Full wwPDB NMR Structure Validation Report (i)

Oct 31, 2021 – 01:47 PM EDT

PDB ID	:	1RKN
Title	:	Solution structure of 1-110 fragment of Staphylococcal Nuclease with G88W mutation
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Deposited on	:	2003-11-22

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:

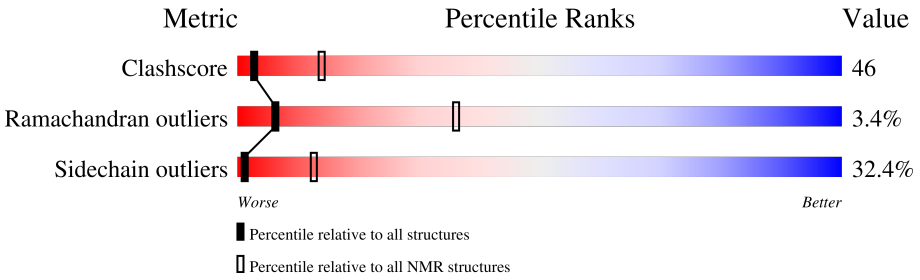
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.23.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (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	110	15% 41% 5% 39%

2 Ensemble composition and analysis (i)

This entry contains 12 models. Model 6 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:36, A:56-A:82, A:88-A:99 (67)	0.39	6

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 3 clusters and 3 single-model clusters were found.

Cluster number	Models
1	1, 4, 6
2	5, 8, 10
3	2, 3, 12
Single-model clusters	7; 9; 11

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1792 atoms, of which 918 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	110	1792	560	918	150	160	4	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	88	TRP	GLY	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: Thermonuclease

Chain A: 15% 41% 5% 39%

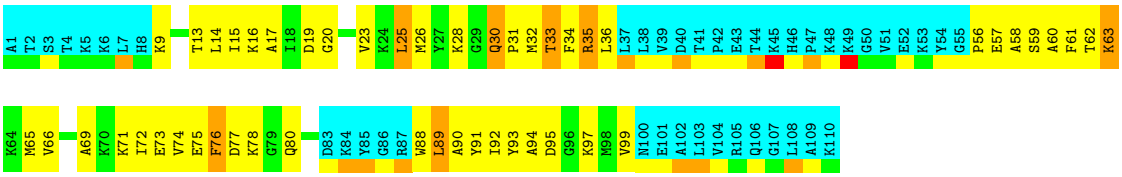
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: Thermonuclease

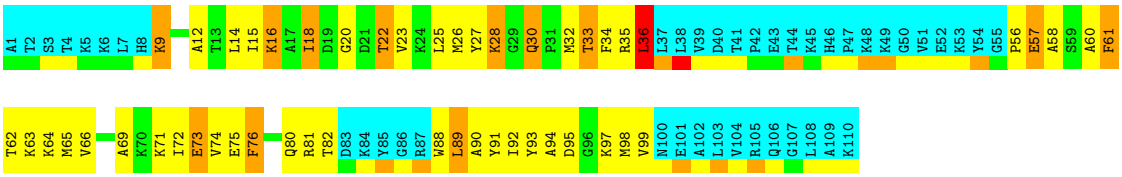
Chain A: 16% 38% 6% 39%



4.2.2 Score per residue for model 2

• Molecule 1: Thermonuclease

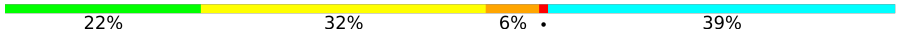
Chain A: 15% 34% 11% • 39%

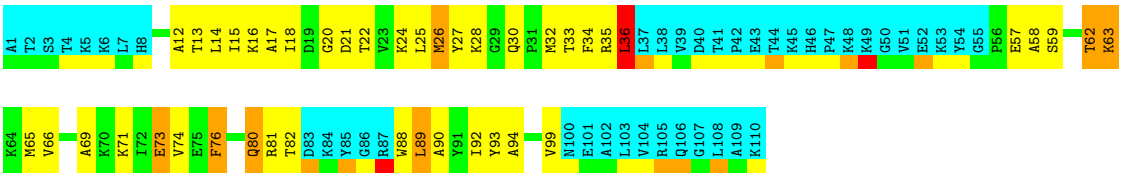


4.2.3 Score per residue for model 3

- Molecule 1: Thermonuclease

Chain A:

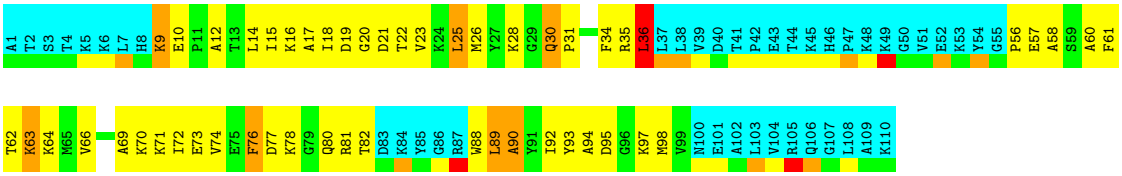




4.2.4 Score per residue for model 4

- Molecule 1: Thermonuclease

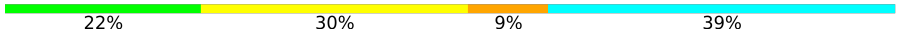
Chain A:

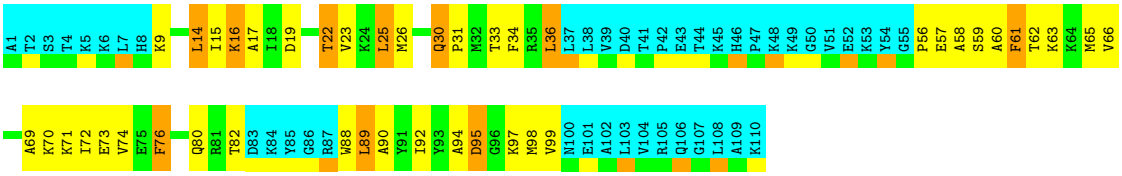


4.2.5 Score per residue for model 5

- Molecule 1: Thermonuclease

Chain A:





4.2.6 Score per residue for model 6 (medoid)

- Molecule 1: Thermonuclease

Chain A: 23% 30% 8% 39%

A1 T2 S3 T4 K5 K6 L7 H8 K9 A12 T13 L14 I15 K16 A17 D21 T22 V23 K24 L25 M26 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

V66 A69 K70 K71 V74 E75 F76 D77 K78 G79 Q80 D83 K84 Y85 G86 R87 W88 L89 A90 Y91 I92 Y93 A94 D95 V99 N100 E101 A102 L103 V104 R105 Q106 G107 L108 A109 K110

4.2.7 Score per residue for model 7

- Molecule 1: Thermonuclease

Chain A: 19% 33% 8% • 39%

A1 T2 S3 T4 K5 K6 L7 H8 K9 A12 T13 L14 I15 K16 A17 I18 T22 V23 K24 L25 M26 Q30 P31 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 K71 I72 E73 V74 E75 F76 D77 Q80 R81 T82 D83 K84 Y85 G86 R87 W88 L89 A90 Y91 I92 Y93 A94 K97 M98 V99 N100 E101 A102 L103 V104 R105 Q106 G107 L108 A109 K110

4.2.8 Score per residue for model 8

- Molecule 1: Thermonuclease

Chain A: 18% 30% 12% • 39%

A1 T2 S3 T4 K5 K6 L7 H8 K9 T13 L14 I15 K16 A17 G20 V23 K24 L25 M26 Y27 Q30 P31 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

A69 K70 K71 I72 E73 F76 D77 K78 G79 Q80 R81 T82 D83 K84 Y85 G86 R87 W88 L89 A90 Y91 I92 Y93 A94 K97 M98 V99 N100 E101 A102 L103 V104 R105 Q106 G107 L108 A109 K110

4.2.9 Score per residue for model 9

- Molecule 1: Thermonuclease

Chain A: 17% 36% 7% 39%

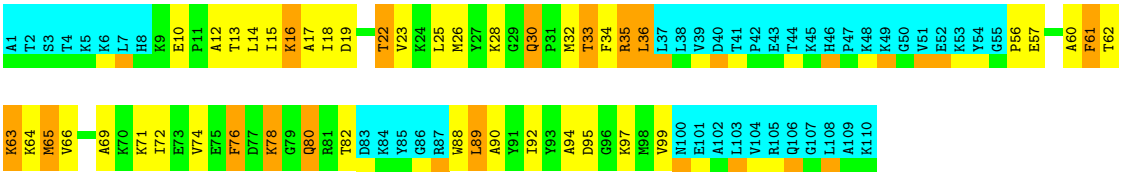
A1 T2 S3 T4 K5 K6 L7 H8 K9 E10 P11 A12 T13 L14 I15 K16 A17 G20 D21 T22 V23 K24 L25 M26 Y27 K28 G29 Q30 P31 M32 T33 F34 R35 L36 L37 L38 V39 D40 T41 P42 E43 T44 K45 H46 P47 K48 K49 G50 V51 E52 K53 Y54 G55 P56 E57 A58 S59 A60 F61

T62 V66 E67 N68 A69 K70 K71 I72 E73 V74 E75 F76 D77 K78 G79 Q80 R81 T82 D83 K84 Y85 G86 R87 W88 L89 A90 Y91 I92 Y93 M98 V99 N100 E101 A102 L103 V104 R105 Q106 G107 L108 A109 K110

4.2.10 Score per residue for model 10

- Molecule 1: Thermonuclease

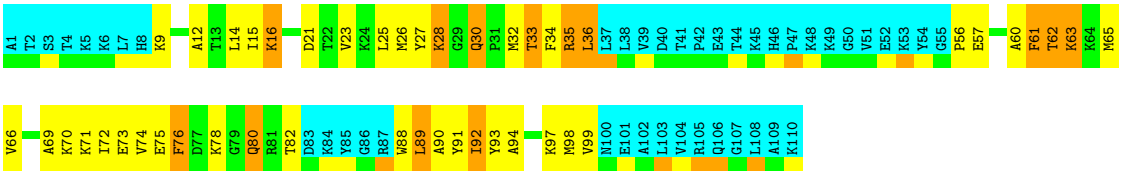
Chain A: 20% 29% 12% 39%



4.2.11 Score per residue for model 11

- Molecule 1: Thermonuclease

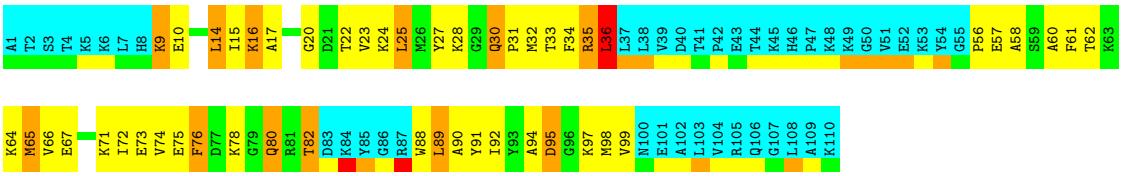
Chain A: 19% 30% 12% 39%



4.2.12 Score per residue for model 12

- Molecule 1: Thermonuclease

Chain A: 16% 33% 11% • 39%



5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *simulated annealing*.

Of the 50 calculated structures, 12 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	structure solution	1.1
CNS	refinement	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	535	556	556	50±5
All	All	6420	6672	6672	596

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 46.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:69:ALA:HB3	1:A:94:ALA:HB1	1.03	1.30	8	10
1:A:17:ALA:HB2	1:A:62:THR:HG21	0.99	1.33	7	8
1:A:25:LEU:HD22	1:A:74:VAL:HG21	0.92	1.40	2	4
1:A:15:ILE:HD12	1:A:16:LYS:N	0.89	1.80	1	11
1:A:82:THR:HG21	1:A:88:TRP:CE2	0.87	2.05	3	2
1:A:82:THR:HG21	1:A:88:TRP:CG	0.85	2.07	9	2
1:A:89:LEU:HD13	1:A:89:LEU:O	0.84	1.72	10	11
1:A:80:GLN:HG3	1:A:89:LEU:HD12	0.84	1.50	2	5
1:A:25:LEU:HD12	1:A:25:LEU:O	0.83	1.74	2	5
1:A:17:ALA:HB2	1:A:62:THR:CG2	0.81	2.04	3	5
1:A:12:ALA:HB3	1:A:25:LEU:HD13	0.81	1.51	3	3
1:A:25:LEU:HG	1:A:34:PHE:CE1	0.80	2.12	11	5
1:A:56:PRO:O	1:A:60:ALA:HB3	0.79	1.77	6	5
1:A:72:ILE:HG23	1:A:93:TYR:O	0.79	1.77	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:20:GLY:HA2	1:A:58:ALA:HB1	0.79	1.55	4	6
1:A:14:LEU:HD12	1:A:66:VAL:HG11	0.79	1.54	2	1
1:A:12:ALA:CB	1:A:25:LEU:HD13	0.78	2.08	3	5
1:A:89:LEU:HD22	1:A:90:ALA:N	0.78	1.93	2	10
1:A:10:GLU:O	1:A:74:VAL:HG12	0.78	1.77	12	1
1:A:10:GLU:O	1:A:74:VAL:HG22	0.77	1.78	9	2
1:A:82:THR:HG21	1:A:88:TRP:CD1	0.77	2.15	12	3
1:A:25:LEU:CD2	1:A:74:VAL:HG21	0.77	2.08	7	3
1:A:25:LEU:HD11	1:A:34:PHE:CZ	0.77	2.15	2	4
1:A:74:VAL:CG1	1:A:90:ALA:HB1	0.76	2.11	3	4
1:A:17:ALA:CB	1:A:62:THR:HG21	0.76	2.10	7	2
1:A:12:ALA:HB1	1:A:25:LEU:HD13	0.73	1.60	9	2
1:A:80:GLN:CG	1:A:89:LEU:HD12	0.73	2.14	2	5
1:A:74:VAL:HG13	1:A:90:ALA:HB1	0.72	1.60	2	6
1:A:14:LEU:HD11	1:A:23:VAL:HB	0.72	1.61	6	3
1:A:14:LEU:HD13	1:A:14:LEU:O	0.71	1.86	7	1
1:A:69:ALA:CB	1:A:94:ALA:HB1	0.70	2.12	6	5
1:A:27:TYR:O	1:A:30:GLN:NE2	0.70	2.24	9	3
1:A:20:GLY:CA	1:A:58:ALA:HB1	0.70	2.16	4	3
1:A:66:VAL:HG13	1:A:72:ILE:HG12	0.69	1.63	5	4
1:A:34:PHE:HA	1:A:88:TRP:O	0.69	1.87	9	9
1:A:76:PHE:HB2	1:A:89:LEU:O	0.69	1.88	1	2
1:A:14:LEU:HD11	1:A:63:LYS:HA	0.69	1.64	11	1
1:A:17:ALA:HB3	1:A:59:SER:HA	0.69	1.65	9	4
1:A:13:THR:HG22	1:A:72:ILE:HD13	0.68	1.66	1	1
1:A:12:ALA:HB1	1:A:26:MET:O	0.68	1.89	3	6
1:A:22:THR:HG22	1:A:33:THR:CG2	0.67	2.20	5	3
1:A:56:PRO:CB	1:A:60:ALA:HB3	0.66	2.21	1	1
1:A:57:GLU:HA	1:A:61:PHE:HB2	0.66	1.67	12	4
1:A:82:THR:HG21	1:A:88:TRP:CD2	0.65	2.25	3	2
1:A:22:THR:HG22	1:A:33:THR:HG21	0.65	1.68	5	2
1:A:15:ILE:HA	1:A:66:VAL:HG11	0.65	1.68	7	1
1:A:14:LEU:HB3	1:A:66:VAL:HG21	0.64	1.70	5	2
1:A:80:GLN:HB2	1:A:89:LEU:HD12	0.64	1.66	9	3
1:A:15:ILE:HD12	1:A:16:LYS:CB	0.64	2.23	4	6
1:A:89:LEU:HD13	1:A:89:LEU:C	0.64	2.13	2	9
1:A:17:ALA:HA	1:A:23:VAL:HG12	0.64	1.69	5	7
1:A:18:ILE:HD12	1:A:22:THR:O	0.63	1.92	10	1
1:A:62:THR:HA	1:A:99:VAL:HG11	0.63	1.70	2	4
1:A:23:VAL:HG22	1:A:34:PHE:O	0.63	1.92	8	2
1:A:36:LEU:HD21	1:A:90:ALA:O	0.63	1.92	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:77:ASP:HB3	1:A:80:GLN:HG2	0.63	1.69	8	3
1:A:15:ILE:HD12	1:A:16:LYS:HB2	0.62	1.70	11	2
1:A:14:LEU:HG	1:A:66:VAL:HG21	0.62	1.72	11	1
1:A:72:ILE:CG2	1:A:92:ILE:HG23	0.62	2.25	8	3
1:A:14:LEU:HD22	1:A:25:LEU:HG	0.61	1.71	12	2
1:A:18:ILE:HD12	1:A:22:THR:HG22	0.61	1.71	4	2
1:A:91:TYR:C	1:A:92:ILE:HD12	0.61	2.15	7	3
1:A:36:LEU:HD11	1:A:90:ALA:O	0.60	1.96	3	1
1:A:17:ALA:CB	1:A:23:VAL:HG12	0.60	2.26	8	3
1:A:25:LEU:O	1:A:31:PRO:HA	0.60	1.96	4	8
1:A:12:ALA:CB	1:A:25:LEU:HD21	0.60	2.26	10	1
1:A:36:LEU:HD22	1:A:89:LEU:HD23	0.60	1.73	6	1
1:A:62:THR:O	1:A:66:VAL:HG23	0.59	1.97	11	1
1:A:12:ALA:HB3	1:A:25:LEU:HD21	0.59	1.75	10	1
1:A:35:ARG:O	1:A:36:LEU:HD12	0.58	1.98	2	2
1:A:36:LEU:HD13	1:A:89:LEU:HB2	0.58	1.74	6	2
1:A:34:PHE:CD2	1:A:88:TRP:HB2	0.58	2.34	6	7
1:A:89:LEU:C	1:A:89:LEU:HD22	0.58	2.19	4	4
1:A:56:PRO:HA	1:A:60:ALA:HB3	0.57	1.75	12	4
1:A:25:LEU:HD12	1:A:25:LEU:C	0.57	2.18	3	5
1:A:14:LEU:CD2	1:A:66:VAL:HG21	0.57	2.30	11	4
1:A:16:LYS:HA	1:A:63:LYS:HB3	0.56	1.77	11	2
1:A:82:THR:HG22	1:A:88:TRP:CE2	0.56	2.34	4	2
1:A:32:MET:O	1:A:34:PHE:CE1	0.56	2.58	9	7
1:A:23:VAL:HG21	1:A:92:ILE:HD13	0.56	1.76	2	1
1:A:66:VAL:HG13	1:A:72:ILE:CG1	0.56	2.31	1	4
1:A:89:LEU:O	1:A:90:ALA:HB2	0.56	2.01	4	7
1:A:62:THR:O	1:A:66:VAL:HG22	0.56	2.00	2	1
1:A:56:PRO:HB2	1:A:60:ALA:HB3	0.56	1.76	7	1
1:A:27:TYR:HB3	1:A:30:GLN:O	0.56	2.00	8	2
1:A:76:PHE:C	1:A:76:PHE:CD1	0.55	2.79	7	5
1:A:12:ALA:HB3	1:A:25:LEU:HD22	0.55	1.79	4	2
1:A:25:LEU:HD22	1:A:74:VAL:CG2	0.55	2.24	2	1
1:A:69:ALA:O	1:A:72:ILE:HD11	0.55	2.01	9	1
1:A:73:GLU:O	1:A:93:TYR:HB2	0.55	2.02	9	1
1:A:14:LEU:HD13	1:A:62:THR:HG22	0.55	1.78	1	1
1:A:15:ILE:HD12	1:A:16:LYS:CG	0.54	2.32	5	4
1:A:25:LEU:HD21	1:A:74:VAL:HG11	0.54	1.78	9	1
1:A:65:MET:CB	1:A:99:VAL:HG12	0.54	2.32	6	2
1:A:25:LEU:CG	1:A:34:PHE:CE1	0.54	2.89	2	4
1:A:62:THR:HG22	1:A:63:LYS:N	0.54	2.18	11	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:82:THR:HG21	1:A:88:TRP:NE1	0.54	2.17	11	2
1:A:80:GLN:CB	1:A:89:LEU:HD12	0.54	2.32	9	2
1:A:36:LEU:HD22	1:A:89:LEU:HB2	0.54	1.80	7	2
1:A:15:ILE:C	1:A:15:ILE:HD12	0.54	2.22	7	1
1:A:92:ILE:HD12	1:A:92:ILE:N	0.54	2.18	8	1
1:A:76:PHE:HB2	1:A:89:LEU:HD13	0.53	1.79	6	4
1:A:27:TYR:CE1	1:A:76:PHE:CE1	0.53	2.96	2	1
1:A:76:PHE:HA	1:A:89:LEU:HD11	0.53	1.80	5	3
1:A:22:THR:HA	1:A:34:PHE:O	0.53	2.03	2	1
1:A:15:ILE:CD1	1:A:16:LYS:N	0.53	2.65	1	10
1:A:62:THR:O	1:A:66:VAL:HG13	0.53	2.04	2	1
1:A:15:ILE:HD12	1:A:16:LYS:HB3	0.53	1.79	6	3
1:A:33:THR:O	1:A:88:TRP:N	0.53	2.40	9	3
1:A:80:GLN:CG	1:A:88:TRP:CE3	0.53	2.92	11	2
1:A:23:VAL:O	1:A:34:PHE:N	0.52	2.42	11	2
1:A:14:LEU:CG	1:A:66:VAL:HG21	0.52	2.34	11	1
1:A:80:GLN:CG	1:A:89:LEU:CD1	0.52	2.87	12	1
1:A:14:LEU:HD11	1:A:23:VAL:CB	0.52	2.33	6	1
1:A:34:PHE:CA	1:A:88:TRP:O	0.52	2.58	7	6
1:A:89:LEU:HD22	1:A:89:LEU:C	0.52	2.25	11	7
1:A:77:ASP:H	1:A:89:LEU:HD11	0.52	1.64	1	3
1:A:25:LEU:HB2	1:A:34:PHE:CD1	0.52	2.39	5	5
1:A:80:GLN:HB2	1:A:88:TRP:CE3	0.52	2.40	2	3
1:A:25:LEU:CD1	1:A:34:PHE:CZ	0.51	2.93	7	3
1:A:35:ARG:O	1:A:36:LEU:HB3	0.51	2.04	3	1
1:A:57:GLU:HA	1:A:61:PHE:CB	0.51	2.35	4	2
1:A:14:LEU:N	1:A:66:VAL:HG11	0.51	2.21	1	1
1:A:14:LEU:HD22	1:A:66:VAL:HG21	0.51	1.82	9	1
1:A:74:VAL:HG12	1:A:76:PHE:HB3	0.51	1.81	10	1
1:A:58:ALA:O	1:A:62:THR:HB	0.51	2.05	5	5
1:A:34:PHE:CD1	1:A:34:PHE:N	0.51	2.79	3	4
1:A:76:PHE:CE2	1:A:88:TRP:CE3	0.50	2.99	10	1
1:A:14:LEU:HD21	1:A:23:VAL:HB	0.50	1.83	7	1
1:A:80:GLN:HG3	1:A:89:LEU:CD1	0.50	2.37	4	3
1:A:14:LEU:CB	1:A:92:ILE:HG21	0.50	2.36	7	1
1:A:14:LEU:HD11	1:A:63:LYS:CA	0.50	2.36	11	1
1:A:30:GLN:O	1:A:30:GLN:HG2	0.50	2.07	9	2
1:A:14:LEU:C	1:A:14:LEU:CD1	0.50	2.80	12	2
1:A:82:THR:CG2	1:A:88:TRP:CE2	0.49	2.91	3	3
1:A:36:LEU:HD13	1:A:89:LEU:CB	0.49	2.36	11	1
1:A:36:LEU:C	1:A:36:LEU:HD13	0.49	2.28	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:35:ARG:N	1:A:88:TRP:O	0.49	2.44	7	8
1:A:25:LEU:CD1	1:A:34:PHE:CD1	0.49	2.95	12	2
1:A:14:LEU:HB3	1:A:66:VAL:HG11	0.49	1.84	3	3
1:A:15:ILE:HD12	1:A:16:LYS:CA	0.48	2.38	4	3
1:A:33:THR:C	1:A:34:PHE:CD1	0.48	2.87	2	3
1:A:34:PHE:HB3	1:A:90:ALA:HB3	0.48	1.85	9	1
1:A:13:THR:HG22	1:A:72:ILE:CD1	0.48	2.36	1	1
1:A:34:PHE:CD2	1:A:88:TRP:CB	0.48	2.96	5	4
1:A:80:GLN:O	1:A:82:THR:N	0.48	2.45	3	1
1:A:89:LEU:O	1:A:89:LEU:HD13	0.48	2.09	4	1
1:A:14:LEU:O	1:A:66:VAL:HG11	0.48	2.09	7	1
1:A:66:VAL:HA	1:A:94:ALA:HB2	0.48	1.84	8	1
1:A:65:MET:SD	1:A:94:ALA:HB3	0.48	2.49	12	2
1:A:15:ILE:HD12	1:A:15:ILE:C	0.47	2.29	6	4
1:A:14:LEU:CG	1:A:92:ILE:HG21	0.47	2.38	7	1
1:A:30:GLN:CG	1:A:30:GLN:O	0.47	2.63	4	4
1:A:66:VAL:HG13	1:A:72:ILE:CD1	0.47	2.39	1	1
1:A:56:PRO:HB2	1:A:60:ALA:CB	0.47	2.40	7	1
1:A:13:THR:HG23	1:A:13:THR:O	0.47	2.10	3	1
1:A:34:PHE:HB3	1:A:88:TRP:O	0.46	2.10	2	1
1:A:25:LEU:HD13	1:A:34:PHE:CD1	0.46	2.45	12	1
1:A:30:GLN:O	1:A:30:GLN:CG	0.46	2.64	5	2
1:A:14:LEU:HD13	1:A:14:LEU:C	0.46	2.30	7	1
1:A:62:THR:HG23	1:A:63:LYS:N	0.46	2.26	8	1
1:A:66:VAL:HG12	1:A:72:ILE:HG12	0.46	1.87	12	1
1:A:73:GLU:HB2	1:A:93:TYR:CE1	0.46	2.45	11	4
1:A:77:ASP:CB	1:A:80:GLN:HG2	0.46	2.40	8	1
1:A:28:LYS:O	1:A:30:GLN:OE1	0.46	2.34	2	2
1:A:15:ILE:O	1:A:63:LYS:HG2	0.46	2.11	7	1
1:A:94:ALA:O	1:A:95:ASP:CB	0.46	2.64	5	3
1:A:80:GLN:HB2	1:A:88:TRP:CZ3	0.46	2.46	2	2
1:A:76:PHE:CD1	1:A:76:PHE:C	0.45	2.89	3	4
1:A:27:TYR:CE2	1:A:76:PHE:CE1	0.45	3.03	3	1
1:A:12:ALA:HB3	1:A:25:LEU:CD2	0.45	2.40	6	1
1:A:74:VAL:HG12	1:A:92:ILE:HG13	0.45	1.88	1	1
1:A:76:PHE:O	1:A:76:PHE:CD1	0.45	2.69	11	3
1:A:74:VAL:HB	1:A:90:ALA:HB1	0.45	1.87	1	1
1:A:80:GLN:O	1:A:81:ARG:C	0.45	2.55	8	1
1:A:27:TYR:CE1	1:A:76:PHE:CZ	0.45	3.04	11	1
1:A:57:GLU:O	1:A:61:PHE:CB	0.45	2.65	5	3
1:A:56:PRO:C	1:A:60:ALA:HB3	0.45	2.31	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:17:ALA:CA	1:A:23:VAL:HG12	0.45	2.40	5	2
1:A:25:LEU:C	1:A:25:LEU:CD1	0.44	2.85	9	2
1:A:16:LYS:HA	1:A:63:LYS:CB	0.44	2.42	1	2
1:A:12:ALA:CB	1:A:25:LEU:CD2	0.44	2.95	10	1
1:A:25:LEU:HD21	1:A:74:VAL:HG21	0.44	1.89	11	1
1:A:74:VAL:CG1	1:A:90:ALA:CB	0.43	2.96	6	2
1:A:76:PHE:CD1	1:A:76:PHE:O	0.43	2.71	4	2
1:A:18:ILE:N	1:A:22:THR:O	0.43	2.50	2	1
1:A:34:PHE:CD2	1:A:90:ALA:HB2	0.43	2.47	3	1
1:A:73:GLU:O	1:A:93:TYR:CZ	0.43	2.71	4	2
1:A:36:LEU:HD23	1:A:36:LEU:N	0.43	2.29	5	1
1:A:61:PHE:CD2	1:A:65:MET:CG	0.43	3.02	11	1
1:A:14:LEU:CD2	1:A:63:LYS:CB	0.43	2.96	4	1
1:A:14:LEU:HD13	1:A:62:THR:CG2	0.43	2.42	1	1
1:A:14:LEU:CD1	1:A:62:THR:CG2	0.43	2.96	1	1
1:A:15:ILE:CD1	1:A:16:LYS:CG	0.43	2.96	12	2
1:A:14:LEU:HB2	1:A:25:LEU:HB3	0.43	1.91	7	1
1:A:65:MET:CB	1:A:99:VAL:HG13	0.43	2.44	8	1
1:A:25:LEU:CD1	1:A:34:PHE:CE1	0.43	3.02	2	3
1:A:82:THR:CG2	1:A:88:TRP:CZ2	0.43	3.01	8	2
1:A:14:LEU:HB3	1:A:92:ILE:HG21	0.43	1.90	7	1
1:A:90:ALA:O	1:A:91:TYR:CD1	0.43	2.72	12	1
1:A:14:LEU:HA	1:A:25:LEU:HA	0.43	1.90	9	3
1:A:80:GLN:HG3	1:A:89:LEU:HD11	0.43	1.89	4	1
1:A:14:LEU:HD22	1:A:63:LYS:HA	0.43	1.89	4	1
1:A:14:LEU:HD11	1:A:23:VAL:CG2	0.43	2.44	6	1
1:A:14:LEU:HD23	1:A:66:VAL:HG21	0.42	1.90	8	1
1:A:63:LYS:O	1:A:66:VAL:HG22	0.42	2.14	8	2
1:A:62:THR:CG2	1:A:63:LYS:N	0.42	2.82	11	1
1:A:73:GLU:HB3	1:A:93:TYR:CZ	0.42	2.50	2	2
1:A:92:ILE:HG22	1:A:93:TYR:N	0.42	2.29	9	1
1:A:66:VAL:HG23	1:A:72:ILE:CD1	0.42	2.44	7	1
1:A:13:THR:HA	1:A:72:ILE:HD13	0.42	1.91	8	1
1:A:12:ALA:CB	1:A:26:MET:O	0.42	2.67	2	1
1:A:93:TYR:HB3	1:A:98:MET:HA	0.42	1.90	2	2
1:A:60:ALA:O	1:A:64:LYS:CB	0.42	2.68	10	1
1:A:57:GLU:OE1	1:A:61:PHE:CG	0.42	2.72	1	1
1:A:56:PRO:O	1:A:60:ALA:CB	0.42	2.62	10	1
1:A:17:ALA:N	1:A:62:THR:HG21	0.42	2.30	10	1
1:A:89:LEU:O	1:A:90:ALA:CB	0.42	2.66	4	1
1:A:69:ALA:HB1	1:A:95:ASP:OD1	0.41	2.15	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:56:PRO:HB3	1:A:60:ALA:HB3	0.41	1.88	1	1
1:A:89:LEU:C	1:A:89:LEU:CD1	0.41	2.87	5	1
1:A:35:ARG:O	1:A:36:LEU:HB2	0.41	2.14	9	1
1:A:74:VAL:HG22	1:A:76:PHE:HB3	0.41	1.89	12	1
1:A:56:PRO:O	1:A:60:ALA:N	0.41	2.52	8	1
1:A:56:PRO:O	1:A:61:PHE:N	0.41	2.53	12	1
1:A:25:LEU:HD13	1:A:74:VAL:CG2	0.41	2.45	10	1
1:A:14:LEU:CD1	1:A:16:LYS:N	0.41	2.84	12	1
1:A:72:ILE:CG2	1:A:92:ILE:CG2	0.41	2.99	12	1
1:A:16:LYS:HG2	1:A:17:ALA:N	0.41	2.31	6	1
1:A:27:TYR:CD1	1:A:27:TYR:C	0.41	2.94	3	1
1:A:25:LEU:CD1	1:A:74:VAL:CG2	0.41	2.98	10	1
1:A:26:MET:O	1:A:26:MET:HG3	0.41	2.16	10	1
1:A:61:PHE:CD2	1:A:65:MET:HG2	0.41	2.51	11	1
1:A:58:ALA:O	1:A:62:THR:CB	0.41	2.69	1	1
1:A:62:THR:CA	1:A:99:VAL:HG11	0.41	2.44	2	1
1:A:36:LEU:N	1:A:36:LEU:CD1	0.41	2.84	3	1
1:A:25:LEU:HD11	1:A:92:ILE:HG12	0.41	1.93	6	1
1:A:17:ALA:HB3	1:A:59:SER:OG	0.41	2.16	8	1
1:A:80:GLN:HG2	1:A:88:TRP:CE3	0.41	2.51	11	1
1:A:80:GLN:HG2	1:A:89:LEU:CD1	0.41	2.46	12	1
1:A:33:THR:O	1:A:88:TRP:HB2	0.40	2.16	9	1
1:A:36:LEU:HB2	1:A:89:LEU:HA	0.40	1.92	7	1
1:A:25:LEU:HB2	1:A:34:PHE:CE1	0.40	2.51	8	1
1:A:76:PHE:CE2	1:A:77:ASP:O	0.40	2.75	9	1
1:A:74:VAL:CG2	1:A:90:ALA:HB1	0.40	2.46	12	1
1:A:32:MET:O	1:A:34:PHE:CD1	0.40	2.75	1	1
1:A:36:LEU:CD1	1:A:90:ALA:O	0.40	2.68	3	1
1:A:12:ALA:O	1:A:72:ILE:O	0.40	2.40	10	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	67/110 (61%)	54±2 (81±3%)	10±2 (16±3%)	2±1 (3±2%)	6 36

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	804/1320 (61%)	652 (81%)	125 (16%)	27 (3%)	6 36

All 7 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	36	LEU	9
1	A	92	ILE	8
1	A	9	LYS	3
1	A	81	ARG	3
1	A	18	ILE	2
1	A	90	ALA	1
1	A	95	ASP	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	56/92 (61%)	38±2 (68±4%)	18±2 (32±4%)	1 12
All	All	672/1104 (61%)	454 (68%)	218 (32%)	1 12

All 41 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	76	PHE	12
1	A	89	LEU	12
1	A	30	GLN	11
1	A	71	LYS	11
1	A	9	LYS	9
1	A	97	LYS	9
1	A	36	LEU	9
1	A	26	MET	8
1	A	28	LYS	8
1	A	63	LYS	8
1	A	65	MET	8
1	A	25	LEU	7

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Mol	Chain	Res	Type	Models (Total)
1	A	78	LYS	7
1	A	35	ARG	6
1	A	16	LYS	6
1	A	61	PHE	6
1	A	33	THR	5
1	A	95	ASP	5
1	A	24	LYS	5
1	A	80	GLN	5
1	A	70	LYS	5
1	A	98	MET	5
1	A	19	ASP	4
1	A	22	THR	4
1	A	64	LYS	4
1	A	73	GLU	4
1	A	21	ASP	4
1	A	14	LEU	4
1	A	57	GLU	3
1	A	75	GLU	3
1	A	81	ARG	3
1	A	67	GLU	3
1	A	62	THR	2
1	A	59	SER	2
1	A	77	ASP	2
1	A	99	VAL	2
1	A	13	THR	2
1	A	82	THR	2
1	A	32	MET	1
1	A	93	TYR	1
1	A	10	GLU	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