



Full wwPDB NMR Structure Validation Report ⓘ

Mar 1, 2026 – 04:11 PM UTC

PDB ID : 2K9M / pdb_00002k9m
Title : Structure of the Core Binding Domain of sigma54
Authors : Hong, E.; Wemmer, D.
Deposited on : 2008-10-19

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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
wwPDB-ShiftChecker : v1.2
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

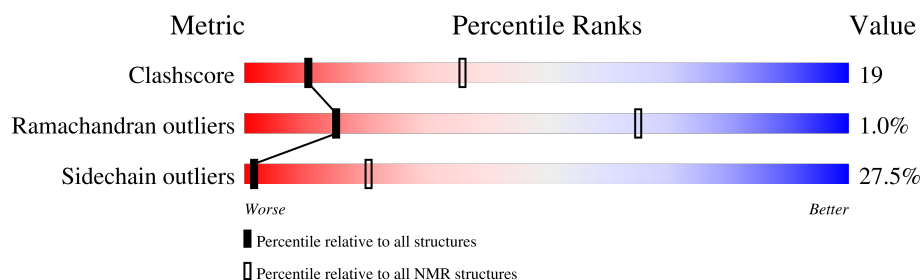
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment was not calculated.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and a grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	130	

2 Ensemble composition and analysis

This entry contains 20 models. Model 3 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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:72-A:185 (114)	0.37	3

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 4 single-model clusters were found.

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

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 2187 atoms, of which 1119 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called RNA polymerase sigma factor RpoN.

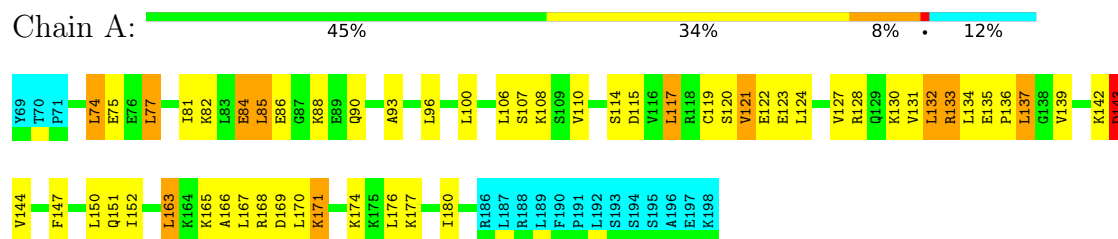
Mol	Chain	Residues	Atoms						Trace
1	A	130	Total	C	H	N	O	S	0
			2187	682	1119	176	208	2	

4 Residue-property plots

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: RNA polymerase sigma factor RpoN

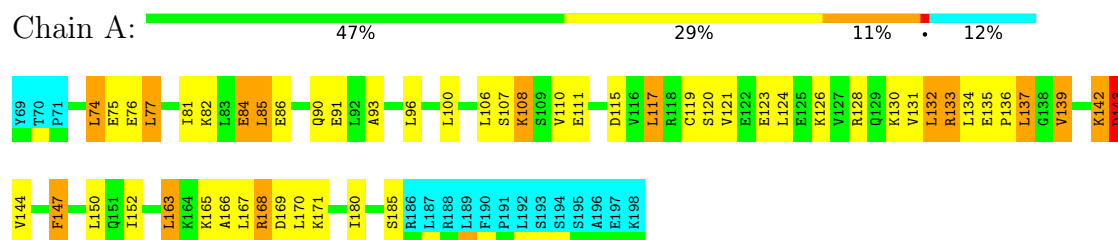


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

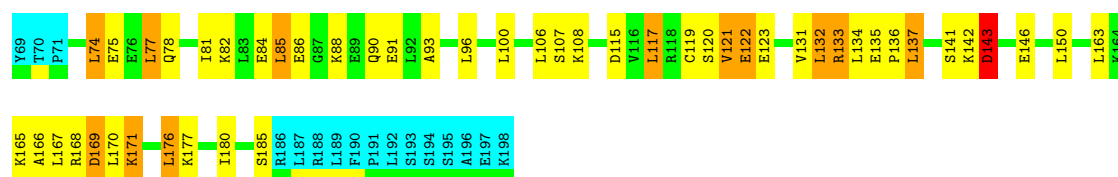
- Molecule 1: RNA polymerase sigma factor RpoN



4.2.2 Score per residue for model 2

- Molecule 1: RNA polymerase sigma factor RpoN

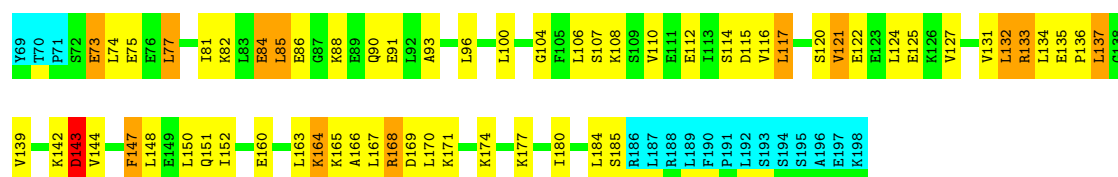




4.2.3 Score per residue for model 3 (medoid)

- Molecule 1: RNA polymerase sigma factor RpoN

Chain A: 40% 38% 9% 12%



4.2.4 Score per residue for model 4

- Molecule 1: RNA polymerase sigma factor RpoN

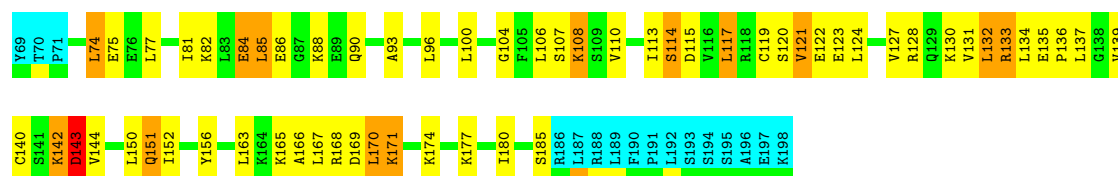
Chain A: 43% 32% 12% 12%



4.2.5 Score per residue for model 5

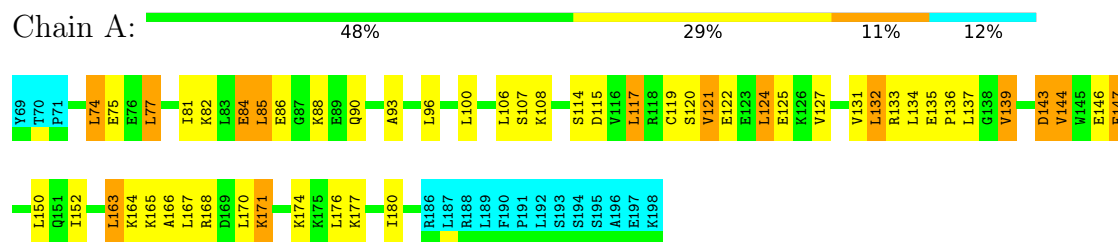
- Molecule 1: RNA polymerase sigma factor RpoN

Chain A: 42% 35% 10% 12%



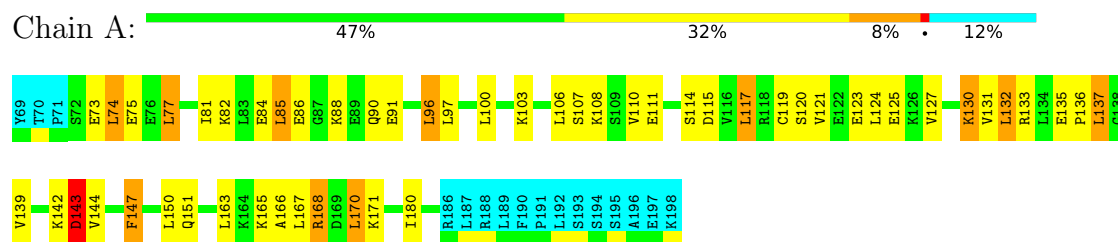
4.2.6 Score per residue for model 6

- Molecule 1: RNA polymerase sigma factor RpoN



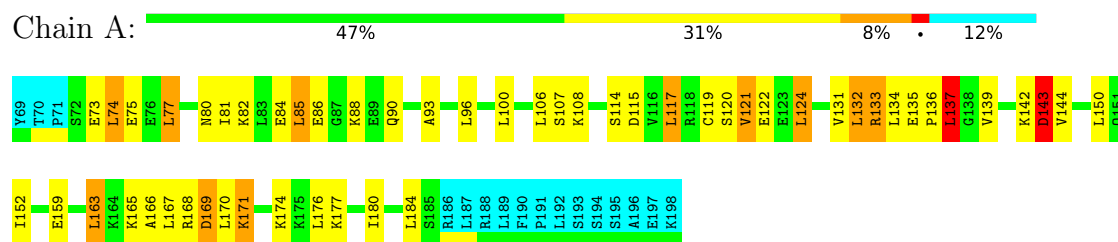
4.2.7 Score per residue for model 7

- Molecule 1: RNA polymerase sigma factor RpoN



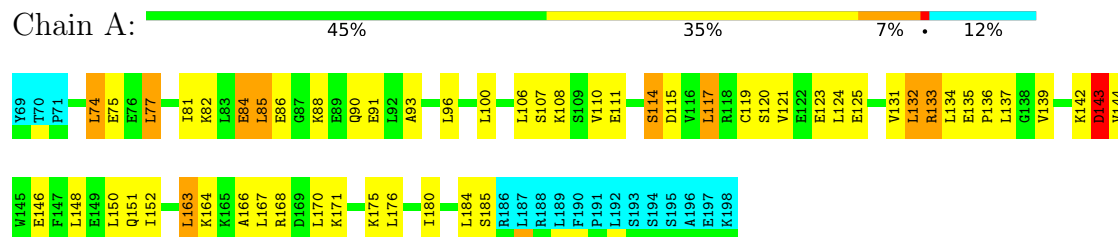
4.2.8 Score per residue for model 8

- Molecule 1: RNA polymerase sigma factor RpoN



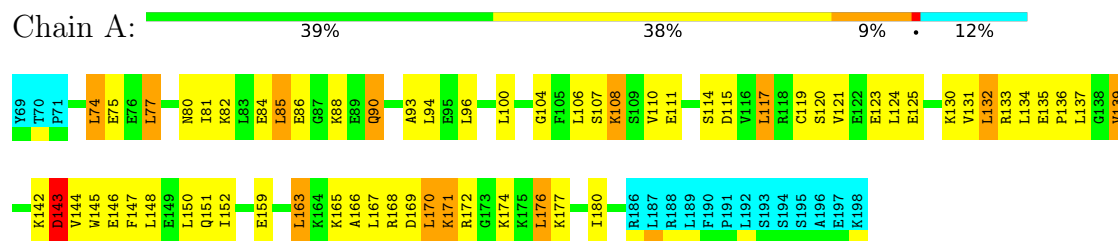
4.2.9 Score per residue for model 9

- Molecule 1: RNA polymerase sigma factor RpoN



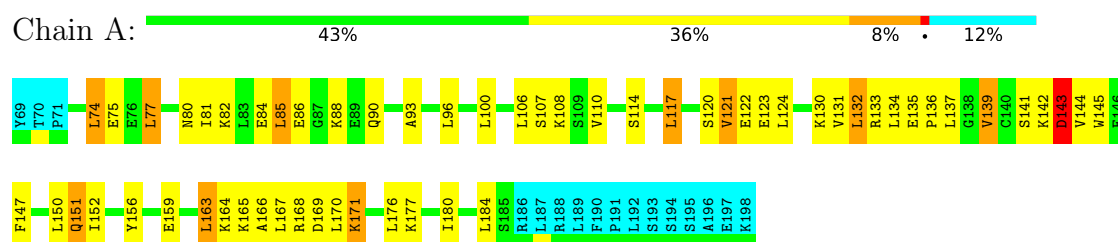
4.2.10 Score per residue for model 10

- Molecule 1: RNA polymerase sigma factor RpoN



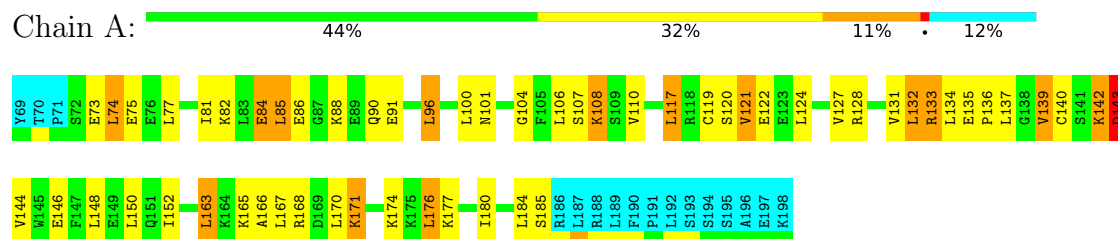
4.2.11 Score per residue for model 11

- Molecule 1: RNA polymerase sigma factor RpoN



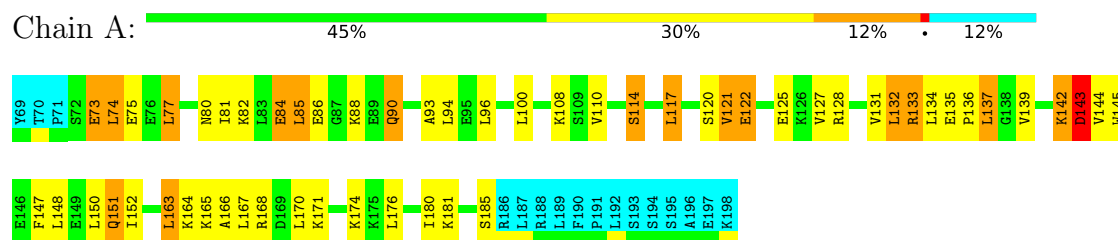
4.2.12 Score per residue for model 12

- Molecule 1: RNA polymerase sigma factor RpoN



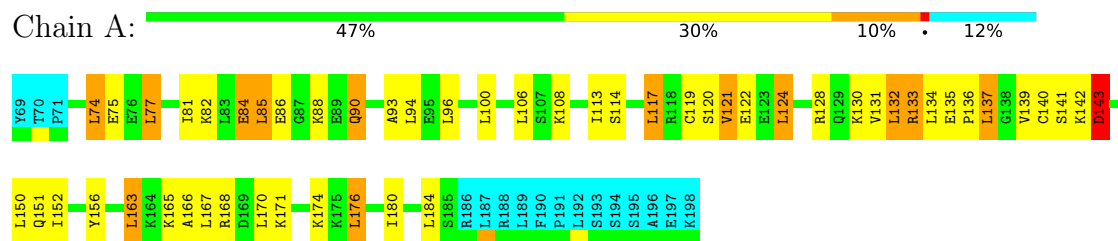
4.2.13 Score per residue for model 13

- Molecule 1: RNA polymerase sigma factor RpoN



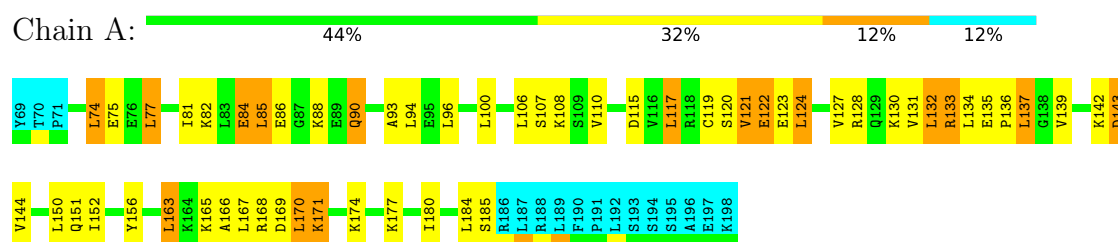
4.2.14 Score per residue for model 14

- Molecule 1: RNA polymerase sigma factor RpoN



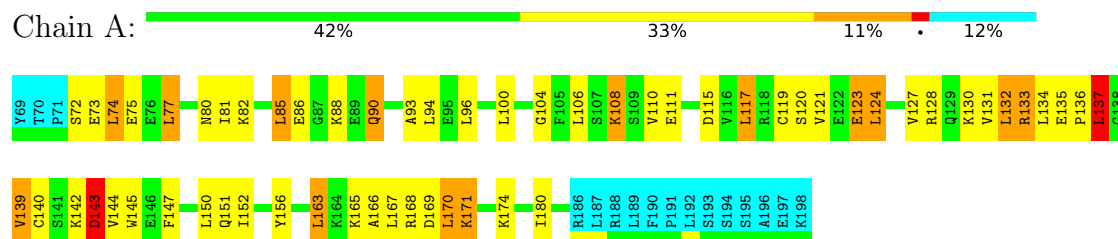
4.2.15 Score per residue for model 15

- Molecule 1: RNA polymerase sigma factor RpoN



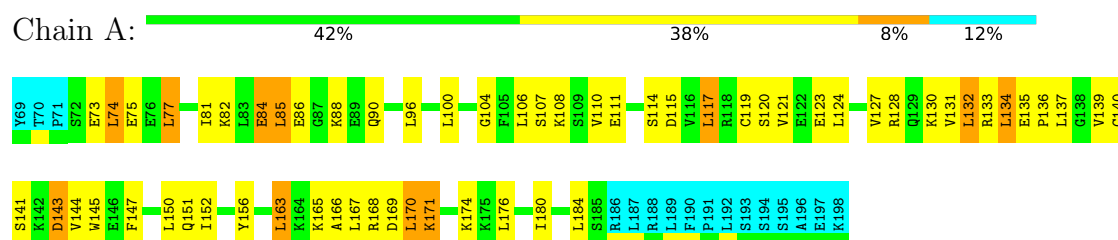
4.2.16 Score per residue for model 16

- Molecule 1: RNA polymerase sigma factor RpoN



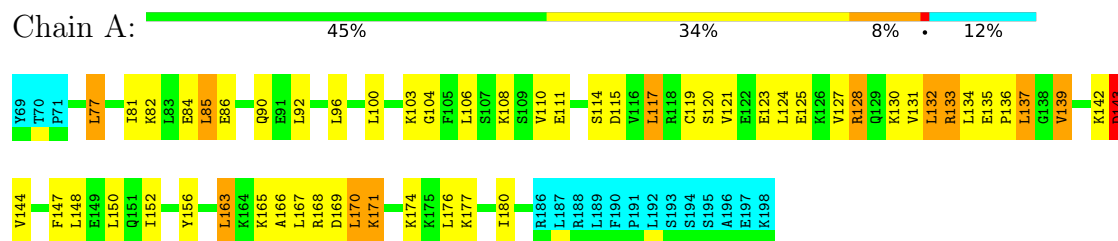
4.2.17 Score per residue for model 17

- Molecule 1: RNA polymerase sigma factor RpoN



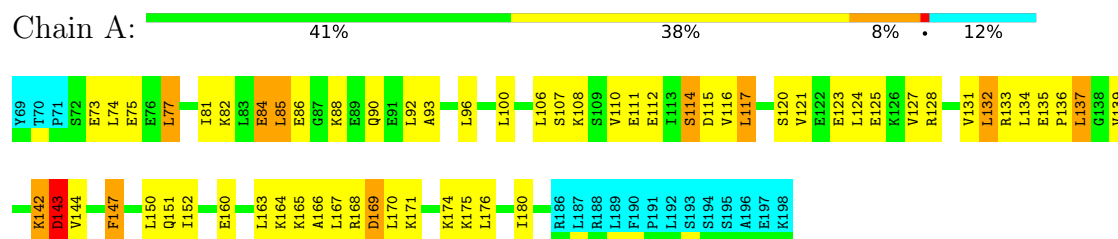
4.2.18 Score per residue for model 18

- Molecule 1: RNA polymerase sigma factor RpoN



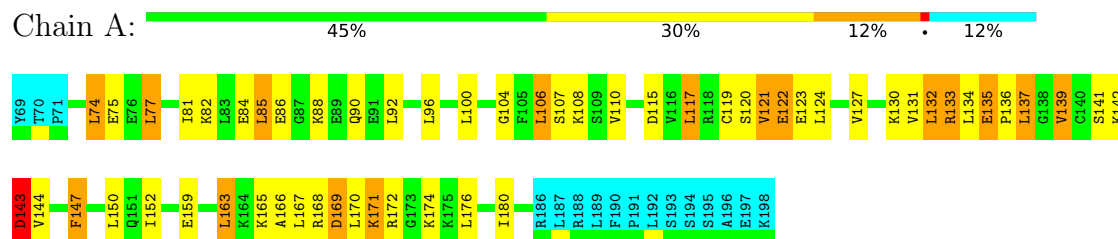
4.2.19 Score per residue for model 19

- Molecule 1: RNA polymerase sigma factor RpoN



4.2.20 Score per residue for model 20

- Molecule 1: RNA polymerase sigma factor RpoN



5 Refinement protocol and experimental data overview ⓘ

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

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *structures with the least restraint violations*.

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

Software name	Classification	Version
CYANA	structure solution	
CYANA	refinement	

No chemical shift data was provided.

6 Model quality

6.1 Standard geometry

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

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	937	982	982	36±5
All	All	18740	19640	19640	722

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:132:LEU:HD11	1:A:150:LEU:HD22	0.92	1.41	11	20
1:A:77:LEU:HD13	1:A:81:ILE:HD11	0.79	1.52	15	16
1:A:163:LEU:HD12	1:A:184:LEU:HD21	0.75	1.57	17	3
1:A:166:ALA:CB	1:A:180:ILE:HG21	0.72	2.15	4	20
1:A:117:LEU:HD12	1:A:117:LEU:O	0.67	1.90	14	20
1:A:96:LEU:HD21	1:A:106:LEU:HD11	0.66	1.66	7	1
1:A:77:LEU:CD1	1:A:81:ILE:HD11	0.66	2.20	2	18
1:A:132:LEU:CD1	1:A:150:LEU:HD22	0.66	2.20	13	20
1:A:84:GLU:CD	1:A:134:LEU:HD21	0.66	2.16	8	5
1:A:137:LEU:HB3	1:A:150:LEU:HD11	0.65	1.69	15	20
1:A:167:LEU:HD12	1:A:168:ARG:N	0.64	2.07	18	20
1:A:93:ALA:CB	1:A:131:VAL:HG11	0.63	2.23	10	15
1:A:170:LEU:HD23	1:A:171:LYS:N	0.63	2.09	18	7
1:A:139:VAL:HG23	1:A:144:VAL:HA	0.62	1.71	16	18

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:93:ALA:HB2	1:A:131:VAL:HG11	0.62	1.72	3	10
1:A:96:LEU:CD1	1:A:110:VAL:HG13	0.62	2.25	17	2
1:A:106:LEU:HD22	1:A:140:CYS:O	0.62	1.93	17	5
1:A:106:LEU:HD13	1:A:108:LYS:O	0.62	1.95	10	2
1:A:170:LEU:HD12	1:A:171:LYS:N	0.61	2.10	13	11
1:A:170:LEU:HD23	1:A:176:LEU:HD21	0.61	1.72	12	2
1:A:84:GLU:OE2	1:A:85:LEU:HD23	0.61	1.96	3	12
1:A:85:LEU:HD22	1:A:130:LYS:HD3	0.60	1.73	20	6
1:A:100:LEU:HD12	1:A:100:LEU:O	0.60	1.96	16	1
1:A:170:LEU:CD2	1:A:176:LEU:HD11	0.59	2.27	4	4
1:A:131:VAL:HA	1:A:134:LEU:HD13	0.58	1.75	4	2
1:A:106:LEU:HD12	1:A:106:LEU:O	0.58	1.98	10	3
1:A:93:ALA:HB1	1:A:131:VAL:HG21	0.58	1.75	13	5
1:A:110:VAL:CG1	1:A:124:LEU:HD22	0.58	2.29	3	5
1:A:124:LEU:HD23	1:A:124:LEU:O	0.58	1.98	19	6
1:A:124:LEU:HD13	1:A:124:LEU:O	0.58	1.98	20	8
1:A:110:VAL:HG21	1:A:128:ARG:NH1	0.57	2.14	15	6
1:A:77:LEU:HD13	1:A:81:ILE:CD1	0.57	2.30	14	16
1:A:110:VAL:CG1	1:A:124:LEU:HD12	0.57	2.29	5	4
1:A:132:LEU:HD21	1:A:150:LEU:HD13	0.57	1.75	5	10
1:A:84:GLU:CD	1:A:134:LEU:HD11	0.57	2.25	18	1
1:A:170:LEU:HD12	1:A:176:LEU:HD11	0.57	1.77	17	1
1:A:96:LEU:HD12	1:A:128:ARG:CZ	0.56	2.31	1	1
1:A:81:ILE:HG23	1:A:85:LEU:HD21	0.55	1.77	2	3
1:A:132:LEU:HD23	1:A:133:ARG:N	0.55	2.17	6	19
1:A:137:LEU:HD23	1:A:147:PHE:CD1	0.55	2.37	4	1
1:A:96:LEU:HD22	1:A:113:ILE:HG21	0.54	1.79	14	2
1:A:170:LEU:C	1:A:170:LEU:HD12	0.54	2.27	1	1
1:A:110:VAL:HG12	1:A:124:LEU:HD23	0.53	1.79	10	2
1:A:110:VAL:CG1	1:A:124:LEU:HD23	0.53	2.33	12	1
1:A:152:ILE:HG23	1:A:163:LEU:HD23	0.53	1.80	14	6
1:A:150:LEU:C	1:A:150:LEU:HD12	0.53	2.28	14	14
1:A:114:SER:HA	1:A:117:LEU:HD23	0.53	1.80	11	11
1:A:152:ILE:HG12	1:A:163:LEU:HD12	0.53	1.79	3	2
1:A:166:ALA:O	1:A:176:LEU:HD21	0.53	2.03	13	4
1:A:117:LEU:HD11	1:A:119:CYS:HB2	0.53	1.80	20	16
1:A:170:LEU:HB3	1:A:176:LEU:HD21	0.52	1.82	20	2
1:A:96:LEU:HD12	1:A:128:ARG:NE	0.52	2.19	14	3
1:A:90:GLN:O	1:A:94:LEU:HD12	0.52	2.04	15	5
1:A:84:GLU:OE2	1:A:134:LEU:HD13	0.52	2.05	20	1
1:A:84:GLU:OE2	1:A:134:LEU:HD21	0.52	2.04	14	7

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:166:ALA:HB1	1:A:180:ILE:HG21	0.52	1.81	11	12
1:A:80:ASN:HB3	1:A:134:LEU:HD23	0.51	1.82	10	1
1:A:100:LEU:HD12	1:A:100:LEU:C	0.51	2.31	7	20
1:A:170:LEU:HD12	1:A:170:LEU:C	0.51	2.30	11	7
1:A:137:LEU:HD23	1:A:147:PHE:CD2	0.50	2.40	3	6
1:A:148:LEU:HD21	1:A:184:LEU:HD22	0.50	1.83	12	1
1:A:137:LEU:HD23	1:A:147:PHE:CZ	0.50	2.42	13	1
1:A:84:GLU:OE2	1:A:134:LEU:HD11	0.50	2.06	18	3
1:A:135:GLU:HA	1:A:136:PRO:C	0.50	2.32	2	20
1:A:170:LEU:CD2	1:A:176:LEU:HD21	0.50	2.35	12	1
1:A:74:LEU:HD12	1:A:75:GLU:N	0.49	2.22	15	18
1:A:133:ARG:HG3	1:A:134:LEU:HD12	0.49	1.82	4	5
1:A:127:VAL:O	1:A:131:VAL:HG13	0.49	2.07	20	7
1:A:166:ALA:HB2	1:A:180:ILE:HG21	0.49	1.84	2	4
1:A:96:LEU:C	1:A:96:LEU:HD13	0.49	2.33	16	9
1:A:176:LEU:HD21	1:A:184:LEU:HD22	0.48	1.83	11	1
1:A:132:LEU:HD12	1:A:141:SER:HB2	0.48	1.84	17	1
1:A:84:GLU:CD	1:A:85:LEU:HD23	0.48	2.34	6	3
1:A:112:GLU:O	1:A:116:VAL:HG13	0.48	2.09	3	2
1:A:124:LEU:HD13	1:A:124:LEU:C	0.47	2.34	5	2
1:A:152:ILE:CG2	1:A:163:LEU:HD23	0.47	2.39	14	1
1:A:123:GLU:O	1:A:127:VAL:HG22	0.47	2.09	16	1
1:A:130:LYS:O	1:A:134:LEU:HD23	0.47	2.09	17	1
1:A:92:LEU:HB2	1:A:127:VAL:HG21	0.47	1.86	19	2
1:A:152:ILE:HG12	1:A:163:LEU:HD23	0.47	1.85	12	9
1:A:132:LEU:CD2	1:A:150:LEU:HD13	0.47	2.39	5	2
1:A:117:LEU:HD11	1:A:119:CYS:CB	0.47	2.40	4	11
1:A:170:LEU:HD23	1:A:176:LEU:HD11	0.47	1.86	13	3
1:A:77:LEU:HD22	1:A:81:ILE:HD11	0.47	1.86	12	2
1:A:84:GLU:HG2	1:A:134:LEU:HD21	0.46	1.87	13	1
1:A:121:VAL:HG12	1:A:122:GLU:N	0.46	2.25	20	11
1:A:114:SER:HB2	1:A:124:LEU:HD13	0.46	1.86	3	1
1:A:148:LEU:HD21	1:A:184:LEU:HD21	0.46	1.86	3	2
1:A:163:LEU:HD23	1:A:163:LEU:N	0.46	2.25	19	2
1:A:81:ILE:CG1	1:A:134:LEU:HD22	0.46	2.41	4	1
1:A:142:LYS:O	1:A:143:ASP:CB	0.45	2.63	8	18
1:A:169:ASP:OD2	1:A:176:LEU:HD12	0.45	2.10	2	1
1:A:150:LEU:HD12	1:A:151:GLN:N	0.45	2.26	17	6
1:A:169:ASP:OD1	1:A:169:ASP:C	0.45	2.59	20	4
1:A:144:VAL:HG13	1:A:145:TRP:N	0.45	2.26	17	6
1:A:137:LEU:HD12	1:A:150:LEU:CD1	0.45	2.42	17	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:170:LEU:C	1:A:170:LEU:HD23	0.45	2.37	3	1
1:A:106:LEU:HD12	1:A:108:LYS:O	0.44	2.11	16	4
1:A:127:VAL:HG23	1:A:128:ARG:N	0.44	2.28	4	5
1:A:167:LEU:HD12	1:A:167:LEU:C	0.44	2.37	9	5
1:A:170:LEU:HB3	1:A:176:LEU:HD11	0.44	1.89	8	1
1:A:85:LEU:HD22	1:A:130:LYS:NZ	0.44	2.27	14	1
1:A:160:GLU:O	1:A:164:LYS:CB	0.44	2.66	19	2
1:A:148:LEU:HD23	1:A:167:LEU:HB2	0.44	1.90	13	2
1:A:96:LEU:HD23	1:A:124:LEU:HD21	0.43	1.88	12	1
1:A:132:LEU:HD23	1:A:132:LEU:C	0.43	2.37	4	3
1:A:131:VAL:O	1:A:134:LEU:HB2	0.43	2.13	12	2
1:A:110:VAL:HG13	1:A:124:LEU:HD23	0.43	1.90	12	1
1:A:151:GLN:CD	1:A:151:GLN:C	0.43	2.86	5	1
1:A:92:LEU:HD13	1:A:119:CYS:SG	0.43	2.54	4	3
1:A:96:LEU:HD22	1:A:128:ARG:CZ	0.43	2.43	17	1
1:A:150:LEU:HD12	1:A:150:LEU:C	0.43	2.39	16	4
1:A:137:LEU:HD21	1:A:151:GLN:HE21	0.43	1.72	13	1
1:A:152:ILE:HG22	1:A:156:TYR:O	0.43	2.13	17	5
1:A:137:LEU:HD21	1:A:151:GLN:HG3	0.43	1.90	16	2
1:A:92:LEU:HD12	1:A:127:VAL:HG11	0.43	1.90	19	1
1:A:96:LEU:O	1:A:96:LEU:HD13	0.42	2.14	19	6
1:A:85:LEU:HD22	1:A:130:LYS:CD	0.42	2.43	10	3
1:A:148:LEU:HD23	1:A:167:LEU:CB	0.42	2.45	10	3
1:A:160:GLU:O	1:A:164:LYS:HB2	0.42	2.14	4	1
1:A:163:LEU:CD1	1:A:180:ILE:HG23	0.42	2.45	16	2
1:A:77:LEU:CD2	1:A:81:ILE:HD11	0.42	2.44	12	2
1:A:78:GLN:HA	1:A:81:ILE:HD12	0.42	1.90	2	1
1:A:96:LEU:CD2	1:A:106:LEU:HD11	0.42	2.42	7	1
1:A:166:ALA:HB1	1:A:176:LEU:CD1	0.42	2.44	10	1
1:A:147:PHE:CD1	1:A:148:LEU:N	0.42	2.88	18	1
1:A:152:ILE:O	1:A:156:TYR:C	0.42	2.63	18	2
1:A:131:VAL:HA	1:A:134:LEU:HD23	0.42	1.91	12	2
1:A:170:LEU:HD22	1:A:176:LEU:HD11	0.42	1.92	4	1
1:A:74:LEU:HG	1:A:75:GLU:N	0.42	2.30	19	1
1:A:96:LEU:HD13	1:A:96:LEU:O	0.41	2.16	2	3
1:A:110:VAL:HG11	1:A:128:ARG:HH11	0.41	1.75	4	1
1:A:96:LEU:HD13	1:A:96:LEU:C	0.41	2.40	19	1
1:A:130:LYS:O	1:A:134:LEU:HD13	0.41	2.15	11	1
1:A:148:LEU:HD12	1:A:148:LEU:O	0.41	2.15	9	1
1:A:137:LEU:HD23	1:A:147:PHE:CE1	0.41	2.51	4	1
1:A:96:LEU:HD11	1:A:110:VAL:HG13	0.41	1.91	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:90:GLN:NE2	1:A:94:LEU:HD11	0.40	2.32	14	1
1:A:180:ILE:HG22	1:A:184:LEU:HG	0.40	1.93	8	1
1:A:92:LEU:HD22	1:A:119:CYS:SG	0.40	2.56	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	114/130 (88%)	104±1 (91±1%)	9±1 (8±1%)	1±0 (1±0%)	15	65
All	All	2280/2600 (88%)	2081 (91%)	177 (8%)	22 (1%)	15	65

All 2 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	143	ASP	20
1	A	137	LEU	2

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	107/122 (88%)	78±2 (73±2%)	29±2 (27±2%)	1	20
All	All	2140/2440 (88%)	1552 (73%)	588 (27%)	1	20

All 62 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	82	LYS	20
1	A	85	LEU	20
1	A	86	GLU	20
1	A	90	GLN	20
1	A	108	LYS	20
1	A	117	LEU	20
1	A	120	SER	20
1	A	121	VAL	20
1	A	132	LEU	20
1	A	143	ASP	19
1	A	165	LYS	19
1	A	77	LEU	18
1	A	163	LEU	18
1	A	74	LEU	17
1	A	88	LYS	17
1	A	107	SER	16
1	A	115	ASP	16
1	A	84	GLU	15
1	A	171	LYS	15
1	A	174	LYS	15
1	A	133	ARG	14
1	A	123	GLU	13
1	A	169	ASP	13
1	A	137	LEU	12
1	A	106	LEU	11
1	A	177	LYS	11
1	A	147	PHE	10
1	A	139	VAL	9
1	A	185	SER	9
1	A	111	GLU	8
1	A	73	GLU	8
1	A	125	GLU	8
1	A	114	SER	7
1	A	170	LEU	7
1	A	91	GLU	6
1	A	164	LYS	6
1	A	124	LEU	6
1	A	142	LYS	5
1	A	146	GLU	5
1	A	176	LEU	5
1	A	80	ASN	5
1	A	151	GLN	5
1	A	130	LYS	4

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Mol	Chain	Res	Type	Models (Total)
1	A	122	GLU	4
1	A	141	SER	4
1	A	159	GLU	4
1	A	168	ARG	3
1	A	135	GLU	2
1	A	128	ARG	2
1	A	96	LEU	2
1	A	103	LYS	2
1	A	175	LYS	2
1	A	172	ARG	2
1	A	76	GLU	1
1	A	126	LYS	1
1	A	144	VAL	1
1	A	97	LEU	1
1	A	101	ASN	1
1	A	181	LYS	1
1	A	140	CYS	1
1	A	72	SER	1
1	A	134	LEU	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.6 Ligand geometry ⓘ

There are no ligands in this entry.

6.7 Other polymers ⓘ

There are no such molecules in this entry.

6.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided