



Full wwPDB NMR Structure Validation Report ⓘ

Feb 13, 2017 – 02:22 am GMT

PDB ID : 2WC2
Title : NMR STRUCTURE OF CATABOLITE ACTIVATOR PROTEIN IN THE UNLIGANDED STATE
Authors : Popovych, N.; Tzeng, S.R.; Kalodimos, C.G.
Deposited on : 2009-03-06

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

Cyrange : Kirchner and Güntert (2011)
NmrClust : Kelley et al. (1996)
MolProbity : 4.02b-467
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : trunk28760
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

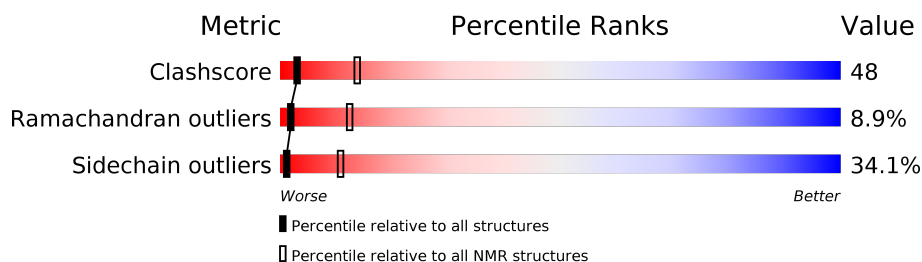
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment 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 (#Entries) | NMR archive (#Entries) |
|-----------------------|-----------------------------|---------------------------|
| Clashscore | 125131 | 11601 |
| Ramachandran outliers | 121729 | 10391 |
| Sidechain outliers | 121581 | 10367 |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for ≥ 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 | 209 | 25% 51% 20% . . |
| 1 | B | 209 | 25% 50% 20% . . |

2 Ensemble composition and analysis ⓘ

This entry contains 20 models. Model 3 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative.

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:8-A:209, B:8-B:209 (404) | 0.64 | 3 |

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

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

NmrClust was unable to cluster the ensemble.

Error message: Inconsistent models

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 6704 atoms, of which 3404 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called CATABOLITE GENE ACTIVATOR.

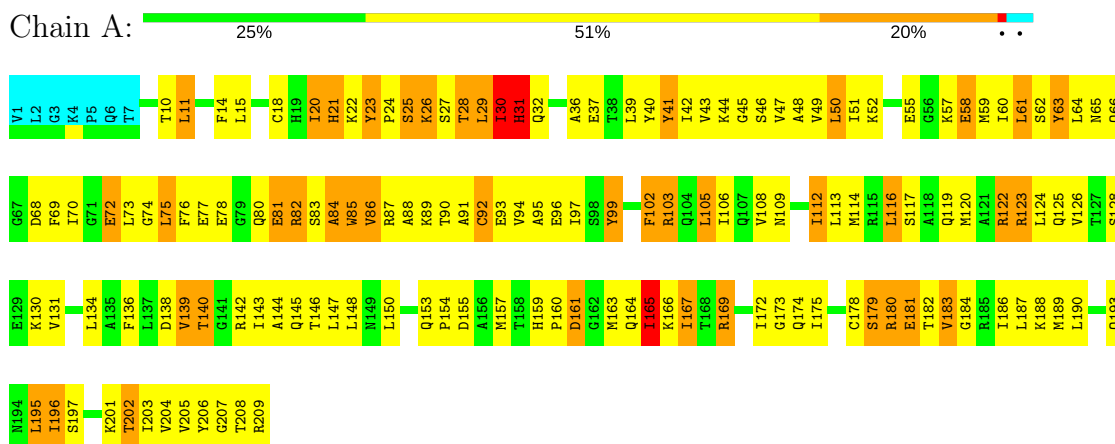
| Mol | Chain | Residues | Atoms | | | | | | Trace |
|-----|-------|----------|-------|------|------|-----|-----|---|-------|
| 1 | A | 209 | Total | C | H | N | O | S | 0 |
| | | | 3352 | 1044 | 1702 | 290 | 307 | 9 | |
| 1 | B | 209 | Total | C | H | N | O | S | 0 |
| | | | 3352 | 1044 | 1702 | 290 | 307 | 9 | |

4 Residue-property plots

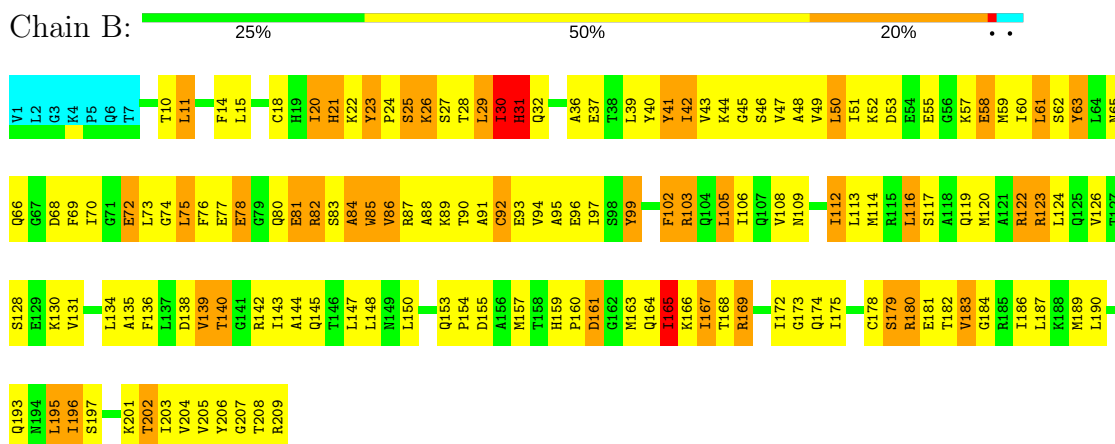
4.1 Average score per residue in the NMR ensemble

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

• Molecule 1: CATABOLITE GENE ACTIVATOR



• Molecule 1: CATABOLITE GENE ACTIVATOR

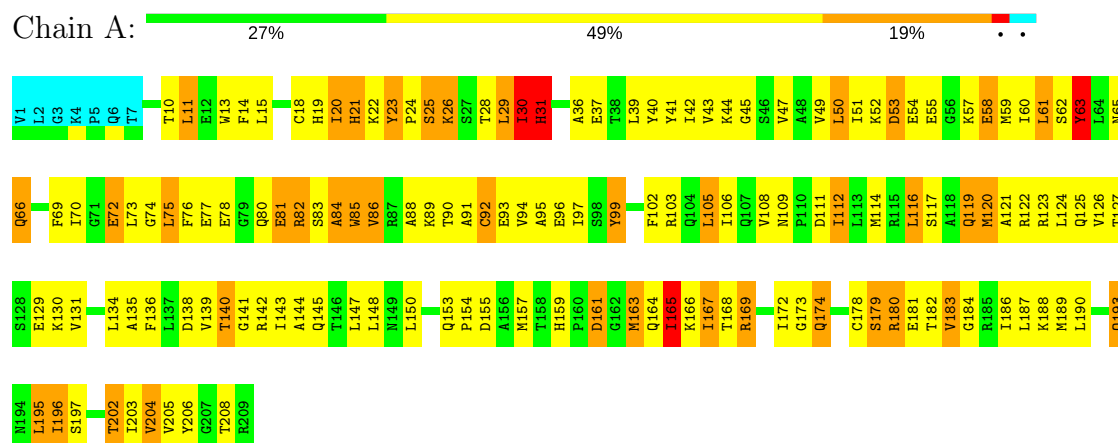


4.2 Scores per residue for each member of the ensemble

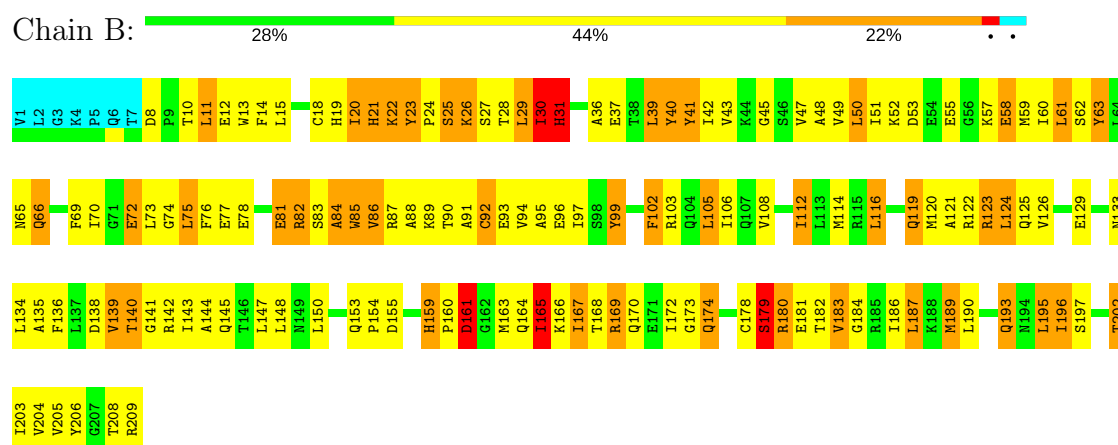
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: CATABOLITE GENE ACTIVATOR



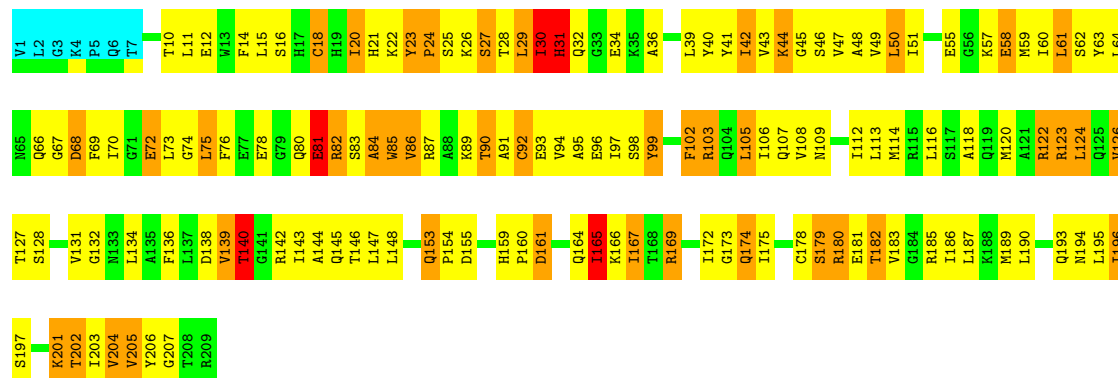
• Molecule 1: CATABOLITE GENE ACTIVATOR



4.2.2 Score per residue for model 2

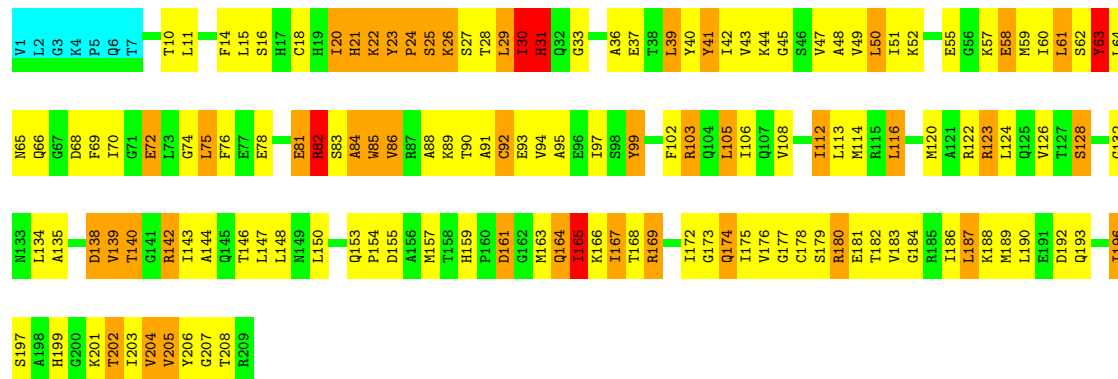
• Molecule 1: CATABOLITE GENE ACTIVATOR



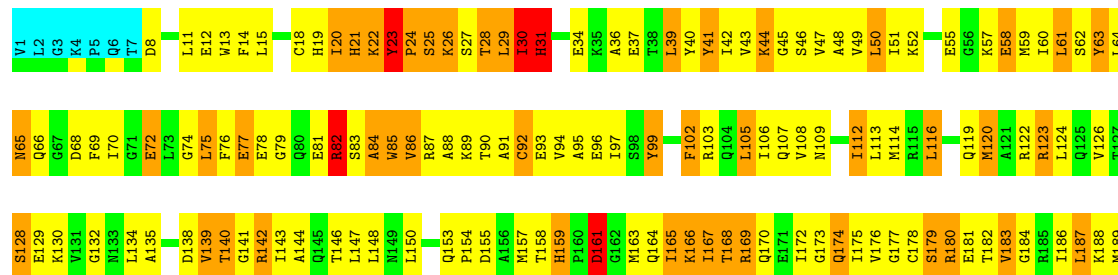


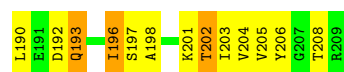
4.2.3 Score per residue for model 3 (medoid)

- Molecule 1: CATABOLITE GENE ACTIVATOR



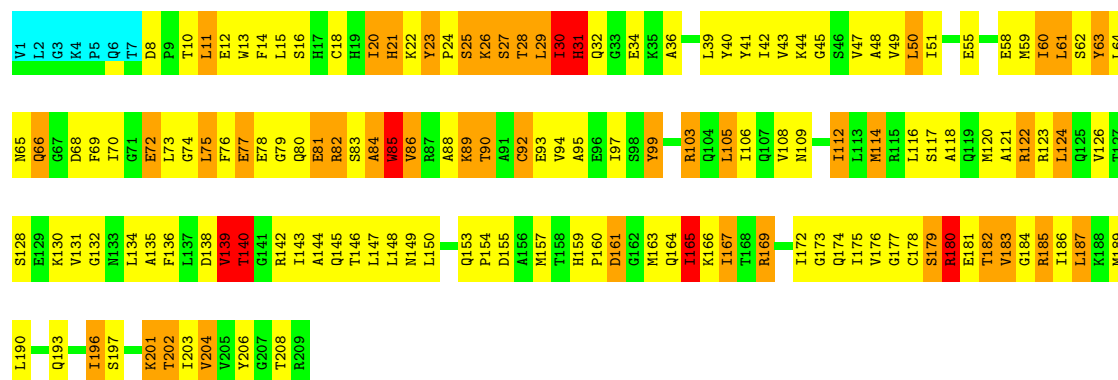
- Molecule 1: CATABOLITE GENE ACTIVATOR



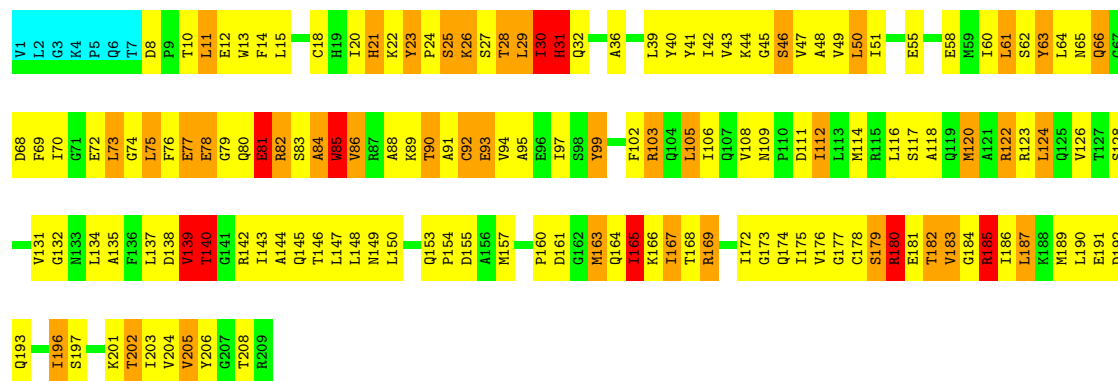


4.2.4 Score per residue for model 4

- Molecule 1: CATABOLITE GENE ACTIVATOR

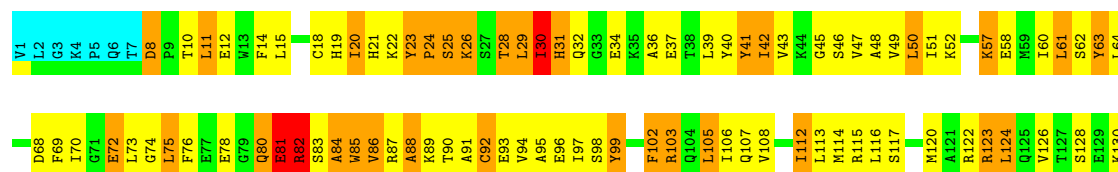


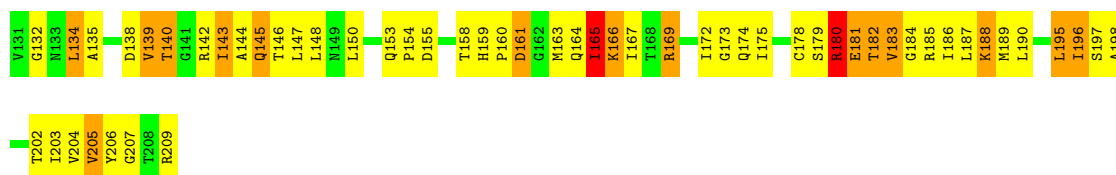
- Molecule 1: CATABOLITE GENE ACTIVATOR



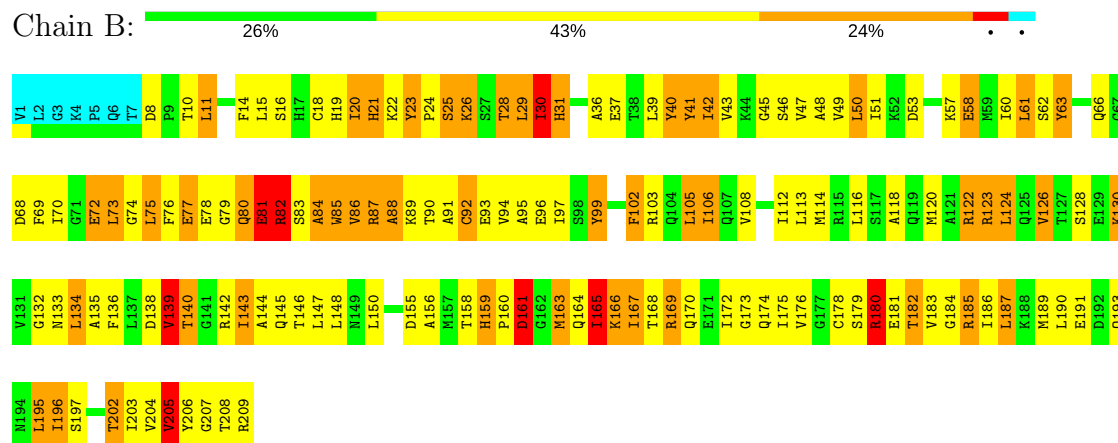
4.2.5 Score per residue for model 5

- Molecule 1: CATABOLITE GENE ACTIVATOR



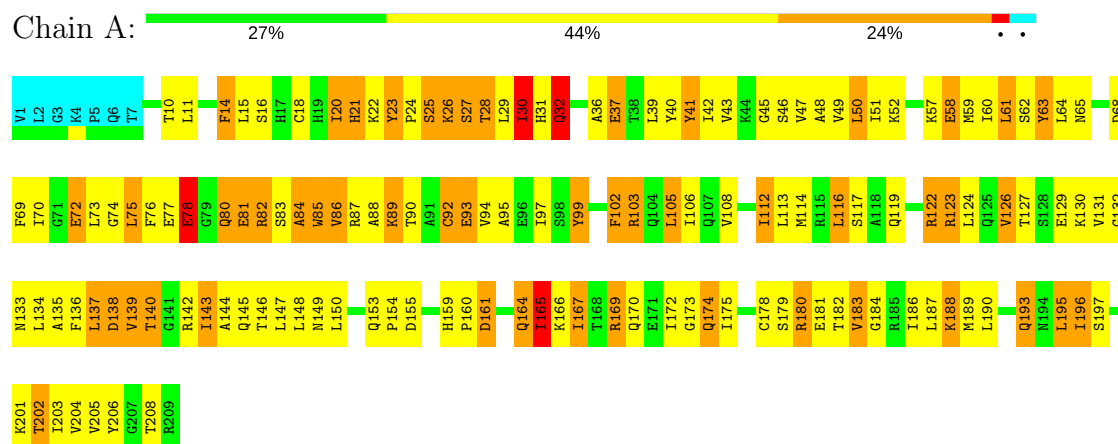


• Molecule 1: CATABOLITE GENE ACTIVATOR

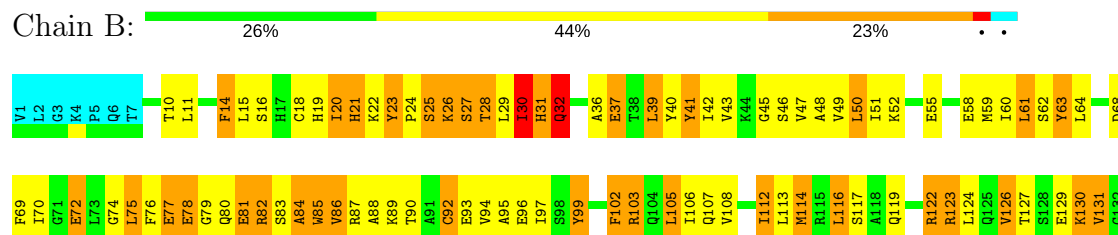


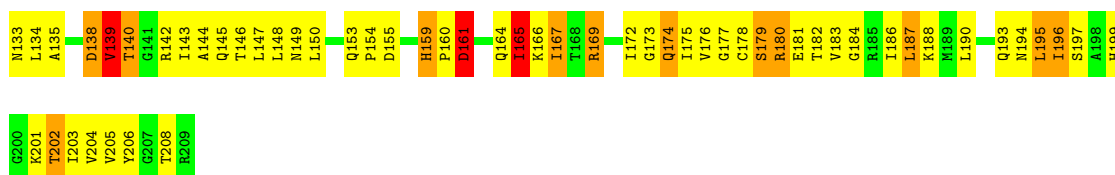
4.2.6 Score per residue for model 6

• Molecule 1: CATABOLITE GENE ACTIVATOR



• Molecule 1: CATABOLITE GENE ACTIVATOR

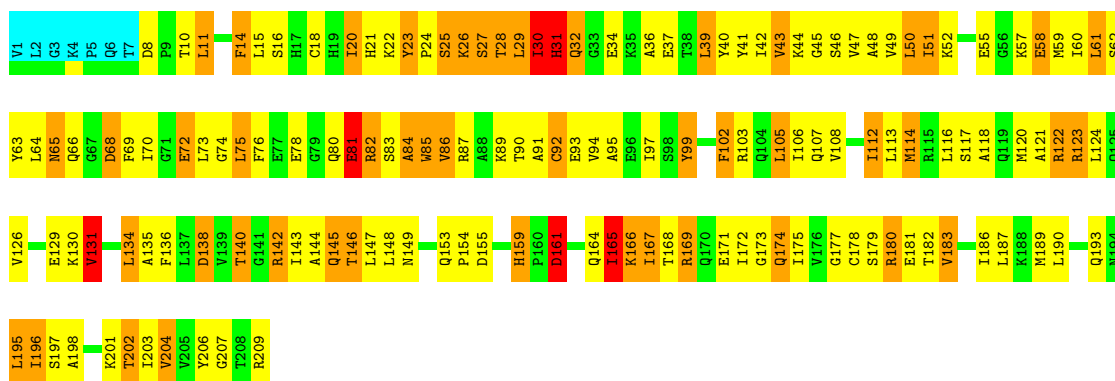




4.2.7 Score per residue for model 7

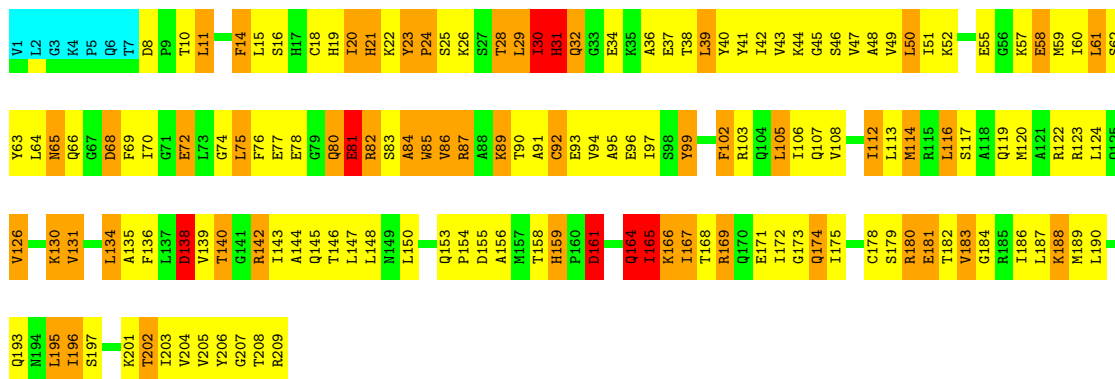
- Molecule 1: CATABOLITE GENE ACTIVATOR

Chain A: 26% 44% 23%



- Molecule 1: CATABOLITE GENE ACTIVATOR

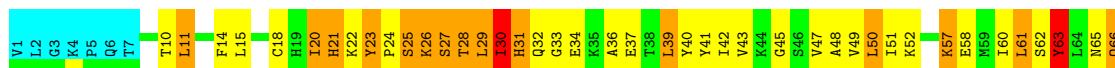
Chain B: 24% 46% 23%

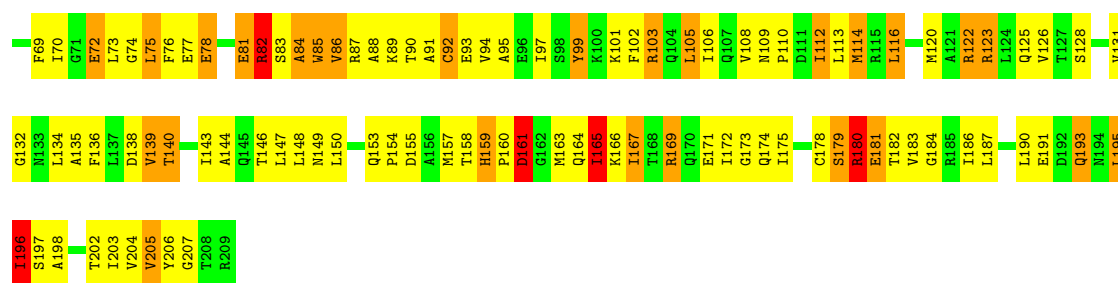


4.2.8 Score per residue for model 8

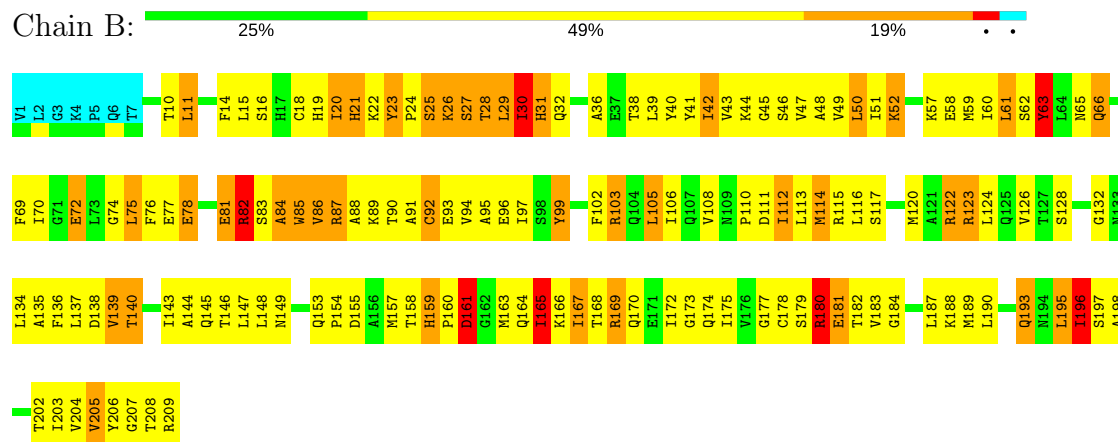
- Molecule 1: CATABOLITE GENE ACTIVATOR

Chain A: 29% 45% 20%



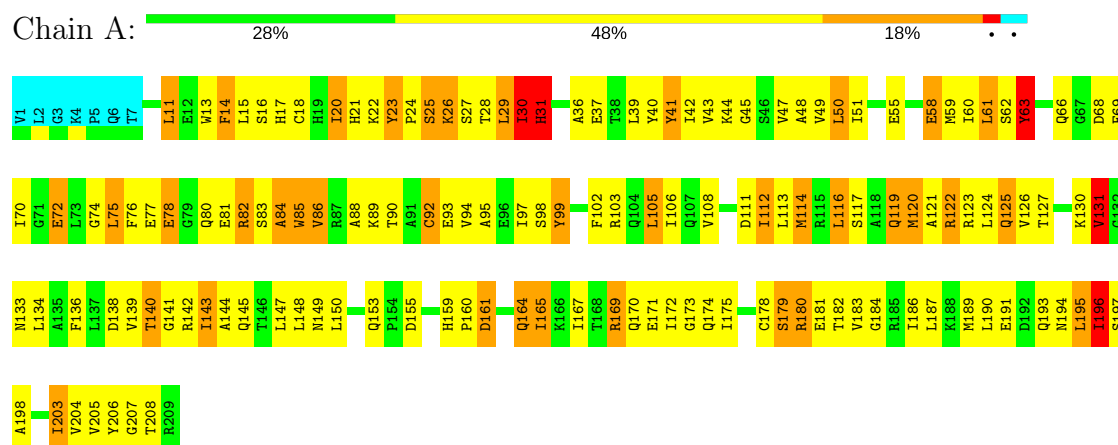


• Molecule 1: CATABOLITE GENE ACTIVATOR

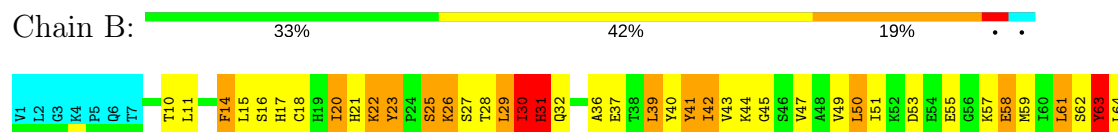


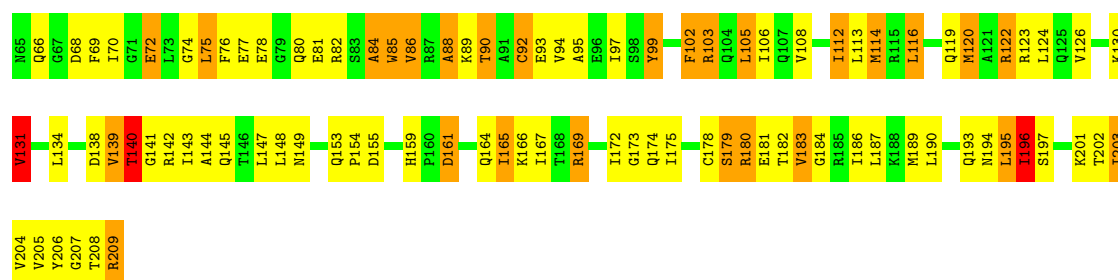
4.2.9 Score per residue for model 9

• Molecule 1: CATABOLITE GENE ACTIVATOR



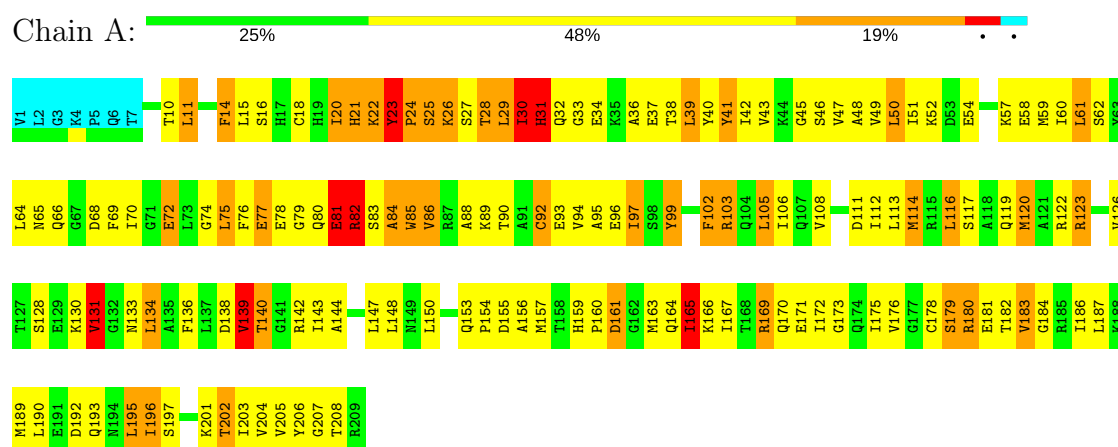
• Molecule 1: CATABOLITE GENE ACTIVATOR



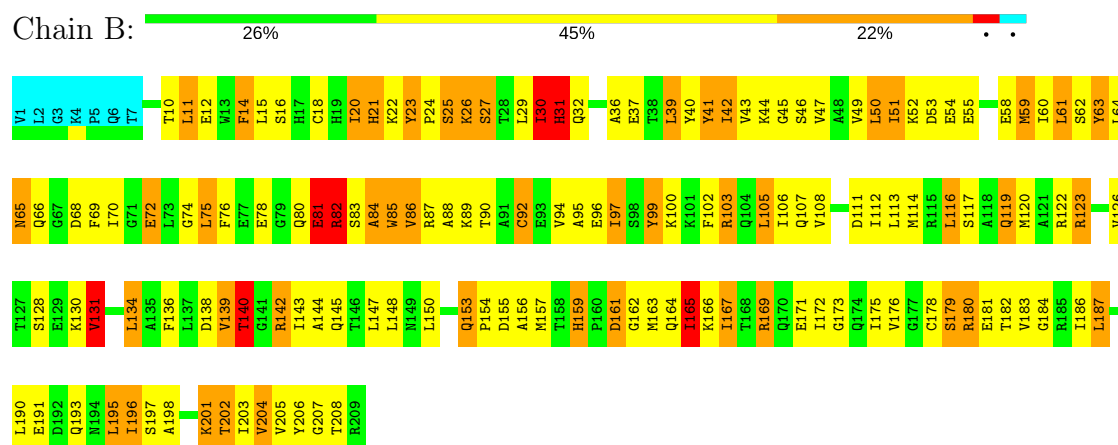


4.2.10 Score per residue for model 10

- Molecule 1: CATABOLITE GENE ACTIVATOR



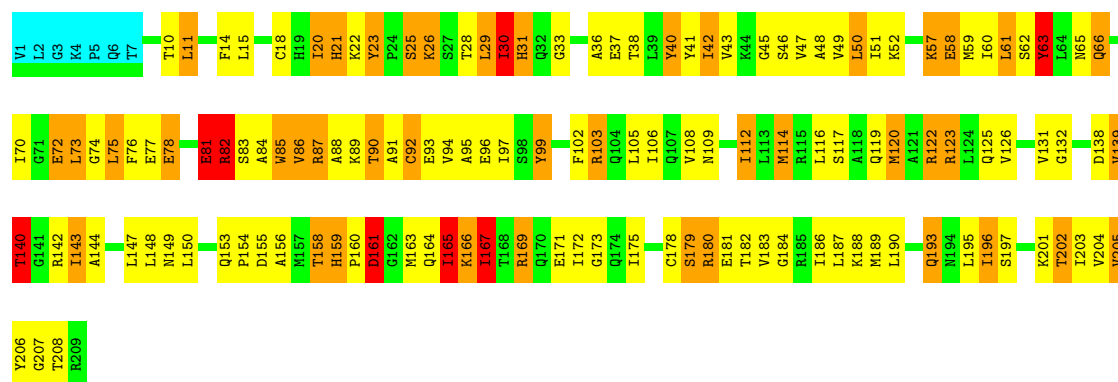
- Molecule 1: CATABOLITE GENE ACTIVATOR



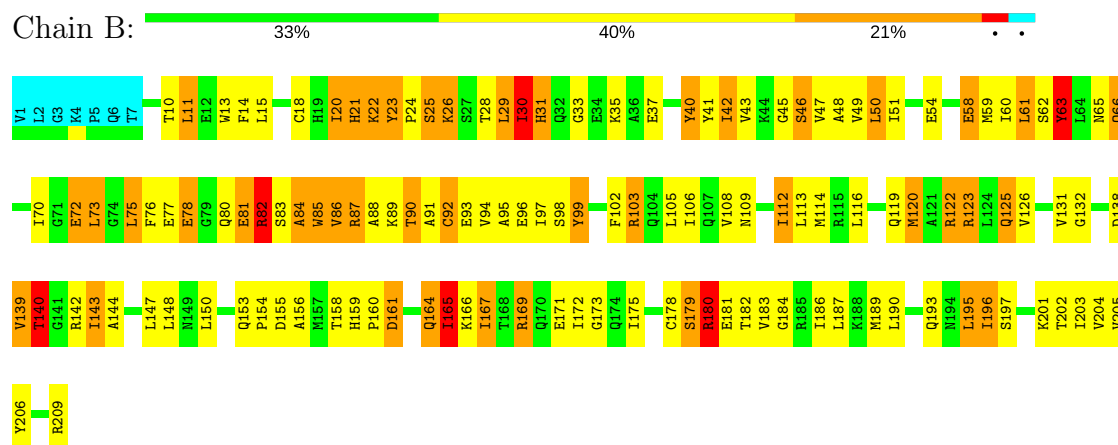
4.2.11 Score per residue for model 11

- Molecule 1: CATABOLITE GENE ACTIVATOR



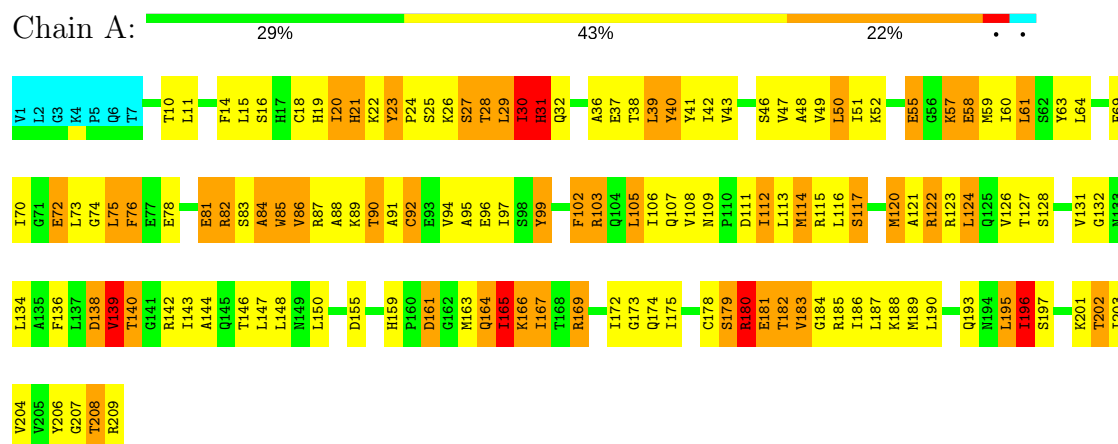


• Molecule 1: CATABOLITE GENE ACTIVATOR

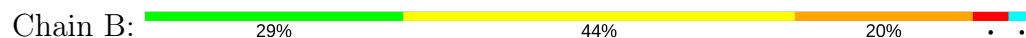


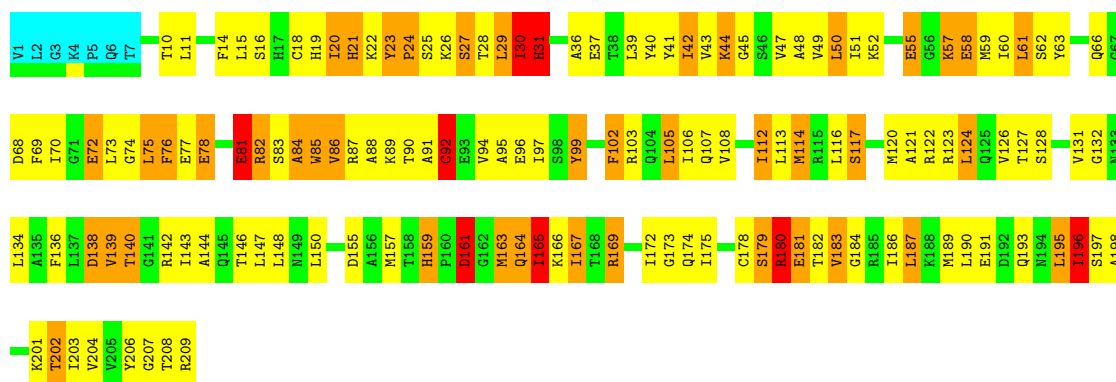
4.2.12 Score per residue for model 12

• Molecule 1: CATABOLITE GENE ACTIVATOR



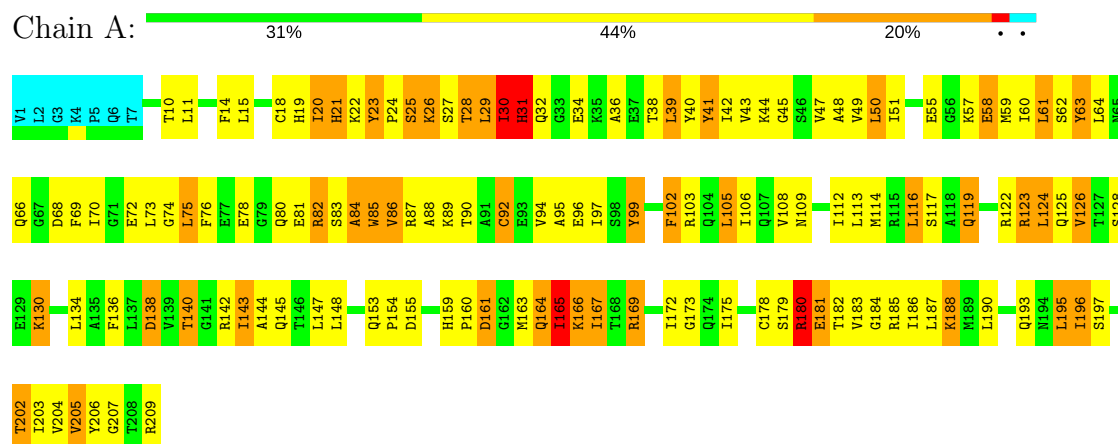
• Molecule 1: CATABOLITE GENE ACTIVATOR



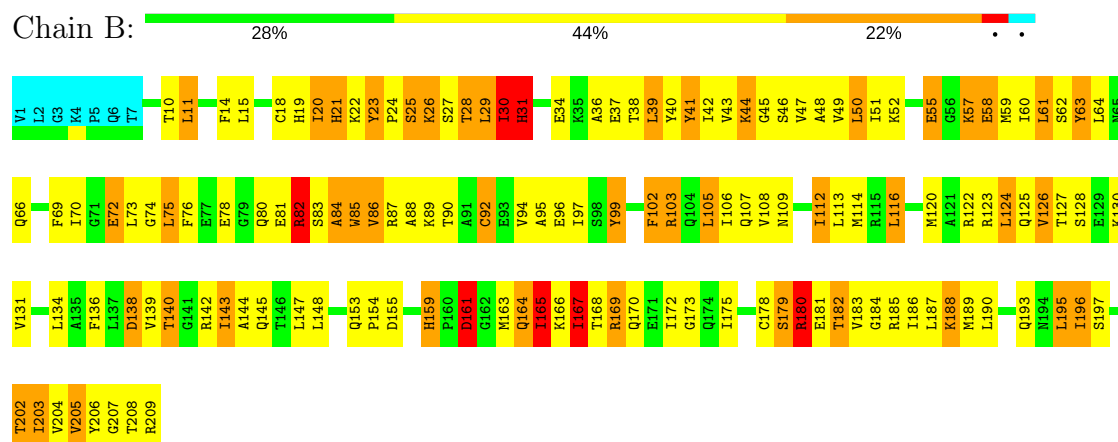


4.2.13 Score per residue for model 13

- Molecule 1: CATABOLITE GENE ACTIVATOR



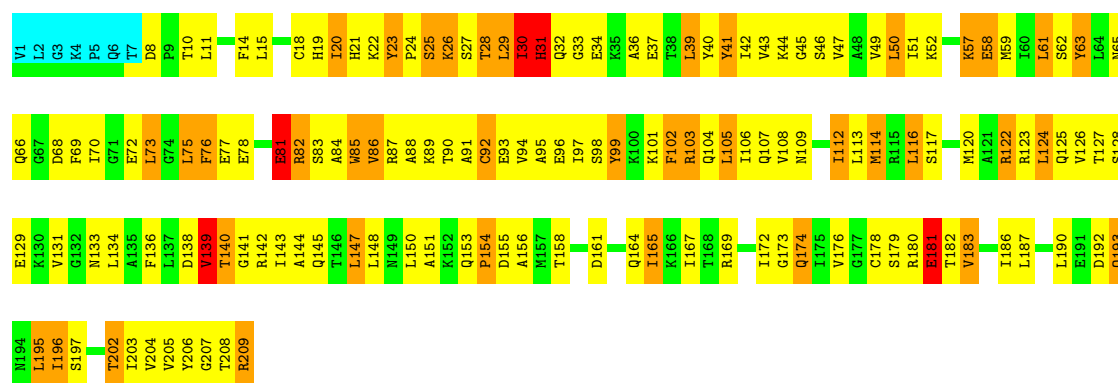
- Molecule 1: CATABOLITE GENE ACTIVATOR



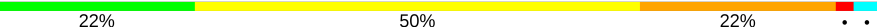
4.2.14 Score per residue for model 14

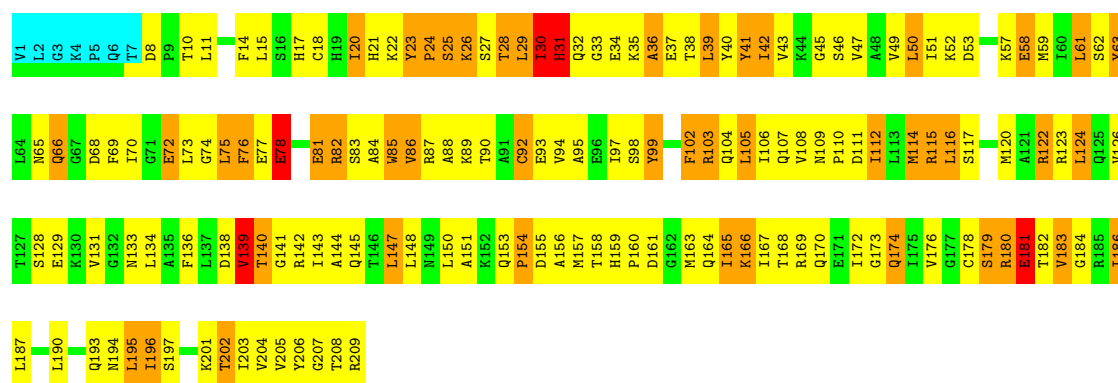
- Molecule 1: CATABOLITE GENE ACTIVATOR

Chain A: 



• Molecule 1: CATABOLITE GENE ACTIVATOR

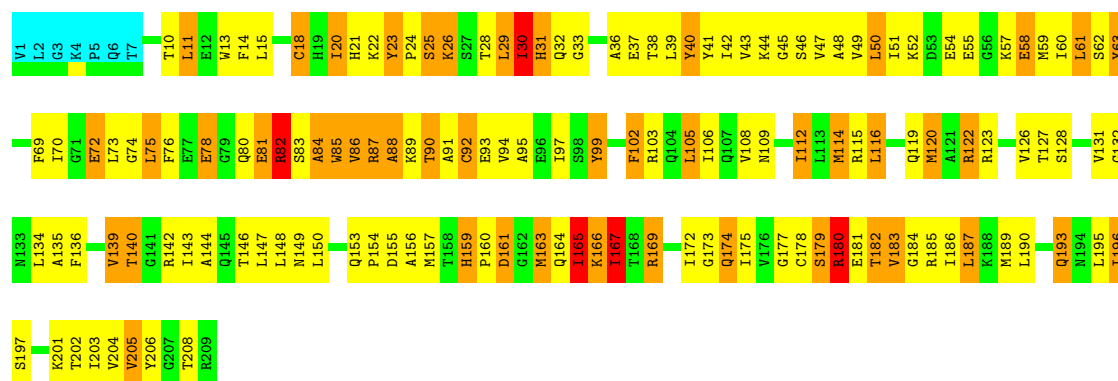
Chain B: 



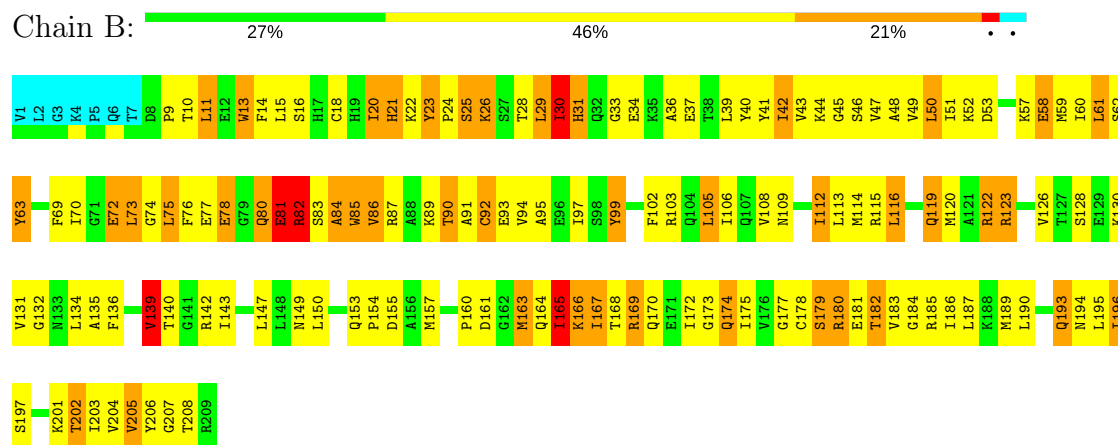
4.2.15 Score per residue for model 15

• Molecule 1: CATABOLITE GENE ACTIVATOR

Chain A: 

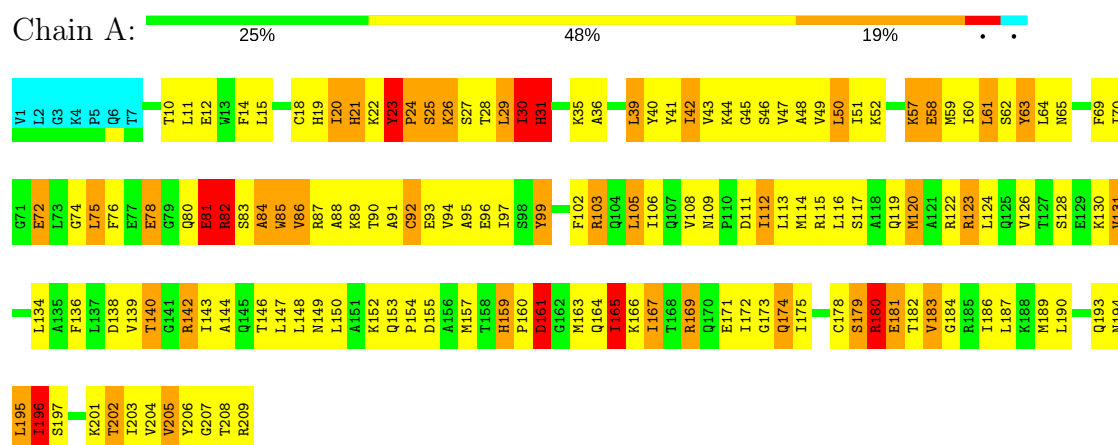


• Molecule 1: CATABOLITE GENE ACTIVATOR

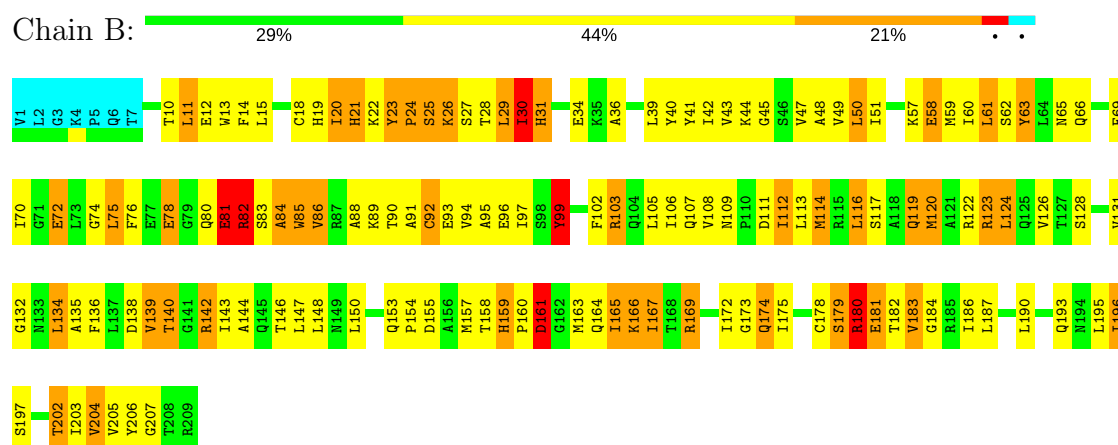


4.2.16 Score per residue for model 16

- Molecule 1: CATABOLITE GENE ACTIVATOR

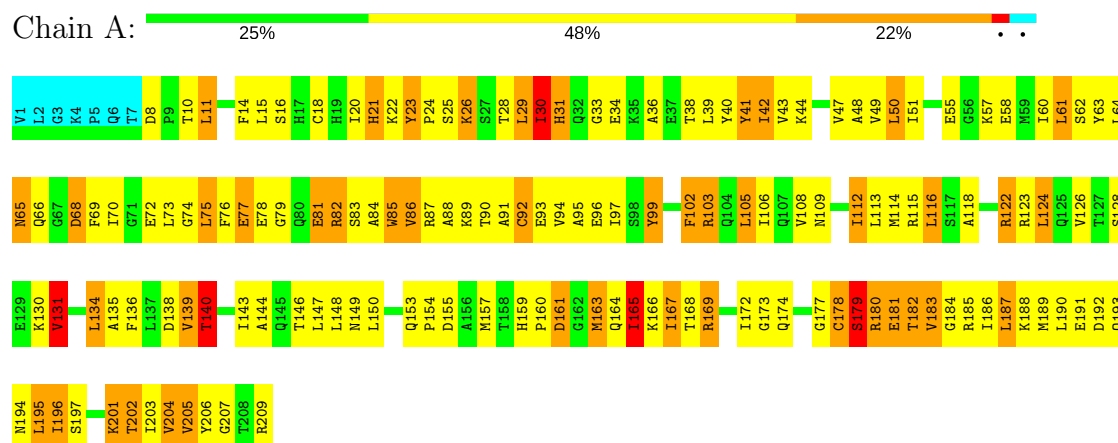


- Molecule 1: CATABOLITE GENE ACTIVATOR

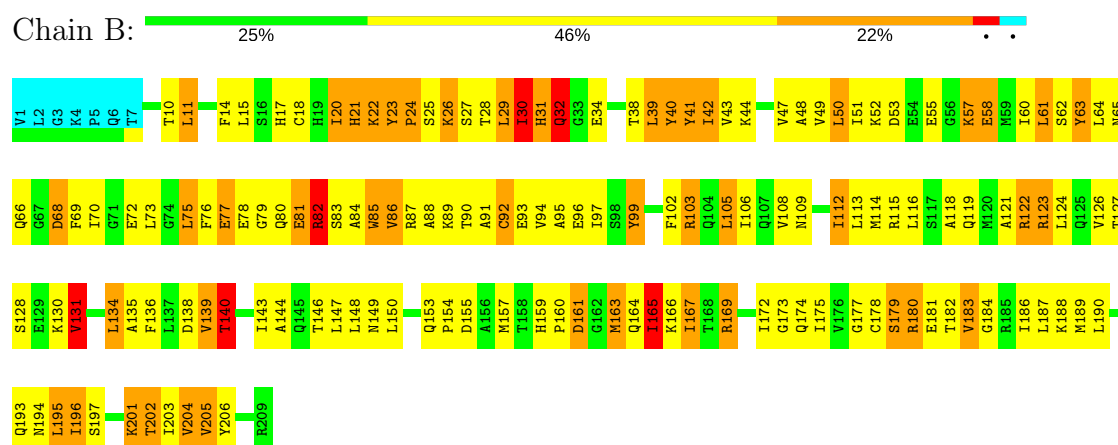


4.2.17 Score per residue for model 17

• Molecule 1: CATABOLITE GENE ACTIVATOR

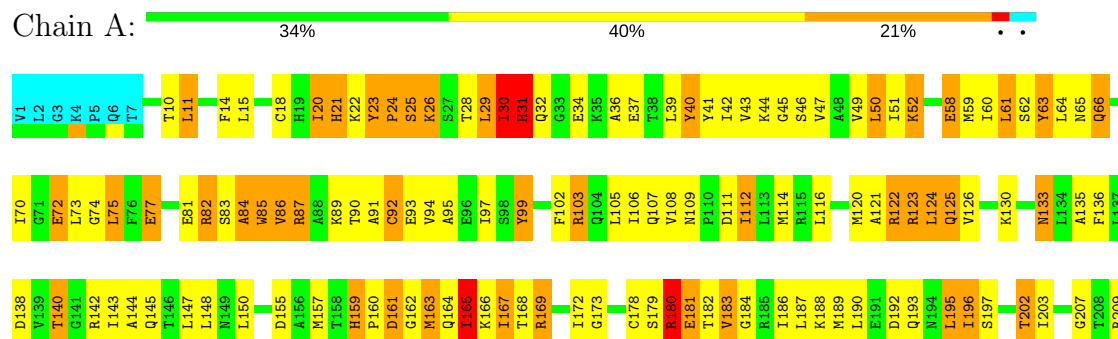


• Molecule 1: CATABOLITE GENE ACTIVATOR

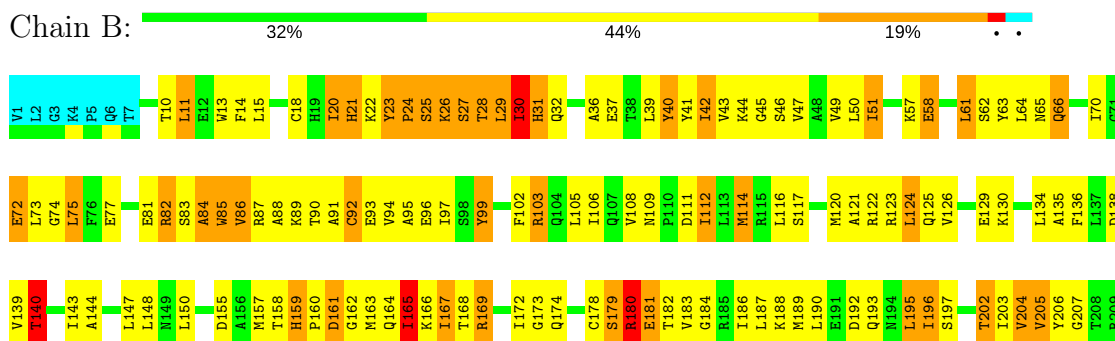


4.2.18 Score per residue for model 18

• Molecule 1: CATABOLITE GENE ACTIVATOR

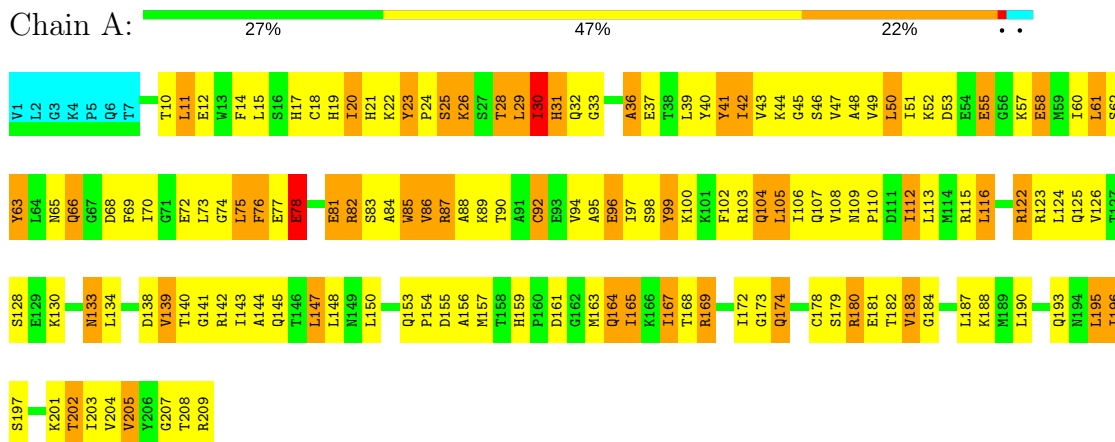


• Molecule 1: CATABOLITE GENE ACTIVATOR

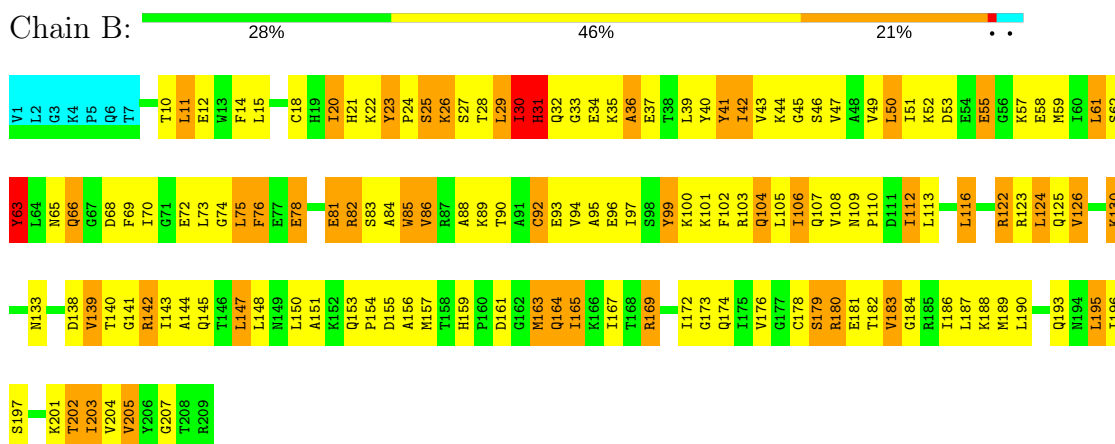


4.2.19 Score per residue for model 19

- Molecule 1: CATABOLITE GENE ACTIVATOR

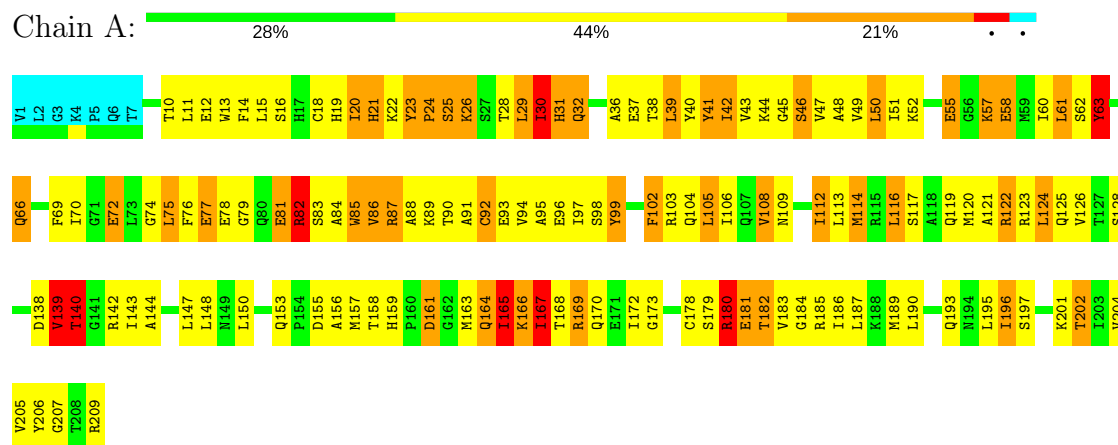


- Molecule 1: CATABOLITE GENE ACTIVATOR



4.2.20 Score per residue for model 20

- Molecule 1: CATABOLITE GENE ACTIVATOR



5 Refinement protocol and experimental data overview

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

Of the 200 calculated structures, 20 were deposited, based on the following criterion: *LOWEST ENERGY*.

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

| Software name | Classification | Version |
|---------------|--------------------|---------|
| HADDOCK-CNS | refinement | |
| NMRVIEW | structure solution | |
| ARIA | structure solution | |
| HADDOCK | structure solution | |
| CNS | structure solution | |

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

6 Model quality i

6.1 Standard geometry i

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 | 0.61±0.02 | 0±0/1624 (0.0±0.0%) | 0.98±0.02 | 2±1/2186 (0.1±0.0%) |
| 1 | B | 0.61±0.01 | 0±0/1624 (0.0±0.0%) | 0.98±0.02 | 3±1/2186 (0.1±0.0%) |
| All | All | 0.61 | 0/64960 (0.0%) | 0.98 | 97/87440 (0.1%) |

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 | 0.7±0.6 |
| 1 | B | 0.0±0.0 | 0.7±0.7 |
| All | All | 0 | 28 |

There are no bond-length outliers.

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 | 205 | VAL | N-CA-C | -8.55 | 87.91 | 111.00 | 11 | 15 |
| 1 | B | 205 | VAL | N-CA-C | -7.64 | 90.37 | 111.00 | 4 | 19 |
| 1 | B | 24 | PRO | CA-C-N | -6.58 | 102.71 | 117.20 | 12 | 8 |
| 1 | A | 28 | THR | CA-C-N | -6.44 | 103.04 | 117.20 | 4 | 4 |
| 1 | A | 24 | PRO | CA-C-N | -6.39 | 103.15 | 117.20 | 5 | 6 |
| 1 | B | 63 | TYR | CA-C-N | -6.16 | 103.66 | 117.20 | 19 | 7 |
| 1 | A | 63 | TYR | CA-C-N | -6.07 | 103.85 | 117.20 | 19 | 9 |
| 1 | B | 28 | THR | CA-C-N | -6.01 | 103.98 | 117.20 | 4 | 3 |
| 1 | B | 187 | LEU | CB-CA-C | 5.63 | 120.91 | 110.20 | 6 | 8 |
| 1 | B | 138 | ASP | N-CA-C | 5.54 | 125.97 | 111.00 | 12 | 3 |
| 1 | A | 187 | LEU | CB-CA-C | 5.42 | 120.49 | 110.20 | 3 | 4 |
| 1 | B | 23 | TYR | CB-CG-CD1 | 5.39 | 124.23 | 121.00 | 3 | 1 |
| 1 | A | 179 | SER | CA-C-N | -5.29 | 105.56 | 117.20 | 17 | 1 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) | Models | |
|-----|-------|-----|------|-----------|-------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 1 | B | 164 | GLN | CA-C-N | -5.25 | 105.64 | 117.20 | 7 | 1 |
| 1 | A | 138 | ASP | N-CA-C | 5.22 | 125.08 | 111.00 | 12 | 2 |
| 1 | B | 30 | ILE | CA-C-N | -5.15 | 105.86 | 117.20 | 17 | 1 |
| 1 | A | 31 | HIS | N-CA-CB | -5.15 | 101.33 | 110.60 | 7 | 1 |
| 1 | A | 30 | ILE | CA-C-N | -5.13 | 105.91 | 117.20 | 17 | 1 |
| 1 | A | 30 | ILE | N-CA-CB | 5.13 | 122.60 | 110.80 | 20 | 1 |
| 1 | A | 23 | TYR | CB-CG-CD1 | 5.11 | 124.06 | 121.00 | 10 | 2 |

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 | 31 | HIS | Mainchain | 13 |
| 1 | B | 31 | HIS | Mainchain | 11 |
| 1 | B | 179 | SER | Mainchain | 1 |
| 1 | B | 138 | ASP | Mainchain | 1 |
| 1 | B | 92 | CYS | Mainchain | 1 |
| 1 | A | 138 | ASP | Mainchain | 1 |

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 | 1599 | 1642 | 1636 | 157±10 |
| 1 | B | 1599 | 1642 | 1636 | 157±11 |
| All | All | 63960 | 65680 | 65439 | 6157 |

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 48.

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

| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|--------------|----------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:43:VAL:O | 1:A:66:GLN:CG | 1.08 | 2.02 | 17 | 2 |
| 1:A:43:VAL:O | 1:A:66:GLN:HG3 | 1.06 | 1.47 | 17 | 3 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:B:43:VAL:O | 1:B:66:GLN:CG | 1.01 | 2.08 | 17 | 2 |
| 1:B:18:CYS:SG | 1:B:95:ALA:HB1 | 0.97 | 2.00 | 4 | 20 |
| 1:A:190:LEU:HD22 | 1:A:196:ILE:HG12 | 0.97 | 1.32 | 13 | 3 |
| 1:B:169:ARG:HB3 | 1:B:187:LEU:HD12 | 0.96 | 1.37 | 20 | 19 |
| 1:A:18:CYS:SG | 1:A:95:ALA:HB1 | 0.96 | 2.01 | 18 | 20 |
| 1:B:44:LYS:HA | 1:B:66:GLN:HG3 | 0.94 | 1.39 | 17 | 6 |
| 1:A:169:ARG:HB3 | 1:A:187:LEU:HD12 | 0.93 | 1.39 | 15 | 20 |
| 1:A:153:GLN:OE1 | 1:A:155:ASP:OD2 | 0.93 | 1.87 | 14 | 1 |
| 1:B:43:VAL:O | 1:B:66:GLN:HG3 | 0.92 | 1.62 | 17 | 2 |
| 1:B:153:GLN:OE1 | 1:B:155:ASP:OD2 | 0.90 | 1.89 | 14 | 1 |
| 1:A:49:VAL:HB | 1:A:62:SER:O | 0.90 | 1.65 | 16 | 4 |
| 1:B:173:GLY:HA2 | 1:B:178:CYS:O | 0.89 | 1.66 | 17 | 19 |
| 1:B:49:VAL:HB | 1:B:62:SER:O | 0.88 | 1.68 | 6 | 3 |
| 1:B:51:ILE:O | 1:B:58:GLU:HA | 0.87 | 1.68 | 20 | 20 |
| 1:A:42:ILE:HD11 | 1:A:46:SER:HA | 0.87 | 1.47 | 11 | 8 |
| 1:A:135:ALA:HB3 | 1:B:135:ALA:HB3 | 0.87 | 1.45 | 3 | 7 |
| 1:A:15:LEU:HA | 1:A:18:CYS:SG | 0.86 | 2.10 | 20 | 20 |
| 1:B:22:LYS:HB3 | 1:B:92:CYS:O | 0.86 | 1.70 | 12 | 19 |
| 1:A:70:ILE:HG23 | 1:A:86:VAL:HG21 | 0.85 | 1.46 | 10 | 15 |
| 1:B:40:TYR:O | 1:B:70:ILE:HB | 0.85 | 1.71 | 2 | 20 |
| 1:B:45:GLY:H | 1:B:66:GLN:HG2 | 0.84 | 1.29 | 8 | 8 |
| 1:B:42:ILE:HD11 | 1:B:46:SER:HA | 0.84 | 1.48 | 11 | 10 |
| 1:A:40:TYR:O | 1:A:70:ILE:HB | 0.84 | 1.73 | 12 | 20 |
| 1:A:45:GLY:H | 1:A:66:GLN:HG2 | 0.84 | 1.33 | 19 | 7 |
| 1:A:15:LEU:HB3 | 1:A:20:ILE:HD11 | 0.84 | 1.50 | 1 | 14 |
| 1:A:190:LEU:HD22 | 1:A:196:ILE:CG1 | 0.84 | 2.03 | 16 | 16 |
| 1:A:124:LEU:HD21 | 1:B:124:LEU:HD21 | 0.83 | 1.48 | 18 | 1 |
| 1:A:173:GLY:HA2 | 1:A:178:CYS:O | 0.83 | 1.72 | 17 | 19 |
| 1:A:51:ILE:O | 1:A:58:GLU:HA | 0.83 | 1.74 | 14 | 20 |
| 1:A:42:ILE:HA | 1:A:94:VAL:HG12 | 0.83 | 1.50 | 6 | 18 |
| 1:B:72:GLU:HB3 | 1:B:116:LEU:HD11 | 0.82 | 1.49 | 7 | 16 |
| 1:B:44:LYS:HA | 1:B:66:GLN:CG | 0.82 | 2.05 | 17 | 1 |
| 1:B:18:CYS:HA | 1:B:97:ILE:HG21 | 0.82 | 1.51 | 11 | 20 |
| 1:A:187:LEU:HD22 | 1:A:190:LEU:HD11 | 0.81 | 1.51 | 13 | 14 |
| 1:B:42:ILE:HA | 1:B:94:VAL:HG12 | 0.81 | 1.51 | 11 | 18 |
| 1:B:42:ILE:HD12 | 1:B:47:VAL:HG13 | 0.81 | 1.50 | 14 | 10 |
| 1:A:41:TYR:HB3 | 1:A:95:ALA:HB3 | 0.81 | 1.52 | 8 | 16 |
| 1:B:193:GLN:HA | 1:B:196:ILE:O | 0.81 | 1.74 | 8 | 20 |
| 1:B:147:LEU:HD22 | 1:B:167:ILE:HD13 | 0.81 | 1.52 | 11 | 5 |
| 1:B:41:TYR:HB3 | 1:B:95:ALA:HB3 | 0.81 | 1.52 | 13 | 16 |
| 1:A:143:ILE:HG12 | 1:A:183:VAL:HG22 | 0.80 | 1.52 | 20 | 4 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:44:LYS:HA | 1:A:66:GLN:HG3 | 0.80 | 1.51 | 17 | 5 |
| 1:A:18:CYS:HA | 1:A:97:ILE:HG21 | 0.80 | 1.54 | 8 | 20 |
| 1:B:15:LEU:HB3 | 1:B:20:ILE:HD11 | 0.80 | 1.52 | 20 | 11 |
| 1:B:164:GLN:HB3 | 1:B:204:VAL:HG23 | 0.80 | 1.51 | 18 | 12 |
| 1:B:47:VAL:HB | 1:B:87:ARG:O | 0.80 | 1.77 | 15 | 6 |
| 1:B:22:LYS:HG2 | 1:B:23:TYR:CD1 | 0.80 | 2.12 | 12 | 19 |
| 1:B:37:GLU:HA | 1:B:99:TYR:CE2 | 0.79 | 2.12 | 15 | 14 |
| 1:A:20:ILE:HD13 | 1:A:95:ALA:HB2 | 0.79 | 1.52 | 18 | 10 |
| 1:B:45:GLY:N | 1:B:66:GLN:HG2 | 0.79 | 1.93 | 11 | 8 |
| 1:B:196:ILE:HG22 | 1:B:197:SER:H | 0.79 | 1.38 | 11 | 14 |
| 1:B:15:LEU:HD22 | 1:B:20:ILE:HD11 | 0.78 | 1.55 | 17 | 5 |
| 1:B:22:LYS:HG3 | 1:B:94:VAL:HG22 | 0.78 | 1.54 | 1 | 17 |
| 1:B:20:ILE:HD13 | 1:B:95:ALA:HB2 | 0.78 | 1.55 | 18 | 9 |
| 1:B:75:LEU:HB2 | 1:B:99:TYR:CD2 | 0.78 | 2.14 | 17 | 18 |
| 1:A:20:ILE:HG13 | 1:A:43:VAL:HG21 | 0.78 | 1.55 | 2 | 1 |
| 1:B:146:THR:HG21 | 1:B:175:ILE:HG21 | 0.77 | 1.55 | 6 | 9 |
| 1:B:43:VAL:O | 1:B:66:GLN:HG2 | 0.77 | 1.77 | 17 | 1 |
| 1:A:196:ILE:HG22 | 1:A:197:SER:H | 0.77 | 1.38 | 2 | 13 |
| 1:B:44:LYS:CA | 1:B:66:GLN:HG3 | 0.77 | 2.09 | 17 | 1 |
| 1:A:128:SER:HB3 | 1:B:51:ILE:HG21 | 0.77 | 1.57 | 15 | 11 |
| 1:A:51:ILE:HG21 | 1:B:128:SER:HB3 | 0.77 | 1.57 | 15 | 9 |
| 1:A:193:GLN:HA | 1:A:196:ILE:O | 0.77 | 1.80 | 1 | 19 |
| 1:A:26:LYS:H | 1:A:88:ALA:HB3 | 0.76 | 1.40 | 6 | 7 |
| 1:A:48:ALA:HB1 | 1:A:60:ILE:HD12 | 0.76 | 1.55 | 8 | 6 |
| 1:B:15:LEU:HA | 1:B:18:CYS:SG | 0.76 | 2.20 | 4 | 20 |
| 1:A:190:LEU:HD22 | 1:A:196:ILE:HG13 | 0.76 | 1.56 | 8 | 11 |
| 1:A:44:LYS:HG2 | 1:A:66:GLN:NE2 | 0.76 | 1.96 | 17 | 2 |
| 1:B:49:VAL:HA | 1:B:85:TRP:O | 0.76 | 1.81 | 4 | 7 |
| 1:B:22:LYS:HG2 | 1:B:23:TYR:CE1 | 0.76 | 2.15 | 12 | 18 |
| 1:B:26:LYS:H | 1:B:88:ALA:HB3 | 0.75 | 1.42 | 10 | 8 |
| 1:A:47:VAL:HB | 1:A:87:ARG:O | 0.75 | 1.81 | 12 | 4 |
| 1:A:72:GLU:HB3 | 1:A:116:LEU:HD11 | 0.75 | 1.56 | 3 | 15 |
| 1:A:75:LEU:HB2 | 1:A:99:TYR:CD2 | 0.75 | 2.17 | 2 | 19 |
| 1:B:167:ILE:HD11 | 1:B:203:ILE:HD12 | 0.74 | 1.59 | 9 | 2 |
| 1:B:172:ILE:HG13 | 1:B:187:LEU:HD11 | 0.74 | 1.59 | 19 | 7 |
| 1:A:49:VAL:HA | 1:A:85:TRP:O | 0.74 | 1.82 | 7 | 9 |
| 1:A:147:LEU:HA | 1:A:150:LEU:HD12 | 0.74 | 1.58 | 16 | 13 |
| 1:A:77:GLU:HA | 1:B:121:ALA:HB1 | 0.74 | 1.58 | 18 | 3 |
| 1:A:164:GLN:HB3 | 1:A:204:VAL:HG23 | 0.74 | 1.57 | 5 | 10 |
| 1:B:139:VAL:HG23 | 1:B:176:VAL:HG11 | 0.74 | 1.60 | 20 | 4 |
| 1:A:22:LYS:HG2 | 1:A:23:TYR:CD1 | 0.74 | 2.18 | 6 | 18 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:B:53:ASP:HB3 | 1:B:55:GLU:OE2 | 0.73 | 1.83 | 19 | 1 |
| 1:A:123:ARG:O | 1:A:126:VAL:HG12 | 0.73 | 1.83 | 14 | 16 |
| 1:B:49:VAL:HG12 | 1:B:61:LEU:HD11 | 0.73 | 1.59 | 19 | 17 |
| 1:A:106:ILE:HD13 | 1:A:113:LEU:HD13 | 0.73 | 1.60 | 3 | 11 |
| 1:B:47:VAL:HG22 | 1:B:64:LEU:HD12 | 0.73 | 1.60 | 6 | 8 |
| 1:B:14:PHE:CD2 | 1:B:105:LEU:HD21 | 0.73 | 2.17 | 2 | 13 |
| 1:A:37:GLU:HA | 1:A:99:TYR:CE2 | 0.73 | 2.17 | 1 | 14 |
| 1:A:45:GLY:N | 1:A:66:GLN:HG2 | 0.73 | 1.98 | 11 | 6 |
| 1:A:14:PHE:CD2 | 1:A:105:LEU:HD21 | 0.73 | 2.19 | 7 | 12 |
| 1:A:11:LEU:O | 1:A:15:LEU:HG | 0.73 | 1.83 | 2 | 20 |
| 1:A:43:VAL:O | 1:A:66:GLN:HG2 | 0.73 | 1.82 | 17 | 1 |
| 1:A:42:ILE:HD12 | 1:A:47:VAL:HG13 | 0.73 | 1.60 | 14 | 11 |
| 1:B:20:ILE:HG12 | 1:B:43:VAL:HG21 | 0.72 | 1.61 | 4 | 3 |
| 1:B:155:ASP:HB3 | 1:B:165:ILE:CG2 | 0.72 | 2.15 | 9 | 7 |
| 1:B:14:PHE:HD2 | 1:B:105:LEU:HD21 | 0.72 | 1.44 | 15 | 4 |
| 1:A:123:ARG:HA | 1:A:126:VAL:HG12 | 0.72 | 1.61 | 3 | 5 |
| 1:B:75:LEU:HG | 1:B:76:PHE:N | 0.72 | 1.98 | 6 | 18 |
| 1:B:138:ASP:O | 1:B:142:ARG:HB2 | 0.72 | 1.85 | 13 | 8 |
| 1:B:99:TYR:O | 1:B:103:ARG:HB3 | 0.71 | 1.84 | 14 | 16 |
| 1:A:138:ASP:O | 1:A:142:ARG:HB2 | 0.71 | 1.85 | 13 | 8 |
| 1:B:44:LYS:HE2 | 1:B:66:GLN:OE1 | 0.71 | 1.85 | 19 | 2 |
| 1:B:169:ARG:CB | 1:B:187:LEU:HD12 | 0.71 | 2.15 | 11 | 18 |
| 1:B:36:ALA:HB3 | 1:B:74:GLY:HA3 | 0.71 | 1.61 | 4 | 16 |
| 1:B:11:LEU:O | 1:B:15:LEU:HG | 0.71 | 1.84 | 9 | 20 |
| 1:A:24:PRO:HA | 1:A:91:ALA:HB2 | 0.71 | 1.60 | 5 | 12 |
| 1:A:75:LEU:HG | 1:A:76:PHE:N | 0.71 | 1.99 | 6 | 19 |
| 1:A:76:PHE:CZ | 1:B:121:ALA:HB2 | 0.71 | 2.20 | 12 | 1 |
| 1:B:31:HIS:CE1 | 1:B:50:LEU:HG | 0.71 | 2.21 | 8 | 15 |
| 1:B:28:THR:HG23 | 1:B:86:VAL:O | 0.71 | 1.86 | 19 | 1 |
| 1:A:190:LEU:HD13 | 1:A:196:ILE:HD11 | 0.71 | 1.62 | 13 | 2 |
| 1:B:155:ASP:HB3 | 1:B:165:ILE:HG22 | 0.71 | 1.63 | 6 | 20 |
| 1:A:172:ILE:HG13 | 1:A:187:LEU:HD11 | 0.71 | 1.63 | 9 | 7 |
| 1:A:22:LYS:C | 1:A:23:TYR:HD1 | 0.70 | 1.89 | 19 | 13 |
| 1:A:44:LYS:HA | 1:A:66:GLN:CG | 0.70 | 2.16 | 17 | 2 |
| 1:B:84:ALA:O | 1:B:85:TRP:HB2 | 0.70 | 1.87 | 9 | 20 |
| 1:B:190:LEU:HD22 | 1:B:196:ILE:CG1 | 0.70 | 2.16 | 12 | 16 |
| 1:A:22:LYS:HB3 | 1:A:92:CYS:O | 0.70 | 1.86 | 14 | 19 |
| 1:B:29:LEU:N | 1:B:29:LEU:HD23 | 0.70 | 2.01 | 17 | 8 |
| 1:A:29:LEU:N | 1:A:29:LEU:HD23 | 0.70 | 2.01 | 17 | 7 |
| 1:B:69:PHE:CD1 | 1:B:116:LEU:HD12 | 0.70 | 2.22 | 6 | 8 |
| 1:A:20:ILE:HD13 | 1:A:43:VAL:HG21 | 0.70 | 1.62 | 15 | 2 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:141:GLY:O | 1:A:145:GLN:HB2 | 0.70 | 1.87 | 1 | 4 |
| 1:B:48:ALA:HB1 | 1:B:60:ILE:HD12 | 0.69 | 1.63 | 8 | 4 |
| 1:B:46:SER:O | 1:B:89:LYS:HB3 | 0.69 | 1.87 | 18 | 9 |
| 1:B:157:MET:O | 1:B:163:MET:HA | 0.69 | 1.87 | 8 | 12 |
| 1:A:169:ARG:CB | 1:A:187:LEU:HD12 | 0.69 | 2.17 | 13 | 17 |
| 1:B:187:LEU:HD22 | 1:B:190:LEU:HD11 | 0.69 | 1.62 | 9 | 13 |
| 1:B:144:ALA:O | 1:B:148:LEU:HG | 0.69 | 1.88 | 1 | 19 |
| 1:A:144:ALA:O | 1:A:148:LEU:HG | 0.69 | 1.87 | 19 | 20 |
| 1:B:22:LYS:C | 1:B:23:TYR:HD1 | 0.69 | 1.90 | 20 | 15 |
| 1:B:72:GLU:HB2 | 1:B:120:MET:SD | 0.69 | 2.28 | 12 | 7 |
| 1:A:47:VAL:HG22 | 1:A:64:LEU:HD12 | 0.69 | 1.62 | 6 | 10 |
| 1:A:29:LEU:HD23 | 1:A:29:LEU:N | 0.69 | 2.03 | 19 | 10 |
| 1:A:36:ALA:HB3 | 1:A:74:GLY:HA3 | 0.69 | 1.63 | 10 | 18 |
| 1:A:22:LYS:HD2 | 1:A:92:CYS:SG | 0.69 | 2.28 | 12 | 9 |
| 1:B:29:LEU:HD23 | 1:B:29:LEU:N | 0.68 | 2.03 | 20 | 9 |
| 1:A:72:GLU:HA | 1:A:75:LEU:HD23 | 0.68 | 1.65 | 1 | 4 |
| 1:A:172:ILE:HG22 | 1:A:183:VAL:HG21 | 0.68 | 1.66 | 10 | 20 |
| 1:A:69:PHE:CD1 | 1:A:116:LEU:HD12 | 0.68 | 2.24 | 6 | 5 |
| 1:A:31:HIS:CD2 | 1:A:31:HIS:O | 0.68 | 2.46 | 12 | 10 |
| 1:A:186:ILE:O | 1:A:189:MET:HG2 | 0.68 | 1.89 | 11 | 14 |
| 1:A:46:SER:O | 1:A:89:LYS:HB3 | 0.68 | 1.88 | 18 | 10 |
| 1:B:11:LEU:HD11 | 1:B:41:TYR:CE2 | 0.68 | 2.24 | 13 | 9 |
| 1:A:76:PHE:CZ | 1:B:117:SER:HB3 | 0.68 | 2.24 | 14 | 1 |
| 1:A:106:ILE:HG22 | 1:A:112:ILE:CG2 | 0.67 | 2.20 | 3 | 16 |
| 1:A:164:GLN:HA | 1:A:203:ILE:O | 0.67 | 1.89 | 9 | 15 |
| 1:A:122:ARG:HD2 | 1:B:77:GLU:OE2 | 0.67 | 1.89 | 7 | 4 |
| 1:B:141:GLY:O | 1:B:145:GLN:HB2 | 0.67 | 1.89 | 1 | 4 |
| 1:A:103:ARG:O | 1:A:106:ILE:HG12 | 0.67 | 1.89 | 19 | 1 |
| 1:A:84:ALA:O | 1:A:85:TRP:HB2 | 0.67 | 1.88 | 17 | 20 |
| 1:B:187:LEU:HD23 | 1:B:190:LEU:HD12 | 0.67 | 1.64 | 10 | 1 |
| 1:A:147:LEU:HD22 | 1:A:167:ILE:HD13 | 0.67 | 1.67 | 11 | 5 |
| 1:A:18:CYS:HA | 1:A:97:ILE:CG2 | 0.67 | 2.20 | 14 | 20 |
| 1:B:28:THR:CA | 1:B:29:LEU:HD23 | 0.67 | 2.20 | 4 | 16 |
| 1:A:53:ASP:HB3 | 1:A:55:GLU:OE2 | 0.67 | 1.90 | 19 | 1 |
| 1:A:22:LYS:HG3 | 1:A:94:VAL:HG22 | 0.67 | 1.64 | 1 | 18 |
| 1:A:106:ILE:HG22 | 1:A:112:ILE:HG22 | 0.67 | 1.65 | 3 | 7 |
| 1:A:157:MET:O | 1:A:163:MET:HA | 0.67 | 1.88 | 8 | 11 |
| 1:B:172:ILE:HG22 | 1:B:183:VAL:HG21 | 0.67 | 1.65 | 20 | 20 |
| 1:A:29:LEU:O | 1:A:30:ILE:HG13 | 0.67 | 1.90 | 20 | 3 |
| 1:A:155:ASP:HB3 | 1:A:165:ILE:HG22 | 0.66 | 1.66 | 10 | 20 |
| 1:A:103:ARG:O | 1:A:107:GLN:HB3 | 0.66 | 1.90 | 14 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:28:THR:HA | 1:A:29:LEU:HD23 | 0.66 | 1.66 | 16 | 9 |
| 1:B:29:LEU:CB | 1:B:86:VAL:HB | 0.66 | 2.20 | 10 | 2 |
| 1:B:44:LYS:HD3 | 1:B:66:GLN:NE2 | 0.66 | 2.05 | 12 | 1 |
| 1:A:186:ILE:HG22 | 1:A:187:LEU:HD23 | 0.66 | 1.67 | 16 | 14 |
| 1:A:33:GLY:N | 1:A:82:ARG:HD3 | 0.66 | 2.05 | 17 | 5 |
| 1:A:117:SER:HA | 1:A:120:MET:SD | 0.66 | 2.31 | 12 | 1 |
| 1:A:69:PHE:CG | 1:A:116:LEU:HD12 | 0.66 | 2.25 | 17 | 15 |
| 1:A:121:ALA:HB2 | 1:B:76:PHE:CZ | 0.66 | 2.26 | 12 | 1 |
| 1:B:31:HIS:CD2 | 1:B:31:HIS:O | 0.66 | 2.49 | 12 | 7 |
| 1:B:24:PRO:HA | 1:B:91:ALA:CB | 0.66 | 2.21 | 3 | 8 |
| 1:B:31:HIS:O | 1:B:31:HIS:CD2 | 0.66 | 2.49 | 14 | 10 |
| 1:A:22:LYS:HG2 | 1:A:23:TYR:CE1 | 0.66 | 2.26 | 9 | 18 |
| 1:B:44:LYS:HG2 | 1:B:66:GLN:NE2 | 0.66 | 2.05 | 17 | 2 |
| 1:A:11:LEU:HD12 | 1:A:15:LEU:HG | 0.66 | 1.67 | 5 | 3 |
| 1:A:171:GLU:HA | 1:A:174:GLN:NE2 | 0.66 | 2.06 | 7 | 1 |
| 1:A:124:LEU:O | 1:A:128:SER:HB2 | 0.66 | 1.91 | 14 | 1 |
| 1:B:186:ILE:O | 1:B:190:LEU:HG | 0.66 | 1.91 | 10 | 13 |
| 1:A:41:TYR:HB2 | 1:A:95:ALA:HB3 | 0.65 | 1.68 | 7 | 1 |
| 1:B:123:ARG:O | 1:B:126:VAL:HG12 | 0.65 | 1.90 | 9 | 16 |
| 1:B:196:ILE:HG22 | 1:B:204:VAL:O | 0.65 | 1.91 | 4 | 10 |
| 1:B:143:ILE:HG12 | 1:B:183:VAL:HG22 | 0.65 | 1.68 | 10 | 5 |
| 1:A:196:ILE:HG22 | 1:A:204:VAL:O | 0.65 | 1.92 | 15 | 4 |
| 1:A:11:LEU:HD21 | 1:A:41:TYR:CE2 | 0.65 | 2.26 | 19 | 6 |
| 1:A:44:LYS:CG | 1:A:66:GLN:NE2 | 0.65 | 2.59 | 17 | 1 |
| 1:A:197:SER:O | 1:A:204:VAL:HB | 0.65 | 1.91 | 9 | 4 |
| 1:B:179:SER:C | 1:B:181:GLU:H | 0.65 | 1.93 | 19 | 20 |
| 1:A:28:THR:CA | 1:A:29:LEU:HD23 | 0.65 | 2.22 | 4 | 16 |
| 1:B:164:GLN:HA | 1:B:203:ILE:O | 0.65 | 1.90 | 9 | 15 |
| 1:A:47:VAL:HA | 1:A:89:LYS:H | 0.65 | 1.51 | 14 | 6 |
| 1:B:143:ILE:O | 1:B:147:LEU:HG | 0.65 | 1.91 | 5 | 18 |
| 1:B:103:ARG:O | 1:B:106:ILE:HG12 | 0.65 | 1.91 | 19 | 1 |
| 1:B:186:ILE:HG22 | 1:B:187:LEU:HD23 | 0.65 | 1.69 | 18 | 10 |
| 1:A:30:ILE:HD12 | 1:A:86:VAL:HG21 | 0.65 | 1.69 | 2 | 3 |
| 1:A:77:GLU:OE2 | 1:B:122:ARG:HD2 | 0.65 | 1.92 | 9 | 1 |
| 1:B:42:ILE:HD11 | 1:B:47:VAL:HG13 | 0.65 | 1.69 | 9 | 1 |
| 1:A:31:HIS:CE1 | 1:A:50:LEU:HG | 0.65 | 2.27 | 17 | 15 |
| 1:A:39:LEU:HD13 | 1:A:102:PHE:CZ | 0.65 | 2.27 | 20 | 2 |
| 1:B:11:LEU:HD21 | 1:B:41:TYR:CE2 | 0.65 | 2.26 | 2 | 8 |
| 1:A:31:HIS:O | 1:A:31:HIS:CD2 | 0.65 | 2.50 | 14 | 7 |
| 1:A:14:PHE:HD2 | 1:A:105:LEU:HD21 | 0.65 | 1.50 | 1 | 5 |
| 1:B:18:CYS:HA | 1:B:97:ILE:CG2 | 0.65 | 2.23 | 2 | 20 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:144:ALA:HB2 | 1:A:195:LEU:HD21 | 0.65 | 1.66 | 13 | 6 |
| 1:B:44:LYS:CG | 1:B:66:GLN:NE2 | 0.64 | 2.60 | 17 | 1 |
| 1:B:103:ARG:O | 1:B:107:GLN:HB3 | 0.64 | 1.92 | 14 | 3 |
| 1:B:23:TYR:N | 1:B:23:TYR:CD1 | 0.64 | 2.64 | 1 | 9 |
| 1:B:24:PRO:HA | 1:B:91:ALA:HB2 | 0.64 | 1.68 | 3 | 12 |
| 1:A:24:PRO:HA | 1:A:91:ALA:CB | 0.64 | 2.22 | 20 | 10 |
| 1:A:20:ILE:O | 1:A:21:HIS:HB2 | 0.64 | 1.91 | 20 | 14 |
| 1:B:47:VAL:HA | 1:B:89:LYS:H | 0.64 | 1.52 | 9 | 7 |
| 1:B:20:ILE:O | 1:B:21:HIS:HB2 | 0.64 | 1.93 | 1 | 15 |
| 1:A:179:SER:C | 1:A:181:GLU:H | 0.64 | 1.94 | 8 | 19 |
| 1:A:187:LEU:HD22 | 1:A:190:LEU:CD1 | 0.64 | 2.23 | 13 | 16 |
| 1:B:20:ILE:HG23 | 1:B:43:VAL:HG21 | 0.64 | 1.68 | 2 | 6 |
| 1:B:190:LEU:HD13 | 1:B:196:ILE:HD11 | 0.64 | 1.69 | 9 | 3 |
| 1:B:69:PHE:CG | 1:B:116:LEU:HD12 | 0.64 | 2.28 | 13 | 16 |
| 1:A:30:ILE:HD12 | 1:A:86:VAL:CG2 | 0.64 | 2.22 | 2 | 8 |
| 1:A:69:PHE:CE2 | 1:A:116:LEU:HA | 0.64 | 2.28 | 16 | 7 |
| 1:B:31:HIS:CE1 | 1:B:58:GLU:HB3 | 0.64 | 2.27 | 8 | 3 |
| 1:A:166:LYS:HB3 | 1:A:202:THR:HG22 | 0.64 | 1.67 | 5 | 1 |
| 1:A:179:SER:HB3 | 1:A:181:GLU:OE2 | 0.64 | 1.93 | 14 | 1 |
| 1:A:42:ILE:HD11 | 1:A:47:VAL:HG13 | 0.64 | 1.70 | 12 | 3 |
| 1:A:146:THR:HG21 | 1:A:175:ILE:HG21 | 0.64 | 1.67 | 6 | 9 |
| 1:A:150:LEU:HD13 | 1:A:167:ILE:HG12 | 0.63 | 1.68 | 4 | 8 |
| 1:B:47:VAL:O | 1:B:63:TYR:HB3 | 0.63 | 1.93 | 9 | 15 |
| 1:B:197:SER:HB2 | 1:B:206:TYR:CE1 | 0.63 | 2.28 | 17 | 13 |
| 1:B:123:ARG:HA | 1:B:126:VAL:HG12 | 0.63 | 1.70 | 14 | 5 |
| 1:B:106:ILE:HD13 | 1:B:113:LEU:HD13 | 0.63 | 1.70 | 7 | 11 |
| 1:A:48:ALA:HB1 | 1:A:60:ILE:HD13 | 0.63 | 1.69 | 16 | 9 |
| 1:A:20:ILE:HG12 | 1:A:43:VAL:HG21 | 0.63 | 1.69 | 10 | 1 |
| 1:B:23:TYR:N | 1:B:23:TYR:HD1 | 0.63 | 1.91 | 1 | 2 |
| 1:A:190:LEU:HD13 | 1:A:196:ILE:HD12 | 0.63 | 1.69 | 14 | 15 |
| 1:B:49:VAL:HG22 | 1:B:85:TRP:O | 0.63 | 1.93 | 13 | 17 |
| 1:B:44:LYS:HD2 | 1:B:66:GLN:CD | 0.63 | 2.14 | 20 | 1 |
| 1:A:18:CYS:CB | 1:A:97:ILE:HG12 | 0.63 | 2.24 | 14 | 12 |
| 1:A:23:TYR:CD1 | 1:A:23:TYR:N | 0.63 | 2.67 | 3 | 17 |
| 1:B:48:ALA:HB1 | 1:B:60:ILE:HD13 | 0.63 | 1.70 | 15 | 11 |
| 1:B:70:ILE:HG23 | 1:B:86:VAL:HG21 | 0.63 | 1.68 | 15 | 12 |
| 1:B:182:THR:O | 1:B:185:ARG:HB2 | 0.63 | 1.94 | 5 | 5 |
| 1:B:134:LEU:HD22 | 1:B:174:GLN:O | 0.63 | 1.94 | 1 | 12 |
| 1:A:143:ILE:O | 1:A:147:LEU:HG | 0.63 | 1.93 | 18 | 17 |
| 1:A:44:LYS:CA | 1:A:66:GLN:HG3 | 0.63 | 2.23 | 17 | 3 |
| 1:B:69:PHE:CE2 | 1:B:116:LEU:HA | 0.63 | 2.28 | 13 | 6 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:11:LEU:HD11 | 1:A:41:TYR:CE2 | 0.63 | 2.28 | 11 | 11 |
| 1:A:44:LYS:O | 1:A:92:CYS:HB3 | 0.63 | 1.94 | 16 | 5 |
| 1:A:82:ARG:HG2 | 1:A:83:SER:N | 0.63 | 2.09 | 17 | 17 |
| 1:A:187:LEU:HA | 1:A:190:LEU:HG | 0.63 | 1.68 | 8 | 19 |
| 1:B:41:TYR:HB2 | 1:B:95:ALA:HB3 | 0.63 | 1.70 | 7 | 1 |
| 1:B:42:ILE:HD11 | 1:B:46:SER:CA | 0.63 | 2.24 | 18 | 8 |
| 1:B:20:ILE:CG1 | 1:B:43:VAL:HG21 | 0.62 | 2.24 | 4 | 4 |
| 1:A:87:ARG:HD3 | 1:A:88:ALA:O | 0.62 | 1.94 | 11 | 1 |
| 1:A:49:VAL:HG22 | 1:A:85:TRP:O | 0.62 | 1.94 | 6 | 15 |
| 1:B:82:ARG:HG2 | 1:B:83:SER:N | 0.62 | 2.08 | 12 | 13 |
| 1:B:187:LEU:HA | 1:B:190:LEU:HG | 0.62 | 1.69 | 9 | 19 |
| 1:A:99:TYR:O | 1:A:103:ARG:HB3 | 0.62 | 1.94 | 2 | 17 |
| 1:A:47:VAL:O | 1:A:63:TYR:HB3 | 0.62 | 1.94 | 9 | 14 |
| 1:B:103:ARG:O | 1:B:106:ILE:HG13 | 0.62 | 1.95 | 18 | 6 |
| 1:B:61:LEU:HD12 | 1:B:62:SER:N | 0.62 | 2.10 | 19 | 1 |
| 1:A:72:GLU:HB2 | 1:A:120:MET:SD | 0.62 | 2.35 | 1 | 8 |
| 1:B:33:GLY:N | 1:B:82:ARG:HD3 | 0.62 | 2.10 | 11 | 2 |
| 1:B:166:LYS:HG2 | 1:B:202:THR:HG22 | 0.62 | 1.70 | 9 | 1 |
| 1:A:155:ASP:HB3 | 1:A:165:ILE:CG2 | 0.62 | 2.24 | 9 | 9 |
| 1:A:134:LEU:HD22 | 1:A:174:GLN:O | 0.62 | 1.94 | 16 | 11 |
| 1:B:180:ARG:HA | 1:B:183:VAL:HG12 | 0.62 | 1.72 | 8 | 7 |
| 1:A:29:LEU:C | 1:A:30:ILE:HG13 | 0.62 | 2.15 | 2 | 18 |
| 1:B:31:HIS:CG | 1:B:31:HIS:O | 0.62 | 2.53 | 2 | 12 |
| 1:B:30:ILE:HD12 | 1:B:86:VAL:CG2 | 0.61 | 2.25 | 1 | 11 |
| 1:B:190:LEU:HD22 | 1:B:196:ILE:HG13 | 0.61 | 1.73 | 17 | 13 |
| 1:A:197:SER:HB2 | 1:A:206:TYR:CE1 | 0.61 | 2.30 | 17 | 13 |
| 1:B:39:LEU:HD11 | 1:B:41:TYR:CE1 | 0.61 | 2.31 | 7 | 1 |
| 1:B:29:LEU:C | 1:B:30:ILE:HG13 | 0.61 | 2.15 | 1 | 16 |
| 1:A:42:ILE:CA | 1:A:94:VAL:HG12 | 0.61 | 2.23 | 20 | 15 |
| 1:A:49:VAL:HG12 | 1:A:61:LEU:HD11 | 0.61 | 1.72 | 10 | 15 |
| 1:A:29:LEU:CB | 1:A:86:VAL:HB | 0.61 | 2.25 | 6 | 1 |
| 1:B:190:LEU:HD13 | 1:B:196:ILE:CD1 | 0.61 | 2.26 | 13 | 3 |
| 1:B:186:ILE:O | 1:B:189:MET:HG2 | 0.61 | 1.94 | 11 | 12 |
| 1:A:42:ILE:HD11 | 1:A:46:SER:CA | 0.61 | 2.25 | 20 | 7 |
| 1:A:117:SER:HB3 | 1:B:76:PHE:CZ | 0.61 | 2.30 | 14 | 1 |
| 1:B:11:LEU:HD12 | 1:B:15:LEU:HG | 0.61 | 1.72 | 5 | 4 |
| 1:B:87:ARG:HD3 | 1:B:88:ALA:O | 0.61 | 1.96 | 11 | 1 |
| 1:B:49:VAL:CG1 | 1:B:61:LEU:HD11 | 0.61 | 2.26 | 19 | 1 |
| 1:A:103:ARG:HA | 1:A:106:ILE:CG1 | 0.61 | 2.26 | 17 | 17 |
| 1:A:31:HIS:O | 1:A:31:HIS:CG | 0.61 | 2.54 | 2 | 9 |
| 1:B:52:LYS:HA | 1:B:57:LYS:O | 0.61 | 1.96 | 7 | 9 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:B:147:LEU:CD2 | 1:B:203:ILE:HG21 | 0.61 | 2.26 | 19 | 1 |
| 1:B:25:SER:O | 1:B:26:LYS:HG3 | 0.61 | 1.96 | 10 | 2 |
| 1:A:134:LEU:O | 1:A:177:GLY:HA3 | 0.61 | 1.96 | 4 | 5 |
| 1:B:190:LEU:HD13 | 1:B:196:ILE:HD12 | 0.60 | 1.73 | 20 | 15 |
| 1:B:42:ILE:CA | 1:B:94:VAL:HG12 | 0.60 | 2.26 | 20 | 16 |
| 1:B:150:LEU:HD13 | 1:B:167:ILE:HG12 | 0.60 | 1.73 | 3 | 10 |
| 1:B:147:LEU:HD22 | 1:B:167:ILE:CD1 | 0.60 | 2.26 | 11 | 4 |
| 1:B:166:LYS:HG3 | 1:B:202:THR:HG23 | 0.60 | 1.73 | 15 | 1 |
| 1:A:49:VAL:HG12 | 1:A:61:LEU:CD1 | 0.60 | 2.27 | 10 | 20 |
| 1:A:147:LEU:HD22 | 1:A:167:ILE:CD1 | 0.60 | 2.25 | 11 | 5 |
| 1:A:117:SER:HB2 | 1:B:76:PHE:CE1 | 0.60 | 2.31 | 4 | 3 |
| 1:A:77:GLU:HG3 | 1:A:79:GLY:N | 0.60 | 2.11 | 20 | 4 |
| 1:B:44:LYS:HA | 1:B:66:GLN:CD | 0.60 | 2.16 | 17 | 1 |
| 1:A:131:VAL:HG12 | 1:B:131:VAL:HG12 | 0.60 | 1.73 | 9 | 4 |
| 1:B:31:HIS:O | 1:B:31:HIS:CG | 0.60 | 2.54 | 10 | 6 |
| 1:B:49:VAL:HG12 | 1:B:61:LEU:CD1 | 0.60 | 2.27 | 9 | 19 |
| 1:A:20:ILE:HA | 1:A:94:VAL:O | 0.60 | 1.97 | 12 | 14 |
| 1:B:20:ILE:HD13 | 1:B:43:VAL:HG21 | 0.60 | 1.72 | 20 | 2 |
| 1:B:103:ARG:HA | 1:B:106:ILE:CG1 | 0.60 | 2.26 | 18 | 19 |
| 1:A:143:ILE:CD1 | 1:A:186:ILE:HD13 | 0.60 | 2.27 | 1 | 3 |
| 1:B:150:LEU:HB3 | 1:B:165:ILE:HG21 | 0.60 | 1.73 | 11 | 4 |
| 1:B:28:THR:HA | 1:B:29:LEU:HD23 | 0.60 | 1.72 | 1 | 7 |
| 1:A:196:ILE:HG22 | 1:A:197:SER:N | 0.60 | 2.11 | 19 | 12 |
| 1:B:50:LEU:CB | 1:B:60:ILE:HA | 0.60 | 2.26 | 10 | 12 |
| 1:B:147:LEU:HA | 1:B:150:LEU:HD12 | 0.60 | 1.74 | 5 | 12 |
| 1:A:23:TYR:N | 1:A:23:TYR:CD1 | 0.60 | 2.70 | 17 | 1 |
| 1:A:44:LYS:HE2 | 1:A:66:GLN:OE1 | 0.60 | 1.95 | 19 | 1 |
| 1:A:72:GLU:HG3 | 1:A:120:MET:HE2 | 0.60 | 1.73 | 14 | 1 |
| 1:A:19:HIS:HB3 | 1:A:96:GLU:O | 0.60 | 1.97 | 1 | 7 |
| 1:B:41:TYR:O | 1:B:43:VAL:HG23 | 0.60 | 1.97 | 11 | 11 |
| 1:A:48:ALA:CB | 1:A:60:ILE:HD12 | 0.60 | 2.27 | 3 | 4 |
| 1:B:59:MET:HE3 | 1:B:174:GLN:HB2 | 0.60 | 1.74 | 3 | 3 |
| 1:B:42:ILE:HD11 | 1:B:64:LEU:HD12 | 0.60 | 1.72 | 10 | 2 |
| 1:B:89:LYS:CE | 1:B:155:ASP:OD1 | 0.60 | 2.50 | 10 | 1 |
| 1:A:37:GLU:HA | 1:A:99:TYR:CZ | 0.60 | 2.31 | 11 | 4 |
| 1:B:28:THR:HA | 1:B:87:ARG:HA | 0.60 | 1.71 | 15 | 4 |
| 1:A:41:TYR:CB | 1:A:95:ALA:HB3 | 0.60 | 2.26 | 7 | 6 |
| 1:A:143:ILE:HD13 | 1:A:186:ILE:HG21 | 0.59 | 1.72 | 8 | 2 |
| 1:A:173:GLY:CA | 1:A:178:CYS:O | 0.59 | 2.50 | 14 | 3 |
| 1:A:180:ARG:O | 1:A:184:GLY:HA3 | 0.59 | 1.97 | 19 | 14 |
| 1:B:196:ILE:HG22 | 1:B:209:ARG:OXT | 0.59 | 1.96 | 9 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:31:HIS:CG | 1:A:31:HIS:O | 0.59 | 2.55 | 10 | 9 |
| 1:B:44:LYS:O | 1:B:92:CYS:HB3 | 0.59 | 1.96 | 16 | 6 |
| 1:B:23:TYR:CD1 | 1:B:23:TYR:N | 0.59 | 2.70 | 18 | 10 |
| 1:A:63:TYR:CD2 | 1:A:89:LYS:HD2 | 0.59 | 2.32 | 18 | 2 |
| 1:B:159:HIS:CE1 | 1:B:161:ASP:HB3 | 0.59 | 2.33 | 18 | 5 |
| 1:A:63:TYR:O | 1:A:64:LEU:HD23 | 0.59 | 1.97 | 12 | 1 |
| 1:A:51:ILE:HD12 | 1:A:61:LEU:HB3 | 0.59 | 1.74 | 7 | 1 |
| 1:A:28:THR:HA | 1:A:87:ARG:HA | 0.59 | 1.73 | 11 | 4 |
| 1:B:179:SER:HB2 | 1:B:181:GLU:OE2 | 0.59 | 1.98 | 14 | 1 |
| 1:A:53:ASP:HB2 | 1:A:57:LYS:HG2 | 0.59 | 1.74 | 1 | 2 |
| 1:B:31:HIS:CE1 | 1:B:58:GLU:HB2 | 0.59 | 2.32 | 1 | 5 |
| 1:B:106:ILE:HG22 | 1:B:112:ILE:CG2 | 0.59 | 2.27 | 17 | 14 |
| 1:A:122:ARG:NH2 | 1:B:78:GLU:HB3 | 0.59 | 2.13 | 19 | 6 |
| 1:A:31:HIS:CE1 | 1:A:58:GLU:HB3 | 0.59 | 2.31 | 8 | 4 |
| 1:A:103:ARG:O | 1:A:106:ILE:HG13 | 0.59 | 1.97 | 1 | 9 |
| 1:B:196:ILE:HG22 | 1:B:197:SER:N | 0.59 | 2.12 | 19 | 10 |
| 1:A:76:PHE:CE2 | 1:A:120:MET:HG3 | 0.59 | 2.33 | 12 | 1 |
| 1:B:27:SER:O | 1:B:88:ALA:N | 0.59 | 2.32 | 13 | 3 |
| 1:A:195:LEU:O | 1:A:209:ARG:HB3 | 0.59 | 1.98 | 20 | 1 |
| 1:B:134:LEU:O | 1:B:177:GLY:HA3 | 0.59 | 1.97 | 4 | 6 |
| 1:B:180:ARG:O | 1:B:184:GLY:HA3 | 0.59 | 1.98 | 12 | 13 |
| 1:A:24:PRO:HA | 1:A:91:ALA:CA | 0.59 | 2.28 | 12 | 10 |
| 1:B:50:LEU:HB3 | 1:B:60:ILE:HG22 | 0.59 | 1.75 | 10 | 1 |
| 1:A:77:GLU:OE2 | 1:B:122:ARG:HA | 0.59 | 1.97 | 9 | 1 |
| 1:A:22:LYS:C | 1:A:23:TYR:CD1 | 0.58 | 2.77 | 2 | 19 |
| 1:B:22:LYS:HD2 | 1:B:92:CYS:SG | 0.58 | 2.38 | 15 | 13 |
| 1:B:47:VAL:HA | 1:B:89:LYS:N | 0.58 | 2.12 | 12 | 15 |
| 1:B:102:PHE:CE1 | 1:B:106:ILE:HG21 | 0.58 | 2.33 | 12 | 9 |
| 1:A:182:THR:O | 1:A:185:ARG:HB2 | 0.58 | 1.97 | 4 | 6 |
| 1:A:102:PHE:CE1 | 1:A:106:ILE:HG21 | 0.58 | 2.32 | 12 | 9 |
| 1:A:27:SER:O | 1:A:88:ALA:N | 0.58 | 2.34 | 13 | 3 |
| 1:B:169:ARG:CB | 1:B:187:LEU:HD13 | 0.58 | 2.28 | 10 | 1 |
| 1:B:51:ILE:HD12 | 1:B:61:LEU:HB3 | 0.58 | 1.72 | 18 | 1 |
| 1:A:23:TYR:N | 1:A:23:TYR:HD1 | 0.58 | 1.96 | 3 | 3 |
| 1:B:196:ILE:HG13 | 1:B:197:SER:N | 0.58 | 2.14 | 13 | 1 |
| 1:B:42:ILE:HG21 | 1:B:45:GLY:O | 0.58 | 1.98 | 2 | 1 |
| 1:B:99:TYR:HA | 1:B:102:PHE:HB3 | 0.58 | 1.76 | 20 | 14 |
| 1:B:172:ILE:CG2 | 1:B:183:VAL:HG21 | 0.58 | 2.28 | 14 | 8 |
| 1:B:69:PHE:CG | 1:B:116:LEU:HD13 | 0.58 | 2.34 | 2 | 1 |
| 1:A:123:ARG:CA | 1:A:126:VAL:HG12 | 0.58 | 2.28 | 3 | 2 |
| 1:A:11:LEU:HD11 | 1:A:41:TYR:HE2 | 0.58 | 1.59 | 5 | 4 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:28:THR:C | 1:A:29:LEU:HD23 | 0.58 | 2.19 | 12 | 14 |
| 1:A:102:PHE:CE2 | 1:A:106:ILE:HG23 | 0.58 | 2.33 | 3 | 1 |
| 1:A:72:GLU:CB | 1:A:116:LEU:HD11 | 0.58 | 2.28 | 7 | 5 |
| 1:B:139:VAL:HA | 1:B:176:VAL:CG1 | 0.58 | 2.29 | 3 | 1 |
| 1:A:30:ILE:HG22 | 1:A:34:GLU:HB2 | 0.58 | 1.74 | 10 | 3 |
| 1:A:143:ILE:HG21 | 1:A:187:LEU:HD21 | 0.58 | 1.75 | 10 | 4 |
| 1:A:20:ILE:CG1 | 1:A:43:VAL:HG21 | 0.58 | 2.29 | 2 | 1 |
| 1:A:123:ARG:HA | 1:A:126:VAL:CG1 | 0.57 | 2.29 | 14 | 2 |
| 1:A:23:TYR:HD1 | 1:A:23:TYR:N | 0.57 | 1.97 | 18 | 5 |
| 1:A:41:TYR:O | 1:A:43:VAL:HG23 | 0.57 | 1.98 | 11 | 9 |
| 1:A:70:ILE:HD13 | 1:A:86:VAL:HG11 | 0.57 | 1.76 | 13 | 14 |
| 1:A:186:ILE:O | 1:A:190:LEU:HG | 0.57 | 2.00 | 17 | 13 |
| 1:B:70:ILE:HD13 | 1:B:86:VAL:HG11 | 0.57 | 1.76 | 20 | 14 |
| 1:A:52:LYS:HA | 1:A:57:LYS:O | 0.57 | 1.98 | 7 | 12 |
| 1:B:28:THR:HA | 1:B:29:LEU:HD22 | 0.57 | 1.77 | 13 | 1 |
| 1:A:117:SER:HB2 | 1:B:76:PHE:CZ | 0.57 | 2.34 | 4 | 5 |
| 1:B:117:SER:HA | 1:B:120:MET:CE | 0.57 | 2.29 | 4 | 1 |
| 1:B:61:LEU:HD22 | 1:B:62:SER:HB2 | 0.57 | 1.75 | 10 | 9 |
| 1:B:190:LEU:CD1 | 1:B:196:ILE:HD12 | 0.57 | 2.29 | 18 | 12 |
| 1:B:174:GLN:HG2 | 1:B:175:ILE:N | 0.57 | 2.14 | 6 | 3 |
| 1:A:15:LEU:HD22 | 1:A:20:ILE:HD11 | 0.57 | 1.76 | 17 | 3 |
| 1:B:169:ARG:CG | 1:B:187:LEU:HD12 | 0.57 | 2.30 | 2 | 2 |
| 1:A:28:THR:HB | 1:A:87:ARG:HA | 0.57 | 1.76 | 2 | 4 |
| 1:B:104:GLN:O | 1:B:107:GLN:HG2 | 0.57 | 2.00 | 19 | 1 |
| 1:A:53:ASP:HB2 | 1:A:57:LYS:CG | 0.56 | 2.30 | 1 | 1 |
| 1:B:187:LEU:HD22 | 1:B:190:LEU:CD1 | 0.56 | 2.30 | 1 | 15 |
| 1:A:41:TYR:O | 1:A:43:VAL:HG13 | 0.56 | 2.00 | 19 | 4 |
| 1:B:169:ARG:HB3 | 1:B:187:LEU:HD13 | 0.56 | 1.75 | 10 | 1 |
| 1:A:72:GLU:CB | 1:A:120:MET:HE1 | 0.56 | 2.30 | 4 | 2 |
| 1:A:172:ILE:CG2 | 1:A:183:VAL:HG21 | 0.56 | 2.30 | 14 | 8 |
| 1:A:60:ILE:HB | 1:A:174:GLN:CD | 0.56 | 2.19 | 3 | 4 |
| 1:B:197:SER:HB3 | 1:B:206:TYR:CE1 | 0.56 | 2.35 | 15 | 6 |
| 1:B:22:LYS:C | 1:B:23:TYR:CD1 | 0.56 | 2.78 | 5 | 19 |
| 1:A:22:LYS:H | 1:A:93:GLU:HA | 0.56 | 1.59 | 17 | 17 |
| 1:B:167:ILE:CD1 | 1:B:203:ILE:HD12 | 0.56 | 2.30 | 10 | 10 |
| 1:B:166:LYS:HA | 1:B:201:LYS:O | 0.56 | 2.01 | 10 | 6 |
| 1:B:144:ALA:HB2 | 1:B:195:LEU:HD21 | 0.56 | 1.77 | 9 | 5 |
| 1:B:114:MET:HA | 1:B:117:SER:OG | 0.56 | 2.00 | 7 | 7 |
| 1:B:190:LEU:HD22 | 1:B:196:ILE:HG12 | 0.56 | 1.77 | 13 | 3 |
| 1:B:11:LEU:HD11 | 1:B:41:TYR:HE2 | 0.56 | 1.61 | 5 | 1 |
| 1:B:18:CYS:CB | 1:B:97:ILE:HG12 | 0.56 | 2.31 | 6 | 16 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:B:37:GLU:HA | 1:B:99:TYR:CZ | 0.56 | 2.36 | 11 | 3 |
| 1:B:119:GLN:O | 1:B:123:ARG:HD3 | 0.56 | 2.00 | 7 | 9 |
| 1:A:113:LEU:HD12 | 1:A:116:LEU:HD23 | 0.56 | 1.76 | 2 | 1 |
| 1:B:39:LEU:HD11 | 1:B:41:TYR:HE1 | 0.56 | 1.61 | 7 | 1 |
| 1:A:147:LEU:CD2 | 1:A:203:ILE:HG21 | 0.56 | 2.30 | 19 | 2 |
| 1:B:23:TYR:HD1 | 1:B:23:TYR:N | 0.56 | 1.98 | 3 | 5 |
| 1:A:49:VAL:N | 1:A:62:SER:O | 0.56 | 2.39 | 14 | 13 |
| 1:A:118:ALA:O | 1:A:122:ARG:HB2 | 0.56 | 2.01 | 2 | 4 |
| 1:B:173:GLY:CA | 1:B:178:CYS:O | 0.56 | 2.54 | 14 | 3 |
| 1:B:65:ASN:O | 1:B:68:ASP:HB2 | 0.56 | 2.01 | 7 | 4 |
| 1:A:89:LYS:CE | 1:A:155:ASP:OD1 | 0.56 | 2.53 | 10 | 1 |
| 1:B:20:ILE:HG13 | 1:B:95:ALA:HB2 | 0.56 | 1.76 | 4 | 1 |
| 1:B:42:ILE:HG22 | 1:B:68:ASP:H | 0.56 | 1.59 | 12 | 2 |
| 1:B:22:LYS:CG | 1:B:94:VAL:HG22 | 0.56 | 2.30 | 1 | 1 |
| 1:B:49:VAL:N | 1:B:62:SER:O | 0.56 | 2.39 | 14 | 14 |
| 1:B:149:ASN:O | 1:B:153:GLN:HG3 | 0.56 | 2.00 | 8 | 2 |
| 1:B:53:ASP:HB2 | 1:B:57:LYS:CG | 0.56 | 2.31 | 1 | 1 |
| 1:B:167:ILE:HD12 | 1:B:203:ILE:HD12 | 0.56 | 1.76 | 11 | 2 |
| 1:A:43:VAL:C | 1:A:66:GLN:HG3 | 0.56 | 2.19 | 17 | 1 |
| 1:B:166:LYS:HG2 | 1:B:202:THR:HG23 | 0.56 | 1.77 | 13 | 1 |
| 1:A:187:LEU:CD2 | 1:A:190:LEU:HD11 | 0.56 | 2.31 | 8 | 4 |
| 1:B:197:SER:O | 1:B:204:VAL:HB | 0.56 | 2.01 | 9 | 3 |
| 1:B:208:THR:O | 1:B:209:ARG:HB2 | 0.56 | 2.01 | 14 | 1 |
| 1:B:63:TYR:CD2 | 1:B:89:LYS:HD2 | 0.55 | 2.35 | 8 | 2 |
| 1:A:29:LEU:HD12 | 1:A:40:TYR:CD1 | 0.55 | 2.36 | 10 | 1 |
| 1:B:183:VAL:HG13 | 1:B:187:LEU:HD12 | 0.55 | 1.77 | 10 | 1 |
| 1:A:149:ASN:O | 1:A:153:GLN:HG3 | 0.55 | 2.01 | 8 | 2 |
| 1:B:20:ILE:HA | 1:B:94:VAL:O | 0.55 | 2.01 | 1 | 16 |
| 1:B:167:ILE:HD11 | 1:B:203:ILE:CD1 | 0.55 | 2.29 | 9 | 1 |
| 1:B:53:ASP:OD1 | 1:B:57:LYS:HB3 | 0.55 | 2.02 | 14 | 1 |
| 1:A:169:ARG:HB2 | 1:A:180:ARG:HB3 | 0.55 | 1.78 | 2 | 14 |
| 1:B:18:CYS:HB3 | 1:B:97:ILE:HG12 | 0.55 | 1.78 | 14 | 14 |
| 1:B:169:ARG:HB2 | 1:B:180:ARG:HB3 | 0.55 | 1.78 | 7 | 11 |
| 1:A:60:ILE:O | 1:A:174:GLN:HG3 | 0.55 | 2.01 | 3 | 3 |
| 1:B:198:ALA:HB2 | 1:B:203:ILE:HG12 | 0.55 | 1.78 | 12 | 4 |
| 1:A:51:ILE:HA | 1:A:84:ALA:HB1 | 0.55 | 1.76 | 15 | 3 |
| 1:B:180:ARG:O | 1:B:184:GLY:CA | 0.55 | 2.55 | 13 | 16 |
| 1:B:45:GLY:HA3 | 1:B:92:CYS:CB | 0.55 | 2.31 | 16 | 5 |
| 1:A:29:LEU:HD12 | 1:A:70:ILE:HG21 | 0.55 | 1.78 | 11 | 8 |
| 1:A:8:ASP:O | 1:A:12:GLU:HB2 | 0.55 | 2.01 | 4 | 1 |
| 1:B:28:THR:C | 1:B:29:LEU:HD23 | 0.55 | 2.22 | 12 | 14 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:47:VAL:HA | 1:A:89:LYS:N | 0.55 | 2.16 | 17 | 14 |
| 1:B:190:LEU:CD2 | 1:B:195:LEU:HB3 | 0.55 | 2.31 | 13 | 10 |
| 1:B:29:LEU:O | 1:B:30:ILE:HG13 | 0.55 | 2.01 | 6 | 5 |
| 1:B:41:TYR:CB | 1:B:95:ALA:HB3 | 0.55 | 2.31 | 15 | 8 |
| 1:A:114:MET:HA | 1:A:117:SER:OG | 0.55 | 2.02 | 12 | 6 |
| 1:A:121:ALA:HB1 | 1:B:77:GLU:HA | 0.55 | 1.76 | 18 | 4 |
| 1:B:124:LEU:HA | 1:B:128:SER:HB2 | 0.55 | 1.79 | 14 | 1 |
| 1:B:143:ILE:HG23 | 1:B:172:ILE:HG21 | 0.55 | 1.77 | 16 | 13 |
| 1:A:171:GLU:O | 1:A:175:ILE:HG13 | 0.55 | 2.02 | 10 | 4 |
| 1:B:143:ILE:HD13 | 1:B:186:ILE:HG12 | 0.55 | 1.79 | 10 | 2 |
| 1:A:76:PHE:HD2 | 1:A:120:MET:SD | 0.55 | 2.25 | 16 | 7 |
| 1:B:189:MET:SD | 1:B:195:LEU:HD13 | 0.55 | 2.42 | 7 | 3 |
| 1:A:164:GLN:HB3 | 1:A:204:VAL:CG2 | 0.55 | 2.32 | 20 | 7 |
| 1:B:11:LEU:O | 1:B:14:PHE:HB3 | 0.54 | 2.02 | 7 | 5 |
| 1:B:143:ILE:HD12 | 1:B:143:ILE:H | 0.54 | 1.62 | 10 | 1 |
| 1:A:24:PRO:HA | 1:A:91:ALA:HA | 0.54 | 1.78 | 12 | 7 |
| 1:A:42:ILE:CD1 | 1:A:47:VAL:HG13 | 0.54 | 2.32 | 8 | 6 |
| 1:A:39:LEU:HB2 | 1:A:75:LEU:HD22 | 0.54 | 1.78 | 13 | 1 |
| 1:B:20:ILE:HD13 | 1:B:95:ALA:CB | 0.54 | 2.32 | 13 | 6 |
| 1:A:139:VAL:HG23 | 1:A:176:VAL:HG11 | 0.54 | 1.78 | 14 | 3 |
| 1:A:99:TYR:HA | 1:A:102:PHE:HB3 | 0.54 | 1.79 | 20 | 11 |
| 1:A:20:ILE:HD13 | 1:A:95:ALA:CB | 0.54 | 2.31 | 16 | 8 |
| 1:A:159:HIS:CE1 | 1:A:161:ASP:HB3 | 0.54 | 2.37 | 18 | 4 |
| 1:A:105:LEU:HG | 1:A:106:ILE:N | 0.54 | 2.17 | 14 | 8 |
| 1:A:42:ILE:HD13 | 1:A:46:SER:HA | 0.54 | 1.79 | 2 | 1 |
| 1:A:52:LYS:O | 1:B:129:GLU:HA | 0.54 | 2.03 | 6 | 3 |
| 1:B:14:PHE:CD2 | 1:B:102:PHE:CE2 | 0.54 | 2.95 | 8 | 8 |
| 1:B:80:GLN:O | 1:B:81:GLU:HB2 | 0.54 | 2.03 | 7 | 8 |
| 1:A:28:THR:HA | 1:A:29:LEU:HD22 | 0.54 | 1.79 | 10 | 2 |
| 1:A:61:LEU:HD13 | 1:A:62:SER:N | 0.54 | 2.18 | 14 | 8 |
| 1:B:72:GLU:O | 1:B:76:PHE:HB3 | 0.54 | 2.03 | 4 | 4 |
| 1:B:8:ASP:O | 1:B:12:GLU:HB2 | 0.54 | 2.03 | 3 | 2 |
| 1:A:20:ILE:HG23 | 1:A:43:VAL:HG21 | 0.54 | 1.80 | 6 | 9 |
| 1:B:105:LEU:HG | 1:B:106:ILE:N | 0.54 | 2.17 | 14 | 7 |
| 1:A:142:ARG:O | 1:A:145:GLN:HB3 | 0.54 | 2.03 | 5 | 4 |
| 1:B:132:GLY:HA2 | 1:B:135:ALA:HB3 | 0.54 | 1.79 | 5 | 1 |
| 1:B:151:ALA:HA | 1:B:156:ALA:HB2 | 0.54 | 1.78 | 19 | 2 |
| 1:A:81:GLU:O | 1:A:82:ARG:HD2 | 0.54 | 2.02 | 14 | 1 |
| 1:B:150:LEU:CD1 | 1:B:167:ILE:HG12 | 0.54 | 2.33 | 15 | 4 |
| 1:A:138:ASP:OD2 | 1:A:142:ARG:HD3 | 0.54 | 2.03 | 11 | 1 |
| 1:B:19:HIS:HB3 | 1:B:96:GLU:O | 0.54 | 2.02 | 1 | 9 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:B:39:LEU:HD22 | 1:B:102:PHE:CD1 | 0.54 | 2.38 | 13 | 7 |
| 1:A:195:LEU:O | 1:A:209:ARG:HG3 | 0.54 | 2.02 | 12 | 4 |
| 1:B:29:LEU:HB3 | 1:B:40:TYR:CZ | 0.54 | 2.38 | 13 | 1 |
| 1:B:113:LEU:HD12 | 1:B:116:LEU:HD23 | 0.54 | 1.78 | 2 | 1 |
| 1:B:134:LEU:HD13 | 1:B:174:GLN:O | 0.54 | 2.03 | 7 | 1 |
| 1:A:197:SER:CB | 1:A:206:TYR:CE1 | 0.53 | 2.91 | 1 | 17 |
| 1:A:180:ARG:O | 1:A:184:GLY:CA | 0.53 | 2.56 | 10 | 17 |
| 1:B:41:TYR:O | 1:B:94:VAL:HA | 0.53 | 2.02 | 11 | 7 |
| 1:B:197:SER:CB | 1:B:206:TYR:CE1 | 0.53 | 2.91 | 1 | 16 |
| 1:B:45:GLY:HA3 | 1:B:92:CYS:HB3 | 0.53 | 1.80 | 10 | 15 |
| 1:B:22:LYS:H | 1:B:93:GLU:HA | 0.53 | 1.62 | 17 | 17 |
| 1:B:123:ARG:HA | 1:B:126:VAL:CG1 | 0.53 | 2.34 | 14 | 2 |
| 1:B:77:GLU:HG3 | 1:B:79:GLY:N | 0.53 | 2.19 | 6 | 5 |
| 1:A:11:LEU:O | 1:A:14:PHE:HB3 | 0.53 | 2.03 | 7 | 3 |
| 1:B:72:GLU:CB | 1:B:116:LEU:HD11 | 0.53 | 2.33 | 18 | 4 |
| 1:A:167:ILE:HD11 | 1:A:203:ILE:CD1 | 0.53 | 2.33 | 9 | 1 |
| 1:B:20:ILE:HG13 | 1:B:43:VAL:HG21 | 0.53 | 1.79 | 15 | 1 |
| 1:B:24:PRO:HA | 1:B:91:ALA:CA | 0.53 | 2.33 | 20 | 9 |
| 1:A:59:MET:HE3 | 1:A:174:GLN:HB2 | 0.53 | 1.79 | 3 | 4 |
| 1:A:183:VAL:O | 1:A:187:LEU:HG | 0.53 | 2.04 | 4 | 3 |
| 1:A:18:CYS:HB3 | 1:A:97:ILE:HG12 | 0.53 | 1.80 | 17 | 14 |
| 1:A:190:LEU:CD1 | 1:A:196:ILE:HD12 | 0.53 | 2.34 | 11 | 14 |
| 1:A:129:GLU:HA | 1:B:52:LYS:O | 0.53 | 2.03 | 6 | 2 |
| 1:A:29:LEU:HD23 | 1:A:86:VAL:HB | 0.53 | 1.79 | 13 | 1 |
| 1:B:156:ALA:HA | 1:B:164:GLN:O | 0.53 | 2.02 | 20 | 4 |
| 1:B:24:PRO:HA | 1:B:91:ALA:HA | 0.53 | 1.80 | 12 | 9 |
| 1:A:45:GLY:HA3 | 1:A:92:CYS:HB3 | 0.53 | 1.81 | 10 | 15 |
| 1:B:49:VAL:HG13 | 1:B:85:TRP:HA | 0.53 | 1.80 | 19 | 5 |
| 1:B:164:GLN:HG3 | 1:B:202:THR:HG22 | 0.53 | 1.81 | 19 | 2 |
| 1:A:174:GLN:HG2 | 1:A:175:ILE:N | 0.53 | 2.18 | 6 | 2 |
| 1:B:143:ILE:HG21 | 1:B:187:LEU:HD21 | 0.53 | 1.79 | 20 | 4 |
| 1:A:143:ILE:HG23 | 1:A:172:ILE:HG21 | 0.53 | 1.80 | 4 | 14 |
| 1:A:80:GLN:O | 1:A:81:GLU:HB2 | 0.53 | 2.03 | 5 | 8 |
| 1:A:180:ARG:HA | 1:A:183:VAL:HG12 | 0.53 | 1.80 | 20 | 6 |
| 1:A:198:ALA:HB2 | 1:A:203:ILE:HG12 | 0.53 | 1.80 | 8 | 3 |
| 1:B:171:GLU:HB3 | 1:B:175:ILE:HD12 | 0.53 | 1.79 | 7 | 1 |
| 1:A:31:HIS:HA | 1:A:82:ARG:HG3 | 0.53 | 1.80 | 17 | 6 |
| 1:A:106:ILE:HG22 | 1:A:112:ILE:HG21 | 0.53 | 1.81 | 7 | 7 |
| 1:A:134:LEU:HB3 | 1:A:175:ILE:O | 0.53 | 2.04 | 9 | 1 |
| 1:B:42:ILE:O | 1:B:42:ILE:HG12 | 0.53 | 2.02 | 5 | 1 |
| 1:A:45:GLY:HA3 | 1:A:92:CYS:CB | 0.53 | 2.34 | 16 | 7 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:41:TYR:O | 1:A:94:VAL:HA | 0.53 | 2.03 | 11 | 6 |
| 1:B:32:GLN:H | 1:B:82:ARG:HG3 | 0.53 | 1.64 | 6 | 2 |
| 1:A:29:LEU:N | 1:A:29:LEU:HD22 | 0.53 | 2.19 | 10 | 2 |
| 1:B:42:ILE:O | 1:B:67:GLY:HA2 | 0.53 | 2.03 | 2 | 1 |
| 1:B:41:TYR:O | 1:B:43:VAL:HG13 | 0.53 | 2.04 | 5 | 3 |
| 1:B:123:ARG:HD3 | 1:B:123:ARG:N | 0.53 | 2.19 | 20 | 1 |
| 1:A:119:GLN:O | 1:A:123:ARG:HD3 | 0.52 | 2.05 | 2 | 8 |
| 1:B:126:VAL:O | 1:B:130:LYS:HB2 | 0.52 | 2.04 | 13 | 1 |
| 1:B:183:VAL:HG13 | 1:B:187:LEU:CD1 | 0.52 | 2.34 | 10 | 1 |
| 1:B:11:LEU:HD11 | 1:B:41:TYR:OH | 0.52 | 2.04 | 19 | 1 |
| 1:A:48:ALA:HB1 | 1:A:60:ILE:HG21 | 0.52 | 1.81 | 4 | 1 |
| 1:B:23:TYR:O | 1:B:91:ALA:HA | 0.52 | 2.05 | 1 | 8 |
| 1:B:22:LYS:CB | 1:B:92:CYS:O | 0.52 | 2.51 | 12 | 1 |
| 1:B:165:ILE:HD12 | 1:B:165:ILE:O | 0.52 | 2.04 | 20 | 1 |
| 1:B:179:SER:C | 1:B:181:GLU:N | 0.52 | 2.61 | 14 | 19 |
| 1:A:196:ILE:CD1 | 1:A:203:ILE:HG23 | 0.52 | 2.35 | 13 | 1 |
| 1:B:139:VAL:HG22 | 1:B:143:ILE:HD11 | 0.52 | 1.81 | 20 | 1 |
| 1:A:73:LEU:HD23 | 1:A:120:MET:SD | 0.52 | 2.44 | 11 | 1 |
| 1:B:138:ASP:CG | 1:B:138:ASP:O | 0.52 | 2.48 | 12 | 1 |
| 1:A:39:LEU:HD11 | 1:A:41:TYR:CE1 | 0.52 | 2.39 | 7 | 1 |
| 1:A:100:LYS:O | 1:A:103:ARG:HG2 | 0.52 | 2.04 | 19 | 1 |
| 1:A:22:LYS:N | 1:A:93:GLU:HA | 0.52 | 2.19 | 2 | 10 |
| 1:A:29:LEU:CD1 | 1:A:70:ILE:HG21 | 0.52 | 2.34 | 19 | 6 |
| 1:B:20:ILE:HD12 | 1:B:43:VAL:HG21 | 0.52 | 1.81 | 9 | 2 |
| 1:B:30:ILE:O | 1:B:86:VAL:HG23 | 0.52 | 2.05 | 2 | 1 |
| 1:A:121:ALA:CB | 1:B:77:GLU:HA | 0.52 | 2.35 | 18 | 1 |
| 1:A:138:ASP:CG | 1:A:138:ASP:O | 0.52 | 2.48 | 20 | 1 |
| 1:B:23:TYR:CB | 1:B:24:PRO:HD2 | 0.52 | 2.34 | 10 | 7 |
| 1:B:25:SER:HB3 | 1:B:90:THR:N | 0.52 | 2.20 | 4 | 2 |
| 1:B:106:ILE:HG22 | 1:B:112:ILE:HG22 | 0.52 | 1.80 | 17 | 6 |
| 1:B:32:GLN:N | 1:B:82:ARG:HG3 | 0.52 | 2.19 | 17 | 3 |
| 1:B:76:PHE:HD2 | 1:B:120:MET:SD | 0.52 | 2.28 | 11 | 6 |
| 1:A:29:LEU:CD2 | 1:A:29:LEU:N | 0.52 | 2.73 | 18 | 9 |
| 1:B:60:ILE:HB | 1:B:174:GLN:CD | 0.52 | 2.25 | 7 | 5 |
| 1:B:76:PHE:CD2 | 1:B:120:MET:SD | 0.52 | 3.03 | 12 | 3 |
| 1:B:196:ILE:CD1 | 1:B:203:ILE:HG23 | 0.52 | 2.34 | 13 | 1 |
| 1:A:14:PHE:C | 1:A:14:PHE:CD1 | 0.52 | 2.83 | 10 | 3 |
| 1:B:134:LEU:HD22 | 1:B:176:VAL:HA | 0.52 | 1.80 | 10 | 1 |
| 1:A:166:LYS:HG3 | 1:A:201:LYS:HB3 | 0.52 | 1.82 | 4 | 1 |
| 1:A:124:LEU:HA | 1:A:128:SER:HB2 | 0.52 | 1.82 | 14 | 1 |
| 1:B:173:GLY:HA3 | 1:B:178:CYS:O | 0.52 | 2.05 | 14 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:138:ASP:O | 1:A:140:THR:N | 0.52 | 2.43 | 8 | 10 |
| 1:A:49:VAL:HG13 | 1:A:85:TRP:HA | 0.52 | 1.81 | 19 | 5 |
| 1:A:65:ASN:O | 1:A:68:ASP:HB2 | 0.52 | 2.05 | 7 | 3 |
| 1:A:142:ARG:O | 1:A:145:GLN:HB2 | 0.52 | 2.04 | 13 | 1 |
| 1:A:15:LEU:HD21 | 1:A:41:TYR:CE2 | 0.52 | 2.40 | 10 | 2 |
| 1:A:23:TYR:HD2 | 1:A:27:SER:CB | 0.52 | 2.17 | 14 | 5 |
| 1:A:124:LEU:HG | 1:B:124:LEU:HD23 | 0.52 | 1.81 | 20 | 1 |
| 1:B:138:ASP:O | 1:B:140:THR:N | 0.51 | 2.44 | 10 | 11 |
| 1:A:44:LYS:HA | 1:A:66:GLN:CD | 0.51 | 2.24 | 17 | 1 |
| 1:B:102:PHE:CE2 | 1:B:106:ILE:HG23 | 0.51 | 2.40 | 17 | 2 |
| 1:B:48:ALA:O | 1:B:87:ARG:HB3 | 0.51 | 2.05 | 15 | 2 |
| 1:A:135:ALA:HA | 1:B:135:ALA:HA | 0.51 | 1.83 | 5 | 1 |
| 1:B:29:LEU:N | 1:B:29:LEU:CD2 | 0.51 | 2.72 | 1 | 6 |
| 1:A:178:CYS:SG | 1:A:183:VAL:HB | 0.51 | 2.44 | 17 | 1 |
| 1:A:197:SER:HB3 | 1:A:206:TYR:CE1 | 0.51 | 2.40 | 13 | 3 |
| 1:A:162:GLY:HA3 | 1:A:204:VAL:CG2 | 0.51 | 2.35 | 2 | 1 |
| 1:A:14:PHE:CD2 | 1:A:102:PHE:CE2 | 0.51 | 2.97 | 3 | 7 |
| 1:B:36:ALA:CB | 1:B:74:GLY:HA3 | 0.51 | 2.34 | 7 | 10 |
| 1:A:96:GLU:O | 1:A:96:GLU:HG3 | 0.51 | 2.05 | 17 | 1 |
| 1:B:50:LEU:HB2 | 1:B:59:MET:O | 0.51 | 2.05 | 11 | 6 |
| 1:B:22:LYS:NZ | 1:B:29:LEU:HD11 | 0.51 | 2.21 | 13 | 1 |
| 1:A:47:VAL:HA | 1:A:89:LYS:CB | 0.51 | 2.35 | 12 | 4 |
| 1:A:51:ILE:HD12 | 1:B:128:SER:HA | 0.51 | 1.81 | 4 | 1 |
| 1:A:42:ILE:HG12 | 1:A:42:ILE:O | 0.51 | 2.05 | 5 | 1 |
| 1:A:33:GLY:HA2 | 1:A:82:ARG:HB3 | 0.51 | 1.82 | 19 | 2 |
| 1:B:179:SER:O | 1:B:181:GLU:N | 0.51 | 2.32 | 1 | 10 |
| 1:A:36:ALA:CB | 1:A:74:GLY:HA3 | 0.51 | 2.35 | 7 | 12 |
| 1:B:43:VAL:C | 1:B:66:GLN:HG3 | 0.51 | 2.23 | 17 | 1 |
| 1:B:51:ILE:HA | 1:B:84:ALA:HB1 | 0.51 | 1.81 | 2 | 5 |
| 1:B:47:VAL:HA | 1:B:89:LYS:CB | 0.51 | 2.35 | 12 | 3 |
| 1:B:193:GLN:HG2 | 1:B:197:SER:OG | 0.51 | 2.05 | 19 | 1 |
| 1:B:106:ILE:HG22 | 1:B:112:ILE:HG21 | 0.51 | 1.82 | 2 | 8 |
| 1:B:30:ILE:HD12 | 1:B:86:VAL:HG23 | 0.51 | 1.81 | 4 | 4 |
| 1:A:165:ILE:O | 1:A:165:ILE:HD12 | 0.51 | 2.05 | 20 | 2 |
| 1:B:63:TYR:OH | 1:B:175:ILE:HD11 | 0.51 | 2.05 | 13 | 1 |
| 1:A:50:LEU:CB | 1:A:60:ILE:HA | 0.51 | 2.36 | 15 | 9 |
| 1:B:183:VAL:O | 1:B:187:LEU:HG | 0.51 | 2.05 | 4 | 4 |
| 1:B:139:VAL:CG2 | 1:B:183:VAL:HG23 | 0.51 | 2.36 | 20 | 2 |
| 1:B:25:SER:O | 1:B:26:LYS:CB | 0.51 | 2.59 | 19 | 15 |
| 1:B:146:THR:O | 1:B:149:ASN:HB3 | 0.51 | 2.06 | 17 | 2 |
| 1:B:47:VAL:CG2 | 1:B:64:LEU:HD12 | 0.51 | 2.35 | 6 | 3 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:B:167:ILE:HG13 | 1:B:203:ILE:HD12 | 0.51 | 1.81 | 14 | 1 |
| 1:B:187:LEU:N | 1:B:187:LEU:HD23 | 0.51 | 2.20 | 1 | 6 |
| 1:B:14:PHE:CE1 | 1:B:41:TYR:CD2 | 0.51 | 2.99 | 17 | 3 |
| 1:A:47:VAL:CG2 | 1:A:64:LEU:HD12 | 0.51 | 2.35 | 6 | 1 |
| 1:B:30:ILE:HG22 | 1:B:34:GLU:HB2 | 0.51 | 1.83 | 13 | 2 |
| 1:A:22:LYS:HE2 | 1:A:27:SER:OG | 0.51 | 2.06 | 10 | 1 |
| 1:A:22:LYS:HB3 | 1:A:92:CYS:C | 0.51 | 2.26 | 2 | 4 |
| 1:A:72:GLU:HB2 | 1:A:120:MET:CE | 0.51 | 2.36 | 5 | 2 |
| 1:A:11:LEU:HD11 | 1:A:41:TYR:OH | 0.51 | 2.06 | 19 | 1 |
| 1:A:208:THR:O | 1:A:209:ARG:HB2 | 0.51 | 2.05 | 19 | 2 |
| 1:B:45:GLY:HA3 | 1:B:92:CYS:HA | 0.51 | 1.83 | 20 | 8 |
| 1:A:153:GLN:HB3 | 1:A:154:PRO:HD2 | 0.51 | 1.83 | 15 | 15 |
| 1:A:78:GLU:HB3 | 1:B:122:ARG:NH2 | 0.51 | 2.21 | 19 | 4 |
| 1:A:102:PHE:CZ | 1:A:106:ILE:HG21 | 0.51 | 2.41 | 15 | 7 |
| 1:A:109:ASN:OD1 | 1:A:112:ILE:HG13 | 0.51 | 2.06 | 19 | 2 |
| 1:B:109:ASN:CG | 1:B:112:ILE:HG13 | 0.51 | 2.25 | 14 | 1 |
| 1:B:31:HIS:HA | 1:B:82:ARG:HG3 | 0.51 | 1.83 | 15 | 5 |
| 1:A:61:LEU:HD22 | 1:A:62:SER:HB2 | 0.51 | 1.81 | 10 | 6 |
| 1:A:139:VAL:CG2 | 1:A:183:VAL:HG23 | 0.51 | 2.36 | 4 | 4 |
| 1:B:14:PHE:C | 1:B:14:PHE:CD1 | 0.51 | 2.85 | 7 | 2 |
| 1:B:164:GLN:HB3 | 1:B:204:VAL:CG2 | 0.50 | 2.36 | 1 | 6 |
| 1:B:82:ARG:CG | 1:B:83:SER:N | 0.50 | 2.73 | 12 | 17 |
| 1:B:166:LYS:CA | 1:B:202:THR:HA | 0.50 | 2.36 | 4 | 7 |
| 1:B:29:LEU:HB2 | 1:B:86:VAL:HB | 0.50 | 1.83 | 10 | 2 |
| 1:B:14:PHE:CD1 | 1:B:15:LEU:HD23 | 0.50 | 2.42 | 19 | 6 |
| 1:A:169:ARG:HG3 | 1:A:180:ARG:HB3 | 0.50 | 1.83 | 20 | 1 |
| 1:B:60:ILE:HG21 | 1:B:63:TYR:CE2 | 0.50 | 2.41 | 1 | 9 |
| 1:A:179:SER:C | 1:A:181:GLU:N | 0.50 | 2.65 | 13 | 19 |
| 1:A:150:LEU:CD1 | 1:A:167:ILE:HG12 | 0.50 | 2.35 | 4 | 7 |
| 1:B:29:LEU:HD22 | 1:B:29:LEU:N | 0.50 | 2.20 | 13 | 1 |
| 1:A:60:ILE:HD11 | 1:A:87:ARG:NH1 | 0.50 | 2.21 | 2 | 1 |
| 1:A:166:LYS:O | 1:A:166:LYS:HD3 | 0.50 | 2.06 | 7 | 1 |
| 1:A:29:LEU:N | 1:A:29:LEU:CD2 | 0.50 | 2.74 | 10 | 6 |
| 1:A:82:ARG:CG | 1:A:83:SER:N | 0.50 | 2.74 | 5 | 18 |
| 1:B:123:ARG:CA | 1:B:126:VAL:HG12 | 0.50 | 2.36 | 3 | 4 |
| 1:A:205:VAL:HG12 | 1:A:209:ARG:OXT | 0.50 | 2.07 | 5 | 2 |
| 1:A:29:LEU:HB3 | 1:A:40:TYR:CZ | 0.50 | 2.41 | 13 | 1 |
| 1:A:191:GLU:HG2 | 1:A:198:ALA:O | 0.50 | 2.06 | 9 | 1 |
| 1:A:166:LYS:HG2 | 1:A:202:THR:HG23 | 0.50 | 1.83 | 20 | 2 |
| 1:A:106:ILE:CD1 | 1:A:113:LEU:HD22 | 0.50 | 2.36 | 19 | 1 |
| 1:B:121:ALA:O | 1:B:124:LEU:HB2 | 0.50 | 2.06 | 18 | 3 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:50:LEU:HB2 | 1:A:59:MET:C | 0.50 | 2.27 | 15 | 11 |
| 1:B:73:LEU:HD23 | 1:B:120:MET:SD | 0.50 | 2.46 | 11 | 1 |
| 1:A:77:GLU:HA | 1:B:121:ALA:CB | 0.50 | 2.34 | 18 | 1 |
| 1:A:103:ARG:HA | 1:A:106:ILE:HG12 | 0.50 | 1.83 | 4 | 7 |
| 1:B:18:CYS:HB3 | 1:B:97:ILE:CD1 | 0.50 | 2.37 | 20 | 8 |
| 1:B:60:ILE:O | 1:B:174:GLN:HG3 | 0.50 | 2.07 | 15 | 4 |
| 1:A:14:PHE:CD1 | 1:A:14:PHE:C | 0.50 | 2.85 | 13 | 3 |
| 1:B:143:ILE:HG12 | 1:B:183:VAL:CG2 | 0.50 | 2.36 | 11 | 1 |
| 1:A:69:PHE:CD1 | 1:A:116:LEU:HD13 | 0.50 | 2.41 | 2 | 1 |
| 1:A:146:THR:HG21 | 1:A:175:ILE:HG23 | 0.50 | 1.84 | 7 | 1 |
| 1:B:72:GLU:HA | 1:B:75:LEU:HD23 | 0.50 | 1.82 | 8 | 6 |
| 1:B:50:LEU:HB2 | 1:B:59:MET:C | 0.50 | 2.27 | 20 | 14 |
| 1:A:23:TYR:CB | 1:A:24:PRO:HD2 | 0.50 | 2.36 | 10 | 7 |
| 1:A:11:LEU:HD23 | 1:A:14:PHE:HB3 | 0.50 | 1.84 | 9 | 4 |
| 1:A:166:LYS:HB3 | 1:A:202:THR:HA | 0.50 | 1.82 | 20 | 2 |
| 1:B:42:ILE:CD1 | 1:B:46:SER:HA | 0.50 | 2.35 | 4 | 3 |
| 1:A:164:GLN:HB2 | 1:A:202:THR:HG22 | 0.50 | 1.84 | 12 | 1 |
| 1:B:146:THR:HG21 | 1:B:175:ILE:HG23 | 0.50 | 1.81 | 7 | 1 |
| 1:B:81:GLU:O | 1:B:82:ARG:HD2 | 0.50 | 2.06 | 14 | 1 |
| 1:A:75:LEU:CB | 1:A:99:TYR:CD2 | 0.50 | 2.95 | 11 | 9 |
| 1:A:196:ILE:CG2 | 1:A:197:SER:H | 0.50 | 2.17 | 18 | 7 |
| 1:A:124:LEU:HG | 1:B:124:LEU:CD2 | 0.50 | 2.37 | 20 | 3 |
| 1:A:129:GLU:O | 1:A:130:LYS:HG2 | 0.50 | 2.07 | 6 | 1 |
| 1:B:23:TYR:CD2 | 1:B:27:SER:HB3 | 0.50 | 2.42 | 6 | 2 |
| 1:A:143:ILE:H | 1:A:143:ILE:HD12 | 0.50 | 1.64 | 10 | 1 |
| 1:A:42:ILE:HG12 | 1:A:94:VAL:HG12 | 0.50 | 1.84 | 2 | 1 |
| 1:B:187:LEU:CD2 | 1:B:190:LEU:HD11 | 0.50 | 2.35 | 9 | 4 |
| 1:B:11:LEU:HD23 | 1:B:14:PHE:HB3 | 0.50 | 1.84 | 19 | 2 |
| 1:A:187:LEU:HA | 1:A:190:LEU:CG | 0.50 | 2.37 | 8 | 1 |
| 1:A:104:GLN:O | 1:A:107:GLN:HG2 | 0.50 | 2.06 | 19 | 1 |
| 1:B:33:GLY:HA2 | 1:B:82:ARG:HB3 | 0.50 | 1.83 | 19 | 1 |
| 1:A:186:ILE:HA | 1:A:189:MET:HG2 | 0.50 | 1.84 | 17 | 1 |
| 1:B:55:GLU:OE1 | 1:B:57:LYS:HB2 | 0.50 | 2.06 | 20 | 3 |
| 1:A:89:LYS:HE2 | 1:A:155:ASP:OD1 | 0.50 | 2.07 | 10 | 1 |
| 1:B:50:LEU:HB3 | 1:B:60:ILE:HA | 0.50 | 1.83 | 10 | 2 |
| 1:B:14:PHE:CD1 | 1:B:14:PHE:C | 0.50 | 2.84 | 9 | 3 |
| 1:A:42:ILE:CD1 | 1:A:46:SER:HA | 0.50 | 2.36 | 5 | 3 |
| 1:B:166:LYS:HA | 1:B:202:THR:HA | 0.49 | 1.84 | 6 | 13 |
| 1:A:169:ARG:HB2 | 1:A:180:ARG:CB | 0.49 | 2.37 | 11 | 7 |
| 1:B:103:ARG:HA | 1:B:106:ILE:HG12 | 0.49 | 1.83 | 4 | 7 |
| 1:B:171:GLU:O | 1:B:175:ILE:HG13 | 0.49 | 2.07 | 10 | 2 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:11:LEU:HD12 | 1:A:15:LEU:CG | 0.49 | 2.38 | 4 | 2 |
| 1:A:196:ILE:HG12 | 1:A:209:ARG:OXT | 0.49 | 2.07 | 7 | 2 |
| 1:A:11:LEU:C | 1:A:13:TRP:H | 0.49 | 2.10 | 20 | 1 |
| 1:A:50:LEU:HB2 | 1:A:59:MET:O | 0.49 | 2.08 | 11 | 5 |
| 1:B:196:ILE:CG2 | 1:B:197:SER:H | 0.49 | 2.16 | 6 | 6 |
| 1:A:31:HIS:CE1 | 1:A:58:GLU:HB2 | 0.49 | 2.42 | 4 | 4 |
| 1:B:47:VAL:HG21 | 1:B:86:VAL:HG12 | 0.49 | 1.83 | 2 | 2 |
| 1:A:128:SER:HB3 | 1:B:51:ILE:CG2 | 0.49 | 2.35 | 5 | 5 |
| 1:B:109:ASN:OD1 | 1:B:112:ILE:HG13 | 0.49 | 2.07 | 19 | 2 |
| 1:A:60:ILE:HG21 | 1:A:63:TYR:CE2 | 0.49 | 2.43 | 16 | 4 |
| 1:B:29:LEU:CD2 | 1:B:29:LEU:N | 0.49 | 2.73 | 17 | 6 |
| 1:B:147:LEU:O | 1:B:150:LEU:HB2 | 0.49 | 2.07 | 20 | 3 |
| 1:B:50:LEU:HA | 1:B:61:LEU:HD12 | 0.49 | 1.84 | 11 | 1 |
| 1:B:61:LEU:HD13 | 1:B:62:SER:N | 0.49 | 2.22 | 15 | 6 |
| 1:A:15:LEU:HA | 1:A:18:CYS:HG | 0.49 | 1.66 | 5 | 2 |
| 1:A:166:LYS:HA | 1:A:202:THR:HA | 0.49 | 1.83 | 12 | 11 |
| 1:B:102:PHE:CZ | 1:B:106:ILE:HG21 | 0.49 | 2.43 | 9 | 7 |
| 1:A:164:GLN:HG3 | 1:A:202:THR:HG22 | 0.49 | 1.83 | 14 | 3 |
| 1:A:25:SER:O | 1:A:26:LYS:CB | 0.49 | 2.60 | 19 | 17 |
| 1:B:50:LEU:HB3 | 1:B:60:ILE:HD13 | 0.49 | 1.84 | 17 | 3 |
| 1:B:29:LEU:HD12 | 1:B:70:ILE:HG21 | 0.49 | 1.84 | 11 | 10 |
| 1:B:143:ILE:HD12 | 1:B:186:ILE:HB | 0.49 | 1.84 | 18 | 2 |
| 1:A:24:PRO:CA | 1:A:91:ALA:HB2 | 0.49 | 2.34 | 5 | 1 |
| 1:A:164:GLN:C | 1:A:165:ILE:HG13 | 0.49 | 2.28 | 12 | 10 |
| 1:B:42:ILE:CD1 | 1:B:47:VAL:HG13 | 0.49 | 2.37 | 13 | 5 |
| 1:A:144:ALA:HB2 | 1:A:195:LEU:CD2 | 0.49 | 2.37 | 18 | 4 |
| 1:A:120:MET:O | 1:A:123:ARG:HB2 | 0.49 | 2.07 | 16 | 2 |
| 1:B:117:SER:HA | 1:B:120:MET:HE3 | 0.49 | 1.85 | 4 | 1 |
| 1:B:22:LYS:HB3 | 1:B:92:CYS:C | 0.49 | 2.28 | 14 | 4 |
| 1:B:23:TYR:HD2 | 1:B:27:SER:CB | 0.49 | 2.20 | 14 | 3 |
| 1:A:50:LEU:HB3 | 1:A:60:ILE:HD13 | 0.49 | 1.84 | 6 | 3 |
| 1:A:190:LEU:HD13 | 1:A:196:ILE:CD1 | 0.49 | 2.37 | 13 | 2 |
| 1:A:41:TYR:HD1 | 1:A:68:ASP:O | 0.49 | 1.91 | 10 | 2 |
| 1:B:169:ARG:HG3 | 1:B:180:ARG:HB2 | 0.49 | 1.85 | 10 | 1 |
| 1:A:49:VAL:CA | 1:A:85:TRP:O | 0.49 | 2.59 | 16 | 2 |
| 1:B:103:ARG:HA | 1:B:106:ILE:HG13 | 0.49 | 1.85 | 13 | 9 |
| 1:B:64:LEU:HB3 | 1:B:68:ASP:CB | 0.49 | 2.37 | 2 | 2 |
| 1:A:146:THR:HG21 | 1:A:175:ILE:CG2 | 0.49 | 2.37 | 7 | 1 |
| 1:B:22:LYS:NZ | 1:B:88:ALA:HB2 | 0.49 | 2.23 | 18 | 2 |
| 1:B:101:LYS:O | 1:B:104:GLN:HG2 | 0.49 | 2.08 | 19 | 1 |
| 1:A:117:SER:HB3 | 1:B:76:PHE:CE2 | 0.49 | 2.43 | 14 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:135:ALA:HB1 | 1:B:135:ALA:HB1 | 0.49 | 1.84 | 1 | 2 |
| 1:B:75:LEU:CB | 1:B:99:TYR:CD2 | 0.49 | 2.95 | 6 | 11 |
| 1:A:41:TYR:CD1 | 1:A:41:TYR:C | 0.49 | 2.85 | 13 | 3 |
| 1:B:138:ASP:O | 1:B:142:ARG:CB | 0.49 | 2.60 | 7 | 1 |
| 1:B:143:ILE:CD1 | 1:B:183:VAL:HA | 0.49 | 2.37 | 18 | 1 |
| 1:A:40:TYR:HB2 | 1:A:70:ILE:HB | 0.49 | 1.83 | 20 | 1 |
| 1:A:135:ALA:CB | 1:B:135:ALA:HB3 | 0.49 | 2.36 | 6 | 2 |
| 1:A:14:PHE:O | 1:A:17:HIS:HB2 | 0.49 | 2.08 | 9 | 1 |
| 1:A:41:TYR:CE1 | 1:A:69:PHE:HD1 | 0.49 | 2.26 | 7 | 1 |
| 1:A:69:PHE:CG | 1:A:116:LEU:HD13 | 0.48 | 2.43 | 2 | 1 |
| 1:A:167:ILE:HG22 | 1:A:171:GLU:HG3 | 0.48 | 1.84 | 8 | 1 |
| 1:B:22:LYS:CG | 1:B:23:TYR:CD1 | 0.48 | 2.96 | 16 | 1 |
| 1:A:184:GLY:O | 1:A:188:LYS:HB2 | 0.48 | 2.08 | 6 | 5 |
| 1:B:22:LYS:N | 1:B:93:GLU:HA | 0.48 | 2.23 | 2 | 11 |
| 1:B:99:TYR:CD1 | 1:B:99:TYR:C | 0.48 | 2.86 | 20 | 7 |
| 1:A:32:GLN:N | 1:A:82:ARG:HG3 | 0.48 | 2.23 | 6 | 3 |
| 1:B:15:LEU:HD21 | 1:B:41:TYR:HE2 | 0.48 | 1.68 | 10 | 1 |
| 1:A:81:GLU:O | 1:A:82:ARG:HD3 | 0.48 | 2.09 | 2 | 3 |
| 1:A:166:LYS:C | 1:A:167:ILE:HG13 | 0.48 | 2.28 | 15 | 2 |
| 1:A:37:GLU:O | 1:A:99:TYR:CD1 | 0.48 | 2.66 | 19 | 1 |
| 1:A:14:PHE:CD1 | 1:A:15:LEU:HD23 | 0.48 | 2.43 | 19 | 7 |
| 1:A:102:PHE:CE2 | 1:A:106:ILE:CG2 | 0.48 | 2.96 | 3 | 4 |
| 1:A:157:MET:O | 1:A:163:MET:HB3 | 0.48 | 2.08 | 3 | 1 |
| 1:B:96:GLU:HG3 | 1:B:96:GLU:O | 0.48 | 2.09 | 17 | 2 |
| 1:B:143:ILE:CG2 | 1:B:187:LEU:HD21 | 0.48 | 2.38 | 5 | 4 |
| 1:A:47:VAL:CG1 | 1:A:88:ALA:HA | 0.48 | 2.38 | 12 | 1 |
| 1:B:180:ARG:HD2 | 1:B:181:GLU:OE2 | 0.48 | 2.07 | 12 | 1 |
| 1:B:31:HIS:HB2 | 1:B:84:ALA:HA | 0.48 | 1.84 | 14 | 1 |
| 1:A:54:GLU:HB2 | 1:B:133:ASN:OD1 | 0.48 | 2.07 | 1 | 1 |
| 1:A:51:ILE:HG21 | 1:B:128:SER:HB2 | 0.48 | 1.85 | 3 | 1 |
| 1:B:140:THR:O | 1:B:142:ARG:N | 0.48 | 2.46 | 3 | 1 |
| 1:A:39:LEU:HD22 | 1:A:102:PHE:CD1 | 0.48 | 2.43 | 20 | 6 |
| 1:A:33:GLY:N | 1:A:82:ARG:HD2 | 0.48 | 2.24 | 10 | 1 |
| 1:B:18:CYS:HA | 1:B:97:ILE:HG23 | 0.48 | 1.84 | 10 | 1 |
| 1:B:11:LEU:HD23 | 1:B:14:PHE:CG | 0.48 | 2.44 | 9 | 1 |
| 1:B:143:ILE:HD13 | 1:B:186:ILE:CG1 | 0.48 | 2.38 | 20 | 1 |
| 1:B:76:PHE:CD1 | 1:B:120:MET:HE1 | 0.48 | 2.44 | 14 | 1 |
| 1:B:143:ILE:HD13 | 1:B:186:ILE:HG13 | 0.48 | 1.85 | 1 | 1 |
| 1:B:143:ILE:HD13 | 1:B:183:VAL:HA | 0.48 | 1.85 | 18 | 2 |
| 1:B:156:ALA:HA | 1:B:165:ILE:HG23 | 0.48 | 1.84 | 20 | 2 |
| 1:B:169:ARG:CA | 1:B:187:LEU:HD12 | 0.48 | 2.38 | 11 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:121:ALA:O | 1:A:124:LEU:HB2 | 0.48 | 2.07 | 18 | 2 |
| 1:A:130:LYS:HG3 | 1:A:133:ASN:OD1 | 0.48 | 2.08 | 19 | 1 |
| 1:A:103:ARG:HA | 1:A:106:ILE:HG13 | 0.48 | 1.85 | 17 | 8 |
| 1:A:34:GLU:OE2 | 1:A:82:ARG:HB2 | 0.48 | 2.08 | 17 | 5 |
| 1:A:18:CYS:HA | 1:A:97:ILE:HG23 | 0.48 | 1.84 | 10 | 3 |
| 1:A:103:ARG:O | 1:A:107:GLN:HG2 | 0.48 | 2.09 | 18 | 1 |
| 1:B:99:TYR:C | 1:B:99:TYR:CD1 | 0.48 | 2.87 | 6 | 6 |
| 1:B:164:GLN:C | 1:B:165:ILE:HG13 | 0.48 | 2.29 | 12 | 9 |
| 1:B:39:LEU:HG | 1:B:40:TYR:N | 0.48 | 2.24 | 3 | 3 |
| 1:A:23:TYR:O | 1:A:91:ALA:HA | 0.48 | 2.08 | 5 | 7 |
| 1:B:118:ALA:O | 1:B:122:ARG:HB2 | 0.48 | 2.08 | 2 | 4 |
| 1:B:48:ALA:CB | 1:B:60:ILE:HD12 | 0.48 | 2.37 | 8 | 3 |
| 1:A:166:LYS:HB3 | 1:A:202:THR:HG23 | 0.48 | 1.86 | 10 | 1 |
| 1:A:156:ALA:HA | 1:A:165:ILE:HG23 | 0.48 | 1.85 | 20 | 4 |
| 1:A:169:ARG:HG3 | 1:A:180:ARG:CB | 0.48 | 2.39 | 20 | 1 |
| 1:A:147:LEU:CD2 | 1:A:167:ILE:HD11 | 0.48 | 2.39 | 19 | 2 |
| 1:A:124:LEU:HA | 1:A:128:SER:CB | 0.48 | 2.38 | 14 | 1 |
| 1:A:190:LEU:CD2 | 1:A:195:LEU:HB3 | 0.48 | 2.39 | 14 | 6 |
| 1:A:122:ARG:CZ | 1:B:78:GLU:HB3 | 0.48 | 2.38 | 20 | 3 |
| 1:A:143:ILE:CG2 | 1:A:187:LEU:HD21 | 0.48 | 2.38 | 8 | 2 |
| 1:B:77:GLU:O | 1:B:78:GLU:HB2 | 0.48 | 2.09 | 14 | 1 |
| 1:A:99:TYR:C | 1:A:99:TYR:CD1 | 0.48 | 2.87 | 3 | 7 |
| 1:B:106:ILE:HD13 | 1:B:113:LEU:HD22 | 0.48 | 1.85 | 15 | 3 |
| 1:A:124:LEU:HG | 1:B:124:LEU:HG | 0.48 | 1.86 | 13 | 4 |
| 1:A:109:ASN:CB | 1:A:112:ILE:HG13 | 0.48 | 2.39 | 11 | 2 |
| 1:A:173:GLY:HA3 | 1:A:178:CYS:O | 0.48 | 2.09 | 14 | 1 |
| 1:A:166:LYS:HA | 1:A:201:LYS:O | 0.47 | 2.10 | 10 | 4 |
| 1:A:11:LEU:HD23 | 1:A:14:PHE:CG | 0.47 | 2.44 | 14 | 4 |
| 1:B:143:ILE:CG1 | 1:B:183:VAL:HG22 | 0.47 | 2.38 | 10 | 1 |
| 1:A:42:ILE:HB | 1:A:68:ASP:O | 0.47 | 2.09 | 2 | 1 |
| 1:B:117:SER:HA | 1:B:120:MET:HE2 | 0.47 | 1.86 | 12 | 1 |
| 1:B:51:ILE:CD1 | 1:B:61:LEU:HB3 | 0.47 | 2.39 | 18 | 1 |
| 1:A:109:ASN:CG | 1:A:112:ILE:HG13 | 0.47 | 2.29 | 14 | 1 |
| 1:A:54:GLU:OE1 | 1:B:130:LYS:HE3 | 0.47 | 2.09 | 15 | 1 |
| 1:A:147:LEU:O | 1:A:150:LEU:HB2 | 0.47 | 2.09 | 20 | 4 |
| 1:A:45:GLY:HA3 | 1:A:92:CYS:HA | 0.47 | 1.85 | 20 | 6 |
| 1:B:143:ILE:HD12 | 1:B:186:ILE:CB | 0.47 | 2.39 | 18 | 2 |
| 1:B:33:GLY:H | 1:B:82:ARG:HB2 | 0.47 | 1.68 | 14 | 1 |
| 1:B:8:ASP:O | 1:B:12:GLU:HG2 | 0.47 | 2.09 | 1 | 1 |
| 1:B:28:THR:HB | 1:B:87:ARG:HA | 0.47 | 1.85 | 17 | 4 |
| 1:A:23:TYR:CD2 | 1:A:27:SER:HB3 | 0.47 | 2.44 | 6 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:B:187:LEU:HD23 | 1:B:187:LEU:N | 0.47 | 2.25 | 20 | 2 |
| 1:B:69:PHE:CB | 1:B:116:LEU:HD12 | 0.47 | 2.39 | 9 | 3 |
| 1:B:138:ASP:OD2 | 1:B:142:ARG:HD3 | 0.47 | 2.09 | 11 | 1 |
| 1:B:14:PHE:CE1 | 1:B:41:TYR:HD2 | 0.47 | 2.27 | 2 | 1 |
| 1:A:51:ILE:HD13 | 1:A:51:ILE:H | 0.47 | 1.69 | 7 | 1 |
| 1:A:109:ASN:HB2 | 1:A:112:ILE:HG13 | 0.47 | 1.86 | 13 | 11 |
| 1:B:75:LEU:CB | 1:B:99:TYR:HD2 | 0.47 | 2.22 | 20 | 2 |
| 1:A:76:PHE:CE1 | 1:B:117:SER:HB2 | 0.47 | 2.45 | 10 | 1 |
| 1:A:27:SER:N | 1:A:88:ALA:HB3 | 0.47 | 2.25 | 14 | 4 |
| 1:B:134:LEU:HB3 | 1:B:175:ILE:O | 0.47 | 2.09 | 9 | 1 |
| 1:B:166:LYS:HB3 | 1:B:202:THR:HG23 | 0.47 | 1.87 | 5 | 1 |
| 1:B:102:PHE:O | 1:B:106:ILE:HG23 | 0.47 | 2.08 | 19 | 1 |
| 1:B:33:GLY:HA2 | 1:B:82:ARG:CB | 0.47 | 2.39 | 14 | 1 |
| 1:B:153:GLN:HB3 | 1:B:154:PRO:HD2 | 0.47 | 1.85 | 17 | 15 |
| 1:A:123:ARG:N | 1:A:123:ARG:HD3 | 0.47 | 2.23 | 7 | 1 |
| 1:A:190:LEU:HD23 | 1:A:195:LEU:HB3 | 0.47 | 1.85 | 19 | 2 |
| 1:B:147:LEU:HD21 | 1:B:203:ILE:HG21 | 0.47 | 1.86 | 14 | 1 |
| 1:B:169:ARG:HB2 | 1:B:180:ARG:CB | 0.47 | 2.39 | 11 | 5 |
| 1:A:179:SER:O | 1:A:181:GLU:N | 0.47 | 2.48 | 13 | 8 |
| 1:A:27:SER:H | 1:A:88:ALA:HB3 | 0.47 | 1.70 | 14 | 3 |
| 1:A:99:TYR:CD1 | 1:A:99:TYR:C | 0.47 | 2.88 | 5 | 5 |
| 1:A:14:PHE:CE1 | 1:A:41:TYR:HD2 | 0.47 | 2.27 | 2 | 3 |
| 1:A:76:PHE:CD2 | 1:A:120:MET:SD | 0.47 | 3.08 | 16 | 5 |
| 1:A:64:LEU:HD13 | 1:A:68:ASP:HB3 | 0.47 | 1.84 | 10 | 1 |
| 1:B:122:ARG:O | 1:B:125:GLN:HG2 | 0.47 | 2.08 | 11 | 1 |
| 1:A:150:LEU:HB3 | 1:A:165:ILE:HG21 | 0.47 | 1.86 | 9 | 3 |
| 1:B:69:PHE:CD1 | 1:B:116:LEU:HD13 | 0.47 | 2.45 | 2 | 1 |
| 1:A:46:SER:HB2 | 1:A:64:LEU:O | 0.47 | 2.09 | 12 | 1 |
| 1:A:157:MET:O | 1:A:163:MET:CA | 0.47 | 2.63 | 8 | 1 |
| 1:A:141:GLY:O | 1:A:145:GLN:CB | 0.47 | 2.63 | 14 | 1 |
| 1:B:147:LEU:CD2 | 1:B:167:ILE:HD11 | 0.47 | 2.40 | 14 | 1 |
| 1:A:20:ILE:HD12 | 1:A:43:VAL:HG21 | 0.47 | 1.86 | 11 | 3 |
| 1:B:76:PHE:CE2 | 1:B:120:MET:HE3 | 0.47 | 2.45 | 2 | 1 |
| 1:A:167:ILE:HD11 | 1:A:203:ILE:HD12 | 0.47 | 1.86 | 9 | 1 |
| 1:A:22:LYS:NZ | 1:A:88:ALA:HB2 | 0.47 | 2.25 | 9 | 3 |
| 1:A:164:GLN:OE1 | 1:A:202:THR:HB | 0.47 | 2.10 | 19 | 1 |
| 1:B:15:LEU:HA | 1:B:18:CYS:HG | 0.47 | 1.69 | 8 | 4 |
| 1:A:61:LEU:HD22 | 1:A:61:LEU:C | 0.47 | 2.30 | 12 | 5 |
| 1:A:60:ILE:HB | 1:A:174:GLN:NE2 | 0.47 | 2.25 | 3 | 2 |
| 1:A:41:TYR:C | 1:A:41:TYR:CD1 | 0.47 | 2.88 | 14 | 3 |
| 1:A:180:ARG:HD2 | 1:A:181:GLU:OE1 | 0.47 | 2.10 | 4 | 3 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:14:PHE:CE1 | 1:A:41:TYR:CD2 | 0.47 | 3.03 | 1 | 6 |
| 1:B:45:GLY:HA3 | 1:B:92:CYS:CA | 0.47 | 2.39 | 16 | 3 |
| 1:B:157:MET:O | 1:B:163:MET:HB3 | 0.47 | 2.09 | 3 | 1 |
| 1:B:60:ILE:HB | 1:B:174:GLN:NE2 | 0.47 | 2.25 | 6 | 4 |
| 1:B:130:LYS:HA | 1:B:133:ASN:OD1 | 0.47 | 2.09 | 5 | 3 |
| 1:A:128:SER:O | 1:B:51:ILE:HG13 | 0.47 | 2.10 | 10 | 1 |
| 1:B:47:VAL:HB | 1:B:88:ALA:HA | 0.47 | 1.85 | 5 | 2 |
| 1:B:124:LEU:O | 1:B:128:SER:HB2 | 0.47 | 2.10 | 14 | 1 |
| 1:B:33:GLY:N | 1:B:82:ARG:HB2 | 0.47 | 2.25 | 14 | 1 |
| 1:A:51:ILE:CG2 | 1:B:128:SER:HB3 | 0.46 | 2.38 | 5 | 4 |
| 1:A:11:LEU:HD13 | 1:A:41:TYR:OH | 0.46 | 2.11 | 10 | 3 |
| 1:B:109:ASN:CB | 1:B:112:ILE:HG13 | 0.46 | 2.40 | 11 | 3 |
| 1:A:143:ILE:CD1 | 1:A:183:VAL:HG22 | 0.46 | 2.41 | 16 | 2 |
| 1:B:102:PHE:CE2 | 1:B:106:ILE:HG22 | 0.46 | 2.45 | 19 | 1 |
| 1:A:77:GLU:OE1 | 1:B:122:ARG:HD2 | 0.46 | 2.10 | 14 | 1 |
| 1:B:64:LEU:HA | 1:B:123:ARG:NH2 | 0.46 | 2.24 | 17 | 2 |
| 1:B:102:PHE:CE2 | 1:B:106:ILE:CG2 | 0.46 | 2.99 | 15 | 3 |
| 1:A:166:LYS:CA | 1:A:202:THR:HA | 0.46 | 2.40 | 4 | 4 |
| 1:B:23:TYR:HB3 | 1:B:24:PRO:HD2 | 0.46 | 1.86 | 13 | 1 |
| 1:B:76:PHE:CE2 | 1:B:116:LEU:HG | 0.46 | 2.45 | 2 | 1 |
| 1:B:178:CYS:SG | 1:B:182:THR:HB | 0.46 | 2.50 | 5 | 1 |
| 1:B:99:TYR:HD1 | 1:B:100:LYS:N | 0.46 | 2.08 | 20 | 1 |
| 1:B:61:LEU:HD22 | 1:B:61:LEU:C | 0.46 | 2.30 | 12 | 5 |
| 1:A:76:PHE:CE1 | 1:A:113:LEU:HD21 | 0.46 | 2.45 | 17 | 1 |
| 1:A:28:THR:CA | 1:A:29:LEU:HD22 | 0.46 | 2.40 | 10 | 1 |
| 1:B:25:SER:O | 1:B:26:LYS:CG | 0.46 | 2.63 | 10 | 1 |
| 1:A:25:SER:HB3 | 1:A:90:THR:N | 0.46 | 2.24 | 19 | 2 |
| 1:A:72:GLU:O | 1:A:76:PHE:HB3 | 0.46 | 2.10 | 12 | 1 |
| 1:A:143:ILE:HG23 | 1:A:172:ILE:CG2 | 0.46 | 2.40 | 8 | 1 |
| 1:B:41:TYR:CE1 | 1:B:69:PHE:HD1 | 0.46 | 2.29 | 7 | 1 |
| 1:A:39:LEU:HD22 | 1:A:102:PHE:CE1 | 0.46 | 2.45 | 20 | 1 |
| 1:B:30:ILE:HD12 | 1:B:86:VAL:HG21 | 0.46 | 1.86 | 1 | 1 |
| 1:B:22:LYS:HG3 | 1:B:94:VAL:CG2 | 0.46 | 2.39 | 19 | 2 |
| 1:A:18:CYS:HB3 | 1:A:97:ILE:CD1 | 0.46 | 2.41 | 13 | 5 |
| 1:A:32:GLN:OE1 | 1:A:32:GLN:HA | 0.46 | 2.09 | 4 | 2 |
| 1:B:96:GLU:O | 1:B:96:GLU:HG3 | 0.46 | 2.11 | 10 | 1 |
| 1:B:142:ARG:O | 1:B:145:GLN:HB3 | 0.46 | 2.10 | 4 | 4 |
| 1:B:103:ARG:C | 1:B:106:ILE:HG13 | 0.46 | 2.31 | 18 | 1 |
| 1:A:167:ILE:CD1 | 1:A:203:ILE:HD12 | 0.46 | 2.40 | 17 | 6 |
| 1:A:28:THR:CB | 1:A:87:ARG:HA | 0.46 | 2.41 | 17 | 2 |
| 1:A:14:PHE:CE2 | 1:A:102:PHE:CE1 | 0.46 | 3.04 | 10 | 2 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:64:LEU:HA | 1:A:123:ARG:NH2 | 0.46 | 2.26 | 10 | 3 |
| 1:A:15:LEU:HD22 | 1:A:20:ILE:CD1 | 0.46 | 2.40 | 11 | 2 |
| 1:A:96:GLU:O | 1:A:97:ILE:HG23 | 0.46 | 2.11 | 11 | 2 |
| 1:A:133:ASN:HD21 | 1:A:142:ARG:NH2 | 0.46 | 2.09 | 2 | 1 |
| 1:A:155:ASP:CB | 1:A:165:ILE:HG22 | 0.46 | 2.41 | 15 | 2 |
| 1:B:27:SER:N | 1:B:88:ALA:HB3 | 0.46 | 2.26 | 9 | 5 |
| 1:B:196:ILE:CG2 | 1:B:197:SER:N | 0.46 | 2.78 | 19 | 3 |
| 1:A:78:GLU:HB3 | 1:B:122:ARG:CZ | 0.46 | 2.40 | 9 | 1 |
| 1:B:187:LEU:HA | 1:B:190:LEU:CG | 0.46 | 2.41 | 9 | 1 |
| 1:B:50:LEU:O | 1:B:50:LEU:HD23 | 0.46 | 2.11 | 5 | 1 |
| 1:B:44:LYS:CE | 1:B:66:GLN:OE1 | 0.46 | 2.59 | 19 | 1 |
| 1:A:34:GLU:O | 1:A:82:ARG:HA | 0.46 | 2.11 | 14 | 1 |
| 1:A:41:TYR:CE2 | 1:A:69:PHE:CE1 | 0.46 | 3.04 | 16 | 4 |
| 1:B:109:ASN:HB2 | 1:B:112:ILE:HG13 | 0.46 | 1.87 | 18 | 9 |
| 1:A:122:ARG:HA | 1:B:77:GLU:OE2 | 0.46 | 2.11 | 8 | 1 |
| 1:B:143:ILE:O | 1:B:147:LEU:HD12 | 0.46 | 2.11 | 19 | 1 |
| 1:A:61:LEU:C | 1:A:61:LEU:HD22 | 0.46 | 2.32 | 6 | 8 |
| 1:A:70:ILE:CG2 | 1:A:86:VAL:HG21 | 0.46 | 2.32 | 10 | 1 |
| 1:B:96:GLU:O | 1:B:97:ILE:HG23 | 0.46 | 2.11 | 11 | 2 |
| 1:B:155:ASP:CB | 1:B:165:ILE:HG22 | 0.46 | 2.41 | 20 | 1 |
| 1:A:146:THR:O | 1:A:149:ASN:HB2 | 0.46 | 2.11 | 16 | 1 |
| 1:A:127:THR:O | 1:A:131:VAL:HG23 | 0.46 | 2.11 | 6 | 2 |
| 1:A:64:LEU:HB3 | 1:A:68:ASP:CB | 0.46 | 2.41 | 2 | 2 |
| 1:A:138:ASP:O | 1:A:138:ASP:CG | 0.46 | 2.54 | 6 | 2 |
| 1:A:113:LEU:HD21 | 1:B:114:MET:HG2 | 0.46 | 1.88 | 9 | 1 |
| 1:B:22:LYS:HZ3 | 1:B:88:ALA:HB2 | 0.46 | 1.71 | 19 | 1 |
| 1:A:76:PHE:CE2 | 1:A:116:LEU:HG | 0.46 | 2.46 | 2 | 1 |
| 1:B:60:ILE:HD11 | 1:B:87:ARG:NH1 | 0.46 | 2.26 | 2 | 1 |
| 1:B:29:LEU:CD1 | 1:B:70:ILE:HG21 | 0.46 | 2.41 | 9 | 3 |
| 1:A:76:PHE:HD2 | 1:A:120:MET:CE | 0.46 | 2.24 | 7 | 1 |
| 1:A:187:LEU:N | 1:A:187:LEU:HD23 | 0.45 | 2.26 | 13 | 6 |
| 1:A:139:VAL:HG21 | 1:A:183:VAL:HG23 | 0.45 | 1.88 | 10 | 1 |
| 1:A:96:GLU:HG3 | 1:A:96:GLU:O | 0.45 | 2.10 | 10 | 3 |
| 1:A:30:ILE:O | 1:A:86:VAL:HG23 | 0.45 | 2.11 | 2 | 1 |
| 1:B:150:LEU:HD13 | 1:B:165:ILE:HD13 | 0.45 | 1.88 | 5 | 1 |
| 1:A:128:SER:HB3 | 1:B:128:SER:HB3 | 0.45 | 1.87 | 14 | 1 |
| 1:A:53:ASP:CB | 1:A:57:LYS:HG2 | 0.45 | 2.42 | 19 | 2 |
| 1:B:184:GLY:O | 1:B:188:LYS:HB2 | 0.45 | 2.11 | 13 | 2 |
| 1:B:89:LYS:NZ | 1:B:155:ASP:OD2 | 0.45 | 2.48 | 10 | 1 |
| 1:B:90:THR:O | 1:B:91:ALA:C | 0.45 | 2.55 | 11 | 2 |
| 1:A:116:LEU:HG | 1:A:120:MET:CE | 0.45 | 2.41 | 18 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:B:47:VAL:HA | 1:B:89:LYS:HB3 | 0.45 | 1.87 | 18 | 1 |
| 1:A:11:LEU:HD21 | 1:A:41:TYR:CZ | 0.45 | 2.46 | 16 | 2 |
| 1:A:31:HIS:CE1 | 1:A:58:GLU:CB | 0.45 | 3.00 | 20 | 5 |
| 1:A:114:MET:HG2 | 1:B:113:LEU:HD21 | 0.45 | 1.88 | 9 | 2 |
| 1:A:125:GLN:O | 1:A:125:GLN:HG3 | 0.45 | 2.10 | 9 | 1 |
| 1:A:22:LYS:HZ1 | 1:A:29:LEU:HD22 | 0.45 | 1.71 | 12 | 1 |
| 1:B:117:SER:HA | 1:B:120:MET:SD | 0.45 | 2.51 | 4 | 1 |
| 1:A:76:PHE:CE2 | 1:A:120:MET:HE3 | 0.45 | 2.46 | 2 | 1 |
| 1:A:46:SER:HB2 | 1:A:64:LEU:C | 0.45 | 2.32 | 12 | 1 |
| 1:B:193:GLN:CA | 1:B:196:ILE:O | 0.45 | 2.59 | 12 | 1 |
| 1:B:147:LEU:HD13 | 1:B:203:ILE:HG21 | 0.45 | 1.87 | 18 | 1 |
| 1:A:147:LEU:HD22 | 1:A:167:ILE:HD11 | 0.45 | 1.89 | 13 | 1 |
| 1:B:76:PHE:CE2 | 1:B:120:MET:SD | 0.45 | 3.10 | 4 | 1 |
| 1:B:142:ARG:O | 1:B:145:GLN:HB2 | 0.45 | 2.12 | 13 | 1 |
| 1:B:196:ILE:CG1 | 1:B:197:SER:N | 0.45 | 2.79 | 13 | 1 |
| 1:A:97:ILE:HD12 | 1:A:102:PHE:HB2 | 0.45 | 1.89 | 10 | 2 |
| 1:A:124:LEU:CD2 | 1:B:124:LEU:HG | 0.45 | 2.42 | 4 | 1 |
| 1:A:164:GLN:CB | 1:A:204:VAL:HG23 | 0.45 | 2.42 | 4 | 1 |
| 1:A:169:ARG:CG | 1:A:187:LEU:HD12 | 0.45 | 2.42 | 5 | 3 |
| 1:B:209:ARG:HG3 | 1:B:209:ARG:OXT | 0.45 | 2.12 | 8 | 1 |
| 1:A:123:ARG:C | 1:A:126:VAL:HG12 | 0.45 | 2.30 | 14 | 1 |
| 1:A:124:LEU:CA | 1:A:128:SER:HB2 | 0.45 | 2.42 | 14 | 1 |
| 1:B:33:GLY:CA | 1:B:82:ARG:HB2 | 0.45 | 2.41 | 14 | 1 |
| 1:B:53:ASP:CB | 1:B:57:LYS:HG2 | 0.45 | 2.41 | 1 | 1 |
| 1:A:131:VAL:HG12 | 1:A:132:GLY:N | 0.45 | 2.26 | 6 | 1 |
| 1:A:81:GLU:O | 1:A:83:SER:N | 0.45 | 2.50 | 11 | 2 |
| 1:B:27:SER:H | 1:B:88:ALA:HB3 | 0.45 | 1.70 | 14 | 2 |
| 1:A:47:VAL:HB | 1:A:88:ALA:HA | 0.45 | 1.87 | 5 | 2 |
| 1:A:180:ARG:NH1 | 1:A:181:GLU:HA | 0.45 | 2.27 | 17 | 1 |
| 1:B:40:TYR:N | 1:B:40:TYR:CD2 | 0.45 | 2.84 | 20 | 3 |
| 1:A:119:GLN:OE1 | 1:A:119:GLN:HA | 0.45 | 2.12 | 6 | 1 |
| 1:A:14:PHE:HD1 | 1:A:15:LEU:HD23 | 0.45 | 1.72 | 14 | 3 |
| 1:B:14:PHE:CE2 | 1:B:102:PHE:CE1 | 0.45 | 3.05 | 10 | 1 |
| 1:A:103:ARG:O | 1:A:107:GLN:HB2 | 0.45 | 2.12 | 12 | 2 |
| 1:A:48:ALA:CB | 1:A:60:ILE:HD13 | 0.45 | 2.40 | 15 | 2 |
| 1:A:47:VAL:HG21 | 1:A:86:VAL:HG12 | 0.45 | 1.89 | 17 | 2 |
| 1:A:196:ILE:CG2 | 1:A:197:SER:N | 0.45 | 2.80 | 19 | 2 |
| 1:A:23:TYR:HB3 | 1:A:24:PRO:HD2 | 0.45 | 1.87 | 13 | 1 |
| 1:B:39:LEU:HB2 | 1:B:75:LEU:HD22 | 0.45 | 1.89 | 13 | 1 |
| 1:B:195:LEU:O | 1:B:209:ARG:HG3 | 0.45 | 2.12 | 7 | 3 |
| 1:B:144:ALA:HB2 | 1:B:195:LEU:CD2 | 0.45 | 2.42 | 18 | 2 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:B:15:LEU:HD21 | 1:B:41:TYR:CE2 | 0.45 | 2.46 | 10 | 1 |
| 1:B:39:LEU:HD13 | 1:B:102:PHE:CZ | 0.45 | 2.46 | 9 | 1 |
| 1:A:11:LEU:O | 1:A:15:LEU:N | 0.45 | 2.50 | 5 | 8 |
| 1:A:63:TYR:OH | 1:A:175:ILE:HD11 | 0.45 | 2.12 | 13 | 1 |
| 1:A:51:ILE:HG21 | 1:B:128:SER:CB | 0.45 | 2.41 | 10 | 1 |
| 1:B:47:VAL:HG21 | 1:B:70:ILE:HD11 | 0.45 | 1.88 | 12 | 1 |
| 1:B:139:VAL:HG23 | 1:B:176:VAL:CG1 | 0.45 | 2.42 | 5 | 1 |
| 1:A:143:ILE:CG1 | 1:A:183:VAL:HG22 | 0.44 | 2.38 | 10 | 1 |
| 1:B:20:ILE:HG21 | 1:B:43:VAL:HG21 | 0.44 | 1.89 | 10 | 1 |
| 1:A:190:LEU:CD1 | 1:A:203:ILE:HD13 | 0.44 | 2.42 | 14 | 2 |
| 1:B:157:MET:O | 1:B:163:MET:CA | 0.44 | 2.62 | 8 | 1 |
| 1:B:27:SER:O | 1:B:88:ALA:HB2 | 0.44 | 2.12 | 18 | 1 |
| 1:A:134:LEU:HD21 | 1:A:174:GLN:O | 0.44 | 2.12 | 14 | 2 |
| 1:A:20:ILE:CD1 | 1:A:95:ALA:HB2 | 0.44 | 2.40 | 16 | 1 |
| 1:B:190:LEU:CD1 | 1:B:203:ILE:HD13 | 0.44 | 2.41 | 16 | 1 |
| 1:A:172:ILE:HB | 1:A:183:VAL:HG11 | 0.44 | 1.88 | 3 | 1 |
| 1:B:41:TYR:CE2 | 1:B:69:PHE:CE1 | 0.44 | 3.04 | 17 | 3 |
| 1:A:135:ALA:HB3 | 1:B:135:ALA:CB | 0.44 | 2.40 | 6 | 1 |
| 1:B:120:MET:O | 1:B:123:ARG:HB2 | 0.44 | 2.11 | 11 | 1 |
| 1:A:143:ILE:HD12 | 1:A:186:ILE:HB | 0.44 | 1.89 | 4 | 2 |
| 1:B:14:PHE:HD1 | 1:B:15:LEU:HD23 | 0.44 | 1.72 | 20 | 3 |
| 1:A:32:GLN:O | 1:A:34:GLU:HG3 | 0.44 | 2.12 | 7 | 2 |
| 1:B:106:ILE:HD12 | 1:B:113:LEU:HB2 | 0.44 | 1.87 | 5 | 2 |
| 1:A:52:LYS:O | 1:B:129:GLU:HG2 | 0.44 | 2.12 | 18 | 1 |
| 1:B:51:ILE:HD13 | 1:B:51:ILE:H | 0.44 | 1.72 | 18 | 1 |
| 1:A:102:PHE:CE2 | 1:A:106:ILE:HG22 | 0.44 | 2.47 | 19 | 1 |
| 1:A:49:VAL:CB | 1:A:62:SER:O | 0.44 | 2.54 | 16 | 1 |
| 1:A:147:LEU:HD21 | 1:A:203:ILE:HG21 | 0.44 | 1.89 | 14 | 1 |
| 1:A:31:HIS:HB2 | 1:A:84:ALA:HA | 0.44 | 1.87 | 14 | 1 |
| 1:A:76:PHE:CZ | 1:B:117:SER:HB2 | 0.44 | 2.46 | 7 | 4 |
| 1:A:196:ILE:HD12 | 1:A:203:ILE:HG23 | 0.44 | 1.88 | 13 | 2 |
| 1:B:189:MET:CG | 1:B:195:LEU:HB2 | 0.44 | 2.42 | 1 | 1 |
| 1:A:20:ILE:O | 1:A:21:HIS:CB | 0.44 | 2.65 | 16 | 8 |
| 1:A:128:SER:HA | 1:B:51:ILE:HD12 | 0.44 | 1.90 | 4 | 1 |
| 1:A:23:TYR:CD2 | 1:A:27:SER:CB | 0.44 | 3.00 | 2 | 2 |
| 1:B:103:ARG:O | 1:B:107:GLN:HB2 | 0.44 | 2.13 | 12 | 4 |
| 1:A:143:ILE:HD13 | 1:A:183:VAL:HG22 | 0.44 | 1.90 | 13 | 2 |
| 1:B:72:GLU:HB2 | 1:B:120:MET:CE | 0.44 | 2.43 | 7 | 3 |
| 1:A:143:ILE:CD1 | 1:A:186:ILE:HG13 | 0.44 | 2.41 | 10 | 1 |
| 1:B:42:ILE:HD11 | 1:B:64:LEU:CD1 | 0.44 | 2.43 | 10 | 1 |
| 1:A:47:VAL:HG21 | 1:A:70:ILE:HD11 | 0.44 | 1.90 | 7 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:104:GLN:O | 1:A:108:VAL:HB | 0.44 | 2.13 | 20 | 1 |
| 1:A:204:VAL:HG12 | 1:A:204:VAL:O | 0.44 | 2.12 | 20 | 1 |
| 1:A:128:SER:HB2 | 1:B:51:ILE:HG21 | 0.44 | 1.90 | 3 | 1 |
| 1:A:90:THR:O | 1:A:91:ALA:C | 0.44 | 2.56 | 11 | 3 |
| 1:B:20:ILE:CD1 | 1:B:43:VAL:HG21 | 0.44 | 2.43 | 11 | 1 |
| 1:A:149:ASN:O | 1:A:153:GLN:HG2 | 0.44 | 2.12 | 4 | 1 |
| 1:A:166:LYS:HB3 | 1:A:202:THR:CG2 | 0.44 | 2.40 | 5 | 1 |
| 1:B:106:ILE:HB | 1:B:113:LEU:HB2 | 0.44 | 1.89 | 15 | 1 |
| 1:B:159:HIS:O | 1:B:161:ASP:N | 0.44 | 2.49 | 8 | 5 |
| 1:B:39:LEU:O | 1:B:96:GLU:HA | 0.44 | 2.13 | 20 | 3 |
| 1:A:110:PRO:HB3 | 1:B:110:PRO:HB3 | 0.44 | 1.90 | 19 | 2 |
| 1:B:76:PHE:HD2 | 1:B:120:MET:CE | 0.44 | 2.25 | 7 | 1 |
| 1:A:189:MET:SD | 1:A:195:LEU:HD13 | 0.44 | 2.53 | 18 | 1 |
| 1:B:11:LEU:HD21 | 1:B:41:TYR:CZ | 0.44 | 2.47 | 20 | 2 |
| 1:A:195:LEU:HA | 1:A:209:ARG:NH2 | 0.44 | 2.27 | 16 | 1 |
| 1:A:134:LEU:HD13 | 1:A:174:GLN:O | 0.44 | 2.12 | 7 | 1 |
| 1:A:51:ILE:HG23 | 1:A:61:LEU:CD1 | 0.44 | 2.42 | 7 | 1 |
| 1:A:72:GLU:CG | 1:A:120:MET:HE2 | 0.44 | 2.41 | 14 | 1 |
| 1:B:11:LEU:O | 1:B:15:LEU:N | 0.44 | 2.48 | 11 | 5 |
| 1:B:169:ARG:HD3 | 1:B:180:ARG:HB3 | 0.44 | 1.90 | 17 | 1 |
| 1:B:41:TYR:CD1 | 1:B:41:TYR:C | 0.44 | 2.91 | 6 | 1 |
| 1:B:169:ARG:HA | 1:B:187:LEU:HD12 | 0.44 | 1.88 | 11 | 1 |
| 1:B:138:ASP:O | 1:B:138:ASP:CG | 0.44 | 2.56 | 20 | 2 |
| 1:A:40:TYR:N | 1:A:40:TYR:CD2 | 0.44 | 2.85 | 12 | 1 |
| 1:A:47:VAL:H | 1:A:64:LEU:HB2 | 0.44 | 1.72 | 12 | 1 |
| 1:A:138:ASP:O | 1:A:142:ARG:CB | 0.44 | 2.65 | 7 | 1 |
| 1:A:40:TYR:O | 1:A:70:ILE:N | 0.44 | 2.51 | 20 | 1 |
| 1:A:105:LEU:HD11 | 1:A:112:ILE:HD12 | 0.44 | 1.89 | 19 | 1 |
| 1:B:100:LYS:O | 1:B:103:ARG:HG2 | 0.44 | 2.13 | 19 | 1 |
| 1:B:106:ILE:HD12 | 1:B:113:LEU:HD22 | 0.44 | 1.88 | 19 | 1 |
| 1:B:169:ARG:HG3 | 1:B:180:ARG:CB | 0.44 | 2.43 | 15 | 1 |
| 1:A:191:GLU:O | 1:A:191:GLU:HG2 | 0.43 | 2.13 | 17 | 2 |
| 1:A:187:LEU:HD23 | 1:A:187:LEU:N | 0.43 | 2.28 | 4 | 5 |
| 1:A:30:ILE:HD12 | 1:A:86:VAL:HG23 | 0.43 | 1.90 | 4 | 4 |
| 1:B:159:HIS:HD2 | 1:B:162:GLY:O | 0.43 | 1.96 | 18 | 2 |
| 1:A:143:ILE:HG12 | 1:A:183:VAL:CG2 | 0.43 | 2.40 | 11 | 1 |
| 1:A:113:LEU:O | 1:A:116:LEU:HB3 | 0.43 | 2.12 | 12 | 1 |
| 1:B:166:LYS:HB2 | 1:B:202:THR:HA | 0.43 | 1.90 | 18 | 1 |
| 1:B:106:ILE:CD1 | 1:B:113:LEU:HD22 | 0.43 | 2.44 | 19 | 1 |
| 1:B:111:ASP:O | 1:B:115:ARG:HB3 | 0.43 | 2.13 | 14 | 1 |
| 1:B:9:PRO:O | 1:B:13:TRP:HB2 | 0.43 | 2.13 | 15 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:18:CYS:HG | 1:A:95:ALA:HB1 | 0.43 | 1.73 | 3 | 2 |
| 1:B:61:LEU:C | 1:B:61:LEU:HD22 | 0.43 | 2.34 | 13 | 6 |
| 1:A:55:GLU:OE1 | 1:A:57:LYS:HB2 | 0.43 | 2.13 | 20 | 2 |
| 1:B:196:ILE:HG12 | 1:B:209:ARG:OXT | 0.43 | 2.12 | 7 | 1 |
| 1:B:156:ALA:HB1 | 1:B:163:MET:SD | 0.43 | 2.52 | 5 | 1 |
| 1:A:18:CYS:SG | 1:A:19:HIS:N | 0.43 | 2.92 | 19 | 1 |
| 1:A:139:VAL:HA | 1:A:176:VAL:CG1 | 0.43 | 2.43 | 3 | 1 |
| 1:A:39:LEU:HG | 1:A:40:TYR:N | 0.43 | 2.27 | 3 | 4 |
| 1:A:146:THR:O | 1:A:149:ASN:HB3 | 0.43 | 2.13 | 6 | 3 |
| 1:B:99:TYR:HD1 | 1:B:99:TYR:C | 0.43 | 2.17 | 5 | 4 |
| 1:A:42:ILE:HG12 | 1:A:94:VAL:CG1 | 0.43 | 2.42 | 2 | 1 |
| 1:B:46:SER:O | 1:B:90:THR:HG23 | 0.43 | 2.14 | 2 | 1 |
| 1:A:143:ILE:HD12 | 1:A:186:ILE:CB | 0.43 | 2.43 | 18 | 1 |
| 1:B:142:ARG:HB3 | 1:B:176:VAL:HG13 | 0.43 | 1.90 | 19 | 1 |
| 1:B:34:GLU:OE2 | 1:B:82:ARG:HB2 | 0.43 | 2.13 | 3 | 3 |
| 1:A:143:ILE:HD13 | 1:A:183:VAL:HA | 0.43 | 1.90 | 17 | 2 |
| 1:A:126:VAL:O | 1:A:130:LYS:HB2 | 0.43 | 2.14 | 13 | 1 |
| 1:B:23:TYR:CD2 | 1:B:27:SER:CB | 0.43 | 3.01 | 2 | 1 |
| 1:B:11:LEU:HD13 | 1:B:41:TYR:OH | 0.43 | 2.13 | 9 | 1 |
| 1:A:151:ALA:HA | 1:A:156:ALA:HB2 | 0.43 | 1.90 | 14 | 1 |
| 1:A:30:ILE:HG21 | 1:A:36:ALA:HA | 0.43 | 1.90 | 14 | 1 |
| 1:A:99:TYR:C | 1:A:99:TYR:HD1 | 0.43 | 2.17 | 3 | 2 |
| 1:B:25:SER:O | 1:B:26:LYS:HB2 | 0.43 | 2.14 | 11 | 2 |
| 1:B:35:LYS:HA | 1:B:81:GLU:HA | 0.43 | 1.89 | 19 | 3 |
| 1:B:180:ARG:HD2 | 1:B:181:GLU:OE1 | 0.43 | 2.14 | 7 | 2 |
| 1:B:153:GLN:CB | 1:B:154:PRO:HD2 | 0.43 | 2.44 | 3 | 2 |
| 1:A:143:ILE:HD12 | 1:A:186:ILE:HD13 | 0.43 | 1.90 | 17 | 1 |
| 1:A:11:LEU:HA | 1:A:14:PHE:HB3 | 0.43 | 1.90 | 6 | 3 |
| 1:A:69:PHE:CB | 1:A:116:LEU:HD12 | 0.43 | 2.44 | 9 | 3 |
| 1:A:187:LEU:O | 1:A:190:LEU:HG | 0.43 | 2.13 | 9 | 1 |
| 1:B:27:SER:O | 1:B:29:LEU:CD2 | 0.43 | 2.65 | 18 | 2 |
| 1:A:190:LEU:O | 1:A:197:SER:HA | 0.43 | 2.12 | 19 | 2 |
| 1:A:132:GLY:HA2 | 1:A:135:ALA:HB3 | 0.43 | 1.89 | 5 | 1 |
| 1:A:127:THR:HG22 | 1:A:127:THR:O | 0.43 | 2.14 | 14 | 1 |
| 1:B:159:HIS:CG | 1:B:160:PRO:HD2 | 0.43 | 2.49 | 14 | 1 |
| 1:B:53:ASP:HB2 | 1:B:57:LYS:HB2 | 0.43 | 1.91 | 15 | 1 |
| 1:B:48:ALA:CB | 1:B:60:ILE:HD13 | 0.43 | 2.42 | 15 | 1 |
| 1:A:156:ALA:HA | 1:A:164:GLN:O | 0.43 | 2.13 | 19 | 1 |
| 1:A:33:GLY:H | 1:A:82:ARG:HB2 | 0.43 | 1.73 | 14 | 1 |
| 1:B:53:ASP:HB2 | 1:B:57:LYS:HG2 | 0.43 | 1.89 | 1 | 1 |
| 1:B:18:CYS:HB3 | 1:B:97:ILE:CG1 | 0.43 | 2.42 | 14 | 3 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:B:143:ILE:HD13 | 1:B:183:VAL:HG22 | 0.43 | 1.90 | 7 | 2 |
| 1:B:22:LYS:HB2 | 1:B:94:VAL:HG22 | 0.43 | 1.89 | 12 | 1 |
| 1:B:32:GLN:O | 1:B:34:GLU:HG3 | 0.43 | 2.14 | 7 | 1 |
| 1:B:166:LYS:CB | 1:B:202:THR:HA | 0.43 | 2.43 | 20 | 1 |
| 1:A:130:LYS:HG2 | 1:A:130:LYS:O | 0.43 | 2.14 | 19 | 1 |
| 1:B:49:VAL:HG13 | 1:B:85:TRP:O | 0.43 | 2.14 | 15 | 1 |
| 1:B:178:CYS:SG | 1:B:183:VAL:HB | 0.43 | 2.54 | 17 | 1 |
| 1:B:30:ILE:CG2 | 1:B:34:GLU:HB2 | 0.43 | 2.43 | 17 | 2 |
| 1:A:196:ILE:HG22 | 1:A:209:ARG:O | 0.43 | 2.13 | 13 | 1 |
| 1:A:50:LEU:HA | 1:A:61:LEU:HD12 | 0.43 | 1.91 | 11 | 2 |
| 1:A:158:THR:HA | 1:A:163:MET:HB3 | 0.43 | 1.91 | 5 | 2 |
| 1:B:137:LEU:HG | 1:B:178:CYS:SG | 0.43 | 2.53 | 4 | 1 |
| 1:A:30:ILE:CG2 | 1:A:34:GLU:HB2 | 0.43 | 2.44 | 2 | 1 |
| 1:B:23:TYR:CD2 | 1:B:27:SER:HB2 | 0.43 | 2.49 | 2 | 1 |
| 1:A:47:VAL:HG12 | 1:A:88:ALA:HA | 0.43 | 1.91 | 12 | 1 |
| 1:A:169:ARG:HB3 | 1:A:187:LEU:CD1 | 0.43 | 2.40 | 16 | 1 |
| 1:A:147:LEU:CG | 1:A:167:ILE:HD11 | 0.43 | 2.44 | 14 | 1 |
| 1:B:11:LEU:HA | 1:B:14:PHE:HB3 | 0.43 | 1.91 | 20 | 2 |
| 1:A:33:GLY:HA2 | 1:A:82:ARG:NH1 | 0.43 | 2.29 | 11 | 1 |
| 1:B:14:PHE:O | 1:B:17:HIS:HB2 | 0.43 | 2.13 | 9 | 1 |
| 1:A:153:GLN:C | 1:A:155:ASP:H | 0.43 | 2.16 | 8 | 1 |
| 1:A:139:VAL:HG22 | 1:A:143:ILE:HD11 | 0.43 | 1.91 | 20 | 1 |
| 1:B:20:ILE:O | 1:B:21:HIS:CB | 0.43 | 2.67 | 15 | 1 |
| 1:A:137:LEU:HG | 1:A:178:CYS:SG | 0.42 | 2.54 | 6 | 1 |
| 1:A:159:HIS:O | 1:A:161:ASP:N | 0.42 | 2.51 | 16 | 4 |
| 1:B:165:ILE:O | 1:B:165:ILE:HD12 | 0.42 | 2.14 | 5 | 1 |
| 1:B:70:ILE:CD1 | 1:B:86:VAL:HG11 | 0.42 | 2.44 | 5 | 1 |
| 1:B:51:ILE:HD12 | 1:B:61:LEU:CB | 0.42 | 2.43 | 18 | 1 |
| 1:B:34:GLU:O | 1:B:82:ARG:HA | 0.42 | 2.14 | 14 | 1 |
| 1:B:31:HIS:CA | 1:B:82:ARG:HG3 | 0.42 | 2.44 | 8 | 1 |
| 1:A:114:MET:O | 1:A:117:SER:HB2 | 0.42 | 2.14 | 14 | 1 |
| 1:A:102:PHE:CD2 | 1:A:103:ARG:N | 0.42 | 2.87 | 17 | 2 |
| 1:A:25:SER:O | 1:A:26:LYS:HG3 | 0.42 | 2.13 | 6 | 1 |
| 1:A:190:LEU:CD2 | 1:A:196:ILE:HG12 | 0.42 | 2.23 | 13 | 1 |
| 1:B:44:LYS:HD3 | 1:B:66:GLN:HB3 | 0.42 | 1.91 | 18 | 1 |
| 1:B:114:MET:O | 1:B:117:SER:HB2 | 0.42 | 2.13 | 14 | 1 |
| 1:A:52:LYS:HG3 | 1:A:58:GLU:HB3 | 0.42 | 1.90 | 1 | 1 |
| 1:A:103:ARG:C | 1:A:106:ILE:HG13 | 0.42 | 2.34 | 18 | 3 |
| 1:B:168:THR:HB | 1:B:170:GLN:OE1 | 0.42 | 2.14 | 15 | 4 |
| 1:A:20:ILE:HG23 | 1:A:43:VAL:CG2 | 0.42 | 2.45 | 7 | 2 |
| 1:A:150:LEU:C | 1:A:152:LYS:N | 0.42 | 2.73 | 16 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:B:41:TYR:O | 1:B:95:ALA:N | 0.42 | 2.49 | 14 | 2 |
| 1:A:31:HIS:CA | 1:A:82:ARG:HG3 | 0.42 | 2.45 | 3 | 1 |
| 1:A:11:LEU:HD22 | 1:A:41:TYR:HE2 | 0.42 | 1.74 | 13 | 2 |
| 1:A:150:LEU:HD13 | 1:A:165:ILE:HD13 | 0.42 | 1.92 | 14 | 2 |
| 1:B:153:GLN:C | 1:B:155:ASP:H | 0.42 | 2.17 | 8 | 1 |
| 1:B:42:ILE:HG23 | 1:B:42:ILE:O | 0.42 | 2.14 | 8 | 1 |
| 1:B:60:ILE:HD11 | 1:B:87:ARG:HD3 | 0.42 | 1.91 | 8 | 1 |
| 1:A:114:MET:CE | 1:B:113:LEU:HD21 | 0.42 | 2.44 | 15 | 2 |
| 1:A:42:ILE:CB | 1:A:94:VAL:HG12 | 0.42 | 2.45 | 5 | 1 |
| 1:A:122:ARG:O | 1:A:125:GLN:HG2 | 0.42 | 2.14 | 18 | 1 |
| 1:A:99:TYR:HA | 1:A:102:PHE:CD2 | 0.42 | 2.50 | 20 | 1 |
| 1:A:166:LYS:CB | 1:A:202:THR:HA | 0.42 | 2.45 | 16 | 2 |
| 1:A:48:ALA:HB1 | 1:A:60:ILE:HG23 | 0.42 | 1.90 | 19 | 1 |
| 1:A:18:CYS:HB2 | 1:A:97:ILE:HG12 | 0.42 | 1.90 | 19 | 1 |
| 1:B:37:GLU:O | 1:B:99:TYR:CD1 | 0.42 | 2.72 | 19 | 1 |
| 1:B:42:ILE:O | 1:B:42:ILE:HG23 | 0.42 | 2.14 | 16 | 1 |
| 1:B:169:ARG:HA | 1:B:172:ILE:HG12 | 0.42 | 1.92 | 15 | 1 |
| 1:A:169:ARG:HD3 | 1:A:180:ARG:HB3 | 0.42 | 1.92 | 17 | 2 |
| 1:B:81:GLU:O | 1:B:83:SER:N | 0.42 | 2.52 | 10 | 3 |
| 1:B:143:ILE:CD1 | 1:B:186:ILE:HD13 | 0.42 | 2.44 | 11 | 1 |
| 1:A:121:ALA:HA | 1:A:124:LEU:HB2 | 0.42 | 1.91 | 4 | 1 |
| 1:A:196:ILE:HD12 | 1:A:203:ILE:CG2 | 0.42 | 2.45 | 16 | 1 |
| 1:A:172:ILE:O | 1:A:176:VAL:HG23 | 0.42 | 2.14 | 14 | 1 |
| 1:A:75:LEU:CG | 1:A:76:PHE:N | 0.42 | 2.81 | 14 | 1 |
| 1:B:143:ILE:HD12 | 1:B:186:ILE:HD12 | 0.42 | 1.91 | 14 | 1 |
| 1:B:14:PHE:HE2 | 1:B:102:PHE:CE1 | 0.42 | 2.32 | 10 | 2 |
| 1:B:167:ILE:HD12 | 1:B:167:ILE:O | 0.42 | 2.14 | 9 | 1 |
| 1:B:21:HIS:HA | 1:B:93:GLU:OE1 | 0.42 | 2.14 | 5 | 1 |
| 1:B:59:MET:HB3 | 1:B:174:GLN:HG2 | 0.42 | 1.91 | 20 | 1 |
| 1:B:179:SER:HB3 | 1:B:180:ARG:H | 0.42 | 1.46 | 14 | 1 |
| 1:B:31:HIS:CE1 | 1:B:58:GLU:CB | 0.42 | 3.03 | 2 | 4 |
| 1:A:42:ILE:HD11 | 1:A:64:LEU:CD1 | 0.42 | 2.44 | 17 | 1 |
| 1:B:76:PHE:CD1 | 1:B:113:LEU:HD11 | 0.42 | 2.50 | 6 | 1 |
| 1:A:41:TYR:CD1 | 1:A:68:ASP:O | 0.42 | 2.73 | 13 | 1 |
| 1:B:189:MET:SD | 1:B:195:LEU:HB2 | 0.42 | 2.55 | 13 | 1 |
| 1:B:41:TYR:HD1 | 1:B:68:ASP:O | 0.42 | 1.98 | 10 | 2 |
| 1:B:81:GLU:O | 1:B:82:ARG:HD3 | 0.42 | 2.15 | 12 | 4 |
| 1:B:77:GLU:O | 1:B:78:GLU:CB | 0.42 | 2.68 | 4 | 2 |
| 1:A:14:PHE:CE2 | 1:A:102:PHE:CD1 | 0.42 | 3.08 | 7 | 2 |
| 1:A:51:ILE:CD1 | 1:A:61:LEU:HB3 | 0.42 | 2.45 | 7 | 1 |
| 1:B:139:VAL:HG21 | 1:B:178:CYS:SG | 0.42 | 2.55 | 5 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:57:LYS:O | 1:A:57:LYS:HG3 | 0.42 | 2.14 | 19 | 1 |
| 1:A:147:LEU:HG | 1:A:167:ILE:HD11 | 0.42 | 1.90 | 14 | 1 |
| 1:A:47:VAL:C | 1:A:89:LYS:HB2 | 0.42 | 2.34 | 14 | 1 |
| 1:B:143:ILE:CD1 | 1:B:186:ILE:HG13 | 0.42 | 2.45 | 1 | 1 |
| 1:B:166:LYS:O | 1:B:167:ILE:HG23 | 0.42 | 2.15 | 13 | 1 |
| 1:B:172:ILE:HG22 | 1:B:183:VAL:CG2 | 0.42 | 2.44 | 10 | 1 |
| 1:B:113:LEU:HG | 1:B:113:LEU:O | 0.42 | 2.14 | 5 | 1 |
| 1:A:39:LEU:O | 1:A:96:GLU:HA | 0.42 | 2.15 | 20 | 1 |
| 1:B:190:LEU:HD22 | 1:B:196:ILE:CB | 0.42 | 2.45 | 16 | 1 |
| 1:B:42:ILE:HD11 | 1:B:64:LEU:CB | 0.42 | 2.45 | 17 | 1 |
| 1:B:147:LEU:HD22 | 1:B:167:ILE:HD11 | 0.42 | 1.92 | 13 | 1 |
| 1:B:41:TYR:C | 1:B:41:TYR:CD1 | 0.42 | 2.93 | 13 | 1 |
| 1:A:22:LYS:HB2 | 1:A:94:VAL:N | 0.42 | 2.30 | 2 | 2 |
| 1:A:129:GLU:O | 1:A:130:LYS:HG3 | 0.42 | 2.15 | 7 | 1 |
| 1:B:14:PHE:CE2 | 1:B:102:PHE:CD1 | 0.42 | 3.08 | 7 | 1 |
| 1:B:116:LEU:HG | 1:B:120:MET:CE | 0.42 | 2.44 | 18 | 1 |
| 1:B:119:GLN:HA | 1:B:119:GLN:OE1 | 0.42 | 2.14 | 20 | 1 |
| 1:A:40:TYR:HB2 | 1:A:70:ILE:CG2 | 0.42 | 2.45 | 16 | 1 |
| 1:B:143:ILE:CD1 | 1:B:183:VAL:HG22 | 0.42 | 2.45 | 16 | 1 |
| 1:A:73:LEU:HD21 | 1:B:124:LEU:CD1 | 0.41 | 2.45 | 2 | 1 |
| 1:B:22:LYS:HB2 | 1:B:94:VAL:N | 0.41 | 2.30 | 2 | 1 |
| 1:B:15:LEU:HB3 | 1:B:20:ILE:CD1 | 0.41 | 2.45 | 15 | 1 |
| 1:B:99:TYR:C | 1:B:99:TYR:HD1 | 0.41 | 2.18 | 18 | 2 |
| 1:B:31:HIS:O | 1:B:32:GLN:HB2 | 0.41 | 2.14 | 17 | 1 |
| 1:A:196:ILE:HG21 | 1:A:203:ILE:HG23 | 0.41 | 1.91 | 11 | 1 |
| 1:B:25:SER:HB3 | 1:B:90:THR:CA | 0.41 | 2.44 | 9 | 2 |
| 1:A:180:ARG:HD2 | 1:A:181:GLU:OE2 | 0.41 | 2.15 | 12 | 1 |
| 1:B:169:ARG:HD2 | 1:B:170:GLN:N | 0.41 | 2.31 | 14 | 1 |
| 1:A:99:TYR:HD1 | 1:A:99:TYR:C | 0.41 | 2.18 | 5 | 4 |
| 1:A:11:LEU:HD23 | 1:A:14:PHE:CB | 0.41 | 2.45 | 13 | 2 |
| 1:B:103:ARG:O | 1:B:107:GLN:HG3 | 0.41 | 2.15 | 13 | 2 |
| 1:A:134:LEU:HD22 | 1:A:176:VAL:HA | 0.41 | 1.92 | 10 | 1 |
| 1:A:77:GLU:O | 1:A:78:GLU:CB | 0.41 | 2.68 | 11 | 1 |
| 1:B:196:ILE:HG21 | 1:B:203:ILE:HG23 | 0.41 | 1.92 | 11 | 1 |
| 1:A:124:LEU:CD1 | 1:B:73:LEU:HD21 | 0.41 | 2.45 | 4 | 2 |
| 1:A:73:LEU:HA | 1:A:77:GLU:HB2 | 0.41 | 1.92 | 8 | 1 |
| 1:A:50:LEU:HD23 | 1:A:50:LEU:O | 0.41 | 2.15 | 5 | 1 |
| 1:A:8:ASP:CG | 1:A:115:ARG:HH12 | 0.41 | 2.19 | 5 | 1 |
| 1:B:205:VAL:HG12 | 1:B:209:ARG:O | 0.41 | 2.15 | 5 | 1 |
| 1:A:159:HIS:HD2 | 1:A:162:GLY:O | 0.41 | 1.98 | 18 | 1 |
| 1:A:85:TRP:CZ2 | 1:A:123:ARG:HG2 | 0.41 | 2.51 | 16 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:B:123:ARG:C | 1:B:126:VAL:HG12 | 0.41 | 2.35 | 14 | 1 |
| 1:A:15:LEU:HD21 | 1:A:41:TYR:HE2 | 0.41 | 1.74 | 10 | 1 |
| 1:A:72:GLU:HG2 | 1:A:116:LEU:HD11 | 0.41 | 1.91 | 4 | 1 |
| 1:A:41:TYR:HB3 | 1:A:95:ALA:CB | 0.41 | 2.37 | 8 | 1 |
| 1:A:45:GLY:HA3 | 1:A:92:CYS:CA | 0.41 | 2.46 | 18 | 1 |
| 1:B:166:LYS:C | 1:B:167:ILE:HG13 | 0.41 | 2.35 | 20 | 1 |
| 1:A:106:ILE:HD12 | 1:A:113:LEU:HD22 | 0.41 | 1.90 | 19 | 1 |
| 1:B:127:THR:O | 1:B:131:VAL:HG22 | 0.41 | 2.15 | 6 | 1 |
| 1:A:14:PHE:HE2 | 1:A:102:PHE:CE1 | 0.41 | 2.34 | 13 | 2 |
| 1:B:164:GLN:CB | 1:B:204:VAL:HG23 | 0.41 | 2.41 | 10 | 1 |
| 1:B:23:TYR:CB | 1:B:24:PRO:CD | 0.41 | 2.99 | 10 | 1 |
| 1:B:52:LYS:HG2 | 1:B:58:GLU:HB3 | 0.41 | 1.91 | 10 | 1 |
| 1:A:14:PHE:HE2 | 1:A:97:ILE:HD11 | 0.41 | 1.75 | 8 | 1 |
| 1:B:147:LEU:HD22 | 1:B:196:ILE:HD13 | 0.41 | 1.91 | 19 | 1 |
| 1:B:134:LEU:HD21 | 1:B:174:GLN:O | 0.41 | 2.15 | 14 | 1 |
| 1:B:73:LEU:HG | 1:B:85:TRP:CD2 | 0.41 | 2.51 | 2 | 2 |
| 1:B:15:LEU:HD22 | 1:B:20:ILE:CD1 | 0.41 | 2.46 | 11 | 1 |
| 1:B:149:ASN:O | 1:B:153:GLN:HG2 | 0.41 | 2.16 | 4 | 1 |
| 1:B:47:VAL:CG1 | 1:B:88:ALA:HA | 0.41 | 2.46 | 12 | 1 |
| 1:A:198:ALA:CB | 1:A:203:ILE:HG12 | 0.41 | 2.46 | 8 | 1 |
| 1:A:8:ASP:O | 1:A:12:GLU:HG3 | 0.41 | 2.15 | 5 | 1 |
| 1:A:102:PHE:O | 1:A:106:ILE:HG23 | 0.41 | 2.15 | 19 | 2 |
| 1:A:72:GLU:HG2 | 1:A:73:LEU:N | 0.41 | 2.31 | 14 | 1 |
| 1:B:190:LEU:HD23 | 1:B:195:LEU:HB3 | 0.41 | 1.91 | 14 | 1 |
| 1:A:184:GLY:O | 1:A:185:ARG:C | 0.41 | 2.59 | 15 | 1 |
| 1:B:180:ARG:HA | 1:B:183:VAL:CG1 | 0.41 | 2.45 | 1 | 1 |
| 1:B:42:ILE:CG2 | 1:B:94:VAL:HG12 | 0.41 | 2.46 | 17 | 1 |
| 1:A:189:MET:SD | 1:A:195:LEU:HB2 | 0.41 | 2.56 | 6 | 1 |
| 1:A:70:ILE:CD1 | 1:A:86:VAL:HG11 | 0.41 | 2.46 | 20 | 3 |
| 1:A:82:ARG:NE | 1:A:83:SER:H | 0.41 | 2.13 | 11 | 1 |
| 1:B:42:ILE:HG22 | 1:B:68:ASP:N | 0.41 | 2.29 | 12 | 1 |
| 1:A:27:SER:O | 1:A:29:LEU:CD2 | 0.41 | 2.69 | 16 | 2 |
| 1:A:41:TYR:CE1 | 1:A:69:PHE:CD1 | 0.41 | 3.08 | 7 | 1 |
| 1:B:166:LYS:HB3 | 1:B:202:THR:HA | 0.41 | 1.92 | 16 | 2 |
| 1:A:147:LEU:HD13 | 1:A:203:ILE:HG21 | 0.41 | 1.92 | 18 | 1 |
| 1:A:75:LEU:HB3 | 1:A:99:TYR:CD2 | 0.41 | 2.51 | 20 | 1 |
| 1:B:139:VAL:HG21 | 1:B:183:VAL:HG23 | 0.41 | 1.91 | 20 | 1 |
| 1:B:172:ILE:HB | 1:B:183:VAL:HG11 | 0.41 | 1.92 | 3 | 1 |
| 1:A:169:ARG:HA | 1:A:172:ILE:CG1 | 0.41 | 2.46 | 17 | 1 |
| 1:A:50:LEU:HB3 | 1:A:60:ILE:HA | 0.41 | 1.93 | 6 | 1 |
| 1:A:196:ILE:HG13 | 1:A:197:SER:N | 0.41 | 2.30 | 13 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:B:113:LEU:O | 1:B:116:LEU:HB3 | 0.41 | 2.15 | 12 | 1 |
| 1:B:127:THR:HG22 | 1:B:131:VAL:HG13 | 0.41 | 1.92 | 20 | 1 |
| 1:B:205:VAL:HG23 | 1:B:205:VAL:O | 0.41 | 2.16 | 19 | 1 |
| 1:A:179:SER:O | 1:A:183:VAL:HB | 0.41 | 2.16 | 16 | 1 |
| 1:B:183:VAL:HG13 | 1:B:187:LEU:HG | 0.41 | 1.92 | 1 | 1 |
| 1:B:140:THR:C | 1:B:142:ARG:N | 0.41 | 2.74 | 3 | 1 |
| 1:B:179:SER:OG | 1:B:181:GLU:HB2 | 0.41 | 2.15 | 17 | 1 |
| 1:A:77:GLU:O | 1:A:78:GLU:HB2 | 0.41 | 2.15 | 6 | 1 |
| 1:B:102:PHE:CD2 | 1:B:103:ARG:N | 0.41 | 2.89 | 13 | 3 |
| 1:A:22:LYS:HE2 | 1:A:88:ALA:HB2 | 0.41 | 1.93 | 13 | 1 |
| 1:A:167:ILE:O | 1:A:167:ILE:HD12 | 0.41 | 2.15 | 10 | 2 |
| 1:A:59:MET:CE | 1:A:175:ILE:HA | 0.41 | 2.46 | 10 | 1 |
| 1:B:186:ILE:HA | 1:B:189:MET:HG2 | 0.41 | 1.93 | 4 | 3 |
| 1:A:164:GLN:HB3 | 1:A:204:VAL:HB | 0.41 | 1.93 | 2 | 1 |
| 1:B:23:TYR:CE2 | 1:B:27:SER:HB2 | 0.41 | 2.51 | 2 | 1 |
| 1:A:61:LEU:HD22 | 1:A:62:SER:HB3 | 0.41 | 1.92 | 2 | 1 |
| 1:B:186:ILE:HG23 | 1:B:195:LEU:HD13 | 0.41 | 1.92 | 12 | 1 |
| 1:A:138:ASP:OD1 | 1:A:142:ARG:HD3 | 0.41 | 2.16 | 18 | 1 |
| 1:A:124:LEU:HB2 | 1:B:124:LEU:HG | 0.41 | 1.92 | 19 | 1 |
| 1:B:170:GLN:O | 1:B:174:GLN:HB2 | 0.41 | 2.16 | 14 | 1 |
| 1:A:25:SER:O | 1:A:26:LYS:HB2 | 0.41 | 2.15 | 15 | 2 |
| 1:A:23:TYR:CD2 | 1:A:27:SER:HB2 | 0.41 | 2.51 | 2 | 3 |
| 1:B:198:ALA:CB | 1:B:203:ILE:HG12 | 0.41 | 2.46 | 8 | 1 |
| 1:A:18:CYS:CA | 1:A:97:ILE:CG2 | 0.41 | 2.98 | 16 | 2 |
| 1:B:35:LYS:HA | 1:B:81:GLU:CA | 0.41 | 2.46 | 19 | 1 |
| 1:A:42:ILE:HG23 | 1:A:42:ILE:O | 0.41 | 2.16 | 15 | 1 |
| 1:B:166:LYS:CG | 1:B:202:THR:HG23 | 0.41 | 2.44 | 15 | 1 |
| 1:B:73:LEU:HD13 | 1:B:77:GLU:HB2 | 0.41 | 1.93 | 15 | 1 |
| 1:B:182:THR:O | 1:B:186:ILE:HD12 | 0.40 | 2.16 | 13 | 1 |
| 1:B:198:ALA:HA | 1:B:203:ILE:HA | 0.40 | 1.91 | 10 | 1 |
| 1:A:78:GLU:HB3 | 1:B:122:ARG:NH1 | 0.40 | 2.31 | 2 | 1 |
| 1:A:73:LEU:HD13 | 1:A:77:GLU:HG3 | 0.40 | 1.93 | 8 | 1 |
| 1:A:14:PHE:HE2 | 1:A:102:PHE:CD1 | 0.40 | 2.34 | 7 | 1 |
| 1:A:124:LEU:CD2 | 1:B:124:LEU:HD21 | 0.40 | 2.33 | 18 | 1 |
| 1:B:169:ARG:HG3 | 1:B:180:ARG:HB3 | 0.40 | 1.92 | 20 | 1 |
| 1:B:186:ILE:O | 1:B:189:MET:HB2 | 0.40 | 2.16 | 19 | 1 |
| 1:B:147:LEU:HD21 | 1:B:167:ILE:HD11 | 0.40 | 1.93 | 14 | 1 |
| 1:A:169:ARG:HA | 1:A:172:ILE:HG12 | 0.40 | 1.92 | 17 | 1 |
| 1:B:11:LEU:HD21 | 1:B:41:TYR:OH | 0.40 | 2.16 | 17 | 1 |
| 1:A:22:LYS:HZ1 | 1:A:29:LEU:HD21 | 0.40 | 1.75 | 6 | 1 |
| 1:A:83:SER:O | 1:A:84:ALA:HB3 | 0.40 | 2.16 | 6 | 2 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:B:59:MET:O | 1:B:59:MET:HG2 | 0.40 | 2.16 | 10 | 1 |
| 1:A:31:HIS:HE2 | 1:A:58:GLU:HB2 | 0.40 | 1.76 | 11 | 1 |
| 1:B:32:GLN:HA | 1:B:32:GLN:OE1 | 0.40 | 2.16 | 4 | 1 |
| 1:A:42:ILE:O | 1:A:67:GLY:HA2 | 0.40 | 2.16 | 2 | 1 |
| 1:B:53:ASP:HB2 | 1:B:57:LYS:HB3 | 0.40 | 1.94 | 9 | 1 |
| 1:B:14:PHE:HE2 | 1:B:102:PHE:CD1 | 0.40 | 2.33 | 7 | 1 |
| 1:B:34:GLU:O | 1:B:82:ARG:N | 0.40 | 2.54 | 20 | 1 |
| 1:A:205:VAL:O | 1:A:205:VAL:HG23 | 0.40 | 2.15 | 19 | 1 |
| 1:B:14:PHE:CE2 | 1:B:97:ILE:HD11 | 0.40 | 2.52 | 19 | 1 |
| 1:B:153:GLN:HB2 | 1:B:154:PRO:HD2 | 0.40 | 1.92 | 14 | 1 |
| 1:B:147:LEU:HD12 | 1:B:196:ILE:CD1 | 0.40 | 2.47 | 6 | 1 |
| 1:B:83:SER:O | 1:B:84:ALA:HB3 | 0.40 | 2.16 | 4 | 1 |
| 1:B:72:GLU:CB | 1:B:120:MET:SD | 0.40 | 3.07 | 12 | 1 |
| 1:A:42:ILE:O | 1:A:42:ILE:HG23 | 0.40 | 2.16 | 8 | 1 |
| 1:A:34:GLU:O | 1:A:82:ARG:N | 0.40 | 2.53 | 5 | 1 |
| 1:B:158:THR:HA | 1:B:163:MET:HB3 | 0.40 | 1.93 | 18 | 1 |
| 1:B:129:GLU:O | 1:B:130:LYS:HG3 | 0.40 | 2.15 | 3 | 1 |
| 1:A:18:CYS:HB3 | 1:A:97:ILE:CG1 | 0.40 | 2.46 | 13 | 1 |
| 1:B:187:LEU:HD23 | 1:B:203:ILE:HD11 | 0.40 | 1.92 | 10 | 1 |
| 1:B:31:HIS:NE2 | 1:B:58:GLU:HB2 | 0.40 | 2.32 | 11 | 1 |
| 1:B:73:LEU:HG | 1:B:85:TRP:CE3 | 0.40 | 2.51 | 2 | 1 |
| 1:A:171:GLU:HB3 | 1:A:175:ILE:HD12 | 0.40 | 1.92 | 7 | 1 |
| 1:A:189:MET:CG | 1:A:195:LEU:HB2 | 0.40 | 2.46 | 5 | 1 |
| 1:B:42:ILE:CB | 1:B:94:VAL:HG12 | 0.40 | 2.47 | 5 | 1 |
| 1:B:179:SER:O | 1:B:183:VAL:HB | 0.40 | 2.16 | 18 | 1 |
| 1:B:110:PRO:O | 1:B:114:MET:HB2 | 0.40 | 2.17 | 14 | 1 |
| 1:B:172:ILE:HG21 | 1:B:183:VAL:CG2 | 0.40 | 2.46 | 14 | 1 |
| 1:B:143:ILE:HG23 | 1:B:172:ILE:CG2 | 0.40 | 2.46 | 1 | 1 |
| 1:A:72:GLU:N | 1:A:72:GLU:OE2 | 0.40 | 2.54 | 17 | 1 |
| 1:B:53:ASP:N | 1:B:57:LYS:O | 0.40 | 2.54 | 17 | 1 |
| 1:B:138:ASP:C | 1:B:138:ASP:OD2 | 0.40 | 2.60 | 6 | 1 |
| 1:B:72:GLU:OE2 | 1:B:72:GLU:N | 0.40 | 2.53 | 10 | 1 |
| 1:A:49:VAL:O | 1:A:61:LEU:HD13 | 0.40 | 2.15 | 4 | 1 |
| 1:B:22:LYS:HZ1 | 1:B:29:LEU:CD1 | 0.40 | 2.29 | 9 | 1 |
| 1:A:124:LEU:HD23 | 1:B:124:LEU:HD23 | 0.40 | 1.91 | 12 | 1 |
| 1:A:41:TYR:CZ | 1:A:69:PHE:CE1 | 0.40 | 3.09 | 7 | 1 |
| 1:A:143:ILE:CD1 | 1:A:183:VAL:HA | 0.40 | 2.46 | 18 | 1 |
| 1:B:49:VAL:HG13 | 1:B:85:TRP:CA | 0.40 | 2.46 | 19 | 1 |
| 1:A:153:GLN:HB2 | 1:A:154:PRO:HD2 | 0.40 | 1.93 | 14 | 1 |
| 1:A:147:LEU:HD21 | 1:A:167:ILE:HD11 | 0.40 | 1.93 | 14 | 1 |
| 1:B:141:GLY:O | 1:B:145:GLN:CB | 0.40 | 2.67 | 14 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|---------------|---------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:B:184:GLY:O | 1:B:185:ARG:C | 0.40 | 2.59 | 15 | 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 | 201/209 (96%) | 157±4 (78±2%) | 26±4 (13±2%) | 18±2 (9±1%) | 2 | 12 |
| 1 | B | 201/209 (96%) | 158±3 (79±2%) | 25±3 (13±2%) | 18±2 (9±1%) | 2 | 12 |
| All | All | 8040/8360 (96%) | 6296 (78%) | 1032 (13%) | 712 (9%) | 2 | 12 |

All 81 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1 | B | 161 | ASP | 20 |
| 1 | A | 81 | GLU | 20 |
| 1 | A | 85 | TRP | 20 |
| 1 | B | 21 | HIS | 20 |
| 1 | A | 30 | ILE | 20 |
| 1 | B | 81 | GLU | 20 |
| 1 | B | 31 | HIS | 20 |
| 1 | A | 196 | ILE | 20 |
| 1 | A | 161 | ASP | 20 |
| 1 | A | 21 | HIS | 20 |
| 1 | B | 30 | ILE | 20 |
| 1 | B | 85 | TRP | 20 |
| 1 | A | 31 | HIS | 20 |
| 1 | B | 26 | LYS | 20 |
| 1 | A | 26 | LYS | 20 |
| 1 | A | 78 | GLU | 19 |
| 1 | B | 196 | ILE | 19 |
| 1 | B | 78 | GLU | 19 |
| 1 | B | 180 | ARG | 18 |
| 1 | B | 139 | VAL | 17 |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1 | A | 180 | ARG | 17 |
| 1 | B | 84 | ALA | 17 |
| 1 | A | 165 | ILE | 17 |
| 1 | A | 139 | VAL | 16 |
| 1 | A | 207 | GLY | 16 |
| 1 | B | 165 | ILE | 15 |
| 1 | A | 84 | ALA | 15 |
| 1 | B | 140 | THR | 15 |
| 1 | A | 140 | THR | 14 |
| 1 | B | 207 | GLY | 14 |
| 1 | A | 160 | PRO | 13 |
| 1 | B | 66 | GLN | 11 |
| 1 | B | 160 | PRO | 11 |
| 1 | B | 82 | ARG | 10 |
| 1 | A | 66 | GLN | 9 |
| 1 | B | 132 | GLY | 8 |
| 1 | A | 82 | ARG | 8 |
| 1 | A | 132 | GLY | 7 |
| 1 | B | 42 | ILE | 7 |
| 1 | A | 131 | VAL | 5 |
| 1 | A | 42 | ILE | 4 |
| 1 | B | 32 | GLN | 4 |
| 1 | A | 32 | GLN | 4 |
| 1 | A | 143 | ILE | 4 |
| 1 | B | 131 | VAL | 4 |
| 1 | A | 201 | LYS | 3 |
| 1 | A | 167 | ILE | 3 |
| 1 | B | 143 | ILE | 3 |
| 1 | B | 130 | LYS | 3 |
| 1 | B | 36 | ALA | 2 |
| 1 | B | 99 | TYR | 2 |
| 1 | A | 88 | ALA | 2 |
| 1 | B | 135 | ALA | 2 |
| 1 | A | 179 | SER | 2 |
| 1 | B | 128 | SER | 2 |
| 1 | B | 167 | ILE | 2 |
| 1 | A | 130 | LYS | 2 |
| 1 | B | 88 | ALA | 2 |
| 1 | B | 185 | ARG | 2 |
| 1 | A | 181 | GLU | 2 |
| 1 | A | 83 | SER | 1 |
| 1 | A | 36 | ALA | 1 |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1 | A | 208 | THR | 1 |
| 1 | A | 136 | PHE | 1 |
| 1 | B | 136 | PHE | 1 |
| 1 | B | 208 | THR | 1 |
| 1 | B | 179 | SER | 1 |
| 1 | B | 137 | LEU | 1 |
| 1 | A | 133 | ASN | 1 |
| 1 | A | 45 | GLY | 1 |
| 1 | A | 28 | THR | 1 |
| 1 | B | 141 | GLY | 1 |
| 1 | A | 138 | ASP | 1 |
| 1 | B | 53 | ASP | 1 |
| 1 | A | 128 | SER | 1 |
| 1 | A | 154 | PRO | 1 |
| 1 | B | 181 | GLU | 1 |
| 1 | B | 28 | THR | 1 |
| 1 | B | 201 | LYS | 1 |
| 1 | A | 185 | ARG | 1 |
| 1 | B | 154 | PRO | 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 | 174/180 (97%) | 115±4 (66±2%) | 59±4 (34±2%) | 1 | 11 |
| 1 | B | 174/180 (97%) | 114±4 (66±2%) | 60±4 (34±2%) | 1 | 10 |
| All | All | 6960/7200 (97%) | 4589 (66%) | 2371 (34%) | 1 | 11 |

All 270 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 | 25 | SER | 20 |
| 1 | A | 30 | ILE | 20 |
| 1 | B | 25 | SER | 20 |
| 1 | B | 92 | CYS | 20 |
| 1 | A | 82 | ARG | 20 |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1 | A | 122 | ARG | 20 |
| 1 | A | 105 | LEU | 20 |
| 1 | B | 82 | ARG | 20 |
| 1 | A | 61 | LEU | 20 |
| 1 | B | 99 | TYR | 20 |
| 1 | A | 92 | CYS | 20 |
| 1 | B | 108 | VAL | 20 |
| 1 | B | 86 | VAL | 20 |
| 1 | A | 75 | LEU | 20 |
| 1 | A | 108 | VAL | 20 |
| 1 | B | 50 | LEU | 20 |
| 1 | A | 182 | THR | 20 |
| 1 | B | 105 | LEU | 20 |
| 1 | B | 122 | ARG | 20 |
| 1 | B | 61 | LEU | 20 |
| 1 | A | 165 | ILE | 20 |
| 1 | B | 165 | ILE | 20 |
| 1 | B | 23 | TYR | 20 |
| 1 | B | 30 | ILE | 20 |
| 1 | B | 182 | THR | 20 |
| 1 | A | 50 | LEU | 20 |
| 1 | A | 86 | VAL | 20 |
| 1 | A | 99 | TYR | 20 |
| 1 | B | 75 | LEU | 20 |
| 1 | A | 23 | TYR | 20 |
| 1 | B | 114 | MET | 19 |
| 1 | A | 29 | LEU | 19 |
| 1 | B | 139 | VAL | 19 |
| 1 | A | 10 | THR | 19 |
| 1 | A | 114 | MET | 19 |
| 1 | B | 140 | THR | 19 |
| 1 | A | 140 | THR | 19 |
| 1 | A | 90 | THR | 19 |
| 1 | B | 169 | ARG | 19 |
| 1 | A | 39 | LEU | 19 |
| 1 | B | 90 | THR | 19 |
| 1 | B | 39 | LEU | 19 |
| 1 | B | 10 | THR | 19 |
| 1 | A | 169 | ARG | 19 |
| 1 | B | 202 | THR | 19 |
| 1 | B | 20 | ILE | 19 |
| 1 | B | 112 | ILE | 18 |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1 | B | 29 | LEU | 18 |
| 1 | B | 195 | LEU | 18 |
| 1 | B | 72 | GLU | 18 |
| 1 | A | 159 | HIS | 18 |
| 1 | B | 167 | ILE | 18 |
| 1 | A | 20 | ILE | 18 |
| 1 | A | 202 | THR | 18 |
| 1 | B | 63 | TYR | 17 |
| 1 | A | 112 | ILE | 17 |
| 1 | A | 195 | LEU | 17 |
| 1 | A | 72 | GLU | 17 |
| 1 | B | 179 | SER | 16 |
| 1 | B | 159 | HIS | 16 |
| 1 | A | 167 | ILE | 16 |
| 1 | B | 124 | LEU | 16 |
| 1 | B | 58 | GLU | 15 |
| 1 | A | 58 | GLU | 15 |
| 1 | A | 63 | TYR | 15 |
| 1 | A | 161 | ASP | 15 |
| 1 | B | 123 | ARG | 15 |
| 1 | A | 183 | VAL | 14 |
| 1 | A | 73 | LEU | 14 |
| 1 | A | 123 | ARG | 14 |
| 1 | B | 161 | ASP | 14 |
| 1 | A | 65 | ASN | 14 |
| 1 | B | 55 | GLU | 13 |
| 1 | B | 131 | VAL | 13 |
| 1 | A | 136 | PHE | 13 |
| 1 | A | 124 | LEU | 13 |
| 1 | A | 180 | ARG | 13 |
| 1 | A | 103 | ARG | 13 |
| 1 | A | 139 | VAL | 13 |
| 1 | B | 11 | LEU | 13 |
| 1 | A | 11 | LEU | 13 |
| 1 | B | 136 | PHE | 12 |
| 1 | A | 131 | VAL | 12 |
| 1 | B | 103 | ARG | 12 |
| 1 | B | 81 | GLU | 12 |
| 1 | A | 116 | LEU | 12 |
| 1 | B | 116 | LEU | 12 |
| 1 | A | 55 | GLU | 11 |
| 1 | A | 81 | GLU | 11 |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1 | A | 208 | THR | 11 |
| 1 | B | 183 | VAL | 11 |
| 1 | A | 102 | PHE | 11 |
| 1 | B | 208 | THR | 11 |
| 1 | A | 87 | ARG | 11 |
| 1 | B | 102 | PHE | 11 |
| 1 | B | 41 | TYR | 11 |
| 1 | B | 65 | ASN | 11 |
| 1 | B | 180 | ARG | 11 |
| 1 | A | 57 | LYS | 11 |
| 1 | B | 27 | SER | 11 |
| 1 | A | 41 | TYR | 10 |
| 1 | A | 142 | ARG | 10 |
| 1 | A | 179 | SER | 10 |
| 1 | B | 142 | ARG | 10 |
| 1 | B | 73 | LEU | 10 |
| 1 | A | 125 | GLN | 10 |
| 1 | A | 16 | SER | 10 |
| 1 | B | 57 | LYS | 9 |
| 1 | B | 126 | VAL | 9 |
| 1 | B | 16 | SER | 9 |
| 1 | A | 181 | GLU | 9 |
| 1 | B | 163 | MET | 9 |
| 1 | A | 166 | LYS | 9 |
| 1 | B | 68 | ASP | 9 |
| 1 | B | 174 | GLN | 9 |
| 1 | A | 201 | LYS | 9 |
| 1 | B | 201 | LYS | 9 |
| 1 | B | 168 | THR | 9 |
| 1 | B | 87 | ARG | 9 |
| 1 | A | 204 | VAL | 8 |
| 1 | B | 205 | VAL | 8 |
| 1 | B | 188 | LYS | 8 |
| 1 | B | 204 | VAL | 8 |
| 1 | A | 32 | GLN | 8 |
| 1 | B | 120 | MET | 8 |
| 1 | A | 174 | GLN | 8 |
| 1 | B | 166 | LYS | 8 |
| 1 | A | 188 | LYS | 8 |
| 1 | B | 32 | GLN | 8 |
| 1 | A | 120 | MET | 7 |
| 1 | A | 126 | VAL | 7 |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1 | A | 168 | THR | 7 |
| 1 | A | 130 | LYS | 7 |
| 1 | A | 164 | GLN | 7 |
| 1 | B | 158 | THR | 7 |
| 1 | A | 27 | SER | 7 |
| 1 | A | 38 | THR | 7 |
| 1 | A | 28 | THR | 7 |
| 1 | A | 68 | ASP | 7 |
| 1 | B | 13 | TRP | 7 |
| 1 | B | 80 | GLN | 7 |
| 1 | B | 28 | THR | 7 |
| 1 | B | 134 | LEU | 7 |
| 1 | A | 163 | MET | 6 |
| 1 | A | 133 | ASN | 6 |
| 1 | B | 130 | LYS | 6 |
| 1 | B | 38 | THR | 6 |
| 1 | B | 194 | ASN | 6 |
| 1 | B | 44 | LYS | 6 |
| 1 | B | 31 | HIS | 6 |
| 1 | B | 40 | TYR | 6 |
| 1 | A | 111 | ASP | 6 |
| 1 | A | 77 | GLU | 6 |
| 1 | A | 193 | GLN | 6 |
| 1 | B | 181 | GLU | 6 |
| 1 | A | 205 | VAL | 6 |
| 1 | B | 125 | GLN | 6 |
| 1 | A | 31 | HIS | 6 |
| 1 | A | 44 | LYS | 5 |
| 1 | B | 164 | GLN | 5 |
| 1 | B | 22 | LYS | 5 |
| 1 | A | 134 | LEU | 5 |
| 1 | B | 77 | GLU | 5 |
| 1 | B | 119 | GLN | 5 |
| 1 | B | 111 | ASP | 5 |
| 1 | A | 98 | SER | 5 |
| 1 | B | 12 | GLU | 5 |
| 1 | B | 42 | ILE | 5 |
| 1 | A | 115 | ARG | 5 |
| 1 | A | 119 | GLN | 5 |
| 1 | A | 192 | ASP | 5 |
| 1 | A | 13 | TRP | 4 |
| 1 | A | 194 | ASN | 4 |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1 | A | 117 | SER | 4 |
| 1 | A | 14 | PHE | 4 |
| 1 | B | 127 | THR | 4 |
| 1 | A | 40 | TYR | 4 |
| 1 | A | 158 | THR | 4 |
| 1 | A | 196 | ILE | 4 |
| 1 | A | 80 | GLN | 4 |
| 1 | B | 191 | GLU | 4 |
| 1 | A | 170 | GLN | 4 |
| 1 | A | 12 | GLU | 4 |
| 1 | B | 193 | GLN | 4 |
| 1 | B | 14 | PHE | 4 |
| 1 | A | 8 | ASP | 4 |
| 1 | B | 98 | SER | 4 |
| 1 | B | 115 | ARG | 4 |
| 1 | A | 127 | THR | 3 |
| 1 | B | 203 | ILE | 3 |
| 1 | B | 145 | GLN | 3 |
| 1 | B | 209 | ARG | 3 |
| 1 | B | 78 | GLU | 3 |
| 1 | B | 8 | ASP | 3 |
| 1 | B | 192 | ASP | 3 |
| 1 | A | 101 | LYS | 3 |
| 1 | B | 170 | GLN | 3 |
| 1 | B | 76 | PHE | 3 |
| 1 | A | 78 | GLU | 3 |
| 1 | A | 145 | GLN | 3 |
| 1 | B | 153 | GLN | 3 |
| 1 | B | 53 | ASP | 3 |
| 1 | A | 76 | PHE | 3 |
| 1 | B | 196 | ILE | 3 |
| 1 | B | 106 | ILE | 2 |
| 1 | A | 138 | ASP | 2 |
| 1 | A | 42 | ILE | 2 |
| 1 | A | 104 | GLN | 2 |
| 1 | A | 18 | CYS | 2 |
| 1 | B | 147 | LEU | 2 |
| 1 | A | 149 | ASN | 2 |
| 1 | B | 104 | GLN | 2 |
| 1 | B | 17 | HIS | 2 |
| 1 | A | 22 | LYS | 2 |
| 1 | A | 52 | LYS | 2 |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1 | A | 89 | LYS | 2 |
| 1 | B | 189 | MET | 2 |
| 1 | B | 52 | LYS | 2 |
| 1 | B | 46 | SER | 2 |
| 1 | B | 185 | ARG | 2 |
| 1 | A | 147 | LEU | 2 |
| 1 | B | 138 | ASP | 2 |
| 1 | B | 51 | ILE | 2 |
| 1 | B | 54 | GLU | 2 |
| 1 | A | 209 | ARG | 2 |
| 1 | A | 199 | HIS | 1 |
| 1 | B | 83 | SER | 1 |
| 1 | A | 43 | VAL | 1 |
| 1 | B | 18 | CYS | 1 |
| 1 | B | 186 | ILE | 1 |
| 1 | B | 129 | GLU | 1 |
| 1 | A | 143 | ILE | 1 |
| 1 | B | 199 | HIS | 1 |
| 1 | B | 37 | GLU | 1 |
| 1 | A | 171 | GLU | 1 |
| 1 | A | 17 | HIS | 1 |
| 1 | A | 37 | GLU | 1 |
| 1 | B | 117 | SER | 1 |
| 1 | A | 96 | GLU | 1 |
| 1 | A | 60 | ILE | 1 |
| 1 | A | 46 | SER | 1 |
| 1 | A | 137 | LEU | 1 |
| 1 | A | 97 | ILE | 1 |
| 1 | B | 24 | PRO | 1 |
| 1 | B | 107 | GLN | 1 |
| 1 | A | 178 | CYS | 1 |
| 1 | B | 133 | ASN | 1 |
| 1 | A | 203 | ILE | 1 |
| 1 | B | 59 | MET | 1 |
| 1 | A | 107 | GLN | 1 |
| 1 | A | 129 | GLU | 1 |
| 1 | B | 97 | ILE | 1 |
| 1 | B | 89 | LYS | 1 |
| 1 | B | 85 | TRP | 1 |
| 1 | A | 85 | TRP | 1 |
| 1 | A | 53 | ASP | 1 |
| 1 | A | 186 | ILE | 1 |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1 | A | 35 | LYS | 1 |
| 1 | B | 93 | GLU | 1 |
| 1 | A | 54 | GLU | 1 |
| 1 | A | 185 | ARG | 1 |
| 1 | A | 24 | PRO | 1 |
| 1 | A | 153 | GLN | 1 |
| 1 | B | 96 | GLU | 1 |
| 1 | B | 149 | ASN | 1 |
| 1 | A | 93 | GLU | 1 |
| 1 | B | 34 | GLU | 1 |
| 1 | B | 100 | LYS | 1 |
| 1 | A | 146 | THR | 1 |
| 1 | A | 51 | ILE | 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 carbohydrates in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided