



# Full wwPDB NMR Structure Validation Report ⓘ

Mar 4, 2026 – 10:48 PM UTC

PDB ID : 1ATY / pdb\_00001aty  
Title : DETERMINATION OF LOCAL PROTEIN STRUCTURE BY SPIN LABEL  
DIFFERENCE 2D NMR: THE REGION NEIGHBORING ASP61 OF SUB-  
UNIT C OF THE F1FO ATP SYNTHASE  
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Deposited on : 1994-10-05

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                                                             |

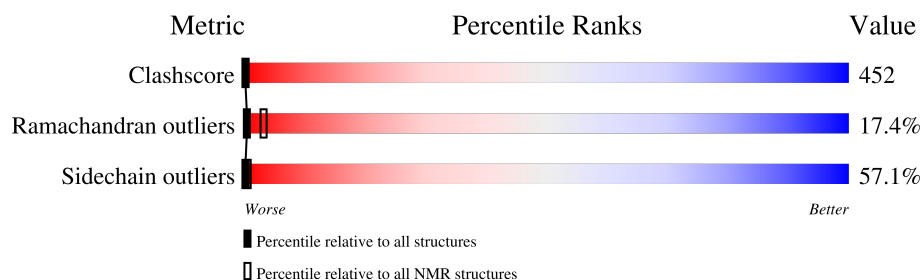
# 1 Overall quality at a glance

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     | 79     |                  |

## 2 Ensemble composition and analysis

This entry contains 9 models. Model 1 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:9-A:25, A:63-A:78 (33) | 0.61              | 1            |

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

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

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

| Cluster number | Models           |
|----------------|------------------|
| 1              | 1, 2, 3, 5, 7, 8 |
| 2              | 4, 6, 9          |

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

There is only 1 type of molecule in this entry. The entry contains 679 atoms, of which 351 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called F1F0 ATP SYNTHASE (SUBUNIT C).

| Mol | Chain | Residues | Atoms |     |     |    |    |   | Trace |
|-----|-------|----------|-------|-----|-----|----|----|---|-------|
| 1   | A     | 46       | Total | C   | H   | N  | O  | S | 0     |
|     |       |          | 679   | 222 | 351 | 47 | 52 | 7 |       |

There is a discrepancy between the modelled and reference sequences:

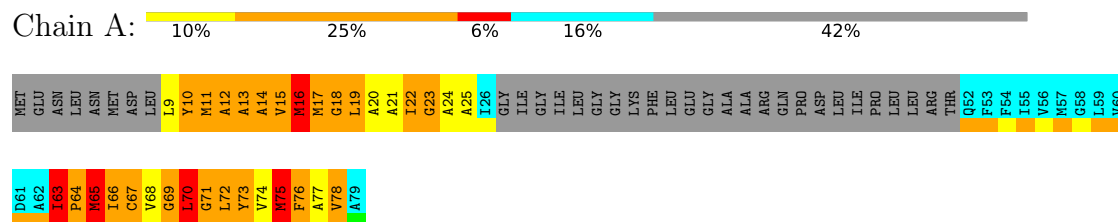
| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| A     | 67      | CYS      | ALA    | conflict | UNP P68699 |

## 4 Residue-property plots [i](#)

### 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: F1F0 ATP SYNTHASE (SUBUNIT C)

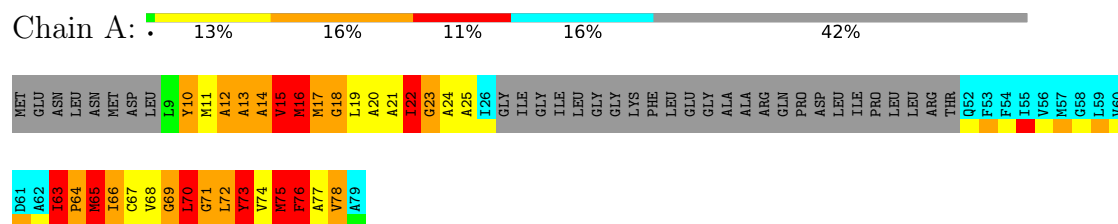


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

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

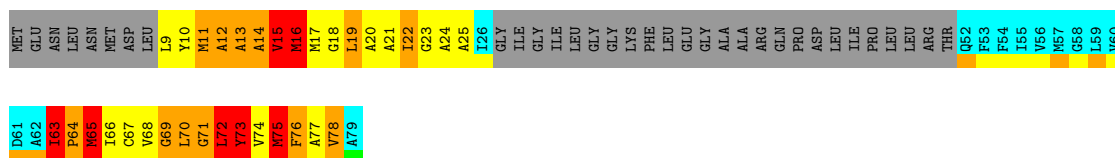
- Molecule 1: F1F0 ATP SYNTHASE (SUBUNIT C)



#### 4.2.2 Score per residue for model 2

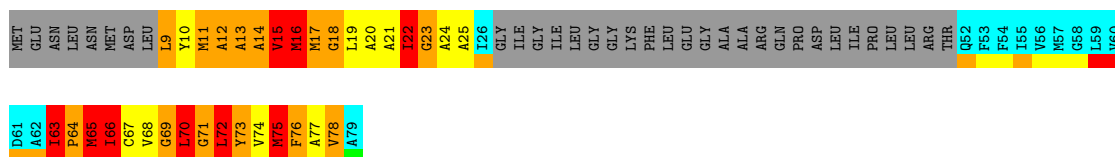
- Molecule 1: F1F0 ATP SYNTHASE (SUBUNIT C)





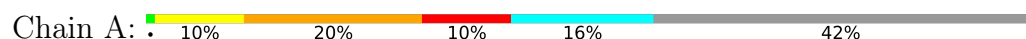
### 4.2.3 Score per residue for model 3

- Molecule 1: F1F0 ATP SYNTHASE (SUBUNIT C)



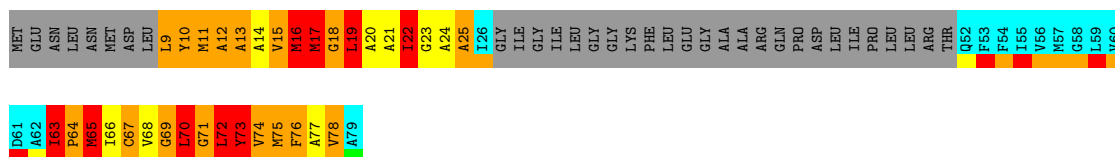
### 4.2.4 Score per residue for model 4

- Molecule 1: F1F0 ATP SYNTHASE (SUBUNIT C)



### 4.2.5 Score per residue for model 5

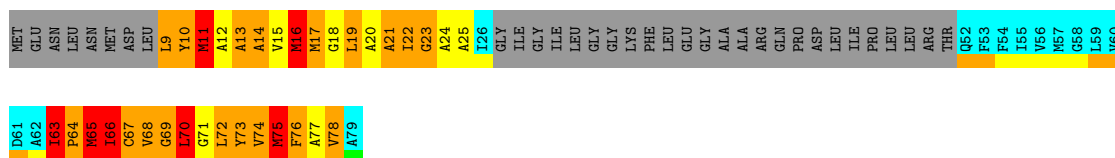
- Molecule 1: F1F0 ATP SYNTHASE (SUBUNIT C)



### 4.2.6 Score per residue for model 6

- Molecule 1: F1F0 ATP SYNTHASE (SUBUNIT C)





#### 4.2.7 Score per residue for model 7

- Molecule 1: F1F0 ATP SYNTHASE (SUBUNIT C)

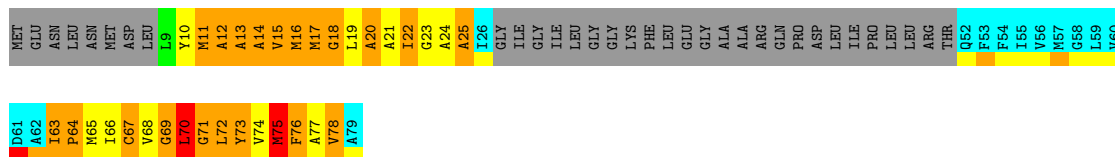
Chain A: 13% 18% 11% 16% 42%



#### 4.2.8 Score per residue for model 8

- Molecule 1: F1F0 ATP SYNTHASE (SUBUNIT C)

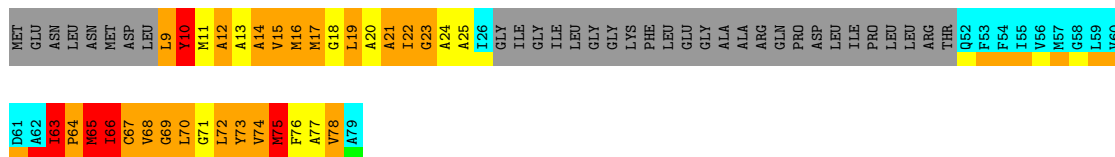
Chain A: 13% 25% 16% 42%



#### 4.2.9 Score per residue for model 9

- Molecule 1: F1F0 ATP SYNTHASE (SUBUNIT C)

Chain A: 11% 24% 6% 16% 42%



## 5 Refinement protocol and experimental data overview

Of the ? calculated structures, 9 were deposited, based on the following criterion: ?.

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

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

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     | 1.75±0.05    | 3±1/232 ( 1.5± 0.6%) | 2.07±0.08   | 12±2/315 ( 3.9± 0.5%) |
| All | All   | 1.75         | 31/2088 ( 1.5%)      | 2.08        | 111/2835 ( 3.9%)      |

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   | 0.3±0.5   |
| All | All   | 0         | 3         |

All unique bond 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(Å) | Ideal(Å) | Models |       |
|-----|-------|-----|------|-------|-------|-------------|----------|--------|-------|
|     |       |     |      |       |       |             |          | Worst  | Total |
| 1   | A     | 65  | MET  | C-N   | -8.86 | 1.21        | 1.33     | 4      | 6     |
| 1   | A     | 71  | GLY  | C-N   | -6.99 | 1.24        | 1.33     | 3      | 6     |
| 1   | A     | 16  | MET  | N-CA  | 6.86  | 1.55        | 1.46     | 5      | 2     |
| 1   | A     | 67  | CYS  | C-N   | -6.25 | 1.26        | 1.34     | 4      | 3     |
| 1   | A     | 21  | ALA  | CA-CB | -5.91 | 1.44        | 1.53     | 6      | 4     |
| 1   | A     | 65  | MET  | N-CA  | 5.67  | 1.53        | 1.46     | 6      | 5     |
| 1   | A     | 75  | MET  | N-CA  | 5.20  | 1.52        | 1.46     | 7      | 3     |
| 1   | A     | 71  | GLY  | N-CA  | 5.14  | 1.51        | 1.45     | 3      | 2     |

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     | 69  | GLY  | N-CA-C | -12.38 | 99.18       | 114.16   | 2      | 9     |
| 1   | A     | 72  | LEU  | N-CA-C | -11.65 | 97.18       | 112.68   | 1      | 9     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) | Models |       |
|-----|-------|-----|------|---------|-------|-------------|----------|--------|-------|
|     |       |     |      |         |       |             |          | Worst  | Total |
| 1   | A     | 64  | PRO  | N-CA-C  | -9.16 | 101.44      | 114.18   | 5      | 2     |
| 1   | A     | 75  | MET  | N-CA-C  | -8.62 | 100.72      | 111.75   | 9      | 3     |
| 1   | A     | 14  | ALA  | N-CA-C  | -8.44 | 101.12      | 111.33   | 3      | 8     |
| 1   | A     | 19  | LEU  | N-CA-C  | -8.33 | 102.16      | 111.07   | 2      | 1     |
| 1   | A     | 73  | TYR  | N-CA-C  | -7.76 | 101.82      | 111.75   | 2      | 6     |
| 1   | A     | 70  | LEU  | N-CA-C  | -7.62 | 102.91      | 111.07   | 8      | 8     |
| 1   | A     | 63  | ILE  | N-CA-CB | -7.51 | 100.69      | 111.21   | 7      | 6     |
| 1   | A     | 12  | ALA  | N-CA-C  | -7.32 | 103.38      | 111.36   | 6      | 9     |
| 1   | A     | 23  | GLY  | N-CA-C  | -7.30 | 106.64      | 114.67   | 3      | 6     |
| 1   | A     | 15  | VAL  | N-CA-C  | -6.90 | 103.61      | 110.30   | 5      | 8     |
| 1   | A     | 64  | PRO  | CB-CA-C | -6.86 | 100.24      | 111.56   | 8      | 3     |
| 1   | A     | 74  | VAL  | N-CA-C  | -6.82 | 106.00      | 113.43   | 4      | 4     |
| 1   | A     | 11  | MET  | N-CA-C  | -6.77 | 101.19      | 111.56   | 6      | 3     |
| 1   | A     | 65  | MET  | N-CA-CB | -6.48 | 100.55      | 110.07   | 2      | 2     |
| 1   | A     | 67  | CYS  | N-CA-C  | -6.16 | 103.18      | 112.04   | 8      | 2     |
| 1   | A     | 13  | ALA  | N-CA-C  | -5.92 | 104.95      | 111.82   | 5      | 8     |
| 1   | A     | 72  | LEU  | CB-CA-C | 5.75  | 119.04      | 109.56   | 2      | 3     |
| 1   | A     | 76  | PHE  | N-CA-C  | -5.41 | 107.23      | 113.88   | 3      | 5     |
| 1   | A     | 72  | LEU  | N-CA-CB | 5.35  | 117.94      | 110.07   | 4      | 2     |
| 1   | A     | 68  | VAL  | O-C-N   | -5.27 | 116.93      | 122.20   | 4      | 1     |
| 1   | A     | 22  | ILE  | N-CA-C  | -5.16 | 104.64      | 111.09   | 3      | 3     |

There are no chirality outliers.

All unique planar outliers are listed below.

| Mol | Chain | Res | Type | Group     | Models (Total) |
|-----|-------|-----|------|-----------|----------------|
| 1   | A     | 10  | TYR  | Sidechain | 3              |

## 6.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes |
|-----|-------|-------|----------|----------|---------|
| 1   | A     | 228   | 249      | 248      | 215±8   |
| All | All   | 2052  | 2241     | 2232     | 1937    |

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 452.

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

| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:13:ALA:O    | 1:A:72:LEU:HD11 | 1.09     | 1.48        | 5      | 1     |
| 1:A:72:LEU:HD21 | 1:A:73:TYR:CZ   | 1.07     | 1.83        | 6      | 3     |
| 1:A:72:LEU:HD21 | 1:A:73:TYR:CE1  | 1.06     | 1.86        | 6      | 3     |
| 1:A:21:ALA:HB1  | 1:A:65:MET:CB   | 1.05     | 1.79        | 3      | 5     |
| 1:A:18:GLY:CA   | 1:A:72:LEU:HD13 | 1.04     | 1.82        | 9      | 3     |
| 1:A:16:MET:CG   | 1:A:72:LEU:HD12 | 1.04     | 1.81        | 2      | 2     |
| 1:A:10:TYR:HA   | 1:A:13:ALA:HB3  | 1.04     | 1.30        | 3      | 8     |
| 1:A:70:LEU:O    | 1:A:74:VAL:HG23 | 1.03     | 1.53        | 1      | 9     |
| 1:A:68:VAL:HG12 | 1:A:72:LEU:CD2  | 1.03     | 1.84        | 1      | 3     |
| 1:A:18:GLY:HA3  | 1:A:72:LEU:HD13 | 1.00     | 1.26        | 4      | 3     |
| 1:A:17:MET:CG   | 1:A:68:VAL:HG12 | 1.00     | 1.87        | 6      | 3     |
| 1:A:64:PRO:CG   | 1:A:65:MET:HE2  | 0.98     | 1.87        | 5      | 3     |
| 1:A:74:VAL:HG13 | 1:A:77:ALA:O    | 0.96     | 1.60        | 8      | 7     |
| 1:A:25:ALA:HB2  | 1:A:65:MET:CG   | 0.95     | 1.91        | 1      | 3     |
| 1:A:10:TYR:CD1  | 1:A:72:LEU:HD13 | 0.95     | 1.95        | 5      | 1     |
| 1:A:21:ALA:HB2  | 1:A:65:MET:HA   | 0.95     | 1.36        | 5      | 5     |
| 1:A:71:GLY:C    | 1:A:72:LEU:HD23 | 0.94     | 1.86        | 7      | 3     |
| 1:A:17:MET:CG   | 1:A:68:VAL:O    | 0.94     | 2.16        | 4      | 3     |
| 1:A:10:TYR:CG   | 1:A:72:LEU:O    | 0.94     | 2.21        | 9      | 9     |
| 1:A:17:MET:HG3  | 1:A:68:VAL:HG12 | 0.94     | 1.39        | 9      | 3     |
| 1:A:21:ALA:HB2  | 1:A:65:MET:CA   | 0.93     | 1.94        | 5      | 7     |
| 1:A:10:TYR:CE1  | 1:A:72:LEU:HD13 | 0.93     | 1.98        | 5      | 1     |
| 1:A:15:VAL:HG12 | 1:A:19:LEU:HD12 | 0.91     | 1.42        | 5      | 3     |
| 1:A:68:VAL:O    | 1:A:72:LEU:HG   | 0.91     | 1.65        | 8      | 2     |
| 1:A:74:VAL:O    | 1:A:78:VAL:HG13 | 0.91     | 1.65        | 9      | 9     |
| 1:A:68:VAL:HG12 | 1:A:72:LEU:HD21 | 0.90     | 1.42        | 1      | 2     |
| 1:A:17:MET:SD   | 1:A:68:VAL:HG12 | 0.90     | 2.07        | 4      | 3     |
| 1:A:21:ALA:HB1  | 1:A:65:MET:CA   | 0.89     | 1.97        | 7      | 6     |
| 1:A:16:MET:SD   | 1:A:72:LEU:HD22 | 0.89     | 2.07        | 8      | 1     |
| 1:A:16:MET:HG3  | 1:A:72:LEU:HD13 | 0.88     | 1.43        | 8      | 2     |
| 1:A:17:MET:CB   | 1:A:72:LEU:HB3  | 0.88     | 1.99        | 6      | 3     |
| 1:A:72:LEU:HD11 | 1:A:73:TYR:CE1  | 0.87     | 2.04        | 9      | 2     |
| 1:A:17:MET:SD   | 1:A:21:ALA:HB2  | 0.87     | 2.09        | 7      | 3     |
| 1:A:63:ILE:HA   | 1:A:66:ILE:HD11 | 0.87     | 1.47        | 9      | 1     |
| 1:A:13:ALA:HB1  | 1:A:72:LEU:HD21 | 0.86     | 1.47        | 5      | 1     |
| 1:A:13:ALA:O    | 1:A:16:MET:HB3  | 0.86     | 1.71        | 5      | 7     |
| 1:A:15:VAL:CG1  | 1:A:19:LEU:HD12 | 0.85     | 1.99        | 5      | 3     |
| 1:A:10:TYR:O    | 1:A:14:ALA:HB2  | 0.85     | 1.69        | 2      | 9     |
| 1:A:17:MET:O    | 1:A:20:ALA:N    | 0.85     | 2.10        | 8      | 5     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:10:TYR:O    | 1:A:10:TYR:CD1  | 0.84     | 2.31        | 9      | 3     |
| 1:A:65:MET:HE3  | 1:A:66:ILE:HG12 | 0.84     | 1.48        | 1      | 3     |
| 1:A:17:MET:O    | 1:A:21:ALA:HB3  | 0.84     | 1.71        | 2      | 2     |
| 1:A:69:GLY:O    | 1:A:72:LEU:HD23 | 0.83     | 1.72        | 9      | 3     |
| 1:A:14:ALA:HA   | 1:A:72:LEU:HD12 | 0.83     | 1.49        | 6      | 1     |
| 1:A:21:ALA:HA   | 1:A:24:ALA:HB3  | 0.83     | 1.50        | 3      | 3     |
| 1:A:21:ALA:CB   | 1:A:65:MET:HA   | 0.82     | 2.04        | 6      | 7     |
| 1:A:65:MET:O    | 1:A:69:GLY:HA3  | 0.82     | 1.74        | 5      | 9     |
| 1:A:16:MET:HG2  | 1:A:72:LEU:HD12 | 0.82     | 1.50        | 2      | 2     |
| 1:A:17:MET:HB2  | 1:A:72:LEU:CG   | 0.81     | 2.04        | 5      | 3     |
| 1:A:25:ALA:HB2  | 1:A:65:MET:HG3  | 0.81     | 1.49        | 1      | 1     |
| 1:A:10:TYR:HE1  | 1:A:72:LEU:HD12 | 0.81     | 1.36        | 4      | 2     |
| 1:A:69:GLY:HA2  | 1:A:72:LEU:HD23 | 0.81     | 1.53        | 4      | 2     |
| 1:A:21:ALA:HB1  | 1:A:65:MET:HA   | 0.81     | 1.53        | 7      | 6     |
| 1:A:13:ALA:HB1  | 1:A:75:MET:HG3  | 0.81     | 1.53        | 6      | 6     |
| 1:A:10:TYR:CD2  | 1:A:73:TYR:HA   | 0.80     | 2.11        | 2      | 6     |
| 1:A:10:TYR:CD1  | 1:A:72:LEU:C    | 0.80     | 2.59        | 8      | 9     |
| 1:A:10:TYR:HB2  | 1:A:75:MET:CB   | 0.80     | 2.06        | 8      | 9     |
| 1:A:21:ALA:HB2  | 1:A:65:MET:CB   | 0.80     | 2.07        | 2      | 2     |
| 1:A:71:GLY:O    | 1:A:75:MET:N    | 0.79     | 2.16        | 9      | 9     |
| 1:A:64:PRO:HG2  | 1:A:65:MET:HE2  | 0.79     | 1.55        | 2      | 2     |
| 1:A:17:MET:HB2  | 1:A:72:LEU:HB2  | 0.79     | 1.54        | 8      | 4     |
| 1:A:22:ILE:HD13 | 1:A:22:ILE:N    | 0.79     | 1.92        | 4      | 1     |
| 1:A:21:ALA:CB   | 1:A:65:MET:CB   | 0.78     | 2.60        | 3      | 6     |
| 1:A:72:LEU:O    | 1:A:75:MET:N    | 0.78     | 2.16        | 2      | 9     |
| 1:A:10:TYR:CE1  | 1:A:72:LEU:HB3  | 0.78     | 2.14        | 3      | 5     |
| 1:A:21:ALA:O    | 1:A:25:ALA:N    | 0.78     | 2.16        | 8      | 9     |
| 1:A:69:GLY:HA2  | 1:A:72:LEU:CD2  | 0.78     | 2.09        | 9      | 3     |
| 1:A:21:ALA:CB   | 1:A:65:MET:HB3  | 0.78     | 2.08        | 2      | 5     |
| 1:A:18:GLY:O    | 1:A:19:LEU:C    | 0.78     | 2.26        | 9      | 5     |
| 1:A:10:TYR:CE1  | 1:A:72:LEU:CB   | 0.77     | 2.67        | 8      | 6     |
| 1:A:17:MET:HG2  | 1:A:68:VAL:O    | 0.77     | 1.78        | 4      | 3     |
| 1:A:21:ALA:HB1  | 1:A:65:MET:HB2  | 0.76     | 1.56        | 3      | 2     |
| 1:A:65:MET:HA   | 1:A:69:GLY:HA3  | 0.76     | 1.58        | 4      | 6     |
| 1:A:64:PRO:HG3  | 1:A:65:MET:HE2  | 0.76     | 1.57        | 5      | 2     |
| 1:A:13:ALA:O    | 1:A:16:MET:N    | 0.76     | 2.18        | 5      | 8     |
| 1:A:69:GLY:O    | 1:A:73:TYR:CD1  | 0.76     | 2.39        | 2      | 3     |
| 1:A:11:MET:O    | 1:A:14:ALA:HB3  | 0.75     | 1.81        | 6      | 9     |
| 1:A:17:MET:HG3  | 1:A:69:GLY:CA   | 0.75     | 2.11        | 3      | 6     |
| 1:A:64:PRO:C    | 1:A:69:GLY:H    | 0.75     | 1.90        | 9      | 6     |
| 1:A:69:GLY:O    | 1:A:73:TYR:CD2  | 0.75     | 2.40        | 4      | 4     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:15:VAL:O    | 1:A:19:LEU:CB   | 0.74     | 2.35        | 7      | 9     |
| 1:A:17:MET:O    | 1:A:21:ALA:CB   | 0.74     | 2.35        | 2      | 4     |
| 1:A:21:ALA:CB   | 1:A:65:MET:CA   | 0.74     | 2.65        | 9      | 9     |
| 1:A:63:ILE:N    | 1:A:64:PRO:HD2  | 0.74     | 1.97        | 6      | 7     |
| 1:A:13:ALA:HA   | 1:A:16:MET:HB3  | 0.74     | 1.57        | 2      | 6     |
| 1:A:13:ALA:O    | 1:A:16:MET:HB2  | 0.74     | 1.82        | 3      | 1     |
| 1:A:18:GLY:O    | 1:A:21:ALA:N    | 0.74     | 2.21        | 6      | 3     |
| 1:A:10:TYR:HB2  | 1:A:76:PHE:N    | 0.74     | 1.97        | 2      | 8     |
| 1:A:17:MET:HB2  | 1:A:72:LEU:CB   | 0.74     | 2.12        | 1      | 7     |
| 1:A:17:MET:HE3  | 1:A:68:VAL:CG1  | 0.74     | 2.12        | 2      | 3     |
| 1:A:72:LEU:CD2  | 1:A:73:TYR:CE1  | 0.74     | 2.71        | 9      | 3     |
| 1:A:17:MET:HE3  | 1:A:68:VAL:HB   | 0.73     | 1.60        | 2      | 2     |
| 1:A:68:VAL:HG12 | 1:A:72:LEU:HD11 | 0.73     | 1.61        | 8      | 1     |
| 1:A:66:ILE:O    | 1:A:70:LEU:HB2  | 0.73     | 1.83        | 7      | 9     |
| 1:A:17:MET:O    | 1:A:18:GLY:C    | 0.73     | 2.32        | 8      | 5     |
| 1:A:17:MET:HE3  | 1:A:68:VAL:CB   | 0.73     | 2.14        | 2      | 1     |
| 1:A:25:ALA:HB2  | 1:A:65:MET:HG2  | 0.73     | 1.58        | 3      | 2     |
| 1:A:74:VAL:HA   | 1:A:77:ALA:HB3  | 0.72     | 1.60        | 2      | 9     |
| 1:A:67:CYS:O    | 1:A:70:LEU:CB   | 0.72     | 2.37        | 8      | 9     |
| 1:A:71:GLY:HA2  | 1:A:74:VAL:HB   | 0.72     | 1.61        | 1      | 6     |
| 1:A:18:GLY:O    | 1:A:22:ILE:N    | 0.72     | 2.23        | 4      | 9     |
| 1:A:17:MET:HB3  | 1:A:72:LEU:N    | 0.72     | 1.98        | 9      | 3     |
| 1:A:72:LEU:HD23 | 1:A:72:LEU:N    | 0.72     | 1.97        | 7      | 2     |
| 1:A:16:MET:CG   | 1:A:72:LEU:HD13 | 0.72     | 2.15        | 8      | 2     |
| 1:A:66:ILE:O    | 1:A:70:LEU:HD13 | 0.71     | 1.86        | 2      | 1     |
| 1:A:10:TYR:CE2  | 1:A:76:PHE:CD1  | 0.71     | 2.78        | 6      | 1     |
| 1:A:13:ALA:CA   | 1:A:16:MET:HB3  | 0.71     | 2.14        | 7      | 6     |
| 1:A:10:TYR:CE1  | 1:A:72:LEU:HD12 | 0.71     | 2.19        | 4      | 2     |
| 1:A:17:MET:HE3  | 1:A:68:VAL:HG12 | 0.71     | 1.63        | 5      | 2     |
| 1:A:68:VAL:O    | 1:A:72:LEU:N    | 0.71     | 2.24        | 5      | 8     |
| 1:A:72:LEU:HG   | 1:A:73:TYR:N    | 0.71     | 2.00        | 9      | 3     |
| 1:A:63:ILE:CA   | 1:A:66:ILE:HD11 | 0.71     | 2.16        | 9      | 1     |
| 1:A:10:TYR:CZ   | 1:A:73:TYR:CD1  | 0.71     | 2.78        | 1      | 5     |
| 1:A:17:MET:CG   | 1:A:69:GLY:CA   | 0.71     | 2.69        | 2      | 6     |
| 1:A:18:GLY:H    | 1:A:72:LEU:HD12 | 0.71     | 1.46        | 5      | 1     |
| 1:A:10:TYR:CE2  | 1:A:73:TYR:HA   | 0.70     | 2.21        | 8      | 9     |
| 1:A:65:MET:O    | 1:A:69:GLY:CA   | 0.70     | 2.40        | 2      | 9     |
| 1:A:10:TYR:O    | 1:A:14:ALA:CB   | 0.70     | 2.40        | 2      | 9     |
| 1:A:25:ALA:HB2  | 1:A:65:MET:SD   | 0.70     | 2.27        | 3      | 2     |
| 1:A:9:LEU:O     | 1:A:13:ALA:HB3  | 0.70     | 1.85        | 5      | 2     |
| 1:A:10:TYR:CB   | 1:A:75:MET:CB   | 0.70     | 2.69        | 6      | 9     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:20:ALA:HB1  | 1:A:64:PRO:HG3  | 0.70     | 1.63        | 4      | 3     |
| 1:A:17:MET:CB   | 1:A:72:LEU:HB2  | 0.70     | 2.17        | 2      | 3     |
| 1:A:70:LEU:O    | 1:A:74:VAL:CB   | 0.70     | 2.40        | 4      | 6     |
| 1:A:10:TYR:CE1  | 1:A:72:LEU:CG   | 0.70     | 2.75        | 9      | 3     |
| 1:A:72:LEU:HD23 | 1:A:75:MET:CG   | 0.69     | 2.16        | 5      | 1     |
| 1:A:10:TYR:CG   | 1:A:72:LEU:C    | 0.69     | 2.69        | 8      | 7     |
| 1:A:76:PHE:CD1  | 1:A:76:PHE:C    | 0.69     | 2.70        | 2      | 6     |
| 1:A:12:ALA:O    | 1:A:15:VAL:HG22 | 0.69     | 1.87        | 2      | 2     |
| 1:A:10:TYR:CD2  | 1:A:76:PHE:CD1  | 0.69     | 2.79        | 6      | 4     |
| 1:A:17:MET:HE2  | 1:A:72:LEU:CD2  | 0.69     | 2.17        | 3      | 1     |
| 1:A:21:ALA:C    | 1:A:25:ALA:HB3  | 0.69     | 2.12        | 8      | 1     |
| 1:A:17:MET:CG   | 1:A:69:GLY:N    | 0.69     | 2.55        | 5      | 5     |
| 1:A:13:ALA:O    | 1:A:16:MET:CB   | 0.69     | 2.40        | 5      | 6     |
| 1:A:15:VAL:O    | 1:A:16:MET:C    | 0.69     | 2.35        | 5      | 8     |
| 1:A:13:ALA:HB1  | 1:A:72:LEU:CD2  | 0.69     | 2.17        | 5      | 1     |
| 1:A:17:MET:HE2  | 1:A:72:LEU:HD12 | 0.69     | 1.63        | 7      | 1     |
| 1:A:64:PRO:O    | 1:A:65:MET:C    | 0.69     | 2.36        | 1      | 6     |
| 1:A:17:MET:HE2  | 1:A:72:LEU:CD1  | 0.68     | 2.18        | 7      | 1     |
| 1:A:17:MET:CB   | 1:A:72:LEU:N    | 0.68     | 2.57        | 9      | 3     |
| 1:A:18:GLY:O    | 1:A:22:ILE:HB   | 0.68     | 1.89        | 1      | 6     |
| 1:A:17:MET:SD   | 1:A:64:PRO:HB2  | 0.68     | 2.28        | 3      | 3     |
| 1:A:65:MET:CA   | 1:A:69:GLY:HA3  | 0.68     | 2.18        | 4      | 4     |
| 1:A:64:PRO:O    | 1:A:66:ILE:N    | 0.68     | 2.27        | 4      | 6     |
| 1:A:13:ALA:HB1  | 1:A:16:MET:HG2  | 0.68     | 1.66        | 8      | 1     |
| 1:A:69:GLY:CA   | 1:A:72:LEU:HD23 | 0.67     | 2.19        | 4      | 3     |
| 1:A:22:ILE:CD1  | 1:A:73:TYR:CZ   | 0.67     | 2.77        | 5      | 3     |
| 1:A:74:VAL:HG12 | 1:A:78:VAL:HG13 | 0.67     | 1.65        | 8      | 6     |
| 1:A:10:TYR:CB   | 1:A:75:MET:HB2  | 0.67     | 2.20        | 6      | 3     |
| 1:A:73:TYR:N    | 1:A:73:TYR:CD1  | 0.67     | 2.62        | 5      | 1     |
| 1:A:70:LEU:HD23 | 1:A:74:VAL:HG21 | 0.67     | 1.66        | 6      | 1     |
| 1:A:63:ILE:HG22 | 1:A:64:PRO:HD3  | 0.67     | 1.65        | 8      | 7     |
| 1:A:72:LEU:HA   | 1:A:75:MET:HB2  | 0.67     | 1.66        | 8      | 7     |
| 1:A:16:MET:HB3  | 1:A:72:LEU:HD21 | 0.67     | 1.65        | 5      | 1     |
| 1:A:76:PHE:CD1  | 1:A:77:ALA:N    | 0.66     | 2.63        | 6      | 9     |
| 1:A:73:TYR:O    | 1:A:76:PHE:CD1  | 0.66     | 2.48        | 9      | 4     |
| 1:A:21:ALA:HA   | 1:A:65:MET:SD   | 0.66     | 2.30        | 8      | 1     |
| 1:A:70:LEU:O    | 1:A:74:VAL:N    | 0.66     | 2.28        | 4      | 4     |
| 1:A:21:ALA:O    | 1:A:24:ALA:N    | 0.66     | 2.28        | 6      | 7     |
| 1:A:69:GLY:O    | 1:A:73:TYR:CG   | 0.66     | 2.48        | 7      | 4     |
| 1:A:74:VAL:HG13 | 1:A:77:ALA:C    | 0.66     | 2.15        | 5      | 5     |
| 1:A:13:ALA:HA   | 1:A:16:MET:HB2  | 0.66     | 1.65        | 5      | 1     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:10:TYR:HB2  | 1:A:75:MET:HB3  | 0.66     | 1.67        | 4      | 7     |
| 1:A:13:ALA:HA   | 1:A:16:MET:HG2  | 0.66     | 1.68        | 3      | 1     |
| 1:A:17:MET:HB2  | 1:A:72:LEU:CD1  | 0.66     | 2.20        | 5      | 1     |
| 1:A:10:TYR:CE1  | 1:A:14:ALA:HA   | 0.66     | 2.25        | 4      | 8     |
| 1:A:22:ILE:CD1  | 1:A:73:TYR:OH   | 0.66     | 2.44        | 7      | 8     |
| 1:A:22:ILE:HD13 | 1:A:73:TYR:CE1  | 0.66     | 2.26        | 3      | 2     |
| 1:A:17:MET:CG   | 1:A:69:GLY:HA2  | 0.65     | 2.21        | 2      | 5     |
| 1:A:17:MET:HB2  | 1:A:72:LEU:HD12 | 0.65     | 1.68        | 5      | 2     |
| 1:A:17:MET:O    | 1:A:21:ALA:N    | 0.65     | 2.29        | 3      | 5     |
| 1:A:68:VAL:HG12 | 1:A:72:LEU:HD23 | 0.65     | 1.64        | 1      | 1     |
| 1:A:74:VAL:HG12 | 1:A:78:VAL:CG1  | 0.65     | 2.22        | 8      | 6     |
| 1:A:64:PRO:C    | 1:A:69:GLY:N    | 0.65     | 2.54        | 4      | 3     |
| 1:A:73:TYR:O    | 1:A:76:PHE:CE1  | 0.65     | 2.49        | 5      | 4     |
| 1:A:24:ALA:HB3  | 1:A:65:MET:HG3  | 0.65     | 1.69        | 8      | 3     |
| 1:A:64:PRO:O    | 1:A:67:CYS:N    | 0.65     | 2.29        | 3      | 6     |
| 1:A:10:TYR:HB3  | 1:A:75:MET:CB   | 0.65     | 2.21        | 6      | 1     |
| 1:A:72:LEU:CD2  | 1:A:75:MET:CG   | 0.65     | 2.75        | 5      | 1     |
| 1:A:21:ALA:O    | 1:A:22:ILE:C    | 0.65     | 2.36        | 2      | 6     |
| 1:A:72:LEU:O    | 1:A:73:TYR:C    | 0.65     | 2.40        | 3      | 7     |
| 1:A:17:MET:CB   | 1:A:72:LEU:CB   | 0.65     | 2.75        | 6      | 4     |
| 1:A:10:TYR:OH   | 1:A:73:TYR:CE1  | 0.64     | 2.47        | 1      | 4     |
| 1:A:10:TYR:HB2  | 1:A:75:MET:HB2  | 0.64     | 1.68        | 6      | 4     |
| 1:A:17:MET:HG2  | 1:A:68:VAL:C    | 0.64     | 2.17        | 5      | 3     |
| 1:A:64:PRO:HA   | 1:A:68:VAL:CB   | 0.64     | 2.23        | 6      | 3     |
| 1:A:13:ALA:CB   | 1:A:72:LEU:HD21 | 0.64     | 2.20        | 5      | 1     |
| 1:A:64:PRO:O    | 1:A:69:GLY:N    | 0.64     | 2.30        | 2      | 2     |
| 1:A:21:ALA:HB2  | 1:A:65:MET:N    | 0.64     | 2.07        | 9      | 3     |
| 1:A:21:ALA:HB1  | 1:A:65:MET:CG   | 0.64     | 2.22        | 1      | 3     |
| 1:A:10:TYR:CD1  | 1:A:72:LEU:HB3  | 0.64     | 2.27        | 2      | 5     |
| 1:A:13:ALA:O    | 1:A:14:ALA:C    | 0.64     | 2.39        | 5      | 7     |
| 1:A:17:MET:HG2  | 1:A:69:GLY:N    | 0.64     | 2.08        | 5      | 6     |
| 1:A:69:GLY:CA   | 1:A:73:TYR:CE1  | 0.64     | 2.81        | 7      | 2     |
| 1:A:71:GLY:O    | 1:A:75:MET:HG2  | 0.64     | 1.93        | 9      | 4     |
| 1:A:22:ILE:HA   | 1:A:25:ALA:HB3  | 0.64     | 1.69        | 6      | 2     |
| 1:A:10:TYR:HB3  | 1:A:76:PHE:HB3  | 0.64     | 1.69        | 4      | 7     |
| 1:A:17:MET:HB3  | 1:A:72:LEU:HB3  | 0.64     | 1.70        | 4      | 3     |
| 1:A:72:LEU:CG   | 1:A:73:TYR:CD1  | 0.64     | 2.81        | 9      | 3     |
| 1:A:65:MET:HG3  | 1:A:66:ILE:HG12 | 0.63     | 1.71        | 7      | 2     |
| 1:A:72:LEU:CD1  | 1:A:73:TYR:CE1  | 0.63     | 2.81        | 9      | 1     |
| 1:A:63:ILE:N    | 1:A:64:PRO:CD   | 0.63     | 2.61        | 6      | 6     |
| 1:A:72:LEU:HD13 | 1:A:75:MET:HG2  | 0.63     | 1.68        | 1      | 2     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:10:TYR:CB   | 1:A:72:LEU:O    | 0.63     | 2.45        | 7      | 7     |
| 1:A:17:MET:CE   | 1:A:72:LEU:CD2  | 0.63     | 2.76        | 3      | 1     |
| 1:A:68:VAL:HG12 | 1:A:72:LEU:HD22 | 0.63     | 1.71        | 3      | 1     |
| 1:A:68:VAL:O    | 1:A:72:LEU:HD23 | 0.63     | 1.94        | 1      | 2     |
| 1:A:72:LEU:HA   | 1:A:75:MET:CB   | 0.63     | 2.24        | 8      | 5     |
| 1:A:72:LEU:HD23 | 1:A:75:MET:HG2  | 0.63     | 1.69        | 5      | 1     |
| 1:A:63:ILE:CB   | 1:A:64:PRO:CD   | 0.62     | 2.77        | 5      | 9     |
| 1:A:63:ILE:HG22 | 1:A:64:PRO:CD   | 0.62     | 2.24        | 5      | 7     |
| 1:A:70:LEU:O    | 1:A:74:VAL:CG2  | 0.62     | 2.47        | 9      | 6     |
| 1:A:9:LEU:O     | 1:A:13:ALA:CB   | 0.62     | 2.47        | 5      | 2     |
| 1:A:10:TYR:CB   | 1:A:76:PHE:N    | 0.62     | 2.62        | 7      | 5     |
| 1:A:17:MET:HG2  | 1:A:72:LEU:HD22 | 0.62     | 1.70        | 3      | 1     |
| 1:A:22:ILE:HD11 | 1:A:72:LEU:HD11 | 0.62     | 1.70        | 4      | 1     |
| 1:A:74:VAL:O    | 1:A:75:MET:C    | 0.62     | 2.43        | 8      | 9     |
| 1:A:10:TYR:CZ   | 1:A:14:ALA:HA   | 0.62     | 2.29        | 3      | 5     |
| 1:A:65:MET:C    | 1:A:65:MET:SD   | 0.62     | 2.83        | 1      | 4     |
| 1:A:16:MET:HG3  | 1:A:17:MET:SD   | 0.62     | 2.35        | 4      | 3     |
| 1:A:10:TYR:CD1  | 1:A:72:LEU:O    | 0.62     | 2.53        | 4      | 3     |
| 1:A:10:TYR:HE1  | 1:A:72:LEU:CD1  | 0.62     | 2.08        | 4      | 2     |
| 1:A:10:TYR:CE1  | 1:A:72:LEU:HB2  | 0.62     | 2.30        | 9      | 3     |
| 1:A:72:LEU:HG   | 1:A:73:TYR:CD1  | 0.62     | 2.29        | 9      | 3     |
| 1:A:17:MET:HG3  | 1:A:68:VAL:CG1  | 0.62     | 2.20        | 9      | 3     |
| 1:A:24:ALA:HB3  | 1:A:65:MET:SD   | 0.62     | 2.35        | 8      | 1     |
| 1:A:72:LEU:HD11 | 1:A:73:TYR:HE1  | 0.61     | 1.53        | 9      | 1     |
| 1:A:21:ALA:HA   | 1:A:65:MET:HB3  | 0.61     | 1.70        | 8      | 2     |
| 1:A:68:VAL:O    | 1:A:72:LEU:CD2  | 0.61     | 2.48        | 1      | 1     |
| 1:A:72:LEU:N    | 1:A:72:LEU:CD2  | 0.61     | 2.62        | 2      | 2     |
| 1:A:73:TYR:CD1  | 1:A:73:TYR:N    | 0.61     | 2.69        | 7      | 3     |
| 1:A:10:TYR:CD1  | 1:A:72:LEU:CG   | 0.61     | 2.84        | 6      | 1     |
| 1:A:16:MET:CG   | 1:A:72:LEU:CD1  | 0.61     | 2.79        | 7      | 2     |
| 1:A:72:LEU:HD21 | 1:A:73:TYR:CE2  | 0.61     | 2.31        | 9      | 3     |
| 1:A:66:ILE:O    | 1:A:70:LEU:CB   | 0.61     | 2.48        | 7      | 6     |
| 1:A:64:PRO:HG2  | 1:A:65:MET:N    | 0.61     | 2.11        | 8      | 3     |
| 1:A:10:TYR:HA   | 1:A:13:ALA:CB   | 0.61     | 2.20        | 6      | 1     |
| 1:A:72:LEU:CA   | 1:A:75:MET:HB2  | 0.61     | 2.25        | 2      | 7     |
| 1:A:72:LEU:N    | 1:A:72:LEU:HD23 | 0.61     | 2.10        | 2      | 1     |
| 1:A:16:MET:HG3  | 1:A:17:MET:HE2  | 0.60     | 1.72        | 5      | 1     |
| 1:A:10:TYR:CD1  | 1:A:72:LEU:CB   | 0.60     | 2.84        | 8      | 5     |
| 1:A:10:TYR:CA   | 1:A:75:MET:HB3  | 0.60     | 2.26        | 9      | 7     |
| 1:A:71:GLY:O    | 1:A:72:LEU:HD12 | 0.60     | 1.95        | 3      | 1     |
| 1:A:17:MET:O    | 1:A:19:LEU:N    | 0.60     | 2.35        | 5      | 5     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:69:GLY:C    | 1:A:73:TYR:CD2  | 0.60     | 2.79        | 6      | 4     |
| 1:A:10:TYR:CD1  | 1:A:14:ALA:HA   | 0.60     | 2.32        | 9      | 2     |
| 1:A:10:TYR:HB2  | 1:A:72:LEU:O    | 0.60     | 1.97        | 1      | 6     |
| 1:A:70:LEU:O    | 1:A:74:VAL:HB   | 0.60     | 1.96        | 5      | 6     |
| 1:A:10:TYR:O    | 1:A:14:ALA:N    | 0.60     | 2.35        | 4      | 9     |
| 1:A:10:TYR:O    | 1:A:14:ALA:CA   | 0.60     | 2.50        | 6      | 9     |
| 1:A:69:GLY:HA3  | 1:A:73:TYR:CE2  | 0.59     | 2.32        | 3      | 3     |
| 1:A:71:GLY:HA2  | 1:A:74:VAL:CB   | 0.59     | 2.26        | 1      | 3     |
| 1:A:17:MET:CG   | 1:A:72:LEU:HD12 | 0.59     | 2.27        | 8      | 1     |
| 1:A:69:GLY:HA3  | 1:A:73:TYR:CE1  | 0.59     | 2.32        | 7      | 2     |
| 1:A:68:VAL:C    | 1:A:72:LEU:HG   | 0.59     | 2.23        | 8      | 2     |
| 1:A:16:MET:SD   | 1:A:72:LEU:CD1  | 0.59     | 2.91        | 7      | 1     |
| 1:A:65:MET:HB2  | 1:A:73:TYR:OH   | 0.59     | 1.96        | 7      | 1     |
| 1:A:17:MET:HG3  | 1:A:21:ALA:CB   | 0.59     | 2.27        | 7      | 2     |
| 1:A:63:ILE:CG2  | 1:A:64:PRO:HD3  | 0.59     | 2.27        | 8      | 7     |
| 1:A:13:ALA:CB   | 1:A:75:MET:CG   | 0.59     | 2.80        | 3      | 1     |
| 1:A:64:PRO:CG   | 1:A:65:MET:CE   | 0.59     | 2.80        | 8      | 2     |
| 1:A:72:LEU:HD13 | 1:A:75:MET:SD   | 0.59     | 2.37        | 2      | 1     |
| 1:A:15:VAL:O    | 1:A:19:LEU:HB2  | 0.59     | 1.97        | 8      | 9     |
| 1:A:64:PRO:CG   | 1:A:65:MET:N    | 0.59     | 2.65        | 8      | 3     |
| 1:A:64:PRO:O    | 1:A:68:VAL:HB   | 0.59     | 1.97        | 2      | 3     |
| 1:A:17:MET:HB3  | 1:A:72:LEU:HB2  | 0.59     | 1.73        | 2      | 1     |
| 1:A:24:ALA:HB3  | 1:A:65:MET:CG   | 0.59     | 2.27        | 8      | 1     |
| 1:A:74:VAL:O    | 1:A:76:PHE:N    | 0.59     | 2.36        | 3      | 6     |
| 1:A:14:ALA:O    | 1:A:18:GLY:CA   | 0.58     | 2.51        | 6      | 9     |
| 1:A:16:MET:CG   | 1:A:17:MET:N    | 0.58     | 2.65        | 9      | 6     |
| 1:A:69:GLY:O    | 1:A:73:TYR:N    | 0.58     | 2.36        | 2      | 4     |
| 1:A:10:TYR:CD2  | 1:A:72:LEU:O    | 0.58     | 2.56        | 9      | 3     |
| 1:A:69:GLY:CA   | 1:A:72:LEU:CD2  | 0.58     | 2.81        | 9      | 2     |
| 1:A:64:PRO:HG2  | 1:A:65:MET:SD   | 0.58     | 2.38        | 8      | 2     |
| 1:A:11:MET:O    | 1:A:14:ALA:CB   | 0.58     | 2.51        | 5      | 9     |
| 1:A:17:MET:HG3  | 1:A:69:GLY:N    | 0.58     | 2.13        | 8      | 3     |
| 1:A:68:VAL:C    | 1:A:72:LEU:HD23 | 0.58     | 2.24        | 1      | 1     |
| 1:A:71:GLY:O    | 1:A:72:LEU:HD23 | 0.58     | 1.98        | 8      | 1     |
| 1:A:10:TYR:CD1  | 1:A:72:LEU:CA   | 0.58     | 2.87        | 8      | 4     |
| 1:A:17:MET:HG2  | 1:A:71:GLY:CA   | 0.58     | 2.28        | 9      | 3     |
| 1:A:64:PRO:HG2  | 1:A:65:MET:CE   | 0.58     | 2.29        | 5      | 2     |
| 1:A:17:MET:HG2  | 1:A:71:GLY:C    | 0.58     | 2.23        | 9      | 3     |
| 1:A:17:MET:SD   | 1:A:20:ALA:HB3  | 0.58     | 2.38        | 8      | 1     |
| 1:A:10:TYR:HB2  | 1:A:75:MET:C    | 0.58     | 2.24        | 4      | 7     |
| 1:A:65:MET:O    | 1:A:70:LEU:N    | 0.58     | 2.37        | 1      | 2     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:65:MET:SD   | 1:A:66:ILE:N    | 0.58     | 2.76        | 7      | 2     |
| 1:A:10:TYR:CD1  | 1:A:13:ALA:C    | 0.58     | 2.81        | 3      | 2     |
| 1:A:71:GLY:O    | 1:A:75:MET:CG   | 0.58     | 2.52        | 4      | 3     |
| 1:A:71:GLY:O    | 1:A:75:MET:CA   | 0.58     | 2.51        | 9      | 4     |
| 1:A:74:VAL:O    | 1:A:77:ALA:N    | 0.57     | 2.37        | 2      | 5     |
| 1:A:21:ALA:HA   | 1:A:65:MET:HG3  | 0.57     | 1.75        | 2      | 2     |
| 1:A:10:TYR:CE1  | 1:A:72:LEU:CD1  | 0.57     | 2.87        | 4      | 4     |
| 1:A:15:VAL:O    | 1:A:16:MET:O    | 0.57     | 2.22        | 5      | 6     |
| 1:A:22:ILE:N    | 1:A:22:ILE:CD1  | 0.57     | 2.67        | 2      | 4     |
| 1:A:64:PRO:CB   | 1:A:68:VAL:HB   | 0.57     | 2.30        | 1      | 6     |
| 1:A:68:VAL:CG1  | 1:A:72:LEU:HD21 | 0.57     | 2.26        | 1      | 2     |
| 1:A:63:ILE:O    | 1:A:66:ILE:HG13 | 0.57     | 1.99        | 9      | 1     |
| 1:A:19:LEU:C    | 1:A:19:LEU:HD23 | 0.57     | 2.24        | 8      | 3     |
| 1:A:72:LEU:O    | 1:A:75:MET:HB2  | 0.57     | 2.00        | 7      | 7     |
| 1:A:10:TYR:HD1  | 1:A:72:LEU:HD13 | 0.57     | 1.54        | 5      | 1     |
| 1:A:72:LEU:CD2  | 1:A:75:MET:HG3  | 0.57     | 2.29        | 5      | 1     |
| 1:A:16:MET:SD   | 1:A:17:MET:HE2  | 0.57     | 2.40        | 1      | 1     |
| 1:A:10:TYR:CE1  | 1:A:13:ALA:O    | 0.57     | 2.58        | 3      | 2     |
| 1:A:20:ALA:O    | 1:A:24:ALA:N    | 0.57     | 2.38        | 3      | 4     |
| 1:A:22:ILE:HD13 | 1:A:73:TYR:HE1  | 0.57     | 1.58        | 3      | 1     |
| 1:A:15:VAL:HG13 | 1:A:19:LEU:HB2  | 0.57     | 1.75        | 4      | 1     |
| 1:A:17:MET:CB   | 1:A:72:LEU:HD12 | 0.57     | 2.29        | 8      | 2     |
| 1:A:10:TYR:CE1  | 1:A:72:LEU:HG   | 0.57     | 2.35        | 9      | 3     |
| 1:A:10:TYR:OH   | 1:A:18:GLY:N    | 0.57     | 2.37        | 2      | 4     |
| 1:A:71:GLY:O    | 1:A:75:MET:CB   | 0.57     | 2.53        | 4      | 3     |
| 1:A:12:ALA:O    | 1:A:15:VAL:HG13 | 0.57     | 2.00        | 7      | 1     |
| 1:A:17:MET:HG2  | 1:A:69:GLY:CA   | 0.56     | 2.31        | 2      | 4     |
| 1:A:21:ALA:CB   | 1:A:65:MET:HB2  | 0.56     | 2.30        | 1      | 1     |
| 1:A:16:MET:SD   | 1:A:17:MET:N    | 0.56     | 2.78        | 2      | 1     |
| 1:A:17:MET:CB   | 1:A:68:VAL:O    | 0.56     | 2.52        | 9      | 3     |
| 1:A:10:TYR:CD1  | 1:A:10:TYR:O    | 0.56     | 2.57        | 5      | 1     |
| 1:A:68:VAL:HG12 | 1:A:72:LEU:CD1  | 0.56     | 2.30        | 8      | 1     |
| 1:A:15:VAL:O    | 1:A:19:LEU:N    | 0.56     | 2.38        | 9      | 3     |
| 1:A:16:MET:HG2  | 1:A:72:LEU:CD1  | 0.56     | 2.29        | 1      | 2     |
| 1:A:71:GLY:C    | 1:A:75:MET:H    | 0.56     | 2.08        | 5      | 2     |
| 1:A:63:ILE:H    | 1:A:64:PRO:HD2  | 0.56     | 1.60        | 2      | 2     |
| 1:A:18:GLY:O    | 1:A:22:ILE:CB   | 0.56     | 2.54        | 3      | 5     |
| 1:A:64:PRO:O    | 1:A:68:VAL:N    | 0.56     | 2.39        | 3      | 7     |
| 1:A:17:MET:CB   | 1:A:21:ALA:HB3  | 0.56     | 2.31        | 3      | 2     |
| 1:A:10:TYR:CB   | 1:A:75:MET:HB3  | 0.56     | 2.31        | 2      | 7     |
| 1:A:17:MET:CE   | 1:A:68:VAL:CG1  | 0.56     | 2.83        | 2      | 1     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:17:MET:HB3  | 1:A:72:LEU:CB   | 0.56     | 2.31        | 9      | 3     |
| 1:A:72:LEU:CG   | 1:A:73:TYR:N    | 0.55     | 2.69        | 9      | 3     |
| 1:A:74:VAL:C    | 1:A:76:PHE:N    | 0.55     | 2.64        | 7      | 9     |
| 1:A:64:PRO:CD   | 1:A:65:MET:HE2  | 0.55     | 2.32        | 8      | 1     |
| 1:A:67:CYS:C    | 1:A:70:LEU:HB2  | 0.55     | 2.27        | 7      | 9     |
| 1:A:10:TYR:CE2  | 1:A:73:TYR:CD1  | 0.55     | 2.94        | 2      | 4     |
| 1:A:71:GLY:C    | 1:A:72:LEU:CD2  | 0.55     | 2.80        | 2      | 2     |
| 1:A:63:ILE:O    | 1:A:67:CYS:CB   | 0.55     | 2.54        | 8      | 1     |
| 1:A:13:ALA:CA   | 1:A:16:MET:HG2  | 0.55     | 2.32        | 8      | 2     |
| 1:A:13:ALA:O    | 1:A:16:MET:HG2  | 0.55     | 2.01        | 8      | 1     |
| 1:A:17:MET:SD   | 1:A:68:VAL:CG1  | 0.55     | 2.92        | 4      | 3     |
| 1:A:67:CYS:O    | 1:A:70:LEU:HB3  | 0.55     | 2.00        | 8      | 9     |
| 1:A:10:TYR:CD1  | 1:A:75:MET:HB2  | 0.55     | 2.37        | 7      | 3     |
| 1:A:13:ALA:CB   | 1:A:16:MET:HG2  | 0.55     | 2.30        | 8      | 2     |
| 1:A:17:MET:CB   | 1:A:72:LEU:CA   | 0.55     | 2.84        | 4      | 3     |
| 1:A:68:VAL:O    | 1:A:71:GLY:N    | 0.55     | 2.39        | 7      | 7     |
| 1:A:10:TYR:CD2  | 1:A:73:TYR:CA   | 0.55     | 2.90        | 2      | 3     |
| 1:A:21:ALA:O    | 1:A:23:GLY:N    | 0.55     | 2.40        | 8      | 2     |
| 1:A:64:PRO:O    | 1:A:68:VAL:CB   | 0.55     | 2.55        | 5      | 2     |
| 1:A:10:TYR:CE1  | 1:A:72:LEU:C    | 0.55     | 2.85        | 4      | 2     |
| 1:A:66:ILE:O    | 1:A:70:LEU:CD1  | 0.54     | 2.55        | 2      | 2     |
| 1:A:10:TYR:HE1  | 1:A:72:LEU:HD13 | 0.54     | 1.59        | 5      | 1     |
| 1:A:71:GLY:C    | 1:A:75:MET:N    | 0.54     | 2.65        | 5      | 1     |
| 1:A:21:ALA:HB1  | 1:A:65:MET:HG2  | 0.54     | 1.79        | 1      | 1     |
| 1:A:64:PRO:CD   | 1:A:65:MET:H    | 0.54     | 2.15        | 5      | 3     |
| 1:A:72:LEU:HD21 | 1:A:73:TYR:CD1  | 0.54     | 2.34        | 9      | 1     |
| 1:A:10:TYR:OH   | 1:A:73:TYR:CD1  | 0.54     | 2.60        | 1      | 4     |
| 1:A:67:CYS:O    | 1:A:70:LEU:HB2  | 0.54     | 2.01        | 8      | 9     |
| 1:A:12:ALA:O    | 1:A:15:VAL:HB   | 0.54     | 2.02        | 5      | 6     |
| 1:A:13:ALA:HB1  | 1:A:75:MET:CG   | 0.54     | 2.32        | 3      | 3     |
| 1:A:66:ILE:O    | 1:A:70:LEU:HD12 | 0.54     | 2.02        | 3      | 2     |
| 1:A:69:GLY:C    | 1:A:72:LEU:HD23 | 0.54     | 2.28        | 9      | 1     |
| 1:A:10:TYR:CD1  | 1:A:72:LEU:HD12 | 0.54     | 2.38        | 6      | 1     |
| 1:A:10:TYR:CZ   | 1:A:73:TYR:HA   | 0.54     | 2.38        | 6      | 1     |
| 1:A:64:PRO:HA   | 1:A:68:VAL:HB   | 0.54     | 1.80        | 6      | 3     |
| 1:A:65:MET:C    | 1:A:69:GLY:HA3  | 0.54     | 2.27        | 4      | 3     |
| 1:A:12:ALA:O    | 1:A:15:VAL:CB   | 0.54     | 2.56        | 5      | 2     |
| 1:A:72:LEU:CD1  | 1:A:75:MET:HG2  | 0.54     | 2.33        | 1      | 1     |
| 1:A:16:MET:HB3  | 1:A:72:LEU:CD2  | 0.54     | 2.33        | 3      | 2     |
| 1:A:16:MET:SD   | 1:A:17:MET:HE1  | 0.54     | 2.43        | 5      | 1     |
| 1:A:16:MET:HG3  | 1:A:72:LEU:CD1  | 0.54     | 2.32        | 7      | 2     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:16:MET:CG   | 1:A:17:MET:SD   | 0.54     | 2.96        | 4      | 3     |
| 1:A:10:TYR:HB3  | 1:A:76:PHE:CD2  | 0.53     | 2.38        | 2      | 5     |
| 1:A:17:MET:CG   | 1:A:21:ALA:CB   | 0.53     | 2.86        | 7      | 3     |
| 1:A:69:GLY:O    | 1:A:73:TYR:CB   | 0.53     | 2.56        | 2      | 2     |
| 1:A:69:GLY:O    | 1:A:70:LEU:C    | 0.53     | 2.50        | 8      | 9     |
| 1:A:13:ALA:HA   | 1:A:16:MET:CB   | 0.53     | 2.32        | 9      | 4     |
| 1:A:14:ALA:HA   | 1:A:72:LEU:CD1  | 0.53     | 2.29        | 6      | 1     |
| 1:A:17:MET:HG2  | 1:A:72:LEU:HG   | 0.53     | 1.80        | 7      | 1     |
| 1:A:14:ALA:O    | 1:A:18:GLY:N    | 0.53     | 2.41        | 8      | 7     |
| 1:A:17:MET:CE   | 1:A:68:VAL:HG12 | 0.53     | 2.33        | 2      | 1     |
| 1:A:17:MET:HB2  | 1:A:72:LEU:HB3  | 0.53     | 1.80        | 6      | 2     |
| 1:A:17:MET:HB2  | 1:A:72:LEU:CA   | 0.53     | 2.33        | 6      | 3     |
| 1:A:21:ALA:C    | 1:A:23:GLY:N    | 0.53     | 2.63        | 8      | 6     |
| 1:A:63:ILE:CG2  | 1:A:64:PRO:CD   | 0.53     | 2.87        | 8      | 7     |
| 1:A:72:LEU:C    | 1:A:74:VAL:N    | 0.53     | 2.65        | 3      | 6     |
| 1:A:13:ALA:HB2  | 1:A:75:MET:SD   | 0.53     | 2.43        | 3      | 1     |
| 1:A:69:GLY:HA3  | 1:A:73:TYR:CD2  | 0.53     | 2.38        | 8      | 1     |
| 1:A:18:GLY:C    | 1:A:22:ILE:HB   | 0.53     | 2.29        | 5      | 5     |
| 1:A:21:ALA:HB1  | 1:A:65:MET:HB3  | 0.53     | 1.74        | 7      | 2     |
| 1:A:17:MET:HG3  | 1:A:65:MET:HA   | 0.53     | 1.81        | 3      | 1     |
| 1:A:17:MET:HE2  | 1:A:72:LEU:HD23 | 0.53     | 1.81        | 3      | 1     |
| 1:A:11:MET:O    | 1:A:14:ALA:N    | 0.53     | 2.41        | 5      | 3     |
| 1:A:21:ALA:CA   | 1:A:65:MET:HB3  | 0.53     | 2.33        | 8      | 3     |
| 1:A:10:TYR:OH   | 1:A:18:GLY:CA   | 0.53     | 2.57        | 2      | 1     |
| 1:A:17:MET:HB3  | 1:A:21:ALA:HB3  | 0.53     | 1.81        | 3      | 2     |
| 1:A:22:ILE:HD12 | 1:A:73:TYR:OH   | 0.53     | 2.03        | 7      | 2     |
| 1:A:16:MET:CB   | 1:A:72:LEU:HD21 | 0.53     | 2.34        | 5      | 1     |
| 1:A:65:MET:O    | 1:A:66:ILE:C    | 0.53     | 2.52        | 9      | 1     |
| 1:A:63:ILE:HB   | 1:A:64:PRO:CD   | 0.53     | 2.33        | 8      | 9     |
| 1:A:64:PRO:O    | 1:A:68:VAL:CA   | 0.53     | 2.56        | 2      | 1     |
| 1:A:15:VAL:HG12 | 1:A:19:LEU:CD1  | 0.53     | 2.32        | 9      | 3     |
| 1:A:22:ILE:CD1  | 1:A:73:TYR:CE1  | 0.53     | 2.92        | 3      | 2     |
| 1:A:25:ALA:CB   | 1:A:65:MET:CG   | 0.53     | 2.78        | 1      | 1     |
| 1:A:13:ALA:CB   | 1:A:75:MET:SD   | 0.53     | 2.97        | 3      | 3     |
| 1:A:16:MET:SD   | 1:A:17:MET:CE   | 0.53     | 2.97        | 5      | 1     |
| 1:A:10:TYR:CD1  | 1:A:72:LEU:HG   | 0.53     | 2.39        | 6      | 1     |
| 1:A:72:LEU:CD2  | 1:A:73:TYR:CD1  | 0.52     | 2.92        | 9      | 2     |
| 1:A:13:ALA:O    | 1:A:16:MET:CG   | 0.52     | 2.57        | 8      | 1     |
| 1:A:17:MET:SD   | 1:A:21:ALA:CB   | 0.52     | 2.93        | 3      | 3     |
| 1:A:13:ALA:HA   | 1:A:16:MET:CG   | 0.52     | 2.34        | 3      | 1     |
| 1:A:10:TYR:CD1  | 1:A:72:LEU:HB2  | 0.52     | 2.39        | 9      | 2     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:65:MET:CA   | 1:A:69:GLY:CA   | 0.52     | 2.87        | 4      | 3     |
| 1:A:17:MET:CE   | 1:A:72:LEU:CD1  | 0.52     | 2.87        | 7      | 2     |
| 1:A:10:TYR:HD2  | 1:A:76:PHE:CD2  | 0.52     | 2.22        | 3      | 4     |
| 1:A:15:VAL:O    | 1:A:19:LEU:HB3  | 0.52     | 2.03        | 7      | 4     |
| 1:A:24:ALA:O    | 1:A:25:ALA:C    | 0.52     | 2.52        | 8      | 4     |
| 1:A:16:MET:HG3  | 1:A:72:LEU:HD12 | 0.52     | 1.72        | 2      | 1     |
| 1:A:14:ALA:CA   | 1:A:72:LEU:HD12 | 0.52     | 2.29        | 6      | 1     |
| 1:A:10:TYR:CG   | 1:A:10:TYR:O    | 0.52     | 2.62        | 1      | 8     |
| 1:A:21:ALA:N    | 1:A:65:MET:SD   | 0.52     | 2.82        | 5      | 2     |
| 1:A:17:MET:HG3  | 1:A:68:VAL:O    | 0.52     | 2.03        | 4      | 3     |
| 1:A:68:VAL:C    | 1:A:70:LEU:N    | 0.52     | 2.64        | 7      | 4     |
| 1:A:17:MET:HE2  | 1:A:72:LEU:HG   | 0.52     | 1.80        | 2      | 1     |
| 1:A:17:MET:SD   | 1:A:65:MET:SD   | 0.52     | 3.08        | 5      | 2     |
| 1:A:74:VAL:O    | 1:A:78:VAL:CG1  | 0.52     | 2.52        | 4      | 4     |
| 1:A:13:ALA:C    | 1:A:16:MET:HB3  | 0.52     | 2.29        | 4      | 7     |
| 1:A:64:PRO:HG2  | 1:A:65:MET:HG2  | 0.52     | 1.82        | 2      | 1     |
| 1:A:72:LEU:HA   | 1:A:75:MET:CG   | 0.52     | 2.33        | 7      | 3     |
| 1:A:18:GLY:HA3  | 1:A:72:LEU:CD1  | 0.52     | 2.24        | 6      | 2     |
| 1:A:74:VAL:O    | 1:A:78:VAL:N    | 0.52     | 2.43        | 4      | 8     |
| 1:A:16:MET:SD   | 1:A:16:MET:C    | 0.52     | 2.93        | 2      | 4     |
| 1:A:16:MET:C    | 1:A:16:MET:SD   | 0.52     | 2.93        | 1      | 2     |
| 1:A:20:ALA:CB   | 1:A:65:MET:SD   | 0.52     | 2.98        | 2      | 2     |
| 1:A:71:GLY:C    | 1:A:72:LEU:CD1  | 0.52     | 2.83        | 3      | 1     |
| 1:A:13:ALA:CA   | 1:A:16:MET:HB2  | 0.51     | 2.34        | 3      | 2     |
| 1:A:15:VAL:HG12 | 1:A:16:MET:N    | 0.51     | 2.18        | 1      | 1     |
| 1:A:10:TYR:OH   | 1:A:17:MET:C    | 0.51     | 2.53        | 2      | 1     |
| 1:A:10:TYR:HB3  | 1:A:75:MET:HB3  | 0.51     | 1.80        | 6      | 1     |
| 1:A:73:TYR:N    | 1:A:73:TYR:HD1  | 0.51     | 2.03        | 7      | 2     |
| 1:A:70:LEU:HD23 | 1:A:74:VAL:CG2  | 0.51     | 2.35        | 6      | 1     |
| 1:A:17:MET:CG   | 1:A:21:ALA:HB2  | 0.51     | 2.36        | 3      | 3     |
| 1:A:72:LEU:C    | 1:A:75:MET:H    | 0.51     | 2.14        | 5      | 6     |
| 1:A:16:MET:HG3  | 1:A:17:MET:H    | 0.51     | 1.65        | 2      | 4     |
| 1:A:21:ALA:HA   | 1:A:65:MET:CG   | 0.51     | 2.36        | 2      | 2     |
| 1:A:18:GLY:N    | 1:A:72:LEU:HD12 | 0.51     | 2.19        | 5      | 1     |
| 1:A:17:MET:HG3  | 1:A:65:MET:O    | 0.51     | 2.06        | 8      | 1     |
| 1:A:65:MET:O    | 1:A:69:GLY:C    | 0.51     | 2.54        | 1      | 3     |
| 1:A:72:LEU:CD1  | 1:A:75:MET:CG   | 0.51     | 2.89        | 1      | 1     |
| 1:A:72:LEU:HD13 | 1:A:75:MET:CG   | 0.51     | 2.36        | 2      | 1     |
| 1:A:18:GLY:CA   | 1:A:22:ILE:HB   | 0.51     | 2.36        | 7      | 3     |
| 1:A:10:TYR:C    | 1:A:14:ALA:N    | 0.51     | 2.69        | 6      | 6     |
| 1:A:72:LEU:HD22 | 1:A:75:MET:SD   | 0.51     | 2.46        | 2      | 1     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:17:MET:HG2  | 1:A:72:LEU:HD12 | 0.51     | 1.83        | 8      | 1     |
| 1:A:17:MET:O    | 1:A:19:LEU:C    | 0.50     | 2.53        | 5      | 4     |
| 1:A:69:GLY:CA   | 1:A:73:TYR:CD1  | 0.50     | 2.94        | 7      | 2     |
| 1:A:69:GLY:HA2  | 1:A:72:LEU:HD22 | 0.50     | 1.79        | 9      | 1     |
| 1:A:68:VAL:CG1  | 1:A:72:LEU:CD2  | 0.50     | 2.76        | 1      | 1     |
| 1:A:20:ALA:C    | 1:A:65:MET:SD   | 0.50     | 2.95        | 8      | 2     |
| 1:A:15:VAL:HA   | 1:A:19:LEU:HB2  | 0.50     | 1.84        | 5      | 1     |
| 1:A:17:MET:HA   | 1:A:17:MET:HE2  | 0.50     | 1.84        | 8      | 1     |
| 1:A:19:LEU:C    | 1:A:19:LEU:CD2  | 0.50     | 2.85        | 8      | 3     |
| 1:A:16:MET:HG3  | 1:A:17:MET:N    | 0.50     | 2.21        | 9      | 3     |
| 1:A:17:MET:C    | 1:A:72:LEU:HD22 | 0.50     | 2.30        | 6      | 3     |
| 1:A:16:MET:HG3  | 1:A:17:MET:CE   | 0.50     | 2.37        | 5      | 1     |
| 1:A:18:GLY:O    | 1:A:20:ALA:N    | 0.50     | 2.45        | 9      | 3     |
| 1:A:74:VAL:CG1  | 1:A:77:ALA:O    | 0.50     | 2.57        | 7      | 1     |
| 1:A:72:LEU:CG   | 1:A:73:TYR:CE1  | 0.50     | 2.95        | 9      | 1     |
| 1:A:72:LEU:CD2  | 1:A:73:TYR:CZ   | 0.49     | 2.78        | 6      | 1     |
| 1:A:22:ILE:HD13 | 1:A:22:ILE:H    | 0.49     | 1.67        | 4      | 2     |
| 1:A:13:ALA:C    | 1:A:16:MET:HB2  | 0.49     | 2.32        | 3      | 1     |
| 1:A:17:MET:SD   | 1:A:64:PRO:O    | 0.49     | 2.70        | 8      | 1     |
| 1:A:19:LEU:O    | 1:A:23:GLY:N    | 0.49     | 2.46        | 8      | 1     |
| 1:A:13:ALA:HB1  | 1:A:75:MET:SD   | 0.49     | 2.47        | 4      | 2     |
| 1:A:10:TYR:CE2  | 1:A:73:TYR:CA   | 0.49     | 2.95        | 8      | 2     |
| 1:A:15:VAL:CG1  | 1:A:19:LEU:HB2  | 0.49     | 2.38        | 9      | 3     |
| 1:A:17:MET:HB3  | 1:A:72:LEU:CA   | 0.49     | 2.37        | 9      | 2     |
| 1:A:17:MET:H    | 1:A:72:LEU:HG   | 0.49     | 1.66        | 5      | 1     |
| 1:A:65:MET:SD   | 1:A:73:TYR:OH   | 0.49     | 2.71        | 1      | 1     |
| 1:A:17:MET:HB3  | 1:A:68:VAL:O    | 0.49     | 2.08        | 9      | 3     |
| 1:A:13:ALA:CB   | 1:A:72:LEU:CD2  | 0.49     | 2.88        | 5      | 1     |
| 1:A:65:MET:SD   | 1:A:65:MET:C    | 0.49     | 2.96        | 3      | 1     |
| 1:A:63:ILE:CB   | 1:A:64:PRO:HD3  | 0.49     | 2.38        | 3      | 3     |
| 1:A:10:TYR:CE1  | 1:A:73:TYR:HD1  | 0.49     | 2.26        | 5      | 1     |
| 1:A:17:MET:HB2  | 1:A:72:LEU:HG   | 0.49     | 1.84        | 5      | 1     |
| 1:A:17:MET:HA   | 1:A:17:MET:CE   | 0.49     | 2.37        | 8      | 1     |
| 1:A:64:PRO:HB2  | 1:A:68:VAL:HB   | 0.49     | 1.85        | 3      | 2     |
| 1:A:10:TYR:HD2  | 1:A:76:PHE:CD1  | 0.49     | 2.25        | 5      | 3     |
| 1:A:21:ALA:HA   | 1:A:65:MET:CB   | 0.49     | 2.38        | 8      | 2     |
| 1:A:67:CYS:CA   | 1:A:70:LEU:HB2  | 0.48     | 2.39        | 3      | 7     |
| 1:A:63:ILE:HB   | 1:A:64:PRO:HD2  | 0.48     | 1.85        | 8      | 3     |
| 1:A:71:GLY:C    | 1:A:72:LEU:HD12 | 0.48     | 2.33        | 3      | 1     |
| 1:A:18:GLY:HA2  | 1:A:21:ALA:HB3  | 0.48     | 1.84        | 6      | 2     |
| 1:A:69:GLY:C    | 1:A:73:TYR:CD1  | 0.48     | 2.91        | 2      | 1     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:68:VAL:HG12 | 1:A:72:LEU:CG   | 0.48     | 2.38        | 7      | 1     |
| 1:A:64:PRO:HG2  | 1:A:65:MET:CG   | 0.48     | 2.39        | 5      | 2     |
| 1:A:17:MET:HG2  | 1:A:72:LEU:CD2  | 0.48     | 2.36        | 3      | 1     |
| 1:A:68:VAL:C    | 1:A:71:GLY:H    | 0.48     | 2.16        | 6      | 2     |
| 1:A:24:ALA:CB   | 1:A:65:MET:HG3  | 0.48     | 2.36        | 2      | 3     |
| 1:A:13:ALA:C    | 1:A:72:LEU:HD11 | 0.48     | 2.26        | 5      | 1     |
| 1:A:22:ILE:HD11 | 1:A:73:TYR:CZ   | 0.48     | 2.44        | 5      | 1     |
| 1:A:17:MET:N    | 1:A:72:LEU:HD23 | 0.48     | 2.23        | 3      | 1     |
| 1:A:65:MET:CG   | 1:A:66:ILE:N    | 0.48     | 2.76        | 7      | 2     |
| 1:A:17:MET:SD   | 1:A:65:MET:HA   | 0.48     | 2.49        | 8      | 1     |
| 1:A:14:ALA:O    | 1:A:18:GLY:HA3  | 0.48     | 2.08        | 2      | 9     |
| 1:A:64:PRO:HA   | 1:A:68:VAL:CG2  | 0.47     | 2.39        | 9      | 3     |
| 1:A:13:ALA:CB   | 1:A:75:MET:HG3  | 0.47     | 2.39        | 1      | 2     |
| 1:A:16:MET:CG   | 1:A:17:MET:HE2  | 0.47     | 2.39        | 5      | 1     |
| 1:A:17:MET:CE   | 1:A:72:LEU:HD12 | 0.47     | 2.38        | 8      | 1     |
| 1:A:16:MET:SD   | 1:A:17:MET:SD   | 0.47     | 3.12        | 6      | 3     |
| 1:A:9:LEU:HD13  | 1:A:9:LEU:O     | 0.47     | 2.09        | 6      | 1     |
| 1:A:25:ALA:CB   | 1:A:65:MET:HG3  | 0.47     | 2.32        | 1      | 1     |
| 1:A:72:LEU:C    | 1:A:75:MET:HB2  | 0.47     | 2.34        | 2      | 3     |
| 1:A:74:VAL:O    | 1:A:78:VAL:HG22 | 0.47     | 2.09        | 6      | 8     |
| 1:A:17:MET:SD   | 1:A:65:MET:CE   | 0.47     | 3.03        | 2      | 1     |
| 1:A:17:MET:C    | 1:A:72:LEU:HB3  | 0.47     | 2.35        | 4      | 2     |
| 1:A:10:TYR:C    | 1:A:14:ALA:H    | 0.47     | 2.17        | 3      | 7     |
| 1:A:16:MET:SD   | 1:A:72:LEU:HD12 | 0.47     | 2.49        | 2      | 2     |
| 1:A:21:ALA:HB2  | 1:A:65:MET:SD   | 0.47     | 2.50        | 2      | 2     |
| 1:A:69:GLY:CA   | 1:A:73:TYR:CE2  | 0.47     | 2.97        | 4      | 3     |
| 1:A:16:MET:SD   | 1:A:72:LEU:CD2  | 0.47     | 2.95        | 8      | 1     |
| 1:A:10:TYR:N    | 1:A:75:MET:HB3  | 0.47     | 2.25        | 5      | 1     |
| 1:A:17:MET:HE2  | 1:A:17:MET:N    | 0.47     | 2.24        | 5      | 1     |
| 1:A:21:ALA:C    | 1:A:25:ALA:CB   | 0.47     | 2.86        | 8      | 1     |
| 1:A:10:TYR:HB3  | 1:A:76:PHE:CB   | 0.47     | 2.40        | 7      | 3     |
| 1:A:16:MET:CB   | 1:A:72:LEU:HG   | 0.47     | 2.39        | 3      | 1     |
| 1:A:65:MET:HG2  | 1:A:73:TYR:OH   | 0.46     | 2.10        | 1      | 1     |
| 1:A:21:ALA:O    | 1:A:24:ALA:C    | 0.46     | 2.59        | 4      | 2     |
| 1:A:15:VAL:CG1  | 1:A:16:MET:N    | 0.46     | 2.77        | 1      | 1     |
| 1:A:10:TYR:HA   | 1:A:75:MET:HB3  | 0.46     | 1.88        | 9      | 2     |
| 1:A:64:PRO:CA   | 1:A:68:VAL:HB   | 0.46     | 2.40        | 9      | 3     |
| 1:A:13:ALA:C    | 1:A:15:VAL:N    | 0.46     | 2.68        | 5      | 1     |
| 1:A:15:VAL:HG13 | 1:A:19:LEU:HD13 | 0.46     | 1.86        | 4      | 1     |
| 1:A:15:VAL:CA   | 1:A:19:LEU:HB2  | 0.46     | 2.41        | 9      | 4     |
| 1:A:10:TYR:CZ   | 1:A:73:TYR:HD1  | 0.46     | 2.28        | 7      | 1     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:16:MET:CG   | 1:A:72:LEU:HG   | 0.46     | 2.41        | 1      | 1     |
| 1:A:72:LEU:O    | 1:A:75:MET:CB   | 0.46     | 2.64        | 1      | 2     |
| 1:A:19:LEU:O    | 1:A:23:GLY:HA3  | 0.46     | 2.10        | 9      | 3     |
| 1:A:76:PHE:C    | 1:A:78:VAL:H    | 0.46     | 2.19        | 4      | 2     |
| 1:A:17:MET:H    | 1:A:72:LEU:CG   | 0.46     | 2.23        | 5      | 1     |
| 1:A:15:VAL:HG12 | 1:A:19:LEU:HB2  | 0.46     | 1.86        | 9      | 1     |
| 1:A:10:TYR:CA   | 1:A:13:ALA:HB3  | 0.46     | 2.32        | 4      | 1     |
| 1:A:66:ILE:O    | 1:A:70:LEU:N    | 0.46     | 2.49        | 8      | 2     |
| 1:A:16:MET:HG3  | 1:A:72:LEU:CG   | 0.46     | 2.40        | 1      | 1     |
| 1:A:10:TYR:CD1  | 1:A:72:LEU:CD1  | 0.46     | 2.99        | 6      | 2     |
| 1:A:63:ILE:HG22 | 1:A:64:PRO:N    | 0.45     | 2.26        | 2      | 6     |
| 1:A:74:VAL:HA   | 1:A:77:ALA:CB   | 0.45     | 2.39        | 8      | 5     |
| 1:A:18:GLY:CA   | 1:A:22:ILE:HG12 | 0.45     | 2.40        | 4      | 1     |
| 1:A:68:VAL:O    | 1:A:69:GLY:C    | 0.45     | 2.57        | 7      | 3     |
| 1:A:13:ALA:C    | 1:A:16:MET:HG2  | 0.45     | 2.35        | 8      | 1     |
| 1:A:65:MET:CG   | 1:A:66:ILE:HG12 | 0.45     | 2.40        | 7      | 2     |
| 1:A:10:TYR:CE2  | 1:A:76:PHE:CE1  | 0.45     | 3.04        | 6      | 1     |
| 1:A:22:ILE:HD11 | 1:A:73:TYR:HE1  | 0.45     | 1.72        | 6      | 1     |
| 1:A:21:ALA:HB1  | 1:A:73:TYR:OH   | 0.45     | 2.12        | 5      | 1     |
| 1:A:69:GLY:HA2  | 1:A:72:LEU:HB2  | 0.45     | 1.88        | 3      | 1     |
| 1:A:72:LEU:O    | 1:A:74:VAL:N    | 0.45     | 2.50        | 3      | 1     |
| 1:A:17:MET:CE   | 1:A:71:GLY:HA3  | 0.45     | 2.41        | 9      | 2     |
| 1:A:22:ILE:HD11 | 1:A:73:TYR:CE1  | 0.45     | 2.47        | 6      | 2     |
| 1:A:72:LEU:CA   | 1:A:75:MET:H    | 0.45     | 2.25        | 2      | 2     |
| 1:A:74:VAL:CG1  | 1:A:78:VAL:HA   | 0.45     | 2.42        | 3      | 3     |
| 1:A:15:VAL:HG13 | 1:A:19:LEU:CB   | 0.45     | 2.42        | 4      | 1     |
| 1:A:75:MET:O    | 1:A:78:VAL:CG2  | 0.45     | 2.64        | 6      | 3     |
| 1:A:18:GLY:HA2  | 1:A:22:ILE:HD13 | 0.45     | 1.88        | 7      | 3     |
| 1:A:17:MET:CE   | 1:A:64:PRO:HB2  | 0.45     | 2.41        | 3      | 1     |
| 1:A:17:MET:SD   | 1:A:68:VAL:HB   | 0.45     | 2.53        | 5      | 1     |
| 1:A:20:ALA:HB1  | 1:A:65:MET:SD   | 0.45     | 2.52        | 5      | 1     |
| 1:A:18:GLY:HA2  | 1:A:22:ILE:CB   | 0.44     | 2.42        | 5      | 1     |
| 1:A:16:MET:O    | 1:A:20:ALA:CB   | 0.44     | 2.65        | 2      | 1     |
| 1:A:64:PRO:O    | 1:A:66:ILE:C    | 0.44     | 2.60        | 3      | 3     |
| 1:A:68:VAL:O    | 1:A:72:LEU:HD13 | 0.44     | 2.13        | 3      | 1     |
| 1:A:71:GLY:HA2  | 1:A:74:VAL:CG2  | 0.44     | 2.42        | 1      | 3     |
| 1:A:74:VAL:C    | 1:A:78:VAL:HG13 | 0.44     | 2.37        | 2      | 4     |
| 1:A:17:MET:HG3  | 1:A:68:VAL:C    | 0.44     | 2.38        | 6      | 3     |
| 1:A:18:GLY:N    | 1:A:72:LEU:HB3  | 0.44     | 2.27        | 4      | 2     |
| 1:A:65:MET:HA   | 1:A:69:GLY:CA   | 0.44     | 2.35        | 4      | 2     |
| 1:A:24:ALA:CB   | 1:A:65:MET:SD   | 0.44     | 3.05        | 8      | 1     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:64:PRO:HD2  | 1:A:65:MET:HG2  | 0.44     | 1.88        | 8      | 1     |
| 1:A:66:ILE:O    | 1:A:70:LEU:CA   | 0.44     | 2.66        | 8      | 1     |
| 1:A:16:MET:HG3  | 1:A:72:LEU:HG   | 0.43     | 1.90        | 1      | 1     |
| 1:A:64:PRO:CB   | 1:A:65:MET:HE2  | 0.43     | 2.43        | 2      | 1     |
| 1:A:63:ILE:HB   | 1:A:64:PRO:HD3  | 0.43     | 1.89        | 3      | 1     |
| 1:A:12:ALA:O    | 1:A:15:VAL:CG2  | 0.43     | 2.66        | 5      | 1     |
| 1:A:13:ALA:CA   | 1:A:16:MET:CB   | 0.43     | 2.96        | 5      | 1     |
| 1:A:22:ILE:HD13 | 1:A:73:TYR:OH   | 0.43     | 2.13        | 8      | 1     |
| 1:A:65:MET:SD   | 1:A:73:TYR:CZ   | 0.43     | 3.10        | 1      | 1     |
| 1:A:64:PRO:O    | 1:A:68:VAL:C    | 0.43     | 2.61        | 2      | 1     |
| 1:A:21:ALA:CB   | 1:A:73:TYR:OH   | 0.43     | 2.66        | 5      | 1     |
| 1:A:12:ALA:O    | 1:A:15:VAL:HG23 | 0.43     | 2.13        | 5      | 1     |
| 1:A:18:GLY:HA2  | 1:A:22:ILE:CG1  | 0.43     | 2.44        | 5      | 1     |
| 1:A:21:ALA:CB   | 1:A:65:MET:N    | 0.43     | 2.79        | 9      | 1     |
| 1:A:18:GLY:O    | 1:A:22:ILE:CA   | 0.43     | 2.67        | 1      | 2     |
| 1:A:21:ALA:CB   | 1:A:65:MET:O    | 0.43     | 2.67        | 5      | 1     |
| 1:A:17:MET:CG   | 1:A:68:VAL:CG1  | 0.43     | 2.80        | 9      | 1     |
| 1:A:18:GLY:O    | 1:A:20:ALA:C    | 0.43     | 2.62        | 9      | 1     |
| 1:A:10:TYR:HB2  | 1:A:76:PHE:H    | 0.43     | 1.72        | 2      | 1     |
| 1:A:65:MET:CE   | 1:A:66:ILE:HG12 | 0.43     | 2.44        | 3      | 1     |
| 1:A:13:ALA:HB1  | 1:A:16:MET:CG   | 0.43     | 2.40        | 8      | 1     |
| 1:A:17:MET:HG2  | 1:A:69:GLY:HA2  | 0.43     | 1.89        | 5      | 4     |
| 1:A:17:MET:CE   | 1:A:17:MET:HA   | 0.43     | 2.43        | 1      | 1     |
| 1:A:17:MET:SD   | 1:A:65:MET:HE1  | 0.43     | 2.54        | 2      | 1     |
| 1:A:17:MET:H    | 1:A:72:LEU:CD1  | 0.43     | 2.26        | 5      | 1     |
| 1:A:21:ALA:HB1  | 1:A:65:MET:O    | 0.43     | 2.14        | 5      | 1     |
| 1:A:16:MET:HB3  | 1:A:72:LEU:HG   | 0.43     | 1.90        | 3      | 1     |
| 1:A:68:VAL:O    | 1:A:72:LEU:CG   | 0.43     | 2.67        | 7      | 1     |
| 1:A:21:ALA:HB2  | 1:A:65:MET:C    | 0.43     | 2.39        | 8      | 1     |
| 1:A:17:MET:C    | 1:A:19:LEU:N    | 0.43     | 2.76        | 3      | 1     |
| 1:A:68:VAL:O    | 1:A:72:LEU:HB2  | 0.43     | 2.14        | 3      | 1     |
| 1:A:69:GLY:C    | 1:A:73:TYR:CE2  | 0.43     | 2.97        | 9      | 2     |
| 1:A:16:MET:CE   | 1:A:17:MET:HE1  | 0.42     | 2.44        | 5      | 1     |
| 1:A:18:GLY:N    | 1:A:72:LEU:HD13 | 0.42     | 2.29        | 6      | 1     |
| 1:A:16:MET:CG   | 1:A:17:MET:H    | 0.42     | 2.24        | 2      | 1     |
| 1:A:17:MET:SD   | 1:A:64:PRO:CB   | 0.42     | 3.04        | 3      | 1     |
| 1:A:67:CYS:SG   | 1:A:68:VAL:HG23 | 0.42     | 2.54        | 7      | 1     |
| 1:A:69:GLY:O    | 1:A:73:TYR:HB2  | 0.42     | 2.14        | 8      | 1     |
| 1:A:65:MET:O    | 1:A:69:GLY:N    | 0.42     | 2.52        | 2      | 1     |
| 1:A:17:MET:CG   | 1:A:68:VAL:C    | 0.42     | 2.90        | 4      | 1     |
| 1:A:18:GLY:C    | 1:A:20:ALA:N    | 0.42     | 2.78        | 6      | 3     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:20:ALA:HB1  | 1:A:65:MET:CE   | 0.42     | 2.43        | 2      | 2     |
| 1:A:69:GLY:HA3  | 1:A:73:TYR:CZ   | 0.42     | 2.48        | 5      | 1     |
| 1:A:18:GLY:HA2  | 1:A:22:ILE:HB   | 0.42     | 1.91        | 7      | 2     |
| 1:A:21:ALA:CA   | 1:A:65:MET:SD   | 0.42     | 3.05        | 8      | 1     |
| 1:A:63:ILE:O    | 1:A:67:CYS:HB2  | 0.42     | 2.15        | 8      | 1     |
| 1:A:69:GLY:CA   | 1:A:73:TYR:CD2  | 0.42     | 3.03        | 8      | 1     |
| 1:A:18:GLY:C    | 1:A:22:ILE:H    | 0.42     | 2.23        | 7      | 1     |
| 1:A:17:MET:SD   | 1:A:64:PRO:HG2  | 0.42     | 2.55        | 3      | 1     |
| 1:A:72:LEU:N    | 1:A:72:LEU:CD1  | 0.42     | 2.83        | 3      | 1     |
| 1:A:16:MET:SD   | 1:A:75:MET:HG3  | 0.42     | 2.55        | 8      | 1     |
| 1:A:14:ALA:HA   | 1:A:72:LEU:HB2  | 0.42     | 1.91        | 9      | 1     |
| 1:A:20:ALA:O    | 1:A:65:MET:HG3  | 0.42     | 2.15        | 2      | 1     |
| 1:A:21:ALA:HB1  | 1:A:25:ALA:HB2  | 0.42     | 1.91        | 8      | 1     |
| 1:A:64:PRO:C    | 1:A:66:ILE:N    | 0.42     | 2.78        | 7      | 2     |
| 1:A:10:TYR:CB   | 1:A:76:PHE:HB3  | 0.42     | 2.44        | 9      | 1     |
| 1:A:16:MET:CG   | 1:A:72:LEU:CG   | 0.42     | 2.98        | 1      | 1     |
| 1:A:22:ILE:HD11 | 1:A:72:LEU:CD1  | 0.41     | 2.44        | 4      | 1     |
| 1:A:64:PRO:HG3  | 1:A:65:MET:CE   | 0.41     | 2.44        | 8      | 1     |
| 1:A:65:MET:C    | 1:A:69:GLY:CA   | 0.41     | 2.92        | 4      | 2     |
| 1:A:13:ALA:HB1  | 1:A:75:MET:HG2  | 0.41     | 1.91        | 2      | 1     |
| 1:A:16:MET:HB3  | 1:A:72:LEU:CG   | 0.41     | 2.45        | 3      | 1     |
| 1:A:21:ALA:HB2  | 1:A:65:MET:H    | 0.41     | 1.74        | 4      | 1     |
| 1:A:65:MET:SD   | 1:A:73:TYR:CE2  | 0.41     | 3.14        | 1      | 1     |
| 1:A:14:ALA:O    | 1:A:15:VAL:C    | 0.41     | 2.62        | 6      | 1     |
| 1:A:17:MET:HE2  | 1:A:75:MET:HG2  | 0.41     | 1.91        | 4      | 2     |
| 1:A:72:LEU:HD23 | 1:A:72:LEU:H    | 0.41     | 1.75        | 9      | 1     |
| 1:A:17:MET:CB   | 1:A:69:GLY:HA2  | 0.41     | 2.45        | 2      | 1     |
| 1:A:65:MET:SD   | 1:A:66:ILE:HG12 | 0.41     | 2.55        | 3      | 1     |
| 1:A:18:GLY:CA   | 1:A:22:ILE:H    | 0.41     | 2.28        | 1      | 2     |
| 1:A:19:LEU:O    | 1:A:20:ALA:C    | 0.41     | 2.63        | 8      | 1     |
| 1:A:69:GLY:O    | 1:A:72:LEU:CD2  | 0.41     | 2.57        | 9      | 1     |
| 1:A:65:MET:N    | 1:A:69:GLY:N    | 0.41     | 2.69        | 4      | 1     |
| 1:A:17:MET:HE3  | 1:A:71:GLY:HA3  | 0.41     | 1.93        | 9      | 1     |
| 1:A:15:VAL:C    | 1:A:19:LEU:HB2  | 0.40     | 2.41        | 9      | 1     |
| 1:A:9:LEU:HD22  | 1:A:9:LEU:HA    | 0.40     | 1.78        | 3      | 1     |
| 1:A:10:TYR:CA   | 1:A:75:MET:CB   | 0.40     | 2.99        | 5      | 1     |
| 1:A:13:ALA:O    | 1:A:16:MET:CA   | 0.40     | 2.68        | 5      | 1     |
| 1:A:16:MET:SD   | 1:A:72:LEU:HG   | 0.40     | 2.57        | 1      | 1     |
| 1:A:17:MET:CA   | 1:A:72:LEU:HB3  | 0.40     | 2.45        | 6      | 1     |
| 1:A:19:LEU:O    | 1:A:23:GLY:CA   | 0.40     | 2.69        | 9      | 1     |
| 1:A:22:ILE:CD1  | 1:A:22:ILE:N    | 0.40     | 2.83        | 5      | 1     |

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| Atom-1         | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|----------------|-----------------|----------|-------------|--------|-------|
|                |                 |          |             | Worst  | Total |
| 1:A:64:PRO:HA  | 1:A:68:VAL:HG23 | 0.40     | 1.93        | 9      | 1     |
| 1:A:64:PRO:HB3 | 1:A:68:VAL:HB   | 0.40     | 1.94        | 9      | 1     |
| 1:A:10:TYR:HD1 | 1:A:72:LEU:HD22 | 0.40     | 1.77        | 5      | 1     |

## 6.3 Torsion angles [i](#)

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

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

| Mol | Chain | Analysed      | Favoured     | Allowed     | Outliers    | Percentiles |   |
|-----|-------|---------------|--------------|-------------|-------------|-------------|---|
| 1   | A     | 32/79 (41%)   | 19±3 (58±8%) | 8±2 (24±5%) | 6±1 (17±4%) | 0           | 3 |
| All | All   | 288/711 (41%) | 168 (58%)    | 70 (24%)    | 50 (17%)    | 0           | 3 |

All 12 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     | 16  | MET  | 9              |
| 1   | A     | 63  | ILE  | 6              |
| 1   | A     | 64  | PRO  | 6              |
| 1   | A     | 65  | MET  | 6              |
| 1   | A     | 18  | GLY  | 5              |
| 1   | A     | 75  | MET  | 5              |
| 1   | A     | 66  | ILE  | 5              |
| 1   | A     | 10  | TYR  | 3              |
| 1   | A     | 25  | ALA  | 2              |
| 1   | A     | 17  | MET  | 1              |
| 1   | A     | 19  | LEU  | 1              |
| 1   | A     | 20  | ALA  | 1              |

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

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

| Mol | Chain | Analysed      | Rotameric    | Outliers      | Percentiles |   |
|-----|-------|---------------|--------------|---------------|-------------|---|
| 1   | A     | 21/57 (37%)   | 9±3 (43±13%) | 12±3 (57±13%) | 0           | 0 |
| All | All   | 189/513 (37%) | 81 (43%)     | 108 (57%)     | 0           | 0 |

All 18 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     | 22  | ILE  | 9              |
| 1   | A     | 75  | MET  | 9              |
| 1   | A     | 78  | VAL  | 9              |
| 1   | A     | 17  | MET  | 8              |
| 1   | A     | 63  | ILE  | 8              |
| 1   | A     | 70  | LEU  | 8              |
| 1   | A     | 16  | MET  | 7              |
| 1   | A     | 65  | MET  | 7              |
| 1   | A     | 73  | TYR  | 7              |
| 1   | A     | 66  | ILE  | 6              |
| 1   | A     | 9   | LEU  | 6              |
| 1   | A     | 11  | MET  | 5              |
| 1   | A     | 15  | VAL  | 4              |
| 1   | A     | 72  | LEU  | 4              |
| 1   | A     | 19  | LEU  | 4              |
| 1   | A     | 76  | PHE  | 3              |
| 1   | A     | 68  | VAL  | 3              |
| 1   | A     | 10  | TYR  | 1              |

### 6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.6 Ligand geometry

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