



Full wwPDB NMR Structure Validation Report ⓘ

Mar 5, 2026 – 07:29 PM UTC

PDB ID : 6G4A / pdb_00006g4a
BMRB ID : 34249
Title : FLN5 (full length)
Authors : Waudby, C.A.; Wlodarski, T.; Karyadi, M.-E.; Cassaignau, A.M.E.; Chan, S.H.S.; Wentink, A.S.; Schmidt-Engler, J.M.; Camilloni, C.; Vendruscolo, M.; Cabrita, L.D.; Christodoulou, J.
Deposited on : 2018-03-27

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

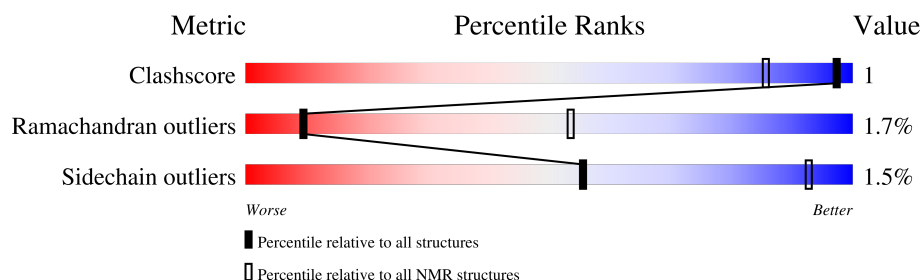
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 43%.

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	114	

2 Ensemble composition and analysis

This entry contains 10 models. Model 1 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:11-A:62, A:66-A:114 (101)	0.55	1

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. No single-model clusters were found.

Cluster number	Models
1	1, 4, 5, 6, 7, 10
2	8, 9
3	2, 3

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1659 atoms, of which 804 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Gelation factor.

Mol	Chain	Residues	Atoms						Trace
1	A	114	Total	C	H	N	O	S	0
			1659	534	804	149	169	3	

There are 9 discrepancies between the modelled and reference sequences:

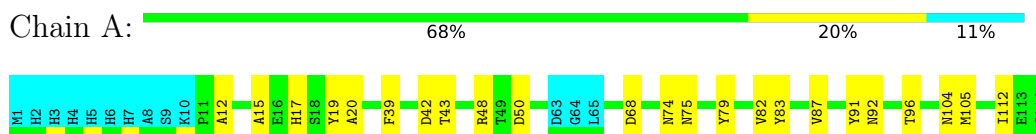
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP P13466
A	2	HIS	-	expression tag	UNP P13466
A	3	HIS	-	expression tag	UNP P13466
A	4	HIS	-	expression tag	UNP P13466
A	5	HIS	-	expression tag	UNP P13466
A	6	HIS	-	expression tag	UNP P13466
A	7	HIS	-	expression tag	UNP P13466
A	8	ALA	-	expression tag	UNP P13466
A	9	SER	-	expression tag	UNP P13466

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: Gelation factor

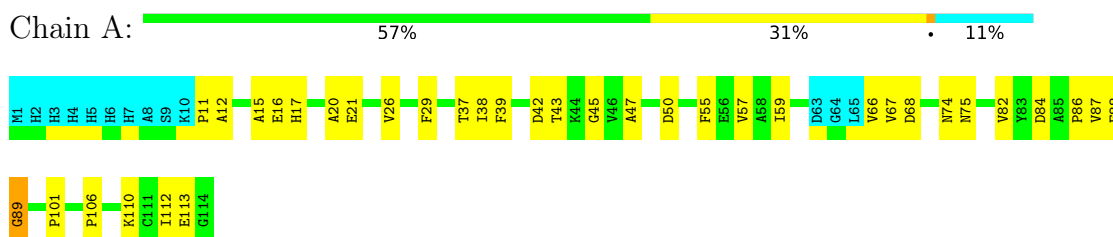


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

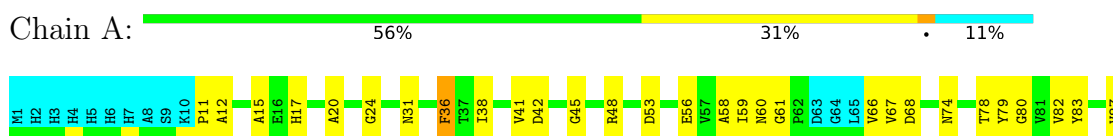
4.2.1 Score per residue for model 1 (medoid)

- Molecule 1: Gelation factor



4.2.2 Score per residue for model 2

- Molecule 1: Gelation factor





4.2.3 Score per residue for model 3

- Molecule 1: Gelation factor

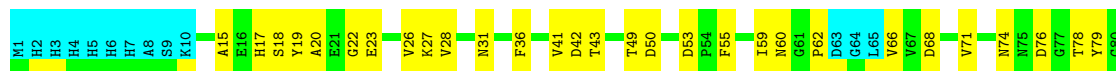
Chain A: 61% 24% 11%



4.2.4 Score per residue for model 4

- Molecule 1: Gelation factor

Chain A: 52% 36% 11%



4.2.5 Score per residue for model 5

- Molecule 1: Gelation factor

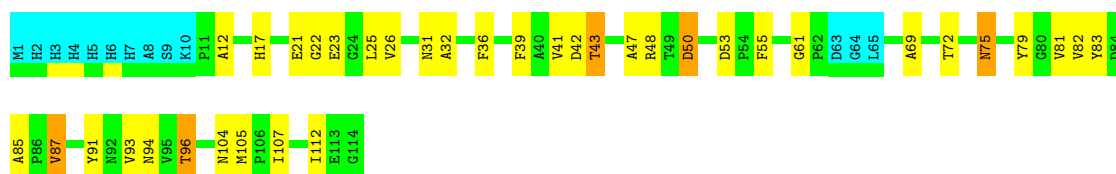
Chain A: 48% 34% 6% 11%



4.2.6 Score per residue for model 6

- Molecule 1: Gelation factor

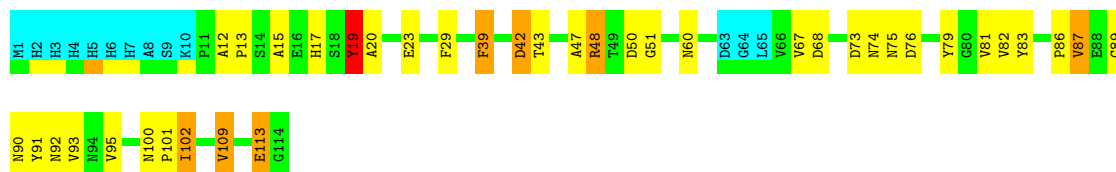
Chain A: 56% 28% 11%



4.2.7 Score per residue for model 7

- Molecule 1: Gelation factor

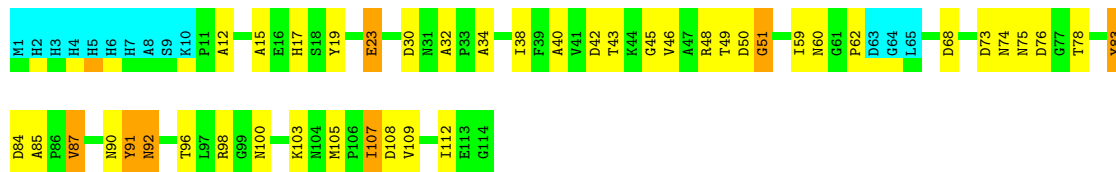
Chain A: 54% 27% 6% 11%



4.2.8 Score per residue for model 8

- Molecule 1: Gelation factor

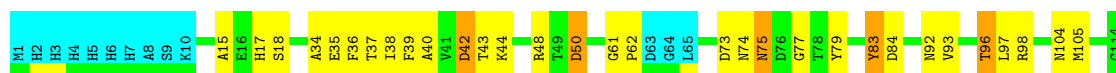
Chain A: 51% 32% 6% 11%



4.2.9 Score per residue for model 9

- Molecule 1: Gelation factor

Chain A: 61% 23% 1% 11%



4.2.10 Score per residue for model 10

- Molecule 1: Gelation factor

Chain A: 58% 29% 1% 11%



5 Refinement protocol and experimental data overview

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

Of the 572 calculated structures, 10 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
GROMACS	structure calculation	4.6.5

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	556
Number of shifts mapped to atoms	556
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	43%

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	0.64±0.03	0±0/763 (0.0± 0.0%)	2.42±0.10	45±8/1043 (4.3± 0.8%)
All	All	0.64	0/7630 (0.0%)	2.42	448/10430 (4.3%)

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	5.8±1.4
All	All	0	58

There are no bond-length outliers.

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	74	ASN	CA-CB-CG	13.17	125.77	112.60	4	4
1	A	12	ALA	CA-C-N	11.93	132.06	119.89	1	4
1	A	12	ALA	C-N-CA	11.93	132.06	119.89	1	4
1	A	75	ASN	CA-CB-CG	11.66	124.26	112.60	9	3
1	A	50	ASP	CA-CB-CG	11.44	124.04	112.60	5	4
1	A	62	PRO	N-CA-CB	10.63	110.35	103.23	4	3
1	A	79	TYR	CA-C-N	10.47	130.99	120.31	5	4
1	A	79	TYR	C-N-CA	10.47	130.99	120.31	5	4
1	A	68	ASP	CA-CB-CG	10.11	122.71	112.60	2	3
1	A	17	HIS	CB-CG-CD2	-9.29	119.12	131.20	1	4
1	A	61	GLY	CA-C-N	9.25	129.82	119.83	5	4
1	A	61	GLY	C-N-CA	9.25	129.82	119.83	5	4
1	A	30	ASP	CA-CB-CG	9.18	121.78	112.60	8	1
1	A	29	PHE	N-CA-C	9.18	120.36	108.34	1	2
1	A	81	VAL	CA-C-O	-9.12	110.81	120.48	7	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	84	ASP	CA-C-N	9.03	133.92	122.64	8	1
1	A	84	ASP	C-N-CA	9.03	133.92	122.64	8	1
1	A	98	ARG	NE-CZ-NH1	9.00	130.50	121.50	10	1
1	A	92	ASN	OD1-CG-ND2	-8.87	113.73	122.60	8	3
1	A	48	ARG	NE-CZ-NH2	8.70	127.03	119.20	10	1
1	A	69	ALA	O-C-N	-8.66	113.23	122.94	10	1
1	A	76	ASP	CA-C-N	8.45	133.41	122.00	7	1
1	A	76	ASP	C-N-CA	8.45	133.41	122.00	7	1
1	A	39	PHE	CA-CB-CG	8.29	122.09	113.80	9	3
1	A	68	ASP	CA-C-O	8.26	128.99	120.24	5	2
1	A	90	ASN	OD1-CG-ND2	-8.17	114.43	122.60	8	4
1	A	104	ASN	CA-CB-CG	8.12	120.72	112.60	6	3
1	A	100	ASN	OD1-CG-ND2	-8.10	114.50	122.60	5	1
1	A	87	VAL	N-CA-C	8.01	120.40	108.46	5	2
1	A	32	ALA	CA-C-N	8.01	129.85	119.84	5	2
1	A	32	ALA	C-N-CA	8.01	129.85	119.84	5	2
1	A	29	PHE	CA-CB-CG	8.01	121.81	113.80	3	1
1	A	43	THR	CA-CB-CG2	7.94	124.00	110.50	6	2
1	A	60	ASN	OD1-CG-ND2	-7.94	114.66	122.60	7	5
1	A	68	ASP	CA-C-N	7.89	133.32	122.19	2	1
1	A	68	ASP	C-N-CA	7.89	133.32	122.19	2	1
1	A	31	ASN	OD1-CG-ND2	-7.80	114.80	122.60	5	1
1	A	42	ASP	CA-CB-CG	7.80	120.40	112.60	6	6
1	A	112	ILE	O-C-N	-7.77	114.43	123.05	1	4
1	A	105	MET	O-C-N	-7.71	116.41	121.88	9	3
1	A	89	GLY	O-C-N	-7.67	117.43	123.80	1	1
1	A	67	VAL	CA-CB-CG1	7.66	123.42	110.40	5	2
1	A	110	LYS	O-C-N	7.61	131.99	123.01	3	1
1	A	107	ILE	O-C-N	-7.55	114.75	122.75	6	1
1	A	100	ASN	CA-C-N	7.54	127.45	120.21	7	1
1	A	100	ASN	C-N-CA	7.54	127.45	120.21	7	1
1	A	82	VAL	CA-CB-CG2	7.47	123.09	110.40	5	1
1	A	11	PRO	CB-CA-C	7.46	120.73	110.95	10	3
1	A	23	GLU	N-CA-C	7.43	119.38	111.28	6	3
1	A	55	PHE	N-CA-C	7.43	120.97	110.50	10	1
1	A	55	PHE	CA-CB-CG	7.40	121.20	113.80	6	2
1	A	66	VAL	CA-CB-CG1	7.29	122.80	110.40	4	1
1	A	100	ASN	CA-C-O	-7.25	114.08	120.60	10	2
1	A	82	VAL	O-C-N	7.21	130.82	123.10	2	3
1	A	49	THR	CA-C-N	7.21	133.70	121.87	4	2
1	A	49	THR	C-N-CA	7.21	133.70	121.87	4	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	48	ARG	NH1-CZ-NH2	-7.21	109.93	119.30	10	4
1	A	112	ILE	CA-CB-CG1	7.13	122.53	110.40	6	2
1	A	48	ARG	CA-C-N	7.09	136.48	122.31	6	4
1	A	48	ARG	C-N-CA	7.09	136.48	122.31	6	4
1	A	42	ASP	CA-C-N	7.07	135.04	121.54	6	6
1	A	42	ASP	C-N-CA	7.07	135.04	121.54	6	6
1	A	104	ASN	OD1-CG-ND2	-7.04	115.56	122.60	4	2
1	A	85	ALA	CA-C-N	7.00	128.22	120.45	5	1
1	A	85	ALA	C-N-CA	7.00	128.22	120.45	5	1
1	A	14	SER	CA-C-N	6.98	129.94	120.44	5	2
1	A	14	SER	C-N-CA	6.98	129.94	120.44	5	2
1	A	41	VAL	CA-CB-CG1	6.98	122.27	110.40	4	4
1	A	12	ALA	N-CA-C	6.97	118.43	109.65	8	3
1	A	21	GLU	N-CA-C	6.96	119.92	108.99	3	2
1	A	96	THR	CA-CB-CG2	6.88	122.20	110.50	6	3
1	A	15	ALA	CA-C-O	-6.88	113.60	120.82	4	1
1	A	94	ASN	OD1-CG-ND2	-6.81	115.79	122.60	6	3
1	A	39	PHE	N-CA-C	6.81	119.22	108.67	10	2
1	A	43	THR	CA-C-O	-6.80	110.79	120.51	9	2
1	A	72	THR	CA-C-N	6.79	131.08	121.02	5	2
1	A	72	THR	C-N-CA	6.79	131.08	121.02	5	2
1	A	105	MET	CA-C-O	-6.73	113.35	120.28	6	1
1	A	20	ALA	N-CA-C	6.70	119.62	109.23	2	6
1	A	73	ASP	CA-CB-CG	6.70	119.30	112.60	9	3
1	A	15	ALA	CA-C-N	6.69	129.55	120.38	2	4
1	A	15	ALA	C-N-CA	6.69	129.55	120.38	2	4
1	A	40	ALA	CA-C-N	6.69	132.24	122.94	9	2
1	A	40	ALA	C-N-CA	6.69	132.24	122.94	9	2
1	A	78	THR	CA-CB-CG2	6.67	121.85	110.50	4	2
1	A	66	VAL	CB-CA-C	6.65	119.70	111.25	1	2
1	A	107	ILE	CA-C-O	-6.64	115.06	121.63	5	1
1	A	41	VAL	O-C-N	-6.60	115.94	123.00	6	1
1	A	100	ASN	N-CA-C	6.51	119.07	109.50	7	1
1	A	113	GLU	CA-C-O	6.48	129.78	120.51	7	1
1	A	113	GLU	CB-CA-C	6.41	119.77	111.50	1	2
1	A	98	ARG	CD-NE-CZ	6.41	133.37	124.40	8	1
1	A	107	ILE	N-CA-C	6.40	118.14	108.80	8	1
1	A	17	HIS	CA-CB-CG	-6.39	107.41	113.80	9	3
1	A	18	SER	CB-CA-C	6.39	120.27	110.62	5	1
1	A	23	GLU	CA-C-O	-6.36	112.65	119.97	4	1
1	A	48	ARG	NE-CZ-NH1	6.33	127.83	121.50	6	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	38	ILE	N-CA-CB	6.33	118.73	111.90	2	1
1	A	17	HIS	O-C-N	-6.31	113.61	122.26	8	1
1	A	90	ASN	CA-CB-CG	-6.28	106.32	112.60	10	1
1	A	83	TYR	N-CA-C	6.27	117.76	108.60	5	2
1	A	20	ALA	O-C-N	-6.25	116.02	123.27	5	1
1	A	81	VAL	CG1-CB-CG2	-6.24	97.08	110.80	6	1
1	A	36	PHE	CA-C-N	6.21	131.53	122.77	4	1
1	A	36	PHE	C-N-CA	6.21	131.53	122.77	4	1
1	A	71	VAL	N-CA-C	6.20	117.64	109.21	10	1
1	A	93	VAL	N-CA-C	6.20	117.52	108.53	7	2
1	A	71	VAL	CB-CA-C	-6.19	102.25	110.98	5	1
1	A	81	VAL	N-CA-C	6.18	117.19	108.36	3	1
1	A	31	ASN	N-CA-C	6.17	120.51	112.92	4	1
1	A	32	ALA	CB-CA-C	6.16	122.31	110.17	6	1
1	A	49	THR	CA-C-O	6.15	126.76	119.56	8	1
1	A	74	ASN	CA-C-N	6.15	131.59	122.74	9	2
1	A	74	ASN	C-N-CA	6.15	131.59	122.74	9	2
1	A	69	ALA	CA-C-O	6.12	127.46	120.54	5	1
1	A	88	GLU	O-C-N	-6.12	114.45	122.59	1	1
1	A	78	THR	N-CA-C	6.12	118.25	109.14	8	1
1	A	71	VAL	CA-CB-CG1	6.11	120.79	110.40	3	2
1	A	95	VAL	CA-CB-CG1	6.08	120.73	110.40	7	1
1	A	37	THR	CA-C-O	-6.07	113.81	120.36	9	1
1	A	92	ASN	CA-CB-CG	-6.06	106.54	112.60	5	1
1	A	68	ASP	CB-CA-C	6.04	120.63	109.70	8	1
1	A	81	VAL	CA-CB-CG2	6.02	120.63	110.40	6	3
1	A	60	ASN	CA-C-O	-6.00	114.22	120.70	7	1
1	A	91	TYR	CA-CB-CG	5.99	124.68	113.90	4	1
1	A	62	PRO	O-C-N	-5.98	116.14	123.01	5	1
1	A	102	ILE	N-CA-CB	-5.98	105.44	112.32	7	1
1	A	31	ASN	CA-C-O	5.97	126.64	119.59	2	1
1	A	76	ASP	CA-CB-CG	5.96	118.56	112.60	8	2
1	A	46	VAL	CA-CB-CG1	5.96	120.53	110.40	8	2
1	A	33	PRO	N-CA-CB	5.96	108.87	103.33	3	2
1	A	113	GLU	O-C-N	-5.95	114.68	122.59	7	1
1	A	56	GLU	CA-C-N	5.94	130.77	123.17	3	2
1	A	56	GLU	C-N-CA	5.94	130.77	123.17	3	2
1	A	86	PRO	CB-CA-C	5.92	118.57	110.52	7	2
1	A	17	HIS	ND1-CE1-NE2	5.92	114.32	108.40	3	1
1	A	87	VAL	CA-CB-CG2	5.88	120.39	110.40	8	3
1	A	12	ALA	O-C-N	-5.86	115.21	121.42	8	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	19	TYR	CA-C-O	-5.85	114.44	120.99	7	2
1	A	75	ASN	CB-CG-ND2	5.81	125.12	116.40	3	1
1	A	93	VAL	CA-C-N	5.80	131.17	122.99	2	2
1	A	93	VAL	C-N-CA	5.80	131.17	122.99	2	2
1	A	53	ASP	CA-C-N	5.80	127.09	119.84	3	1
1	A	53	ASP	C-N-CA	5.80	127.09	119.84	3	1
1	A	98	ARG	CB-CA-C	5.80	120.26	111.80	9	1
1	A	15	ALA	O-C-N	-5.79	114.57	122.33	7	1
1	A	26	VAL	CB-CA-C	-5.76	105.92	111.05	6	1
1	A	34	ALA	N-CA-C	5.76	119.04	110.52	9	1
1	A	53	ASP	CA-CB-CG	5.75	118.35	112.60	2	2
1	A	96	THR	O-C-N	-5.74	116.18	123.24	9	1
1	A	84	ASP	CA-CB-CG	5.73	118.33	112.60	8	2
1	A	15	ALA	N-CA-C	5.72	117.59	111.36	9	1
1	A	78	THR	OG1-CB-CG2	-5.71	97.87	109.30	5	1
1	A	38	ILE	CA-C-O	-5.71	114.00	120.74	1	2
1	A	17	HIS	CE1-NE2-CD2	-5.71	103.29	109.00	5	2
1	A	74	ASN	OD1-CG-ND2	-5.71	116.89	122.60	8	1
1	A	83	TYR	O-C-N	-5.68	116.27	122.92	8	1
1	A	103	LYS	CA-C-O	-5.67	115.25	121.89	4	2
1	A	82	VAL	CA-CB-CG1	5.67	120.04	110.40	3	4
1	A	17	HIS	CA-C-O	5.67	125.52	119.34	5	2
1	A	15	ALA	CB-CA-C	5.66	120.30	110.68	10	1
1	A	27	LYS	CA-C-N	5.65	130.85	123.06	4	1
1	A	27	LYS	C-N-CA	5.65	130.85	123.06	4	1
1	A	59	ILE	CA-C-N	5.64	131.43	122.74	10	1
1	A	59	ILE	C-N-CA	5.64	131.43	122.74	10	1
1	A	59	ILE	O-C-N	-5.63	116.59	123.00	1	1
1	A	101	PRO	N-CA-CB	5.63	109.78	102.86	1	1
1	A	90	ASN	CB-CA-C	5.62	118.80	110.14	7	1
1	A	39	PHE	CB-CA-C	5.60	119.27	110.19	5	3
1	A	109	VAL	CA-CB-CG1	5.59	119.90	110.40	2	1
1	A	62	PRO	CA-C-N	5.59	132.22	121.54	8	1
1	A	62	PRO	C-N-CA	5.59	132.22	121.54	8	1
1	A	78	THR	CA-CB-OG1	-5.58	101.24	109.60	2	1
1	A	26	VAL	CA-CB-CG1	5.57	119.86	110.40	6	1
1	A	45	GLY	CA-C-N	5.56	128.89	120.77	2	1
1	A	45	GLY	C-N-CA	5.56	128.89	120.77	2	1
1	A	43	THR	N-CA-CB	5.56	119.89	110.49	4	1
1	A	83	TYR	CB-CG-CD1	-5.56	112.46	120.80	6	1
1	A	42	ASP	N-CA-C	5.56	117.03	110.97	1	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	17	HIS	CB-CG-ND1	5.53	130.99	122.70	1	1
1	A	75	ASN	CA-C-O	5.52	127.65	120.81	5	1
1	A	53	ASP	N-CA-CB	5.51	117.99	110.05	4	1
1	A	100	ASN	CA-CB-CG	5.50	118.11	112.60	2	1
1	A	51	GLY	O-C-N	-5.50	117.46	123.29	7	1
1	A	84	ASP	N-CA-C	5.49	117.53	109.24	9	1
1	A	13	PRO	N-CA-CB	5.49	108.12	103.35	10	1
1	A	73	ASP	O-C-N	-5.49	116.53	123.01	10	1
1	A	16	GLU	CA-C-N	5.48	131.29	122.14	10	2
1	A	16	GLU	C-N-CA	5.48	131.29	122.14	10	2
1	A	75	ASN	N-CA-CB	-5.47	103.98	112.30	7	1
1	A	32	ALA	O-C-N	-5.47	115.68	121.04	8	1
1	A	86	PRO	N-CD-CG	5.47	111.40	103.20	5	1
1	A	89	GLY	N-CA-C	5.47	117.56	110.45	7	2
1	A	48	ARG	CD-NE-CZ	5.46	132.05	124.40	6	1
1	A	51	GLY	CA-C-N	5.46	128.36	120.11	5	1
1	A	51	GLY	C-N-CA	5.46	128.36	120.11	5	1
1	A	50	ASP	O-C-N	-5.46	117.83	123.29	6	2
1	A	74	ASN	N-CA-C	5.46	119.81	113.20	9	1
1	A	77	GLY	CA-C-O	-5.46	113.49	118.95	10	1
1	A	82	VAL	CA-C-O	-5.44	114.57	120.67	2	1
1	A	72	THR	CA-C-O	5.44	127.23	120.54	5	1
1	A	31	ASN	N-CA-CB	-5.44	102.62	110.56	4	1
1	A	48	ARG	N-CA-C	5.43	118.67	110.64	10	1
1	A	76	ASP	O-C-N	-5.41	116.61	122.19	7	1
1	A	93	VAL	CA-CB-CG1	5.41	119.60	110.40	9	1
1	A	35	GLU	N-CA-C	5.41	117.61	109.23	9	1
1	A	104	ASN	N-CA-CB	-5.38	103.95	112.08	10	2
1	A	109	VAL	CA-C-O	5.37	125.69	120.27	7	1
1	A	106	PRO	N-CA-CB	5.36	108.49	102.60	1	2
1	A	18	SER	N-CA-C	5.36	117.34	108.13	10	2
1	A	28	VAL	N-CA-C	5.35	116.19	108.48	4	1
1	A	73	ASP	N-CA-C	5.32	118.28	110.30	3	1
1	A	13	PRO	N-CD-CG	5.32	111.18	103.20	10	1
1	A	93	VAL	CA-C-O	5.30	126.10	120.48	6	1
1	A	92	ASN	N-CA-C	5.30	117.16	108.52	9	1
1	A	85	ALA	O-C-N	-5.30	115.32	121.47	6	1
1	A	39	PHE	CA-C-N	5.29	130.53	122.65	1	1
1	A	39	PHE	C-N-CA	5.29	130.53	122.65	1	1
1	A	59	ILE	CA-CB-CG1	5.29	119.39	110.40	8	2
1	A	91	TYR	CA-C-O	5.29	127.52	121.28	3	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	104	ASN	N-CA-C	5.27	118.86	111.90	9	1
1	A	22	GLY	O-C-N	-5.27	117.99	123.58	3	1
1	A	70	LYS	CA-C-N	5.25	130.42	122.91	5	1
1	A	70	LYS	C-N-CA	5.25	130.42	122.91	5	1
1	A	104	ASN	CB-CA-C	5.25	119.91	111.66	5	1
1	A	34	ALA	O-C-N	5.25	128.94	123.06	8	1
1	A	50	ASP	CA-C-O	-5.25	115.62	121.23	1	1
1	A	103	LYS	CA-C-N	5.25	129.79	122.08	8	2
1	A	103	LYS	C-N-CA	5.25	129.79	122.08	8	2
1	A	51	GLY	N-CA-C	5.25	118.87	111.42	8	1
1	A	84	ASP	CB-CA-C	5.24	119.14	109.71	4	1
1	A	108	ASP	N-CA-C	5.24	118.02	109.59	8	1
1	A	31	ASN	CA-CB-CG	5.23	117.83	112.60	6	1
1	A	33	PRO	O-C-N	-5.22	117.01	123.01	10	1
1	A	96	THR	N-CA-C	5.21	117.17	108.99	5	1
1	A	47	ALA	CA-C-O	-5.20	116.15	122.03	3	1
1	A	35	GLU	CA-C-O	-5.17	115.12	120.70	5	1
1	A	72	THR	OG1-CB-CG2	-5.17	98.96	109.30	5	1
1	A	83	TYR	CA-C-N	5.17	130.92	122.81	6	1
1	A	83	TYR	C-N-CA	5.17	130.92	122.81	6	1
1	A	87	VAL	O-C-N	-5.15	117.33	123.05	7	1
1	A	109	VAL	CB-CA-C	5.14	118.06	110.77	8	1
1	A	18	SER	CA-C-N	5.13	130.63	121.75	9	1
1	A	18	SER	C-N-CA	5.13	130.63	121.75	9	1
1	A	80	GLY	O-C-N	5.13	127.40	122.99	2	1
1	A	26	VAL	O-C-N	-5.12	116.16	122.57	10	1
1	A	38	ILE	CB-CA-C	5.12	117.15	110.96	5	2
1	A	101	PRO	CB-CA-C	-5.11	102.47	110.96	1	1
1	A	74	ASN	O-C-N	5.11	128.73	122.34	10	1
1	A	37	THR	N-CA-C	5.11	117.23	108.90	1	1
1	A	79	TYR	CB-CG-CD1	-5.11	113.13	120.80	7	1
1	A	22	GLY	N-CA-C	5.11	117.50	111.63	4	2
1	A	44	LYS	CA-CB-CG	5.10	124.30	114.10	9	1
1	A	77	GLY	CA-C-N	5.10	131.39	122.82	9	1
1	A	77	GLY	C-N-CA	5.10	131.39	122.82	9	1
1	A	86	PRO	CA-N-CD	-5.10	104.86	112.00	5	1
1	A	28	VAL	CA-C-O	-5.08	115.17	120.76	5	1
1	A	19	TYR	CB-CG-CD2	-5.08	113.17	120.80	10	1
1	A	31	ASN	O-C-N	-5.08	116.20	122.25	2	1
1	A	49	THR	O-C-N	-5.08	116.24	122.34	8	1
1	A	111	CYS	N-CA-CB	-5.08	102.98	111.20	4	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	66	VAL	O-C-N	-5.07	116.91	122.69	2	1
1	A	71	VAL	CG1-CB-CG2	-5.05	99.68	110.80	5	1
1	A	88	GLU	CB-CG-CD	-5.05	104.01	112.60	4	1
1	A	103	LYS	N-CA-C	5.05	117.91	110.59	4	1
1	A	26	VAL	CA-C-O	-5.05	116.31	120.80	1	1
1	A	36	PHE	CA-CB-CG	5.05	118.85	113.80	9	1
1	A	13	PRO	CA-C-O	-5.04	115.64	121.95	7	1
1	A	109	VAL	CA-CB-CG2	5.04	118.97	110.40	7	1
1	A	98	ARG	N-CA-CB	-5.04	104.34	111.84	9	1
1	A	113	GLU	CA-CB-CG	5.03	124.16	114.10	7	1
1	A	23	GLU	CB-CA-C	5.03	119.94	110.63	8	1
1	A	94	ASN	CB-CA-C	-5.03	103.03	110.62	10	1
1	A	86	PRO	N-CA-CB	5.02	108.21	103.19	3	1
1	A	110	LYS	N-CA-CB	5.01	117.31	109.85	1	1

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	87	VAL	Peptide	6
1	A	96	THR	Peptide	6
1	A	19	TYR	Sidechain	5
1	A	91	TYR	Sidechain,Mainchain	5
1	A	79	TYR	Sidechain	4
1	A	50	ASP	Peptide	4
1	A	83	TYR	Sidechain	3
1	A	29	PHE	Sidechain	2
1	A	48	ARG	Sidechain	2
1	A	57	VAL	Mainchain	1
1	A	86	PRO	Peptide	1
1	A	89	GLY	Mainchain	1
1	A	36	PHE	Sidechain	1
1	A	58	ALA	Mainchain,Peptide	1
1	A	103	LYS	Mainchain	1
1	A	24	GLY	Mainchain	1
1	A	105	MET	Peptide	1
1	A	55	PHE	Sidechain	1
1	A	59	ILE	Peptide	1
1	A	16	GLU	Peptide	1
1	A	17	HIS	Sidechain	1

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Mol	Chain	Res	Type	Group	Models (Total)
1	A	32	ALA	Peptide	1
1	A	21	GLU	Peptide	1
1	A	69	ALA	Mainchain	1
1	A	67	VAL	Peptide	1
1	A	92	ASN	Peptide	1
1	A	97	LEU	Mainchain,Peptide	1
1	A	39	PHE	Sidechain	1

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	747	710	710	1±1
All	All	7470	7100	7100	9

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 1.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:85:ALA:HB2	1:A:91:TYR:CE2	0.52	2.39	8	1
1:A:107:ILE:HD12	1:A:107:ILE:C	0.51	2.30	8	1
1:A:24:GLY:HA3	1:A:36:PHE:CD2	0.44	2.47	2	1
1:A:101:PRO:C	1:A:102:ILE:HG23	0.44	2.38	7	1
1:A:19:TYR:O	1:A:39:PHE:CD2	0.44	2.70	7	1
1:A:105:MET:HG3	1:A:106:PRO:HA	0.42	1.92	4	1
1:A:91:TYR:CD2	1:A:111:CYS:SG	0.41	3.13	3	1
1:A:25:LEU:HD21	1:A:36:PHE:CE1	0.41	2.50	6	1
1:A:29:PHE:HA	1:A:112:ILE:O	0.41	2.16	3	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	100/114 (88%)	90±2 (90±2%)	8±2 (8±2%)	2±1 (2±1%)	9	53
All	All	1000/1140 (88%)	899 (90%)	84 (8%)	17 (2%)	9	53

All 6 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	43	THR	5
1	A	47	ALA	4
1	A	45	GLY	3
1	A	113	GLU	2
1	A	42	ASP	2
1	A	26	VAL	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	80/91 (88%)	79±1 (98±1%)	1±1 (2±1%)	55	93
All	All	800/910 (88%)	788 (98%)	12 (2%)	55	93

All 9 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	75	ASN	3
1	A	83	TYR	2
1	A	67	VAL	1
1	A	26	VAL	1
1	A	97	LEU	1
1	A	42	ASP	1
1	A	109	VAL	1
1	A	23	GLU	1
1	A	46	VAL	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

The completeness of assignment taking into account all chemical shift lists is 43% for the well-defined parts and 39% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list*

7.1.1 Bookkeeping

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	556
Number of shifts mapped to atoms	556
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	91	-0.18 ± 0.10	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	82	-0.11 ± 0.23	None needed (< 0.5 ppm)
$^{13}\text{C}'$	93	0.40 ± 0.16	None needed (< 0.5 ppm)
^{15}N	94	-0.23 ± 0.53	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 43%, i.e. 538 atoms were assigned a chemical shift out of a possible 1257. 0 out of 16 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	458/500 (92%)	189/205 (92%)	178/202 (88%)	91/93 (98%)
Sidechain	80/674 (12%)	0/438 (0%)	80/216 (37%)	0/20 (0%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	0/83 (0%)	0/40 (0%)	0/42 (0%)	0/1 (0%)
Overall	538/1257 (43%)	189/683 (28%)	258/460 (56%)	91/114 (80%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 39%, i.e. 556 atoms were assigned a chemical shift out of a possible 1430. 0 out of 17 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	474/566 (84%)	196/232 (84%)	184/228 (81%)	94/106 (89%)
Sidechain	82/739 (11%)	0/481 (0%)	82/237 (35%)	0/21 (0%)
Aromatic	0/125 (0%)	0/64 (0%)	0/54 (0%)	0/7 (0%)
Overall	556/1430 (39%)	196/777 (25%)	266/519 (51%)	94/134 (70%)

7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

7.1.5 Random Coil Index (RCI) plots [i](#)

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition. If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain A:

