



# Full wwPDB NMR Structure Validation Report ⓘ

Mar 9, 2026 – 03:31 AM UTC

PDB ID : 2ORC / pdb\_00002orc  
Title : CRO REPRESSOR INSERTION MUTANT K56-[DGEVK], NMR, 32  
STRUCTURES  
Authors : Mossing, M.C.  
Deposited on : 1998-01-20

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                                                             |

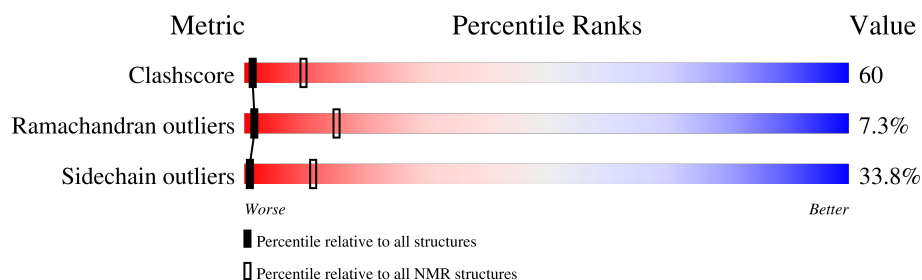
# 1 Overall quality at a glance

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     | 71     | <div> <div></div> <div>13%</div> <div>58%</div> <div>18%</div> <div>11%</div> </div> |

## 2 Ensemble composition and analysis

This entry contains 32 models. Model 26 is the overall representative, medoid model (most similar to other models).

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

| Well-defined (core) protein residues |                       |                   |              |
|--------------------------------------|-----------------------|-------------------|--------------|
| Well-defined core                    | Residue range (total) | Backbone RMSD (Å) | Medoid model |
| 1                                    | A:3-A:60 (58)         | 1.26              | 26           |

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 1 single-model cluster was found.

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

### 3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1124 atoms, of which 569 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called CRO REPRESSOR.

| Mol | Chain | Residues | Atoms |     |     |    |     |   | Trace |
|-----|-------|----------|-------|-----|-----|----|-----|---|-------|
| 1   | A     | 71       | Total | C   | H   | N  | O   | S | 0     |
|     |       |          | 1124  | 350 | 569 | 97 | 106 | 2 |       |

There are 5 discrepancies between the modelled and reference sequences:

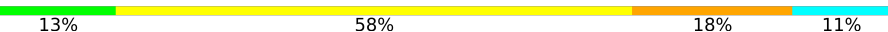
| Chain | Residue | Modelled | Actual | Comment   | Reference  |
|-------|---------|----------|--------|-----------|------------|
| A     | 54      | GLU      | -      | insertion | UNP P03040 |
| A     | 55      | VAL      | -      | insertion | UNP P03040 |
| A     | 56      | LYS      | -      | insertion | UNP P03040 |
| A     | 56A     | ASP      | -      | insertion | UNP P03040 |
| A     | 56B     | GLY      | -      | insertion | UNP P03040 |

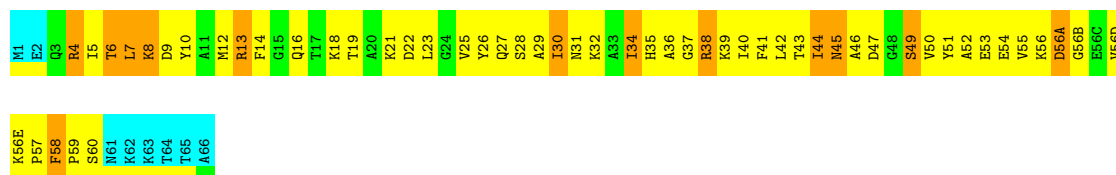
## 4 Residue-property plots

### 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: CRO REPRESSOR

Chain A: 

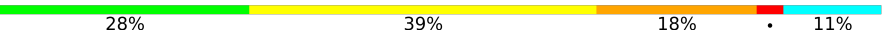


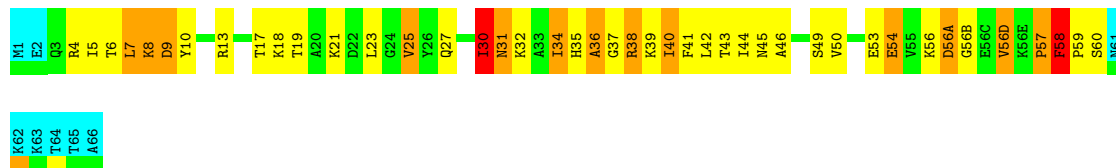
### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

#### 4.2.1 Score per residue for model 1

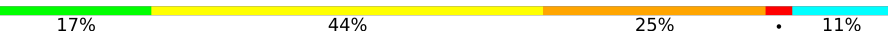
#### • Molecule 1: CRO REPRESSOR

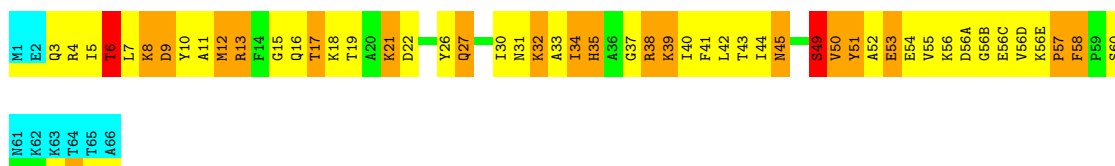
Chain A: 



#### 4.2.2 Score per residue for model 2

#### • Molecule 1: CRO REPRESSOR

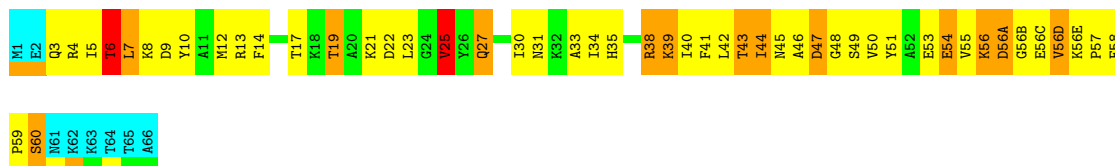
Chain A: 



### 4.2.3 Score per residue for model 3

- Molecule 1: CRO REPRESSOR

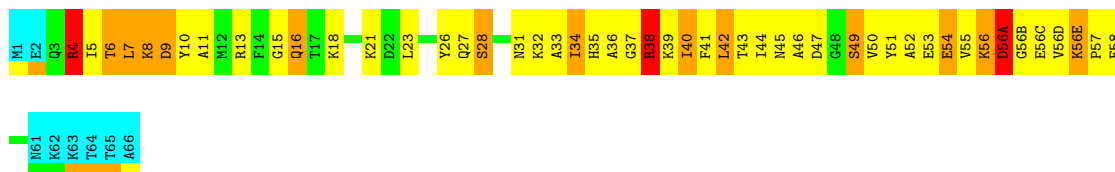
Chain A: 18% 49% 18% • 11%



### 4.2.4 Score per residue for model 4

- Molecule 1: CRO REPRESSOR

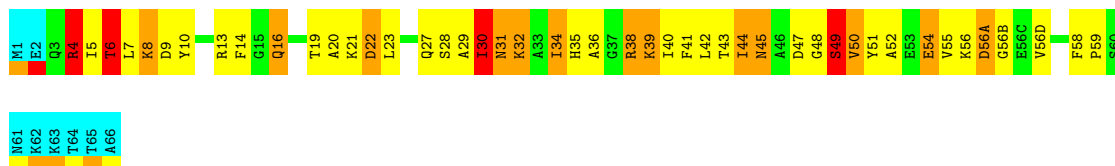
Chain A: 20% 46% 18% • 11%



### 4.2.5 Score per residue for model 5

- Molecule 1: CRO REPRESSOR

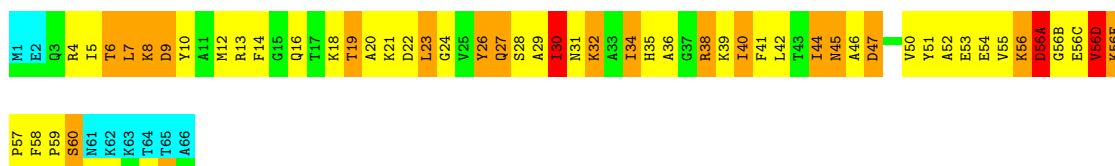
Chain A: 24% 41% 18% 6% 11%



### 4.2.6 Score per residue for model 6

- Molecule 1: CRO REPRESSOR

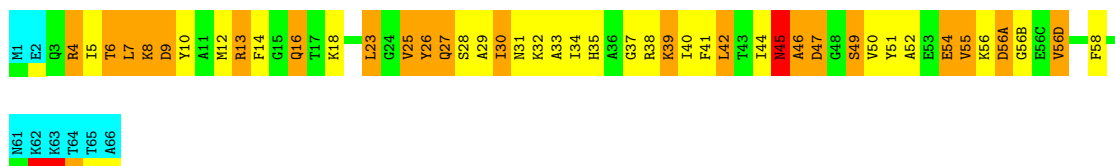
Chain A: 14% 45% 25% • 11%



#### 4.2.7 Score per residue for model 7

- Molecule 1: CRO REPRESSOR

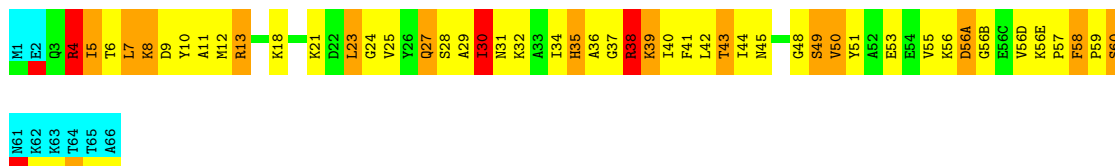
Chain A: 25% 32% 30% 11%



#### 4.2.8 Score per residue for model 8

- Molecule 1: CRO REPRESSOR

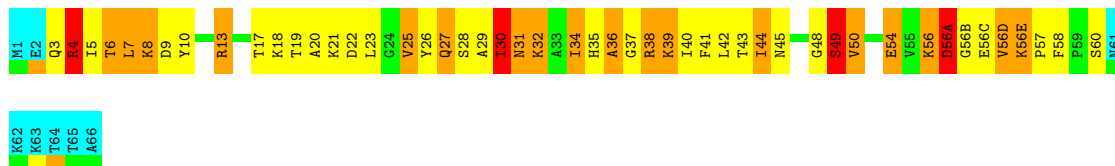
Chain A: 21% 44% 20% 11%



#### 4.2.9 Score per residue for model 9

- Molecule 1: CRO REPRESSOR

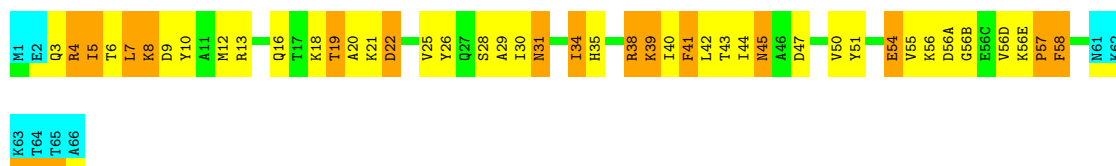
Chain A: 20% 38% 25% 6% 11%



#### 4.2.10 Score per residue for model 10

- Molecule 1: CRO REPRESSOR

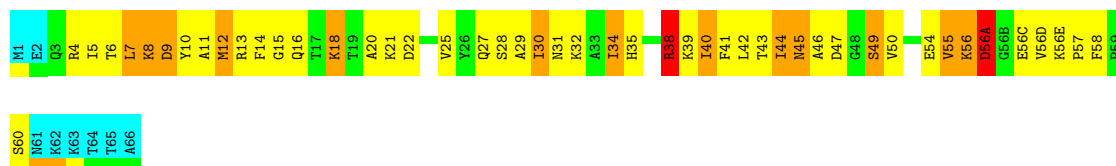
Chain A: 27% 41% 21% 11%



#### 4.2.11 Score per residue for model 11

- Molecule 1: CRO REPRESSOR

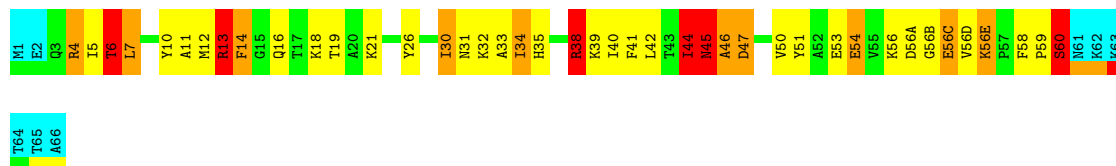
Chain A: 21% 46% 18% • 11%



#### 4.2.12 Score per residue for model 12

- Molecule 1: CRO REPRESSOR

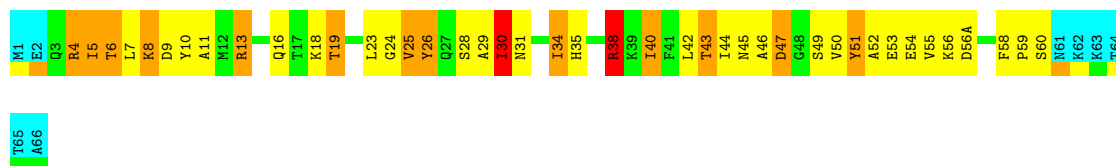
Chain A: 30% 37% 14% 8% 11%



#### 4.2.13 Score per residue for model 13

- Molecule 1: CRO REPRESSOR

Chain A: 30% 38% 18% • 11%

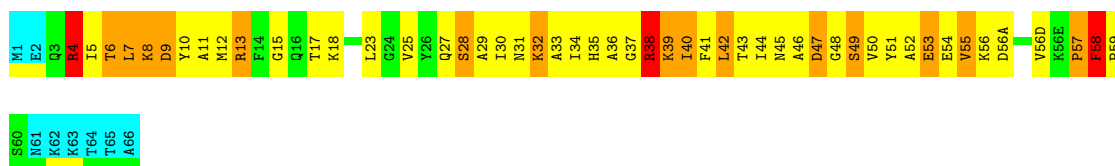


#### 4.2.14 Score per residue for model 14

- Molecule 1: CRO REPRESSOR

Chain A: 18% 45% 21% • 11%

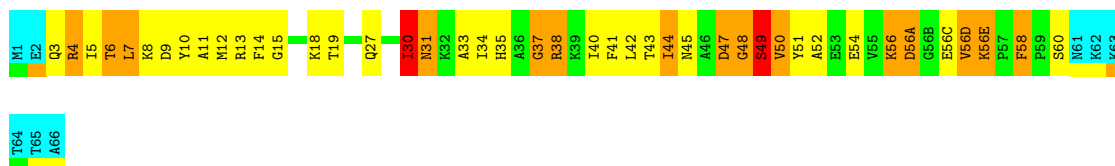




#### 4.2.15 Score per residue for model 15

- Molecule 1: CRO REPRESSOR

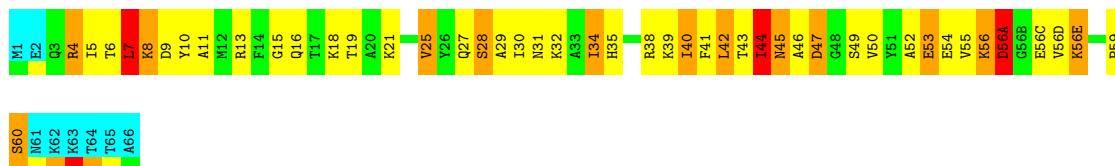
Chain A: 28% 37% 21% • 11%



#### 4.2.16 Score per residue for model 16

- Molecule 1: CRO REPRESSOR

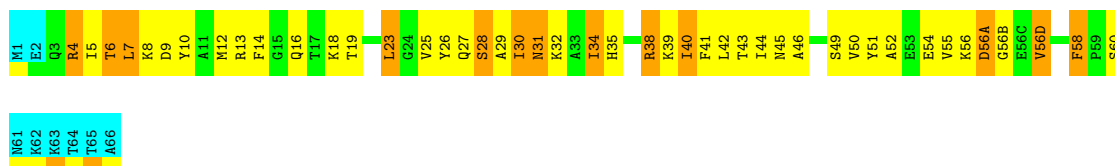
Chain A: 24% 42% 18% • 11%



#### 4.2.17 Score per residue for model 17

- Molecule 1: CRO REPRESSOR

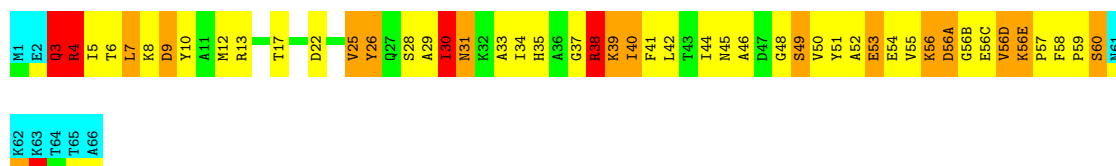
Chain A: 25% 45% 18% 11%



#### 4.2.18 Score per residue for model 18

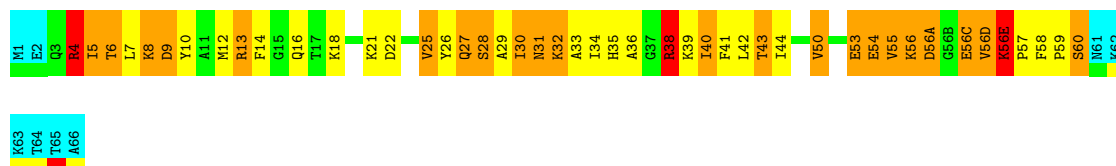
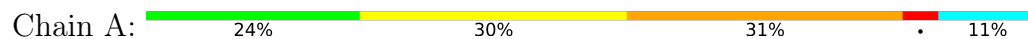
- Molecule 1: CRO REPRESSOR

Chain A: 21% 42% 20% 6% 11%



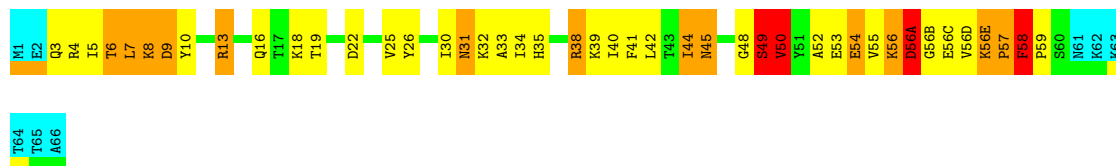
#### 4.2.19 Score per residue for model 19

- Molecule 1: CRO REPRESSOR



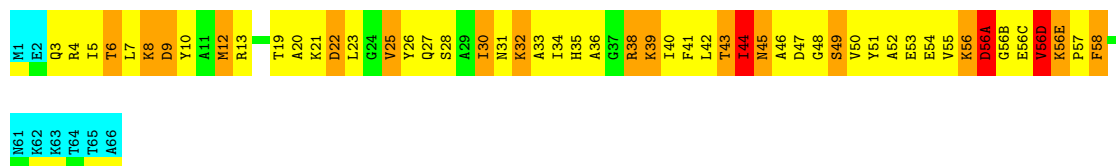
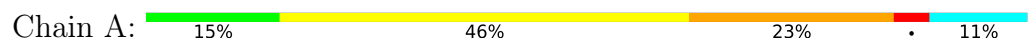
#### 4.2.20 Score per residue for model 20

- Molecule 1: CRO REPRESSOR



#### 4.2.21 Score per residue for model 21

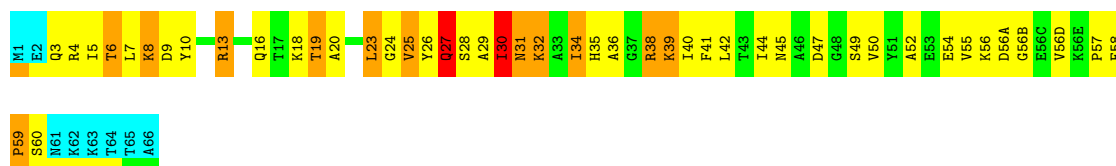
- Molecule 1: CRO REPRESSOR



#### 4.2.22 Score per residue for model 22

- Molecule 1: CRO REPRESSOR

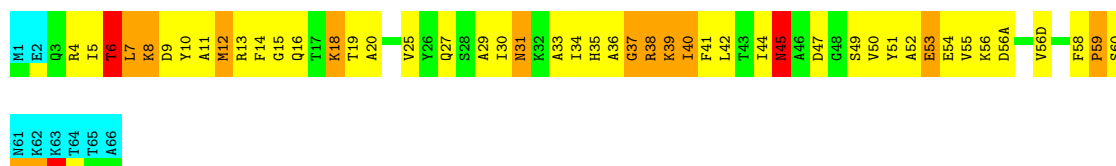




#### 4.2.23 Score per residue for model 23

- Molecule 1: CRO REPRESSOR

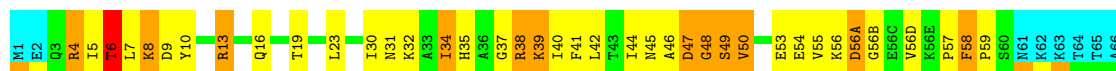
Chain A: 23% 48% 15% • 11%



#### 4.2.24 Score per residue for model 24

- Molecule 1: CRO REPRESSOR

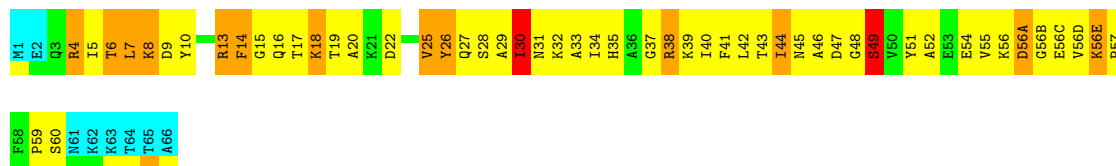
Chain A: 34% 37% 17% • 11%



#### 4.2.25 Score per residue for model 25

- Molecule 1: CRO REPRESSOR

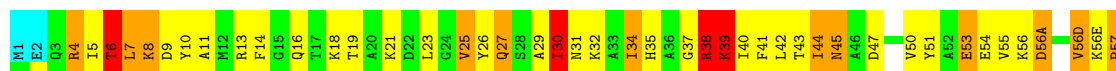
Chain A: 14% 54% 18% • 11%



#### 4.2.26 Score per residue for model 26 (medoid)

- Molecule 1: CRO REPRESSOR

Chain A: 24% 41% 18% 6% 11%

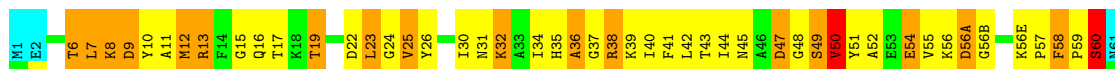




#### 4.2.27 Score per residue for model 27

- Molecule 1: CRO REPRESSOR

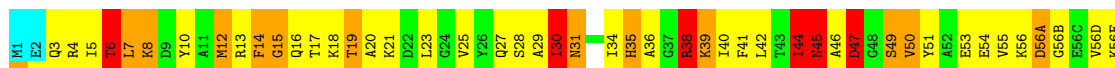
Chain A: 21% 41% 24% • 11%



#### 4.2.28 Score per residue for model 28

- Molecule 1: CRO REPRESSOR

Chain A: 18% 42% 20% 8% 11%



#### 4.2.29 Score per residue for model 29

- Molecule 1: CRO REPRESSOR

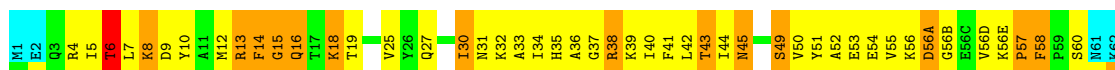
Chain A: 32% 37% 15% • 11%



#### 4.2.30 Score per residue for model 30

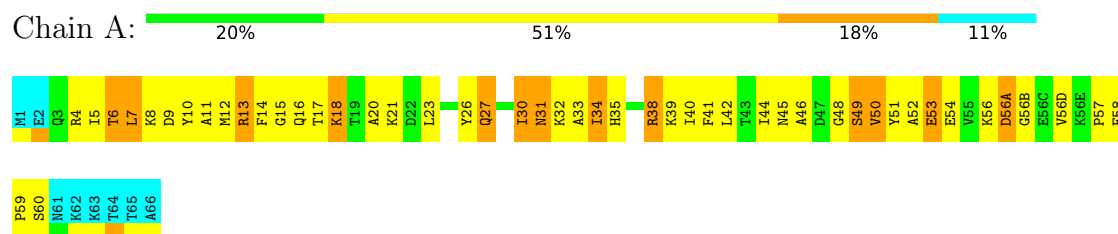
- Molecule 1: CRO REPRESSOR

Chain A: 23% 45% 20% • 11%



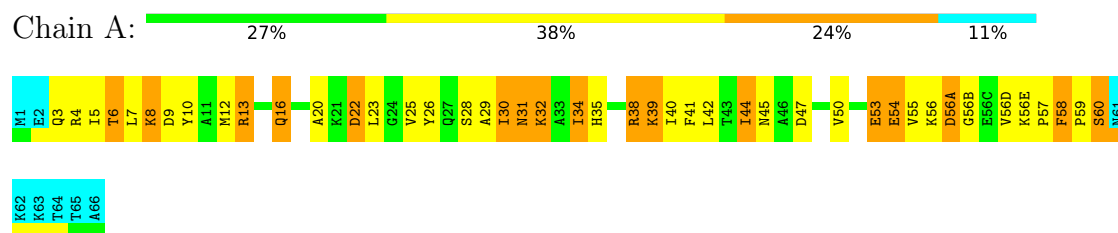
#### 4.2.31 Score per residue for model 31

- Molecule 1: CRO REPRESSOR



#### 4.2.32 Score per residue for model 32

- Molecule 1: CRO REPRESSOR



## 5 Refinement protocol and experimental data overview

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

Of the 50 calculated structures, 32 were deposited, based on the following criterion: *NO DISTANCE VIOLATION > 0.5Å, NO DIHEDRAL VIOLATION > 5 DEGREES*.

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

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

No chemical shift data was provided.

## 6 Model quality

### 6.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the (average) root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Chain | Bond lengths |                      | Bond angles |                      |
|-----|-------|--------------|----------------------|-------------|----------------------|
|     |       | RMSZ         | #Z>5                 | RMSZ        | #Z>5                 |
| 1   | A     | 1.42±0.01    | 0±0/501 ( 0.0± 0.0%) | 1.60±0.02   | 3±2/674 ( 0.4± 0.2%) |
| All | All   | 1.42         | 1/16032 ( 0.0%)      | 1.60        | 95/21568 ( 0.4%)     |

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

| Mol | Chain | Chirality | Planarity |
|-----|-------|-----------|-----------|
| 1   | A     | 0.0±0.0   | 2.8±0.6   |
| All | All   | 0         | 88        |

All unique bond outliers are listed below.

| Mol | Chain | Res   | Type | Atoms | Z    | Observed(Å) | Ideal(Å) | Models |       |
|-----|-------|-------|------|-------|------|-------------|----------|--------|-------|
|     |       |       |      |       |      |             |          | Worst  | Total |
| 1   | A     | 56(E) | LYS  | N-CA  | 5.79 | 1.51        | 1.46     | 25     | 1     |

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

| Mol | Chain | Res   | Type | Atoms   | Z     | Observed(°) | Ideal(°) | Models |       |
|-----|-------|-------|------|---------|-------|-------------|----------|--------|-------|
|     |       |       |      |         |       |             |          | Worst  | Total |
| 1   | A     | 34    | ILE  | N-CA-CB | -8.02 | 105.06      | 111.64   | 31     | 16    |
| 1   | A     | 40    | ILE  | N-CA-CB | -7.25 | 103.81      | 112.07   | 11     | 9     |
| 1   | A     | 44    | ILE  | N-CA-CB | -7.14 | 105.14      | 112.28   | 26     | 7     |
| 1   | A     | 3     | GLN  | N-CA-CB | -6.99 | 101.64      | 110.45   | 18     | 2     |
| 1   | A     | 56(D) | VAL  | N-CA-CB | -6.96 | 104.41      | 112.34   | 21     | 7     |
| 1   | A     | 4     | ARG  | N-CA-CB | -6.69 | 102.37      | 110.53   | 9      | 1     |
| 1   | A     | 25    | VAL  | N-CA-CB | -6.54 | 105.12      | 112.45   | 16     | 8     |
| 1   | A     | 56(E) | LYS  | N-CA-CB | -6.30 | 105.35      | 111.27   | 19     | 3     |
| 1   | A     | 55    | VAL  | N-CA-CB | -5.96 | 104.59      | 112.34   | 10     | 3     |
| 1   | A     | 50    | VAL  | N-CA-CB | -5.89 | 104.56      | 112.10   | 24     | 16    |

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| Mol | Chain | Res   | Type | Atoms    | Z     | Observed(°) | Ideal(°) | Models |       |
|-----|-------|-------|------|----------|-------|-------------|----------|--------|-------|
|     |       |       |      |          |       |             |          | Worst  | Total |
| 1   | A     | 30    | ILE  | N-CA-CB  | -5.87 | 104.02      | 110.65   | 13     | 15    |
| 1   | A     | 39    | LYS  | N-CA-CB  | -5.64 | 105.02      | 111.79   | 23     | 3     |
| 1   | A     | 46    | ALA  | N-CA-C   | -5.27 | 106.43      | 112.86   | 7      | 2     |
| 1   | A     | 56(A) | ASP  | N-CA-CB  | -5.10 | 104.50      | 112.41   | 5      | 1     |
| 1   | A     | 7     | LEU  | N-CA-C   | -5.10 | 106.22      | 112.90   | 16     | 1     |
| 1   | A     | 41    | PHE  | CA-CB-CG | -5.09 | 108.71      | 113.80   | 10     | 1     |

There are no chirality outliers.

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

| Mol | Chain | Res | Type | Group     | Models (Total) |
|-----|-------|-----|------|-----------|----------------|
| 1   | A     | 13  | ARG  | Sidechain | 31             |
| 1   | A     | 38  | ARG  | Sidechain | 29             |
| 1   | A     | 4   | ARG  | Sidechain | 28             |

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

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes |
|-----|-------|-------|----------|----------|---------|
| 1   | A     | 492   | 501      | 501      | 60±12   |
| All | All   | 15744 | 16032    | 16032    | 1904    |

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 60.

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

| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:23:LEU:HD12 | 1:A:25:VAL:HG21 | 1.04     | 1.23        | 7      | 2     |
| 1:A:7:LEU:HD12  | 1:A:40:ILE:HD13 | 0.97     | 1.32        | 23     | 2     |
| 1:A:7:LEU:CD1   | 1:A:42:LEU:HD11 | 0.96     | 1.91        | 4      | 5     |
| 1:A:22:ASP:OD2  | 1:A:50:VAL:HG11 | 0.95     | 1.62        | 19     | 1     |
| 1:A:23:LEU:HD22 | 1:A:42:LEU:HD22 | 0.93     | 1.36        | 22     | 1     |
| 1:A:7:LEU:HD23  | 1:A:40:ILE:HD12 | 0.92     | 1.38        | 18     | 3     |
| 1:A:7:LEU:HD22  | 1:A:40:ILE:HD13 | 0.92     | 1.40        | 21     | 1     |

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| Atom-1          | Atom-2             | Clash(Å) | Distance(Å) | Models |       |
|-----------------|--------------------|----------|-------------|--------|-------|
|                 |                    |          |             | Worst  | Total |
| 1:A:44:ILE:HG23 | 1:A:49:SER:O       | 0.91     | 1.64        | 9      | 12    |
| 1:A:7:LEU:HD13  | 1:A:34:ILE:HG12    | 0.91     | 1.41        | 23     | 1     |
| 1:A:7:LEU:HD22  | 1:A:40:ILE:HD12    | 0.90     | 1.43        | 20     | 11    |
| 1:A:5:ILE:O     | 1:A:42:LEU:HD12    | 0.90     | 1.66        | 16     | 3     |
| 1:A:7:LEU:HD23  | 1:A:40:ILE:HD13    | 0.89     | 1.41        | 3      | 5     |
| 1:A:55:VAL:O    | 1:A:56(D):VAL:HG12 | 0.89     | 1.66        | 25     | 1     |
| 1:A:27:GLN:HA   | 1:A:30:ILE:HD12    | 0.88     | 1.45        | 3      | 1     |
| 1:A:23:LEU:HD11 | 1:A:25:VAL:CG2     | 0.88     | 1.99        | 8      | 2     |
| 1:A:23:LEU:HD12 | 1:A:25:VAL:CG2     | 0.86     | 1.99        | 7      | 2     |
| 1:A:37:GLY:O    | 1:A:40:ILE:HD11    | 0.86     | 1.69        | 2      | 4     |
| 1:A:7:LEU:HB2   | 1:A:34:ILE:HD11    | 0.85     | 1.47        | 4      | 1     |
| 1:A:7:LEU:HD12  | 1:A:42:LEU:HD11    | 0.85     | 1.47        | 21     | 3     |
| 1:A:22:ASP:HB3  | 1:A:50:VAL:HG11    | 0.83     | 1.47        | 32     | 2     |
| 1:A:5:ILE:HG22  | 1:A:10:TYR:HB2     | 0.82     | 1.49        | 14     | 20    |
| 1:A:46:ALA:HB3  | 1:A:49:SER:CB      | 0.82     | 2.03        | 25     | 5     |
| 1:A:7:LEU:HD23  | 1:A:40:ILE:CD1     | 0.82     | 2.05        | 28     | 2     |
| 1:A:23:LEU:HD22 | 1:A:42:LEU:CD2     | 0.81     | 2.03        | 22     | 2     |
| 1:A:7:LEU:HD12  | 1:A:19:THR:HG21    | 0.81     | 1.49        | 25     | 1     |
| 1:A:7:LEU:HD11  | 1:A:42:LEU:HD21    | 0.80     | 1.54        | 10     | 4     |
| 1:A:49:SER:O    | 1:A:50:VAL:HG23    | 0.79     | 1.77        | 9      | 6     |
| 1:A:42:LEU:HD12 | 1:A:42:LEU:N       | 0.77     | 1.95        | 27     | 17    |
| 1:A:7:LEU:CB    | 1:A:34:ILE:HD11    | 0.77     | 2.09        | 4      | 3     |
| 1:A:7:LEU:CD2   | 1:A:40:ILE:HD12    | 0.77     | 2.10        | 20     | 9     |
| 1:A:17:THR:HG23 | 1:A:27:GLN:OE1     | 0.76     | 1.81        | 2      | 1     |
| 1:A:7:LEU:HD21  | 1:A:40:ILE:HG21    | 0.76     | 1.57        | 18     | 5     |
| 1:A:7:LEU:CD1   | 1:A:42:LEU:HD21    | 0.76     | 2.11        | 10     | 5     |
| 1:A:46:ALA:HB3  | 1:A:49:SER:HB2     | 0.76     | 1.58        | 25     | 3     |
| 1:A:8:LYS:HB2   | 1:A:34:ILE:HD13    | 0.75     | 1.57        | 2      | 2     |
| 1:A:7:LEU:HD13  | 1:A:34:ILE:CG1     | 0.75     | 2.10        | 23     | 1     |
| 1:A:30:ILE:HG22 | 1:A:34:ILE:HD12    | 0.74     | 1.58        | 17     | 9     |
| 1:A:40:ILE:HG23 | 1:A:54:GLU:CA      | 0.74     | 2.12        | 30     | 1     |
| 1:A:40:ILE:HG23 | 1:A:54:GLU:HG3     | 0.74     | 1.59        | 13     | 1     |
| 1:A:7:LEU:HB3   | 1:A:34:ILE:HD11    | 0.74     | 1.59        | 16     | 4     |
| 1:A:7:LEU:HD13  | 1:A:40:ILE:HG21    | 0.73     | 1.58        | 21     | 1     |
| 1:A:7:LEU:HD21  | 1:A:40:ILE:CG2     | 0.73     | 2.14        | 8      | 5     |
| 1:A:25:VAL:CG1  | 1:A:30:ILE:HD11    | 0.73     | 2.12        | 17     | 1     |
| 1:A:22:ASP:CB   | 1:A:50:VAL:HG11    | 0.73     | 2.13        | 32     | 1     |
| 1:A:56(D):VAL:O | 1:A:56(D):VAL:HG23 | 0.73     | 1.82        | 2      | 3     |
| 1:A:56(B):GLY:O | 1:A:56(D):VAL:HG13 | 0.73     | 1.82        | 2      | 3     |
| 1:A:7:LEU:HD21  | 1:A:34:ILE:HG12    | 0.73     | 1.60        | 13     | 7     |
| 1:A:43:THR:HG22 | 1:A:48:GLY:HA2     | 0.73     | 1.60        | 15     | 1     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:33:ALA:HB1  | 1:A:40:ILE:CD1  | 0.73     | 2.14        | 31     | 2     |
| 1:A:45:ASN:O    | 1:A:46:ALA:HB3  | 0.73     | 1.84        | 1      | 12    |
| 1:A:30:ILE:HG22 | 1:A:31:ASN:N    | 0.72     | 1.98        | 11     | 13    |
| 1:A:7:LEU:HB2   | 1:A:42:LEU:HD11 | 0.72     | 1.62        | 3      | 5     |
| 1:A:23:LEU:HD21 | 1:A:52:ALA:HB2  | 0.72     | 1.61        | 21     | 1     |
| 1:A:7:LEU:HD11  | 1:A:30:ILE:CD1  | 0.71     | 2.16        | 25     | 3     |
| 1:A:44:ILE:HG12 | 1:A:50:VAL:HG22 | 0.71     | 1.62        | 24     | 2     |
| 1:A:46:ALA:O    | 1:A:47:ASP:CB   | 0.70     | 2.39        | 3      | 11    |
| 1:A:43:THR:HG23 | 1:A:43:THR:O    | 0.70     | 1.86        | 17     | 2     |
| 1:A:40:ILE:HG23 | 1:A:54:GLU:HA   | 0.70     | 1.62        | 30     | 1     |
| 1:A:7:LEU:HD23  | 1:A:34:ILE:CG1  | 0.70     | 2.17        | 21     | 1     |
| 1:A:50:VAL:HG12 | 1:A:50:VAL:O    | 0.70     | 1.84        | 15     | 3     |
| 1:A:22:ASP:OD1  | 1:A:50:VAL:HG21 | 0.70     | 1.87        | 18     | 4     |
| 1:A:7:LEU:HD13  | 1:A:42:LEU:HD11 | 0.70     | 1.63        | 10     | 3     |
| 1:A:26:TYR:O    | 1:A:30:ILE:HD12 | 0.70     | 1.87        | 10     | 4     |
| 1:A:30:ILE:HG22 | 1:A:34:ILE:CD1  | 0.70     | 2.16        | 17     | 3     |
| 1:A:32:LYS:O    | 1:A:36:ALA:HB3  | 0.69     | 1.87        | 19     | 2     |
| 1:A:23:LEU:HD13 | 1:A:42:LEU:HD21 | 0.69     | 1.63        | 6      | 2     |
| 1:A:16:GLN:NE2  | 1:A:30:ILE:HG21 | 0.69     | 2.02        | 31     | 1     |
| 1:A:48:GLY:O    | 1:A:50:VAL:HG23 | 0.69     | 1.87        | 18     | 2     |
| 1:A:7:LEU:HD12  | 1:A:40:ILE:CD1  | 0.69     | 2.15        | 23     | 2     |
| 1:A:30:ILE:HG23 | 1:A:34:ILE:HD12 | 0.69     | 1.63        | 29     | 4     |
| 1:A:7:LEU:HD12  | 1:A:19:THR:CG2  | 0.68     | 2.18        | 25     | 1     |
| 1:A:7:LEU:HD13  | 1:A:42:LEU:CD1  | 0.68     | 2.19        | 10     | 2     |
| 1:A:16:GLN:NE2  | 1:A:30:ILE:HG22 | 0.68     | 2.03        | 23     | 1     |
| 1:A:44:ILE:HG22 | 1:A:46:ALA:H    | 0.68     | 1.48        | 24     | 1     |
| 1:A:30:ILE:HD12 | 1:A:34:ILE:HD11 | 0.67     | 1.64        | 5      | 4     |
| 1:A:23:LEU:HD11 | 1:A:25:VAL:HG21 | 0.67     | 1.65        | 8      | 2     |
| 1:A:30:ILE:N    | 1:A:30:ILE:HD13 | 0.67     | 2.04        | 17     | 4     |
| 1:A:44:ILE:HG22 | 1:A:44:ILE:O    | 0.67     | 1.89        | 25     | 3     |
| 1:A:16:GLN:O    | 1:A:20:ALA:HB2  | 0.67     | 1.89        | 5      | 6     |
| 1:A:33:ALA:O    | 1:A:40:ILE:HD11 | 0.67     | 1.90        | 23     | 3     |
| 1:A:7:LEU:CD1   | 1:A:23:LEU:HD11 | 0.67     | 2.19        | 31     | 1     |
| 1:A:25:VAL:HG12 | 1:A:30:ILE:HD11 | 0.67     | 1.66        | 17     | 1     |
| 1:A:23:LEU:CD2  | 1:A:52:ALA:HB2  | 0.67     | 2.20        | 21     | 1     |
| 1:A:23:LEU:CD1  | 1:A:42:LEU:HD21 | 0.66     | 2.20        | 6      | 1     |
| 1:A:19:THR:O    | 1:A:23:LEU:HD12 | 0.66     | 1.90        | 9      | 6     |
| 1:A:7:LEU:HA    | 1:A:42:LEU:HD13 | 0.66     | 1.68        | 29     | 6     |
| 1:A:23:LEU:HD21 | 1:A:42:LEU:HD23 | 0.66     | 1.67        | 4      | 1     |
| 1:A:45:ASN:O    | 1:A:46:ALA:CB   | 0.65     | 2.44        | 29     | 8     |
| 1:A:5:ILE:HD12  | 1:A:10:TYR:CE1  | 0.65     | 2.26        | 17     | 6     |

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| Atom-1          | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|-----------------|------------------|----------|-------------|--------|-------|
|                 |                  |          |             | Worst  | Total |
| 1:A:54:GLU:O    | 1:A:56(D):VAL:HA | 0.65     | 1.92        | 25     | 16    |
| 1:A:22:ASP:CG   | 1:A:50:VAL:HG21  | 0.65     | 2.16        | 11     | 4     |
| 1:A:33:ALA:CB   | 1:A:58:PHE:CZ    | 0.65     | 2.80        | 7      | 4     |
| 1:A:38:ARG:N    | 1:A:38:ARG:HD2   | 0.65     | 2.06        | 8      | 4     |
| 1:A:40:ILE:C    | 1:A:41:PHE:CG    | 0.65     | 2.75        | 3      | 25    |
| 1:A:30:ILE:O    | 1:A:33:ALA:HB3   | 0.64     | 1.91        | 2      | 1     |
| 1:A:7:LEU:HD12  | 1:A:42:LEU:CD1   | 0.64     | 2.22        | 21     | 2     |
| 1:A:20:ALA:HB1  | 1:A:24:GLY:O     | 0.64     | 1.91        | 22     | 1     |
| 1:A:7:LEU:HG    | 1:A:34:ILE:HD11  | 0.64     | 1.68        | 12     | 3     |
| 1:A:7:LEU:HD11  | 1:A:34:ILE:HD11  | 0.64     | 1.66        | 1      | 6     |
| 1:A:38:ARG:HB2  | 1:A:40:ILE:HD11  | 0.63     | 1.69        | 22     | 1     |
| 1:A:10:TYR:CE1  | 1:A:44:ILE:CD1   | 0.63     | 2.82        | 28     | 1     |
| 1:A:32:LYS:O    | 1:A:36:ALA:HB2   | 0.63     | 1.94        | 14     | 7     |
| 1:A:10:TYR:CZ   | 1:A:14:PHE:CZ    | 0.63     | 2.87        | 25     | 2     |
| 1:A:3:GLN:CG    | 1:A:3:GLN:O      | 0.63     | 2.47        | 18     | 1     |
| 1:A:7:LEU:HD11  | 1:A:34:ILE:CD1   | 0.63     | 2.24        | 32     | 4     |
| 1:A:14:PHE:O    | 1:A:15:GLY:C     | 0.62     | 2.41        | 28     | 1     |
| 1:A:7:LEU:CD2   | 1:A:34:ILE:HD11  | 0.62     | 2.24        | 12     | 1     |
| 1:A:14:PHE:N    | 1:A:14:PHE:CD1   | 0.62     | 2.67        | 12     | 3     |
| 1:A:7:LEU:N     | 1:A:7:LEU:HD13   | 0.62     | 2.09        | 16     | 1     |
| 1:A:40:ILE:O    | 1:A:41:PHE:CG    | 0.61     | 2.54        | 2      | 21    |
| 1:A:7:LEU:CG    | 1:A:34:ILE:HD11  | 0.61     | 2.25        | 12     | 1     |
| 1:A:43:THR:HG22 | 1:A:48:GLY:CA    | 0.61     | 2.24        | 15     | 1     |
| 1:A:46:ALA:HB3  | 1:A:49:SER:OG    | 0.61     | 1.95        | 11     | 1     |
| 1:A:10:TYR:CE2  | 1:A:44:ILE:HD11  | 0.61     | 2.31        | 11     | 8     |
| 1:A:38:ARG:O    | 1:A:39:LYS:C     | 0.61     | 2.44        | 26     | 3     |
| 1:A:41:PHE:C    | 1:A:42:LEU:HD12  | 0.61     | 2.20        | 31     | 4     |
| 1:A:7:LEU:HD11  | 1:A:34:ILE:CG1   | 0.61     | 2.26        | 32     | 1     |
| 1:A:36:ALA:O    | 1:A:37:GLY:C     | 0.60     | 2.44        | 23     | 2     |
| 1:A:10:TYR:CE1  | 1:A:14:PHE:CZ    | 0.60     | 2.89        | 12     | 1     |
| 1:A:7:LEU:HD22  | 1:A:42:LEU:HD11  | 0.60     | 1.72        | 31     | 1     |
| 1:A:44:ILE:CD1  | 1:A:50:VAL:HG22  | 0.60     | 2.26        | 10     | 1     |
| 1:A:56:LYS:O    | 1:A:56(A):ASP:C  | 0.60     | 2.43        | 1      | 19    |
| 1:A:5:ILE:HG21  | 1:A:10:TYR:CG    | 0.60     | 2.31        | 13     | 1     |
| 1:A:23:LEU:C    | 1:A:58:PHE:CZ    | 0.60     | 2.80        | 22     | 1     |
| 1:A:50:VAL:O    | 1:A:51:TYR:CG    | 0.60     | 2.55        | 21     | 1     |
| 1:A:48:GLY:O    | 1:A:50:VAL:N     | 0.60     | 2.34        | 9      | 4     |
| 1:A:11:ALA:HB2  | 1:A:19:THR:HG21  | 0.60     | 1.71        | 13     | 2     |
| 1:A:33:ALA:HB1  | 1:A:40:ILE:HD12  | 0.60     | 1.73        | 31     | 1     |
| 1:A:6:THR:O     | 1:A:10:TYR:CB    | 0.60     | 2.50        | 31     | 30    |
| 1:A:23:LEU:CD1  | 1:A:25:VAL:CG2   | 0.60     | 2.79        | 8      | 1     |

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| Atom-1          | Atom-2             | Clash(Å) | Distance(Å) | Models |       |
|-----------------|--------------------|----------|-------------|--------|-------|
|                 |                    |          |             | Worst  | Total |
| 1:A:37:GLY:O    | 1:A:39:LYS:N       | 0.60     | 2.35        | 8      | 1     |
| 1:A:40:ILE:C    | 1:A:41:PHE:CD1     | 0.60     | 2.80        | 22     | 4     |
| 1:A:7:LEU:CD1   | 1:A:19:THR:HG21    | 0.59     | 2.25        | 25     | 1     |
| 1:A:30:ILE:N    | 1:A:30:ILE:CD1     | 0.59     | 2.66        | 27     | 8     |
| 1:A:31:ASN:O    | 1:A:35:HIS:CB      | 0.59     | 2.50        | 19     | 31    |
| 1:A:26:TYR:O    | 1:A:30:ILE:HD13    | 0.59     | 1.96        | 27     | 3     |
| 1:A:38:ARG:N    | 1:A:38:ARG:CD      | 0.59     | 2.63        | 8      | 1     |
| 1:A:11:ALA:HB2  | 1:A:19:THR:OG1     | 0.59     | 1.96        | 12     | 3     |
| 1:A:5:ILE:HG22  | 1:A:10:TYR:CB      | 0.59     | 2.25        | 14     | 9     |
| 1:A:38:ARG:CD   | 1:A:38:ARG:N       | 0.59     | 2.65        | 22     | 6     |
| 1:A:31:ASN:O    | 1:A:35:HIS:CG      | 0.59     | 2.55        | 8      | 2     |
| 1:A:43:THR:CG2  | 1:A:43:THR:O       | 0.59     | 2.51        | 8      | 1     |
| 1:A:7:LEU:CD1   | 1:A:19:THR:CG2     | 0.59     | 2.80        | 25     | 1     |
| 1:A:31:ASN:OD1  | 1:A:35:HIS:CE1     | 0.59     | 2.55        | 28     | 1     |
| 1:A:40:ILE:C    | 1:A:41:PHE:CD2     | 0.58     | 2.80        | 14     | 16    |
| 1:A:40:ILE:O    | 1:A:41:PHE:CD1     | 0.58     | 2.56        | 1      | 16    |
| 1:A:31:ASN:O    | 1:A:35:HIS:HB2     | 0.58     | 1.98        | 28     | 15    |
| 1:A:3:GLN:CB    | 1:A:45:ASN:ND2     | 0.58     | 2.66        | 15     | 1     |
| 1:A:40:ILE:O    | 1:A:41:PHE:CD2     | 0.58     | 2.56        | 8      | 2     |
| 1:A:4:ARG:NH1   | 1:A:41:PHE:CG      | 0.58     | 2.72        | 29     | 1     |
| 1:A:25:VAL:CG1  | 1:A:30:ILE:CD1     | 0.58     | 2.81        | 17     | 1     |
| 1:A:16:GLN:NE2  | 1:A:30:ILE:CG2     | 0.58     | 2.66        | 31     | 2     |
| 1:A:58:PHE:CG   | 1:A:58:PHE:O       | 0.58     | 2.55        | 1      | 1     |
| 1:A:54:GLU:C    | 1:A:55:VAL:CG2     | 0.58     | 2.77        | 19     | 12    |
| 1:A:44:ILE:HG22 | 1:A:45:ASN:H       | 0.58     | 1.57        | 7      | 5     |
| 1:A:44:ILE:CG2  | 1:A:45:ASN:N       | 0.58     | 2.67        | 21     | 1     |
| 1:A:52:ALA:HB3  | 1:A:58:PHE:O       | 0.58     | 1.99        | 13     | 9     |
| 1:A:42:LEU:N    | 1:A:42:LEU:CD1     | 0.58     | 2.66        | 27     | 11    |
| 1:A:45:ASN:C    | 1:A:47:ASP:H       | 0.58     | 2.06        | 28     | 1     |
| 1:A:10:TYR:CZ   | 1:A:44:ILE:HD11    | 0.58     | 2.33        | 11     | 5     |
| 1:A:10:TYR:CE1  | 1:A:44:ILE:HD11    | 0.58     | 2.34        | 28     | 1     |
| 1:A:39:LYS:O    | 1:A:41:PHE:CE2     | 0.57     | 2.57        | 20     | 4     |
| 1:A:8:LYS:HB2   | 1:A:34:ILE:HG23    | 0.57     | 1.76        | 19     | 3     |
| 1:A:30:ILE:CG2  | 1:A:31:ASN:N       | 0.57     | 2.67        | 11     | 13    |
| 1:A:45:ASN:ND2  | 1:A:45:ASN:N       | 0.57     | 2.52        | 5      | 3     |
| 1:A:7:LEU:HD23  | 1:A:34:ILE:HG13    | 0.57     | 1.76        | 21     | 1     |
| 1:A:55:VAL:HG22 | 1:A:56(D):VAL:HG12 | 0.57     | 1.76        | 26     | 3     |
| 1:A:7:LEU:HD21  | 1:A:34:ILE:HG13    | 0.57     | 1.77        | 14     | 2     |
| 1:A:10:TYR:O    | 1:A:14:PHE:CE2     | 0.57     | 2.58        | 15     | 1     |
| 1:A:8:LYS:CG    | 1:A:34:ILE:CG2     | 0.57     | 2.82        | 25     | 4     |
| 1:A:34:ILE:O    | 1:A:38:ARG:CD      | 0.57     | 2.53        | 14     | 8     |

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| Atom-1          | Atom-2            | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-------------------|----------|-------------|--------|-------|
|                 |                   |          |             | Worst  | Total |
| 1:A:33:ALA:CB   | 1:A:58:PHE:CE1    | 0.57     | 2.88        | 7      | 2     |
| 1:A:30:ILE:HD12 | 1:A:30:ILE:N      | 0.57     | 2.14        | 29     | 2     |
| 1:A:7:LEU:CD1   | 1:A:42:LEU:CD2    | 0.57     | 2.83        | 10     | 4     |
| 1:A:38:ARG:HG3  | 1:A:40:ILE:HD11   | 0.57     | 1.77        | 11     | 2     |
| 1:A:36:ALA:O    | 1:A:38:ARG:N      | 0.57     | 2.38        | 23     | 1     |
| 1:A:23:LEU:HD22 | 1:A:42:LEU:HD23   | 0.57     | 1.76        | 6      | 1     |
| 1:A:22:ASP:OD1  | 1:A:50:VAL:CG1    | 0.57     | 2.52        | 21     | 1     |
| 1:A:7:LEU:CD1   | 1:A:23:LEU:CD1    | 0.57     | 2.83        | 22     | 1     |
| 1:A:23:LEU:CD2  | 1:A:42:LEU:CD2    | 0.56     | 2.83        | 6      | 2     |
| 1:A:8:LYS:HG2   | 1:A:34:ILE:HG21   | 0.56     | 1.77        | 16     | 2     |
| 1:A:40:ILE:HG23 | 1:A:53:GLU:O      | 0.56     | 2.00        | 20     | 1     |
| 1:A:7:LEU:HD11  | 1:A:34:ILE:HG12   | 0.56     | 1.78        | 32     | 2     |
| 1:A:45:ASN:N    | 1:A:45:ASN:OD1    | 0.56     | 2.38        | 9      | 4     |
| 1:A:6:THR:O     | 1:A:10:TYR:HB2    | 0.56     | 2.00        | 24     | 28    |
| 1:A:49:SER:O    | 1:A:50:VAL:CG2    | 0.56     | 2.52        | 15     | 4     |
| 1:A:7:LEU:HD11  | 1:A:42:LEU:CD2    | 0.56     | 2.31        | 18     | 2     |
| 1:A:23:LEU:O    | 1:A:23:LEU:CG     | 0.56     | 2.53        | 22     | 1     |
| 1:A:40:ILE:HD13 | 1:A:54:GLU:HB2    | 0.56     | 1.75        | 32     | 1     |
| 1:A:46:ALA:HB3  | 1:A:49:SER:HB3    | 0.56     | 1.78        | 13     | 4     |
| 1:A:25:VAL:HG11 | 1:A:29:ALA:CB     | 0.56     | 2.29        | 29     | 1     |
| 1:A:46:ALA:O    | 1:A:47:ASP:HB3    | 0.56     | 2.01        | 13     | 10    |
| 1:A:25:VAL:CG1  | 1:A:29:ALA:CB     | 0.56     | 2.84        | 29     | 2     |
| 1:A:8:LYS:CD    | 1:A:8:LYS:C       | 0.56     | 2.78        | 23     | 6     |
| 1:A:45:ASN:CG   | 1:A:46:ALA:N      | 0.56     | 2.61        | 7      | 2     |
| 1:A:7:LEU:H     | 1:A:7:LEU:HD22    | 0.56     | 1.59        | 10     | 1     |
| 1:A:7:LEU:HD11  | 1:A:23:LEU:HD11   | 0.56     | 1.75        | 31     | 1     |
| 1:A:10:TYR:CE1  | 1:A:14:PHE:CE1    | 0.56     | 2.93        | 12     | 1     |
| 1:A:23:LEU:HD21 | 1:A:42:LEU:HD21   | 0.56     | 1.77        | 26     | 1     |
| 1:A:7:LEU:CD2   | 1:A:34:ILE:CG1    | 0.55     | 2.84        | 7      | 4     |
| 1:A:55:VAL:HG22 | 1:A:56(D):VAL:CG2 | 0.55     | 2.31        | 32     | 1     |
| 1:A:58:PHE:CD2  | 1:A:58:PHE:O      | 0.55     | 2.60        | 21     | 2     |
| 1:A:23:LEU:CB   | 1:A:42:LEU:HD21   | 0.55     | 2.31        | 22     | 1     |
| 1:A:25:VAL:HG22 | 1:A:59:PRO:HG3    | 0.55     | 1.77        | 22     | 1     |
| 1:A:7:LEU:CB    | 1:A:40:ILE:HG21   | 0.55     | 2.31        | 3      | 2     |
| 1:A:7:LEU:HB3   | 1:A:40:ILE:HG21   | 0.55     | 1.78        | 14     | 3     |
| 1:A:56:LYS:O    | 1:A:56(B):GLY:N   | 0.55     | 2.39        | 7      | 18    |
| 1:A:24:GLY:C    | 1:A:25:VAL:CG2    | 0.55     | 2.79        | 8      | 3     |
| 1:A:33:ALA:O    | 1:A:40:ILE:CD1    | 0.55     | 2.54        | 23     | 1     |
| 1:A:52:ALA:CB   | 1:A:58:PHE:O      | 0.55     | 2.55        | 31     | 8     |
| 1:A:33:ALA:O    | 1:A:38:ARG:CB     | 0.55     | 2.55        | 19     | 1     |
| 1:A:11:ALA:HB2  | 1:A:19:THR:CB     | 0.54     | 2.32        | 12     | 1     |

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| Atom-1          | Atom-2             | Clash(Å) | Distance(Å) | Models |       |
|-----------------|--------------------|----------|-------------|--------|-------|
|                 |                    |          |             | Worst  | Total |
| 1:A:43:THR:O    | 1:A:49:SER:O       | 0.54     | 2.25        | 21     | 1     |
| 1:A:7:LEU:CD1   | 1:A:42:LEU:CD1     | 0.54     | 2.79        | 4      | 5     |
| 1:A:8:LYS:HG2   | 1:A:34:ILE:HG23    | 0.54     | 1.78        | 10     | 2     |
| 1:A:20:ALA:CB   | 1:A:30:ILE:HD13    | 0.54     | 2.32        | 10     | 1     |
| 1:A:30:ILE:CG2  | 1:A:34:ILE:CD1     | 0.54     | 2.86        | 10     | 3     |
| 1:A:22:ASP:OD1  | 1:A:50:VAL:CG2     | 0.54     | 2.56        | 27     | 1     |
| 1:A:6:THR:OG1   | 1:A:9:ASP:CB       | 0.54     | 2.56        | 21     | 9     |
| 1:A:4:ARG:O     | 1:A:4:ARG:CD       | 0.54     | 2.56        | 5      | 3     |
| 1:A:26:TYR:O    | 1:A:28:SER:N       | 0.54     | 2.41        | 6      | 3     |
| 1:A:44:ILE:O    | 1:A:45:ASN:CB      | 0.54     | 2.56        | 7      | 1     |
| 1:A:43:THR:HG22 | 1:A:48:GLY:O       | 0.54     | 2.03        | 21     | 1     |
| 1:A:44:ILE:CG1  | 1:A:50:VAL:HG22    | 0.54     | 2.32        | 22     | 1     |
| 1:A:55:VAL:C    | 1:A:56(D):VAL:HG12 | 0.54     | 2.27        | 25     | 1     |
| 1:A:40:ILE:HG22 | 1:A:41:PHE:N       | 0.54     | 2.18        | 16     | 4     |
| 1:A:10:TYR:CD1  | 1:A:14:PHE:CE1     | 0.54     | 2.96        | 12     | 1     |
| 1:A:38:ARG:CD   | 1:A:38:ARG:C       | 0.54     | 2.80        | 28     | 2     |
| 1:A:40:ILE:CG2  | 1:A:53:GLU:O       | 0.54     | 2.55        | 20     | 1     |
| 1:A:7:LEU:CD2   | 1:A:42:LEU:HD11    | 0.54     | 2.33        | 31     | 1     |
| 1:A:43:THR:CG2  | 1:A:48:GLY:O       | 0.54     | 2.56        | 21     | 1     |
| 1:A:11:ALA:O    | 1:A:15:GLY:N       | 0.53     | 2.42        | 27     | 8     |
| 1:A:43:THR:OG1  | 1:A:51:TYR:CB      | 0.53     | 2.56        | 2      | 1     |
| 1:A:4:ARG:HA    | 1:A:42:LEU:O       | 0.53     | 2.04        | 4      | 13    |
| 1:A:20:ALA:CA   | 1:A:24:GLY:O       | 0.53     | 2.56        | 22     | 1     |
| 1:A:38:ARG:O    | 1:A:39:LYS:CB      | 0.53     | 2.55        | 14     | 4     |
| 1:A:7:LEU:HD11  | 1:A:30:ILE:HD12    | 0.53     | 1.80        | 25     | 1     |
| 1:A:14:PHE:CE1  | 1:A:18:LYS:HB3     | 0.53     | 2.37        | 25     | 1     |
| 1:A:54:GLU:OE1  | 1:A:56(C):GLU:CB   | 0.53     | 2.57        | 25     | 1     |
| 1:A:34:ILE:HA   | 1:A:38:ARG:CD      | 0.53     | 2.33        | 27     | 1     |
| 1:A:7:LEU:CD2   | 1:A:34:ILE:HG12    | 0.53     | 2.33        | 7      | 8     |
| 1:A:10:TYR:CE2  | 1:A:14:PHE:CZ      | 0.53     | 2.96        | 15     | 1     |
| 1:A:43:THR:O    | 1:A:43:THR:CG2     | 0.53     | 2.56        | 17     | 2     |
| 1:A:7:LEU:HB3   | 1:A:34:ILE:HD12    | 0.53     | 1.79        | 2      | 1     |
| 1:A:59:PRO:O    | 1:A:60:SER:C       | 0.53     | 2.52        | 8      | 8     |
| 1:A:19:THR:O    | 1:A:23:LEU:CD2     | 0.53     | 2.57        | 17     | 2     |
| 1:A:38:ARG:HD3  | 1:A:38:ARG:O       | 0.53     | 2.03        | 28     | 1     |
| 1:A:45:ASN:C    | 1:A:47:ASP:N       | 0.53     | 2.66        | 28     | 9     |
| 1:A:44:ILE:CG2  | 1:A:49:SER:O       | 0.53     | 2.56        | 15     | 6     |
| 1:A:5:ILE:HB    | 1:A:10:TYR:CD1     | 0.53     | 2.38        | 31     | 1     |
| 1:A:26:TYR:O    | 1:A:30:ILE:CD1     | 0.53     | 2.57        | 32     | 1     |
| 1:A:53:GLU:CG   | 1:A:56(E):LYS:O    | 0.53     | 2.57        | 2      | 1     |
| 1:A:4:ARG:O     | 1:A:4:ARG:HD3      | 0.53     | 2.04        | 5      | 4     |

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| Atom-1          | Atom-2            | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-------------------|----------|-------------|--------|-------|
|                 |                   |          |             | Worst  | Total |
| 1:A:5:ILE:HG22  | 1:A:6:THR:H       | 0.53     | 1.64        | 32     | 2     |
| 1:A:5:ILE:CG2   | 1:A:10:TYR:CG     | 0.53     | 2.92        | 13     | 1     |
| 1:A:41:PHE:O    | 1:A:53:GLU:CB     | 0.53     | 2.57        | 29     | 2     |
| 1:A:42:LEU:HD23 | 1:A:50:VAL:HG13   | 0.53     | 1.81        | 27     | 1     |
| 1:A:55:VAL:HG13 | 1:A:56(D):VAL:CG1 | 0.53     | 2.33        | 30     | 1     |
| 1:A:54:GLU:OE2  | 1:A:58:PHE:CD1    | 0.53     | 2.62        | 4      | 1     |
| 1:A:20:ALA:O    | 1:A:24:GLY:C      | 0.53     | 2.52        | 22     | 2     |
| 1:A:54:GLU:CD   | 1:A:58:PHE:CD2    | 0.52     | 2.87        | 14     | 1     |
| 1:A:19:THR:O    | 1:A:23:LEU:HD21   | 0.52     | 2.03        | 17     | 1     |
| 1:A:7:LEU:HD22  | 1:A:40:ILE:HG13   | 0.52     | 1.81        | 32     | 1     |
| 1:A:23:LEU:HD21 | 1:A:42:LEU:CD2    | 0.52     | 2.34        | 1      | 2     |
| 1:A:16:GLN:OE1  | 1:A:30:ILE:HG21   | 0.52     | 2.04        | 7      | 1     |
| 1:A:19:THR:HG23 | 1:A:23:LEU:HD21   | 0.52     | 1.80        | 22     | 1     |
| 1:A:16:GLN:CG   | 1:A:17:THR:N      | 0.52     | 2.72        | 28     | 1     |
| 1:A:7:LEU:HD12  | 1:A:42:LEU:HD21   | 0.52     | 1.81        | 21     | 2     |
| 1:A:39:LYS:CG   | 1:A:39:LYS:O      | 0.52     | 2.57        | 6      | 2     |
| 1:A:38:ARG:O    | 1:A:38:ARG:HD3    | 0.52     | 2.05        | 8      | 1     |
| 1:A:43:THR:O    | 1:A:43:THR:HG23   | 0.52     | 2.03        | 8      | 1     |
| 1:A:38:ARG:C    | 1:A:38:ARG:HD3    | 0.52     | 2.29        | 10     | 3     |
| 1:A:38:ARG:CG   | 1:A:40:ILE:HD11   | 0.52     | 2.34        | 19     | 2     |
| 1:A:38:ARG:NE   | 1:A:40:ILE:HD11   | 0.52     | 2.19        | 8      | 2     |
| 1:A:33:ALA:HB1  | 1:A:58:PHE:CZ     | 0.52     | 2.39        | 15     | 1     |
| 1:A:20:ALA:CB   | 1:A:24:GLY:O      | 0.52     | 2.57        | 22     | 1     |
| 1:A:44:ILE:O    | 1:A:45:ASN:OD1    | 0.52     | 2.27        | 7      | 3     |
| 1:A:44:ILE:O    | 1:A:45:ASN:C      | 0.52     | 2.53        | 16     | 8     |
| 1:A:54:GLU:C    | 1:A:55:VAL:HG23   | 0.52     | 2.29        | 3      | 7     |
| 1:A:57:PRO:O    | 1:A:58:PHE:C      | 0.52     | 2.50        | 4      | 6     |
| 1:A:4:ARG:CZ    | 1:A:41:PHE:CB     | 0.52     | 2.88        | 29     | 1     |
| 1:A:7:LEU:CA    | 1:A:42:LEU:CD1    | 0.52     | 2.88        | 7      | 5     |
| 1:A:5:ILE:HG23  | 1:A:10:TYR:HB2    | 0.52     | 1.82        | 11     | 1     |
| 1:A:10:TYR:CZ   | 1:A:14:PHE:CE2    | 0.52     | 2.98        | 25     | 1     |
| 1:A:5:ILE:O     | 1:A:42:LEU:CD1    | 0.52     | 2.58        | 8      | 1     |
| 1:A:33:ALA:O    | 1:A:34:ILE:HD13   | 0.52     | 2.05        | 30     | 1     |
| 1:A:31:ASN:O    | 1:A:35:HIS:HB3    | 0.52     | 2.05        | 5      | 20    |
| 1:A:5:ILE:HD12  | 1:A:10:TYR:CD1    | 0.52     | 2.40        | 20     | 3     |
| 1:A:3:GLN:HB3   | 1:A:45:ASN:ND2    | 0.51     | 2.21        | 15     | 1     |
| 1:A:58:PHE:CD1  | 1:A:58:PHE:C      | 0.51     | 2.88        | 27     | 6     |
| 1:A:22:ASP:OD1  | 1:A:23:LEU:N      | 0.51     | 2.43        | 9      | 1     |
| 1:A:14:PHE:CD1  | 1:A:14:PHE:O      | 0.51     | 2.62        | 25     | 1     |
| 1:A:32:LYS:O    | 1:A:36:ALA:CB     | 0.51     | 2.58        | 1      | 5     |
| 1:A:6:THR:O     | 1:A:10:TYR:HB3    | 0.51     | 2.05        | 4      | 13    |

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| Atom-1          | Atom-2            | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-------------------|----------|-------------|--------|-------|
|                 |                   |          |             | Worst  | Total |
| 1:A:48:GLY:C    | 1:A:49:SER:HG     | 0.51     | 2.13        | 9      | 1     |
| 1:A:10:TYR:CD1  | 1:A:14:PHE:CZ     | 0.51     | 2.98        | 12     | 1     |
| 1:A:7:LEU:CD2   | 1:A:34:ILE:HG13   | 0.51     | 2.35        | 14     | 1     |
| 1:A:14:PHE:CD1  | 1:A:15:GLY:N      | 0.51     | 2.78        | 15     | 1     |
| 1:A:52:ALA:O    | 1:A:57:PRO:HA     | 0.51     | 2.06        | 20     | 1     |
| 1:A:56(D):VAL:O | 1:A:56(D):VAL:CG2 | 0.51     | 2.56        | 2      | 2     |
| 1:A:42:LEU:HA   | 1:A:51:TYR:O      | 0.51     | 2.06        | 4      | 12    |
| 1:A:7:LEU:HB3   | 1:A:40:ILE:CG2    | 0.51     | 2.36        | 7      | 2     |
| 1:A:26:TYR:CD1  | 1:A:28:SER:HB2    | 0.51     | 2.41        | 4      | 1     |
| 1:A:22:ASP:OD2  | 1:A:50:VAL:CG2    | 0.51     | 2.58        | 5      | 1     |
| 1:A:46:ALA:C    | 1:A:47:ASP:CG     | 0.51     | 2.78        | 28     | 1     |
| 1:A:53:GLU:OE1  | 1:A:56(D):VAL:CG2 | 0.51     | 2.59        | 32     | 1     |
| 1:A:46:ALA:O    | 1:A:47:ASP:HB2    | 0.51     | 2.06        | 12     | 2     |
| 1:A:33:ALA:HB2  | 1:A:58:PHE:CE1    | 0.51     | 2.41        | 7      | 1     |
| 1:A:48:GLY:C    | 1:A:49:SER:OG     | 0.51     | 2.53        | 9      | 1     |
| 1:A:7:LEU:CG    | 1:A:30:ILE:HG23   | 0.51     | 2.36        | 2      | 1     |
| 1:A:34:ILE:HA   | 1:A:40:ILE:HD11   | 0.51     | 1.82        | 7      | 1     |
| 1:A:30:ILE:N    | 1:A:30:ILE:HD12   | 0.51     | 2.20        | 2      | 3     |
| 1:A:23:LEU:HD13 | 1:A:30:ILE:HD11   | 0.51     | 1.82        | 5      | 1     |
| 1:A:37:GLY:O    | 1:A:38:ARG:O      | 0.51     | 2.29        | 14     | 2     |
| 1:A:8:LYS:CD    | 1:A:34:ILE:HG22   | 0.51     | 2.36        | 22     | 1     |
| 1:A:16:GLN:HG3  | 1:A:17:THR:N      | 0.51     | 2.21        | 28     | 1     |
| 1:A:10:TYR:CZ   | 1:A:44:ILE:CD1    | 0.51     | 2.93        | 28     | 5     |
| 1:A:38:ARG:H    | 1:A:38:ARG:HD2    | 0.51     | 1.66        | 10     | 1     |
| 1:A:5:ILE:CD1   | 1:A:10:TYR:CE1    | 0.51     | 2.94        | 17     | 1     |
| 1:A:38:ARG:HG2  | 1:A:40:ILE:CG1    | 0.51     | 2.36        | 18     | 1     |
| 1:A:8:LYS:HG3   | 1:A:34:ILE:CG2    | 0.51     | 2.35        | 25     | 3     |
| 1:A:44:ILE:HD13 | 1:A:50:VAL:HG22   | 0.51     | 1.83        | 10     | 1     |
| 1:A:22:ASP:C    | 1:A:50:VAL:HG11   | 0.51     | 2.30        | 32     | 1     |
| 1:A:57:PRO:O    | 1:A:58:PHE:O      | 0.50     | 2.30        | 26     | 6     |
| 1:A:46:ALA:CB   | 1:A:49:SER:HB2    | 0.50     | 2.33        | 25     | 2     |
| 1:A:16:GLN:O    | 1:A:20:ALA:CB     | 0.50     | 2.59        | 6      | 2     |
| 1:A:37:GLY:O    | 1:A:38:ARG:C      | 0.50     | 2.54        | 27     | 1     |
| 1:A:10:TYR:O    | 1:A:14:PHE:CE1    | 0.50     | 2.64        | 12     | 1     |
| 1:A:43:THR:CG2  | 1:A:48:GLY:HA2    | 0.50     | 2.36        | 15     | 1     |
| 1:A:44:ILE:O    | 1:A:48:GLY:C      | 0.50     | 2.54        | 21     | 1     |
| 1:A:52:ALA:HB1  | 1:A:58:PHE:O      | 0.50     | 2.04        | 17     | 2     |
| 1:A:7:LEU:HD23  | 1:A:34:ILE:CD1    | 0.50     | 2.34        | 21     | 1     |
| 1:A:14:PHE:CD1  | 1:A:14:PHE:C      | 0.50     | 2.89        | 25     | 1     |
| 1:A:42:LEU:HD23 | 1:A:50:VAL:HG21   | 0.50     | 1.82        | 32     | 1     |
| 1:A:34:ILE:O    | 1:A:38:ARG:HD2    | 0.50     | 2.05        | 2      | 6     |

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| Atom-1          | Atom-2             | Clash(Å) | Distance(Å) | Models |       |
|-----------------|--------------------|----------|-------------|--------|-------|
|                 |                    |          |             | Worst  | Total |
| 1:A:22:ASP:OD1  | 1:A:50:VAL:CB      | 0.50     | 2.60        | 27     | 1     |
| 1:A:53:GLU:HA   | 1:A:56(E):LYS:O    | 0.50     | 2.06        | 16     | 9     |
| 1:A:30:ILE:HG23 | 1:A:34:ILE:HD11    | 0.50     | 1.84        | 14     | 1     |
| 1:A:41:PHE:CD1  | 1:A:41:PHE:N       | 0.50     | 2.79        | 30     | 1     |
| 1:A:17:THR:O    | 1:A:21:LYS:CG      | 0.50     | 2.60        | 2      | 1     |
| 1:A:19:THR:O    | 1:A:23:LEU:CD1     | 0.50     | 2.59        | 9      | 1     |
| 1:A:7:LEU:HD11  | 1:A:30:ILE:HD11    | 0.50     | 1.84        | 15     | 2     |
| 1:A:50:VAL:O    | 1:A:50:VAL:CG1     | 0.50     | 2.57        | 15     | 2     |
| 1:A:49:SER:C    | 1:A:50:VAL:HG23    | 0.50     | 2.31        | 30     | 4     |
| 1:A:6:THR:HG22  | 1:A:7:LEU:H        | 0.50     | 1.66        | 22     | 9     |
| 1:A:43:THR:CG2  | 1:A:45:ASN:ND2     | 0.50     | 2.74        | 4      | 1     |
| 1:A:20:ALA:HB2  | 1:A:27:GLN:HG3     | 0.50     | 1.83        | 21     | 1     |
| 1:A:25:VAL:CG2  | 1:A:59:PRO:HG3     | 0.50     | 2.37        | 22     | 1     |
| 1:A:5:ILE:CG2   | 1:A:10:TYR:HB2     | 0.50     | 2.37        | 16     | 8     |
| 1:A:26:TYR:O    | 1:A:27:GLN:C       | 0.49     | 2.54        | 6      | 7     |
| 1:A:56(D):VAL:C | 1:A:56(E):LYS:CG   | 0.49     | 2.84        | 10     | 5     |
| 1:A:23:LEU:HD23 | 1:A:23:LEU:N       | 0.49     | 2.22        | 7      | 3     |
| 1:A:55:VAL:HG13 | 1:A:56(D):VAL:HG12 | 0.49     | 1.83        | 23     | 3     |
| 1:A:51:TYR:O    | 1:A:52:ALA:C       | 0.49     | 2.54        | 29     | 1     |
| 1:A:22:ASP:O    | 1:A:50:VAL:CG1     | 0.49     | 2.60        | 32     | 1     |
| 1:A:8:LYS:O     | 1:A:9:ASP:C        | 0.49     | 2.53        | 11     | 24    |
| 1:A:7:LEU:HD21  | 1:A:34:ILE:HD11    | 0.49     | 1.84        | 24     | 2     |
| 1:A:23:LEU:O    | 1:A:23:LEU:HD12    | 0.49     | 2.05        | 22     | 1     |
| 1:A:25:VAL:HG12 | 1:A:29:ALA:HB3     | 0.49     | 1.82        | 26     | 1     |
| 1:A:42:LEU:HB3  | 1:A:50:VAL:HG23    | 0.49     | 1.83        | 32     | 1     |
| 1:A:8:LYS:HG2   | 1:A:34:ILE:CG2     | 0.49     | 2.37        | 28     | 8     |
| 1:A:38:ARG:HD2  | 1:A:38:ARG:N       | 0.49     | 2.22        | 2      | 3     |
| 1:A:23:LEU:CD1  | 1:A:25:VAL:HG23    | 0.49     | 2.37        | 8      | 1     |
| 1:A:34:ILE:O    | 1:A:35:HIS:C       | 0.49     | 2.54        | 8      | 2     |
| 1:A:38:ARG:CD   | 1:A:40:ILE:CG1     | 0.49     | 2.90        | 8      | 1     |
| 1:A:38:ARG:HD3  | 1:A:40:ILE:CG1     | 0.49     | 2.37        | 8      | 1     |
| 1:A:7:LEU:CD2   | 1:A:40:ILE:HB      | 0.49     | 2.37        | 16     | 2     |
| 1:A:42:LEU:HD12 | 1:A:42:LEU:H       | 0.49     | 1.67        | 23     | 1     |
| 1:A:10:TYR:CZ   | 1:A:44:ILE:HD12    | 0.49     | 2.42        | 9      | 2     |
| 1:A:58:PHE:O    | 1:A:58:PHE:CG      | 0.49     | 2.66        | 20     | 2     |
| 1:A:44:ILE:HG23 | 1:A:45:ASN:N       | 0.49     | 2.23        | 21     | 1     |
| 1:A:40:ILE:HG23 | 1:A:54:GLU:N       | 0.49     | 2.22        | 30     | 1     |
| 1:A:33:ALA:O    | 1:A:37:GLY:O       | 0.49     | 2.30        | 25     | 3     |
| 1:A:11:ALA:CB   | 1:A:19:THR:OG1     | 0.49     | 2.60        | 27     | 3     |
| 1:A:3:GLN:O     | 1:A:3:GLN:HG2      | 0.49     | 2.06        | 18     | 1     |
| 1:A:44:ILE:O    | 1:A:45:ASN:CG      | 0.49     | 2.55        | 7      | 1     |

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| Atom-1            | Atom-2             | Clash(Å) | Distance(Å) | Models |       |
|-------------------|--------------------|----------|-------------|--------|-------|
|                   |                    |          |             | Worst  | Total |
| 1:A:48:GLY:O      | 1:A:49:SER:O       | 0.49     | 2.30        | 21     | 3     |
| 1:A:54:GLU:O      | 1:A:56(D):VAL:C    | 0.49     | 2.56        | 25     | 1     |
| 1:A:40:ILE:CG2    | 1:A:41:PHE:N       | 0.49     | 2.76        | 16     | 2     |
| 1:A:45:ASN:O      | 1:A:46:ALA:C       | 0.49     | 2.56        | 11     | 5     |
| 1:A:30:ILE:HG23   | 1:A:34:ILE:CD1     | 0.49     | 2.37        | 12     | 5     |
| 1:A:42:LEU:HD23   | 1:A:52:ALA:HB2     | 0.49     | 1.84        | 16     | 2     |
| 1:A:6:THR:CB      | 1:A:9:ASP:HB2      | 0.49     | 2.38        | 20     | 7     |
| 1:A:7:LEU:HD13    | 1:A:7:LEU:N        | 0.49     | 2.23        | 10     | 3     |
| 1:A:11:ALA:HB1    | 1:A:16:GLN:HA      | 0.49     | 1.84        | 4      | 1     |
| 1:A:28:SER:O      | 1:A:29:ALA:C       | 0.49     | 2.55        | 5      | 17    |
| 1:A:24:GLY:C      | 1:A:25:VAL:HG23    | 0.49     | 2.33        | 8      | 1     |
| 1:A:8:LYS:CG      | 1:A:34:ILE:HG21    | 0.49     | 2.37        | 29     | 3     |
| 1:A:56(E):LYS:HB3 | 1:A:57:PRO:CD      | 0.48     | 2.38        | 9      | 4     |
| 1:A:23:LEU:CD1    | 1:A:30:ILE:HD11    | 0.48     | 2.37        | 5      | 1     |
| 1:A:45:ASN:OD1    | 1:A:45:ASN:C       | 0.48     | 2.56        | 7      | 3     |
| 1:A:56(D):VAL:O   | 1:A:56(E):LYS:HG2  | 0.48     | 2.08        | 25     | 5     |
| 1:A:54:GLU:O      | 1:A:56(D):VAL:CA   | 0.48     | 2.61        | 25     | 1     |
| 1:A:7:LEU:CD1     | 1:A:7:LEU:N        | 0.48     | 2.75        | 16     | 2     |
| 1:A:44:ILE:C      | 1:A:45:ASN:OD1     | 0.48     | 2.56        | 28     | 4     |
| 1:A:25:VAL:HG12   | 1:A:30:ILE:CD1     | 0.48     | 2.37        | 17     | 1     |
| 1:A:14:PHE:O      | 1:A:15:GLY:O       | 0.48     | 2.31        | 28     | 2     |
| 1:A:43:THR:O      | 1:A:43:THR:OG1     | 0.48     | 2.31        | 3      | 2     |
| 1:A:38:ARG:O      | 1:A:39:LYS:HB2     | 0.48     | 2.08        | 28     | 3     |
| 1:A:25:VAL:HG12   | 1:A:26:TYR:H       | 0.48     | 1.68        | 27     | 1     |
| 1:A:43:THR:OG1    | 1:A:51:TYR:HB2     | 0.48     | 2.08        | 2      | 3     |
| 1:A:7:LEU:HG      | 1:A:34:ILE:CD1     | 0.48     | 2.38        | 12     | 4     |
| 1:A:5:ILE:O       | 1:A:6:THR:O        | 0.48     | 2.31        | 14     | 8     |
| 1:A:38:ARG:HG2    | 1:A:40:ILE:HG13    | 0.48     | 1.85        | 18     | 1     |
| 1:A:22:ASP:OD2    | 1:A:50:VAL:HG21    | 0.48     | 2.09        | 20     | 2     |
| 1:A:8:LYS:HD3     | 1:A:34:ILE:CG2     | 0.48     | 2.38        | 32     | 2     |
| 1:A:39:LYS:CG     | 1:A:55:VAL:O       | 0.48     | 2.61        | 8      | 1     |
| 1:A:7:LEU:HD23    | 1:A:34:ILE:HD11    | 0.48     | 1.85        | 21     | 1     |
| 1:A:19:THR:O      | 1:A:23:LEU:HG      | 0.48     | 2.09        | 22     | 2     |
| 1:A:45:ASN:OD1    | 1:A:46:ALA:N       | 0.48     | 2.46        | 21     | 2     |
| 1:A:7:LEU:HB2     | 1:A:42:LEU:CD1     | 0.48     | 2.38        | 7      | 2     |
| 1:A:44:ILE:O      | 1:A:45:ASN:O       | 0.48     | 2.32        | 28     | 5     |
| 1:A:54:GLU:N      | 1:A:56(E):LYS:O    | 0.48     | 2.47        | 25     | 3     |
| 1:A:35:HIS:CD2    | 1:A:35:HIS:C       | 0.48     | 2.91        | 15     | 1     |
| 1:A:55:VAL:HB     | 1:A:56(D):VAL:HG12 | 0.48     | 1.86        | 14     | 1     |
| 1:A:25:VAL:HG11   | 1:A:59:PRO:HG2     | 0.48     | 1.85        | 16     | 1     |
| 1:A:9:ASP:O       | 1:A:10:TYR:C       | 0.48     | 2.56        | 16     | 7     |

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| Atom-1            | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|-------------------|------------------|----------|-------------|--------|-------|
|                   |                  |          |             | Worst  | Total |
| 1:A:31:ASN:O      | 1:A:32:LYS:C     | 0.48     | 2.53        | 2      | 1     |
| 1:A:45:ASN:ND2    | 1:A:49:SER:CB    | 0.48     | 2.76        | 2      | 2     |
| 1:A:59:PRO:C      | 1:A:60:SER:OG    | 0.48     | 2.56        | 16     | 1     |
| 1:A:22:ASP:C      | 1:A:22:ASP:OD1   | 0.47     | 2.57        | 10     | 2     |
| 1:A:38:ARG:O      | 1:A:38:ARG:HG2   | 0.47     | 2.08        | 10     | 1     |
| 1:A:56(A):ASP:OD1 | 1:A:56(A):ASP:C  | 0.47     | 2.57        | 25     | 1     |
| 1:A:44:ILE:HA     | 1:A:49:SER:O     | 0.47     | 2.09        | 4      | 6     |
| 1:A:53:GLU:CA     | 1:A:56(E):LYS:O  | 0.47     | 2.61        | 4      | 1     |
| 1:A:13:ARG:HB3    | 1:A:14:PHE:CD1   | 0.47     | 2.44        | 12     | 1     |
| 1:A:40:ILE:CD1    | 1:A:54:GLU:HB2   | 0.47     | 2.40        | 32     | 1     |
| 1:A:23:LEU:CD1    | 1:A:25:VAL:HG21  | 0.47     | 2.35        | 17     | 1     |
| 1:A:38:ARG:CG     | 1:A:40:ILE:HG13  | 0.47     | 2.39        | 18     | 1     |
| 1:A:5:ILE:O       | 1:A:42:LEU:HD13  | 0.47     | 2.09        | 8      | 1     |
| 1:A:19:THR:O      | 1:A:22:ASP:OD2   | 0.47     | 2.32        | 29     | 2     |
| 1:A:10:TYR:CE2    | 1:A:44:ILE:CD1   | 0.47     | 2.98        | 21     | 2     |
| 1:A:10:TYR:HH     | 1:A:14:PHE:HE2   | 0.47     | 1.52        | 25     | 1     |
| 1:A:14:PHE:CZ     | 1:A:19:THR:OG1   | 0.47     | 2.66        | 15     | 1     |
| 1:A:38:ARG:CG     | 1:A:40:ILE:CG1   | 0.47     | 2.93        | 18     | 1     |
| 1:A:45:ASN:OD1    | 1:A:45:ASN:N     | 0.47     | 2.48        | 10     | 2     |
| 1:A:23:LEU:HD22   | 1:A:58:PHE:CE1   | 0.47     | 2.45        | 5      | 1     |
| 1:A:20:ALA:HB2    | 1:A:30:ILE:HG13  | 0.47     | 1.86        | 11     | 2     |
| 1:A:54:GLU:C      | 1:A:56(D):VAL:HA | 0.47     | 2.35        | 25     | 1     |
| 1:A:56(E):LYS:HB2 | 1:A:57:PRO:CD    | 0.47     | 2.40        | 30     | 1     |
| 1:A:57:PRO:O      | 1:A:58:PHE:HB2   | 0.47     | 2.10        | 22     | 7     |
| 1:A:56(A):ASP:O   | 1:A:56(B):GLY:C  | 0.47     | 2.57        | 20     | 3     |
| 1:A:19:THR:O      | 1:A:22:ASP:OD1   | 0.47     | 2.32        | 9      | 1     |
| 1:A:20:ALA:HB1    | 1:A:30:ILE:HD13  | 0.47     | 1.87        | 10     | 1     |
| 1:A:3:GLN:HB2     | 1:A:45:ASN:ND2   | 0.47     | 2.25        | 15     | 1     |
| 1:A:6:THR:C       | 1:A:42:LEU:CD1   | 0.47     | 2.88        | 15     | 1     |
| 1:A:28:SER:OG     | 1:A:29:ALA:N     | 0.47     | 2.46        | 17     | 1     |
| 1:A:33:ALA:O      | 1:A:38:ARG:HB3   | 0.47     | 2.10        | 19     | 1     |
| 1:A:23:LEU:HG     | 1:A:24:GLY:N     | 0.47     | 2.24        | 27     | 1     |
| 1:A:56(A):ASP:OD1 | 1:A:56(A):ASP:O  | 0.47     | 2.33        | 5      | 1     |
| 1:A:52:ALA:O      | 1:A:58:PHE:O     | 0.47     | 2.33        | 4      | 1     |
| 1:A:47:ASP:O      | 1:A:47:ASP:OD1   | 0.47     | 2.33        | 12     | 1     |
| 1:A:34:ILE:HA     | 1:A:38:ARG:HD2   | 0.47     | 1.86        | 27     | 1     |
| 1:A:7:LEU:CD2     | 1:A:40:ILE:HG13  | 0.47     | 2.39        | 32     | 1     |
| 1:A:7:LEU:CB      | 1:A:40:ILE:CG2   | 0.46     | 2.92        | 3      | 2     |
| 1:A:42:LEU:CA     | 1:A:51:TYR:O     | 0.46     | 2.63        | 4      | 2     |
| 1:A:44:ILE:HG22   | 1:A:45:ASN:N     | 0.46     | 2.25        | 7      | 1     |
| 1:A:59:PRO:O      | 1:A:60:SER:O     | 0.46     | 2.33        | 27     | 3     |

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| Atom-1          | Atom-2             | Clash(Å) | Distance(Å) | Models |       |
|-----------------|--------------------|----------|-------------|--------|-------|
|                 |                    |          |             | Worst  | Total |
| 1:A:30:ILE:HG23 | 1:A:34:ILE:HG13    | 0.46     | 1.87        | 30     | 1     |
| 1:A:7:LEU:HD21  | 1:A:34:ILE:CG1     | 0.46     | 2.41        | 7      | 3     |
| 1:A:51:TYR:C    | 1:A:51:TYR:CD1     | 0.46     | 2.92        | 27     | 2     |
| 1:A:22:ASP:C    | 1:A:50:VAL:CG1     | 0.46     | 2.89        | 32     | 1     |
| 1:A:43:THR:OG1  | 1:A:43:THR:O       | 0.46     | 2.34        | 2      | 1     |
| 1:A:57:PRO:HB2  | 1:A:60:SER:C       | 0.46     | 2.35        | 9      | 1     |
| 1:A:31:ASN:O    | 1:A:35:HIS:CD2     | 0.46     | 2.69        | 8      | 1     |
| 1:A:30:ILE:CG2  | 1:A:34:ILE:HD12    | 0.46     | 2.40        | 27     | 4     |
| 1:A:23:LEU:HG   | 1:A:25:VAL:HG23    | 0.46     | 1.86        | 27     | 1     |
| 1:A:45:ASN:O    | 1:A:47:ASP:OD1     | 0.46     | 2.33        | 28     | 1     |
| 1:A:19:THR:O    | 1:A:23:LEU:HD23    | 0.46     | 2.10        | 27     | 1     |
| 1:A:19:THR:HA   | 1:A:22:ASP:OD2     | 0.46     | 2.11        | 29     | 2     |
| 1:A:45:ASN:CG   | 1:A:49:SER:HB3     | 0.46     | 2.36        | 1      | 2     |
| 1:A:7:LEU:HA    | 1:A:42:LEU:CD1     | 0.46     | 2.41        | 24     | 9     |
| 1:A:48:GLY:O    | 1:A:49:SER:C       | 0.46     | 2.58        | 9      | 2     |
| 1:A:45:ASN:HB2  | 1:A:48:GLY:N       | 0.46     | 2.26        | 24     | 1     |
| 1:A:45:ASN:O    | 1:A:47:ASP:N       | 0.46     | 2.49        | 4      | 2     |
| 1:A:7:LEU:CD2   | 1:A:19:THR:HG21    | 0.46     | 2.40        | 23     | 1     |
| 1:A:6:THR:OG1   | 1:A:9:ASP:HB3      | 0.46     | 2.11        | 21     | 7     |
| 1:A:23:LEU:O    | 1:A:25:VAL:CG2     | 0.46     | 2.64        | 3      | 1     |
| 1:A:7:LEU:HD21  | 1:A:34:ILE:HA      | 0.46     | 1.88        | 5      | 1     |
| 1:A:5:ILE:CG2   | 1:A:10:TYR:CB      | 0.46     | 2.93        | 8      | 2     |
| 1:A:7:LEU:HD13  | 1:A:23:LEU:CD1     | 0.46     | 2.41        | 22     | 1     |
| 1:A:8:LYS:CB    | 1:A:34:ILE:HD13    | 0.46     | 2.42        | 27     | 1     |
| 1:A:34:ILE:O    | 1:A:38:ARG:HD3     | 0.46     | 2.10        | 27     | 1     |
| 1:A:55:VAL:HG22 | 1:A:56(D):VAL:HG23 | 0.46     | 1.87        | 32     | 1     |
| 1:A:6:THR:OG1   | 1:A:9:ASP:N        | 0.45     | 2.50        | 15     | 4     |
| 1:A:39:LYS:HG3  | 1:A:55:VAL:O       | 0.45     | 2.11        | 8      | 1     |
| 1:A:7:LEU:HD11  | 1:A:30:ILE:HG13    | 0.45     | 1.87        | 2      | 1     |
| 1:A:33:ALA:O    | 1:A:38:ARG:HB2     | 0.45     | 2.11        | 30     | 4     |
| 1:A:54:GLU:O    | 1:A:56(D):VAL:CB   | 0.45     | 2.64        | 10     | 2     |
| 1:A:39:LYS:O    | 1:A:55:VAL:CG2     | 0.45     | 2.65        | 4      | 1     |
| 1:A:22:ASP:OD1  | 1:A:50:VAL:HG13    | 0.45     | 2.11        | 21     | 1     |
| 1:A:40:ILE:HG23 | 1:A:54:GLU:CB      | 0.45     | 2.42        | 24     | 1     |
| 1:A:3:GLN:OE1   | 1:A:44:ILE:O       | 0.45     | 2.35        | 32     | 1     |
| 1:A:22:ASP:N    | 1:A:22:ASP:OD1     | 0.45     | 2.49        | 3      | 1     |
| 1:A:4:ARG:HA    | 1:A:42:LEU:C       | 0.45     | 2.37        | 18     | 3     |
| 1:A:26:TYR:CD1  | 1:A:28:SER:CB      | 0.45     | 2.99        | 4      | 1     |
| 1:A:56:LYS:HG3  | 1:A:56(A):ASP:N    | 0.45     | 2.26        | 4      | 2     |
| 1:A:26:TYR:CD1  | 1:A:26:TYR:N       | 0.45     | 2.84        | 6      | 2     |
| 1:A:50:VAL:C    | 1:A:51:TYR:CD1     | 0.45     | 2.94        | 18     | 1     |

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| Atom-1          | Atom-2            | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-------------------|----------|-------------|--------|-------|
|                 |                   |          |             | Worst  | Total |
| 1:A:42:LEU:HD23 | 1:A:50:VAL:CG1    | 0.45     | 2.42        | 28     | 1     |
| 1:A:26:TYR:C    | 1:A:28:SER:N      | 0.45     | 2.75        | 6      | 3     |
| 1:A:49:SER:O    | 1:A:49:SER:OG     | 0.45     | 2.35        | 7      | 1     |
| 1:A:36:ALA:O    | 1:A:38:ARG:HD2    | 0.45     | 2.11        | 23     | 1     |
| 1:A:56(A):ASP:O | 1:A:56(A):ASP:CG  | 0.45     | 2.60        | 19     | 2     |
| 1:A:45:ASN:ND2  | 1:A:49:SER:HB3    | 0.45     | 2.27        | 2      | 1     |
| 1:A:57:PRO:O    | 1:A:58:PHE:CB     | 0.45     | 2.65        | 22     | 2     |
| 1:A:23:LEU:HD11 | 1:A:42:LEU:HD21   | 0.45     | 1.89        | 13     | 1     |
| 1:A:23:LEU:CD1  | 1:A:23:LEU:O      | 0.45     | 2.65        | 22     | 1     |
| 1:A:38:ARG:O    | 1:A:38:ARG:CG     | 0.45     | 2.65        | 10     | 1     |
| 1:A:52:ALA:O    | 1:A:57:PRO:O      | 0.45     | 2.34        | 20     | 1     |
| 1:A:23:LEU:HD23 | 1:A:50:VAL:HG11   | 0.45     | 1.88        | 1      | 1     |
| 1:A:39:LYS:O    | 1:A:55:VAL:HG23   | 0.45     | 2.12        | 4      | 1     |
| 1:A:25:VAL:O    | 1:A:26:TYR:O      | 0.45     | 2.35        | 18     | 2     |
| 1:A:54:GLU:OE1  | 1:A:58:PHE:HB2    | 0.45     | 2.12        | 19     | 1     |
| 1:A:30:ILE:O    | 1:A:34:ILE:HB     | 0.45     | 2.12        | 30     | 3     |
| 1:A:57:PRO:HD2  | 1:A:60:SER:CB     | 0.45     | 2.42        | 3      | 2     |
| 1:A:40:ILE:HG21 | 1:A:58:PHE:CD2    | 0.45     | 2.47        | 4      | 2     |
| 1:A:7:LEU:CG    | 1:A:34:ILE:HG12   | 0.45     | 2.42        | 32     | 2     |
| 1:A:7:LEU:O     | 1:A:11:ALA:HB2    | 0.45     | 2.12        | 8      | 1     |
| 1:A:20:ALA:CB   | 1:A:27:GLN:HG3    | 0.45     | 2.42        | 9      | 1     |
| 1:A:8:LYS:C     | 1:A:8:LYS:HD3     | 0.45     | 2.37        | 17     | 2     |
| 1:A:54:GLU:HG2  | 1:A:55:VAL:N      | 0.45     | 2.26        | 26     | 1     |
| 1:A:14:PHE:O    | 1:A:18:LYS:HB2    | 0.45     | 2.11        | 30     | 1     |
| 1:A:50:VAL:O    | 1:A:50:VAL:HG12   | 0.44     | 2.12        | 8      | 1     |
| 1:A:39:LYS:HD3  | 1:A:55:VAL:O      | 0.44     | 2.12        | 11     | 1     |
| 1:A:53:GLU:OE1  | 1:A:55:VAL:CG2    | 0.44     | 2.65        | 23     | 1     |
| 1:A:17:THR:O    | 1:A:20:ALA:HB3    | 0.44     | 2.13        | 25     | 1     |
| 1:A:51:TYR:CZ   | 1:A:53:GLU:CG     | 0.44     | 3.00        | 26     | 1     |
| 1:A:39:LYS:CB   | 1:A:55:VAL:O      | 0.44     | 2.65        | 28     | 1     |
| 1:A:53:GLU:HG2  | 1:A:56(E):LYS:O   | 0.44     | 2.12        | 2      | 1     |
| 1:A:55:VAL:HG22 | 1:A:56(D):VAL:CG1 | 0.44     | 2.42        | 3      | 1     |
| 1:A:46:ALA:CB   | 1:A:49:SER:CB     | 0.44     | 2.90        | 4      | 1     |
| 1:A:8:LYS:HD2   | 1:A:8:LYS:C       | 0.44     | 2.38        | 19     | 1     |
| 1:A:7:LEU:HD21  | 1:A:34:ILE:CD1    | 0.44     | 2.42        | 30     | 2     |
| 1:A:8:LYS:HG3   | 1:A:34:ILE:HG21   | 0.44     | 1.88        | 27     | 1     |
| 1:A:6:THR:O     | 1:A:42:LEU:HD13   | 0.44     | 2.13        | 2      | 4     |
| 1:A:7:LEU:HB3   | 1:A:34:ILE:CD1    | 0.44     | 2.41        | 10     | 3     |
| 1:A:38:ARG:HG3  | 1:A:40:ILE:CG1    | 0.44     | 2.43        | 19     | 1     |
| 1:A:10:TYR:C    | 1:A:10:TYR:CD1    | 0.44     | 2.93        | 7      | 3     |
| 1:A:5:ILE:HG22  | 1:A:10:TYR:N      | 0.44     | 2.26        | 10     | 2     |

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| Atom-1          | Atom-2            | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-------------------|----------|-------------|--------|-------|
|                 |                   |          |             | Worst  | Total |
| 1:A:28:SER:C    | 1:A:30:ILE:N      | 0.44     | 2.74        | 7      | 7     |
| 1:A:53:GLU:O    | 1:A:53:GLU:HG3    | 0.44     | 2.13        | 8      | 1     |
| 1:A:25:VAL:HG11 | 1:A:30:ILE:CD1    | 0.44     | 2.42        | 17     | 1     |
| 1:A:40:ILE:HD13 | 1:A:58:PHE:CD1    | 0.44     | 2.48        | 17     | 1     |
| 1:A:8:LYS:C     | 1:A:8:LYS:HD2     | 0.44     | 2.38        | 3      | 2     |
| 1:A:38:ARG:C    | 1:A:38:ARG:CD     | 0.44     | 2.89        | 10     | 1     |
| 1:A:9:ASP:O     | 1:A:12:MET:CB     | 0.44     | 2.66        | 11     | 3     |
| 1:A:34:ILE:C    | 1:A:36:ALA:N      | 0.44     | 2.75        | 21     | 1     |
| 1:A:39:LYS:N    | 1:A:39:LYS:HD2    | 0.44     | 2.27        | 25     | 1     |
| 1:A:7:LEU:HD22  | 1:A:40:ILE:HB     | 0.44     | 1.90        | 30     | 1     |
| 1:A:41:PHE:C    | 1:A:42:LEU:HG     | 0.44     | 2.37        | 4      | 1     |
| 1:A:4:ARG:N     | 1:A:4:ARG:HD2     | 0.44     | 2.28        | 5      | 1     |
| 1:A:20:ALA:O    | 1:A:24:GLY:O      | 0.44     | 2.35        | 6      | 1     |
| 1:A:39:LYS:O    | 1:A:39:LYS:HG2    | 0.44     | 2.12        | 6      | 2     |
| 1:A:42:LEU:CB   | 1:A:51:TYR:O      | 0.44     | 2.65        | 30     | 2     |
| 1:A:10:TYR:CD2  | 1:A:14:PHE:CZ     | 0.44     | 3.06        | 15     | 1     |
| 1:A:48:GLY:O    | 1:A:49:SER:HB2    | 0.44     | 2.13        | 15     | 4     |
| 1:A:5:ILE:HG21  | 1:A:10:TYR:HA     | 0.44     | 1.89        | 31     | 2     |
| 1:A:42:LEU:HB3  | 1:A:50:VAL:CG1    | 0.44     | 2.42        | 24     | 1     |
| 1:A:58:PHE:CA   | 1:A:59:PRO:C      | 0.44     | 2.91        | 1      | 1     |
| 1:A:56:LYS:O    | 1:A:56(A):ASP:HB3 | 0.44     | 2.13        | 23     | 7     |
| 1:A:3:GLN:O     | 1:A:43:THR:HA     | 0.44     | 2.13        | 10     | 2     |
| 1:A:38:ARG:NE   | 1:A:38:ARG:HA     | 0.44     | 2.28        | 23     | 1     |
| 1:A:7:LEU:C     | 1:A:7:LEU:CD2     | 0.44     | 2.91        | 27     | 1     |
| 1:A:8:LYS:HD2   | 1:A:9:ASP:N       | 0.43     | 2.28        | 3      | 2     |
| 1:A:41:PHE:C    | 1:A:42:LEU:CG     | 0.43     | 2.91        | 4      | 1     |
| 1:A:54:GLU:CD   | 1:A:55:VAL:N      | 0.43     | 2.76        | 16     | 2     |
| 1:A:23:LEU:O    | 1:A:23:LEU:HG     | 0.43     | 2.12        | 22     | 1     |
| 1:A:38:ARG:NH1  | 1:A:54:GLU:HB2    | 0.43     | 2.28        | 28     | 1     |
| 1:A:7:LEU:CD1   | 1:A:34:ILE:HG12   | 0.43     | 2.43        | 32     | 1     |
| 1:A:57:PRO:O    | 1:A:58:PHE:CD2    | 0.43     | 2.72        | 1      | 1     |
| 1:A:58:PHE:O    | 1:A:58:PHE:CD2    | 0.43     | 2.70        | 1      | 2     |
| 1:A:9:ASP:O     | 1:A:12:MET:HB3    | 0.43     | 2.14        | 19     | 4     |
| 1:A:38:ARG:HE   | 1:A:40:ILE:HD11   | 0.43     | 1.73        | 8      | 1     |
| 1:A:23:LEU:HD22 | 1:A:59:PRO:HD3    | 0.43     | 1.89        | 14     | 1     |
| 1:A:8:LYS:HB2   | 1:A:34:ILE:CG2    | 0.43     | 2.43        | 17     | 2     |
| 1:A:40:ILE:HG12 | 1:A:54:GLU:CG     | 0.43     | 2.43        | 21     | 1     |
| 1:A:26:TYR:N    | 1:A:26:TYR:CD1    | 0.43     | 2.82        | 31     | 1     |
| 1:A:58:PHE:HA   | 1:A:59:PRO:C      | 0.43     | 2.35        | 1      | 1     |
| 1:A:22:ASP:CB   | 1:A:50:VAL:HG21   | 0.43     | 2.42        | 2      | 1     |
| 1:A:57:PRO:HB2  | 1:A:60:SER:CA     | 0.43     | 2.42        | 9      | 1     |

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| Atom-1           | Atom-2             | Clash(Å) | Distance(Å) | Models |       |
|------------------|--------------------|----------|-------------|--------|-------|
|                  |                    |          |             | Worst  | Total |
| 1:A:22:ASP:CA    | 1:A:50:VAL:HG11    | 0.43     | 2.43        | 32     | 1     |
| 1:A:55:VAL:HG23  | 1:A:56(D):VAL:HG12 | 0.43     | 1.90        | 2      | 1     |
| 1:A:57:PRO:O     | 1:A:58:PHE:HB3     | 0.43     | 2.13        | 28     | 5     |
| 1:A:58:PHE:CD2   | 1:A:59:PRO:HA      | 0.43     | 2.48        | 5      | 1     |
| 1:A:33:ALA:O     | 1:A:38:ARG:CD      | 0.43     | 2.66        | 18     | 1     |
| 1:A:5:ILE:CG2    | 1:A:10:TYR:HA      | 0.43     | 2.44        | 19     | 1     |
| 1:A:14:PHE:CZ    | 1:A:18:LYS:HB3     | 0.43     | 2.48        | 25     | 1     |
| 1:A:36:ALA:O     | 1:A:38:ARG:HG2     | 0.43     | 2.13        | 23     | 1     |
| 1:A:54:GLU:O     | 1:A:56(D):VAL:HB   | 0.43     | 2.13        | 31     | 1     |
| 1:A:39:LYS:CE    | 1:A:56:LYS:HB2     | 0.43     | 2.44        | 3      | 1     |
| 1:A:56(E):LYS:CB | 1:A:57:PRO:CD      | 0.43     | 2.97        | 9      | 2     |
| 1:A:46:ALA:O     | 1:A:49:SER:OG      | 0.43     | 2.32        | 14     | 1     |
| 1:A:53:GLU:O     | 1:A:53:GLU:OE2     | 0.43     | 2.37        | 16     | 1     |
| 1:A:23:LEU:HB2   | 1:A:25:VAL:HG23    | 0.43     | 1.90        | 32     | 1     |
| 1:A:53:GLU:CB    | 1:A:56(E):LYS:O    | 0.43     | 2.67        | 4      | 1     |
| 1:A:39:LYS:HB3   | 1:A:55:VAL:O       | 0.43     | 2.14        | 7      | 1     |
| 1:A:34:ILE:O     | 1:A:38:ARG:NE      | 0.43     | 2.52        | 14     | 1     |
| 1:A:31:ASN:C     | 1:A:33:ALA:N       | 0.43     | 2.74        | 2      | 1     |
| 1:A:25:VAL:O     | 1:A:26:TYR:C       | 0.43     | 2.61        | 7      | 3     |
| 1:A:5:ILE:CG2    | 1:A:10:TYR:CA      | 0.43     | 2.96        | 31     | 2     |
| 1:A:10:TYR:HD2   | 1:A:42:LEU:HD22    | 0.43     | 1.73        | 20     | 1     |
| 1:A:34:ILE:HG13  | 1:A:40:ILE:HD12    | 0.43     | 1.91        | 2      | 1     |
| 1:A:51:TYR:CD1   | 1:A:51:TYR:N       | 0.43     | 2.84        | 18     | 1     |
| 1:A:30:ILE:O     | 1:A:34:ILE:CB      | 0.43     | 2.66        | 30     | 1     |
| 1:A:28:SER:O     | 1:A:30:ILE:N       | 0.43     | 2.52        | 5      | 1     |
| 1:A:27:GLN:O     | 1:A:30:ILE:HB      | 0.43     | 2.14        | 15     | 4     |
| 1:A:59:PRO:C     | 1:A:60:SER:HG      | 0.43     | 2.22        | 16     | 1     |
| 1:A:42:LEU:CD1   | 1:A:42:LEU:N       | 0.43     | 2.81        | 21     | 1     |
| 1:A:43:THR:CG2   | 1:A:45:ASN:CG      | 0.43     | 2.92        | 25     | 1     |
| 1:A:27:GLN:HA    | 1:A:30:ILE:HG12    | 0.43     | 1.90        | 31     | 1     |
| 1:A:23:LEU:C     | 1:A:25:VAL:HG23    | 0.42     | 2.38        | 3      | 1     |
| 1:A:39:LYS:C     | 1:A:41:PHE:CE2     | 0.42     | 2.97        | 3      | 1     |
| 1:A:51:TYR:CD1   | 1:A:52:ALA:N       | 0.42     | 2.87        | 14     | 1     |
| 1:A:7:LEU:CB     | 1:A:34:ILE:HG12    | 0.42     | 2.44        | 8      | 1     |
| 1:A:56:LYS:CG    | 1:A:56(A):ASP:OD2  | 0.42     | 2.67        | 22     | 1     |
| 1:A:38:ARG:CZ    | 1:A:40:ILE:HG12    | 0.42     | 2.43        | 28     | 1     |
| 1:A:23:LEU:CB    | 1:A:52:ALA:HB2     | 0.42     | 2.44        | 6      | 1     |
| 1:A:56:LYS:HG3   | 1:A:56(A):ASP:OD2  | 0.42     | 2.14        | 22     | 1     |
| 1:A:14:PHE:CE1   | 1:A:18:LYS:CB      | 0.42     | 3.03        | 25     | 1     |
| 1:A:55:VAL:CA    | 1:A:56(D):VAL:HA   | 0.42     | 2.44        | 25     | 1     |
| 1:A:43:THR:O     | 1:A:43:THR:HG22    | 0.42     | 2.13        | 25     | 2     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:10:TYR:CE1  | 1:A:44:ILE:HD12 | 0.42     | 2.48        | 28     | 1     |
| 1:A:16:GLN:OE1  | 1:A:31:ASN:OD1  | 0.42     | 2.37        | 30     | 1     |
| 1:A:52:ALA:O    | 1:A:53:GLU:HG2  | 0.42     | 2.15        | 30     | 1     |
| 1:A:45:ASN:ND2  | 1:A:47:ASP:HB3  | 0.42     | 2.30        | 22     | 1     |
| 1:A:22:ASP:OD1  | 1:A:50:VAL:HG11 | 0.42     | 2.13        | 29     | 1     |
| 1:A:39:LYS:O    | 1:A:39:LYS:HG3  | 0.42     | 2.14        | 1      | 3     |
| 1:A:7:LEU:HG    | 1:A:30:ILE:HG23 | 0.42     | 1.90        | 2      | 1     |
| 1:A:38:ARG:O    | 1:A:39:LYS:HB3  | 0.42     | 2.15        | 21     | 2     |
| 1:A:43:THR:HB   | 1:A:51:TYR:CB   | 0.42     | 2.44        | 10     | 2     |
| 1:A:34:ILE:HA   | 1:A:40:ILE:CD1  | 0.42     | 2.44        | 7      | 1     |
| 1:A:22:ASP:HB3  | 1:A:50:VAL:CG1  | 0.42     | 2.43        | 20     | 1     |
| 1:A:44:ILE:O    | 1:A:48:GLY:HA3  | 0.42     | 2.15        | 21     | 1     |
| 1:A:7:LEU:CD2   | 1:A:40:ILE:HG21 | 0.42     | 2.45        | 3      | 1     |
| 1:A:39:LYS:C    | 1:A:40:ILE:CG1  | 0.42     | 2.91        | 10     | 1     |
| 1:A:43:THR:CG2  | 1:A:51:TYR:HB3  | 0.42     | 2.44        | 17     | 1     |
| 1:A:7:LEU:HD22  | 1:A:58:PHE:CE2  | 0.42     | 2.49        | 24     | 1     |
| 1:A:40:ILE:HG23 | 1:A:54:GLU:HB3  | 0.42     | 1.91        | 24     | 1     |
| 1:A:14:PHE:CD1  | 1:A:14:PHE:N    | 0.42     | 2.87        | 25     | 1     |
| 1:A:49:SER:OG   | 1:A:51:TYR:CE2  | 0.42     | 2.71        | 28     | 1     |
| 1:A:45:ASN:OD1  | 1:A:49:SER:HB3  | 0.42     | 2.14        | 30     | 1     |
| 1:A:8:LYS:H     | 1:A:34:ILE:HD13 | 0.42     | 1.73        | 2      | 1     |
| 1:A:27:GLN:O    | 1:A:28:SER:C    | 0.42     | 2.63        | 4      | 1     |
| 1:A:14:PHE:CD2  | 1:A:18:LYS:HE3  | 0.42     | 2.50        | 11     | 1     |
| 1:A:5:ILE:HG21  | 1:A:10:TYR:CD2  | 0.42     | 2.50        | 13     | 1     |
| 1:A:36:ALA:HB3  | 1:A:38:ARG:CZ   | 0.42     | 2.44        | 22     | 1     |
| 1:A:44:ILE:O    | 1:A:44:ILE:CG2  | 0.42     | 2.61        | 25     | 1     |
| 1:A:22:ASP:HB3  | 1:A:50:VAL:HG21 | 0.42     | 1.90        | 2      | 1     |
| 1:A:38:ARG:CD   | 1:A:40:ILE:HD11 | 0.42     | 2.45        | 10     | 1     |
| 1:A:7:LEU:HD11  | 1:A:42:LEU:CD1  | 0.42     | 2.45        | 18     | 1     |
| 1:A:30:ILE:O    | 1:A:34:ILE:CG1  | 0.42     | 2.67        | 27     | 1     |
| 1:A:8:LYS:C     | 1:A:8:LYS:CD    | 0.42     | 2.92        | 19     | 2     |
| 1:A:5:ILE:HG13  | 1:A:44:ILE:CD1  | 0.42     | 2.44        | 8      | 1     |
| 1:A:58:PHE:HA   | 1:A:59:PRO:HA   | 0.42     | 1.77        | 24     | 5     |
| 1:A:24:GLY:C    | 1:A:25:VAL:HG22 | 0.42     | 2.40        | 13     | 1     |
| 1:A:43:THR:O    | 1:A:51:TYR:HB2  | 0.42     | 2.15        | 13     | 1     |
| 1:A:14:PHE:HB3  | 1:A:18:LYS:CB   | 0.42     | 2.44        | 23     | 1     |
| 1:A:8:LYS:CG    | 1:A:34:ILE:HG23 | 0.42     | 2.44        | 25     | 1     |
| 1:A:23:LEU:HB2  | 1:A:52:ALA:CB   | 0.41     | 2.44        | 6      | 1     |
| 1:A:54:GLU:HB2  | 1:A:56(E):LYS:O | 0.41     | 2.14        | 25     | 1     |
| 1:A:23:LEU:HB3  | 1:A:50:VAL:CG1  | 0.41     | 2.45        | 27     | 1     |
| 1:A:52:ALA:O    | 1:A:53:GLU:CG   | 0.41     | 2.68        | 30     | 1     |

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| Atom-1            | Atom-2             | Clash(Å) | Distance(Å) | Models |       |
|-------------------|--------------------|----------|-------------|--------|-------|
|                   |                    |          |             | Worst  | Total |
| 1:A:8:LYS:HD3     | 1:A:34:ILE:HG23    | 0.41     | 1.92        | 32     | 1     |
| 1:A:44:ILE:HG23   | 1:A:50:VAL:HG22    | 0.41     | 1.91        | 4      | 1     |
| 1:A:26:TYR:HB2    | 1:A:29:ALA:HB3     | 0.41     | 1.92        | 6      | 1     |
| 1:A:23:LEU:N      | 1:A:23:LEU:CD2     | 0.41     | 2.83        | 7      | 1     |
| 1:A:8:LYS:CD      | 1:A:9:ASP:N        | 0.41     | 2.83        | 17     | 1     |
| 1:A:35:HIS:CD2    | 1:A:35:HIS:O       | 0.41     | 2.73        | 26     | 1     |
| 1:A:4:ARG:CZ      | 1:A:41:PHE:CG      | 0.41     | 3.03        | 29     | 1     |
| 1:A:49:SER:C      | 1:A:50:VAL:CG2     | 0.41     | 2.93        | 30     | 1     |
| 1:A:54:GLU:O      | 1:A:55:VAL:CG2     | 0.41     | 2.68        | 3      | 1     |
| 1:A:16:GLN:NE2    | 1:A:27:GLN:HG2     | 0.41     | 2.31        | 4      | 1     |
| 1:A:6:THR:OG1     | 1:A:9:ASP:HB2      | 0.41     | 2.15        | 21     | 3     |
| 1:A:43:THR:HG22   | 1:A:45:ASN:ND2     | 0.41     | 2.29        | 11     | 1     |
| 1:A:7:LEU:HD13    | 1:A:40:ILE:CG2     | 0.41     | 2.38        | 21     | 1     |
| 1:A:42:LEU:HD23   | 1:A:50:VAL:HG12    | 0.41     | 1.92        | 24     | 1     |
| 1:A:33:ALA:HB1    | 1:A:40:ILE:HD11    | 0.41     | 1.86        | 31     | 1     |
| 1:A:42:LEU:HB3    | 1:A:50:VAL:CG2     | 0.41     | 2.46        | 32     | 1     |
| 1:A:56(E):LYS:HB2 | 1:A:60:SER:OG      | 0.41     | 2.15        | 32     | 1     |
| 1:A:8:LYS:HB2     | 1:A:34:ILE:CD1     | 0.41     | 2.39        | 2      | 2     |
| 1:A:30:ILE:C      | 1:A:32:LYS:N       | 0.41     | 2.78        | 5      | 3     |
| 1:A:20:ALA:HA     | 1:A:24:GLY:HA3     | 0.41     | 1.91        | 6      | 1     |
| 1:A:39:LYS:HD2    | 1:A:55:VAL:O       | 0.41     | 2.16        | 8      | 1     |
| 1:A:30:ILE:O      | 1:A:34:ILE:HG13    | 0.41     | 2.15        | 29     | 3     |
| 1:A:4:ARG:HG2     | 1:A:41:PHE:HB3     | 0.41     | 1.92        | 15     | 1     |
| 1:A:14:PHE:CE1    | 1:A:18:LYS:HB2     | 0.41     | 2.51        | 15     | 1     |
| 1:A:55:VAL:CB     | 1:A:56(D):VAL:HG12 | 0.41     | 2.46        | 14     | 1     |
| 1:A:10:TYR:CD1    | 1:A:10:TYR:C       | 0.41     | 2.99        | 21     | 1     |
| 1:A:56:LYS:HD2    | 1:A:56:LYS:C       | 0.41     | 2.40        | 24     | 1     |
| 1:A:22:ASP:OD1    | 1:A:22:ASP:C       | 0.41     | 2.63        | 27     | 1     |
| 1:A:22:ASP:OD1    | 1:A:50:VAL:HB      | 0.41     | 2.15        | 27     | 1     |
| 1:A:45:ASN:OD1    | 1:A:49:SER:CB      | 0.41     | 2.69        | 29     | 1     |
| 1:A:5:ILE:CB      | 1:A:10:TYR:CD1     | 0.41     | 3.03        | 31     | 1     |
| 1:A:3:GLN:HB2     | 1:A:44:ILE:O       | 0.41     | 2.15        | 32     | 1     |
| 1:A:58:PHE:C      | 1:A:58:PHE:CD1     | 0.41     | 2.95        | 10     | 1     |
| 1:A:30:ILE:HG22   | 1:A:31:ASN:H       | 0.41     | 1.74        | 13     | 2     |
| 1:A:56(D):VAL:C   | 1:A:56(E):LYS:HG2  | 0.41     | 2.41        | 26     | 2     |
| 1:A:54:GLU:O      | 1:A:55:VAL:HG22    | 0.41     | 2.16        | 19     | 1     |
| 1:A:52:ALA:O      | 1:A:57:PRO:HB3     | 0.41     | 2.15        | 25     | 1     |
| 1:A:54:GLU:OE1    | 1:A:56(C):GLU:HB2  | 0.41     | 2.15        | 25     | 1     |
| 1:A:30:ILE:O      | 1:A:32:LYS:N       | 0.41     | 2.54        | 5      | 1     |
| 1:A:23:LEU:CG     | 1:A:25:VAL:HG23    | 0.41     | 2.46        | 8      | 1     |
| 1:A:56(B):GLY:O   | 1:A:56(C):GLU:HB2  | 0.41     | 2.14        | 25     | 2     |

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| Atom-1          | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|-----------------|------------------|----------|-------------|--------|-------|
|                 |                  |          |             | Worst  | Total |
| 1:A:9:ASP:O     | 1:A:12:MET:HB2   | 0.41     | 2.15        | 27     | 1     |
| 1:A:14:PHE:CD2  | 1:A:18:LYS:HD3   | 0.41     | 2.50        | 31     | 1     |
| 1:A:41:PHE:O    | 1:A:53:GLU:O     | 0.41     | 2.39        | 31     | 1     |
| 1:A:22:ASP:HB3  | 1:A:50:VAL:CG2   | 0.41     | 2.46        | 2      | 1     |
| 1:A:55:VAL:HA   | 1:A:56(C):GLU:O  | 0.41     | 2.16        | 2      | 1     |
| 1:A:41:PHE:O    | 1:A:42:LEU:HG    | 0.41     | 2.16        | 9      | 1     |
| 1:A:7:LEU:CD2   | 1:A:33:ALA:O     | 0.41     | 2.68        | 19     | 1     |
| 1:A:42:LEU:HB3  | 1:A:51:TYR:O     | 0.41     | 2.15        | 21     | 2     |
| 1:A:44:ILE:O    | 1:A:48:GLY:CA    | 0.41     | 2.69        | 21     | 1     |
| 1:A:24:GLY:N    | 1:A:58:PHE:CZ    | 0.41     | 2.89        | 22     | 1     |
| 1:A:43:THR:OG1  | 1:A:51:TYR:HB3   | 0.41     | 2.16        | 26     | 1     |
| 1:A:54:GLU:CD   | 1:A:58:PHE:HB3   | 0.41     | 2.41        | 27     | 1     |
| 1:A:44:ILE:C    | 1:A:45:ASN:CG    | 0.41     | 2.89        | 28     | 1     |
| 1:A:34:ILE:CG2  | 1:A:35:HIS:N     | 0.41     | 2.83        | 2      | 1     |
| 1:A:54:GLU:O    | 1:A:56(C):GLU:O  | 0.41     | 2.38        | 2      | 1     |
| 1:A:4:ARG:HD2   | 1:A:43:THR:HG22  | 0.41     | 1.92        | 19     | 1     |
| 1:A:40:ILE:HG12 | 1:A:54:GLU:CB    | 0.40     | 2.46        | 1      | 1     |
| 1:A:7:LEU:HD11  | 1:A:42:LEU:HD11  | 0.40     | 1.92        | 8      | 1     |
| 1:A:6:THR:CB    | 1:A:9:ASP:HB3    | 0.40     | 2.46        | 9      | 1     |
| 1:A:5:ILE:HG22  | 1:A:6:THR:N      | 0.40     | 2.30        | 21     | 1     |
| 1:A:23:LEU:CB   | 1:A:42:LEU:CD2   | 0.40     | 3.00        | 22     | 1     |
| 1:A:13:ARG:NH1  | 1:A:13:ARG:HG2   | 0.40     | 2.30        | 7      | 1     |
| 1:A:23:LEU:HB3  | 1:A:25:VAL:CG2   | 0.40     | 2.46        | 9      | 1     |
| 1:A:42:LEU:HD23 | 1:A:50:VAL:CG2   | 0.40     | 2.46        | 32     | 1     |
| 1:A:7:LEU:CB    | 1:A:42:LEU:HD11  | 0.40     | 2.42        | 3      | 1     |
| 1:A:5:ILE:O     | 1:A:41:PHE:HA    | 0.40     | 2.16        | 4      | 1     |
| 1:A:23:LEU:HD22 | 1:A:58:PHE:CD1   | 0.40     | 2.51        | 5      | 1     |
| 1:A:34:ILE:HG22 | 1:A:38:ARG:HE    | 0.40     | 1.76        | 14     | 1     |
| 1:A:44:ILE:C    | 1:A:45:ASN:ND2   | 0.40     | 2.79        | 15     | 1     |
| 1:A:5:ILE:CD1   | 1:A:10:TYR:CD1   | 0.40     | 3.04        | 17     | 1     |
| 1:A:7:LEU:HD12  | 1:A:42:LEU:CD2   | 0.40     | 2.46        | 21     | 1     |
| 1:A:8:LYS:CD    | 1:A:34:ILE:CG2   | 0.40     | 2.99        | 22     | 1     |
| 1:A:36:ALA:CB   | 1:A:38:ARG:CZ    | 0.40     | 2.98        | 22     | 1     |
| 1:A:54:GLU:OE2  | 1:A:58:PHE:CB    | 0.40     | 2.69        | 27     | 1     |
| 1:A:4:ARG:NH2   | 1:A:53:GLU:OE1   | 0.40     | 2.55        | 31     | 1     |
| 1:A:57:PRO:HD2  | 1:A:60:SER:OG    | 0.40     | 2.16        | 32     | 1     |
| 1:A:7:LEU:HA    | 1:A:42:LEU:HD11  | 0.40     | 1.93        | 6      | 1     |
| 1:A:5:ILE:HG13  | 1:A:44:ILE:HD12  | 0.40     | 1.93        | 8      | 1     |
| 1:A:5:ILE:HG22  | 1:A:10:TYR:CA    | 0.40     | 2.46        | 10     | 1     |
| 1:A:56:LYS:HB3  | 1:A:56(C):GLU:CB | 0.40     | 2.46        | 19     | 1     |
| 1:A:6:THR:C     | 1:A:42:LEU:HD13  | 0.40     | 2.42        | 21     | 1     |

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| Atom-1         | Atom-2         | Clash(Å) | Distance(Å) | Models |       |
|----------------|----------------|----------|-------------|--------|-------|
|                |                |          |             | Worst  | Total |
| 1:A:10:TYR:C   | 1:A:12:MET:N   | 0.40     | 2.79        | 28     | 1     |
| 1:A:4:ARG:HD2  | 1:A:4:ARG:N    | 0.40     | 2.31        | 4      | 1     |
| 1:A:24:GLY:HA3 | 1:A:30:ILE:CG1 | 0.40     | 2.46        | 6      | 1     |
| 1:A:52:ALA:O   | 1:A:57:PRO:C   | 0.40     | 2.65        | 20     | 1     |
| 1:A:44:ILE:C   | 1:A:46:ALA:N   | 0.40     | 2.79        | 31     | 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     | 63/71 (89%)     | 45±4 (71±6%) | 13±3 (21±5%) | 5±2 (7±4%) | <b>1</b>    | <b>15</b> |
| All | All   | 2016/2272 (89%) | 1441 (71%)   | 428 (21%)    | 147 (7%)   | <b>1</b>    | <b>15</b> |

All 20 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     | 56(A) | ASP  | 21             |
| 1   | A     | 6     | THR  | 14             |
| 1   | A     | 49    | SER  | 12             |
| 1   | A     | 58    | PHE  | 10             |
| 1   | A     | 47    | ASP  | 10             |
| 1   | A     | 45    | ASN  | 10             |
| 1   | A     | 57    | PRO  | 9              |
| 1   | A     | 60    | SER  | 9              |
| 1   | A     | 44    | ILE  | 8              |
| 1   | A     | 36    | ALA  | 6              |
| 1   | A     | 37    | GLY  | 6              |
| 1   | A     | 39    | LYS  | 6              |
| 1   | A     | 50    | VAL  | 5              |
| 1   | A     | 59    | PRO  | 4              |
| 1   | A     | 26    | TYR  | 4              |
| 1   | A     | 38    | ARG  | 4              |
| 1   | A     | 48    | GLY  | 3              |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 15  | GLY  | 3              |
| 1   | A     | 27  | GLN  | 2              |
| 1   | A     | 55  | VAL  | 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     | 51/58 (88%)     | 34±4 (66±8%) | 17±4 (34±8%) | 1           | 11 |
| All | All   | 1632/1856 (88%) | 1081 (66%)   | 551 (34%)    | 1           | 11 |

All 47 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     | 8   | LYS  | 28             |
| 1   | A     | 7   | LEU  | 23             |
| 1   | A     | 18  | LYS  | 23             |
| 1   | A     | 6   | THR  | 22             |
| 1   | A     | 32  | LYS  | 22             |
| 1   | A     | 38  | ARG  | 20             |
| 1   | A     | 27  | GLN  | 19             |
| 1   | A     | 30  | ILE  | 19             |
| 1   | A     | 12  | MET  | 19             |
| 1   | A     | 16  | GLN  | 19             |
| 1   | A     | 21  | LYS  | 17             |
| 1   | A     | 25  | VAL  | 17             |
| 1   | A     | 39  | LYS  | 17             |
| 1   | A     | 13  | ARG  | 16             |
| 1   | A     | 31  | ASN  | 15             |
| 1   | A     | 53  | GLU  | 15             |
| 1   | A     | 49  | SER  | 15             |
| 1   | A     | 19  | THR  | 14             |
| 1   | A     | 9   | ASP  | 13             |
| 1   | A     | 54  | GLU  | 13             |
| 1   | A     | 4   | ARG  | 13             |
| 1   | A     | 56  | LYS  | 12             |

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| Mol | Chain | Res   | Type | Models (Total) |
|-----|-------|-------|------|----------------|
| 1   | A     | 56(A) | ASP  | 12             |
| 1   | A     | 56(C) | GLU  | 12             |
| 1   | A     | 56(D) | VAL  | 12             |
| 1   | A     | 56(E) | LYS  | 12             |
| 1   | A     | 43    | THR  | 9              |
| 1   | A     | 58    | PHE  | 9              |
| 1   | A     | 60    | SER  | 9              |
| 1   | A     | 14    | PHE  | 9              |
| 1   | A     | 17    | THR  | 8              |
| 1   | A     | 45    | ASN  | 8              |
| 1   | A     | 47    | ASP  | 8              |
| 1   | A     | 28    | SER  | 7              |
| 1   | A     | 22    | ASP  | 6              |
| 1   | A     | 23    | LEU  | 6              |
| 1   | A     | 44    | ILE  | 5              |
| 1   | A     | 51    | TYR  | 4              |
| 1   | A     | 42    | LEU  | 4              |
| 1   | A     | 5     | ILE  | 4              |
| 1   | A     | 3     | GLN  | 4              |
| 1   | A     | 35    | HIS  | 3              |
| 1   | A     | 26    | TYR  | 2              |
| 1   | A     | 55    | VAL  | 2              |
| 1   | A     | 40    | ILE  | 2              |
| 1   | A     | 50    | VAL  | 2              |
| 1   | A     | 34    | ILE  | 1              |

### 6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 6.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 6.6 Ligand geometry

There are no ligands in this entry.

## 6.7 Other polymers

There are no such molecules in this entry.

## 6.8 Polymer linkage issues

There are no chain breaks in this entry.

## 7 Chemical shift validation

No chemical shift data were provided