# Full wwPDB NMR Structure Validation Report (i)

Oct 11, 2021 – 12:45 AM EDT

| | | |
|---|---|---|
| PDB ID | : | 2PQE |
| Title | : | Solution structure of proline-free mutant of staphylococcal nuclease |
| Authors | : | Shan, L.; Tong, Y.; Xie, T.; Wang, M.; Wang, J. |
| Deposited on | : | 2007-05-01 |

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
https://www.wwpdb.org/validation/2017/NMRValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

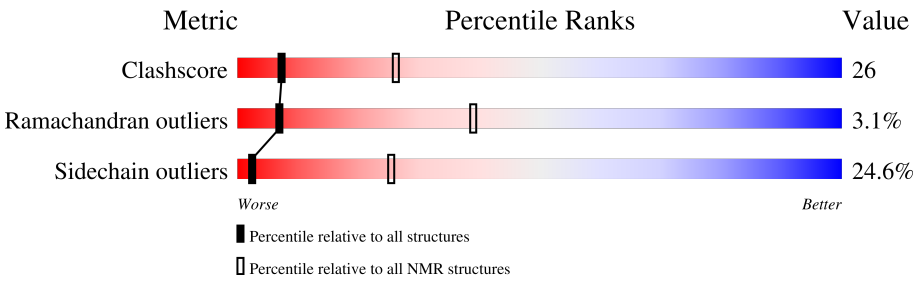
| | | |
|---|---|---|
| MolProbity | : | 4.02b-467 |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| RCI | : | v_1n_11_5_13_A (Berjanski et al., 2005) |
| PANAV | : | Wang et al. (2010) |
| ShiftChecker | : | 2.23.2 |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.23.2 |

# 1 Overall quality at a glance (i)

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 | 158937 | 12864 |
| Ramachandran outliers | 154571 | 11451 |
| Sidechain outliers | 154315 | 11428 |

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 <=5%

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | A | 149 | 32% 44% • 21% |

# 2 Ensemble composition and analysis (i)

This entry contains 21 models. Model 1 is the overall representative, medoid model (most similar to other models).

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

| Well-defined (core) protein residues | | | |
|---|---|---|---|
| **Well-defined core** | **Residue range (total)** | **Backbone RMSD (Å)** | **Medoid model** |
| 1 | A:9-A:42, A:53-A:112, A:118-A:141 (118) | 0.25 | 1 |

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

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

The models can be grouped into 4 clusters and 6 single-model clusters were found.

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

# 3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 2377 atoms, of which 1207 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Thermonuclease.

| Mol | Chain | Residues | Atoms | | | | | | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | H | N | O | S | |
| 1 | A | 149 | 2377 | 735 | 1207 | 206 | 225 | 4 | 0 |

There are 6 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| A | 11 | ALA | PRO | engineered mutation | UNP Q8NXI6 |
| A | 31 | ALA | PRO | engineered mutation | UNP Q8NXI6 |
| A | 42 | ALA | PRO | engineered mutation | UNP Q8NXI6 |
| A | 47 | THR | PRO | engineered mutation | UNP Q8NXI6 |
| A | 56 | ALA | PRO | engineered mutation | UNP Q8NXI6 |
| A | 117 | GLY | PRO | engineered mutation | UNP Q8NXI6 |

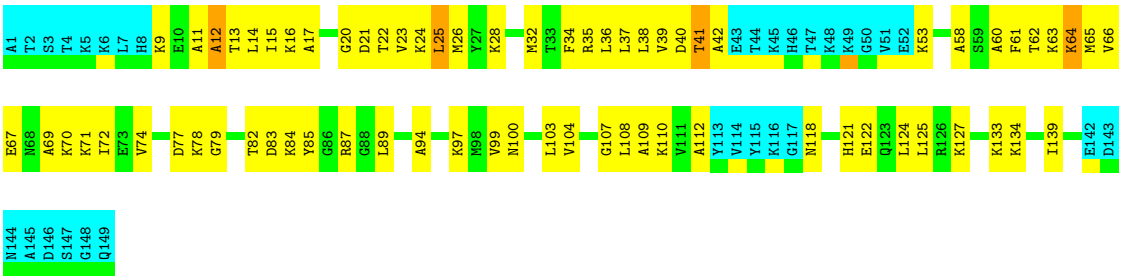
# 4 Residue-property plots (i)

## 4.1 Average score per residue in the NMR ensemble

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

• Molecule 1: Thermonuclease

Chain A: 32% 44% • 21%




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

Colouring as in section 4.1 above.

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

• Molecule 1: Thermonuclease

Chain A: 36% 38% 5% 21%

### 4.2.2 Score per residue for model 2

- Molecule 1: Thermonuclease

Chain A: 39% 36% • 21%

A1 T2 S3 T4 K5 K6 L7 H8 K9 E10 A11 A12 T13 L14 I15 K16 A17 D21 T22 V23 K24 L25 M26 Y27 K28 M32 T33 F34 R35 L36 L37 L38 V39 D40 T41 A42 E43 T44 K45 H46 T47 K48 K49 G50 V51 E52 K53 Y54 G55 A58 F61 T62 K63 K64 M65 V66

E67 N68 A69 K70 K71 I72 E73 V74 E75 F76 D77 K78 G79 T82 D83 K84 Y85 G86 R87 G88 L89 A90 V99 N100 L103 V104 R105 Q106 G107 L108 A109 Y113 V114 Y115 K116 G117 N118 N119 T120 H121 E122 K133 L137 E142 D143 N144 A145 D146 S147 G148 Q149

### 4.2.3 Score per residue for model 3

- Molecule 1: Thermonuclease

Chain A: 37% 36% 6% 21%

A1 T2 S3 T4 K5 K6 L7 H8 K9 E10 A11 A12 T13 L14 I15 K16 A17 G20 V23 K24 L25 M26 Y27 K28 R35 L36 L37 L38 V39 D40 T41 A42 E43 T44 K45 H46 T47 K48 K49 G50 V51 E52 K53 Y54 G55 A56 E57 A58 F61 T62 K63 K64 M65 V66 E67 N68

A69 K70 K71 I72 E73 V74 E75 F76 D77 Q80 K84 R87 G88 L89 Y93 A94 K97 M98 V99 N100 L103 V104 R105 Q106 G107 L108 A109 A112 Y113 V114 Y115 K116 G117 N118 H121 L124 L125 R126 K127 K133 K134 S141 E142 D143 N144 A145 D146 S147 G148

Q149

### 4.2.4 Score per residue for model 4

- Molecule 1: Thermonuclease

Chain A: 32% 38% 9% 21%

A1 T2 S3 T4 K5 K6 L7 H8 K9 E10 A11 A12 T13 L14 I15 K16 A17 I18 D19 G20 D21 T22 L25 M26 Y27 K28 F34 R35 L36 L37 L38 V39 D40 T41 A42 E43 T44 K45 H46 T47 K48 K49 G50 V51 E52 K53 E57 A58 S59 A60 F61 T62 K63 K64 M65 V66 E67

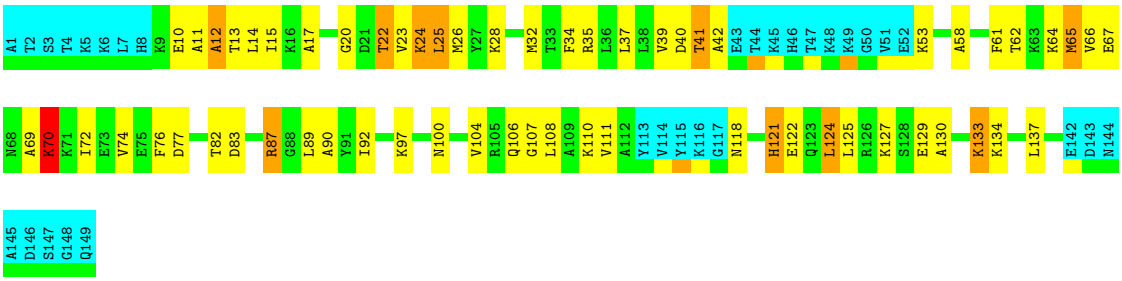
N68 A69 K70 K71 I72 E73 V74 D77 K78 G79 Q80 R81 T82 D83 K84 R87 G88 L89 A90 Y91 I92 Y93 A94 K97 M98 V99 N100 E101 A102 L103 V104 G107 L108 A109 K110 V111 A112 Y113 V114 Y115 K116 G117 H121 E122 Q123 L124 L125 R126 K127 K133 K134 E135 K136

I139 W140 S141 E142 D143 N144 A145 D146 S147 G148 Q149

### 4.2.5 Score per residue for model 5

- Molecule 1: Thermonuclease

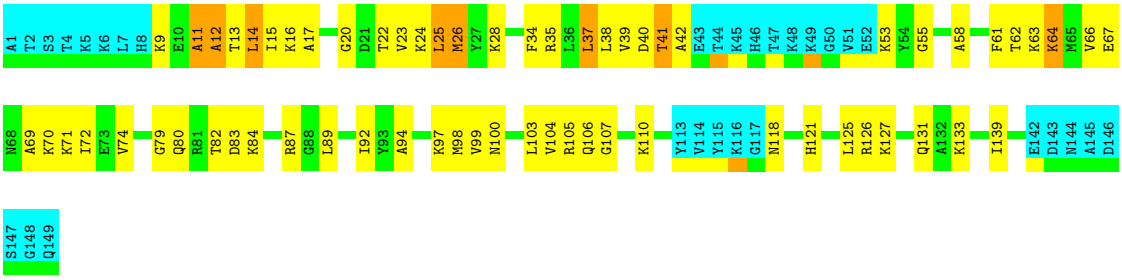
Chain A: 38% 34% 7% • 21%




### 4.2.6 Score per residue for model 6

- Molecule 1: Thermonuclease

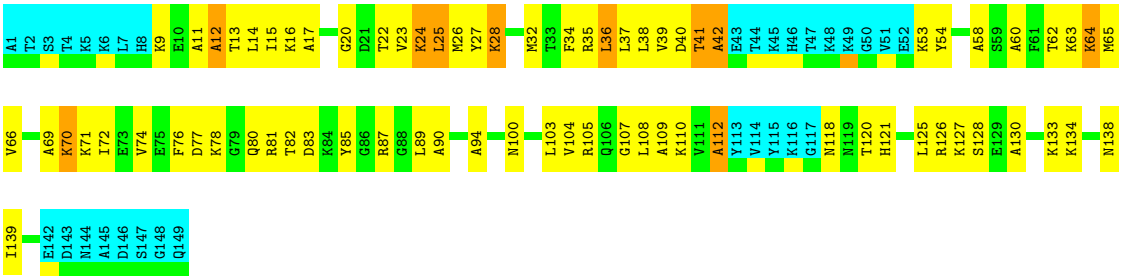
Chain A: 36% 38% 5% 21%




### 4.2.7 Score per residue for model 7

- Molecule 1: Thermonuclease

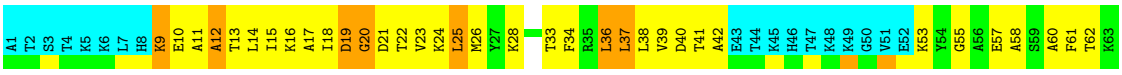
Chain A: 30% 42% 7% 21%

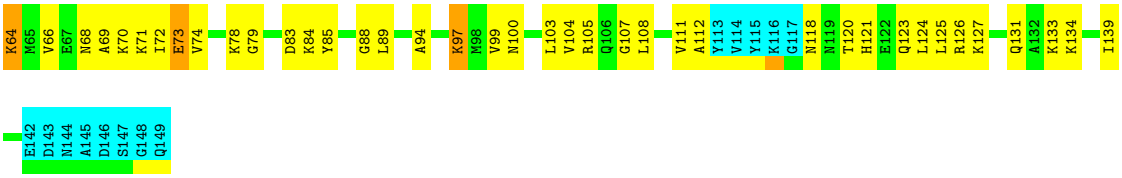



### 4.2.8 Score per residue for model 8

- Molecule 1: Thermonuclease

Chain A: 30% 43% 7% 21%






### 4.2.9 Score per residue for model 9

- Molecule 1: Thermonuclease

Chain A: 35% 39% 5% 21%

### 4.2.10 Score per residue for model 10

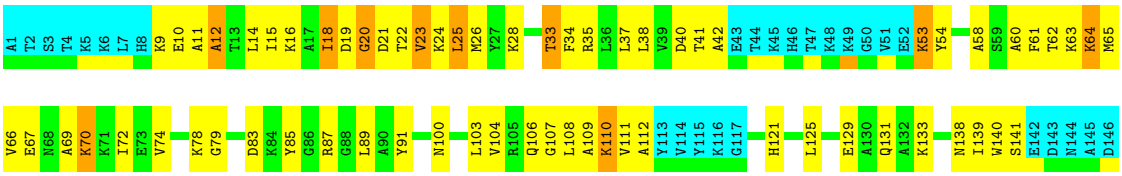
- Molecule 1: Thermonuclease

Chain A: 35% 38% 6% 21%

### 4.2.11 Score per residue for model 11

- Molecule 1: Thermonuclease

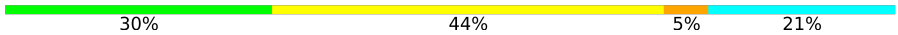
Chain A: 35% 38% 7% 21%

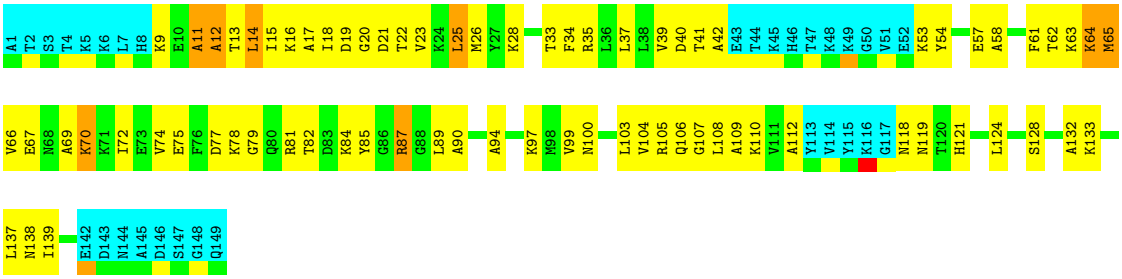


### 4.2.12 Score per residue for model 12

- Molecule 1: Thermonuclease

Chain A:

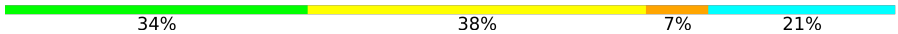


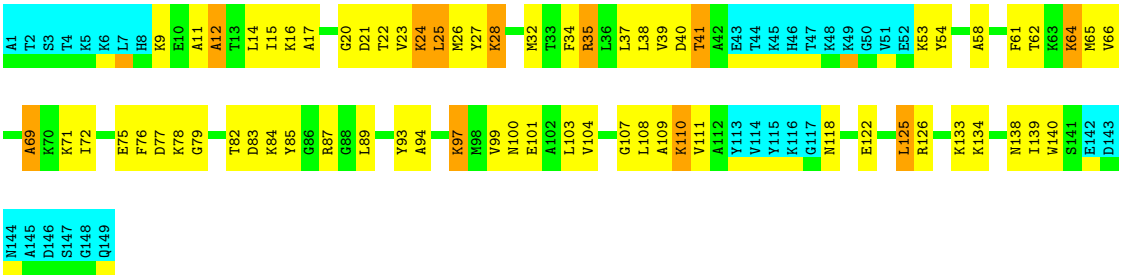




### 4.2.13 Score per residue for model 13

- Molecule 1: Thermonuclease

Chain A:

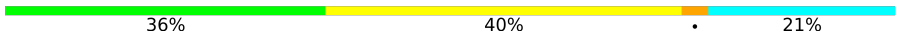



### 4.2.14 Score per residue for model 14

- Molecule 1: Thermonuclease

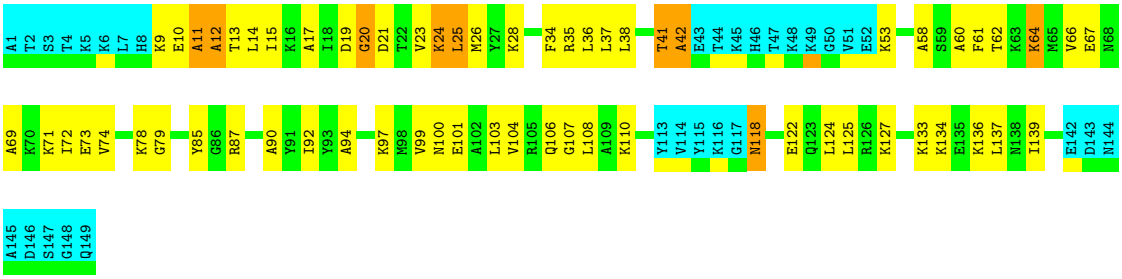
Chain A:



### 4.2.15 Score per residue for model 15

- Molecule 1: Thermonuclease

Chain A: 37% 36% 6% 21%




### 4.2.16 Score per residue for model 16

- Molecule 1: Thermonuclease

Chain A: 33% 40% 6% 21%

### 4.2.17 Score per residue for model 17

- Molecule 1: Thermonuclease

Chain A: 34% 38% 7% 21%

### 4.2.18 Score per residue for model 18

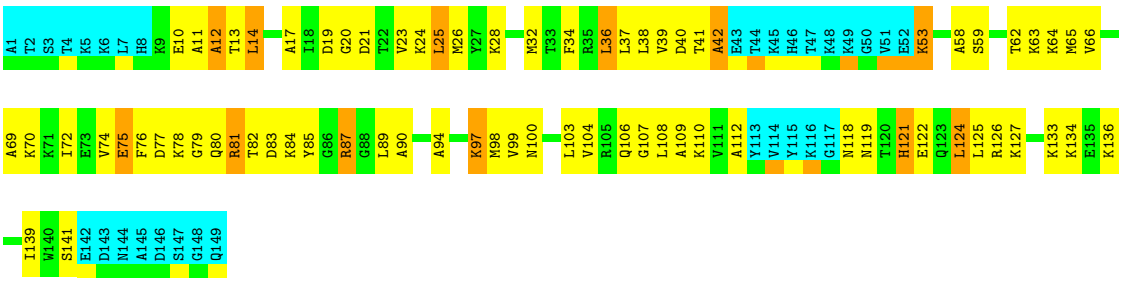
- Molecule 1: Thermonuclease

Chain A: 37% 38% 5% 21%

### 4.2.19 Score per residue for model 19

- Molecule 1: Thermonuclease

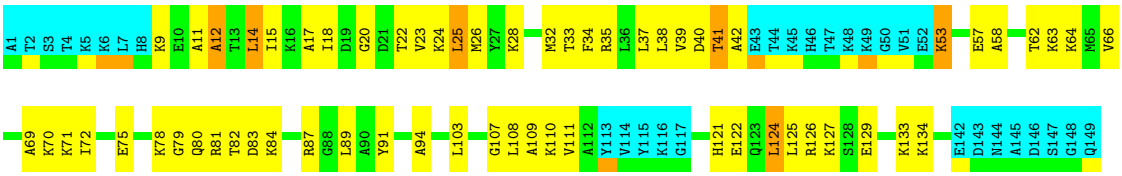
Chain A: 29% 42% 8% 21%




### 4.2.20 Score per residue for model 20

- Molecule 1: Thermonuclease

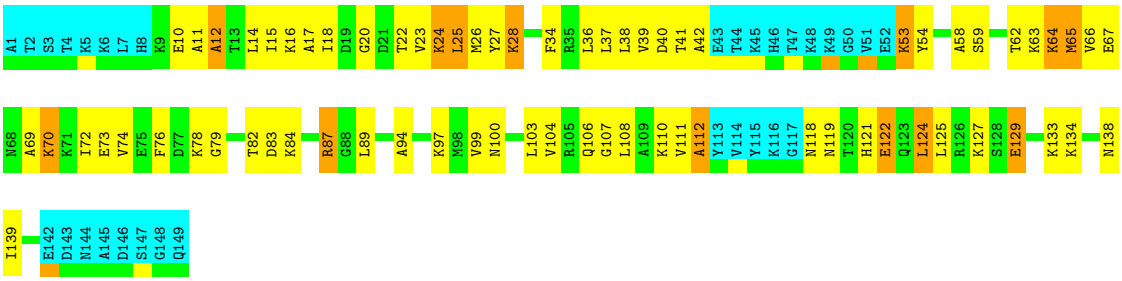
Chain A: 38% 38% • 21%




### 4.2.21 Score per residue for model 21

- Molecule 1: Thermonuclease

Chain A: 32% 39% 9% 21%


A1 T2 S3 T4 K5 K6 L7 H8 K9 E10 A11 A12 T13 L14 I15 K16 A17 I18 D19 G20 D21 T22 V23 K24 L25 M26 Y27 K28 F34 R35 L36 L37 L38 V39 D40 T41 A42 E43 T44 K45 H46 T47 K48 K49 G50 V51 E52 K53 Y54 A58 S59 T62 K63 K64 M65 V66 E67
N68 A69 K70 K71 I72 E73 V74 E75 F76 D77 K78 G79 T82 D83 K84 R87 G88 L89 A94 K97 M98 V99 N100 L103 V104 R105 Q106 G107 L108 A109 K110 V111 A112 Y113 V114 Y115 K116 G117 N118 N119 T120 H121 E122 Q123 L124 L125 R126 K127 S128 E129 K133 K134 N138
I139 E142 D143 N144 A145 D146 S147 G148 Q149

# 5 Refinement protocol and experimental data overview (i)

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

Of the 200 calculated structures, 21 were deposited, based on the following criterion: *structures with the lowest energy*.

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

| Software name | Classification | Version |
|---|---|---|
| CNS | refinement | 1.1 |
| CNS | structure solution | 1.1 |

No chemical shift data was provided.

# 6 Model quality (i)

## 6.1 Standard geometry (i)

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

## 6.2 Too-close contacts (i)

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes |
|---|---|---|---|---|---|
| 1 | A | 927 | 967 | 966 | 50±5 |
| All | All | 19467 | 20307 | 20286 | 1048 |

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 26.

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

| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|---|---|---|---|---|---|
| | | | | Worst | Total |
| 1:A:41:THR:HG22 | 1:A:58:ALA:HB1 | 1.08 | 1.15 | 13 | 21 |
| 1:A:14:LEU:HD13 | 1:A:66:VAL:HG21 | 0.91 | 1.40 | 12 | 1 |
| 1:A:14:LEU:HD13 | 1:A:66:VAL:CG2 | 0.82 | 2.04 | 12 | 1 |
| 1:A:41:THR:HG22 | 1:A:58:ALA:CB | 0.82 | 2.05 | 15 | 9 |
| 1:A:69:ALA:CB | 1:A:94:ALA:HB1 | 0.81 | 2.05 | 17 | 15 |
| 1:A:12:ALA:HB3 | 1:A:26:MET:O | 0.81 | 1.75 | 6 | 20 |
| 1:A:37:LEU:HD13 | 1:A:118:ASN:ND2 | 0.80 | 1.91 | 14 | 2 |
| 1:A:34:PHE:CE2 | 1:A:74:VAL:HG21 | 0.79 | 2.12 | 8 | 14 |
| 1:A:20:GLY:O | 1:A:62:THR:HG21 | 0.78 | 1.78 | 15 | 17 |
| 1:A:11:ALA:HB2 | 1:A:74:VAL:HG22 | 0.77 | 1.56 | 15 | 12 |
| 1:A:107:GLY:O | 1:A:139:ILE:HG23 | 0.77 | 1.79 | 14 | 16 |
| 1:A:69:ALA:HB2 | 1:A:94:ALA:HB1 | 0.77 | 1.56 | 20 | 15 |
| 1:A:37:LEU:HD22 | 1:A:118:ASN:ND2 | 0.77 | 1.94 | 12 | 3 |
| 1:A:18:ILE:HD12 | 1:A:22:THR:HG22 | 0.77 | 1.56 | 10 | 4 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|---|---|---|---|---|---|
| | | | | Worst | Total |
| 1:A:89:LEU:HD12 | 1:A:89:LEU:O | 0.76 | 1.80 | 17 | 4 |
| 1:A:36:LEU:HD22 | 1:A:39:VAL:HG21 | 0.76 | 1.57 | 10 | 5 |
| 1:A:41:THR:CG2 | 1:A:58:ALA:HB1 | 0.74 | 2.13 | 7 | 14 |
| 1:A:37:LEU:HD13 | 1:A:118:ASN:CG | 0.74 | 2.03 | 1 | 3 |
| 1:A:82:THR:HG22 | 1:A:87:ARG:O | 0.73 | 1.82 | 4 | 13 |
| 1:A:100:ASN:O | 1:A:104:VAL:HG23 | 0.73 | 1.83 | 3 | 18 |
| 1:A:121:HIS:O | 1:A:125:LEU:HD12 | 0.73 | 1.83 | 16 | 10 |
| 1:A:13:THR:O | 1:A:25:LEU:HD23 | 0.72 | 1.83 | 17 | 6 |
| 1:A:17:ALA:HB1 | 1:A:23:VAL:HG12 | 0.72 | 1.62 | 13 | 16 |
| 1:A:80:GLN:O | 1:A:89:LEU:HD11 | 0.71 | 1.85 | 20 | 4 |
| 1:A:17:ALA:CB | 1:A:23:VAL:HG12 | 0.71 | 2.16 | 9 | 16 |
| 1:A:111:VAL:HG23 | 1:A:129:GLU:HG3 | 0.71 | 1.62 | 5 | 1 |
| 1:A:25:LEU:HD11 | 1:A:72:ILE:CG2 | 0.71 | 2.15 | 17 | 17 |
| 1:A:37:LEU:O | 1:A:39:VAL:HG23 | 0.70 | 1.87 | 9 | 17 |
| 1:A:37:LEU:HD13 | 1:A:118:ASN:OD1 | 0.70 | 1.86 | 1 | 1 |
| 1:A:104:VAL:HG22 | 1:A:109:ALA:O | 0.70 | 1.87 | 11 | 5 |
| 1:A:18:ILE:O | 1:A:18:ILE:HD13 | 0.70 | 1.85 | 11 | 1 |
| 1:A:14:LEU:HD22 | 1:A:66:VAL:HB | 0.70 | 1.63 | 4 | 2 |
| 1:A:38:LEU:HD11 | 1:A:118:ASN:O | 0.69 | 1.87 | 16 | 4 |
| 1:A:25:LEU:HD11 | 1:A:72:ILE:HG21 | 0.69 | 1.65 | 11 | 16 |
| 1:A:62:THR:OG1 | 1:A:103:LEU:HD11 | 0.69 | 1.87 | 21 | 3 |
| 1:A:39:VAL:CG1 | 1:A:109:ALA:HB1 | 0.69 | 2.18 | 3 | 7 |
| 1:A:122:GLU:HA | 1:A:125:LEU:HD12 | 0.69 | 1.63 | 21 | 5 |
| 1:A:107:GLY:C | 1:A:108:LEU:HD12 | 0.69 | 2.08 | 16 | 7 |
| 1:A:38:LEU:HA | 1:A:112:ALA:HB3 | 0.68 | 1.65 | 17 | 7 |
| 1:A:14:LEU:HG | 1:A:66:VAL:HG22 | 0.68 | 1.64 | 8 | 2 |
| 1:A:74:VAL:HG12 | 1:A:92:ILE:HD13 | 0.68 | 1.64 | 14 | 6 |
| 1:A:34:PHE:CE2 | 1:A:74:VAL:HG11 | 0.68 | 2.23 | 5 | 4 |
| 1:A:39:VAL:HG12 | 1:A:109:ALA:HB1 | 0.67 | 1.65 | 17 | 9 |
| 1:A:14:LEU:HD13 | 1:A:14:LEU:O | 0.67 | 1.88 | 17 | 3 |
| 1:A:37:LEU:HD21 | 1:A:89:LEU:HD13 | 0.67 | 1.65 | 20 | 4 |
| 1:A:37:LEU:HD21 | 1:A:118:ASN:HB3 | 0.67 | 1.67 | 17 | 3 |
| 1:A:14:LEU:HD13 | 1:A:66:VAL:HB | 0.67 | 1.66 | 2 | 3 |
| 1:A:41:THR:HG21 | 1:A:103:LEU:HD22 | 0.66 | 1.65 | 20 | 2 |
| 1:A:14:LEU:HD21 | 1:A:23:VAL:CG2 | 0.65 | 2.21 | 11 | 1 |
| 1:A:38:LEU:HB3 | 1:A:125:LEU:HD13 | 0.65 | 1.67 | 4 | 5 |
| 1:A:15:ILE:HD11 | 1:A:26:MET:HG3 | 0.64 | 1.69 | 4 | 1 |
| 1:A:36:LEU:HD22 | 1:A:39:VAL:CG2 | 0.64 | 2.22 | 18 | 3 |
| 1:A:83:ASP:HB3 | 1:A:89:LEU:HD11 | 0.64 | 1.69 | 5 | 6 |
| 1:A:62:THR:O | 1:A:66:VAL:HG13 | 0.63 | 1.93 | 4 | 13 |
| 1:A:58:ALA:HA | 1:A:108:LEU:HD12 | 0.63 | 1.70 | 17 | 7 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|---|---|---|---|---|---|
| | | | | Worst | Total |
| 1:A:11:ALA:HB1 | 1:A:25:LEU:HD22 | 0.63 | 1.70 | 8 | 8 |
| 1:A:37:LEU:HD22 | 1:A:118:ASN:OD1 | 0.63 | 1.93 | 18 | 2 |
| 1:A:105:ARG:O | 1:A:137:LEU:HD13 | 0.63 | 1.94 | 16 | 1 |
| 1:A:25:LEU:HD13 | 1:A:74:VAL:CG1 | 0.63 | 2.22 | 14 | 4 |
| 1:A:111:VAL:HG23 | 1:A:129:GLU:CG | 0.62 | 2.24 | 5 | 2 |
| 1:A:38:LEU:HD12 | 1:A:118:ASN:ND2 | 0.62 | 2.09 | 3 | 1 |
| 1:A:11:ALA:HB3 | 1:A:73:GLU:HA | 0.62 | 1.69 | 8 | 3 |
| 1:A:22:THR:HG23 | 1:A:35:ARG:NE | 0.62 | 2.08 | 11 | 1 |
| 1:A:14:LEU:N | 1:A:72:ILE:HD13 | 0.62 | 2.10 | 8 | 5 |
| 1:A:121:HIS:CB | 1:A:124:LEU:HD21 | 0.62 | 2.23 | 5 | 4 |
| 1:A:15:ILE:HD11 | 1:A:26:MET:HB2 | 0.62 | 1.72 | 12 | 5 |
| 1:A:121:HIS:CG | 1:A:124:LEU:HD21 | 0.62 | 2.29 | 3 | 2 |
| 1:A:121:HIS:HB3 | 1:A:124:LEU:HD21 | 0.62 | 1.70 | 21 | 4 |
| 1:A:14:LEU:HD22 | 1:A:15:ILE:N | 0.62 | 2.08 | 13 | 14 |
| 1:A:37:LEU:HD21 | 1:A:118:ASN:CB | 0.62 | 2.25 | 13 | 1 |
| 1:A:72:ILE:HD12 | 1:A:72:ILE:N | 0.62 | 2.10 | 8 | 21 |
| 1:A:38:LEU:HD11 | 1:A:119:ASN:HA | 0.61 | 1.73 | 14 | 2 |
| 1:A:37:LEU:HD21 | 1:A:89:LEU:HD22 | 0.61 | 1.70 | 7 | 2 |
| 1:A:42:ALA:HB2 | 1:A:55:GLY:O | 0.61 | 1.95 | 8 | 4 |
| 1:A:25:LEU:HD11 | 1:A:72:ILE:HG22 | 0.61 | 1.71 | 17 | 5 |
| 1:A:65:MET:O | 1:A:69:ALA:HB2 | 0.61 | 1.96 | 5 | 10 |
| 1:A:42:ALA:HB2 | 1:A:55:GLY:HA2 | 0.61 | 1.71 | 2 | 1 |
| 1:A:62:THR:HG23 | 1:A:99:VAL:HG11 | 0.60 | 1.71 | 6 | 3 |
| 1:A:101:GLU:CD | 1:A:124:LEU:HD13 | 0.60 | 2.15 | 15 | 1 |
| 1:A:42:ALA:HB2 | 1:A:58:ALA:HB3 | 0.60 | 1.73 | 19 | 9 |
| 1:A:37:LEU:HD11 | 1:A:77:ASP:OD1 | 0.60 | 1.97 | 3 | 1 |
| 1:A:15:ILE:HD11 | 1:A:26:MET:CB | 0.60 | 2.26 | 13 | 2 |
| 1:A:62:THR:O | 1:A:66:VAL:HG22 | 0.60 | 1.97 | 2 | 14 |
| 1:A:99:VAL:HG12 | 1:A:103:LEU:CD1 | 0.59 | 2.27 | 1 | 11 |
| 1:A:18:ILE:CD1 | 1:A:33:THR:HG23 | 0.59 | 2.27 | 8 | 3 |
| 1:A:83:ASP:HB2 | 1:A:89:LEU:HD11 | 0.58 | 1.75 | 16 | 6 |
| 1:A:14:LEU:HD11 | 1:A:23:VAL:HG21 | 0.58 | 1.76 | 2 | 1 |
| 1:A:37:LEU:HD12 | 1:A:89:LEU:HD13 | 0.58 | 1.74 | 19 | 2 |
| 1:A:15:ILE:HD11 | 1:A:26:MET:CG | 0.58 | 2.29 | 4 | 1 |
| 1:A:107:GLY:O | 1:A:108:LEU:HD22 | 0.58 | 1.99 | 17 | 3 |
| 1:A:18:ILE:HG22 | 1:A:22:THR:O | 0.58 | 1.99 | 11 | 2 |
| 1:A:34:PHE:CZ | 1:A:74:VAL:HG21 | 0.57 | 2.34 | 4 | 4 |
| 1:A:121:HIS:C | 1:A:125:LEU:HD12 | 0.57 | 2.19 | 5 | 4 |
| 1:A:133:LYS:HG3 | 1:A:134:LYS:N | 0.57 | 2.14 | 5 | 1 |
| 1:A:36:LEU:HD22 | 1:A:92:ILE:HG12 | 0.57 | 1.74 | 16 | 1 |
| 1:A:14:LEU:HD22 | 1:A:15:ILE:H | 0.57 | 1.59 | 8 | 2 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|---|---|---|---|---|---|
| | | | | Worst | Total |
| 1:A:107:GLY:C | 1:A:108:LEU:HD22 | 0.57 | 2.19 | 20 | 11 |
| 1:A:38:LEU:HD12 | 1:A:91:TYR:OH | 0.57 | 1.99 | 1 | 1 |
| 1:A:33:THR:HG21 | 1:A:87:ARG:NH1 | 0.56 | 2.15 | 2 | 1 |
| 1:A:11:ALA:O | 1:A:12:ALA:HB2 | 0.56 | 2.00 | 17 | 19 |
| 1:A:57:GLU:HG2 | 1:A:108:LEU:HD21 | 0.56 | 1.77 | 9 | 1 |
| 1:A:83:ASP:HB2 | 1:A:89:LEU:HD23 | 0.56 | 1.77 | 17 | 4 |
| 1:A:14:LEU:HD13 | 1:A:66:VAL:CB | 0.55 | 2.32 | 2 | 3 |
| 1:A:38:LEU:HD22 | 1:A:122:GLU:OE1 | 0.55 | 2.01 | 15 | 1 |
| 1:A:39:VAL:HG13 | 1:A:109:ALA:HB1 | 0.55 | 1.77 | 18 | 1 |
| 1:A:37:LEU:CD2 | 1:A:89:LEU:HD22 | 0.54 | 2.31 | 16 | 4 |
| 1:A:37:LEU:HD11 | 1:A:118:ASN:ND2 | 0.54 | 2.17 | 13 | 2 |
| 1:A:75:GLU:O | 1:A:90:ALA:HB1 | 0.54 | 2.01 | 9 | 3 |
| 1:A:14:LEU:HD23 | 1:A:72:ILE:HD11 | 0.54 | 1.78 | 10 | 2 |
| 1:A:132:ALA:CB | 1:A:137:LEU:HD12 | 0.54 | 2.33 | 12 | 1 |
| 1:A:130:ALA:HB1 | 1:A:134:LYS:HE3 | 0.54 | 1.78 | 5 | 1 |
| 1:A:14:LEU:HD13 | 1:A:14:LEU:C | 0.53 | 2.23 | 17 | 2 |
| 1:A:21:ASP:O | 1:A:35:ARG:HA | 0.53 | 2.03 | 10 | 5 |
| 1:A:14:LEU:H | 1:A:72:ILE:HD13 | 0.53 | 1.62 | 21 | 9 |
| 1:A:14:LEU:CD1 | 1:A:23:VAL:HG21 | 0.53 | 2.34 | 2 | 1 |
| 1:A:17:ALA:HA | 1:A:23:VAL:HG12 | 0.53 | 1.81 | 6 | 13 |
| 1:A:17:ALA:CA | 1:A:23:VAL:HG12 | 0.53 | 2.34 | 6 | 13 |
| 1:A:14:LEU:C | 1:A:14:LEU:HD13 | 0.53 | 2.22 | 13 | 6 |
| 1:A:41:THR:O | 1:A:42:ALA:HB2 | 0.52 | 2.04 | 15 | 4 |
| 1:A:11:ALA:HB2 | 1:A:74:VAL:CG2 | 0.52 | 2.34 | 8 | 3 |
| 1:A:36:LEU:HD22 | 1:A:92:ILE:CG1 | 0.52 | 2.35 | 16 | 1 |
| 1:A:38:LEU:O | 1:A:125:LEU:HD23 | 0.51 | 2.05 | 10 | 1 |
| 1:A:111:VAL:O | 1:A:111:VAL:HG13 | 0.51 | 2.05 | 8 | 4 |
| 1:A:64:LYS:CD | 1:A:64:LYS:N | 0.51 | 2.73 | 13 | 4 |
| 1:A:69:ALA:O | 1:A:72:ILE:HD11 | 0.51 | 2.05 | 3 | 6 |
| 1:A:62:THR:O | 1:A:66:VAL:HG12 | 0.51 | 2.05 | 6 | 4 |
| 1:A:37:LEU:HD22 | 1:A:118:ASN:HD22 | 0.51 | 1.61 | 12 | 2 |
| 1:A:104:VAL:CG2 | 1:A:109:ALA:HB3 | 0.51 | 2.35 | 9 | 1 |
| 1:A:61:PHE:CD2 | 1:A:103:LEU:HD23 | 0.51 | 2.40 | 16 | 2 |
| 1:A:34:PHE:HB3 | 1:A:92:ILE:HD11 | 0.51 | 1.82 | 5 | 1 |
| 1:A:37:LEU:HD23 | 1:A:89:LEU:HD22 | 0.51 | 1.82 | 18 | 2 |
| 1:A:91:TYR:OH | 1:A:125:LEU:HD11 | 0.51 | 2.06 | 1 | 1 |
| 1:A:18:ILE:CD1 | 1:A:22:THR:HG22 | 0.51 | 2.36 | 8 | 1 |
| 1:A:41:THR:O | 1:A:42:ALA:HB3 | 0.51 | 2.06 | 4 | 9 |
| 1:A:10:GLU:O | 1:A:74:VAL:HG22 | 0.50 | 2.05 | 5 | 3 |
| 1:A:80:GLN:HG2 | 1:A:89:LEU:HD12 | 0.50 | 1.84 | 10 | 1 |
| 1:A:14:LEU:CG | 1:A:66:VAL:HG22 | 0.50 | 2.34 | 8 | 2 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|---|---|---|---|---|---|
| | | | | Worst | Total |
| 1:A:11:ALA:HB1 | 1:A:25:LEU:CD2 | 0.50 | 2.35 | 8 | 1 |
| 1:A:14:LEU:HD22 | 1:A:24:LYS:O | 0.50 | 2.07 | 3 | 10 |
| 1:A:61:PHE:HD2 | 1:A:108:LEU:HD22 | 0.50 | 1.67 | 16 | 1 |
| 1:A:37:LEU:HD11 | 1:A:89:LEU:HD13 | 0.50 | 1.83 | 7 | 1 |
| 1:A:37:LEU:HD23 | 1:A:38:LEU:HG | 0.49 | 1.83 | 17 | 2 |
| 1:A:132:ALA:HA | 1:A:137:LEU:HD12 | 0.49 | 1.83 | 10 | 1 |
| 1:A:54:TYR:HB2 | 1:A:139:ILE:HG22 | 0.49 | 1.83 | 12 | 1 |
| 1:A:121:HIS:HB3 | 1:A:124:LEU:HD12 | 0.49 | 1.82 | 17 | 3 |
| 1:A:37:LEU:CD2 | 1:A:89:LEU:HD13 | 0.49 | 2.37 | 20 | 1 |
| 1:A:99:VAL:HG12 | 1:A:103:LEU:HD11 | 0.48 | 1.86 | 1 | 1 |
| 1:A:99:VAL:HG12 | 1:A:103:LEU:HD12 | 0.48 | 1.85 | 12 | 7 |
| 1:A:69:ALA:O | 1:A:70:LYS:HB2 | 0.48 | 2.08 | 19 | 4 |
| 1:A:18:ILE:HD13 | 1:A:18:ILE:C | 0.48 | 2.27 | 11 | 1 |
| 1:A:62:THR:HG1 | 1:A:103:LEU:HD11 | 0.48 | 1.66 | 21 | 1 |
| 1:A:19:ASP:O | 1:A:21:ASP:N | 0.48 | 2.47 | 4 | 5 |
| 1:A:103:LEU:HD23 | 1:A:108:LEU:HB2 | 0.48 | 1.86 | 7 | 1 |
| 1:A:38:LEU:HD13 | 1:A:125:LEU:CD1 | 0.48 | 2.39 | 21 | 1 |
| 1:A:120:THR:HG22 | 1:A:121:HIS:CD2 | 0.48 | 2.44 | 8 | 1 |
| 1:A:37:LEU:HD12 | 1:A:90:ALA:HA | 0.48 | 1.86 | 15 | 4 |
| 1:A:22:THR:HG23 | 1:A:35:ARG:HG2 | 0.48 | 1.84 | 5 | 2 |
| 1:A:64:LYS:N | 1:A:64:LYS:HD2 | 0.48 | 2.24 | 12 | 1 |
| 1:A:36:LEU:HD13 | 1:A:39:VAL:HG11 | 0.47 | 1.86 | 4 | 2 |
| 1:A:61:PHE:CD2 | 1:A:108:LEU:HD22 | 0.47 | 2.44 | 16 | 1 |
| 1:A:111:VAL:HG23 | 1:A:129:GLU:OE2 | 0.47 | 2.09 | 20 | 1 |
| 1:A:65:MET:SD | 1:A:99:VAL:HG22 | 0.47 | 2.49 | 3 | 1 |
| 1:A:25:LEU:CB | 1:A:34:PHE:CD1 | 0.47 | 2.98 | 17 | 4 |
| 1:A:17:ALA:HB3 | 1:A:63:LYS:HB3 | 0.47 | 1.85 | 17 | 1 |
| 1:A:25:LEU:HD13 | 1:A:74:VAL:HG13 | 0.47 | 1.86 | 14 | 1 |
| 1:A:103:LEU:HD23 | 1:A:108:LEU:CB | 0.47 | 2.39 | 7 | 1 |
| 1:A:17:ALA:HA | 1:A:23:VAL:HG23 | 0.47 | 1.87 | 10 | 2 |
| 1:A:42:ALA:HB2 | 1:A:55:GLY:CA | 0.47 | 2.40 | 2 | 1 |
| 1:A:121:HIS:O | 1:A:125:LEU:HD13 | 0.47 | 2.09 | 11 | 1 |
| 1:A:32:MET:CG | 1:A:34:PHE:CE1 | 0.47 | 2.98 | 20 | 11 |
| 1:A:10:GLU:O | 1:A:11:ALA:HB3 | 0.46 | 2.09 | 15 | 2 |
| 1:A:89:LEU:O | 1:A:90:ALA:HB2 | 0.46 | 2.11 | 14 | 7 |
| 1:A:14:LEU:CD2 | 1:A:23:VAL:CG2 | 0.46 | 2.93 | 11 | 1 |
| 1:A:41:THR:CG2 | 1:A:103:LEU:HD22 | 0.46 | 2.38 | 20 | 1 |
| 1:A:11:ALA:HB2 | 1:A:74:VAL:HG13 | 0.46 | 1.88 | 17 | 1 |
| 1:A:72:ILE:HG23 | 1:A:93:TYR:O | 0.46 | 2.10 | 3 | 4 |
| 1:A:58:ALA:CA | 1:A:108:LEU:HD12 | 0.46 | 2.41 | 17 | 1 |
| 1:A:111:VAL:HG23 | 1:A:129:GLU:CD | 0.46 | 2.31 | 14 | 2 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|---|---|---|---|---|---|
| | | | | Worst | Total |
| 1:A:61:PHE:CD1 | 1:A:103:LEU:CD2 | 0.46 | 2.99 | 17 | 13 |
| 1:A:61:PHE:HD2 | 1:A:103:LEU:HD23 | 0.46 | 1.71 | 16 | 2 |
| 1:A:69:ALA:O | 1:A:70:LYS:CB | 0.45 | 2.64 | 11 | 11 |
| 1:A:107:GLY:O | 1:A:108:LEU:HD12 | 0.45 | 2.10 | 16 | 3 |
| 1:A:66:VAL:HG23 | 1:A:67:GLU:N | 0.45 | 2.26 | 15 | 11 |
| 1:A:36:LEU:HB3 | 1:A:39:VAL:HB | 0.45 | 1.88 | 19 | 1 |
| 1:A:37:LEU:HG | 1:A:89:LEU:HD22 | 0.45 | 1.87 | 2 | 1 |
| 1:A:121:HIS:CD2 | 1:A:124:LEU:HD21 | 0.45 | 2.47 | 4 | 2 |
| 1:A:57:GLU:HG2 | 1:A:108:LEU:HD11 | 0.45 | 1.89 | 1 | 1 |
| 1:A:108:LEU:HD12 | 1:A:108:LEU:N | 0.45 | 2.26 | 11 | 2 |
| 1:A:11:ALA:O | 1:A:12:ALA:CB | 0.45 | 2.65 | 17 | 9 |
| 1:A:91:TYR:CZ | 1:A:121:HIS:ND1 | 0.45 | 2.85 | 11 | 1 |
| 1:A:60:ALA:O | 1:A:64:LYS:HG2 | 0.45 | 2.12 | 17 | 2 |
| 1:A:64:LYS:N | 1:A:64:LYS:HD3 | 0.45 | 2.27 | 21 | 3 |
| 1:A:63:LYS:CD | 1:A:64:LYS:CD | 0.45 | 2.94 | 12 | 1 |
| 1:A:22:THR:HG23 | 1:A:35:ARG:CD | 0.45 | 2.41 | 11 | 1 |
| 1:A:110:LYS:CB | 1:A:140:TRP:CZ2 | 0.44 | 3.00 | 13 | 3 |
| 1:A:76:PHE:CE1 | 1:A:81:ARG:CG | 0.44 | 3.00 | 7 | 2 |
| 1:A:89:LEU:HD12 | 1:A:89:LEU:C | 0.44 | 2.32 | 19 | 3 |
| 1:A:54:TYR:CE1 | 1:A:138:ASN:ND2 | 0.44 | 2.86 | 12 | 2 |
| 1:A:15:ILE:CD1 | 1:A:26:MET:N | 0.44 | 2.80 | 8 | 5 |
| 1:A:85:TYR:CD2 | 1:A:87:ARG:NH2 | 0.44 | 2.85 | 11 | 1 |
| 1:A:58:ALA:HA | 1:A:108:LEU:HD23 | 0.44 | 1.89 | 16 | 1 |
| 1:A:39:VAL:HG22 | 1:A:125:LEU:HD23 | 0.44 | 1.88 | 14 | 1 |
| 1:A:13:THR:O | 1:A:26:MET:N | 0.44 | 2.48 | 15 | 9 |
| 1:A:41:THR:HG23 | 1:A:58:ALA:HB1 | 0.44 | 1.89 | 8 | 1 |
| 1:A:92:ILE:O | 1:A:99:VAL:HG23 | 0.44 | 2.13 | 16 | 1 |
| 1:A:69:ALA:HB1 | 1:A:95:ASP:N | 0.43 | 2.28 | 17 | 1 |
| 1:A:37:LEU:HD13 | 1:A:118:ASN:HD22 | 0.43 | 1.71 | 14 | 1 |
| 1:A:101:GLU:OE2 | 1:A:124:LEU:HD13 | 0.43 | 2.13 | 15 | 1 |
| 1:A:38:LEU:HD13 | 1:A:125:LEU:HD13 | 0.43 | 1.90 | 18 | 1 |
| 1:A:100:ASN:ND2 | 1:A:124:LEU:HD11 | 0.43 | 2.28 | 4 | 1 |
| 1:A:14:LEU:HG | 1:A:66:VAL:CG2 | 0.43 | 2.44 | 21 | 2 |
| 1:A:54:TYR:O | 1:A:58:ALA:HB2 | 0.43 | 2.13 | 17 | 1 |
| 1:A:11:ALA:CB | 1:A:74:VAL:HG22 | 0.43 | 2.38 | 8 | 1 |
| 1:A:36:LEU:HD13 | 1:A:39:VAL:CG1 | 0.43 | 2.43 | 4 | 1 |
| 1:A:60:ALA:O | 1:A:64:LYS:CG | 0.42 | 2.67 | 4 | 10 |
| 1:A:61:PHE:CB | 1:A:108:LEU:CD2 | 0.42 | 2.97 | 11 | 1 |
| 1:A:17:ALA:HB3 | 1:A:63:LYS:HG2 | 0.42 | 1.91 | 20 | 1 |
| 1:A:27:TYR:O | 1:A:28:LYS:HG3 | 0.42 | 2.14 | 21 | 3 |
| 1:A:93:TYR:CE2 | 1:A:98:MET:HE2 | 0.42 | 2.49 | 3 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|---|---|---|---|---|---|
| | | | | Worst | Total |
| 1:A:98:MET:CE | 1:A:124:LEU:HD13 | 0.42 | 2.44 | 18 | 1 |
| 1:A:123:GLN:NE2 | 1:A:124:LEU:HD21 | 0.42 | 2.30 | 10 | 1 |
| 1:A:111:VAL:HG23 | 1:A:129:GLU:CB | 0.42 | 2.45 | 5 | 1 |
| 1:A:121:HIS:CG | 1:A:124:LEU:HD12 | 0.42 | 2.50 | 8 | 1 |
| 1:A:72:ILE:N | 1:A:72:ILE:CD1 | 0.42 | 2.82 | 5 | 6 |
| 1:A:94:ALA:O | 1:A:97:LYS:N | 0.42 | 2.52 | 18 | 11 |
| 1:A:41:THR:HG23 | 1:A:108:LEU:O | 0.42 | 2.15 | 14 | 1 |
| 1:A:62:THR:O | 1:A:66:VAL:CG1 | 0.42 | 2.67 | 12 | 1 |
| 1:A:36:LEU:HD21 | 1:A:100:ASN:HB3 | 0.41 | 1.92 | 4 | 1 |
| 1:A:66:VAL:HG13 | 1:A:67:GLU:N | 0.41 | 2.30 | 6 | 1 |
| 1:A:27:TYR:CD2 | 1:A:28:LYS:HD3 | 0.41 | 2.49 | 7 | 1 |
| 1:A:59:SER:O | 1:A:63:LYS:CB | 0.41 | 2.68 | 21 | 1 |
| 1:A:32:MET:HG3 | 1:A:34:PHE:CE1 | 0.41 | 2.50 | 2 | 4 |
| 1:A:54:TYR:CZ | 1:A:138:ASN:OD1 | 0.41 | 2.73 | 14 | 1 |
| 1:A:9:LYS:HB3 | 1:A:93:TYR:CD1 | 0.41 | 2.51 | 1 | 1 |
| 1:A:76:PHE:CE2 | 1:A:89:LEU:O | 0.41 | 2.74 | 17 | 3 |
| 1:A:76:PHE:CD2 | 1:A:89:LEU:O | 0.41 | 2.73 | 18 | 3 |
| 1:A:25:LEU:HB3 | 1:A:34:PHE:CD1 | 0.41 | 2.50 | 15 | 5 |
| 1:A:37:LEU:CD1 | 1:A:89:LEU:HD13 | 0.41 | 2.45 | 19 | 2 |
| 1:A:36:LEU:HD22 | 1:A:100:ASN:HB3 | 0.41 | 1.93 | 9 | 2 |
| 1:A:130:ALA:HB1 | 1:A:134:LYS:CE | 0.41 | 2.45 | 7 | 1 |
| 1:A:38:LEU:CA | 1:A:112:ALA:HB3 | 0.41 | 2.46 | 8 | 1 |
| 1:A:61:PHE:O | 1:A:61:PHE:CD1 | 0.41 | 2.74 | 5 | 1 |
| 1:A:9:LYS:CD | 1:A:9:LYS:N | 0.41 | 2.84 | 3 | 1 |
| 1:A:71:LYS:CE | 1:A:73:GLU:CG | 0.41 | 2.99 | 3 | 1 |
| 1:A:54:TYR:CZ | 1:A:138:ASN:CB | 0.41 | 3.04 | 10 | 4 |
| 1:A:33:THR:CG2 | 1:A:35:ARG:NH1 | 0.41 | 2.83 | 11 | 1 |
| 1:A:41:THR:O | 1:A:42:ALA:CB | 0.41 | 2.69 | 15 | 1 |
| 1:A:41:THR:HG23 | 1:A:109:ALA:HB2 | 0.41 | 1.92 | 17 | 1 |
| 1:A:76:PHE:CE1 | 1:A:81:ARG:HG2 | 0.41 | 2.51 | 1 | 1 |
| 1:A:76:PHE:CD1 | 1:A:89:LEU:O | 0.41 | 2.74 | 13 | 3 |
| 1:A:83:ASP:O | 1:A:85:TYR:CD2 | 0.41 | 2.74 | 8 | 2 |
| 1:A:39:VAL:HG22 | 1:A:125:LEU:CD2 | 0.41 | 2.46 | 16 | 1 |
| 1:A:84:LYS:O | 1:A:85:TYR:CD1 | 0.41 | 2.74 | 12 | 2 |
| 1:A:69:ALA:HB1 | 1:A:95:ASP:HB2 | 0.41 | 1.91 | 17 | 1 |
| 1:A:91:TYR:HE2 | 1:A:125:LEU:HD21 | 0.41 | 1.75 | 20 | 1 |
| 1:A:76:PHE:CE1 | 1:A:89:LEU:O | 0.40 | 2.74 | 2 | 1 |
| 1:A:38:LEU:CD1 | 1:A:125:LEU:CD1 | 0.40 | 2.99 | 20 | 1 |
| 1:A:98:MET:CB | 1:A:101:GLU:CG | 0.40 | 3.00 | 10 | 1 |
| 1:A:21:ASP:OD1 | 1:A:36:LEU:HD12 | 0.40 | 2.16 | 15 | 1 |
| 1:A:130:ALA:O | 1:A:134:LYS:N | 0.40 | 2.54 | 16 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|---|---|---|---|---|---|
| | | | | Worst | Total |
| 1:A:66:VAL:CG1 | 1:A:67:GLU:N | 0.40 | 2.84 | 6 | 1 |
| 1:A:14:LEU:HD22 | 1:A:14:LEU:C | 0.40 | 2.35 | 20 | 1 |
| 1:A:76:PHE:CE2 | 1:A:81:ARG:HG3 | 0.40 | 2.51 | 19 | 1 |
| 1:A:17:ALA:HB3 | 1:A:63:LYS:CG | 0.40 | 2.46 | 20 | 1 |

## 6.3 Torsion angles (i)

### 6.3.1 Protein backbone (i)

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 1 | A | 118/149 (79%) | 95±2 (80±2%) | 19±3 (16±2%) | 4±1 (3±1%) | 7 | 39 |
| All | All | 2478/3129 (79%) | 1993 (80%) | 407 (16%) | 78 (3%) | 7 | 39 |

All 13 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

| Mol | Chain | Res | Type | Models (Total) |
|---|---|---|---|---|
| 1 | A | 12 | ALA | 21 |
| 1 | A | 79 | GLY | 12 |
| 1 | A | 112 | ALA | 8 |
| 1 | A | 42 | ALA | 7 |
| 1 | A | 20 | GLY | 5 |
| 1 | A | 53 | LYS | 5 |
| 1 | A | 84 | LYS | 4 |
| 1 | A | 70 | LYS | 4 |
| 1 | A | 137 | LEU | 3 |
| 1 | A | 118 | ASN | 3 |
| 1 | A | 11 | ALA | 3 |
| 1 | A | 88 | GLY | 2 |
| 1 | A | 69 | ALA | 1 |

### 6.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR

entries. The Analysed column shows the number of residues for which the sidechain conformation was analysed and the total number of residues.

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|---|---|---|---|---|---|
| 1 | A | 94/120 (78%) | 71±3 (75±3%) | 23±3 (25±3%) | 2 25 |
| All | All | 1974/2520 (78%) | 1489 (75%) | 485 (25%) | 2 25 |

All 61 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 | LEU | 21 |
| 1 | A | 28 | LYS | 21 |
| 1 | A | 64 | LYS | 21 |
| 1 | A | 133 | LYS | 21 |
| 1 | A | 53 | LYS | 20 |
| 1 | A | 9 | LYS | 17 |
| 1 | A | 16 | LYS | 17 |
| 1 | A | 40 | ASP | 17 |
| 1 | A | 110 | LYS | 17 |
| 1 | A | 127 | LYS | 17 |
| 1 | A | 78 | LYS | 14 |
| 1 | A | 41 | THR | 13 |
| 1 | A | 24 | LYS | 13 |
| 1 | A | 134 | LYS | 11 |
| 1 | A | 71 | LYS | 11 |
| 1 | A | 35 | ARG | 10 |
| 1 | A | 77 | ASP | 10 |
| 1 | A | 63 | LYS | 10 |
| 1 | A | 87 | ARG | 10 |
| 1 | A | 84 | LYS | 10 |
| 1 | A | 106 | GLN | 10 |
| 1 | A | 65 | MET | 9 |
| 1 | A | 126 | ARG | 9 |
| 1 | A | 36 | LEU | 9 |
| 1 | A | 22 | THR | 8 |
| 1 | A | 14 | LEU | 8 |
| 1 | A | 97 | LYS | 8 |
| 1 | A | 57 | GLU | 7 |
| 1 | A | 105 | ARG | 7 |
| 1 | A | 136 | LYS | 7 |
| 1 | A | 85 | TYR | 7 |
| 1 | A | 81 | ARG | 6 |
| 1 | A | 122 | GLU | 6 |

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| Mol | Chain | Res | Type | Models (Total) |
|---|---|---|---|---|
| 1 | A | 131 | GLN | 6 |
| 1 | A | 141 | SER | 6 |
| 1 | A | 75 | GLU | 6 |
| 1 | A | 70 | LYS | 6 |
| 1 | A | 124 | LEU | 5 |
| 1 | A | 67 | GLU | 5 |
| 1 | A | 98 | MET | 5 |
| 1 | A | 121 | HIS | 4 |
| 1 | A | 80 | GLN | 4 |
| 1 | A | 101 | GLU | 3 |
| 1 | A | 128 | SER | 3 |
| 1 | A | 19 | ASP | 3 |
| 1 | A | 123 | GLN | 3 |
| 1 | A | 120 | THR | 2 |
| 1 | A | 26 | MET | 2 |
| 1 | A | 37 | LEU | 2 |
| 1 | A | 10 | GLU | 2 |
| 1 | A | 68 | ASN | 2 |
| 1 | A | 33 | THR | 2 |
| 1 | A | 129 | GLU | 2 |
| 1 | A | 119 | ASN | 2 |
| 1 | A | 59 | SER | 2 |
| 1 | A | 89 | LEU | 1 |
| 1 | A | 73 | GLU | 1 |
| 1 | A | 30 | GLN | 1 |
| 1 | A | 18 | ILE | 1 |
| 1 | A | 23 | VAL | 1 |
| 1 | A | 125 | LEU | 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 monosaccharides 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 (i)

No chemical shift data were provided