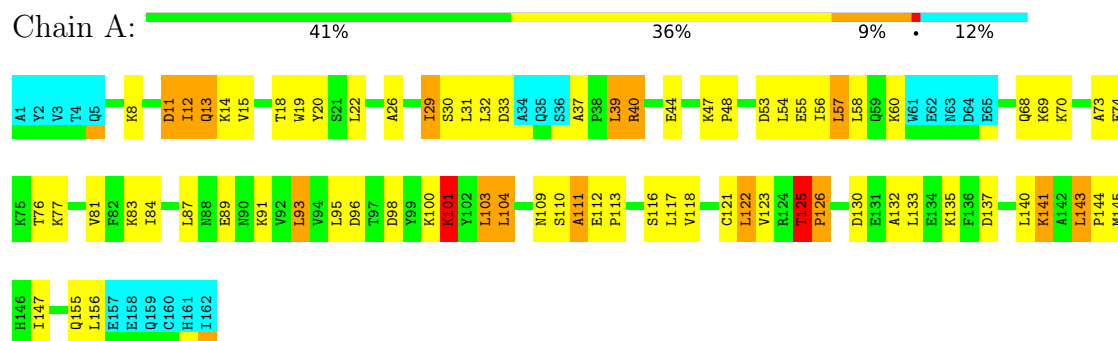
## 4 Residue-property plots

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

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

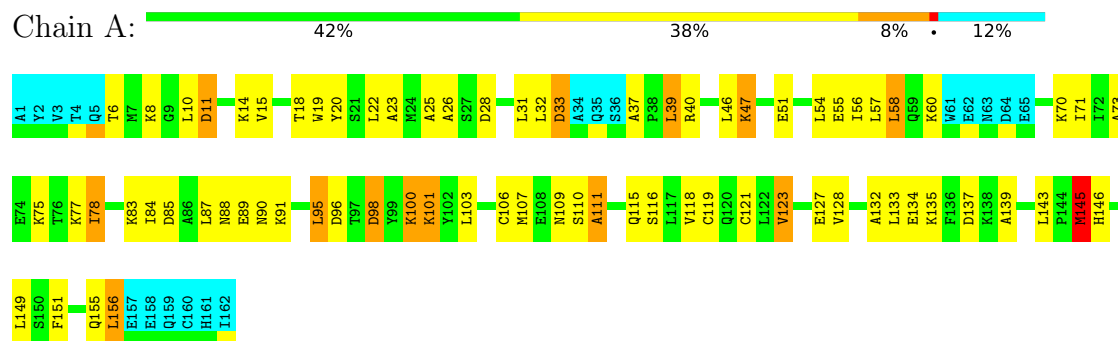
#### • Molecule 1: BETA-LACTOGLOBULIN





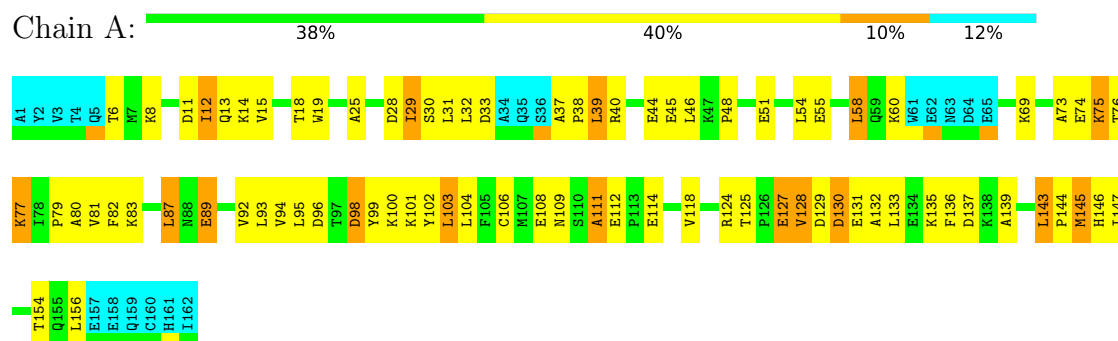
#### 4.2.3 Score per residue for model 3

- Molecule 1: BETA-LACTOGLOBULIN



#### 4.2.4 Score per residue for model 4

- Molecule 1: BETA-LACTOGLOBULIN



#### 4.2.5 Score per residue for model 5 (medoid)

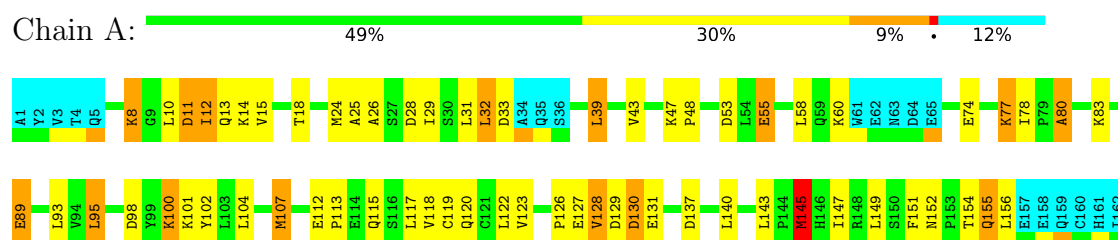
- Molecule 1: BETA-LACTOGLOBULIN





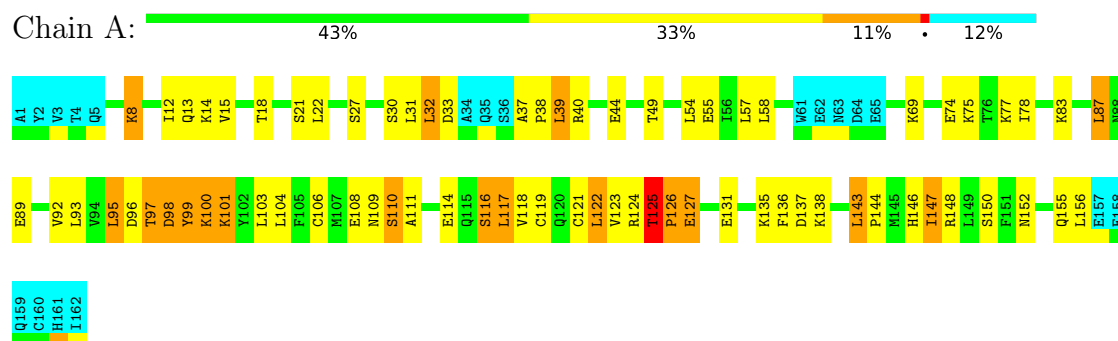
#### 4.2.6 Score per residue for model 6

- Molecule 1: BETA-LACTOGLOBULIN



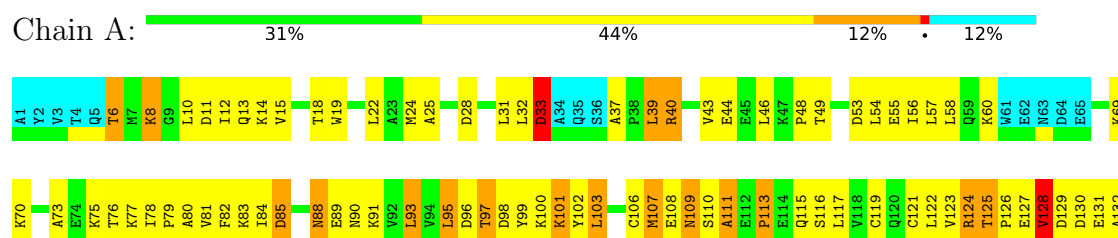
#### 4.2.7 Score per residue for model 7

- Molecule 1: BETA-LACTOGLOBULIN



#### 4.2.8 Score per residue for model 8

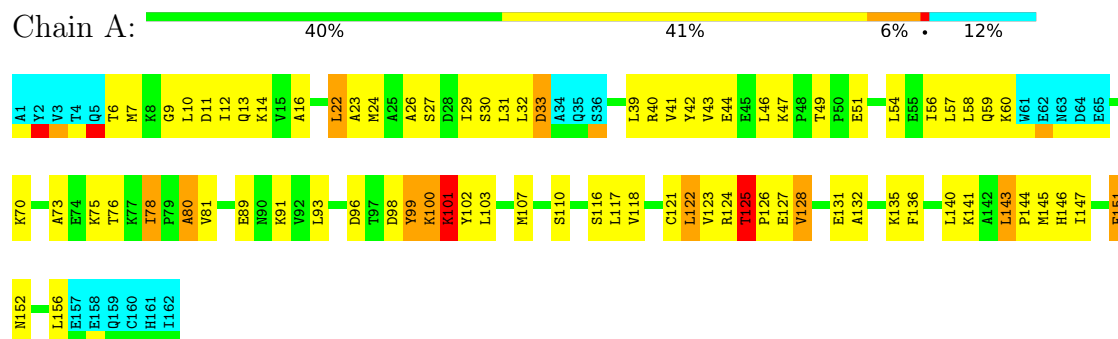
- Molecule 1: BETA-LACTOGLOBULIN





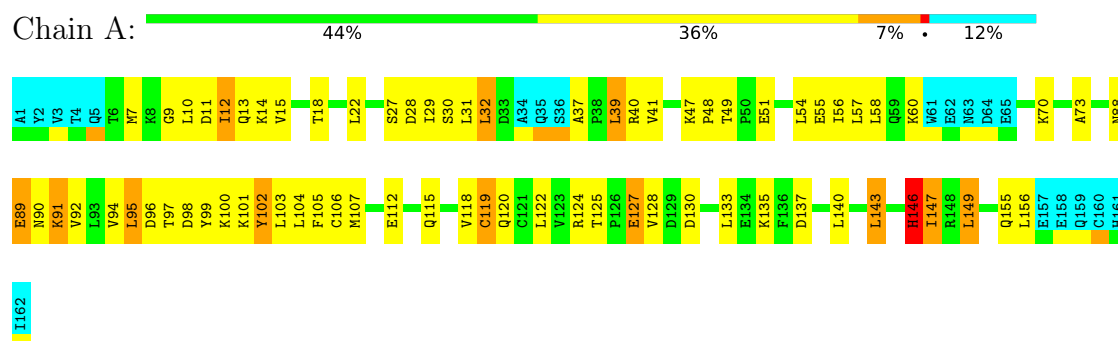
#### 4.2.9 Score per residue for model 9

- Molecule 1: BETA-LACTOGLOBULIN



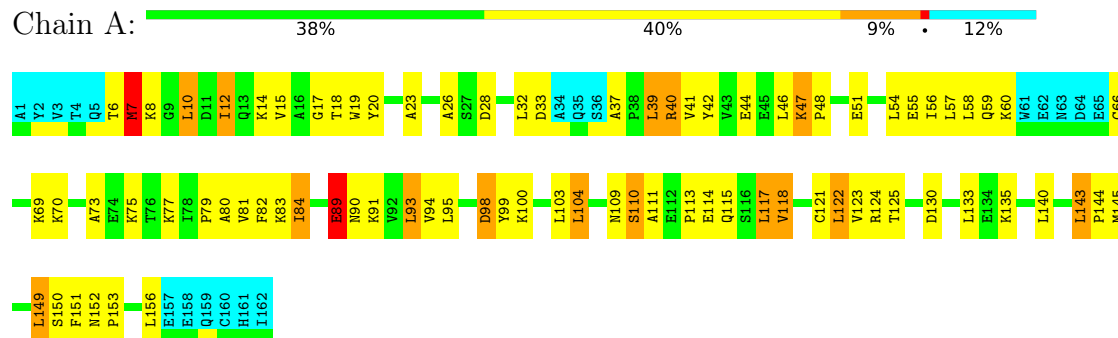
#### 4.2.10 Score per residue for model 10

- Molecule 1: BETA-LACTOGLOBULIN



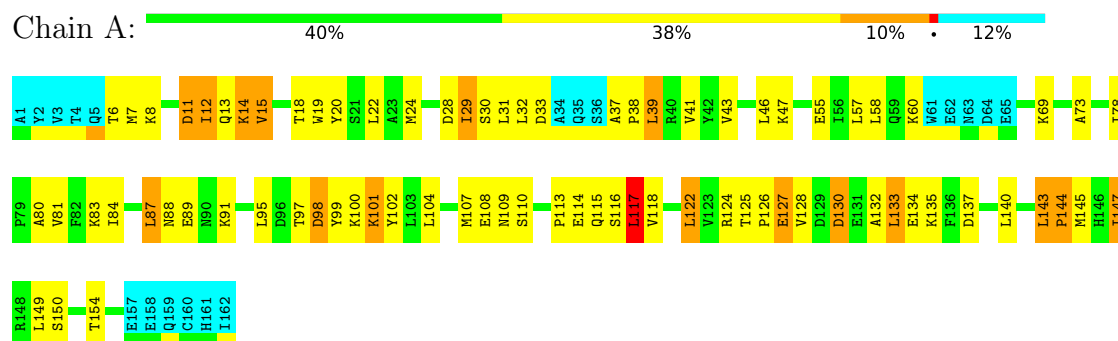
#### 4.2.11 Score per residue for model 11

- Molecule 1: BETA-LACTOGLOBULIN



### 4.2.12 Score per residue for model 12

#### • Molecule 1: BETA-LACTOGLOBULIN



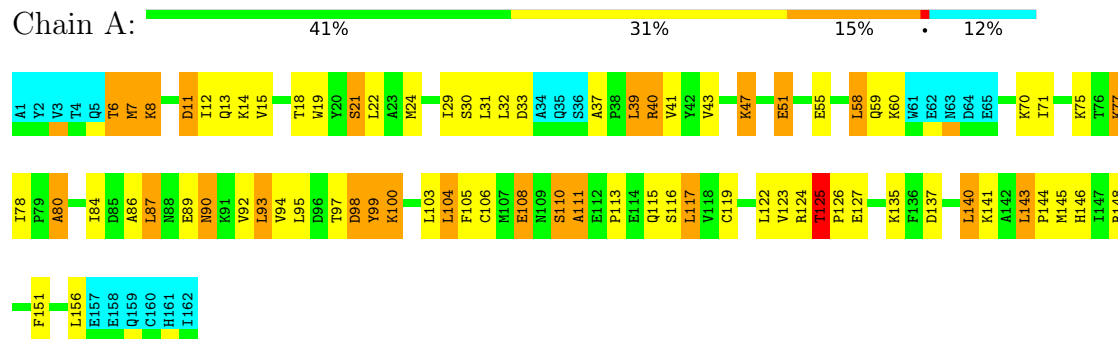
### 4.2.13 Score per residue for model 13

#### • Molecule 1: BETA-LACTOGLOBULIN



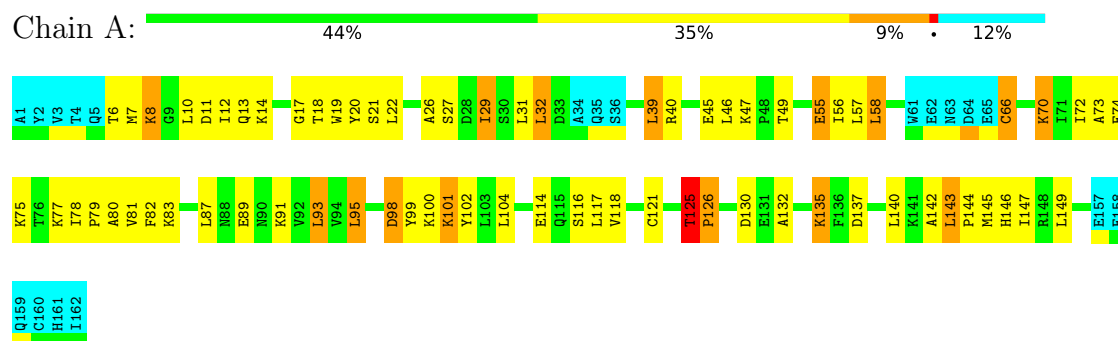
### 4.2.14 Score per residue for model 14

#### • Molecule 1: BETA-LACTOGLOBULIN



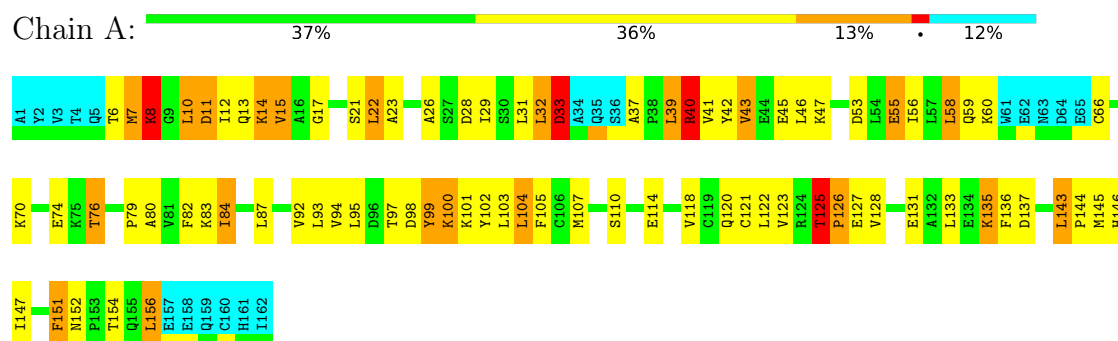
### 4.2.15 Score per residue for model 15

- Molecule 1: BETA-LACTOGLOBULIN



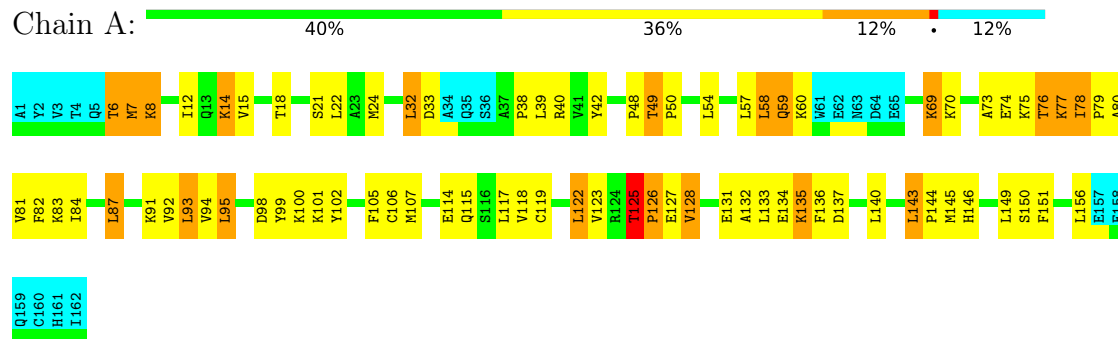
### 4.2.16 Score per residue for model 16

- Molecule 1: BETA-LACTOGLOBULIN



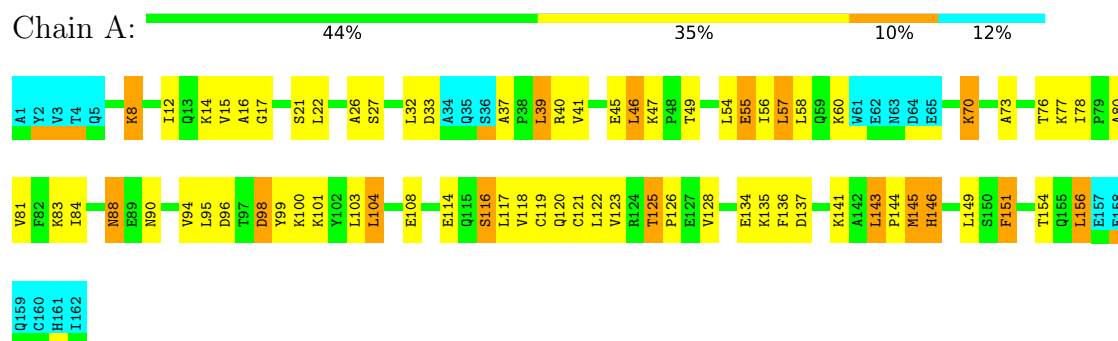
### 4.2.17 Score per residue for model 17

- Molecule 1: BETA-LACTOGLOBULIN



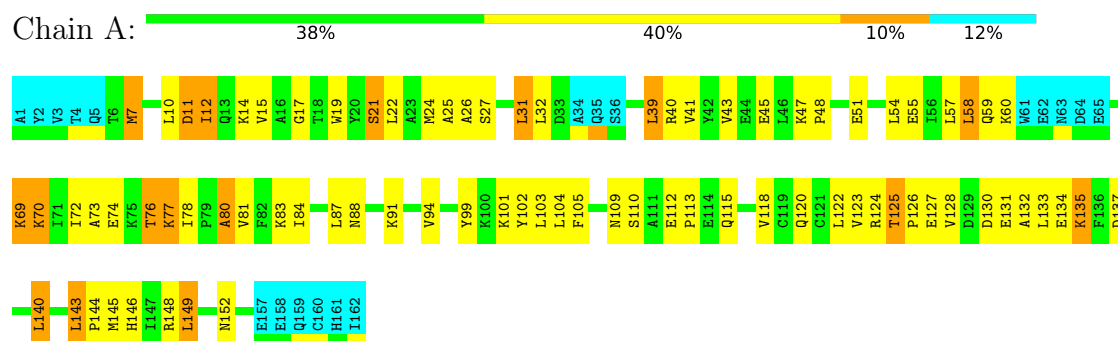
### 4.2.18 Score per residue for model 18

#### • Molecule 1: BETA-LACTOGLOBULIN



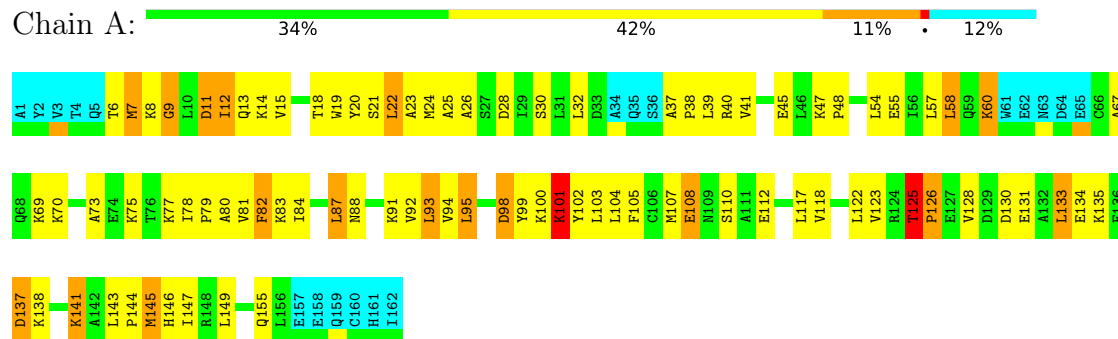
### 4.2.19 Score per residue for model 19

#### • Molecule 1: BETA-LACTOGLOBULIN



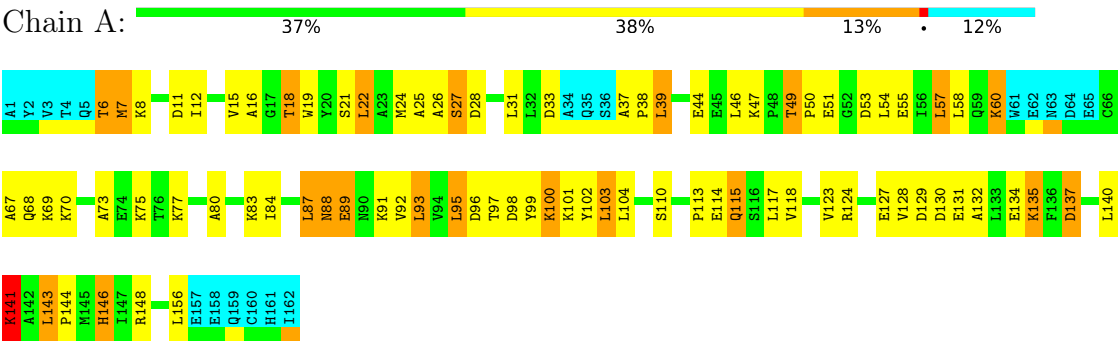
### 4.2.20 Score per residue for model 20

#### • Molecule 1: BETA-LACTOGLOBULIN



4.2.21 Score per residue for model 21

● Molecule 1: BETA-LACTOGLOBULIN



## 5 Refinement protocol and experimental data overview ⓘ

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

Of the 60 calculated structures, 21 were deposited, based on the following criterion: *lowest total energy*.

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

| Software name | Classification     | Version |
|---------------|--------------------|---------|
| X-PLOR        | structure solution | ARIA    |
| CNS           | structure solution | 0.9     |
| CNS           | refinement         | 0.9     |

No chemical shift data was provided.

## 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     | 1127  | 1170     | 1169     | 43±9    |
| All | All   | 23667 | 24570    | 24549    | 912     |

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 19.

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

| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:39:LEU:HD21  | 1:A:118:VAL:HG21 | 1.09     | 1.22        | 19     | 4     |
| 1:A:29:ILE:HG23  | 1:A:147:ILE:HD13 | 0.95     | 1.33        | 12     | 5     |
| 1:A:26:ALA:HB2   | 1:A:118:VAL:HG23 | 0.89     | 1.44        | 20     | 6     |
| 1:A:39:LEU:HD21  | 1:A:118:VAL:HG11 | 0.88     | 1.44        | 3      | 3     |
| 1:A:12:ILE:O     | 1:A:15:VAL:HG22  | 0.87     | 1.69        | 18     | 10    |
| 1:A:46:LEU:CD2   | 1:A:56:ILE:HG23  | 0.87     | 2.00        | 16     | 2     |
| 1:A:26:ALA:CB    | 1:A:118:VAL:HG12 | 0.87     | 2.00        | 9      | 3     |
| 1:A:123:VAL:HG21 | 1:A:127:GLU:O    | 0.84     | 1.72        | 14     | 1     |
| 1:A:41:VAL:CG2   | 1:A:58:LEU:HD13  | 0.84     | 2.03        | 11     | 1     |
| 1:A:39:LEU:HD11  | 1:A:118:VAL:HG11 | 0.81     | 1.51        | 7      | 3     |
| 1:A:26:ALA:HB1   | 1:A:118:VAL:HG12 | 0.81     | 1.52        | 9      | 1     |
| 1:A:23:ALA:HB3   | 1:A:121:CYS:SG   | 0.81     | 2.16        | 11     | 3     |
| 1:A:31:LEU:O     | 1:A:37:ALA:HB1   | 0.80     | 1.75        | 21     | 8     |
| 1:A:81:VAL:HG13  | 1:A:93:LEU:CD1   | 0.79     | 2.06        | 11     | 2     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:92:VAL:C     | 1:A:93:LEU:HD12  | 0.79     | 2.02        | 5      | 1     |
| 1:A:25:ALA:HB1   | 1:A:145:MET:SD   | 0.79     | 2.18        | 6      | 6     |
| 1:A:12:ILE:HD11  | 1:A:54:LEU:HD13  | 0.79     | 1.53        | 21     | 4     |
| 1:A:39:LEU:CD2   | 1:A:118:VAL:HG21 | 0.78     | 2.08        | 15     | 3     |
| 1:A:93:LEU:HD21  | 1:A:108:GLU:OE2  | 0.78     | 1.78        | 20     | 1     |
| 1:A:28:ASP:HB2   | 1:A:31:LEU:HD22  | 0.78     | 1.53        | 1      | 1     |
| 1:A:103:LEU:HD11 | 1:A:122:LEU:HD12 | 0.78     | 1.54        | 2      | 1     |
| 1:A:32:LEU:HD22  | 1:A:149:LEU:CD1  | 0.77     | 2.10        | 17     | 1     |
| 1:A:92:VAL:C     | 1:A:93:LEU:HD13  | 0.77     | 2.05        | 21     | 2     |
| 1:A:123:VAL:HG11 | 1:A:126:PRO:O    | 0.77     | 1.80        | 2      | 1     |
| 1:A:43:VAL:HG11  | 1:A:122:LEU:HD11 | 0.76     | 1.58        | 6      | 1     |
| 1:A:46:LEU:HD21  | 1:A:56:ILE:HG23  | 0.74     | 1.59        | 16     | 1     |
| 1:A:103:LEU:HD13 | 1:A:103:LEU:O    | 0.74     | 1.80        | 2      | 1     |
| 1:A:46:LEU:HD11  | 1:A:54:LEU:HD11  | 0.74     | 1.59        | 4      | 1     |
| 1:A:93:LEU:HD11  | 1:A:108:GLU:OE2  | 0.74     | 1.83        | 14     | 2     |
| 1:A:10:LEU:HD11  | 1:A:79:PRO:CB    | 0.73     | 2.13        | 16     | 1     |
| 1:A:10:LEU:HD11  | 1:A:79:PRO:HB2   | 0.73     | 1.60        | 16     | 1     |
| 1:A:81:VAL:HG12  | 1:A:93:LEU:HG    | 0.71     | 1.62        | 15     | 1     |
| 1:A:39:LEU:HD23  | 1:A:118:VAL:HG11 | 0.71     | 1.58        | 16     | 1     |
| 1:A:10:LEU:HD23  | 1:A:10:LEU:O     | 0.71     | 1.84        | 13     | 2     |
| 1:A:39:LEU:HD22  | 1:A:118:VAL:HG21 | 0.71     | 1.60        | 16     | 3     |
| 1:A:73:ALA:HB1   | 1:A:82:PHE:HB3   | 0.71     | 1.59        | 17     | 2     |
| 1:A:56:ILE:HG22  | 1:A:58:LEU:CD2   | 0.71     | 2.16        | 15     | 1     |
| 1:A:41:VAL:HG21  | 1:A:58:LEU:HD13  | 0.70     | 1.60        | 11     | 1     |
| 1:A:101:LYS:O    | 1:A:123:VAL:HG23 | 0.70     | 1.85        | 8      | 2     |
| 1:A:81:VAL:HG22  | 1:A:93:LEU:CD1   | 0.70     | 2.17        | 4      | 1     |
| 1:A:139:ALA:O    | 1:A:143:LEU:HD21 | 0.70     | 1.87        | 4      | 1     |
| 1:A:144:PRO:O    | 1:A:145:MET:HE2  | 0.69     | 1.86        | 8      | 2     |
| 1:A:31:LEU:HD22  | 1:A:39:LEU:HD23  | 0.69     | 1.62        | 7      | 1     |
| 1:A:22:LEU:HD11  | 1:A:128:VAL:HG23 | 0.69     | 1.64        | 5      | 2     |
| 1:A:20:TYR:O     | 1:A:122:LEU:HD23 | 0.69     | 1.87        | 13     | 2     |
| 1:A:54:LEU:HB3   | 1:A:73:ALA:HB3   | 0.68     | 1.65        | 11     | 14    |
| 1:A:31:LEU:HD13  | 1:A:118:VAL:CG2  | 0.68     | 2.19        | 6      | 1     |
| 1:A:46:LEU:CD1   | 1:A:56:ILE:HG23  | 0.68     | 2.18        | 15     | 3     |
| 1:A:58:LEU:HD12  | 1:A:69:LYS:O     | 0.68     | 1.88        | 19     | 4     |
| 1:A:31:LEU:HB3   | 1:A:39:LEU:HD13  | 0.67     | 1.64        | 3      | 1     |
| 1:A:22:LEU:CD1   | 1:A:128:VAL:HG22 | 0.67     | 2.18        | 19     | 1     |
| 1:A:39:LEU:CD2   | 1:A:118:VAL:HG11 | 0.67     | 2.18        | 16     | 3     |
| 1:A:10:LEU:HD12  | 1:A:94:VAL:HG11  | 0.67     | 1.67        | 19     | 1     |
| 1:A:121:CYS:O    | 1:A:122:LEU:HD23 | 0.67     | 1.90        | 2      | 1     |
| 1:A:57:LEU:HD22  | 1:A:70:LYS:HB3   | 0.67     | 1.65        | 21     | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:19:TRP:CE3   | 1:A:103:LEU:HD12 | 0.67     | 2.25        | 2      | 1     |
| 1:A:81:VAL:HG22  | 1:A:93:LEU:HG    | 0.66     | 1.67        | 5      | 1     |
| 1:A:39:LEU:HD22  | 1:A:118:VAL:HG11 | 0.66     | 1.67        | 6      | 2     |
| 1:A:81:VAL:HG22  | 1:A:93:LEU:HD12  | 0.66     | 1.65        | 17     | 2     |
| 1:A:38:PRO:O     | 1:A:87:LEU:HD22  | 0.66     | 1.91        | 12     | 2     |
| 1:A:31:LEU:HD22  | 1:A:39:LEU:CD1   | 0.66     | 2.21        | 3      | 1     |
| 1:A:12:ILE:HG22  | 1:A:48:PRO:CG    | 0.66     | 2.20        | 4      | 5     |
| 1:A:12:ILE:HG22  | 1:A:48:PRO:HG3   | 0.66     | 1.66        | 4      | 4     |
| 1:A:11:ASP:O     | 1:A:15:VAL:HG23  | 0.66     | 1.91        | 19     | 1     |
| 1:A:92:VAL:O     | 1:A:93:LEU:HD13  | 0.66     | 1.91        | 17     | 1     |
| 1:A:121:CYS:C    | 1:A:122:LEU:HD23 | 0.65     | 2.17        | 2      | 2     |
| 1:A:12:ILE:HD11  | 1:A:79:PRO:O     | 0.65     | 1.91        | 11     | 1     |
| 1:A:26:ALA:HB2   | 1:A:118:VAL:HG13 | 0.65     | 1.68        | 16     | 1     |
| 1:A:143:LEU:HD22 | 1:A:143:LEU:N    | 0.65     | 2.07        | 10     | 1     |
| 1:A:95:LEU:HD11  | 1:A:104:LEU:HB3  | 0.65     | 1.67        | 20     | 2     |
| 1:A:77:LYS:C     | 1:A:78:ILE:HD12  | 0.65     | 2.17        | 17     | 1     |
| 1:A:121:CYS:SG   | 1:A:132:ALA:HB1  | 0.65     | 2.32        | 15     | 3     |
| 1:A:29:ILE:HG23  | 1:A:147:ILE:HD12 | 0.65     | 1.69        | 9      | 1     |
| 1:A:19:TRP:CD1   | 1:A:46:LEU:HD12  | 0.65     | 2.26        | 11     | 2     |
| 1:A:93:LEU:HD22  | 1:A:93:LEU:N     | 0.65     | 2.07        | 17     | 2     |
| 1:A:93:LEU:HD13  | 1:A:93:LEU:N     | 0.65     | 2.06        | 21     | 1     |
| 1:A:28:ASP:CB    | 1:A:31:LEU:HD22  | 0.64     | 2.22        | 1      | 1     |
| 1:A:39:LEU:O     | 1:A:41:VAL:HG22  | 0.64     | 1.93        | 14     | 4     |
| 1:A:22:LEU:O     | 1:A:22:LEU:HD22  | 0.64     | 1.93        | 20     | 1     |
| 1:A:142:ALA:C    | 1:A:143:LEU:HD23 | 0.64     | 2.17        | 15     | 1     |
| 1:A:46:LEU:HD23  | 1:A:56:ILE:HG23  | 0.64     | 1.70        | 16     | 1     |
| 1:A:20:TYR:C     | 1:A:122:LEU:HD23 | 0.64     | 2.17        | 13     | 2     |
| 1:A:125:THR:HG22 | 1:A:126:PRO:HD2  | 0.63     | 1.70        | 19     | 2     |
| 1:A:127:GLU:O    | 1:A:128:VAL:HG12 | 0.63     | 1.93        | 6      | 2     |
| 1:A:39:LEU:HD13  | 1:A:118:VAL:HG21 | 0.63     | 1.70        | 6      | 1     |
| 1:A:95:LEU:HD23  | 1:A:95:LEU:N     | 0.63     | 2.09        | 8      | 5     |
| 1:A:22:LEU:HD11  | 1:A:128:VAL:HG13 | 0.63     | 1.71        | 19     | 1     |
| 1:A:22:LEU:HD21  | 1:A:133:LEU:CD2  | 0.62     | 2.24        | 12     | 2     |
| 1:A:15:VAL:HG11  | 1:A:103:LEU:CD1  | 0.62     | 2.24        | 16     | 1     |
| 1:A:78:ILE:HD12  | 1:A:78:ILE:N     | 0.62     | 2.08        | 3      | 2     |
| 1:A:38:PRO:O     | 1:A:87:LEU:HD21  | 0.62     | 1.93        | 7      | 3     |
| 1:A:116:SER:O    | 1:A:118:VAL:HG22 | 0.62     | 1.95        | 18     | 1     |
| 1:A:32:LEU:HD11  | 1:A:39:LEU:HD23  | 0.62     | 1.70        | 9      | 1     |
| 1:A:54:LEU:HD23  | 1:A:56:ILE:CG1   | 0.62     | 2.25        | 2      | 1     |
| 1:A:39:LEU:CD1   | 1:A:118:VAL:HG11 | 0.61     | 2.23        | 7      | 2     |
| 1:A:18:THR:HG23  | 1:A:45:GLU:OE1   | 0.61     | 1.95        | 13     | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:31:LEU:HD12  | 1:A:118:VAL:CG2  | 0.61     | 2.25        | 16     | 1     |
| 1:A:37:ALA:HB1   | 1:A:40:ARG:CB    | 0.61     | 2.25        | 11     | 2     |
| 1:A:73:ALA:HA    | 1:A:84:ILE:HG22  | 0.61     | 1.72        | 8      | 11    |
| 1:A:45:GLU:OE1   | 1:A:57:LEU:HD12  | 0.61     | 1.95        | 5      | 1     |
| 1:A:43:VAL:HG21  | 1:A:122:LEU:HD21 | 0.61     | 1.72        | 6      | 2     |
| 1:A:26:ALA:N     | 1:A:145:MET:HE2  | 0.61     | 2.10        | 20     | 1     |
| 1:A:15:VAL:HG23  | 1:A:48:PRO:HD3   | 0.61     | 1.71        | 1      | 1     |
| 1:A:33:ASP:O     | 1:A:37:ALA:HB2   | 0.61     | 1.96        | 8      | 6     |
| 1:A:12:ILE:HD13  | 1:A:82:PHE:CZ    | 0.60     | 2.31        | 8      | 1     |
| 1:A:81:VAL:HG13  | 1:A:93:LEU:HD13  | 0.60     | 1.72        | 11     | 1     |
| 1:A:121:CYS:C    | 1:A:122:LEU:HD12 | 0.60     | 2.21        | 18     | 1     |
| 1:A:93:LEU:N     | 1:A:93:LEU:HD23  | 0.60     | 2.11        | 20     | 2     |
| 1:A:103:LEU:C    | 1:A:103:LEU:HD22 | 0.60     | 2.21        | 13     | 2     |
| 1:A:22:LEU:C     | 1:A:22:LEU:HD13  | 0.60     | 2.22        | 20     | 2     |
| 1:A:19:TRP:C     | 1:A:122:LEU:HD12 | 0.60     | 2.21        | 11     | 1     |
| 1:A:39:LEU:HD21  | 1:A:89:GLU:OE2   | 0.60     | 1.96        | 8      | 1     |
| 1:A:103:LEU:C    | 1:A:103:LEU:HD13 | 0.60     | 2.22        | 9      | 3     |
| 1:A:22:LEU:HD12  | 1:A:127:GLU:O    | 0.59     | 1.97        | 14     | 2     |
| 1:A:22:LEU:HD13  | 1:A:128:VAL:HG12 | 0.59     | 1.74        | 18     | 1     |
| 1:A:156:LEU:C    | 1:A:156:LEU:HD23 | 0.59     | 2.23        | 6      | 1     |
| 1:A:143:LEU:HD23 | 1:A:143:LEU:N    | 0.59     | 2.12        | 15     | 1     |
| 1:A:38:PRO:CB    | 1:A:87:LEU:HD13  | 0.59     | 2.27        | 17     | 1     |
| 1:A:46:LEU:CD1   | 1:A:54:LEU:HD11  | 0.59     | 2.27        | 4      | 1     |
| 1:A:128:VAL:HG13 | 1:A:128:VAL:O    | 0.59     | 1.97        | 16     | 1     |
| 1:A:31:LEU:HD12  | 1:A:39:LEU:HD23  | 0.59     | 1.74        | 19     | 1     |
| 1:A:29:ILE:HG22  | 1:A:33:ASP:HB3   | 0.59     | 1.75        | 6      | 1     |
| 1:A:129:ASP:CG   | 1:A:132:ALA:HB3  | 0.59     | 2.23        | 21     | 1     |
| 1:A:127:GLU:C    | 1:A:128:VAL:HG23 | 0.58     | 2.23        | 8      | 2     |
| 1:A:22:LEU:HD21  | 1:A:128:VAL:HG13 | 0.58     | 1.75        | 17     | 1     |
| 1:A:84:ILE:HD11  | 1:A:89:GLU:O     | 0.58     | 1.97        | 11     | 4     |
| 1:A:156:LEU:C    | 1:A:156:LEU:HD12 | 0.58     | 2.24        | 14     | 1     |
| 1:A:26:ALA:O     | 1:A:147:ILE:HG22 | 0.58     | 1.98        | 15     | 2     |
| 1:A:37:ALA:HB1   | 1:A:40:ARG:HB2   | 0.58     | 1.76        | 20     | 4     |
| 1:A:56:ILE:HD12  | 1:A:71:ILE:O     | 0.58     | 1.98        | 13     | 1     |
| 1:A:80:ALA:O     | 1:A:94:VAL:HG23  | 0.58     | 1.98        | 18     | 5     |
| 1:A:118:VAL:HG13 | 1:A:118:VAL:O    | 0.57     | 1.99        | 21     | 4     |
| 1:A:22:LEU:C     | 1:A:22:LEU:HD23  | 0.57     | 2.24        | 5      | 3     |
| 1:A:7:MET:HE2    | 1:A:99:TYR:OH    | 0.57     | 1.99        | 9      | 1     |
| 1:A:143:LEU:N    | 1:A:143:LEU:HD23 | 0.57     | 2.14        | 8      | 7     |
| 1:A:84:ILE:HD11  | 1:A:89:GLU:OE1   | 0.57     | 1.99        | 21     | 1     |
| 1:A:10:LEU:CD1   | 1:A:94:VAL:HG11  | 0.57     | 2.29        | 19     | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:89:GLU:OE2   | 1:A:107:MET:HE2  | 0.57     | 1.99        | 6      | 1     |
| 1:A:26:ALA:HB2   | 1:A:118:VAL:CG2  | 0.57     | 2.30        | 5      | 2     |
| 1:A:152:ASN:O    | 1:A:156:LEU:HD23 | 0.57     | 2.00        | 7      | 1     |
| 1:A:81:VAL:O     | 1:A:81:VAL:HG13  | 0.57     | 2.00        | 9      | 1     |
| 1:A:39:LEU:O     | 1:A:39:LEU:HD13  | 0.56     | 2.01        | 2      | 2     |
| 1:A:32:LEU:HD22  | 1:A:149:LEU:HD13 | 0.56     | 1.77        | 10     | 1     |
| 1:A:39:LEU:HD21  | 1:A:118:VAL:CG2  | 0.56     | 2.31        | 18     | 2     |
| 1:A:41:VAL:HG21  | 1:A:58:LEU:HD22  | 0.56     | 1.77        | 5      | 1     |
| 1:A:84:ILE:HD13  | 1:A:84:ILE:H     | 0.56     | 1.59        | 11     | 2     |
| 1:A:22:LEU:CD2   | 1:A:132:ALA:HB3  | 0.56     | 2.31        | 19     | 1     |
| 1:A:7:MET:SD     | 1:A:97:THR:HG22  | 0.55     | 2.41        | 10     | 1     |
| 1:A:31:LEU:HD22  | 1:A:39:LEU:CD2   | 0.55     | 2.31        | 7      | 1     |
| 1:A:31:LEU:HD13  | 1:A:118:VAL:HG11 | 0.55     | 1.76        | 9      | 1     |
| 1:A:6:THR:O      | 1:A:80:ALA:HB1   | 0.55     | 2.01        | 11     | 1     |
| 1:A:24:MET:HE1   | 1:A:41:VAL:O     | 0.55     | 2.00        | 1      | 5     |
| 1:A:78:ILE:HB    | 1:A:81:VAL:HG22  | 0.55     | 1.77        | 15     | 1     |
| 1:A:29:ILE:CG2   | 1:A:147:ILE:HD13 | 0.55     | 2.22        | 12     | 1     |
| 1:A:39:LEU:HG    | 1:A:118:VAL:HG11 | 0.55     | 1.78        | 11     | 1     |
| 1:A:15:VAL:HG13  | 1:A:19:TRP:CZ2   | 0.55     | 2.37        | 3      | 2     |
| 1:A:46:LEU:HD22  | 1:A:46:LEU:N     | 0.55     | 2.17        | 15     | 1     |
| 1:A:31:LEU:C     | 1:A:37:ALA:HB1   | 0.54     | 2.26        | 1      | 3     |
| 1:A:24:MET:SD    | 1:A:32:LEU:HD11  | 0.54     | 2.42        | 19     | 1     |
| 1:A:21:SER:HA    | 1:A:122:LEU:HD23 | 0.54     | 1.78        | 17     | 2     |
| 1:A:87:LEU:HD13  | 1:A:89:GLU:OE2   | 0.54     | 2.02        | 21     | 1     |
| 1:A:43:VAL:HG11  | 1:A:122:LEU:CD1  | 0.54     | 2.31        | 6      | 1     |
| 1:A:31:LEU:HD22  | 1:A:39:LEU:HD12  | 0.54     | 1.79        | 4      | 2     |
| 1:A:84:ILE:HD13  | 1:A:84:ILE:N     | 0.54     | 2.17        | 11     | 2     |
| 1:A:38:PRO:CB    | 1:A:87:LEU:HD12  | 0.54     | 2.32        | 20     | 1     |
| 1:A:38:PRO:HB3   | 1:A:87:LEU:HD13  | 0.54     | 1.79        | 17     | 1     |
| 1:A:19:TRP:CZ3   | 1:A:103:LEU:HD12 | 0.53     | 2.37        | 2      | 2     |
| 1:A:151:PHE:CB   | 1:A:156:LEU:HD12 | 0.53     | 2.33        | 6      | 1     |
| 1:A:22:LEU:HD12  | 1:A:123:VAL:HG21 | 0.53     | 1.78        | 21     | 1     |
| 1:A:46:LEU:HD11  | 1:A:56:ILE:HG23  | 0.53     | 1.78        | 15     | 2     |
| 1:A:86:ALA:C     | 1:A:87:LEU:HD23  | 0.53     | 2.29        | 14     | 1     |
| 1:A:147:ILE:HG23 | 1:A:147:ILE:O    | 0.53     | 2.04        | 7      | 3     |
| 1:A:7:MET:HE1    | 1:A:10:LEU:HA    | 0.53     | 1.79        | 19     | 1     |
| 1:A:105:PHE:CE1  | 1:A:122:LEU:HD12 | 0.53     | 2.39        | 13     | 1     |
| 1:A:121:CYS:O    | 1:A:122:LEU:HD12 | 0.52     | 2.04        | 8      | 1     |
| 1:A:92:VAL:C     | 1:A:93:LEU:HD22  | 0.52     | 2.30        | 4      | 2     |
| 1:A:97:THR:HG21  | 1:A:103:LEU:HD12 | 0.52     | 1.80        | 14     | 1     |
| 1:A:12:ILE:HG22  | 1:A:48:PRO:HG2   | 0.52     | 1.81        | 1      | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:49:THR:HG1   | 1:A:53:ASP:CG    | 0.52     | 2.13        | 8      | 1     |
| 1:A:14:LYS:CD    | 1:A:99:TYR:CE1   | 0.52     | 2.92        | 16     | 1     |
| 1:A:12:ILE:HD12  | 1:A:82:PHE:CZ    | 0.52     | 2.39        | 11     | 1     |
| 1:A:156:LEU:O    | 1:A:156:LEU:HD23 | 0.52     | 2.05        | 10     | 1     |
| 1:A:10:LEU:HD21  | 1:A:80:ALA:HA    | 0.52     | 1.81        | 11     | 1     |
| 1:A:57:LEU:HD23  | 1:A:69:LYS:O     | 0.52     | 2.04        | 2      | 1     |
| 1:A:105:PHE:CE2  | 1:A:120:GLN:CG   | 0.52     | 2.93        | 10     | 1     |
| 1:A:105:PHE:CE1  | 1:A:122:LEU:HD11 | 0.52     | 2.40        | 17     | 1     |
| 1:A:97:THR:O     | 1:A:102:TYR:CE1  | 0.52     | 2.63        | 8      | 1     |
| 1:A:149:LEU:HD12 | 1:A:151:PHE:CE1  | 0.52     | 2.40        | 11     | 1     |
| 1:A:19:TRP:CE3   | 1:A:103:LEU:HD23 | 0.51     | 2.39        | 4      | 1     |
| 1:A:29:ILE:HA    | 1:A:147:ILE:HG21 | 0.51     | 1.81        | 15     | 1     |
| 1:A:37:ALA:HB3   | 1:A:40:ARG:HB2   | 0.51     | 1.82        | 7      | 1     |
| 1:A:76:THR:HG22  | 1:A:76:THR:O     | 0.51     | 2.04        | 18     | 1     |
| 1:A:44:GLU:OE2   | 1:A:57:LEU:HD22  | 0.51     | 2.05        | 2      | 1     |
| 1:A:22:LEU:HD11  | 1:A:128:VAL:HG22 | 0.51     | 1.82        | 10     | 1     |
| 1:A:84:ILE:HD12  | 1:A:92:VAL:CG2   | 0.51     | 2.36        | 16     | 1     |
| 1:A:14:LYS:NZ    | 1:A:99:TYR:CE2   | 0.51     | 2.79        | 17     | 1     |
| 1:A:82:PHE:N     | 1:A:82:PHE:CD1   | 0.51     | 2.78        | 20     | 1     |
| 1:A:18:THR:O     | 1:A:18:THR:HG23  | 0.51     | 2.05        | 5      | 2     |
| 1:A:29:ILE:HG22  | 1:A:33:ASP:HB2   | 0.51     | 1.83        | 2      | 2     |
| 1:A:105:PHE:CZ   | 1:A:120:GLN:CG   | 0.51     | 2.94        | 10     | 2     |
| 1:A:22:LEU:HD21  | 1:A:133:LEU:HD22 | 0.51     | 1.83        | 12     | 1     |
| 1:A:81:VAL:HG22  | 1:A:93:LEU:HD11  | 0.50     | 1.83        | 4      | 1     |
| 1:A:93:LEU:HD13  | 1:A:108:GLU:OE2  | 0.50     | 2.05        | 5      | 1     |
| 1:A:41:VAL:HG12  | 1:A:60:LYS:CB    | 0.50     | 2.36        | 9      | 1     |
| 1:A:26:ALA:HA    | 1:A:118:VAL:HG12 | 0.50     | 1.82        | 18     | 2     |
| 1:A:128:VAL:HG22 | 1:A:128:VAL:O    | 0.50     | 2.05        | 9      | 1     |
| 1:A:103:LEU:HD11 | 1:A:122:LEU:CB   | 0.50     | 2.36        | 13     | 1     |
| 1:A:39:LEU:HD21  | 1:A:118:VAL:CG1  | 0.50     | 2.29        | 3      | 1     |
| 1:A:104:LEU:HD22 | 1:A:121:CYS:SG   | 0.50     | 2.46        | 2      | 1     |
| 1:A:107:MET:O    | 1:A:118:VAL:HG12 | 0.50     | 2.06        | 13     | 1     |
| 1:A:151:PHE:N    | 1:A:151:PHE:CD1  | 0.50     | 2.80        | 16     | 3     |
| 1:A:10:LEU:HD23  | 1:A:10:LEU:C     | 0.50     | 2.32        | 19     | 1     |
| 1:A:151:PHE:HB3  | 1:A:156:LEU:HD12 | 0.50     | 1.84        | 6      | 2     |
| 1:A:28:ASP:HB3   | 1:A:31:LEU:HD22  | 0.50     | 1.84        | 8      | 1     |
| 1:A:43:VAL:HG11  | 1:A:122:LEU:HD21 | 0.50     | 1.83        | 12     | 2     |
| 1:A:15:VAL:HG11  | 1:A:103:LEU:HD13 | 0.50     | 1.83        | 8      | 2     |
| 1:A:28:ASP:OD2   | 1:A:31:LEU:HD13  | 0.50     | 2.07        | 8      | 1     |
| 1:A:56:ILE:O     | 1:A:58:LEU:HD23  | 0.49     | 2.07        | 13     | 1     |
| 1:A:8:LYS:H      | 1:A:80:ALA:HB2   | 0.49     | 1.66        | 1      | 3     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:7:MET:SD     | 1:A:10:LEU:HD12  | 0.49     | 2.47        | 19     | 1     |
| 1:A:48:PRO:HG3   | 1:A:54:LEU:HD12  | 0.49     | 1.85        | 2      | 1     |
| 1:A:32:LEU:HD12  | 1:A:32:LEU:O     | 0.49     | 2.07        | 6      | 1     |
| 1:A:39:LEU:CD1   | 1:A:118:VAL:HG21 | 0.49     | 2.38        | 2      | 3     |
| 1:A:31:LEU:HD13  | 1:A:39:LEU:HD13  | 0.49     | 1.85        | 6      | 1     |
| 1:A:143:LEU:CB   | 1:A:144:PRO:CD   | 0.49     | 2.90        | 2      | 6     |
| 1:A:123:VAL:HG21 | 1:A:127:GLU:HA   | 0.49     | 1.83        | 17     | 1     |
| 1:A:21:SER:HB3   | 1:A:24:MET:HE3   | 0.49     | 1.85        | 21     | 1     |
| 1:A:31:LEU:HD22  | 1:A:39:LEU:HD13  | 0.49     | 1.84        | 3      | 1     |
| 1:A:78:ILE:HB    | 1:A:81:VAL:HG12  | 0.49     | 1.85        | 18     | 3     |
| 1:A:128:VAL:O    | 1:A:128:VAL:HG23 | 0.49     | 2.08        | 20     | 1     |
| 1:A:10:LEU:HD23  | 1:A:79:PRO:O     | 0.49     | 2.07        | 15     | 1     |
| 1:A:12:ILE:HD12  | 1:A:82:PHE:HZ    | 0.48     | 1.67        | 11     | 1     |
| 1:A:103:LEU:N    | 1:A:103:LEU:CD1  | 0.48     | 2.76        | 13     | 1     |
| 1:A:21:SER:O     | 1:A:156:LEU:HD21 | 0.48     | 2.08        | 16     | 1     |
| 1:A:7:MET:HB3    | 1:A:80:ALA:HB2   | 0.48     | 1.85        | 21     | 1     |
| 1:A:125:THR:N    | 1:A:126:PRO:CD   | 0.48     | 2.76        | 8      | 1     |
| 1:A:14:LYS:CD    | 1:A:99:TYR:CD1   | 0.48     | 2.96        | 12     | 1     |
| 1:A:81:VAL:HG23  | 1:A:93:LEU:HD21  | 0.48     | 1.84        | 9      | 1     |
| 1:A:43:VAL:HG22  | 1:A:58:LEU:CD1   | 0.48     | 2.38        | 16     | 1     |
| 1:A:84:ILE:N     | 1:A:84:ILE:CD1   | 0.48     | 2.77        | 16     | 1     |
| 1:A:32:LEU:HD21  | 1:A:149:LEU:HG   | 0.48     | 1.84        | 19     | 1     |
| 1:A:104:LEU:HD11 | 1:A:121:CYS:SG   | 0.48     | 2.49        | 7      | 2     |
| 1:A:21:SER:CB    | 1:A:24:MET:HE3   | 0.48     | 2.38        | 21     | 1     |
| 1:A:22:LEU:HD11  | 1:A:133:LEU:HD12 | 0.48     | 1.86        | 20     | 1     |
| 1:A:41:VAL:HG23  | 1:A:41:VAL:O     | 0.48     | 2.08        | 10     | 1     |
| 1:A:103:LEU:HD22 | 1:A:103:LEU:O    | 0.48     | 2.09        | 13     | 1     |
| 1:A:54:LEU:HD23  | 1:A:56:ILE:HG12  | 0.48     | 1.84        | 2      | 1     |
| 1:A:116:SER:O    | 1:A:118:VAL:HG12 | 0.48     | 2.08        | 7      | 1     |
| 1:A:19:TRP:C     | 1:A:20:TYR:CD1   | 0.48     | 2.92        | 2      | 5     |
| 1:A:125:THR:CB   | 1:A:126:PRO:CD   | 0.48     | 2.92        | 2      | 8     |
| 1:A:41:VAL:CG1   | 1:A:58:LEU:HD13  | 0.47     | 2.39        | 1      | 1     |
| 1:A:31:LEU:CD1   | 1:A:118:VAL:CG2  | 0.47     | 2.92        | 6      | 2     |
| 1:A:32:LEU:HD23  | 1:A:40:ARG:HB2   | 0.47     | 1.85        | 9      | 1     |
| 1:A:17:GLY:O     | 1:A:19:TRP:CD1   | 0.47     | 2.68        | 11     | 2     |
| 1:A:81:VAL:HG22  | 1:A:93:LEU:CG    | 0.47     | 2.39        | 5      | 1     |
| 1:A:19:TRP:CH2   | 1:A:103:LEU:HD12 | 0.47     | 2.44        | 13     | 1     |
| 1:A:150:SER:C    | 1:A:151:PHE:CD1  | 0.47     | 2.92        | 13     | 1     |
| 1:A:7:MET:HE3    | 1:A:9:GLY:O      | 0.47     | 2.08        | 20     | 1     |
| 1:A:23:ALA:HB1   | 1:A:149:LEU:O    | 0.47     | 2.09        | 3      | 1     |
| 1:A:27:SER:O     | 1:A:146:HIS:CG   | 0.47     | 2.67        | 21     | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:105:PHE:CD1  | 1:A:105:PHE:N    | 0.47     | 2.81        | 13     | 2     |
| 1:A:14:LYS:HD2   | 1:A:99:TYR:CE1   | 0.47     | 2.45        | 16     | 1     |
| 1:A:26:ALA:CA    | 1:A:145:MET:HE2  | 0.47     | 2.39        | 20     | 1     |
| 1:A:78:ILE:N     | 1:A:78:ILE:CD1   | 0.47     | 2.77        | 17     | 2     |
| 1:A:79:PRO:O     | 1:A:82:PHE:CZ    | 0.47     | 2.68        | 17     | 3     |
| 1:A:71:ILE:HD11  | 1:A:87:LEU:HD13  | 0.47     | 1.85        | 5      | 1     |
| 1:A:105:PHE:CZ   | 1:A:120:GLN:CD   | 0.47     | 2.93        | 19     | 1     |
| 1:A:143:LEU:HD12 | 1:A:145:MET:CE   | 0.47     | 2.40        | 4      | 1     |
| 1:A:143:LEU:HD23 | 1:A:144:PRO:HD2  | 0.47     | 1.87        | 18     | 2     |
| 1:A:19:TRP:CH2   | 1:A:99:TYR:O     | 0.47     | 2.67        | 5      | 5     |
| 1:A:98:ASP:CG    | 1:A:102:TYR:CE2  | 0.47     | 2.92        | 5      | 1     |
| 1:A:31:LEU:HD13  | 1:A:118:VAL:HG21 | 0.47     | 1.87        | 6      | 1     |
| 1:A:39:LEU:HD21  | 1:A:89:GLU:CD    | 0.47     | 2.35        | 8      | 1     |
| 1:A:26:ALA:HB2   | 1:A:118:VAL:HG12 | 0.47     | 1.84        | 9      | 1     |
| 1:A:41:VAL:HG11  | 1:A:58:LEU:HD21  | 0.47     | 1.86        | 16     | 1     |
| 1:A:10:LEU:HD22  | 1:A:12:ILE:HD13  | 0.47     | 1.86        | 19     | 1     |
| 1:A:12:ILE:HG22  | 1:A:48:PRO:CB    | 0.47     | 2.39        | 19     | 1     |
| 1:A:57:LEU:HD12  | 1:A:70:LYS:HB3   | 0.47     | 1.86        | 19     | 1     |
| 1:A:38:PRO:CA    | 1:A:87:LEU:CD1   | 0.47     | 2.92        | 20     | 1     |
| 1:A:19:TRP:CZ2   | 1:A:99:TYR:O     | 0.47     | 2.68        | 20     | 2     |
| 1:A:32:LEU:CD1   | 1:A:40:ARG:N     | 0.47     | 2.78        | 7      | 1     |
| 1:A:16:ALA:HB1   | 1:A:47:LYS:HG3   | 0.47     | 1.86        | 21     | 3     |
| 1:A:92:VAL:C     | 1:A:93:LEU:HD23  | 0.47     | 2.35        | 20     | 1     |
| 1:A:81:VAL:HG23  | 1:A:93:LEU:CD2   | 0.47     | 2.40        | 2      | 2     |
| 1:A:22:LEU:HD13  | 1:A:127:GLU:O    | 0.47     | 2.09        | 9      | 1     |
| 1:A:28:ASP:HB3   | 1:A:31:LEU:HD13  | 0.47     | 1.86        | 1      | 1     |
| 1:A:24:MET:CB    | 1:A:32:LEU:HD21  | 0.47     | 2.40        | 14     | 1     |
| 1:A:39:LEU:CD2   | 1:A:118:VAL:CG1  | 0.47     | 2.93        | 16     | 1     |
| 1:A:84:ILE:CD1   | 1:A:88:ASN:ND2   | 0.47     | 2.78        | 20     | 1     |
| 1:A:18:THR:O     | 1:A:19:TRP:CG    | 0.47     | 2.68        | 21     | 1     |
| 1:A:46:LEU:HD12  | 1:A:56:ILE:HG13  | 0.46     | 1.86        | 9      | 1     |
| 1:A:24:MET:HE3   | 1:A:151:PHE:CE1  | 0.46     | 2.44        | 17     | 1     |
| 1:A:156:LEU:HD23 | 1:A:156:LEU:O    | 0.46     | 2.10        | 6      | 1     |
| 1:A:14:LYS:CB    | 1:A:99:TYR:CD1   | 0.46     | 2.98        | 13     | 1     |
| 1:A:103:LEU:N    | 1:A:103:LEU:HD13 | 0.46     | 2.25        | 13     | 1     |
| 1:A:79:PRO:O     | 1:A:82:PHE:CE1   | 0.46     | 2.68        | 8      | 1     |
| 1:A:31:LEU:O     | 1:A:32:LEU:HD12  | 0.46     | 2.10        | 7      | 1     |
| 1:A:103:LEU:C    | 1:A:103:LEU:HD23 | 0.46     | 2.36        | 16     | 1     |
| 1:A:152:ASN:CB   | 1:A:153:PRO:CD   | 0.46     | 2.93        | 5      | 2     |
| 1:A:94:VAL:HG13  | 1:A:104:LEU:O    | 0.46     | 2.11        | 10     | 2     |
| 1:A:103:LEU:C    | 1:A:104:LEU:HD23 | 0.46     | 2.36        | 14     | 2     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:76:THR:CG2   | 1:A:81:VAL:HG13  | 0.46     | 2.40        | 18     | 1     |
| 1:A:25:ALA:HB2   | 1:A:148:ARG:HG3  | 0.46     | 1.87        | 21     | 1     |
| 1:A:31:LEU:CB    | 1:A:39:LEU:HD13  | 0.46     | 2.38        | 3      | 1     |
| 1:A:10:LEU:HD23  | 1:A:12:ILE:N     | 0.46     | 2.26        | 19     | 1     |
| 1:A:39:LEU:HD21  | 1:A:89:GLU:OE1   | 0.46     | 2.11        | 11     | 1     |
| 1:A:22:LEU:CD2   | 1:A:132:ALA:CB   | 0.46     | 2.93        | 19     | 1     |
| 1:A:79:PRO:O     | 1:A:82:PHE:CE2   | 0.46     | 2.68        | 15     | 3     |
| 1:A:125:THR:N    | 1:A:126:PRO:HD3  | 0.46     | 2.25        | 8      | 1     |
| 1:A:112:GLU:N    | 1:A:113:PRO:CD   | 0.46     | 2.79        | 19     | 1     |
| 1:A:21:SER:HB3   | 1:A:43:VAL:HG12  | 0.46     | 1.87        | 14     | 2     |
| 1:A:122:LEU:HD12 | 1:A:122:LEU:N    | 0.46     | 2.26        | 14     | 1     |
| 1:A:105:PHE:CE1  | 1:A:120:GLN:CG   | 0.46     | 2.98        | 16     | 1     |
| 1:A:6:THR:O      | 1:A:6:THR:HG23   | 0.45     | 2.12        | 11     | 1     |
| 1:A:76:THR:HG21  | 1:A:81:VAL:HG13  | 0.45     | 1.88        | 18     | 2     |
| 1:A:11:ASP:O     | 1:A:13:GLN:N     | 0.45     | 2.49        | 16     | 11    |
| 1:A:58:LEU:HD21  | 1:A:71:ILE:CD1   | 0.45     | 2.41        | 3      | 1     |
| 1:A:104:LEU:N    | 1:A:104:LEU:HD23 | 0.45     | 2.26        | 11     | 1     |
| 1:A:49:THR:HG22  | 1:A:50:PRO:HD2   | 0.45     | 1.87        | 13     | 3     |
| 1:A:143:LEU:CB   | 1:A:144:PRO:HD2  | 0.45     | 2.41        | 16     | 14    |
| 1:A:32:LEU:HD11  | 1:A:40:ARG:N     | 0.45     | 2.26        | 7      | 1     |
| 1:A:93:LEU:CD2   | 1:A:93:LEU:N     | 0.45     | 2.78        | 13     | 2     |
| 1:A:105:PHE:CZ   | 1:A:120:GLN:HG2  | 0.45     | 2.45        | 13     | 1     |
| 1:A:105:PHE:CZ   | 1:A:120:GLN:NE2  | 0.45     | 2.83        | 19     | 1     |
| 1:A:57:LEU:HD22  | 1:A:70:LYS:CB    | 0.45     | 2.42        | 18     | 1     |
| 1:A:19:TRP:CZ3   | 1:A:103:LEU:HD23 | 0.45     | 2.46        | 21     | 1     |
| 1:A:58:LEU:HD11  | 1:A:71:ILE:CD1   | 0.45     | 2.41        | 14     | 1     |
| 1:A:42:TYR:CE2   | 1:A:44:GLU:OE2   | 0.45     | 2.70        | 9      | 1     |
| 1:A:48:PRO:HG3   | 1:A:54:LEU:HD13  | 0.45     | 1.89        | 8      | 1     |
| 1:A:20:TYR:O     | 1:A:122:LEU:HD13 | 0.45     | 2.11        | 11     | 1     |
| 1:A:26:ALA:CA    | 1:A:118:VAL:HG12 | 0.45     | 2.42        | 18     | 1     |
| 1:A:95:LEU:N     | 1:A:95:LEU:CD2   | 0.45     | 2.78        | 8      | 2     |
| 1:A:78:ILE:O     | 1:A:78:ILE:HG23  | 0.45     | 2.10        | 5      | 1     |
| 1:A:76:THR:HG23  | 1:A:81:VAL:HG13  | 0.45     | 1.88        | 8      | 1     |
| 1:A:32:LEU:HD13  | 1:A:40:ARG:HG2   | 0.45     | 1.88        | 16     | 1     |
| 1:A:22:LEU:HD23  | 1:A:22:LEU:O     | 0.45     | 2.12        | 21     | 1     |
| 1:A:140:LEU:O    | 1:A:143:LEU:HD12 | 0.45     | 2.12        | 21     | 2     |
| 1:A:143:LEU:HB3  | 1:A:144:PRO:CD   | 0.45     | 2.42        | 2      | 2     |
| 1:A:43:VAL:CG1   | 1:A:122:LEU:HD11 | 0.45     | 2.38        | 6      | 1     |
| 1:A:109:ASN:C    | 1:A:110:SER:HG   | 0.45     | 2.19        | 7      | 1     |
| 1:A:31:LEU:HD13  | 1:A:39:LEU:CD1   | 0.45     | 2.42        | 4      | 1     |
| 1:A:105:PHE:CZ   | 1:A:120:GLN:HG3  | 0.45     | 2.47        | 10     | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:143:LEU:N    | 1:A:143:LEU:CD2  | 0.45     | 2.78        | 10     | 1     |
| 1:A:14:LYS:HD2   | 1:A:99:TYR:CG    | 0.44     | 2.47        | 12     | 2     |
| 1:A:39:LEU:HD22  | 1:A:118:VAL:CG1  | 0.44     | 2.40        | 6      | 1     |
| 1:A:105:PHE:CE1  | 1:A:120:GLN:HG3  | 0.44     | 2.47        | 16     | 1     |
| 1:A:11:ASP:OD2   | 1:A:99:TYR:CZ    | 0.44     | 2.70        | 19     | 1     |
| 1:A:32:LEU:HB2   | 1:A:147:ILE:HD13 | 0.44     | 1.87        | 20     | 1     |
| 1:A:19:TRP:CZ3   | 1:A:103:LEU:HB2  | 0.44     | 2.48        | 5      | 1     |
| 1:A:39:LEU:HD11  | 1:A:118:VAL:CG1  | 0.44     | 2.42        | 5      | 1     |
| 1:A:125:THR:CB   | 1:A:126:PRO:HD3  | 0.44     | 2.42        | 20     | 6     |
| 1:A:46:LEU:HD23  | 1:A:56:ILE:HA    | 0.44     | 1.88        | 3      | 2     |
| 1:A:41:VAL:CG1   | 1:A:58:LEU:HD21  | 0.44     | 2.42        | 16     | 1     |
| 1:A:20:TYR:CD1   | 1:A:20:TYR:N     | 0.44     | 2.86        | 20     | 1     |
| 1:A:38:PRO:CB    | 1:A:87:LEU:CD1   | 0.44     | 2.95        | 20     | 1     |
| 1:A:121:CYS:SG   | 1:A:136:PHE:CD1  | 0.44     | 3.10        | 1      | 2     |
| 1:A:79:PRO:O     | 1:A:80:ALA:HB2   | 0.44     | 2.13        | 5      | 1     |
| 1:A:152:ASN:O    | 1:A:156:LEU:N    | 0.44     | 2.51        | 9      | 1     |
| 1:A:121:CYS:HB2  | 1:A:136:PHE:CD1  | 0.44     | 2.48        | 7      | 4     |
| 1:A:56:ILE:HG22  | 1:A:58:LEU:HD22  | 0.44     | 1.89        | 15     | 1     |
| 1:A:127:GLU:O    | 1:A:128:VAL:CG1  | 0.44     | 2.66        | 4      | 2     |
| 1:A:93:LEU:N     | 1:A:93:LEU:HD22  | 0.44     | 2.27        | 13     | 1     |
| 1:A:57:LEU:C     | 1:A:57:LEU:HD13  | 0.44     | 2.38        | 20     | 1     |
| 1:A:29:ILE:O     | 1:A:33:ASP:N     | 0.43     | 2.51        | 16     | 3     |
| 1:A:125:THR:HG23 | 1:A:127:GLU:O    | 0.43     | 2.13        | 5      | 1     |
| 1:A:109:ASN:O    | 1:A:111:ALA:N    | 0.43     | 2.52        | 7      | 7     |
| 1:A:149:LEU:HD22 | 1:A:149:LEU:N    | 0.43     | 2.29        | 6      | 1     |
| 1:A:95:LEU:HD11  | 1:A:104:LEU:CB   | 0.43     | 2.40        | 20     | 2     |
| 1:A:98:ASP:OD1   | 1:A:102:TYR:CZ   | 0.43     | 2.71        | 15     | 1     |
| 1:A:32:LEU:HD12  | 1:A:32:LEU:N     | 0.43     | 2.28        | 4      | 1     |
| 1:A:25:ALA:HB3   | 1:A:140:LEU:HD21 | 0.43     | 1.89        | 21     | 2     |
| 1:A:121:CYS:SG   | 1:A:136:PHE:CG   | 0.43     | 3.11        | 16     | 1     |
| 1:A:31:LEU:HB2   | 1:A:32:LEU:HD12  | 0.43     | 1.90        | 4      | 1     |
| 1:A:102:TYR:CD2  | 1:A:132:ALA:CB   | 0.43     | 3.01        | 8      | 1     |
| 1:A:102:TYR:CD1  | 1:A:102:TYR:C    | 0.43     | 2.94        | 10     | 2     |
| 1:A:22:LEU:HD13  | 1:A:132:ALA:HB3  | 0.43     | 1.91        | 1      | 2     |
| 1:A:23:ALA:CB    | 1:A:136:PHE:CE2  | 0.43     | 3.02        | 5      | 1     |
| 1:A:110:SER:O    | 1:A:111:ALA:HB2  | 0.43     | 2.14        | 8      | 2     |
| 1:A:103:LEU:HD13 | 1:A:103:LEU:C    | 0.43     | 2.36        | 2      | 1     |
| 1:A:6:THR:O      | 1:A:8:LYS:N      | 0.43     | 2.52        | 5      | 6     |
| 1:A:127:GLU:C    | 1:A:128:VAL:CG2  | 0.43     | 2.92        | 8      | 1     |
| 1:A:152:ASN:O    | 1:A:156:LEU:CB   | 0.43     | 2.67        | 6      | 1     |
| 1:A:154:THR:O    | 1:A:155:GLN:CB   | 0.43     | 2.66        | 6      | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:93:LEU:N     | 1:A:93:LEU:CD2   | 0.43     | 2.79        | 20     | 2     |
| 1:A:25:ALA:C     | 1:A:145:MET:HE2  | 0.43     | 2.39        | 20     | 1     |
| 1:A:47:LYS:O     | 1:A:55:GLU:CB    | 0.43     | 2.67        | 14     | 13    |
| 1:A:104:LEU:HD22 | 1:A:136:PHE:CD1  | 0.43     | 2.49        | 4      | 1     |
| 1:A:78:ILE:O     | 1:A:80:ALA:N     | 0.43     | 2.49        | 14     | 5     |
| 1:A:22:LEU:HD21  | 1:A:133:LEU:HD12 | 0.43     | 1.90        | 1      | 1     |
| 1:A:48:PRO:CB    | 1:A:53:ASP:O     | 0.43     | 2.67        | 6      | 1     |
| 1:A:132:ALA:O    | 1:A:136:PHE:CB   | 0.43     | 2.67        | 17     | 2     |
| 1:A:7:MET:N      | 1:A:94:VAL:O     | 0.43     | 2.52        | 11     | 4     |
| 1:A:105:PHE:CD1  | 1:A:105:PHE:C    | 0.43     | 2.97        | 14     | 1     |
| 1:A:76:THR:O     | 1:A:77:LYS:CB    | 0.43     | 2.67        | 18     | 1     |
| 1:A:22:LEU:HD21  | 1:A:133:LEU:CD1  | 0.43     | 2.43        | 20     | 1     |
| 1:A:98:ASP:O     | 1:A:100:LYS:N    | 0.42     | 2.53        | 7      | 16    |
| 1:A:54:LEU:HD23  | 1:A:56:ILE:HD11  | 0.42     | 1.91        | 10     | 1     |
| 1:A:19:TRP:CZ3   | 1:A:124:ARG:N    | 0.42     | 2.87        | 13     | 1     |
| 1:A:32:LEU:O     | 1:A:37:ALA:CB    | 0.42     | 2.67        | 16     | 1     |
| 1:A:137:ASP:O    | 1:A:141:LYS:N    | 0.42     | 2.52        | 20     | 3     |
| 1:A:102:TYR:CD2  | 1:A:132:ALA:HB2  | 0.42     | 2.50        | 12     | 2     |
| 1:A:129:ASP:O    | 1:A:131:GLU:N    | 0.42     | 2.52        | 6      | 4     |
| 1:A:103:LEU:CD1  | 1:A:122:LEU:CB   | 0.42     | 2.97        | 13     | 1     |
| 1:A:113:PRO:O    | 1:A:115:GLN:N    | 0.42     | 2.52        | 21     | 2     |
| 1:A:104:LEU:HD22 | 1:A:121:CYS:HB3  | 0.42     | 1.90        | 16     | 1     |
| 1:A:143:LEU:O    | 1:A:145:MET:N    | 0.42     | 2.52        | 20     | 1     |
| 1:A:113:PRO:O    | 1:A:117:LEU:N    | 0.42     | 2.52        | 11     | 5     |
| 1:A:24:MET:O     | 1:A:149:LEU:N    | 0.42     | 2.53        | 8      | 2     |
| 1:A:103:LEU:HD11 | 1:A:122:LEU:HB3  | 0.42     | 1.90        | 13     | 1     |
| 1:A:39:LEU:O     | 1:A:39:LEU:CD1   | 0.42     | 2.68        | 19     | 1     |
| 1:A:140:LEU:HG   | 1:A:145:MET:HE3  | 0.42     | 1.90        | 19     | 1     |
| 1:A:101:LYS:CG   | 1:A:131:GLU:OE1  | 0.42     | 2.68        | 20     | 1     |
| 1:A:140:LEU:O    | 1:A:143:LEU:CD1  | 0.42     | 2.67        | 2      | 2     |
| 1:A:22:LEU:CD1   | 1:A:127:GLU:O    | 0.42     | 2.68        | 7      | 3     |
| 1:A:128:VAL:O    | 1:A:128:VAL:HG13 | 0.42     | 2.15        | 9      | 1     |
| 1:A:31:LEU:O     | 1:A:39:LEU:CB    | 0.42     | 2.68        | 10     | 3     |
| 1:A:6:THR:O      | 1:A:80:ALA:CB    | 0.42     | 2.68        | 16     | 5     |
| 1:A:19:TRP:CD1   | 1:A:19:TRP:N     | 0.42     | 2.87        | 14     | 1     |
| 1:A:7:MET:CE     | 1:A:99:TYR:OH    | 0.42     | 2.68        | 16     | 1     |
| 1:A:145:MET:O    | 1:A:146:HIS:CG   | 0.42     | 2.73        | 18     | 1     |
| 1:A:96:ASP:C     | 1:A:97:THR:CG2   | 0.42     | 2.93        | 21     | 1     |
| 1:A:12:ILE:CG2   | 1:A:48:PRO:CG    | 0.42     | 2.95        | 1      | 1     |
| 1:A:81:VAL:O     | 1:A:82:PHE:CG    | 0.42     | 2.72        | 4      | 1     |
| 1:A:89:GLU:OE2   | 1:A:107:MET:HE3  | 0.42     | 2.13        | 8      | 1     |

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| Atom-1          | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|-----------------|------------------|----------|-------------|--------|-------|
|                 |                  |          |             | Worst  | Total |
| 1:A:42:TYR:CE1  | 1:A:156:LEU:HD11 | 0.42     | 2.50        | 9      | 1     |
| 1:A:44:GLU:OE2  | 1:A:59:GLN:CG    | 0.42     | 2.68        | 11     | 1     |
| 1:A:19:TRP:O    | 1:A:20:TYR:CG    | 0.42     | 2.73        | 15     | 1     |
| 1:A:42:TYR:CB   | 1:A:59:GLN:O     | 0.42     | 2.68        | 17     | 1     |
| 1:A:21:SER:O    | 1:A:156:LEU:CD1  | 0.42     | 2.68        | 18     | 1     |
| 1:A:84:ILE:CD1  | 1:A:89:GLU:O     | 0.42     | 2.68        | 1      | 1     |
| 1:A:125:THR:O   | 1:A:127:GLU:N    | 0.42     | 2.53        | 12     | 2     |
| 1:A:143:LEU:HB3 | 1:A:144:PRO:HD2  | 0.42     | 1.91        | 2      | 2     |
| 1:A:100:LYS:O   | 1:A:101:LYS:CD   | 0.42     | 2.68        | 4      | 1     |
| 1:A:18:THR:O    | 1:A:18:THR:CG2   | 0.42     | 2.68        | 5      | 1     |
| 1:A:27:SER:O    | 1:A:146:HIS:CB   | 0.42     | 2.68        | 9      | 3     |
| 1:A:27:SER:O    | 1:A:146:HIS:ND1  | 0.42     | 2.53        | 10     | 1     |
| 1:A:80:ALA:O    | 1:A:94:VAL:N     | 0.42     | 2.53        | 18     | 1     |
| 1:A:131:GLU:O   | 1:A:135:LYS:CE   | 0.42     | 2.68        | 1      | 2     |
| 1:A:117:LEU:C   | 1:A:117:LEU:HD13 | 0.42     | 2.39        | 7      | 1     |
| 1:A:102:TYR:CB  | 1:A:122:LEU:O    | 0.42     | 2.68        | 19     | 2     |
| 1:A:20:TYR:C    | 1:A:122:LEU:CD1  | 0.42     | 2.92        | 11     | 1     |
| 1:A:117:LEU:C   | 1:A:117:LEU:CD1  | 0.42     | 2.93        | 12     | 1     |
| 1:A:22:LEU:O    | 1:A:151:PHE:N    | 0.42     | 2.53        | 13     | 1     |
| 1:A:17:GLY:O    | 1:A:45:GLU:CG    | 0.42     | 2.68        | 16     | 2     |
| 1:A:95:LEU:CD1  | 1:A:104:LEU:CB   | 0.42     | 2.98        | 15     | 1     |
| 1:A:102:TYR:CZ  | 1:A:135:LYS:HD2  | 0.42     | 2.50        | 16     | 2     |
| 1:A:123:VAL:CG1 | 1:A:129:ASP:OD2  | 0.42     | 2.68        | 21     | 1     |
| 1:A:53:ASP:CB   | 1:A:73:ALA:O     | 0.42     | 2.68        | 2      | 2     |
| 1:A:22:LEU:C    | 1:A:22:LEU:CD2   | 0.42     | 2.93        | 5      | 2     |
| 1:A:126:PRO:C   | 1:A:127:GLU:CG   | 0.42     | 2.93        | 6      | 1     |
| 1:A:98:ASP:O    | 1:A:100:LYS:CG   | 0.42     | 2.67        | 9      | 2     |
| 1:A:101:LYS:O   | 1:A:124:ARG:N    | 0.42     | 2.53        | 9      | 1     |
| 1:A:14:LYS:HD3  | 1:A:99:TYR:CE1   | 0.42     | 2.50        | 16     | 1     |
| 1:A:31:LEU:CD1  | 1:A:118:VAL:HG21 | 0.42     | 2.45        | 16     | 1     |
| 1:A:39:LEU:O    | 1:A:41:VAL:N     | 0.42     | 2.53        | 18     | 1     |
| 1:A:22:LEU:HD12 | 1:A:123:VAL:HG11 | 0.42     | 1.91        | 3      | 1     |
| 1:A:75:LYS:O    | 1:A:76:THR:CG2   | 0.42     | 2.68        | 4      | 1     |
| 1:A:103:LEU:C   | 1:A:103:LEU:CD1  | 0.42     | 2.92        | 9      | 2     |
| 1:A:32:LEU:HD13 | 1:A:40:ARG:HA    | 0.42     | 1.90        | 14     | 1     |
| 1:A:103:LEU:C   | 1:A:103:LEU:CD2  | 0.42     | 2.92        | 13     | 2     |
| 1:A:14:LYS:HB3  | 1:A:99:TYR:CD1   | 0.42     | 2.50        | 7      | 1     |
| 1:A:95:LEU:HD11 | 1:A:119:CYS:SG   | 0.42     | 2.55        | 10     | 1     |
| 1:A:12:ILE:O    | 1:A:15:VAL:CG2   | 0.42     | 2.68        | 20     | 2     |
| 1:A:18:THR:O    | 1:A:124:ARG:CG   | 0.42     | 2.68        | 12     | 1     |
| 1:A:109:ASN:O   | 1:A:113:PRO:CD   | 0.42     | 2.68        | 12     | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:98:ASP:CG    | 1:A:102:TYR:CZ   | 0.42     | 2.98        | 21     | 1     |
| 1:A:82:PHE:CD1   | 1:A:82:PHE:N     | 0.41     | 2.87        | 5      | 1     |
| 1:A:102:TYR:OH   | 1:A:135:LYS:CD   | 0.41     | 2.68        | 21     | 4     |
| 1:A:28:ASP:CG    | 1:A:31:LEU:HD13  | 0.41     | 2.39        | 8      | 1     |
| 1:A:97:THR:HG23  | 1:A:99:TYR:CE1   | 0.41     | 2.50        | 16     | 1     |
| 1:A:12:ILE:CG2   | 1:A:48:PRO:HB3   | 0.41     | 2.45        | 19     | 1     |
| 1:A:46:LEU:HD12  | 1:A:55:GLU:O     | 0.41     | 2.15        | 4      | 1     |
| 1:A:32:LEU:O     | 1:A:32:LEU:CD1   | 0.41     | 2.68        | 6      | 1     |
| 1:A:41:VAL:HG23  | 1:A:58:LEU:HD13  | 0.41     | 1.86        | 11     | 1     |
| 1:A:44:GLU:CD    | 1:A:59:GLN:CG    | 0.41     | 2.93        | 11     | 1     |
| 1:A:15:VAL:O     | 1:A:17:GLY:N     | 0.41     | 2.53        | 13     | 2     |
| 1:A:22:LEU:HD13  | 1:A:23:ALA:CB    | 0.41     | 2.45        | 20     | 1     |
| 1:A:129:ASP:CG   | 1:A:132:ALA:CB   | 0.41     | 2.92        | 21     | 1     |
| 1:A:41:VAL:HG11  | 1:A:58:LEU:HD13  | 0.41     | 1.92        | 1      | 1     |
| 1:A:140:LEU:HD13 | 1:A:143:LEU:HD12 | 0.41     | 1.91        | 14     | 1     |
| 1:A:32:LEU:HD12  | 1:A:39:LEU:HD22  | 0.41     | 1.92        | 15     | 1     |
| 1:A:119:CYS:C    | 1:A:120:GLN:CG   | 0.41     | 2.93        | 18     | 1     |
| 1:A:129:ASP:C    | 1:A:131:GLU:N    | 0.41     | 2.78        | 8      | 2     |
| 1:A:31:LEU:O     | 1:A:37:ALA:CB    | 0.41     | 2.67        | 5      | 1     |
| 1:A:95:LEU:HD11  | 1:A:104:LEU:HD23 | 0.41     | 1.91        | 7      | 1     |
| 1:A:110:SER:OG   | 1:A:111:ALA:N    | 0.41     | 2.53        | 7      | 1     |
| 1:A:80:ALA:C     | 1:A:81:VAL:CG2   | 0.41     | 2.94        | 1      | 2     |
| 1:A:156:LEU:HD23 | 1:A:156:LEU:C    | 0.41     | 2.41        | 10     | 1     |
| 1:A:39:LEU:CD2   | 1:A:118:VAL:CG2  | 0.41     | 2.97        | 16     | 1     |
| 1:A:22:LEU:C     | 1:A:22:LEU:CD1   | 0.41     | 2.92        | 20     | 1     |
| 1:A:23:ALA:HB1   | 1:A:136:PHE:CE2  | 0.41     | 2.50        | 5      | 1     |
| 1:A:124:ARG:O    | 1:A:125:THR:CB   | 0.41     | 2.69        | 8      | 1     |
| 1:A:7:MET:HE3    | 1:A:9:GLY:C      | 0.41     | 2.40        | 20     | 1     |
| 1:A:60:LYS:O     | 1:A:67:ALA:N     | 0.41     | 2.53        | 20     | 2     |
| 1:A:14:LYS:HE3   | 1:A:99:TYR:CD2   | 0.41     | 2.50        | 5      | 1     |
| 1:A:24:MET:CE    | 1:A:41:VAL:O     | 0.41     | 2.68        | 12     | 2     |
| 1:A:46:LEU:HD12  | 1:A:56:ILE:HA    | 0.41     | 1.93        | 13     | 1     |
| 1:A:103:LEU:CD1  | 1:A:122:LEU:HB2  | 0.41     | 2.46        | 13     | 1     |
| 1:A:45:GLU:C     | 1:A:46:LEU:HD22  | 0.41     | 2.40        | 15     | 1     |
| 1:A:129:ASP:OD1  | 1:A:132:ALA:HB3  | 0.41     | 2.15        | 21     | 1     |
| 1:A:98:ASP:O     | 1:A:99:TYR:CB    | 0.41     | 2.69        | 4      | 1     |
| 1:A:152:ASN:OD1  | 1:A:153:PRO:CD   | 0.41     | 2.69        | 11     | 1     |
| 1:A:78:ILE:HG22  | 1:A:80:ALA:H     | 0.41     | 1.75        | 12     | 1     |
| 1:A:107:MET:N    | 1:A:118:VAL:O    | 0.41     | 2.54        | 13     | 1     |
| 1:A:84:ILE:HD13  | 1:A:92:VAL:HG21  | 0.41     | 1.93        | 14     | 1     |
| 1:A:95:LEU:CD2   | 1:A:104:LEU:O    | 0.41     | 2.69        | 21     | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:101:LYS:CG   | 1:A:131:GLU:OE2  | 0.41     | 2.68        | 1      | 1     |
| 1:A:44:GLU:CD    | 1:A:57:LEU:HD22  | 0.41     | 2.41        | 2      | 1     |
| 1:A:58:LEU:CD1   | 1:A:69:LYS:O     | 0.41     | 2.67        | 4      | 1     |
| 1:A:12:ILE:CG2   | 1:A:48:PRO:CB    | 0.41     | 2.99        | 5      | 1     |
| 1:A:39:LEU:HD12  | 1:A:118:VAL:HG21 | 0.41     | 1.92        | 5      | 1     |
| 1:A:119:CYS:O    | 1:A:120:GLN:CG   | 0.41     | 2.68        | 6      | 1     |
| 1:A:127:GLU:O    | 1:A:128:VAL:O    | 0.41     | 2.39        | 6      | 1     |
| 1:A:10:LEU:CD2   | 1:A:79:PRO:O     | 0.41     | 2.69        | 15     | 1     |
| 1:A:56:ILE:O     | 1:A:70:LYS:CB    | 0.41     | 2.69        | 15     | 1     |
| 1:A:32:LEU:O     | 1:A:37:ALA:HB2   | 0.41     | 2.15        | 16     | 1     |
| 1:A:121:CYS:HB3  | 1:A:136:PHE:CD1  | 0.41     | 2.51        | 16     | 1     |
| 1:A:87:LEU:O     | 1:A:89:GLU:N     | 0.41     | 2.54        | 5      | 1     |
| 1:A:156:LEU:C    | 1:A:156:LEU:CD2  | 0.41     | 2.93        | 6      | 1     |
| 1:A:44:GLU:N     | 1:A:57:LEU:O     | 0.41     | 2.54        | 8      | 1     |
| 1:A:43:VAL:HG22  | 1:A:58:LEU:HD11  | 0.41     | 1.94        | 16     | 1     |
| 1:A:32:LEU:HD23  | 1:A:40:ARG:CB    | 0.40     | 2.46        | 9      | 1     |
| 1:A:97:THR:OG1   | 1:A:98:ASP:N     | 0.40     | 2.54        | 12     | 1     |
| 1:A:75:LYS:O     | 1:A:75:LYS:CG    | 0.40     | 2.69        | 15     | 1     |
| 1:A:39:LEU:HD21  | 1:A:118:VAL:CB   | 0.40     | 2.47        | 17     | 1     |
| 1:A:8:LYS:N      | 1:A:80:ALA:HB2   | 0.40     | 2.30        | 18     | 1     |
| 1:A:76:THR:OG1   | 1:A:77:LYS:N     | 0.40     | 2.54        | 19     | 2     |
| 1:A:43:VAL:HG21  | 1:A:122:LEU:CD2  | 0.40     | 2.46        | 14     | 1     |
| 1:A:103:LEU:O    | 1:A:104:LEU:HD23 | 0.40     | 2.16        | 14     | 1     |
| 1:A:128:VAL:O    | 1:A:128:VAL:CG1  | 0.40     | 2.68        | 16     | 1     |
| 1:A:31:LEU:CD2   | 1:A:88:ASN:CB    | 0.40     | 2.99        | 21     | 1     |
| 1:A:98:ASP:OD2   | 1:A:101:LYS:CD   | 0.40     | 2.69        | 2      | 1     |
| 1:A:48:PRO:CA    | 1:A:53:ASP:O     | 0.40     | 2.69        | 6      | 1     |
| 1:A:103:LEU:O    | 1:A:122:LEU:N    | 0.40     | 2.53        | 11     | 1     |
| 1:A:123:VAL:HG11 | 1:A:128:VAL:H    | 0.40     | 1.75        | 17     | 1     |
| 1:A:7:MET:CE     | 1:A:9:GLY:O      | 0.40     | 2.69        | 20     | 1     |
| 1:A:15:VAL:HG12  | 1:A:15:VAL:O     | 0.40     | 2.17        | 3      | 1     |
| 1:A:112:GLU:O    | 1:A:112:GLU:CG   | 0.40     | 2.69        | 10     | 1     |
| 1:A:123:VAL:HG12 | 1:A:124:ARG:N    | 0.40     | 2.31        | 14     | 1     |
| 1:A:39:LEU:CD2   | 1:A:118:VAL:CB   | 0.40     | 2.98        | 16     | 1     |
| 1:A:95:LEU:N     | 1:A:95:LEU:HD23  | 0.40     | 2.32        | 6      | 1     |
| 1:A:102:TYR:C    | 1:A:102:TYR:CD1  | 0.40     | 3.00        | 6      | 1     |
| 1:A:91:LYS:C     | 1:A:92:VAL:CG2   | 0.40     | 2.95        | 10     | 1     |
| 1:A:56:ILE:HG22  | 1:A:58:LEU:HD23  | 0.40     | 1.91        | 15     | 1     |
| 1:A:104:LEU:CD2  | 1:A:121:CYS:SG   | 0.40     | 3.10        | 18     | 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     | 143/162 (88%)   | 108±3 (75±2%) | 26±4 (18±3%) | 9±3 (7±2%) | 2           | 17 |
| All | All   | 3003/3402 (88%) | 2259 (75%)    | 545 (18%)    | 199 (7%)   | 2           | 17 |

All 51 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     | 8   | LYS  | 14             |
| 1   | A     | 12  | ILE  | 13             |
| 1   | A     | 40  | ARG  | 11             |
| 1   | A     | 99  | TYR  | 10             |
| 1   | A     | 101 | LYS  | 10             |
| 1   | A     | 125 | THR  | 9              |
| 1   | A     | 128 | VAL  | 8              |
| 1   | A     | 126 | PRO  | 7              |
| 1   | A     | 145 | MET  | 7              |
| 1   | A     | 7   | MET  | 7              |
| 1   | A     | 77  | LYS  | 5              |
| 1   | A     | 127 | GLU  | 5              |
| 1   | A     | 146 | HIS  | 5              |
| 1   | A     | 110 | SER  | 5              |
| 1   | A     | 111 | ALA  | 5              |
| 1   | A     | 130 | ASP  | 5              |
| 1   | A     | 80  | ALA  | 5              |
| 1   | A     | 33  | ASP  | 4              |
| 1   | A     | 89  | GLU  | 4              |
| 1   | A     | 9   | GLY  | 4              |
| 1   | A     | 6   | THR  | 4              |
| 1   | A     | 95  | LEU  | 3              |
| 1   | A     | 144 | PRO  | 3              |
| 1   | A     | 78  | ILE  | 3              |
| 1   | A     | 76  | THR  | 3              |
| 1   | A     | 141 | LYS  | 2              |
| 1   | A     | 11  | ASP  | 2              |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 87  | LEU  | 2              |
| 1   | A     | 113 | PRO  | 2              |
| 1   | A     | 116 | SER  | 2              |
| 1   | A     | 85  | ASP  | 2              |
| 1   | A     | 88  | ASN  | 2              |
| 1   | A     | 43  | VAL  | 2              |
| 1   | A     | 100 | LYS  | 2              |
| 1   | A     | 51  | GLU  | 2              |
| 1   | A     | 66  | CYS  | 2              |
| 1   | A     | 117 | LEU  | 2              |
| 1   | A     | 16  | ALA  | 2              |
| 1   | A     | 53  | ASP  | 2              |
| 1   | A     | 79  | PRO  | 1              |
| 1   | A     | 112 | GLU  | 1              |
| 1   | A     | 97  | THR  | 1              |
| 1   | A     | 22  | LEU  | 1              |
| 1   | A     | 15  | VAL  | 1              |
| 1   | A     | 114 | GLU  | 1              |
| 1   | A     | 90  | ASN  | 1              |
| 1   | A     | 151 | PHE  | 1              |
| 1   | A     | 14  | LYS  | 1              |
| 1   | A     | 152 | ASN  | 1              |
| 1   | A     | 48  | PRO  | 1              |
| 1   | A     | 115 | GLN  | 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     | 127/144 (88%)   | 88±4 (69±3%) | 39±4 (31±3%) | 1           | 15 |
| All | All   | 2667/3024 (88%) | 1847 (69%)   | 820 (31%)    | 1           | 15 |

All 103 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     | 58  | LEU  | 20             |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 135 | LYS  | 20             |
| 1   | A     | 143 | LEU  | 19             |
| 1   | A     | 14  | LYS  | 18             |
| 1   | A     | 39  | LEU  | 18             |
| 1   | A     | 137 | ASP  | 18             |
| 1   | A     | 60  | LYS  | 17             |
| 1   | A     | 83  | LYS  | 17             |
| 1   | A     | 101 | LYS  | 16             |
| 1   | A     | 91  | LYS  | 15             |
| 1   | A     | 125 | THR  | 15             |
| 1   | A     | 95  | LEU  | 15             |
| 1   | A     | 18  | THR  | 14             |
| 1   | A     | 70  | LYS  | 14             |
| 1   | A     | 32  | LEU  | 14             |
| 1   | A     | 77  | LYS  | 14             |
| 1   | A     | 57  | LEU  | 13             |
| 1   | A     | 133 | LEU  | 13             |
| 1   | A     | 28  | ASP  | 12             |
| 1   | A     | 89  | GLU  | 12             |
| 1   | A     | 87  | LEU  | 12             |
| 1   | A     | 75  | LYS  | 12             |
| 1   | A     | 55  | GLU  | 11             |
| 1   | A     | 93  | LEU  | 11             |
| 1   | A     | 96  | ASP  | 11             |
| 1   | A     | 117 | LEU  | 11             |
| 1   | A     | 145 | MET  | 11             |
| 1   | A     | 11  | ASP  | 11             |
| 1   | A     | 140 | LEU  | 11             |
| 1   | A     | 30  | SER  | 10             |
| 1   | A     | 74  | GLU  | 10             |
| 1   | A     | 98  | ASP  | 10             |
| 1   | A     | 146 | HIS  | 10             |
| 1   | A     | 123 | VAL  | 10             |
| 1   | A     | 6   | THR  | 9              |
| 1   | A     | 124 | ARG  | 9              |
| 1   | A     | 103 | LEU  | 9              |
| 1   | A     | 104 | LEU  | 9              |
| 1   | A     | 116 | SER  | 9              |
| 1   | A     | 130 | ASP  | 9              |
| 1   | A     | 156 | LEU  | 9              |
| 1   | A     | 107 | MET  | 9              |
| 1   | A     | 115 | GLN  | 9              |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 114 | GLU  | 9              |
| 1   | A     | 106 | CYS  | 8              |
| 1   | A     | 147 | ILE  | 8              |
| 1   | A     | 155 | GLN  | 8              |
| 1   | A     | 122 | LEU  | 8              |
| 1   | A     | 51  | GLU  | 8              |
| 1   | A     | 88  | ASN  | 8              |
| 1   | A     | 110 | SER  | 8              |
| 1   | A     | 134 | GLU  | 8              |
| 1   | A     | 108 | GLU  | 8              |
| 1   | A     | 49  | THR  | 8              |
| 1   | A     | 59  | GLN  | 7              |
| 1   | A     | 90  | ASN  | 7              |
| 1   | A     | 119 | CYS  | 7              |
| 1   | A     | 127 | GLU  | 7              |
| 1   | A     | 141 | LYS  | 7              |
| 1   | A     | 100 | LYS  | 7              |
| 1   | A     | 69  | LYS  | 7              |
| 1   | A     | 33  | ASP  | 6              |
| 1   | A     | 15  | VAL  | 6              |
| 1   | A     | 8   | LYS  | 6              |
| 1   | A     | 10  | LEU  | 6              |
| 1   | A     | 149 | LEU  | 6              |
| 1   | A     | 22  | LEU  | 5              |
| 1   | A     | 29  | ILE  | 5              |
| 1   | A     | 47  | LYS  | 5              |
| 1   | A     | 45  | GLU  | 5              |
| 1   | A     | 154 | THR  | 5              |
| 1   | A     | 13  | GLN  | 4              |
| 1   | A     | 40  | ARG  | 4              |
| 1   | A     | 76  | THR  | 4              |
| 1   | A     | 112 | GLU  | 4              |
| 1   | A     | 151 | PHE  | 4              |
| 1   | A     | 131 | GLU  | 4              |
| 1   | A     | 150 | SER  | 4              |
| 1   | A     | 21  | SER  | 4              |
| 1   | A     | 46  | LEU  | 3              |
| 1   | A     | 72  | ILE  | 3              |
| 1   | A     | 44  | GLU  | 3              |
| 1   | A     | 42  | TYR  | 3              |
| 1   | A     | 27  | SER  | 3              |
| 1   | A     | 138 | LYS  | 3              |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 148 | ARG  | 3              |
| 1   | A     | 7   | MET  | 3              |
| 1   | A     | 68  | GLN  | 2              |
| 1   | A     | 78  | ILE  | 2              |
| 1   | A     | 85  | ASP  | 2              |
| 1   | A     | 66  | CYS  | 2              |
| 1   | A     | 24  | MET  | 2              |
| 1   | A     | 97  | THR  | 2              |
| 1   | A     | 109 | ASN  | 2              |
| 1   | A     | 102 | TYR  | 2              |
| 1   | A     | 84  | ILE  | 2              |
| 1   | A     | 128 | VAL  | 1              |
| 1   | A     | 118 | VAL  | 1              |
| 1   | A     | 120 | GLN  | 1              |
| 1   | A     | 31  | LEU  | 1              |
| 1   | A     | 152 | ASN  | 1              |
| 1   | A     | 41  | VAL  | 1              |
| 1   | A     | 82  | PHE  | 1              |

### 6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

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

There are no ligands in this entry.

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

There are no such molecules in this entry.

## 6.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 7 Chemical shift validation

No chemical shift data were provided