# Full wwPDB NMR Structure Validation Report (i)

Oct 17, 2021 – 09:20 AM EDT

| | | |
|---|---|---|
| PDB ID | : | 1JOR |
| Title | : | Ensemble structures for unligated Staphylococcal nuclease-H124L |
| Authors | : | Wang, J.; Truckses, D.M.; Abildgaard, F.; Dzakula, Z.; Zolnai, Z.; Markley, J.L. |
| Deposited on | : | 2001-07-30 |

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:

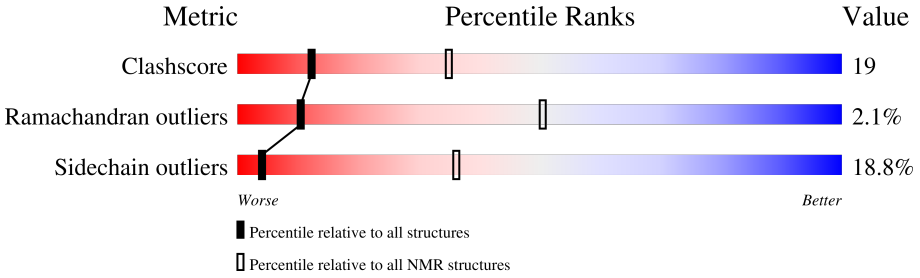
| | | |
|---|---|---|
| MolProbity | : | 4.02b-467 |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| RCI | : | v_1n_11_5_13_A (Berjanski et al., 2005) |
| PANAV | : | Wang et al. (2010) |
| ShiftChecker | : | 2.23.2 |
| Ideal geometry (proteins) | : | 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 | 40% 37% • 21% |

# 2 Ensemble composition and analysis (i)

This entry contains 30 models. Model 16 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:41, A:57-A:141 (118) | 0.34 | 16 |

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 7 clusters and 7 single-model clusters were found.

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

# 3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 2397 atoms, of which 1216 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called staphylococcal nuclease.

| Mol | Chain | Residues | Atoms | | | | | | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | H | N | O | S | |
| 1 | A | 149 | 2397 | 747 | 1216 | 206 | 224 | 4 | 0 |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| A | 124 | LEU | HIS | engineered mutation | UNP P00644 |

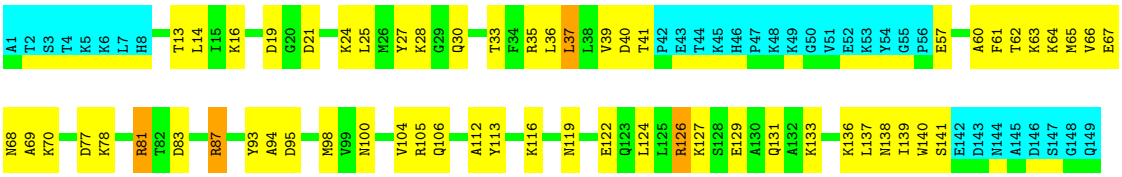
# 4 Residue-property plots (i)

## 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: staphylococcal nuclease

Chain A: 40% 37% • 21%



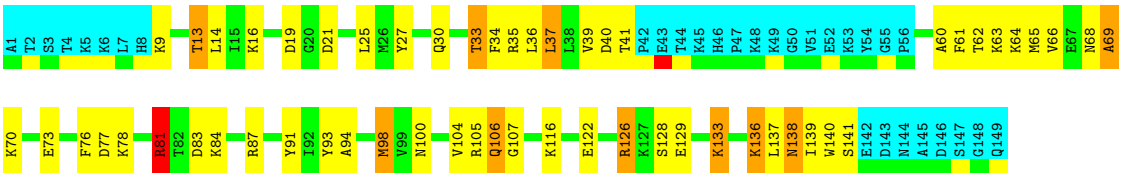

## 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

### 4.2.1 Score per residue for model 1

• Molecule 1: staphylococcal nuclease

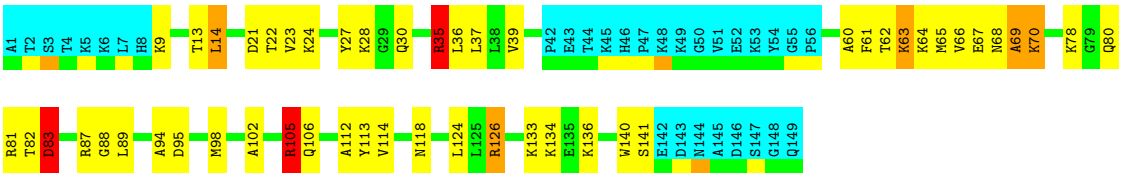
Chain A: 42% 30% 7% • 21%




### 4.2.2 Score per residue for model 2

• Molecule 1: staphylococcal nuclease

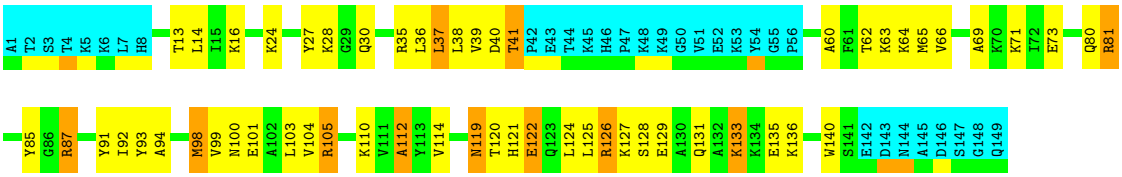
Chain A: 46% 28% • • 21%




### 4.2.3 Score per residue for model 3

- Molecule 1: staphylococcal nuclease

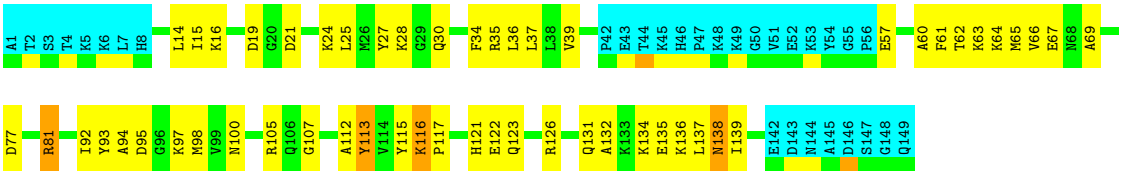
Chain A: 42% 30% 7% 21%




### 4.2.4 Score per residue for model 4

- Molecule 1: staphylococcal nuclease

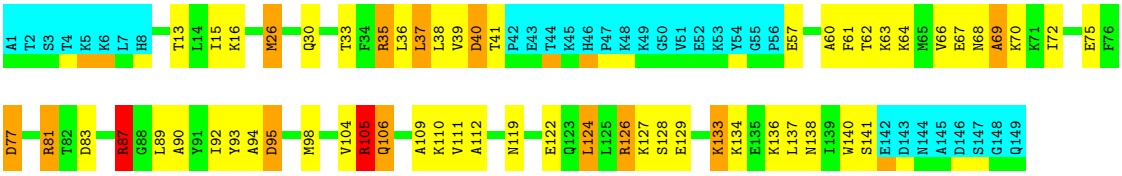
Chain A: 44% 33% • 21%




### 4.2.5 Score per residue for model 5

- Molecule 1: staphylococcal nuclease

Chain A: 40% 30% 8% • 21%




### 4.2.6 Score per residue for model 6

- Molecule 1: staphylococcal nuclease

Chain A: 44% 30% 5% • 21%

A1 T2 S3 T4 K5 K6 L7 H8 L14 I15 K16 D19 V23 K24 L25 M26 Y27 K28 L36 L37 L38 V39 D40 T41 P42 E43 T44 K45 H46 P47 K48 K49 G50 V51 E52 K53 Y54 G55 P56 E57 A58 S59 A60 F61 T62 K63 K64 M65 V66 E67 N68 A69 K70 E73

K78 G79 Q80 R81 T82 D83 K84 Y85 G86 R87 G88 L89 Y93 A94 D95 M98 L103 V104 R105 Q106 G107 L108 A109 Y113 V114 Y115 K116 N119 E122 Q123 L124 L125 R126 Q131 L137 N138 E142 D143 N144 A145 D146 S147 G148 Q149

### 4.2.7 Score per residue for model 7

- Molecule 1: staphylococcal nuclease

Chain A: 42% 30% 8% 21%

A1 T2 S3 T4 K5 K6 L7 H8 K9 L14 I15 K16 D21 K24 T33 F34 R35 L36 L37 L38 V39 D40 T41 P42 E43 T44 K45 H46 P47 K48 K49 G50 V51 E52 K53 Y54 G55 P56 E57 A58 S59 A60 F61 T62 K63 K64 M65 V66 E67 N68 A69 K70 D77 K78

R81 T82 D83 K84 R87 G88 Y91 I92 Y93 A94 D95 M98 V99 N100 E101 V104 R105 Q106 A109 K110 V111 A112 K116 P117 N118 N119 E122 Q123 L124 L125 R126 K127 A132 K133 W140 S141 E142 D143 N144 A145 D146 S147 G148 Q149

### 4.2.8 Score per residue for model 8

- Molecule 1: staphylococcal nuclease

Chain A: 40% 32% 7% • 21%

A1 T2 S3 T4 K5 K6 L7 H8 K9 T13 K16 D19 L25 M26 Y27 K28 T33 F34 R35 L36 L37 L38 V39 D40 T41 P42 E43 T44 K45 H46 P47 K48 K49 G50 V51 E52 K53 Y54 G55 P56 A60 F61 T62 K63 K64 M65 V66 E67 N68 A69 K70 E73 V74

E75 F76 D77 R81 T82 D83 K84 R87 A90 Y91 I92 Y93 A94 D95 M98 V99 N100 E101 A102 L103 V104 R105 Q106 G107 L108 A109 K110 V111 A112 N119 T120 L124 L125 R126 K127 S128 K133 K134 E135 K136 L137 N138 I139 W140 S141 E142 D143 N144 A145 D146 S147 G148 Q149

### 4.2.9 Score per residue for model 9

- Molecule 1: staphylococcal nuclease

Chain A: 45% 27% 7% 21%

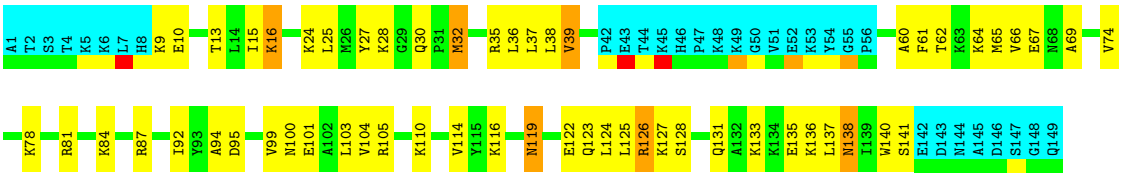
A1 T2 S3 T4 K5 K6 L7 H8 L14 I15 K16 K24 L25 M26 Y27 K28 P31 F34 R35 L36 L37 L38 V39 P42 E43 T44 K45 H46 P47 K48 K49 G50 V51 E52 K53 Y54 G55 P56 E57 A60 F61 T62 K63 K64 M65 V66 E67 N68 A69 K70 E73 V74

K78 G79 Q80 R81 T82 D83 R87 I92 Y93 A94 D95 G96 K97 M98 V99 N100 E101 R105 K110 V114 Y115 K116 N119 E122 R126 K127 S128 K133 K134 L137 N138 I139 W140 S141 E142 D143 N144 A145 D146 S147 G148 Q149

### 4.2.10 Score per residue for model 10

- Molecule 1: staphylococcal nuclease

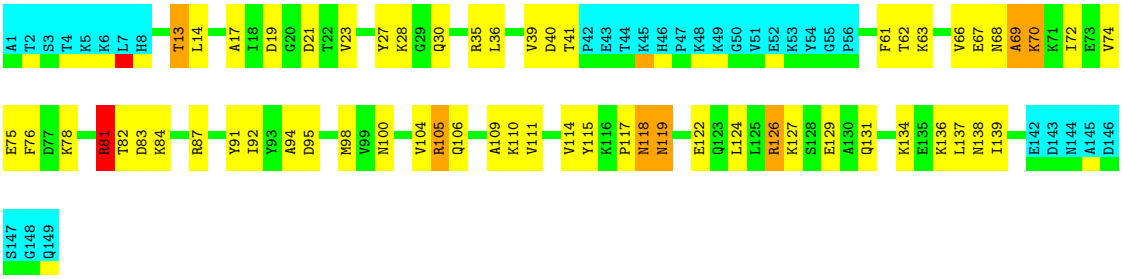
Chain A: 41% 34% • 21%




### 4.2.11 Score per residue for model 11

- Molecule 1: staphylococcal nuclease

Chain A: 39% 35% 5% • 21%




### 4.2.12 Score per residue for model 12

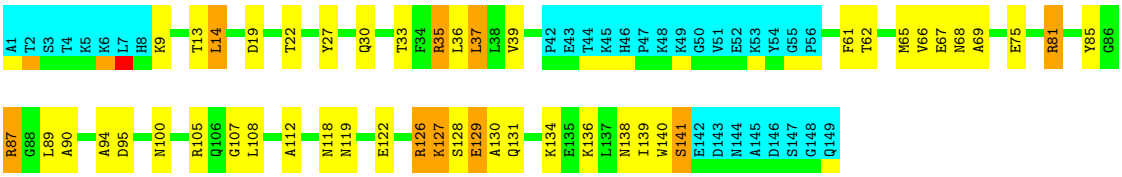
- Molecule 1: staphylococcal nuclease

Chain A: 40% 32% 7% 21%

### 4.2.13 Score per residue for model 13

- Molecule 1: staphylococcal nuclease

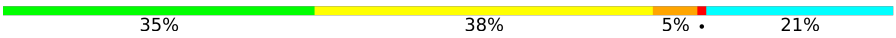
Chain A: 48% 26% 6% 21%

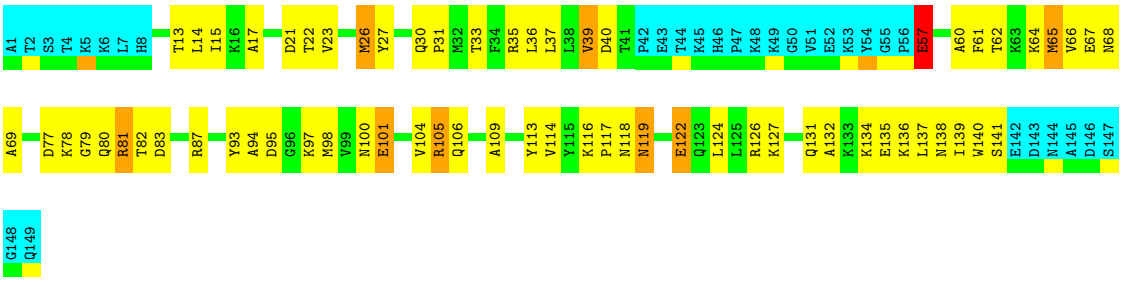



### 4.2.14 Score per residue for model 14

- Molecule 1: staphylococcal nuclease

Chain A:

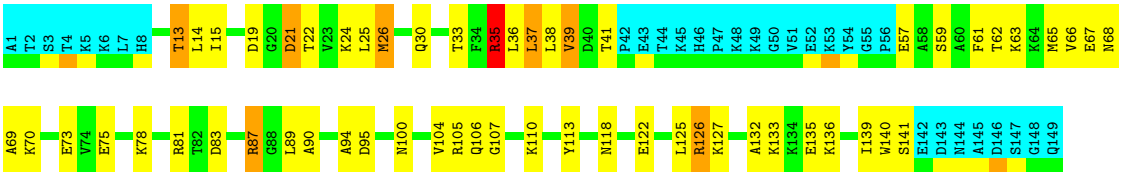



### 4.2.15 Score per residue for model 15

- Molecule 1: staphylococcal nuclease

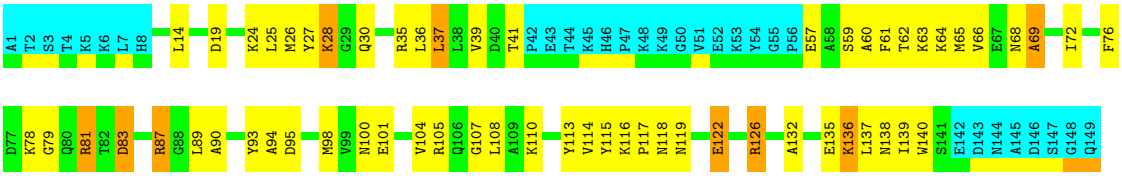
Chain A:




### 4.2.16 Score per residue for model 16 (medoid)

- Molecule 1: staphylococcal nuclease

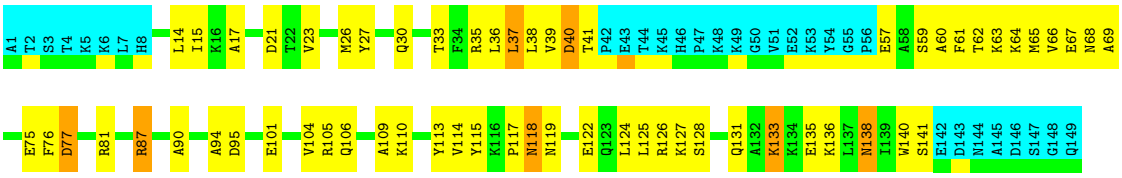
Chain A:



### 4.2.17 Score per residue for model 17

- Molecule 1: staphylococcal nuclease

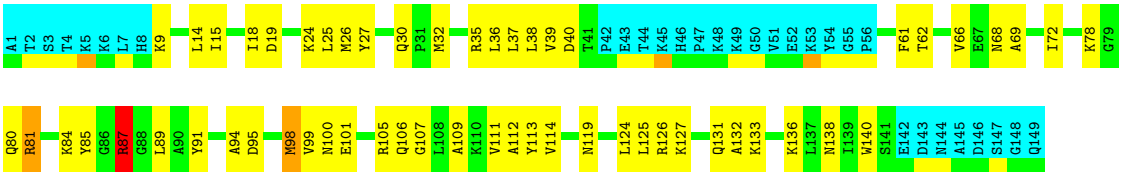
Chain A: 38% 36% 5% 21%




### 4.2.18 Score per residue for model 18

- Molecule 1: staphylococcal nuclease

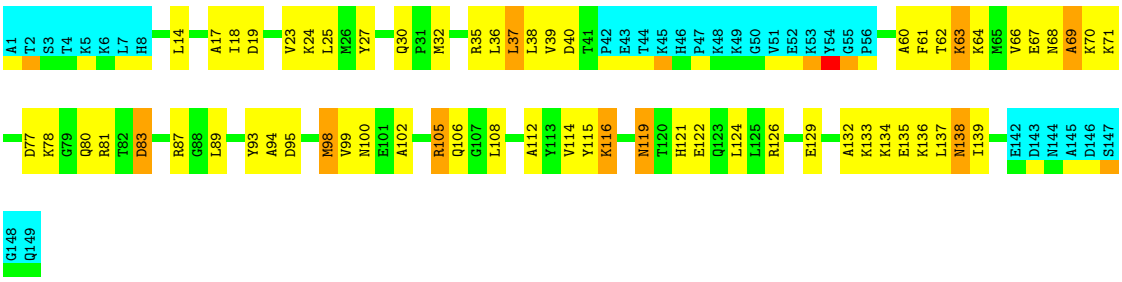
Chain A: 42% 36% •• 21%




### 4.2.19 Score per residue for model 19

- Molecule 1: staphylococcal nuclease

Chain A: 38% 36% 6% 21%




### 4.2.20 Score per residue for model 20

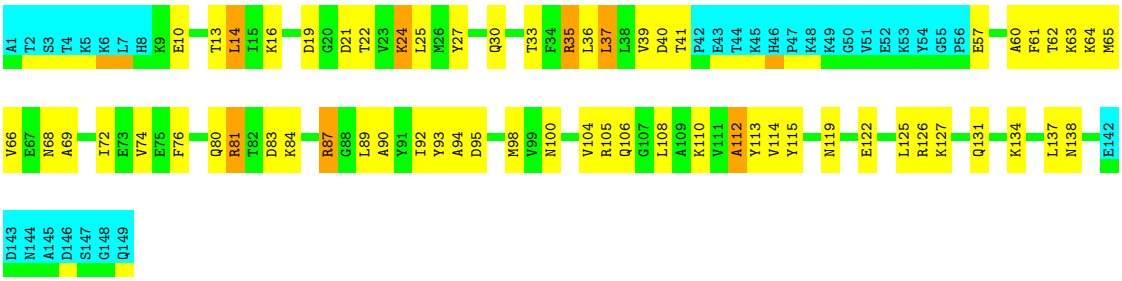
- Molecule 1: staphylococcal nuclease

Chain A: 42% 30% 7% 21%

### 4.2.21 Score per residue for model 21

- Molecule 1: staphylococcal nuclease

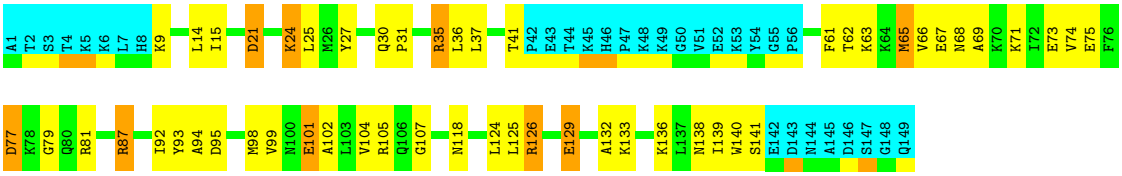
Chain A: 38% 37% 5% 21%




### 4.2.22 Score per residue for model 22

- Molecule 1: staphylococcal nuclease

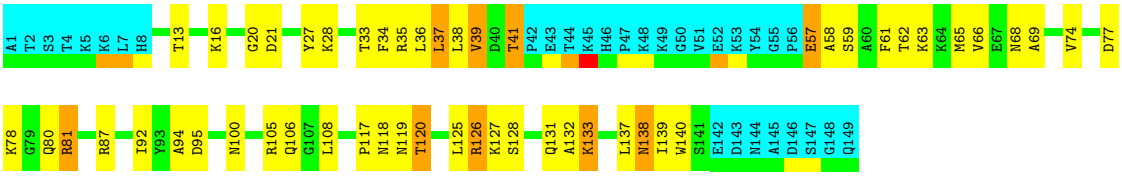
Chain A: 44% 29% 6% 21%




### 4.2.23 Score per residue for model 23

- Molecule 1: staphylococcal nuclease

Chain A: 44% 29% 6% 21%




### 4.2.24 Score per residue for model 24

- Molecule 1: staphylococcal nuclease

Chain A: 34% 40% 5% 21%

A1 T2 S3 T4 K5 K6 L7 H8 T13 L14 I15 K16 A17 V23 K24 L25 M26 Y27 Q30 P31 M32 T33 F34 R35 L36 L37 L38 V39 D40 T41 P42 E43 T44 K45 H46 P47 K48 K49 G50 V51 E52 K53 Y54 G55 P56 E57 A60 F61 T62 K63 K64 M65 V66 E67 N68 A69

I72 E73 D77 K78 G79 Q80 R81 K84 Y85 G86 R87 Y93 A94 D95 M98 V99 N100 L103 V104 R105 Q106 G107 L108 A109 K110 V111 A112 Y113 V114 N118 N119 T120 H121 E122 Q123 L124 L125 R126 K133 K134 E135 K136 L137 N138 I139 W140 S141 E142 D143 N144 A145 D146

S147 G148 Q149

### 4.2.25 Score per residue for model 25

- Molecule 1: staphylococcal nuclease

Chain A: 35% 38% 6% 21%

A1 T2 S3 T4 K5 K6 L7 H8 K9 T13 L14 I15 K16 A17 I18 D19 V23 K24 L25 M26 Y27 K28 G29 Q30 T33 F34 R35 L36 L37 L38 V39 D40 T41 P42 E43 T44 K45 H46 P47 K48 K49 G50 V51 E52 K53 Y54 G55 P56 E57 F61 T62 K63 K64 M65 V66 E67

N68 A69 E73 V74 E75 F76 D77 R81 K84 R87 G88 L89 A90 A94 D95 N100 V104 R105 L108 A109 K110 V111 A112 Y113 V114 Y115 N119 T120 H121 E122 R126 K127 S128 E129 A132 K133 K134 E135 K136 L137 N138 I139 W140 S141 E142 D143 N144 A145 D146

S147 G148 Q149

### 4.2.26 Score per residue for model 26

- Molecule 1: staphylococcal nuclease

Chain A: 38% 35% 7% 21%

A1 T2 S3 T4 K5 K6 L7 H8 L14 I15 K24 L25 M26 Y27 K28 G29 Q30 P31 M32 R35 L36 L37 L38 V39 D40 T41 P42 E43 T44 K45 H46 P47 K48 K49 G50 V51 E52 K53 Y54 G55 P56 E57 A60 F61 T62 K63 K64 M65 N68 A69 V74 E75 K78

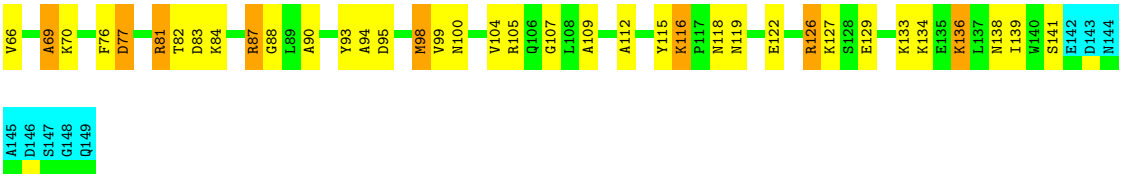
G79 Q80 R81 T82 D83 R87 A90 Y91 I92 Y93 A94 D95 M98 V99 N100 E101 V104 R105 K110 V111 A112 Y113 V114 Y115 K116 N119 T120 H121 E122 R126 K127 S128 E129 A130 Q131 A132 K133 K134 E135 K136 L137 N138 I139 W140 S141 E142 D143 N144 A145 D146 S147 G148 Q149

### 4.2.27 Score per residue for model 27

- Molecule 1: staphylococcal nuclease

Chain A: 36% 34% 9% 21%

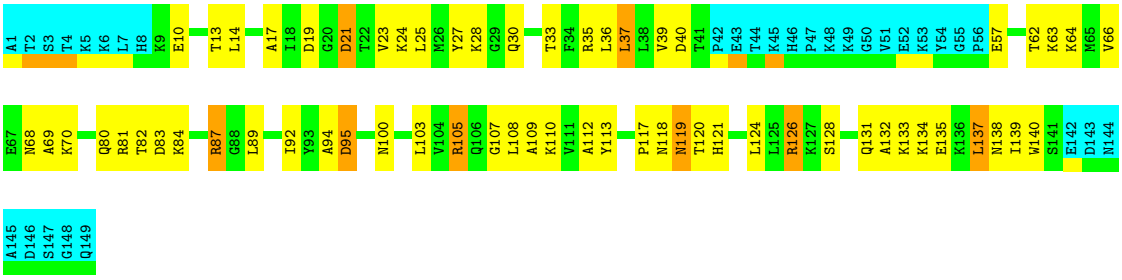
A1 T2 S3 T4 K5 K6 L7 H8 K9 L14 I15 K16 A17 I18 D19 V23 K24 L25 M26 Y27 K28 G29 Q30 P31 M32 T33 F34 R35 L36 L37 L38 V39 D40 T41 P42 E43 T44 K45 H46 P47 K48 K49 G50 V51 E52 K53 Y54 G55 P56 E57 A58 S59 A60 F61 T62 K63 K64 M65




### 4.2.28 Score per residue for model 28

- Molecule 1: staphylococcal nuclease

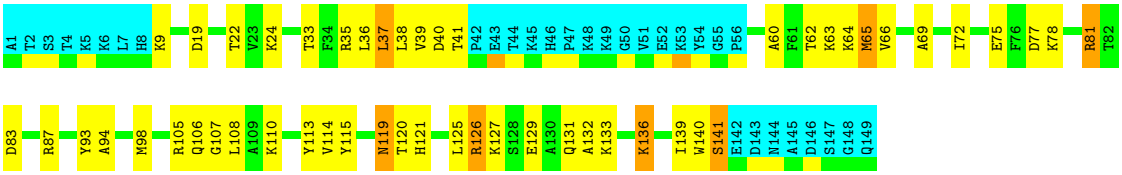
Chain A: 38% 36% 5% 21%




### 4.2.29 Score per residue for model 29

- Molecule 1: staphylococcal nuclease

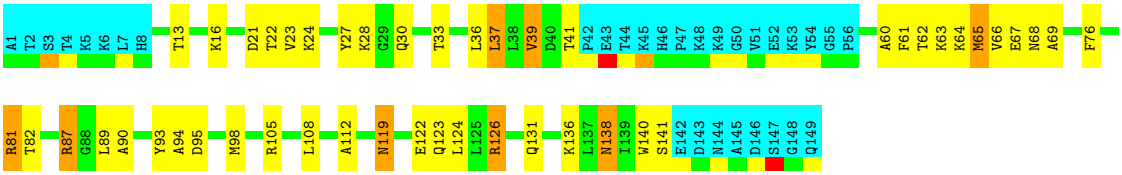
Chain A: 45% 30% 5% 21%




### 4.2.30 Score per residue for model 30

- Molecule 1: staphylococcal nuclease

Chain A: 48% 26% 5% 21%



# 5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *Distance, hydrogen bond and torsion angle constraints.*

Of the 90 calculated structures, 30 were deposited, based on the following criterion: *structures with acceptable covalent geometry,structures with the least restraint violations.*

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

| Software name | Classification | Version |
|---|---|---|
| X-PLOR | structure solution | 3.1 |
| Insight II | structure solution | 2.3 |
| HBPLUS | structure solution | |
| X-PLOR | refinement | 3.1 |

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.

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 | 4.8±0.4 |
| All | All | 0 | 144 |

There are no bond-length outliers.

There are no bond-angle outliers.

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 | 81 | ARG | Sidechain | 30 |
| 1 | A | 105 | ARG | Sidechain | 30 |
| 1 | A | 126 | ARG | Sidechain | 30 |
| 1 | A | 35 | ARG | Sidechain | 28 |
| 1 | A | 87 | ARG | Sidechain | 26 |

## 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 | 943 | 982 | 982 | 37±6 |
| All | All | 28290 | 29460 | 29460 | 1101 |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 19.

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

| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|---|---|---|---|---|---|
| | | | | Worst | Total |
| 1:A:14:LEU:HD12 | 1:A:25:LEU:CD2 | 0.96 | 1.89 | 1 | 4 |
| 1:A:107:GLY:O | 1:A:139:ILE:HD12 | 0.89 | 1.67 | 16 | 8 |
| 1:A:135:GLU:HB3 | 1:A:137:LEU:HD21 | 0.89 | 1.45 | 26 | 7 |
| 1:A:69:ALA:CB | 1:A:94:ALA:HB1 | 0.88 | 1.99 | 6 | 12 |
| 1:A:14:LEU:HD12 | 1:A:25:LEU:HD22 | 0.84 | 1.47 | 1 | 1 |
| 1:A:36:LEU:HD22 | 1:A:100:ASN:OD1 | 0.84 | 1.71 | 4 | 10 |
| 1:A:83:ASP:OD1 | 1:A:89:LEU:HD11 | 0.83 | 1.73 | 2 | 3 |
| 1:A:24:LYS:O | 1:A:25:LEU:HD23 | 0.83 | 1.73 | 16 | 8 |
| 1:A:14:LEU:HD13 | 1:A:15:ILE:N | 0.82 | 1.90 | 26 | 6 |
| 1:A:100:ASN:O | 1:A:104:VAL:HG23 | 0.81 | 1.75 | 8 | 11 |
| 1:A:65:MET:O | 1:A:69:ALA:HB2 | 0.81 | 1.74 | 13 | 12 |
| 1:A:25:LEU:HD12 | 1:A:34:PHE:CG | 0.79 | 2.13 | 27 | 5 |
| 1:A:62:THR:O | 1:A:66:VAL:HG22 | 0.77 | 1.80 | 25 | 21 |
| 1:A:124:LEU:HD13 | 1:A:124:LEU:O | 0.76 | 1.80 | 17 | 2 |
| 1:A:69:ALA:HB2 | 1:A:94:ALA:HB1 | 0.76 | 1.57 | 28 | 13 |
| 1:A:62:THR:O | 1:A:66:VAL:HG13 | 0.75 | 1.81 | 13 | 25 |
| 1:A:83:ASP:CG | 1:A:89:LEU:HD11 | 0.75 | 2.02 | 12 | 4 |
| 1:A:40:ASP:O | 1:A:109:ALA:HB1 | 0.75 | 1.81 | 25 | 12 |
| 1:A:105:ARG:O | 1:A:137:LEU:HD13 | 0.74 | 1.82 | 5 | 1 |
| 1:A:135:GLU:CB | 1:A:137:LEU:HD21 | 0.72 | 2.13 | 26 | 3 |
| 1:A:104:VAL:HG21 | 1:A:125:LEU:CD2 | 0.72 | 2.14 | 22 | 2 |
| 1:A:104:VAL:HG13 | 1:A:129:GLU:OE1 | 0.71 | 1.85 | 27 | 2 |
| 1:A:14:LEU:HD22 | 1:A:66:VAL:O | 0.71 | 1.84 | 16 | 2 |
| 1:A:25:LEU:HD12 | 1:A:34:PHE:CD1 | 0.71 | 2.20 | 27 | 2 |
| 1:A:82:THR:HG22 | 1:A:88:GLY:HA2 | 0.71 | 1.59 | 27 | 1 |
| 1:A:38:LEU:HD22 | 1:A:114:VAL:HG22 | 0.71 | 1.62 | 17 | 2 |
| 1:A:33:THR:HG21 | 1:A:87:ARG:CZ | 0.69 | 2.18 | 28 | 1 |
| 1:A:39:VAL:O | 1:A:112:ALA:HB2 | 0.69 | 1.88 | 21 | 11 |
| 1:A:38:LEU:HD23 | 1:A:114:VAL:HG21 | 0.69 | 1.63 | 18 | 1 |
| 1:A:72:ILE:HD12 | 1:A:72:ILE:N | 0.69 | 2.03 | 5 | 1 |
| 1:A:104:VAL:HG21 | 1:A:125:LEU:HD22 | 0.68 | 1.64 | 6 | 6 |
| 1:A:83:ASP:HB3 | 1:A:89:LEU:HD11 | 0.67 | 1.66 | 16 | 3 |
| 1:A:21:ASP:OD2 | 1:A:41:THR:HG23 | 0.67 | 1.88 | 21 | 2 |
| 1:A:33:THR:HG21 | 1:A:87:ARG:NH2 | 0.67 | 2.05 | 28 | 1 |
| 1:A:14:LEU:C | 1:A:14:LEU:HD13 | 0.67 | 2.09 | 4 | 3 |
| 1:A:37:LEU:O | 1:A:39:VAL:HG23 | 0.67 | 1.88 | 9 | 23 |
| 1:A:114:VAL:HG11 | 1:A:122:GLU:HG3 | 0.67 | 1.67 | 14 | 1 |
| 1:A:17:ALA:CB | 1:A:23:VAL:HG12 | 0.67 | 2.20 | 19 | 5 |
| 1:A:36:LEU:HB3 | 1:A:39:VAL:HG21 | 0.66 | 1.67 | 3 | 24 |
| 1:A:114:VAL:HG12 | 1:A:119:ASN:OD1 | 0.66 | 1.91 | 14 | 1 |
| 1:A:69:ALA:O | 1:A:72:ILE:HD11 | 0.66 | 1.91 | 18 | 3 |
| 1:A:74:VAL:HG12 | 1:A:92:ILE:HD12 | 0.66 | 1.67 | 26 | 3 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|---|---|---|---|---|---|
| | | | | Worst | Total |
| 1:A:108:LEU:HD21 | 1:A:138:ASN:OD1 | 0.65 | 1.90 | 16 | 7 |
| 1:A:21:ASP:CG | 1:A:41:THR:HG23 | 0.65 | 2.11 | 21 | 2 |
| 1:A:14:LEU:HD13 | 1:A:14:LEU:C | 0.65 | 2.12 | 22 | 4 |
| 1:A:74:VAL:HG12 | 1:A:92:ILE:CD1 | 0.64 | 2.22 | 26 | 4 |
| 1:A:106:GLN:HB3 | 1:A:108:LEU:HD12 | 0.64 | 1.69 | 29 | 1 |
| 1:A:14:LEU:HD13 | 1:A:66:VAL:HB | 0.64 | 1.70 | 2 | 4 |
| 1:A:41:THR:O | 1:A:41:THR:HG23 | 0.63 | 1.92 | 17 | 1 |
| 1:A:114:VAL:HG21 | 1:A:122:GLU:OE2 | 0.63 | 1.94 | 21 | 1 |
| 1:A:36:LEU:CB | 1:A:39:VAL:HG21 | 0.62 | 2.24 | 11 | 1 |
| 1:A:104:VAL:HG13 | 1:A:129:GLU:CD | 0.62 | 2.16 | 5 | 1 |
| 1:A:124:LEU:HD13 | 1:A:124:LEU:C | 0.61 | 2.15 | 17 | 2 |
| 1:A:120:THR:HG22 | 1:A:121:HIS:CE1 | 0.61 | 2.31 | 25 | 1 |
| 1:A:37:LEU:HD12 | 1:A:89:LEU:C | 0.61 | 2.16 | 13 | 1 |
| 1:A:17:ALA:HB1 | 1:A:23:VAL:HG12 | 0.61 | 1.73 | 27 | 7 |
| 1:A:99:VAL:O | 1:A:103:LEU:HD12 | 0.60 | 1.97 | 10 | 2 |
| 1:A:33:THR:HG21 | 1:A:87:ARG:NH1 | 0.60 | 2.12 | 25 | 2 |
| 1:A:101:GLU:OE1 | 1:A:124:LEU:HD21 | 0.60 | 1.97 | 18 | 1 |
| 1:A:133:LYS:CG | 1:A:140:TRP:CD2 | 0.60 | 2.84 | 17 | 4 |
| 1:A:38:LEU:HD11 | 1:A:119:ASN:HA | 0.60 | 1.74 | 19 | 2 |
| 1:A:69:ALA:HB1 | 1:A:95:ASP:N | 0.59 | 2.13 | 2 | 1 |
| 1:A:36:LEU:CB | 1:A:39:VAL:CG2 | 0.59 | 2.80 | 11 | 2 |
| 1:A:133:LYS:CG | 1:A:140:TRP:CE3 | 0.58 | 2.85 | 3 | 5 |
| 1:A:15:ILE:HD11 | 1:A:26:MET:SD | 0.58 | 2.38 | 14 | 2 |
| 1:A:33:THR:O | 1:A:34:PHE:CD1 | 0.56 | 2.58 | 1 | 1 |
| 1:A:23:VAL:HG23 | 1:A:25:LEU:HD21 | 0.56 | 1.77 | 12 | 1 |
| 1:A:66:VAL:HG23 | 1:A:67:GLU:N | 0.56 | 2.15 | 13 | 7 |
| 1:A:75:GLU:O | 1:A:90:ALA:HB1 | 0.56 | 1.99 | 8 | 5 |
| 1:A:132:ALA:HB1 | 1:A:140:TRP:CD1 | 0.56 | 2.35 | 7 | 8 |
| 1:A:101:GLU:HG3 | 1:A:124:LEU:HD21 | 0.56 | 1.77 | 14 | 3 |
| 1:A:135:GLU:HB2 | 1:A:137:LEU:HD12 | 0.56 | 1.76 | 28 | 1 |
| 1:A:61:PHE:CZ | 1:A:65:MET:SD | 0.56 | 2.99 | 13 | 1 |
| 1:A:93:TYR:CZ | 1:A:98:MET:SD | 0.56 | 2.99 | 16 | 7 |
| 1:A:114:VAL:HG11 | 1:A:122:GLU:OE1 | 0.56 | 2.01 | 11 | 1 |
| 1:A:124:LEU:C | 1:A:124:LEU:HD23 | 0.56 | 2.20 | 24 | 1 |
| 1:A:14:LEU:HD22 | 1:A:25:LEU:HD23 | 0.56 | 1.75 | 27 | 1 |
| 1:A:126:ARG:O | 1:A:130:ALA:HB2 | 0.56 | 1.99 | 26 | 1 |
| 1:A:133:LYS:HG2 | 1:A:140:TRP:CD2 | 0.56 | 2.35 | 17 | 8 |
| 1:A:66:VAL:O | 1:A:72:ILE:HD11 | 0.56 | 2.01 | 24 | 3 |
| 1:A:133:LYS:HG3 | 1:A:140:TRP:CD2 | 0.55 | 2.36 | 20 | 7 |
| 1:A:37:LEU:HD12 | 1:A:90:ALA:HA | 0.55 | 1.78 | 27 | 2 |
| 1:A:133:LYS:HG2 | 1:A:140:TRP:CE3 | 0.55 | 2.36 | 3 | 6 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|---|---|---|---|---|---|
| | | | | Worst | Total |
| 1:A:83:ASP:HB3 | 1:A:89:LEU:HD21 | 0.55 | 1.76 | 15 | 1 |
| 1:A:24:LYS:C | 1:A:25:LEU:HD23 | 0.55 | 2.22 | 21 | 4 |
| 1:A:98:MET:SD | 1:A:124:LEU:HD21 | 0.55 | 2.41 | 22 | 1 |
| 1:A:114:VAL:HG21 | 1:A:122:GLU:CG | 0.54 | 2.32 | 14 | 1 |
| 1:A:65:MET:CE | 1:A:94:ALA:HB3 | 0.54 | 2.32 | 21 | 1 |
| 1:A:18:ILE:HG22 | 1:A:19:ASP:OD1 | 0.54 | 2.02 | 18 | 2 |
| 1:A:72:ILE:HD12 | 1:A:72:ILE:H | 0.54 | 1.62 | 5 | 2 |
| 1:A:38:LEU:HD23 | 1:A:114:VAL:CG2 | 0.54 | 2.31 | 18 | 1 |
| 1:A:132:ALA:C | 1:A:140:TRP:CD1 | 0.54 | 2.81 | 7 | 6 |
| 1:A:61:PHE:CD1 | 1:A:103:LEU:HD21 | 0.54 | 2.38 | 24 | 1 |
| 1:A:136:LYS:O | 1:A:141:SER:CB | 0.54 | 2.56 | 26 | 8 |
| 1:A:27:TYR:O | 1:A:30:GLN:CG | 0.54 | 2.56 | 13 | 16 |
| 1:A:132:ALA:HA | 1:A:137:LEU:HD12 | 0.54 | 1.80 | 25 | 2 |
| 1:A:15:ILE:HD12 | 1:A:25:LEU:O | 0.54 | 2.03 | 22 | 5 |
| 1:A:76:PHE:CD2 | 1:A:90:ALA:HB2 | 0.54 | 2.37 | 27 | 2 |
| 1:A:91:TYR:CD1 | 1:A:91:TYR:N | 0.54 | 2.76 | 8 | 4 |
| 1:A:38:LEU:HD22 | 1:A:114:VAL:HG13 | 0.54 | 1.79 | 9 | 1 |
| 1:A:38:LEU:HB3 | 1:A:125:LEU:HD12 | 0.54 | 1.79 | 20 | 1 |
| 1:A:76:PHE:CD1 | 1:A:90:ALA:HB2 | 0.53 | 2.38 | 30 | 3 |
| 1:A:62:THR:O | 1:A:66:VAL:CG1 | 0.53 | 2.56 | 19 | 9 |
| 1:A:114:VAL:HG13 | 1:A:119:ASN:HB3 | 0.53 | 1.81 | 29 | 2 |
| 1:A:61:PHE:O | 1:A:61:PHE:CD1 | 0.53 | 2.61 | 5 | 2 |
| 1:A:63:LYS:O | 1:A:67:GLU:CG | 0.53 | 2.57 | 17 | 6 |
| 1:A:14:LEU:HD22 | 1:A:25:LEU:CD2 | 0.53 | 2.34 | 27 | 3 |
| 1:A:68:ASN:O | 1:A:70:LYS:N | 0.52 | 2.42 | 12 | 9 |
| 1:A:37:LEU:O | 1:A:39:VAL:CG2 | 0.52 | 2.58 | 25 | 6 |
| 1:A:60:ALA:O | 1:A:64:LYS:CB | 0.52 | 2.57 | 14 | 8 |
| 1:A:65:MET:HE2 | 1:A:94:ALA:HB3 | 0.52 | 1.81 | 6 | 1 |
| 1:A:83:ASP:OD2 | 1:A:87:ARG:CZ | 0.52 | 2.57 | 1 | 1 |
| 1:A:107:GLY:O | 1:A:138:ASN:CB | 0.52 | 2.57 | 24 | 6 |
| 1:A:101:GLU:CG | 1:A:128:SER:OG | 0.52 | 2.58 | 9 | 1 |
| 1:A:21:ASP:OD1 | 1:A:41:THR:HG23 | 0.52 | 2.04 | 15 | 2 |
| 1:A:40:ASP:O | 1:A:109:ALA:CB | 0.52 | 2.57 | 7 | 2 |
| 1:A:65:MET:O | 1:A:69:ALA:CB | 0.52 | 2.56 | 13 | 10 |
| 1:A:15:ILE:HD12 | 1:A:25:LEU:C | 0.52 | 2.25 | 24 | 2 |
| 1:A:61:PHE:C | 1:A:61:PHE:CD1 | 0.52 | 2.82 | 19 | 9 |
| 1:A:110:LYS:HD3 | 1:A:140:TRP:CH2 | 0.52 | 2.40 | 15 | 1 |
| 1:A:61:PHE:CE2 | 1:A:106:GLN:OE1 | 0.52 | 2.63 | 5 | 1 |
| 1:A:136:LYS:O | 1:A:141:SER:CA | 0.52 | 2.58 | 14 | 7 |
| 1:A:85:TYR:CD1 | 1:A:85:TYR:N | 0.52 | 2.76 | 3 | 1 |
| 1:A:92:ILE:C | 1:A:93:TYR:CD1 | 0.52 | 2.83 | 4 | 4 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|---|---|---|---|---|---|
| | | | | Worst | Total |
| 1:A:93:TYR:CD1 | 1:A:98:MET:HA | 0.52 | 2.40 | 6 | 2 |
| 1:A:64:LYS:O | 1:A:68:ASN:ND2 | 0.52 | 2.43 | 1 | 4 |
| 1:A:114:VAL:CG1 | 1:A:119:ASN:OD1 | 0.52 | 2.57 | 3 | 2 |
| 1:A:106:GLN:O | 1:A:138:ASN:ND2 | 0.52 | 2.43 | 24 | 1 |
| 1:A:101:GLU:OE1 | 1:A:124:LEU:CD2 | 0.52 | 2.57 | 3 | 1 |
| 1:A:133:LYS:HG3 | 1:A:140:TRP:CE2 | 0.52 | 2.39 | 17 | 5 |
| 1:A:113:TYR:HB3 | 1:A:115:TYR:CE1 | 0.52 | 2.40 | 17 | 1 |
| 1:A:21:ASP:OD2 | 1:A:41:THR:CG2 | 0.51 | 2.58 | 21 | 1 |
| 1:A:62:THR:O | 1:A:66:VAL:CG2 | 0.51 | 2.57 | 3 | 8 |
| 1:A:114:VAL:HG21 | 1:A:122:GLU:HG3 | 0.51 | 1.82 | 14 | 4 |
| 1:A:21:ASP:OD1 | 1:A:22:THR:N | 0.51 | 2.44 | 14 | 1 |
| 1:A:14:LEU:HA | 1:A:25:LEU:HD23 | 0.51 | 1.81 | 20 | 1 |
| 1:A:137:LEU:O | 1:A:139:ILE:N | 0.51 | 2.44 | 23 | 8 |
| 1:A:61:PHE:CD1 | 1:A:61:PHE:C | 0.51 | 2.83 | 5 | 12 |
| 1:A:113:TYR:HB3 | 1:A:115:TYR:CZ | 0.51 | 2.41 | 17 | 5 |
| 1:A:69:ALA:CB | 1:A:95:ASP:OD1 | 0.51 | 2.59 | 27 | 3 |
| 1:A:38:LEU:HB2 | 1:A:125:LEU:CD1 | 0.51 | 2.36 | 18 | 5 |
| 1:A:10:GLU:CB | 1:A:27:TYR:OH | 0.51 | 2.59 | 28 | 1 |
| 1:A:60:ALA:O | 1:A:64:LYS:CG | 0.50 | 2.59 | 1 | 5 |
| 1:A:81:ARG:O | 1:A:82:THR:HG23 | 0.50 | 2.06 | 11 | 1 |
| 1:A:95:ASP:OD1 | 1:A:95:ASP:N | 0.50 | 2.43 | 27 | 1 |
| 1:A:40:ASP:OD2 | 1:A:112:ALA:CB | 0.50 | 2.59 | 18 | 2 |
| 1:A:14:LEU:C | 1:A:14:LEU:CD1 | 0.50 | 2.80 | 22 | 7 |
| 1:A:97:LYS:O | 1:A:99:VAL:N | 0.50 | 2.45 | 9 | 1 |
| 1:A:120:THR:HG23 | 1:A:121:HIS:N | 0.50 | 2.20 | 12 | 3 |
| 1:A:100:ASN:O | 1:A:104:VAL:CG2 | 0.50 | 2.59 | 24 | 1 |
| 1:A:60:ALA:O | 1:A:64:LYS:CD | 0.50 | 2.60 | 30 | 2 |
| 1:A:119:ASN:OD1 | 1:A:122:GLU:CB | 0.50 | 2.60 | 30 | 6 |
| 1:A:30:GLN:NE2 | 1:A:32:MET:SD | 0.50 | 2.85 | 12 | 1 |
| 1:A:113:TYR:HB3 | 1:A:115:TYR:CE2 | 0.50 | 2.41 | 20 | 4 |
| 1:A:124:LEU:CD1 | 1:A:124:LEU:C | 0.50 | 2.79 | 5 | 1 |
| 1:A:98:MET:SD | 1:A:101:GLU:CB | 0.49 | 3.00 | 22 | 2 |
| 1:A:27:TYR:CD2 | 1:A:28:LYS:HG3 | 0.49 | 2.42 | 28 | 1 |
| 1:A:85:TYR:HB2 | 1:A:87:ARG:CD | 0.49 | 2.37 | 6 | 2 |
| 1:A:27:TYR:CE2 | 1:A:28:LYS:CD | 0.49 | 2.96 | 6 | 1 |
| 1:A:105:ARG:O | 1:A:137:LEU:CD1 | 0.49 | 2.59 | 5 | 1 |
| 1:A:85:TYR:CB | 1:A:87:ARG:CD | 0.49 | 2.90 | 6 | 1 |
| 1:A:26:MET:SD | 1:A:30:GLN:N | 0.49 | 2.86 | 15 | 1 |
| 1:A:14:LEU:HD12 | 1:A:25:LEU:HD23 | 0.49 | 1.84 | 25 | 1 |
| 1:A:85:TYR:CB | 1:A:87:ARG:HD2 | 0.49 | 2.38 | 6 | 1 |
| 1:A:66:VAL:CG2 | 1:A:67:GLU:N | 0.49 | 2.76 | 13 | 3 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|---|---|---|---|---|---|
| | | | | Worst | Total |
| 1:A:14:LEU:CD2 | 1:A:66:VAL:O | 0.49 | 2.59 | 16 | 1 |
| 1:A:113:TYR:O | 1:A:115:TYR:CE1 | 0.49 | 2.65 | 29 | 1 |
| 1:A:36:LEU:HB2 | 1:A:39:VAL:CG2 | 0.49 | 2.37 | 11 | 2 |
| 1:A:117:PRO:O | 1:A:119:ASN:N | 0.49 | 2.45 | 11 | 6 |
| 1:A:124:LEU:C | 1:A:124:LEU:CD1 | 0.49 | 2.81 | 17 | 1 |
| 1:A:133:LYS:HD3 | 1:A:140:TRP:CE3 | 0.48 | 2.43 | 12 | 1 |
| 1:A:39:VAL:CG1 | 1:A:104:VAL:CG2 | 0.48 | 2.90 | 15 | 1 |
| 1:A:99:VAL:O | 1:A:102:ALA:HB3 | 0.48 | 2.08 | 19 | 2 |
| 1:A:36:LEU:HB3 | 1:A:39:VAL:CG2 | 0.48 | 2.37 | 11 | 19 |
| 1:A:133:LYS:HA | 1:A:140:TRP:CG | 0.48 | 2.42 | 9 | 4 |
| 1:A:36:LEU:CD2 | 1:A:92:ILE:HG12 | 0.48 | 2.39 | 7 | 4 |
| 1:A:9:LYS:CG | 1:A:75:GLU:OE1 | 0.48 | 2.61 | 29 | 1 |
| 1:A:95:ASP:N | 1:A:95:ASP:OD1 | 0.48 | 2.47 | 24 | 2 |
| 1:A:93:TYR:CZ | 1:A:98:MET:HG3 | 0.48 | 2.43 | 3 | 2 |
| 1:A:102:ALA:O | 1:A:106:GLN:CG | 0.48 | 2.62 | 2 | 1 |
| 1:A:37:LEU:CD1 | 1:A:77:ASP:OD2 | 0.48 | 2.61 | 22 | 3 |
| 1:A:98:MET:CE | 1:A:121:HIS:ND1 | 0.48 | 2.76 | 19 | 1 |
| 1:A:61:PHE:CD1 | 1:A:61:PHE:O | 0.48 | 2.66 | 15 | 5 |
| 1:A:124:LEU:O | 1:A:124:LEU:CD1 | 0.48 | 2.62 | 5 | 1 |
| 1:A:21:ASP:CG | 1:A:41:THR:CG2 | 0.48 | 2.82 | 21 | 1 |
| 1:A:36:LEU:HB2 | 1:A:39:VAL:HG23 | 0.48 | 1.86 | 18 | 1 |
| 1:A:57:GLU:CD | 1:A:58:ALA:N | 0.48 | 2.67 | 23 | 1 |
| 1:A:14:LEU:CD2 | 1:A:25:LEU:CD2 | 0.47 | 2.92 | 27 | 1 |
| 1:A:113:TYR:CD1 | 1:A:114:VAL:N | 0.47 | 2.82 | 2 | 1 |
| 1:A:87:ARG:CD | 1:A:87:ARG:N | 0.47 | 2.77 | 5 | 2 |
| 1:A:119:ASN:O | 1:A:119:ASN:OD1 | 0.47 | 2.32 | 11 | 2 |
| 1:A:93:TYR:CD1 | 1:A:93:TYR:N | 0.47 | 2.82 | 9 | 1 |
| 1:A:114:VAL:HG11 | 1:A:119:ASN:ND2 | 0.47 | 2.24 | 25 | 1 |
| 1:A:63:LYS:HA | 1:A:66:VAL:CG2 | 0.47 | 2.40 | 25 | 8 |
| 1:A:25:LEU:HD12 | 1:A:34:PHE:CD2 | 0.47 | 2.45 | 4 | 1 |
| 1:A:83:ASP:OD1 | 1:A:89:LEU:CD1 | 0.47 | 2.61 | 5 | 1 |
| 1:A:68:ASN:ND2 | 1:A:68:ASN:N | 0.47 | 2.62 | 17 | 6 |
| 1:A:77:ASP:OD2 | 1:A:91:TYR:OH | 0.47 | 2.33 | 7 | 1 |
| 1:A:21:ASP:OD2 | 1:A:39:VAL:O | 0.47 | 2.32 | 11 | 1 |
| 1:A:69:ALA:O | 1:A:72:ILE:CD1 | 0.47 | 2.60 | 18 | 1 |
| 1:A:22:THR:CG2 | 1:A:33:THR:CG2 | 0.47 | 2.93 | 21 | 2 |
| 1:A:61:PHE:O | 1:A:65:MET:CB | 0.47 | 2.62 | 27 | 1 |
| 1:A:10:GLU:CG | 1:A:27:TYR:OH | 0.47 | 2.63 | 28 | 1 |
| 1:A:101:GLU:OE1 | 1:A:124:LEU:HD23 | 0.47 | 2.08 | 3 | 1 |
| 1:A:132:ALA:CB | 1:A:140:TRP:CD1 | 0.47 | 2.98 | 7 | 3 |
| 1:A:92:ILE:HG22 | 1:A:93:TYR:N | 0.47 | 2.24 | 21 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|---|---|---|---|---|---|
| | | | | Worst | Total |
| 1:A:83:ASP:OD2 | 1:A:89:LEU:HD21 | 0.47 | 2.10 | 12 | 2 |
| 1:A:133:LYS:HG2 | 1:A:140:TRP:CE2 | 0.46 | 2.45 | 22 | 3 |
| 1:A:94:ALA:CB | 1:A:99:VAL:HG22 | 0.46 | 2.40 | 27 | 1 |
| 1:A:133:LYS:HE2 | 1:A:140:TRP:CZ3 | 0.46 | 2.46 | 7 | 1 |
| 1:A:93:TYR:CE2 | 1:A:98:MET:HB3 | 0.46 | 2.45 | 22 | 1 |
| 1:A:33:THR:HG22 | 1:A:34:PHE:N | 0.46 | 2.26 | 23 | 1 |
| 1:A:60:ALA:O | 1:A:64:LYS:HB2 | 0.46 | 2.11 | 14 | 10 |
| 1:A:107:GLY:O | 1:A:138:ASN:HB2 | 0.46 | 2.11 | 18 | 7 |
| 1:A:27:TYR:CE2 | 1:A:28:LYS:HG3 | 0.46 | 2.45 | 27 | 2 |
| 1:A:38:LEU:CB | 1:A:125:LEU:CD1 | 0.46 | 2.93 | 18 | 1 |
| 1:A:37:LEU:CD2 | 1:A:89:LEU:HD22 | 0.46 | 2.40 | 25 | 1 |
| 1:A:116:LYS:CB | 1:A:117:PRO:HA | 0.46 | 2.41 | 4 | 1 |
| 1:A:39:VAL:O | 1:A:40:ASP:OD1 | 0.46 | 2.33 | 1 | 2 |
| 1:A:21:ASP:OD1 | 1:A:36:LEU:HD12 | 0.46 | 2.11 | 28 | 1 |
| 1:A:27:TYR:O | 1:A:30:GLN:HG2 | 0.46 | 2.11 | 24 | 12 |
| 1:A:77:ASP:OD1 | 1:A:118:ASN:OD1 | 0.46 | 2.34 | 24 | 1 |
| 1:A:77:ASP:OD2 | 1:A:118:ASN:OD1 | 0.46 | 2.34 | 7 | 1 |
| 1:A:115:TYR:O | 1:A:116:LYS:C | 0.45 | 2.55 | 16 | 7 |
| 1:A:76:PHE:CD2 | 1:A:81:ARG:HB3 | 0.45 | 2.47 | 11 | 1 |
| 1:A:136:LYS:HA | 1:A:140:TRP:O | 0.45 | 2.11 | 12 | 10 |
| 1:A:93:TYR:CE1 | 1:A:98:MET:HB3 | 0.45 | 2.46 | 7 | 1 |
| 1:A:83:ASP:OD1 | 1:A:87:ARG:O | 0.45 | 2.34 | 16 | 1 |
| 1:A:104:VAL:HG13 | 1:A:129:GLU:HB2 | 0.45 | 1.87 | 26 | 1 |
| 1:A:121:HIS:CD2 | 1:A:121:HIS:N | 0.45 | 2.84 | 4 | 1 |
| 1:A:133:LYS:HG3 | 1:A:140:TRP:CE3 | 0.45 | 2.46 | 5 | 1 |
| 1:A:57:GLU:OE1 | 1:A:108:LEU:HD22 | 0.45 | 2.12 | 23 | 1 |
| 1:A:114:VAL:HG13 | 1:A:119:ASN:CB | 0.45 | 2.41 | 29 | 1 |
| 1:A:27:TYR:O | 1:A:30:GLN:HG3 | 0.45 | 2.12 | 25 | 8 |
| 1:A:135:GLU:O | 1:A:136:LYS:CB | 0.45 | 2.63 | 4 | 5 |
| 1:A:119:ASN:OD1 | 1:A:122:GLU:HB3 | 0.45 | 2.11 | 6 | 2 |
| 1:A:38:LEU:CD2 | 1:A:114:VAL:HB | 0.45 | 2.41 | 18 | 1 |
| 1:A:73:GLU:OE1 | 1:A:73:GLU:N | 0.45 | 2.50 | 24 | 1 |
| 1:A:133:LYS:HD2 | 1:A:140:TRP:CZ3 | 0.45 | 2.46 | 1 | 1 |
| 1:A:133:LYS:HD2 | 1:A:140:TRP:CH2 | 0.45 | 2.47 | 1 | 1 |
| 1:A:60:ALA:O | 1:A:64:LYS:HB3 | 0.45 | 2.12 | 27 | 2 |
| 1:A:127:LYS:O | 1:A:130:ALA:HB3 | 0.45 | 2.11 | 13 | 1 |
| 1:A:57:GLU:OE2 | 1:A:138:ASN:OD1 | 0.45 | 2.34 | 17 | 1 |
| 1:A:23:VAL:HG11 | 1:A:62:THR:CG2 | 0.45 | 2.42 | 24 | 1 |
| 1:A:100:ASN:N | 1:A:100:ASN:OD1 | 0.45 | 2.50 | 3 | 3 |
| 1:A:128:SER:O | 1:A:130:ALA:N | 0.45 | 2.50 | 13 | 1 |
| 1:A:30:GLN:OE1 | 1:A:32:MET:CG | 0.44 | 2.65 | 10 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|---|---|---|---|---|---|
| | | | | Worst | Total |
| 1:A:135:GLU:CB | 1:A:137:LEU:HD11 | 0.44 | 2.41 | 14 | 1 |
| 1:A:115:TYR:O | 1:A:116:LYS:O | 0.44 | 2.35 | 4 | 1 |
| 1:A:106:GLN:O | 1:A:106:GLN:OE1 | 0.44 | 2.35 | 20 | 1 |
| 1:A:136:LYS:HA | 1:A:140:TRP:CB | 0.44 | 2.42 | 13 | 9 |
| 1:A:78:LYS:C | 1:A:78:LYS:CD | 0.44 | 2.85 | 26 | 1 |
| 1:A:101:GLU:HG3 | 1:A:128:SER:OG | 0.44 | 2.12 | 9 | 1 |
| 1:A:71:LYS:O | 1:A:73:GLU:OE2 | 0.44 | 2.34 | 22 | 1 |
| 1:A:38:LEU:O | 1:A:125:LEU:HD13 | 0.44 | 2.12 | 23 | 1 |
| 1:A:132:ALA:HA | 1:A:137:LEU:CD1 | 0.44 | 2.42 | 4 | 1 |
| 1:A:87:ARG:N | 1:A:87:ARG:HD3 | 0.44 | 2.28 | 5 | 1 |
| 1:A:111:VAL:HG11 | 1:A:122:GLU:OE2 | 0.44 | 2.13 | 5 | 1 |
| 1:A:27:TYR:CZ | 1:A:28:LYS:HG3 | 0.44 | 2.48 | 11 | 1 |
| 1:A:83:ASP:OD1 | 1:A:83:ASP:N | 0.44 | 2.49 | 16 | 1 |
| 1:A:93:TYR:OH | 1:A:98:MET:SD | 0.44 | 2.75 | 30 | 2 |
| 1:A:77:ASP:HB3 | 1:A:118:ASN:OD1 | 0.44 | 2.13 | 27 | 1 |
| 1:A:85:TYR:O | 1:A:87:ARG:NH1 | 0.44 | 2.50 | 13 | 1 |
| 1:A:106:GLN:OE1 | 1:A:106:GLN:CA | 0.44 | 2.65 | 20 | 1 |
| 1:A:137:LEU:O | 1:A:138:ASN:C | 0.44 | 2.56 | 23 | 7 |
| 1:A:37:LEU:O | 1:A:38:LEU:CB | 0.44 | 2.66 | 6 | 1 |
| 1:A:14:LEU:HD22 | 1:A:66:VAL:HG23 | 0.44 | 1.90 | 9 | 1 |
| 1:A:13:THR:CB | 1:A:26:MET:HB3 | 0.44 | 2.43 | 20 | 1 |
| 1:A:98:MET:SD | 1:A:101:GLU:HB2 | 0.44 | 2.52 | 22 | 1 |
| 1:A:69:ALA:HB1 | 1:A:95:ASP:OD1 | 0.44 | 2.13 | 26 | 1 |
| 1:A:68:ASN:O | 1:A:69:ALA:C | 0.44 | 2.57 | 18 | 11 |
| 1:A:111:VAL:O | 1:A:112:ALA:O | 0.44 | 2.35 | 7 | 1 |
| 1:A:132:ALA:O | 1:A:140:TRP:CD1 | 0.44 | 2.71 | 7 | 1 |
| 1:A:37:LEU:HD12 | 1:A:90:ALA:N | 0.44 | 2.26 | 13 | 1 |
| 1:A:15:ILE:CD1 | 1:A:25:LEU:C | 0.44 | 2.86 | 24 | 1 |
| 1:A:33:THR:HG21 | 1:A:87:ARG:HH11 | 0.44 | 1.70 | 27 | 1 |
| 1:A:22:THR:HG22 | 1:A:33:THR:CG2 | 0.44 | 2.43 | 29 | 1 |
| 1:A:76:PHE:CD2 | 1:A:81:ARG:HG2 | 0.43 | 2.47 | 1 | 1 |
| 1:A:100:ASN:OD1 | 1:A:100:ASN:N | 0.43 | 2.51 | 4 | 3 |
| 1:A:141:SER:O | 1:A:141:SER:OG | 0.43 | 2.34 | 15 | 2 |
| 1:A:60:ALA:O | 1:A:64:LYS:HD2 | 0.43 | 2.13 | 30 | 1 |
| 1:A:136:LYS:O | 1:A:141:SER:HA | 0.43 | 2.13 | 1 | 6 |
| 1:A:111:VAL:HG23 | 1:A:129:GLU:OE1 | 0.43 | 2.13 | 11 | 2 |
| 1:A:128:SER:O | 1:A:129:GLU:C | 0.43 | 2.55 | 13 | 1 |
| 1:A:84:LYS:O | 1:A:85:TYR:CD1 | 0.43 | 2.71 | 24 | 1 |
| 1:A:108:LEU:CD2 | 1:A:138:ASN:OD1 | 0.43 | 2.63 | 16 | 1 |
| 1:A:77:ASP:CB | 1:A:118:ASN:OD1 | 0.43 | 2.65 | 17 | 2 |
| 1:A:13:THR:O | 1:A:14:LEU:C | 0.43 | 2.56 | 11 | 3 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|---|---|---|---|---|---|
| | | | | Worst | Total |
| 1:A:94:ALA:O | 1:A:95:ASP:HB2 | 0.43 | 2.12 | 22 | 23 |
| 1:A:14:LEU:CD2 | 1:A:67:GLU:HA | 0.43 | 2.44 | 7 | 1 |
| 1:A:39:VAL:HG21 | 1:A:100:ASN:ND2 | 0.43 | 2.28 | 21 | 4 |
| 1:A:122:GLU:O | 1:A:123:GLN:C | 0.43 | 2.57 | 4 | 2 |
| 1:A:15:ILE:CD1 | 1:A:31:PRO:HB3 | 0.43 | 2.43 | 12 | 3 |
| 1:A:35:ARG:O | 1:A:36:LEU:C | 0.43 | 2.57 | 25 | 5 |
| 1:A:20:GLY:HA3 | 1:A:41:THR:HG21 | 0.43 | 1.90 | 23 | 1 |
| 1:A:106:GLN:O | 1:A:107:GLY:C | 0.43 | 2.57 | 1 | 2 |
| 1:A:69:ALA:CB | 1:A:94:ALA:CB | 0.43 | 2.89 | 2 | 1 |
| 1:A:21:ASP:OD1 | 1:A:21:ASP:C | 0.43 | 2.57 | 7 | 1 |
| 1:A:67:GLU:OE1 | 1:A:67:GLU:CA | 0.43 | 2.67 | 12 | 1 |
| 1:A:122:GLU:HA | 1:A:122:GLU:OE1 | 0.43 | 2.14 | 27 | 1 |
| 1:A:120:THR:HG23 | 1:A:121:HIS:CD2 | 0.43 | 2.49 | 3 | 2 |
| 1:A:77:ASP:OD1 | 1:A:120:THR:CG2 | 0.43 | 2.66 | 8 | 1 |
| 1:A:98:MET:O | 1:A:99:VAL:C | 0.43 | 2.57 | 9 | 3 |
| 1:A:33:THR:O | 1:A:88:GLY:N | 0.43 | 2.52 | 7 | 1 |
| 1:A:93:TYR:CE1 | 1:A:98:MET:HG3 | 0.43 | 2.48 | 19 | 1 |
| 1:A:27:TYR:O | 1:A:28:LYS:HB2 | 0.42 | 2.14 | 27 | 11 |
| 1:A:104:VAL:HG13 | 1:A:129:GLU:OE2 | 0.42 | 2.13 | 5 | 1 |
| 1:A:14:LEU:HG | 1:A:15:ILE:N | 0.42 | 2.28 | 6 | 1 |
| 1:A:102:ALA:O | 1:A:106:GLN:HG2 | 0.42 | 2.14 | 8 | 1 |
| 1:A:120:THR:CG2 | 1:A:121:HIS:N | 0.42 | 2.82 | 12 | 1 |
| 1:A:69:ALA:HA | 1:A:95:ASP:OD1 | 0.42 | 2.14 | 26 | 1 |
| 1:A:108:LEU:HD21 | 1:A:138:ASN:CG | 0.42 | 2.34 | 30 | 1 |
| 1:A:136:LYS:HA | 1:A:140:TRP:HB2 | 0.42 | 1.92 | 29 | 1 |
| 1:A:93:TYR:OH | 1:A:98:MET:CE | 0.42 | 2.68 | 14 | 1 |
| 1:A:119:ASN:OD1 | 1:A:119:ASN:C | 0.42 | 2.58 | 19 | 2 |
| 1:A:119:ASN:O | 1:A:119:ASN:CG | 0.42 | 2.58 | 10 | 1 |
| 1:A:13:THR:HB | 1:A:26:MET:CB | 0.42 | 2.44 | 20 | 1 |
| 1:A:77:ASP:OD1 | 1:A:120:THR:OG1 | 0.42 | 2.37 | 23 | 1 |
| 1:A:10:GLU:HB2 | 1:A:74:VAL:CG2 | 0.42 | 2.44 | 10 | 1 |
| 1:A:27:TYR:O | 1:A:30:GLN:OE1 | 0.42 | 2.38 | 1 | 1 |
| 1:A:37:LEU:O | 1:A:38:LEU:HB2 | 0.42 | 2.15 | 15 | 4 |
| 1:A:136:LYS:O | 1:A:141:SER:HB2 | 0.42 | 2.15 | 8 | 7 |
| 1:A:129:GLU:OE2 | 1:A:133:LYS:CG | 0.42 | 2.68 | 12 | 1 |
| 1:A:39:VAL:HG12 | 1:A:104:VAL:CG2 | 0.42 | 2.45 | 15 | 1 |
| 1:A:138:ASN:N | 1:A:141:SER:HB2 | 0.42 | 2.29 | 26 | 1 |
| 1:A:113:TYR:CB | 1:A:115:TYR:CZ | 0.42 | 3.02 | 6 | 1 |
| 1:A:63:LYS:O | 1:A:67:GLU:CB | 0.42 | 2.67 | 19 | 1 |
| 1:A:83:ASP:OD2 | 1:A:89:LEU:HD11 | 0.42 | 2.14 | 6 | 1 |
| 1:A:134:LYS:O | 1:A:134:LYS:CG | 0.42 | 2.68 | 9 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|---|---|---|---|---|---|
| | | | | Worst | Total |
| 1:A:85:TYR:HB3 | 1:A:87:ARG:CZ | 0.42 | 2.45 | 13 | 1 |
| 1:A:79:GLY:O | 1:A:80:GLN:C | 0.42 | 2.58 | 14 | 1 |
| 1:A:82:THR:HG22 | 1:A:87:ARG:O | 0.42 | 2.15 | 30 | 1 |
| 1:A:27:TYR:O | 1:A:28:LYS:C | 0.42 | 2.58 | 26 | 1 |
| 1:A:72:ILE:N | 1:A:72:ILE:CD1 | 0.41 | 2.75 | 5 | 1 |
| 1:A:67:GLU:OE1 | 1:A:67:GLU:HA | 0.41 | 2.14 | 12 | 1 |
| 1:A:101:GLU:HG3 | 1:A:124:LEU:CD2 | 0.41 | 2.43 | 12 | 1 |
| 1:A:74:VAL:HG13 | 1:A:92:ILE:HD13 | 0.41 | 1.91 | 23 | 1 |
| 1:A:101:GLU:OE2 | 1:A:128:SER:HB2 | 0.41 | 2.15 | 26 | 1 |
| 1:A:112:ALA:O | 1:A:113:TYR:C | 0.41 | 2.57 | 4 | 2 |
| 1:A:14:LEU:HD22 | 1:A:66:VAL:C | 0.41 | 2.36 | 18 | 1 |
| 1:A:111:VAL:O | 1:A:112:ALA:C | 0.41 | 2.58 | 18 | 1 |
| 1:A:9:LYS:HG2 | 1:A:75:GLU:OE1 | 0.41 | 2.15 | 29 | 1 |
| 1:A:23:VAL:HG23 | 1:A:23:VAL:O | 0.41 | 2.15 | 30 | 1 |
| 1:A:35:ARG:HD2 | 1:A:87:ARG:NH1 | 0.41 | 2.30 | 7 | 1 |
| 1:A:119:ASN:CG | 1:A:119:ASN:O | 0.41 | 2.58 | 12 | 1 |
| 1:A:38:LEU:HB3 | 1:A:125:LEU:CD1 | 0.41 | 2.45 | 20 | 1 |
| 1:A:115:TYR:O | 1:A:118:ASN:HB2 | 0.41 | 2.16 | 11 | 1 |
| 1:A:85:TYR:HB3 | 1:A:87:ARG:CD | 0.41 | 2.45 | 18 | 1 |
| 1:A:133:LYS:HE3 | 1:A:140:TRP:CZ3 | 0.41 | 2.50 | 20 | 1 |
| 1:A:124:LEU:C | 1:A:124:LEU:CD2 | 0.41 | 2.89 | 24 | 1 |
| 1:A:13:THR:HG22 | 1:A:14:LEU:N | 0.41 | 2.31 | 3 | 1 |
| 1:A:91:TYR:O | 1:A:92:ILE:HD13 | 0.41 | 2.16 | 11 | 1 |
| 1:A:37:LEU:CD1 | 1:A:89:LEU:HB3 | 0.41 | 2.46 | 15 | 1 |
| 1:A:24:LYS:NZ | 1:A:31:PRO:HB2 | 0.41 | 2.31 | 22 | 1 |
| 1:A:104:VAL:CG1 | 1:A:129:GLU:HB2 | 0.41 | 2.45 | 20 | 2 |
| 1:A:10:GLU:OE1 | 1:A:27:TYR:OH | 0.41 | 2.34 | 21 | 1 |
| 1:A:114:VAL:CG1 | 1:A:119:ASN:CB | 0.41 | 2.98 | 29 | 1 |
| 1:A:63:LYS:HA | 1:A:66:VAL:HG22 | 0.41 | 1.93 | 4 | 2 |
| 1:A:114:VAL:CG1 | 1:A:122:GLU:OE1 | 0.41 | 2.68 | 11 | 1 |
| 1:A:37:LEU:HD12 | 1:A:77:ASP:OD2 | 0.41 | 2.15 | 22 | 1 |
| 1:A:16:LYS:O | 1:A:24:LYS:CB | 0.41 | 2.69 | 4 | 1 |
| 1:A:38:LEU:HD22 | 1:A:122:GLU:OE1 | 0.41 | 2.16 | 5 | 1 |
| 1:A:21:ASP:OD1 | 1:A:21:ASP:O | 0.41 | 2.39 | 7 | 1 |
| 1:A:14:LEU:HB2 | 1:A:72:ILE:HD13 | 0.41 | 1.93 | 11 | 1 |
| 1:A:37:LEU:HD13 | 1:A:118:ASN:OD1 | 0.41 | 2.16 | 22 | 1 |
| 1:A:119:ASN:ND2 | 1:A:122:GLU:CB | 0.41 | 2.83 | 3 | 1 |
| 1:A:135:GLU:O | 1:A:136:LYS:HB2 | 0.41 | 2.16 | 25 | 3 |
| 1:A:68:ASN:N | 1:A:68:ASN:ND2 | 0.41 | 2.66 | 5 | 1 |
| 1:A:85:TYR:HB3 | 1:A:87:ARG:HD2 | 0.41 | 1.93 | 6 | 1 |
| 1:A:133:LYS:CE | 1:A:140:TRP:CZ3 | 0.41 | 3.04 | 7 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|---|---|---|---|---|---|
| | | | | Worst | Total |
| 1:A:137:LEU:N | 1:A:137:LEU:HD23 | 0.41 | 2.31 | 10 | 1 |
| 1:A:129:GLU:O | 1:A:133:LYS:HG3 | 0.41 | 2.16 | 22 | 1 |
| 1:A:61:PHE:O | 1:A:65:MET:HB3 | 0.41 | 2.16 | 27 | 1 |
| 1:A:106:GLN:O | 1:A:108:LEU:N | 0.41 | 2.54 | 29 | 1 |
| 1:A:83:ASP:HB2 | 1:A:87:ARG:CG | 0.41 | 2.46 | 1 | 1 |
| 1:A:40:ASP:OD2 | 1:A:112:ALA:HB2 | 0.41 | 2.15 | 18 | 1 |
| 1:A:135:GLU:C | 1:A:136:LYS:CG | 0.41 | 2.90 | 20 | 1 |
| 1:A:105:ARG:O | 1:A:105:ARG:CG | 0.40 | 2.70 | 2 | 1 |
| 1:A:35:ARG:NH2 | 1:A:85:TYR:CD2 | 0.40 | 2.90 | 12 | 1 |
| 1:A:36:LEU:CD2 | 1:A:92:ILE:CG1 | 0.40 | 3.00 | 10 | 1 |
| 1:A:14:LEU:CD2 | 1:A:67:GLU:CD | 0.40 | 2.89 | 13 | 1 |
| 1:A:37:LEU:HD11 | 1:A:89:LEU:HB3 | 0.40 | 1.94 | 18 | 1 |
| 1:A:64:LYS:O | 1:A:68:ASN:CG | 0.40 | 2.60 | 25 | 1 |
| 1:A:120:THR:HG22 | 1:A:121:HIS:ND1 | 0.40 | 2.31 | 28 | 2 |
| 1:A:114:VAL:CG1 | 1:A:119:ASN:HB3 | 0.40 | 2.45 | 29 | 1 |
| 1:A:65:MET:CE | 1:A:97:LYS:NZ | 0.40 | 2.85 | 14 | 1 |
| 1:A:114:VAL:HG11 | 1:A:119:ASN:OD1 | 0.40 | 2.16 | 16 | 1 |
| 1:A:60:ALA:O | 1:A:64:LYS:HG3 | 0.40 | 2.17 | 20 | 1 |
| 1:A:38:LEU:CD2 | 1:A:114:VAL:HG13 | 0.40 | 2.46 | 24 | 1 |
| 1:A:124:LEU:HD23 | 1:A:124:LEU:C | 0.40 | 2.36 | 28 | 1 |
| 1:A:82:THR:C | 1:A:89:LEU:CD1 | 0.40 | 2.89 | 30 | 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%) | 103±3 (87±2%) | 13±3 (11±2%) | 2±1 (2±1%) | 10 | 50 |
| All | All | 3540/4470 (79%) | 3085 (87%) | 380 (11%) | 75 (2%) | 10 | 50 |

All 14 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 | 138 | ASN | 12 |

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| Mol | Chain | Res | Type | Models (Total) |
|---|---|---|---|---|
| 1 | A | 119 | ASN | 12 |
| 1 | A | 69 | ALA | 11 |
| 1 | A | 118 | ASN | 9 |
| 1 | A | 57 | GLU | 9 |
| 1 | A | 98 | MET | 7 |
| 1 | A | 112 | ALA | 4 |
| 1 | A | 79 | GLY | 3 |
| 1 | A | 83 | ASP | 2 |
| 1 | A | 16 | LYS | 2 |
| 1 | A | 88 | GLY | 1 |
| 1 | A | 141 | SER | 1 |
| 1 | A | 80 | GLN | 1 |
| 1 | A | 109 | 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 | 99/125 (79%) | 80±4 (81±4%) | 19±4 (19±4%) | 4 36 |
| All | All | 2970/3750 (79%) | 2412 (81%) | 558 (19%) | 4 36 |

All 65 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 | 126 | ARG | 21 |
| 1 | A | 37 | LEU | 20 |
| 1 | A | 81 | ARG | 18 |
| 1 | A | 13 | THR | 17 |
| 1 | A | 127 | LYS | 16 |
| 1 | A | 131 | GLN | 16 |
| 1 | A | 16 | LYS | 15 |
| 1 | A | 19 | ASP | 15 |
| 1 | A | 63 | LYS | 15 |
| 1 | A | 65 | MET | 15 |
| 1 | A | 78 | LYS | 15 |
| 1 | A | 106 | GLN | 14 |

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| Mol | Chain | Res | Type | Models (Total) |
|---|---|---|---|---|
| 1 | A | 24 | LYS | 13 |
| 1 | A | 110 | LYS | 13 |
| 1 | A | 87 | ARG | 13 |
| 1 | A | 33 | THR | 12 |
| 1 | A | 9 | LYS | 11 |
| 1 | A | 41 | THR | 11 |
| 1 | A | 77 | ASP | 11 |
| 1 | A | 84 | LYS | 11 |
| 1 | A | 83 | ASP | 11 |
| 1 | A | 134 | LYS | 11 |
| 1 | A | 40 | ASP | 11 |
| 1 | A | 116 | LYS | 10 |
| 1 | A | 122 | GLU | 10 |
| 1 | A | 133 | LYS | 10 |
| 1 | A | 80 | GLN | 10 |
| 1 | A | 105 | ARG | 10 |
| 1 | A | 128 | SER | 9 |
| 1 | A | 136 | LYS | 9 |
| 1 | A | 124 | LEU | 9 |
| 1 | A | 39 | VAL | 9 |
| 1 | A | 21 | ASP | 8 |
| 1 | A | 73 | GLU | 8 |
| 1 | A | 35 | ARG | 8 |
| 1 | A | 70 | LYS | 8 |
| 1 | A | 57 | GLU | 8 |
| 1 | A | 59 | SER | 8 |
| 1 | A | 129 | GLU | 7 |
| 1 | A | 113 | TYR | 7 |
| 1 | A | 26 | MET | 7 |
| 1 | A | 22 | THR | 6 |
| 1 | A | 82 | THR | 6 |
| 1 | A | 119 | ASN | 6 |
| 1 | A | 98 | MET | 6 |
| 1 | A | 32 | MET | 6 |
| 1 | A | 95 | ASP | 5 |
| 1 | A | 101 | GLU | 5 |
| 1 | A | 14 | LEU | 4 |
| 1 | A | 64 | LYS | 4 |
| 1 | A | 71 | LYS | 3 |
| 1 | A | 137 | LEU | 3 |
| 1 | A | 67 | GLU | 3 |
| 1 | A | 28 | LYS | 3 |

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| Mol | Chain | Res | Type | Models (Total) |
|---|---|---|---|---|
| 1 | A | 23 | VAL | 2 |
| 1 | A | 97 | LYS | 2 |
| 1 | A | 103 | LEU | 2 |
| 1 | A | 123 | GLN | 2 |
| 1 | A | 74 | VAL | 2 |
| 1 | A | 75 | GLU | 2 |
| 1 | A | 141 | SER | 2 |
| 1 | A | 30 | GLN | 1 |
| 1 | A | 135 | GLU | 1 |
| 1 | A | 138 | ASN | 1 |
| 1 | A | 120 | THR | 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