



Full wwPDB NMR Structure Validation Report ⓘ

Mar 26, 2026 – 10:56 AM UTC

PDB ID : 2KXI / pdb_00002kxi
Title : Solution NMR structure of the apoform of NarE (NMB1343)
Authors : Koehler, C.; Carlier, L.; Veggi, D.; Soriani, M.; Pizza, M.; Boelens, R.; Bonvin, A.M.J.J.
Deposited on : 2010-05-06

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

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

A user guide is available at

<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

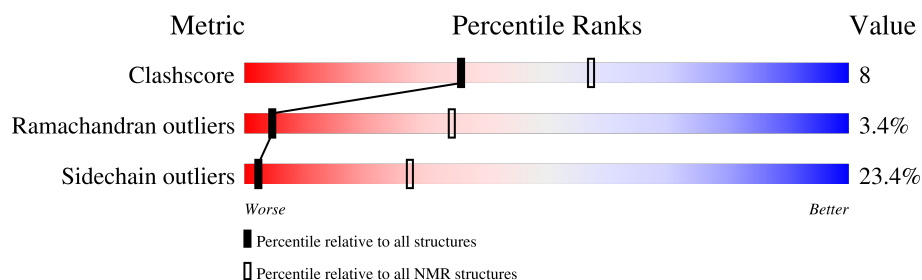
1 Overall quality at a glance

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	153	

2 Ensemble composition and analysis ⓘ

This entry contains 20 models. Model 18 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:3-A:24, A:51-A:144 (116)	1.66	18

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

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

The models can be grouped into 4 clusters and 2 single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2398 atoms, of which 1171 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms						Trace
1	A	153	Total	C	H	N	O	S	0
			2398	770	1171	211	241	5	

There are 8 discrepancies between the modelled and reference sequences:

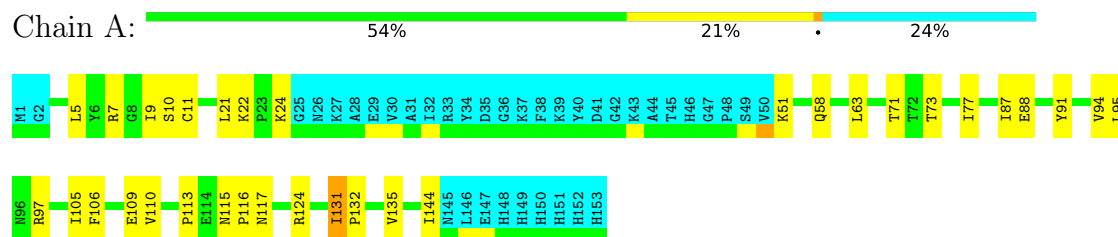
Chain	Residue	Modelled	Actual	Comment	Reference
A	146	LEU	-	expression tag	UNP Q9JZ10
A	147	GLU	-	expression tag	UNP Q9JZ10
A	148	HIS	-	expression tag	UNP Q9JZ10
A	149	HIS	-	expression tag	UNP Q9JZ10
A	150	HIS	-	expression tag	UNP Q9JZ10
A	151	HIS	-	expression tag	UNP Q9JZ10
A	152	HIS	-	expression tag	UNP Q9JZ10
A	153	HIS	-	expression tag	UNP Q9JZ10

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: Uncharacterized protein

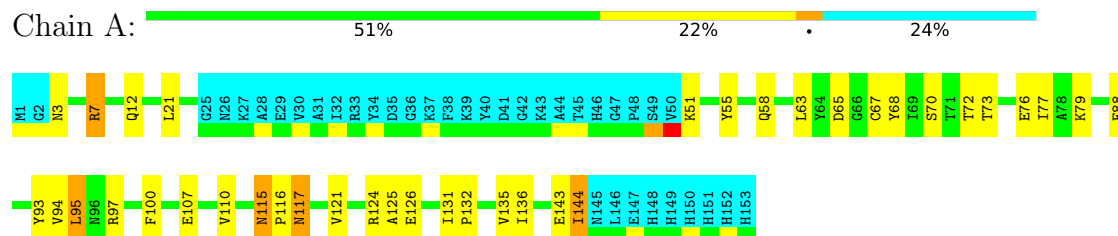


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

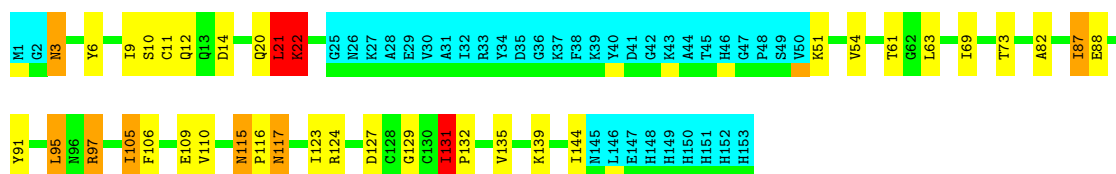
- Molecule 1: Uncharacterized protein



4.2.2 Score per residue for model 2

- Molecule 1: Uncharacterized protein

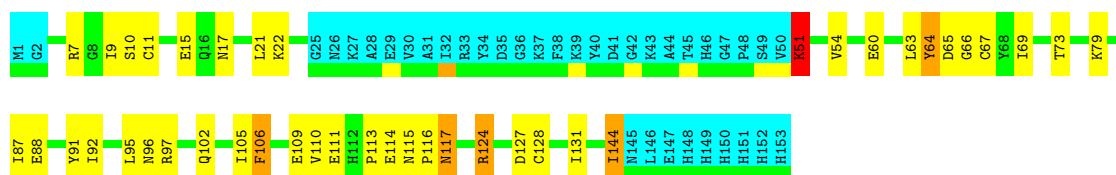




4.2.3 Score per residue for model 3

- Molecule 1: Uncharacterized protein

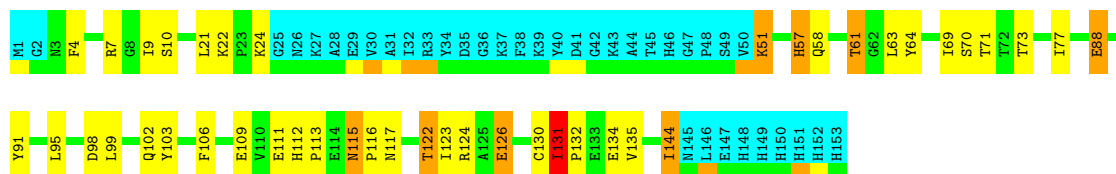
Chain A: 48% 24% • • 24%



4.2.4 Score per residue for model 4

- Molecule 1: Uncharacterized protein

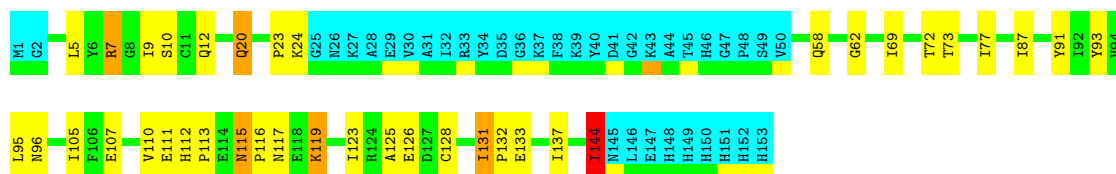
Chain A: 48% 22% 5% • 24%



4.2.5 Score per residue for model 5

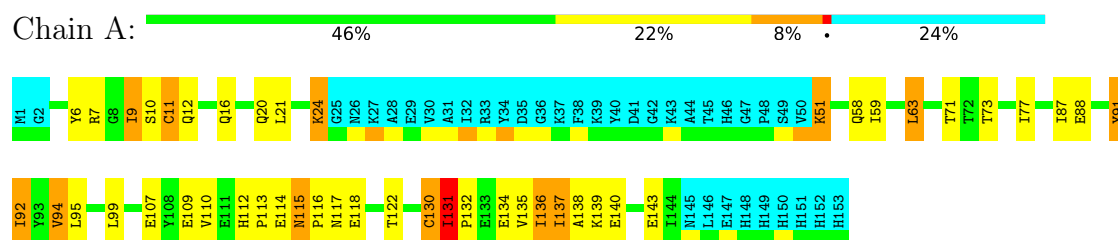
- Molecule 1: Uncharacterized protein

Chain A: 51% 21% • • 24%



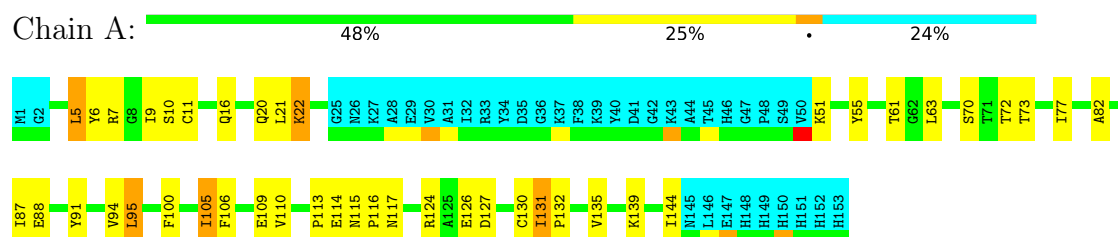
4.2.6 Score per residue for model 6

- Molecule 1: Uncharacterized protein



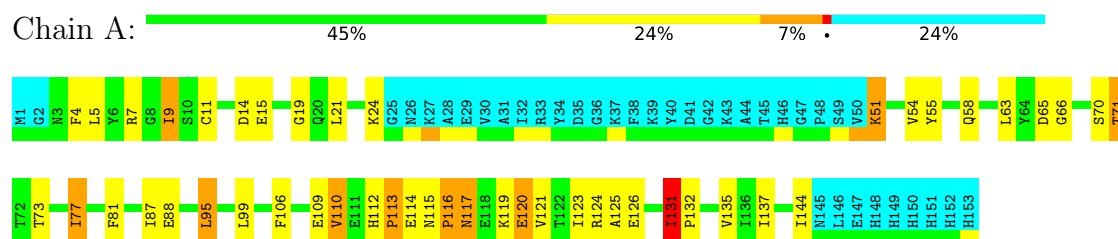
4.2.7 Score per residue for model 7

- Molecule 1: Uncharacterized protein



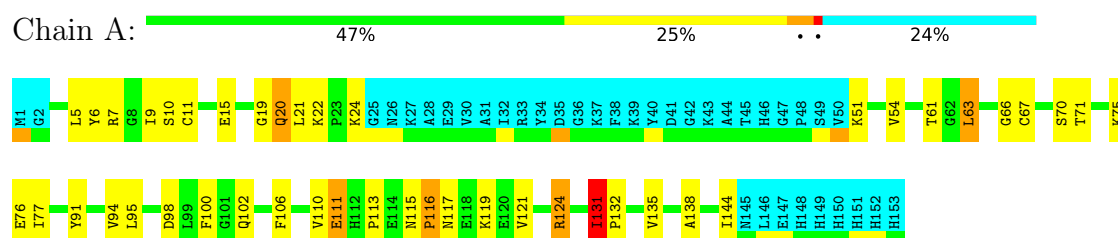
4.2.8 Score per residue for model 8

- Molecule 1: Uncharacterized protein



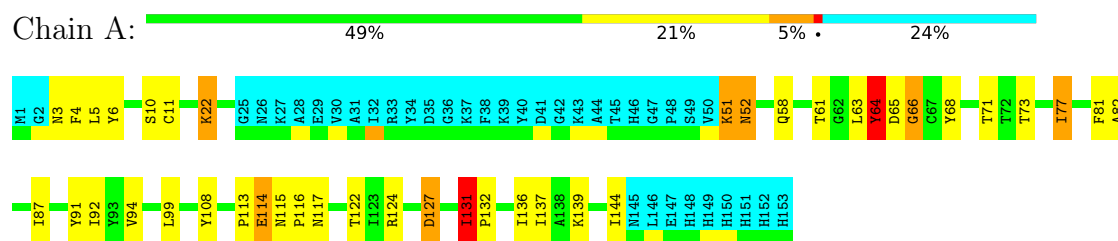
4.2.9 Score per residue for model 9

- Molecule 1: Uncharacterized protein



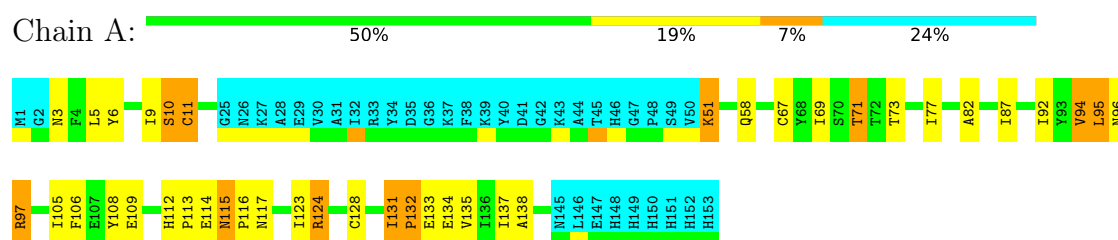
4.2.10 Score per residue for model 10

- Molecule 1: Uncharacterized protein



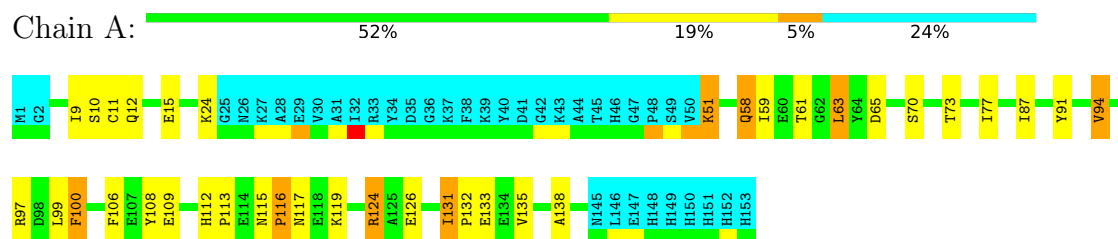
4.2.11 Score per residue for model 11

- Molecule 1: Uncharacterized protein



4.2.12 Score per residue for model 12

- Molecule 1: Uncharacterized protein



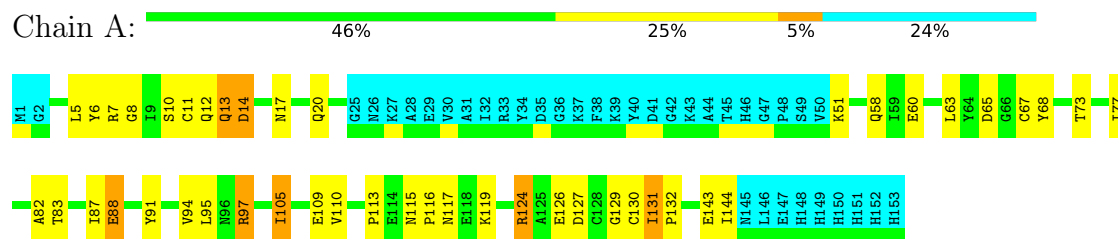
4.2.13 Score per residue for model 13

- Molecule 1: Uncharacterized protein



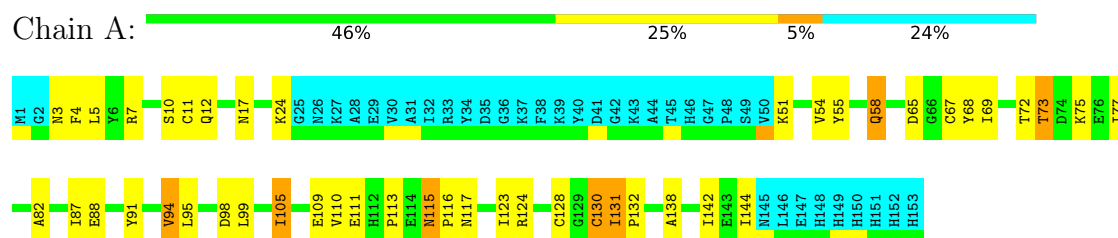
4.2.14 Score per residue for model 14

- Molecule 1: Uncharacterized protein



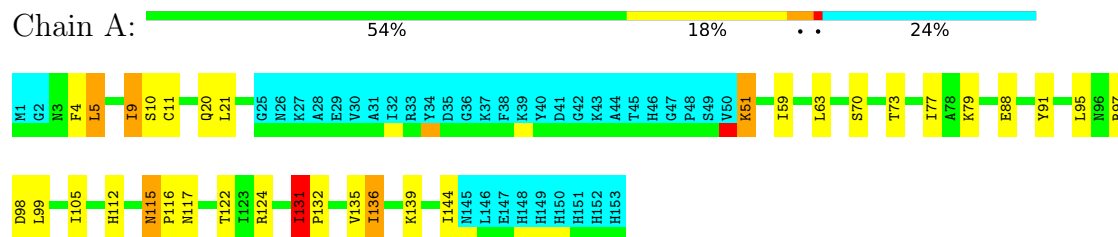
4.2.15 Score per residue for model 15

- Molecule 1: Uncharacterized protein



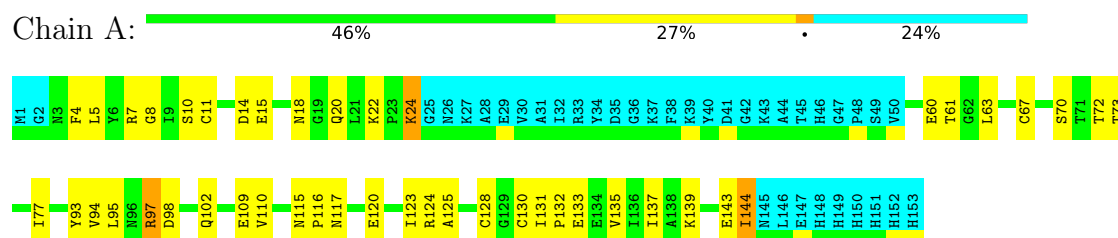
4.2.16 Score per residue for model 16

- Molecule 1: Uncharacterized protein



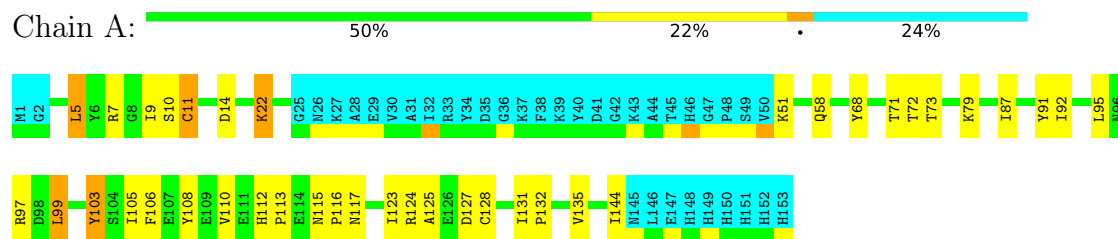
4.2.17 Score per residue for model 17

- Molecule 1: Uncharacterized protein



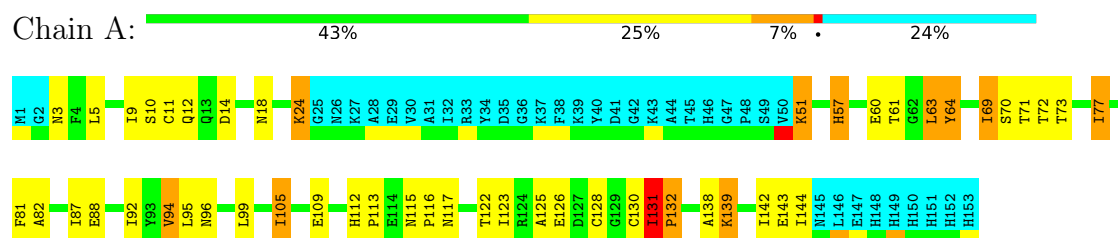
4.2.18 Score per residue for model 18 (medoid)

- Molecule 1: Uncharacterized protein



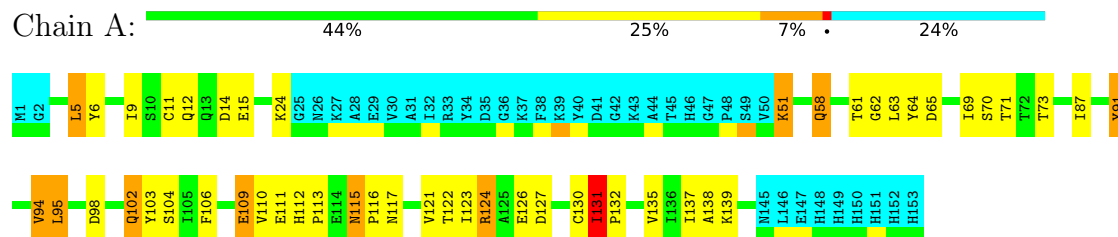
4.2.19 Score per residue for model 19

- Molecule 1: Uncharacterized protein



4.2.20 Score per residue for model 20

- Molecule 1: Uncharacterized protein



5 Refinement protocol and experimental data overview

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

Of the 400 calculated structures, 20 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
CYANA	structure solution	
TALOS	structure solution	
CNS	refinement	

No chemical shift data was provided.

6 Model quality [i](#)

6.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the (average) root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.50±0.03	0±0/949 (0.0± 0.1%)	0.68±0.01	0±0/1284 (0.0± 0.0%)
All	All	0.50	9/18980 (0.0%)	0.68	0/25680 (0.0%)

All unique bond outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	131	ILE	CA-CB	7.66	1.57	1.54	2	9

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	931	892	892	14±3
All	All	18620	17840	17840	285

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 8.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:94:VAL:HG22	1:A:138:ALA:HB3	0.73	1.61	20	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:131:ILE:HG23	1:A:132:PRO:HD3	0.72	1.59	2	18
1:A:127:ASP:HB3	1:A:131:ILE:HB	0.67	1.64	2	5
1:A:15:GLU:HG2	1:A:21:LEU:HB3	0.66	1.68	8	1
1:A:9:ILE:HB	1:A:91:TYR:HB3	0.64	1.68	5	3
1:A:67:CYS:SG	1:A:68:TYR:CZ	0.61	2.94	15	1
1:A:106:PHE:HB2	1:A:124:ARG:HG2	0.61	1.71	12	1
1:A:9:ILE:HG23	1:A:91:TYR:HB3	0.60	1.73	16	5
1:A:94:VAL:HG23	1:A:138:ALA:HB3	0.59	1.73	19	3
1:A:58:GLN:HE22	1:A:67:CYS:HB3	0.59	1.58	14	1
1:A:5:LEU:HB2	1:A:95:LEU:HB2	0.59	1.75	17	1
1:A:5:LEU:HD12	1:A:71:THR:HG21	0.58	1.73	18	1
1:A:95:LEU:HD23	1:A:135:VAL:HG13	0.58	1.74	11	3
1:A:95:LEU:HD23	1:A:135:VAL:HG22	0.58	1.76	8	2
1:A:69:ILE:HG13	1:A:123:ILE:HB	0.56	1.76	5	1
1:A:11:CYS:HB2	1:A:14:ASP:HB2	0.56	1.76	18	1
1:A:55:TYR:HA	1:A:124:ARG:NH1	0.56	2.15	15	1
1:A:106:PHE:HB3	1:A:124:ARG:HB2	0.56	1.77	18	1
1:A:106:PHE:HB2	1:A:124:ARG:HB2	0.56	1.78	4	6
1:A:18:ASN:ND2	1:A:22:LYS:H	0.56	1.98	17	1
1:A:136:ILE:HG12	1:A:136:ILE:O	0.54	2.02	6	1
1:A:69:ILE:HG12	1:A:123:ILE:HB	0.54	1.80	19	1
1:A:111:GLU:HB3	1:A:119:LYS:HG3	0.53	1.78	9	1
1:A:69:ILE:HD12	1:A:123:ILE:HD11	0.53	1.80	20	1
1:A:7:ARG:NH2	1:A:130:CYS:SG	0.53	2.82	6	1
1:A:5:LEU:HD12	1:A:95:LEU:HB2	0.53	1.80	7	1
1:A:131:ILE:CG2	1:A:132:PRO:HD3	0.53	2.33	18	5
1:A:99:LEU:HD22	1:A:137:ILE:HG23	0.53	1.81	6	1
1:A:112:HIS:HB3	1:A:113:PRO:HD2	0.52	1.81	6	3
1:A:58:GLN:NE2	1:A:128:CYS:SG	0.52	2.82	15	1
1:A:82:ALA:HB1	1:A:87:ILE:HG21	0.52	1.82	15	2
1:A:7:ARG:HH11	1:A:7:ARG:HG3	0.52	1.64	17	1
1:A:88:GLU:HG3	1:A:144:ILE:HD13	0.51	1.82	4	1
1:A:99:LEU:HD23	1:A:135:VAL:HA	0.51	1.82	16	3
1:A:143:GLU:O	1:A:144:ILE:HB	0.51	2.05	17	1
1:A:54:VAL:HG21	1:A:67:CYS:SG	0.51	2.46	13	1
1:A:5:LEU:HD11	1:A:97:ARG:HG2	0.51	1.83	17	1
1:A:124:ARG:NH1	1:A:126:GLU:HA	0.51	2.21	1	1
1:A:7:ARG:NH1	1:A:130:CYS:SG	0.51	2.83	14	2
1:A:7:ARG:HH11	1:A:21:LEU:HD12	0.50	1.67	6	1
1:A:106:PHE:HB3	1:A:124:ARG:HB3	0.50	1.82	7	1
1:A:124:ARG:NH2	1:A:126:GLU:HA	0.50	2.21	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:5:LEU:HD21	1:A:123:ILE:HD13	0.50	1.84	11	2
1:A:71:THR:HG22	1:A:121:VAL:HG13	0.50	1.83	8	1
1:A:95:LEU:N	1:A:95:LEU:HD12	0.50	2.22	20	1
1:A:22:LYS:HE3	1:A:128:CYS:SG	0.49	2.47	18	1
1:A:82:ALA:HA	1:A:87:ILE:HD12	0.49	1.82	7	3
1:A:124:ARG:O	1:A:124:ARG:HG3	0.49	2.07	9	1
1:A:21:LEU:O	1:A:22:LYS:HG3	0.49	2.07	2	1
1:A:58:GLN:HB2	1:A:63:LEU:HD12	0.49	1.84	10	1
1:A:124:ARG:HH12	1:A:126:GLU:HA	0.49	1.68	1	1
1:A:139:LYS:HD2	1:A:139:LYS:N	0.49	2.23	19	1
1:A:57:HIS:HB3	1:A:63:LEU:HD22	0.49	1.84	19	1
1:A:51:LYS:NZ	1:A:126:GLU:HA	0.48	2.23	4	1
1:A:105:ILE:HG23	1:A:124:ARG:O	0.48	2.08	14	5
1:A:100:PHE:HB3	1:A:105:ILE:HD12	0.48	1.85	7	1
1:A:20:GLN:HB3	1:A:23:PRO:HD3	0.47	1.86	5	1
1:A:132:PRO:O	1:A:135:VAL:HG22	0.47	2.09	7	1
1:A:88:GLU:HB3	1:A:144:ILE:HG12	0.47	1.85	3	1
1:A:113:PRO:O	1:A:116:PRO:HD2	0.47	2.10	5	2
1:A:58:GLN:HA	1:A:62:GLY:O	0.47	2.09	20	1
1:A:115:ASN:N	1:A:116:PRO:CD	0.47	2.77	4	17
1:A:67:CYS:SG	1:A:129:GLY:N	0.47	2.88	14	1
1:A:7:ARG:NH1	1:A:21:LEU:HD12	0.47	2.24	6	1
1:A:115:ASN:N	1:A:116:PRO:HD2	0.46	2.25	3	15
1:A:3:ASN:HA	1:A:97:ARG:NH1	0.46	2.25	2	1
1:A:77:ILE:O	1:A:81:PHE:HB3	0.46	2.11	10	4
1:A:19:GLY:O	1:A:20:GLN:HB2	0.46	2.11	9	1
1:A:115:ASN:C	1:A:117:ASN:N	0.46	2.73	1	19
1:A:125:ALA:HB1	1:A:131:ILE:HG22	0.46	1.86	1	4
1:A:94:VAL:CG2	1:A:138:ALA:HB3	0.46	2.41	6	2
1:A:5:LEU:HD23	1:A:71:THR:HB	0.46	1.88	11	1
1:A:64:TYR:O	1:A:66:GLY:N	0.46	2.49	10	1
1:A:7:ARG:HG3	1:A:7:ARG:NH1	0.45	2.26	17	1
1:A:69:ILE:HB	1:A:123:ILE:HB	0.45	1.88	15	2
1:A:96:ASN:HB2	1:A:137:ILE:HD13	0.45	1.87	5	2
1:A:58:GLN:NE2	1:A:67:CYS:HB3	0.45	2.26	14	1
1:A:19:GLY:O	1:A:24:LYS:NZ	0.45	2.50	8	1
1:A:108:TYR:HB3	1:A:124:ARG:NE	0.45	2.26	18	2
1:A:7:ARG:HB3	1:A:93:TYR:CE2	0.45	2.47	17	2
1:A:11:CYS:HB2	1:A:14:ASP:HB3	0.45	1.88	14	1
1:A:3:ASN:HB2	1:A:97:ARG:HD2	0.44	1.89	1	1
1:A:100:PHE:CZ	1:A:135:VAL:HG21	0.44	2.47	9	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:58:GLN:HG3	1:A:68:TYR:CD2	0.44	2.47	18	1
1:A:88:GLU:HG2	1:A:144:ILE:HA	0.44	1.88	1	1
1:A:131:ILE:N	1:A:132:PRO:CD	0.44	2.81	1	4
1:A:106:PHE:HD2	1:A:124:ARG:HD2	0.44	1.71	18	1
1:A:63:LEU:HD13	1:A:70:SER:HB3	0.44	1.89	20	1
1:A:5:LEU:HD21	1:A:123:ILE:HG13	0.44	1.89	17	1
1:A:8:GLY:HA3	1:A:87:ILE:HD13	0.44	1.89	14	1
1:A:13:GLN:HG3	1:A:14:ASP:N	0.44	2.28	14	1
1:A:108:TYR:HB2	1:A:124:ARG:HD3	0.44	1.90	12	1
1:A:64:TYR:CE2	1:A:128:CYS:SG	0.43	3.11	19	1
1:A:127:ASP:H	1:A:131:ILE:HG21	0.43	1.72	14	2
1:A:136:ILE:HD11	1:A:139:LYS:HB3	0.43	1.89	16	1
1:A:7:ARG:NH1	1:A:8:GLY:O	0.43	2.51	17	1
1:A:67:CYS:SG	1:A:68:TYR:CE1	0.43	3.12	1	1
1:A:63:LEU:HD22	1:A:64:TYR:CE1	0.43	2.49	3	1
1:A:87:ILE:HD12	1:A:142:ILE:HG21	0.43	1.90	19	1
1:A:59:ILE:HD11	1:A:124:ARG:NH2	0.43	2.29	12	1
1:A:82:ALA:O	1:A:87:ILE:HG23	0.43	2.13	2	1
1:A:61:THR:HB	1:A:63:LEU:HD22	0.43	1.90	4	1
1:A:112:HIS:HB2	1:A:118:GLU:HB3	0.43	1.88	6	1
1:A:5:LEU:HA	1:A:71:THR:OG1	0.43	2.14	8	1
1:A:112:HIS:HB3	1:A:113:PRO:CD	0.43	2.44	6	2
1:A:24:LYS:O	1:A:131:ILE:HA	0.43	2.13	6	1
1:A:5:LEU:HG	1:A:71:THR:HB	0.43	1.91	8	1
1:A:82:ALA:HB1	1:A:87:ILE:HG12	0.42	1.91	19	1
1:A:7:ARG:HB3	1:A:93:TYR:CE1	0.42	2.49	5	1
1:A:59:ILE:HA	1:A:63:LEU:HA	0.42	1.89	6	1
1:A:87:ILE:O	1:A:88:GLU:C	0.42	2.62	15	4
1:A:125:ALA:HB1	1:A:131:ILE:CG2	0.42	2.45	8	1
1:A:68:TYR:CD1	1:A:124:ARG:HA	0.42	2.50	10	1
1:A:113:PRO:HB2	1:A:116:PRO:HG2	0.42	1.90	7	1
1:A:96:ASN:HB3	1:A:99:LEU:HD12	0.42	1.91	19	1
1:A:21:LEU:HD23	1:A:21:LEU:H	0.42	1.74	6	1
1:A:109:GLU:HG2	1:A:121:VAL:HG22	0.42	1.92	20	1
1:A:22:LYS:NZ	1:A:129:GLY:O	0.42	2.53	2	1
1:A:72:THR:H	1:A:77:ILE:HD12	0.42	1.74	13	1
1:A:21:LEU:H	1:A:21:LEU:HD23	0.42	1.75	7	1
1:A:92:ILE:HG13	1:A:140:GLU:HG3	0.42	1.92	6	1
1:A:71:THR:HG23	1:A:77:ILE:HD12	0.42	1.90	19	1
1:A:9:ILE:HG12	1:A:11:CYS:H	0.41	1.75	6	2
1:A:9:ILE:HG12	1:A:10:SER:N	0.41	2.29	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:100:PHE:CE1	1:A:135:VAL:HG11	0.41	2.50	12	1
1:A:5:LEU:HG	1:A:95:LEU:O	0.41	2.15	16	1
1:A:103:TYR:OH	1:A:134:GLU:HB2	0.41	2.15	4	1
1:A:132:PRO:HG2	1:A:135:VAL:HB	0.41	1.92	6	2
1:A:110:VAL:HG13	1:A:120:GLU:HB3	0.41	1.92	8	1
1:A:13:GLN:O	1:A:17:ASN:HB2	0.41	2.15	14	1
1:A:99:LEU:O	1:A:103:TYR:HB2	0.41	2.15	18	1
1:A:12:GLN:NE2	1:A:91:TYR:HB2	0.41	2.30	6	1
1:A:22:LYS:NZ	1:A:128:CYS:O	0.41	2.54	3	1
1:A:64:TYR:N	1:A:64:TYR:CD1	0.41	2.88	10	1
1:A:12:GLN:HB2	1:A:91:TYR:HB2	0.41	1.91	12	1
1:A:122:THR:HB	1:A:124:ARG:NE	0.41	2.30	4	1
1:A:117:ASN:O	1:A:119:LYS:NZ	0.41	2.54	5	1
1:A:20:GLN:HG2	1:A:21:LEU:N	0.41	2.31	16	1
1:A:105:ILE:HG13	1:A:125:ALA:HA	0.41	1.93	19	1
1:A:58:GLN:O	1:A:63:LEU:HA	0.41	2.16	12	1
1:A:95:LEU:HD23	1:A:135:VAL:HB	0.41	1.93	17	1
1:A:100:PHE:HB3	1:A:105:ILE:CD1	0.41	2.46	7	1
1:A:114:GLU:HG2	1:A:115:ASN:N	0.41	2.31	10	1
1:A:55:TYR:HA	1:A:124:ARG:CZ	0.41	2.46	15	1
1:A:5:LEU:HD23	1:A:97:ARG:HB2	0.41	1.93	16	1
1:A:21:LEU:HD11	1:A:136:ILE:HD13	0.40	1.91	1	1
1:A:5:LEU:HB2	1:A:71:THR:HG21	0.40	1.92	20	1
1:A:57:HIS:NE2	1:A:63:LEU:HD11	0.40	2.30	4	1
1:A:71:THR:O	1:A:121:VAL:N	0.40	2.54	9	1
1:A:102:GLN:HG3	1:A:103:TYR:N	0.40	2.32	20	1
1:A:6:TYR:HA	1:A:94:VAL:HG12	0.40	1.92	9	1
1:A:12:GLN:HB3	1:A:91:TYR:HB2	0.40	1.93	2	1
1:A:69:ILE:HG23	1:A:123:ILE:HB	0.40	1.92	2	1
1:A:21:LEU:O	1:A:22:LYS:HB2	0.40	2.16	4	1
1:A:9:ILE:HG13	1:A:21:LEU:HD22	0.40	1.92	8	1
1:A:124:ARG:HD2	1:A:124:ARG:N	0.40	2.31	12	1
1:A:58:GLN:HG2	1:A:68:TYR:HD2	0.40	1.76	14	1

6.3 Torsion angles ⓘ

6.3.1 Protein backbone ⓘ

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	116/153 (76%)	98±3 (85±2%)	14±2 (12±2%)	4±2 (3±1%)	4	34
All	All	2320/3060 (76%)	1968 (85%)	273 (12%)	79 (3%)	4	34

All 18 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	144	ILE	15
1	A	113	PRO	12
1	A	63	LEU	8
1	A	22	LYS	6
1	A	88	GLU	5
1	A	65	ASP	5
1	A	3	ASN	4
1	A	66	GLY	4
1	A	116	PRO	3
1	A	132	PRO	3
1	A	21	LEU	2
1	A	51	LYS	2
1	A	64	TYR	2
1	A	4	PHE	2
1	A	11	CYS	2
1	A	20	GLN	2
1	A	62	GLY	1
1	A	24	LYS	1

6.3.2 Protein sidechains ⓘ

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	102/131 (78%)	78±4 (77±4%)	24±4 (23±4%)	2	27
All	All	2040/2620 (78%)	1562 (77%)	478 (23%)	2	27

All 86 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	73	THR	18
1	A	10	SER	17
1	A	131	ILE	17
1	A	77	ILE	16
1	A	95	LEU	16
1	A	11	CYS	14
1	A	109	GLU	14
1	A	110	VAL	13
1	A	94	VAL	12
1	A	51	LYS	12
1	A	5	LEU	11
1	A	105	ILE	10
1	A	24	LYS	10
1	A	7	ARG	9
1	A	58	GLN	9
1	A	70	SER	9
1	A	115	ASN	9
1	A	61	THR	9
1	A	72	THR	8
1	A	6	TYR	7
1	A	87	ILE	7
1	A	97	ARG	7
1	A	139	LYS	7
1	A	111	GLU	7
1	A	124	ARG	7
1	A	112	HIS	7
1	A	122	THR	7
1	A	130	CYS	7
1	A	91	TYR	7
1	A	12	GLN	6
1	A	14	ASP	6
1	A	92	ILE	6
1	A	114	GLU	6
1	A	98	ASP	6
1	A	126	GLU	6
1	A	9	ILE	6
1	A	117	ASN	5
1	A	20	GLN	5
1	A	63	LEU	5
1	A	15	GLU	5
1	A	102	GLN	5
1	A	71	THR	5
1	A	137	ILE	5

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Mol	Chain	Res	Type	Models (Total)
1	A	4	PHE	5
1	A	65	ASP	4
1	A	79	LYS	4
1	A	54	VAL	4
1	A	60	GLU	4
1	A	67	CYS	4
1	A	64	TYR	4
1	A	119	LYS	4
1	A	133	GLU	4
1	A	99	LEU	4
1	A	55	TYR	3
1	A	107	GLU	3
1	A	21	LEU	3
1	A	22	LYS	3
1	A	69	ILE	3
1	A	128	CYS	3
1	A	136	ILE	3
1	A	76	GLU	2
1	A	143	GLU	2
1	A	17	ASN	2
1	A	127	ASP	2
1	A	57	HIS	2
1	A	16	GLN	2
1	A	134	GLU	2
1	A	120	GLU	2
1	A	75	LYS	2
1	A	108	TYR	2
1	A	121	VAL	1
1	A	96	ASN	1
1	A	106	PHE	1
1	A	144	ILE	1
1	A	88	GLU	1
1	A	52	ASN	1
1	A	100	PHE	1
1	A	74	ASP	1
1	A	89	ASN	1
1	A	13	GLN	1
1	A	83	THR	1
1	A	59	ILE	1
1	A	103	TYR	1
1	A	123	ILE	1
1	A	3	ASN	1

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Mol	Chain	Res	Type	Models (Total)
1	A	18	ASN	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 oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided