



Full wwPDB NMR Structure Validation Report ⓘ

Mar 5, 2026 – 07:01 PM UTC

PDB ID : 1BYN / pdb_00001byn
Title : SOLUTION STRUCTURE OF THE CALCIUM-BOUND FIRST C2-DOMAIN OF SYNAPTOTAGMIN I
Authors : Shao, X.; Fernandez, I.; Sudhof, T.C.; Rizo, J.
Deposited on : 1998-10-18

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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

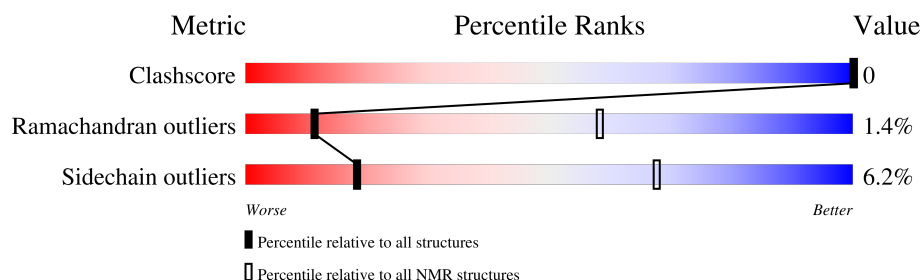
1 Overall quality at a glance

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	128	 87% 9% . .

2 Ensemble composition and analysis

This entry contains 20 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:142-A:264 (123)	0.43	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 2 clusters and 3 single-model clusters were found.

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

3 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 2084 atoms, of which 1038 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called PROTEIN (SYNAPTOTAGMIN I).

Mol	Chain	Residues	Atoms						Trace
1	A	128	Total	C	H	N	O	S	0
			2081	677	1038	169	194	3	

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	188	ASP	GLU	conflict	UNP P21707

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

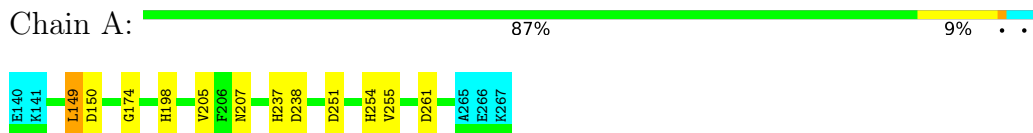
Mol	Chain	Residues	Atoms	
2	A	3	Total	Ca
			3	3

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: PROTEIN (SYNAPTOTAGMIN I)

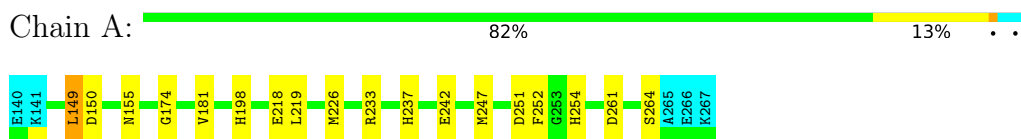


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

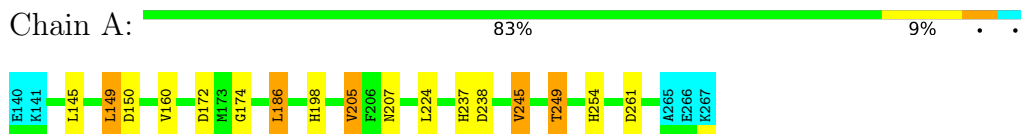
4.2.1 Score per residue for model 1

- Molecule 1: PROTEIN (SYNAPTOTAGMIN I)



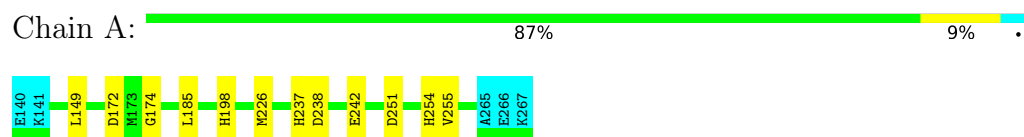
4.2.2 Score per residue for model 2

- Molecule 1: PROTEIN (SYNAPTOTAGMIN I)



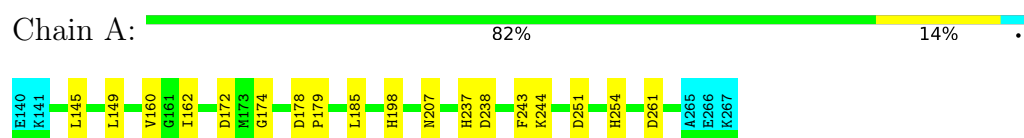
4.2.3 Score per residue for model 3

- Molecule 1: PROTEIN (SYNAPTOTAGMIN I)



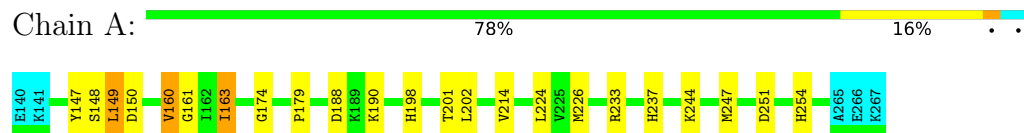
4.2.4 Score per residue for model 4

- Molecule 1: PROTEIN (SYNAPTOTAGMIN I)



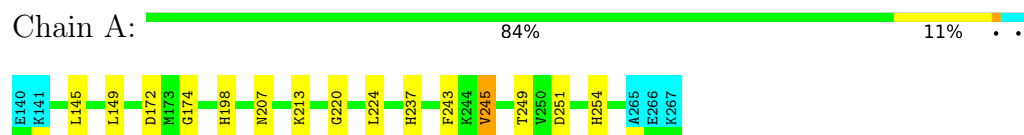
4.2.5 Score per residue for model 5

- Molecule 1: PROTEIN (SYNAPTOTAGMIN I)



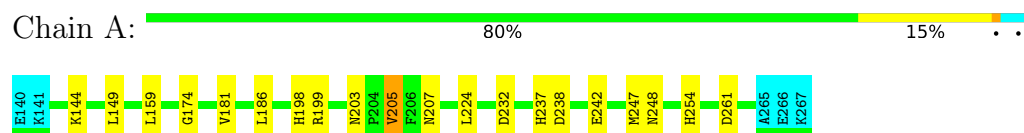
4.2.6 Score per residue for model 6 (medoid)

- Molecule 1: PROTEIN (SYNAPTOTAGMIN I)



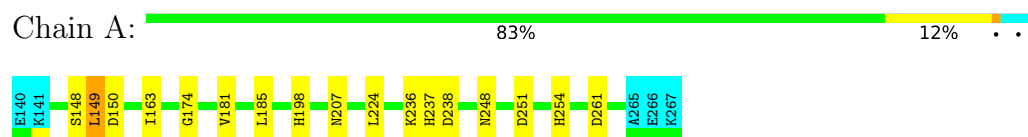
4.2.7 Score per residue for model 7

- Molecule 1: PROTEIN (SYNAPTOTAGMIN I)



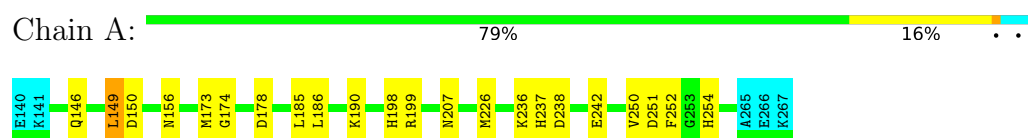
4.2.8 Score per residue for model 8

- Molecule 1: PROTEIN (SYNAPTOTAGMIN I)



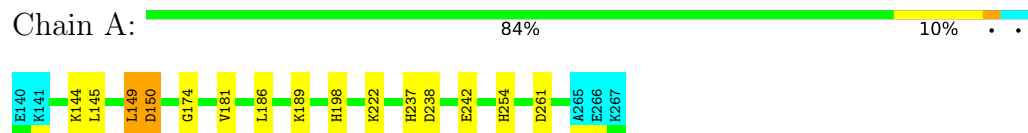
4.2.9 Score per residue for model 9

- Molecule 1: PROTEIN (SYNAPTOTAGMIN I)



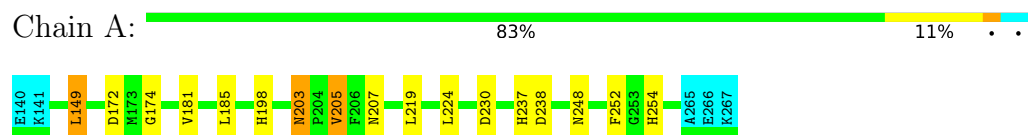
4.2.10 Score per residue for model 10

- Molecule 1: PROTEIN (SYNAPTOTAGMIN I)



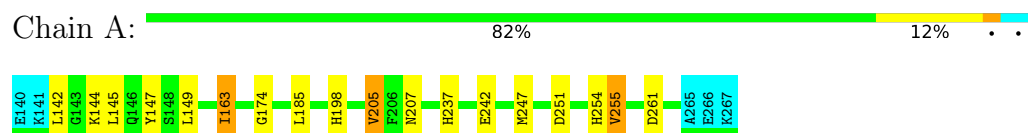
4.2.11 Score per residue for model 11

- Molecule 1: PROTEIN (SYNAPTOTAGMIN I)



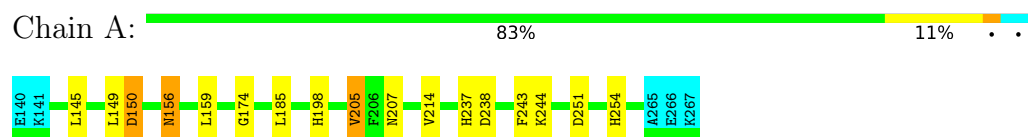
4.2.12 Score per residue for model 12

- Molecule 1: PROTEIN (SYNAPTOTAGMIN I)



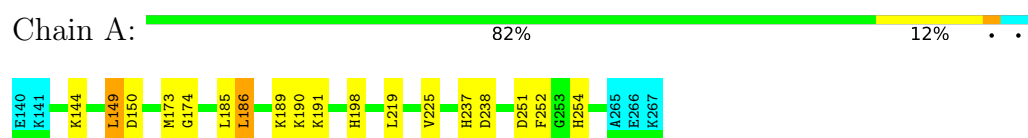
4.2.13 Score per residue for model 13

- Molecule 1: PROTEIN (SYNAPTOTAGMIN I)



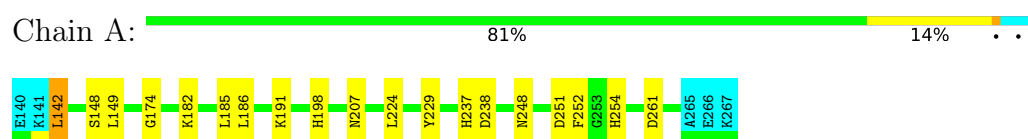
4.2.14 Score per residue for model 14

- Molecule 1: PROTEIN (SYNAPTOTAGMIN I)



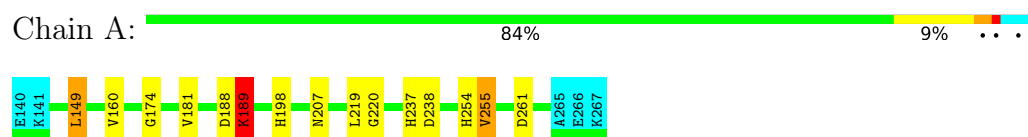
4.2.15 Score per residue for model 15

- Molecule 1: PROTEIN (SYNAPTOTAGMIN I)



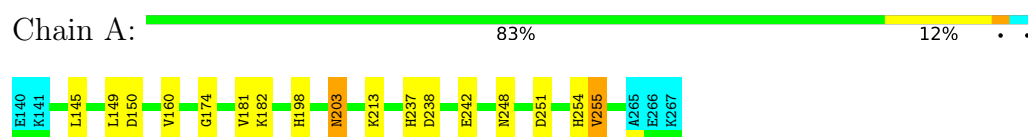
4.2.16 Score per residue for model 16

- Molecule 1: PROTEIN (SYNAPTOTAGMIN I)



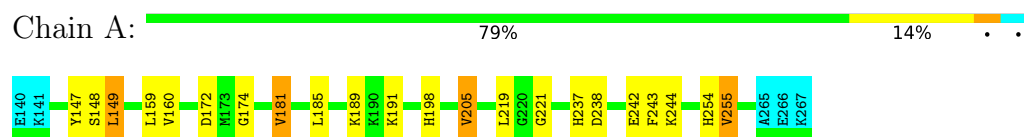
4.2.17 Score per residue for model 17

- Molecule 1: PROTEIN (SYNAPTOTAGMIN I)



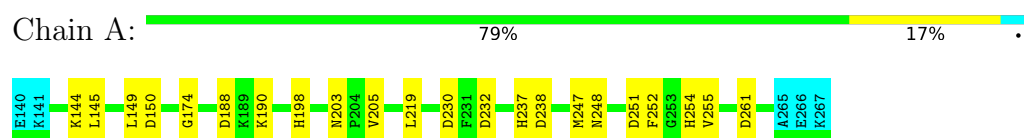
4.2.18 Score per residue for model 18

- Molecule 1: PROTEIN (SYNAPTOTAGMIN I)



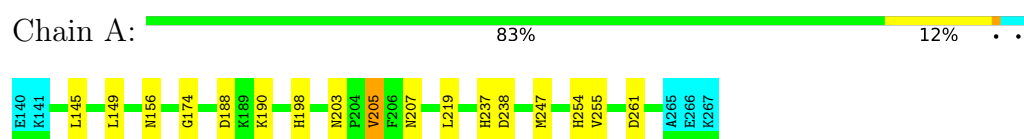
4.2.19 Score per residue for model 19

- Molecule 1: PROTEIN (SYNAPTOTAGMIN I)



4.2.20 Score per residue for model 20

- Molecule 1: PROTEIN (SYNAPTOTAGMIN I)



5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *FEWEST RESTRAINTS VIOLATIONS*.

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

Software name	Classification	Version
Discover	refinement	
Discover	structure solution	
NMRCHITECT	structure solution	

No chemical shift data was provided.

6 Model quality [i](#)

6.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CA

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	1.52±0.01	5±1/1028 (0.5± 0.1%)	1.58±0.04	18±3/1390 (1.3± 0.2%)
All	All	1.52	102/20560 (0.5%)	1.58	354/27800 (1.3%)

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	0.1±0.4
All	All	0	3

All unique bond outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	237	HIS	CG-CD2	6.47	1.43	1.35	1	20
1	A	254	HIS	CG-CD2	6.16	1.42	1.35	17	20
1	A	202	LEU	CA-C	5.84	1.60	1.52	5	1
1	A	163	ILE	CA-CB	5.79	1.62	1.54	12	1
1	A	198	HIS	CG-CD2	5.70	1.42	1.35	5	14
1	A	189	LYS	CA-C	5.66	1.60	1.52	16	1
1	A	198	HIS	ND1-CE1	5.39	1.38	1.32	19	20
1	A	214	VAL	CA-C	5.33	1.57	1.52	5	2
1	A	160	VAL	CA-C	5.27	1.59	1.52	5	1
1	A	150	ASP	CA-C	5.13	1.59	1.52	10	2
1	A	254	HIS	ND1-CE1	5.13	1.37	1.32	17	17
1	A	254	HIS	CA-C	5.12	1.58	1.52	3	2
1	A	203	ASN	CA-C	5.07	1.58	1.52	20	1

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	150	ASP	CA-CB-CG	13.01	125.61	112.60	13	10
1	A	198	HIS	ND1-CE1-NE2	12.02	120.42	108.40	15	20
1	A	237	HIS	ND1-CE1-NE2	11.92	120.32	108.40	1	20
1	A	254	HIS	ND1-CE1-NE2	11.82	120.22	108.40	17	20
1	A	207	ASN	CA-CB-CG	10.72	123.32	112.60	9	12
1	A	238	ASP	CA-CB-CG	10.58	123.18	112.60	20	16
1	A	252	PHE	N-CA-CB	-10.04	98.81	110.35	14	6
1	A	251	ASP	CA-CB-CG	9.45	122.05	112.60	19	13
1	A	198	HIS	CE1-NE2-CD2	-9.22	99.78	109.00	15	20
1	A	237	HIS	CE1-NE2-CD2	-9.08	99.92	109.00	1	20
1	A	254	HIS	CE1-NE2-CD2	-8.95	100.05	109.00	13	20
1	A	261	ASP	CA-CB-CG	7.93	120.53	112.60	12	11
1	A	248	ASN	CA-CB-CG	7.90	120.50	112.60	11	6
1	A	178	ASP	N-CA-CB	-7.56	98.76	110.11	9	2
1	A	156	ASN	CA-CB-CG	7.48	120.08	112.60	9	2
1	A	149	LEU	N-CA-CB	-7.39	99.17	110.77	20	13
1	A	236	LYS	N-CA-CB	-7.18	99.48	110.04	8	1
1	A	203	ASN	N-CA-CB	-6.77	101.99	110.79	17	4
1	A	155	ASN	CA-CB-CG	6.56	119.16	112.60	1	1
1	A	149	LEU	CB-CA-C	6.44	119.36	110.34	5	4
1	A	190	LYS	N-CA-CB	-6.29	100.70	110.39	9	2
1	A	186	LEU	N-CA-CB	-6.25	99.72	110.72	14	4
1	A	198	HIS	CG-ND1-CE1	-6.20	98.75	109.30	19	20
1	A	160	VAL	CA-CB-CG1	6.12	120.80	110.40	16	1
1	A	201	THR	CA-CB-CG2	6.09	120.86	110.50	5	1
1	A	254	HIS	CG-ND1-CE1	-6.03	99.06	109.30	16	20
1	A	205	VAL	CB-CA-C	6.01	119.01	110.84	2	7
1	A	144	LYS	CA-CB-CG	5.99	126.08	114.10	14	4
1	A	237	HIS	CA-CB-CG	5.90	119.70	113.80	11	4
1	A	159	LEU	N-CA-CB	-5.90	98.72	110.64	18	2
1	A	249	THR	N-CA-CB	-5.88	100.82	110.40	2	1
1	A	245	VAL	CA-CB-CG1	5.86	120.36	110.40	2	1
1	A	188	ASP	N-CA-C	5.86	117.34	111.07	20	2
1	A	245	VAL	CA-CB-CG2	5.84	120.32	110.40	6	2
1	A	237	HIS	CG-ND1-CE1	-5.80	99.45	109.30	19	20
1	A	254	HIS	CB-CA-C	5.75	121.87	110.42	14	2
1	A	254	HIS	N-CA-CB	-5.70	106.29	111.59	7	1
1	A	142	LEU	CB-CA-C	5.67	118.46	111.43	15	1
1	A	213	LYS	N-CA-CB	-5.61	102.99	110.57	6	2
1	A	230	ASP	CA-CB-CG	5.59	118.19	112.60	11	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	172	ASP	N-CA-C	5.47	119.95	113.28	2	1
1	A	172	ASP	CA-CB-CG	5.47	118.07	112.60	4	1
1	A	199	ARG	N-CA-C	5.45	118.22	110.10	9	1
1	A	179	PRO	N-CA-C	5.41	120.56	111.32	4	2
1	A	181	VAL	N-CA-CB	5.38	116.39	110.53	18	1
1	A	163	ILE	CB-CG1-CD1	5.37	125.07	113.80	5	1
1	A	178	ASP	CA-CB-CG	5.33	117.93	112.60	4	2
1	A	198	HIS	CB-CG-CD2	-5.33	124.27	131.20	19	1
1	A	254	HIS	CA-C-O	5.28	121.66	118.33	6	1
1	A	220	GLY	N-CA-C	5.27	119.02	112.64	6	2
1	A	243	PHE	CA-CB-CG	5.24	119.04	113.80	6	4
1	A	252	PHE	N-CA-C	5.24	118.79	112.93	9	1
1	A	163	ILE	CA-CB-CG1	5.23	119.29	110.40	5	1
1	A	144	LYS	N-CA-CB	-5.22	103.31	111.56	10	1
1	A	219	LEU	N-CA-CB	-5.20	102.53	110.07	19	3
1	A	254	HIS	CA-C-N	5.19	127.54	120.63	13	2
1	A	254	HIS	C-N-CA	5.19	127.54	120.63	13	2
1	A	173	MET	N-CA-CB	-5.19	104.20	110.53	14	2
1	A	218	GLU	N-CA-CB	-5.13	102.41	110.30	1	1
1	A	224	LEU	N-CA-CB	-5.12	102.07	110.21	6	2
1	A	190	LYS	CB-CA-C	5.08	120.53	110.42	19	1
1	A	188	ASP	CA-CB-CG	5.06	117.66	112.60	19	1

There are no chirality outliers.

All unique planar outliers are listed below.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	147	TYR	Sidechain	3

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	1002	994	994	0±0
All	All	20100	19880	19880	1

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 0.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:186:LEU:HD13	1:A:225:VAL:HG21	0.47	1.85	14	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	123/128 (96%)	109±2 (89±1%)	12±2 (10±2%)	2±1 (1±1%)	11	58
All	All	2460/2560 (96%)	2184 (89%)	242 (10%)	34 (1%)	11	58

All 8 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	174	GLY	20
1	A	255	VAL	6
1	A	233	ARG	2
1	A	156	ASN	2
1	A	161	GLY	1
1	A	188	ASP	1
1	A	189	LYS	1
1	A	221	GLY	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	111/115 (97%)	104±2 (94±2%)	7±2 (6±2%)	18	68
All	All	2220/2300 (97%)	2082 (94%)	138 (6%)	18	68

All 36 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	149	LEU	15
1	A	185	LEU	10
1	A	145	LEU	9
1	A	181	VAL	8
1	A	242	GLU	8
1	A	205	VAL	8
1	A	247	MET	6
1	A	160	VAL	5
1	A	224	LEU	5
1	A	255	VAL	5
1	A	219	LEU	4
1	A	226	MET	4
1	A	172	ASP	4
1	A	244	LYS	4
1	A	148	SER	4
1	A	189	LYS	4
1	A	186	LEU	3
1	A	163	ILE	3
1	A	190	LYS	3
1	A	191	LYS	3
1	A	245	VAL	2
1	A	249	THR	2
1	A	232	ASP	2
1	A	150	ASP	2
1	A	203	ASN	2
1	A	142	LEU	2
1	A	182	LYS	2
1	A	264	SER	1
1	A	162	ILE	1
1	A	199	ARG	1
1	A	146	GLN	1
1	A	236	LYS	1
1	A	250	VAL	1
1	A	222	LYS	1
1	A	159	LEU	1
1	A	229	TYR	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](#)

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

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