



Full wwPDB NMR Structure Validation Report ⓘ

Mar 5, 2026 – 05:59 PM UTC

PDB ID : 2MEZ / pdb_00002mez
BMRB ID : 19028
Title : Flexible anchoring of archaeal MBF1 on ribosomes suggests role as recruitment factor
Authors : Launay, H.; Blombarch, F.; Camilloni, C.; Vendruscolo, M.; van des Oost, J.; Christodoulou, J.
Deposited on : 2013-10-03

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

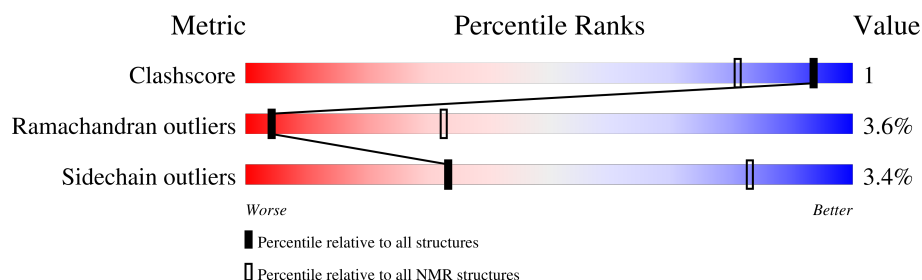
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 30%.

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	106	26% 26% 43% .

2 Ensemble composition and analysis

This entry contains 16 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: *minimized average structure*.

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:23-A:78 (56)	2.54	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 1 single-model cluster was found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1667 atoms, of which 850 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Multiprotein Bridging Factor (MBP-like).

Mol	Chain	Residues	Atoms					Trace
1	A	102	Total	C	H	N	O	0
			1667	514	850	140	163	

There are 8 discrepancies between the modelled and reference sequences:

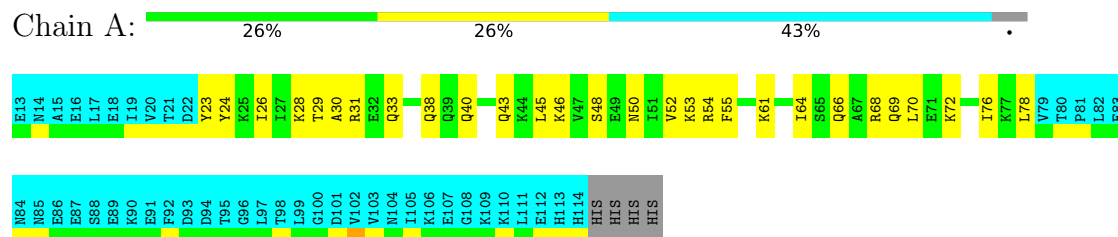
Chain	Residue	Modelled	Actual	Comment	Reference
A	111	LEU	-	expression tag	UNP Q980M2
A	112	GLU	-	expression tag	UNP Q980M2
A	113	HIS	-	expression tag	UNP Q980M2
A	114	HIS	-	expression tag	UNP Q980M2
A	115	HIS	-	expression tag	UNP Q980M2
A	116	HIS	-	expression tag	UNP Q980M2
A	117	HIS	-	expression tag	UNP Q980M2
A	118	HIS	-	expression tag	UNP Q980M2

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: Multiprotein Bridging Factor (MBP-like)

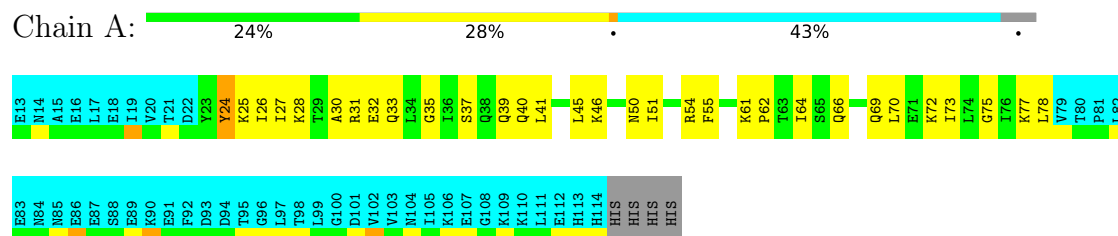


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

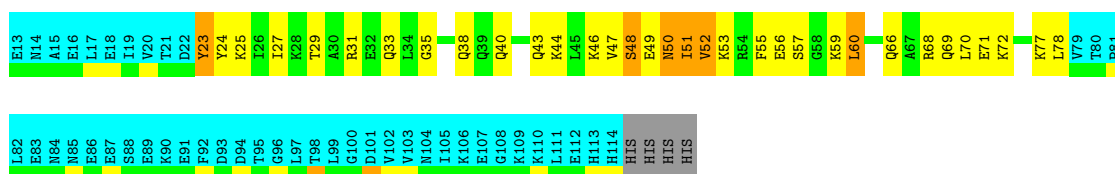
- Molecule 1: Multiprotein Bridging Factor (MBP-like)



4.2.2 Score per residue for model 2

- Molecule 1: Multiprotein Bridging Factor (MBP-like)

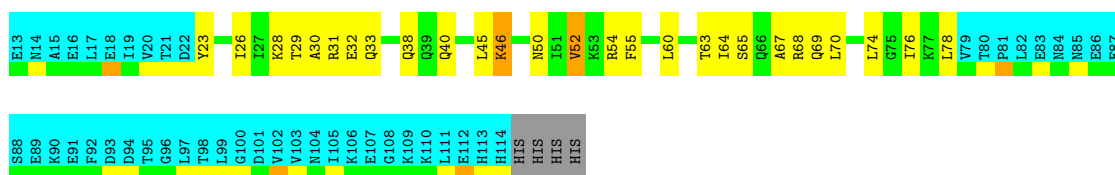




4.2.3 Score per residue for model 3 (medoid)

- Molecule 1: Multiprotein Bridging Factor (MBP-like)

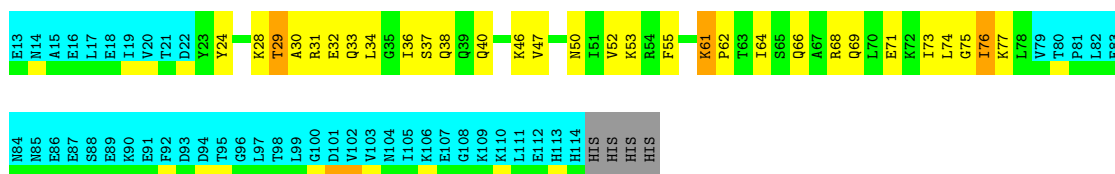
Chain A: 27% 24% 43%



4.2.4 Score per residue for model 4

- Molecule 1: Multiprotein Bridging Factor (MBP-like)

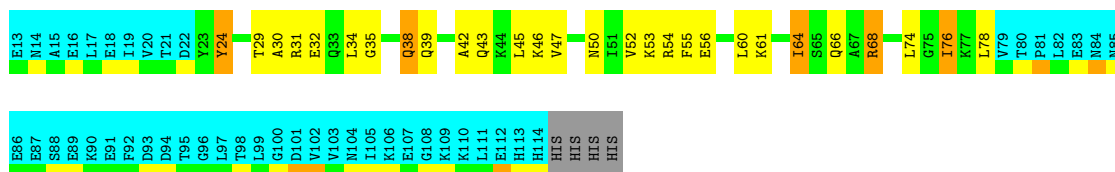
Chain A: 25% 25% 43%



4.2.5 Score per residue for model 5

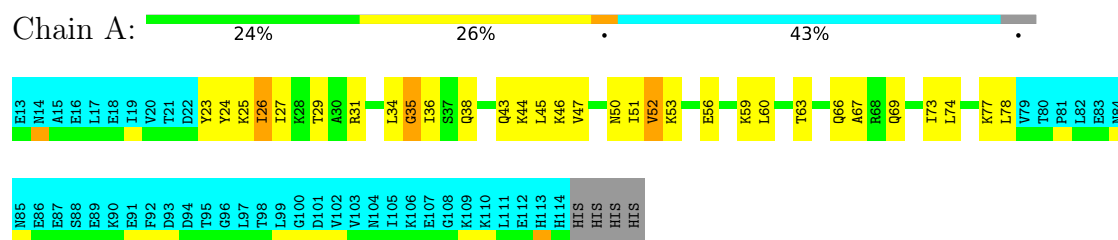
- Molecule 1: Multiprotein Bridging Factor (MBP-like)

Chain A: 26% 22% 5% 43%



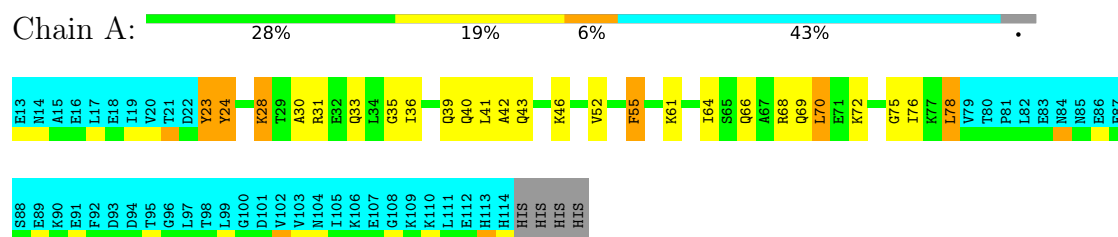
4.2.6 Score per residue for model 6

- Molecule 1: Multiprotein Bridging Factor (MBP-like)



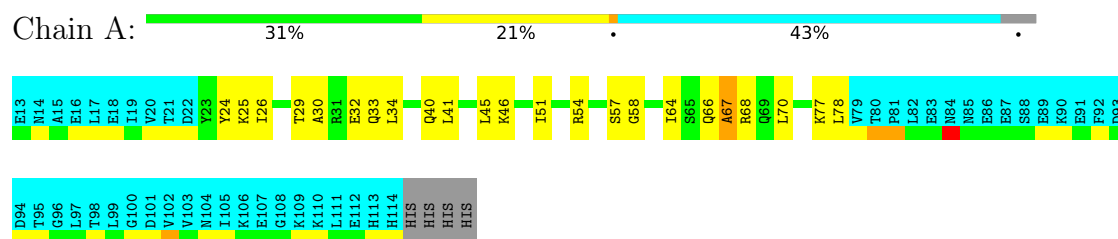
4.2.7 Score per residue for model 7

- Molecule 1: Multiprotein Bridging Factor (MBP-like)



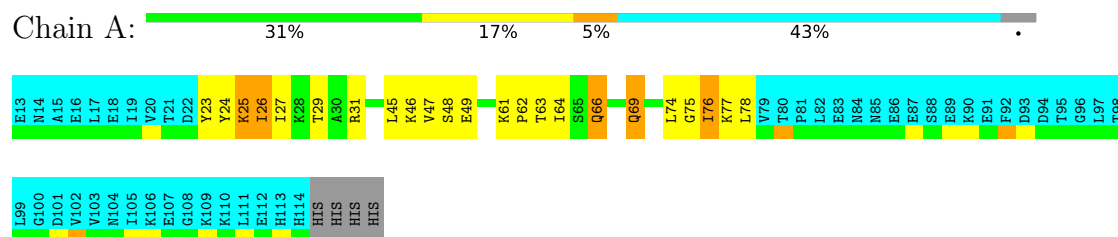
4.2.8 Score per residue for model 8

- Molecule 1: Multiprotein Bridging Factor (MBP-like)



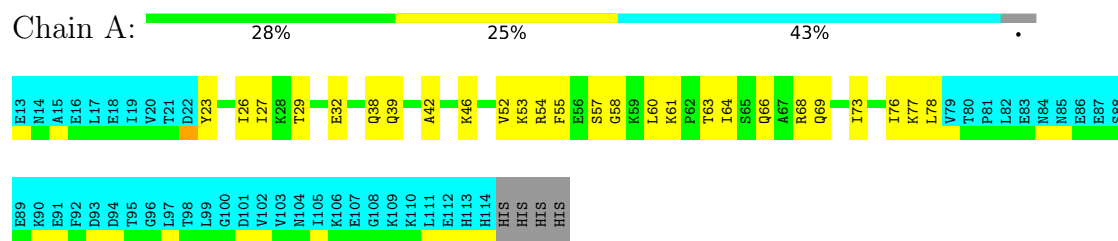
4.2.9 Score per residue for model 9

- Molecule 1: Multiprotein Bridging Factor (MBP-like)



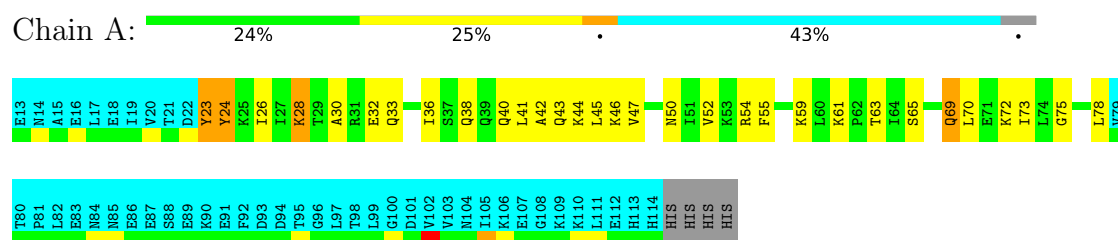
4.2.10 Score per residue for model 10

- Molecule 1: Multiprotein Bridging Factor (MBP-like)



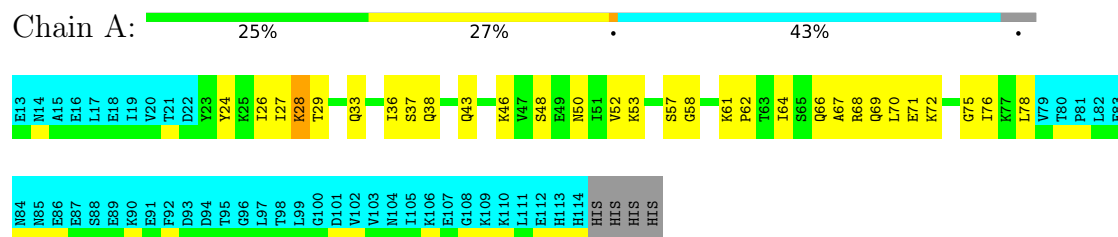
4.2.11 Score per residue for model 11

- Molecule 1: Multiprotein Bridging Factor (MBP-like)



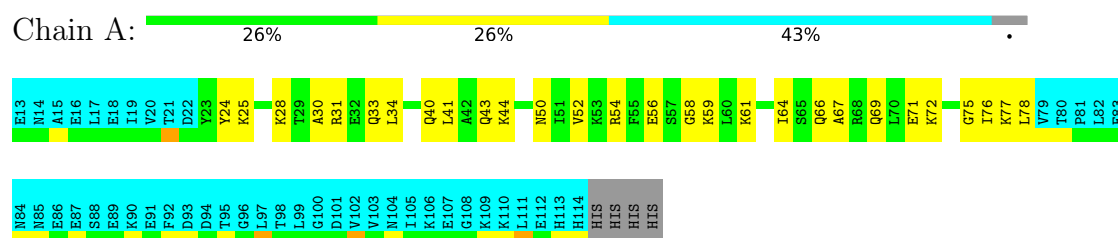
4.2.12 Score per residue for model 12

- Molecule 1: Multiprotein Bridging Factor (MBP-like)



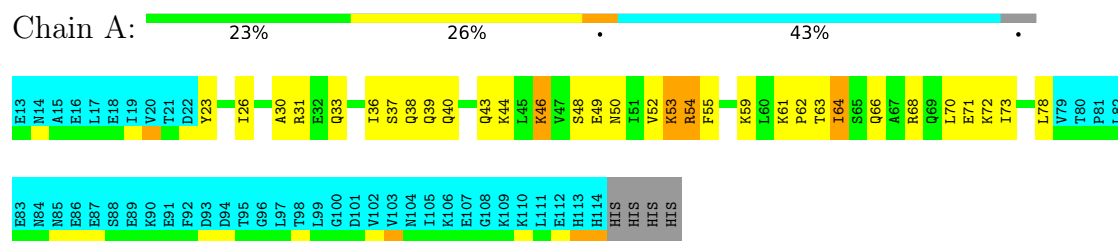
4.2.13 Score per residue for model 13

- Molecule 1: Multiprotein Bridging Factor (MBP-like)



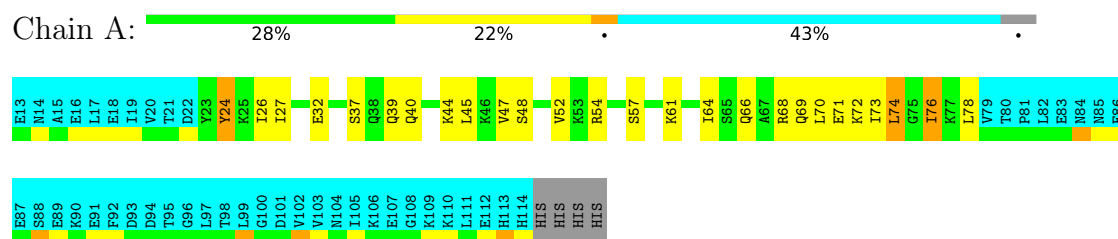
4.2.14 Score per residue for model 14

- Molecule 1: Multiprotein Bridging Factor (MBP-like)



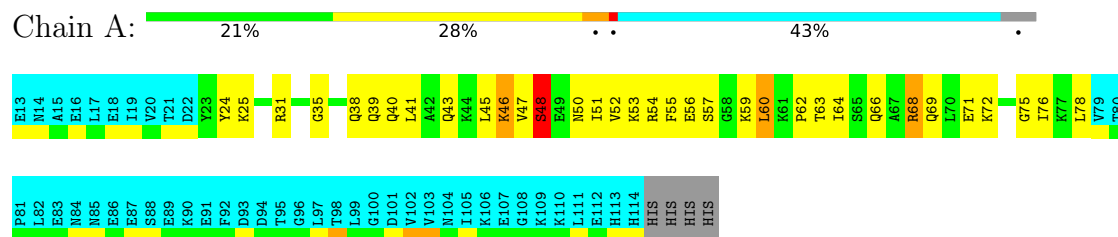
4.2.15 Score per residue for model 15

- Molecule 1: Multiprotein Bridging Factor (MBP-like)



4.2.16 Score per residue for model 16

- Molecule 1: Multiprotein Bridging Factor (MBP-like)



5 Refinement protocol and experimental data overview

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

Of the 1756 calculated structures, 16 were deposited, based on the following criterion: *one structure per cluster*.

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

Software name	Classification	Version
CamShift-MD	refinement	

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	392
Number of shifts mapped to atoms	392
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	30%

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	0.61±0.02	0±0/458 (0.0± 0.0%)	2.63±0.10	39±7/610 (6.3± 1.2%)
All	All	0.61	0/7328 (0.0%)	2.63	619/9760 (6.3%)

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	2.3±1.5
All	All	0	37

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	43	GLN	OE1-CD-NE2	-12.21	110.39	122.60	13	6
1	A	73	ILE	N-CA-C	12.07	122.00	110.42	14	1
1	A	78	LEU	CA-C-N	11.26	141.97	121.70	11	8
1	A	78	LEU	C-N-CA	11.26	141.97	121.70	11	8
1	A	29	THR	CA-CB-OG1	-11.26	92.71	109.60	3	2
1	A	66	GLN	OE1-CD-NE2	-11.06	111.54	122.60	6	9
1	A	36	ILE	N-CA-C	10.63	123.94	109.80	7	3
1	A	51	ILE	CA-C-N	10.44	133.72	120.56	1	1
1	A	51	ILE	C-N-CA	10.44	133.72	120.56	1	1
1	A	68	ARG	NE-CZ-NH2	-10.44	109.80	119.20	12	4
1	A	69	GLN	OE1-CD-NE2	-10.22	112.38	122.60	1	5
1	A	55	PHE	CA-CB-CG	10.15	123.95	113.80	4	9
1	A	28	LYS	N-CA-C	9.79	121.89	111.03	13	3
1	A	64	ILE	CB-CA-C	9.67	124.08	111.70	3	1
1	A	77	LYS	CA-C-O	-9.59	111.10	121.56	9	5

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	54	ARG	NE-CZ-NH2	9.59	127.83	119.20	8	5
1	A	66	GLN	CA-C-O	-9.57	110.31	120.55	5	4
1	A	65	SER	O-C-N	-9.52	111.30	122.15	11	2
1	A	30	ALA	O-C-N	-9.17	112.40	122.12	14	1
1	A	64	ILE	O-C-N	-9.14	112.64	121.87	13	2
1	A	50	ASN	CA-C-N	9.01	137.93	121.70	2	4
1	A	50	ASN	C-N-CA	9.01	137.93	121.70	2	4
1	A	56	GLU	N-CA-C	9.01	123.28	111.75	6	1
1	A	40	GLN	OE1-CD-NE2	-8.82	113.78	122.60	15	5
1	A	48	SER	N-CA-C	8.81	122.44	110.55	9	3
1	A	33	GLN	OE1-CD-NE2	-8.79	113.81	122.60	4	7
1	A	27	ILE	CB-CA-C	8.68	123.85	112.14	10	4
1	A	69	GLN	CA-C-N	8.62	131.65	120.44	12	6
1	A	69	GLN	C-N-CA	8.62	131.65	120.44	12	6
1	A	78	LEU	O-C-N	-8.58	112.00	123.15	5	10
1	A	46	LYS	CA-C-N	8.54	133.16	120.95	3	6
1	A	46	LYS	C-N-CA	8.54	133.16	120.95	3	6
1	A	61	LYS	CA-C-N	8.53	128.48	120.03	15	6
1	A	61	LYS	C-N-CA	8.53	128.48	120.03	15	6
1	A	53	LYS	N-CA-C	8.48	120.52	111.28	2	3
1	A	39	GLN	OE1-CD-NE2	-8.45	114.15	122.60	15	4
1	A	35	GLY	CA-C-N	8.44	133.07	120.75	7	5
1	A	35	GLY	C-N-CA	8.44	133.07	120.75	7	5
1	A	32	GLU	CA-C-O	-8.37	111.55	120.42	3	5
1	A	50	ASN	CA-CB-CG	-8.36	104.24	112.60	3	4
1	A	29	THR	CA-C-N	8.36	133.97	120.60	12	6
1	A	29	THR	C-N-CA	8.36	133.97	120.60	12	6
1	A	45	LEU	CA-C-O	8.35	128.30	118.69	16	3
1	A	71	GLU	CA-C-N	8.34	131.79	120.44	16	1
1	A	71	GLU	C-N-CA	8.34	131.79	120.44	16	1
1	A	50	ASN	OD1-CG-ND2	-8.21	114.39	122.60	14	3
1	A	41	LEU	CA-C-N	8.19	131.60	120.54	11	3
1	A	41	LEU	C-N-CA	8.19	131.60	120.54	11	3
1	A	32	GLU	N-CA-CB	-8.18	98.06	110.16	10	1
1	A	51	ILE	O-C-N	-8.14	113.43	121.90	1	2
1	A	35	GLY	CA-C-O	8.09	127.61	119.04	2	2
1	A	64	ILE	N-CA-CB	8.03	119.94	110.55	9	4
1	A	55	PHE	N-CA-C	-7.96	101.69	111.40	5	2
1	A	38	GLN	OE1-CD-NE2	-7.57	115.03	122.60	4	4
1	A	61	LYS	N-CA-C	7.55	119.16	109.72	11	2
1	A	53	LYS	CA-C-N	7.54	130.69	120.44	14	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	53	LYS	C-N-CA	7.54	130.69	120.44	14	2
1	A	40	GLN	CA-C-O	-7.50	111.62	120.10	16	3
1	A	44	LYS	CA-C-N	7.48	135.20	122.26	13	2
1	A	44	LYS	C-N-CA	7.48	135.20	122.26	13	2
1	A	40	GLN	CA-C-N	7.47	130.29	120.28	7	6
1	A	40	GLN	C-N-CA	7.47	130.29	120.28	7	6
1	A	63	THR	CA-C-N	7.46	130.55	120.77	16	4
1	A	63	THR	C-N-CA	7.46	130.55	120.77	16	4
1	A	50	ASN	N-CA-C	7.43	122.43	111.96	16	4
1	A	66	GLN	CA-C-N	7.40	131.92	120.82	1	5
1	A	66	GLN	C-N-CA	7.40	131.92	120.82	1	5
1	A	30	ALA	N-CA-C	7.35	118.94	111.07	7	4
1	A	75	GLY	CA-C-N	7.35	135.20	121.97	4	4
1	A	75	GLY	C-N-CA	7.35	135.20	121.97	4	4
1	A	64	ILE	CA-C-O	-7.34	113.43	121.29	1	5
1	A	23	TYR	CA-C-N	7.30	131.19	120.90	11	3
1	A	23	TYR	C-N-CA	7.30	131.19	120.90	11	3
1	A	58	GLY	CA-C-O	-7.22	110.19	119.58	12	1
1	A	50	ASN	O-C-N	-7.20	113.69	122.19	16	3
1	A	28	LYS	CA-C-O	-7.15	113.54	120.90	13	2
1	A	24	TYR	O-C-N	-7.13	114.19	122.89	16	1
1	A	68	ARG	NE-CZ-NH1	-7.12	114.39	121.50	4	2
1	A	57	SER	N-CA-C	7.09	121.94	113.28	16	3
1	A	69	GLN	CA-C-O	-7.02	111.51	119.79	13	1
1	A	62	PRO	N-CA-CB	6.98	109.92	103.15	16	2
1	A	44	LYS	CA-CB-CG	-6.95	100.20	114.10	15	1
1	A	52	VAL	CA-C-N	6.92	129.87	120.38	13	5
1	A	52	VAL	C-N-CA	6.92	129.87	120.38	13	5
1	A	27	ILE	CA-C-N	6.92	129.56	120.28	2	6
1	A	27	ILE	C-N-CA	6.92	129.56	120.28	2	6
1	A	47	VAL	CB-CA-C	-6.92	101.66	111.34	6	3
1	A	62	PRO	CB-CA-C	6.90	122.03	111.40	1	2
1	A	31	ARG	NE-CZ-NH1	6.90	128.40	121.50	4	3
1	A	26	ILE	CA-C-N	6.86	129.34	120.56	6	4
1	A	26	ILE	C-N-CA	6.86	129.34	120.56	6	4
1	A	45	LEU	CB-CA-C	6.85	120.92	110.37	5	1
1	A	66	GLN	CB-CG-CD	-6.82	101.01	112.60	7	1
1	A	38	GLN	CA-C-N	6.79	129.27	120.44	16	1
1	A	38	GLN	C-N-CA	6.79	129.27	120.44	16	1
1	A	26	ILE	CA-C-O	-6.75	113.18	120.47	12	3
1	A	24	TYR	CA-C-N	6.69	129.91	120.28	7	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	24	TYR	C-N-CA	6.69	129.91	120.28	7	1
1	A	38	GLN	CA-C-O	-6.66	113.44	120.63	10	2
1	A	45	LEU	CA-C-N	6.66	134.25	121.54	9	6
1	A	45	LEU	C-N-CA	6.66	134.25	121.54	9	6
1	A	54	ARG	NE-CZ-NH1	6.65	128.15	121.50	3	4
1	A	54	ARG	NH1-CZ-NH2	-6.63	110.68	119.30	5	1
1	A	44	LYS	N-CA-C	-6.62	105.17	113.18	11	1
1	A	46	LYS	N-CA-CB	-6.58	101.70	111.71	12	1
1	A	43	GLN	CA-C-O	-6.56	112.42	119.97	7	1
1	A	41	LEU	CB-CA-C	6.52	121.61	110.79	7	3
1	A	70	LEU	CA-C-O	6.52	127.84	121.00	15	4
1	A	24	TYR	N-CA-C	6.51	119.74	109.39	15	4
1	A	31	ARG	CA-C-N	6.49	129.51	120.29	9	5
1	A	31	ARG	C-N-CA	6.49	129.51	120.29	9	5
1	A	71	GLU	O-C-N	-6.49	115.24	122.12	15	3
1	A	66	GLN	N-CA-C	6.49	118.43	111.36	13	2
1	A	28	LYS	CA-C-N	6.40	129.15	120.38	7	3
1	A	28	LYS	C-N-CA	6.40	129.15	120.38	7	3
1	A	33	GLN	CA-C-N	6.39	131.54	120.68	11	1
1	A	33	GLN	C-N-CA	6.39	131.54	120.68	11	1
1	A	37	SER	N-CA-C	6.37	118.94	110.53	1	3
1	A	73	ILE	O-C-N	-6.31	115.33	121.83	6	1
1	A	64	ILE	CB-CG1-CD1	6.30	127.02	113.80	15	1
1	A	43	GLN	CG-CD-NE2	6.29	125.84	116.40	11	2
1	A	59	LYS	O-C-N	6.26	129.85	122.34	14	1
1	A	43	GLN	N-CA-C	-6.25	104.09	111.03	16	2
1	A	52	VAL	CA-CB-CG2	6.22	120.98	110.40	14	1
1	A	31	ARG	O-C-N	-6.22	115.53	122.12	7	2
1	A	73	ILE	CA-C-N	6.21	133.41	121.54	4	3
1	A	73	ILE	C-N-CA	6.21	133.41	121.54	4	3
1	A	25	LYS	N-CA-CB	-6.20	102.06	110.67	13	1
1	A	76	ILE	CA-C-N	6.18	130.65	120.94	9	2
1	A	76	ILE	C-N-CA	6.18	130.65	120.94	9	2
1	A	30	ALA	CA-C-O	-6.17	114.54	120.90	11	2
1	A	44	LYS	CA-C-O	6.15	127.09	120.20	14	2
1	A	53	LYS	CA-C-O	-6.14	114.55	121.00	4	1
1	A	29	THR	CA-CB-CG2	6.13	120.92	110.50	10	2
1	A	52	VAL	N-CA-CB	6.13	117.30	110.62	10	2
1	A	74	LEU	CD1-CG-CD2	-6.12	97.34	110.80	6	1
1	A	42	ALA	CA-C-O	-6.12	114.35	120.90	11	1
1	A	27	ILE	O-C-N	6.11	128.23	121.94	15	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	45	LEU	N-CA-C	-6.09	105.02	112.88	15	2
1	A	66	GLN	CB-CA-C	6.08	120.37	110.95	6	1
1	A	46	LYS	N-CA-C	6.07	123.72	110.80	14	3
1	A	68	ARG	CD-NE-CZ	-6.06	115.92	124.40	3	1
1	A	31	ARG	N-CA-C	-6.05	103.84	111.11	16	2
1	A	67	ALA	CA-C-O	-6.05	114.47	120.82	3	2
1	A	50	ASN	CA-C-O	-6.04	112.45	119.64	2	1
1	A	66	GLN	CG-CD-NE2	6.04	125.45	116.40	7	2
1	A	76	ILE	O-C-N	5.96	127.66	122.12	5	1
1	A	63	THR	CA-CB-OG1	5.96	118.53	109.60	3	1
1	A	34	LEU	N-CA-CB	-5.95	100.42	110.41	6	1
1	A	70	LEU	CA-C-N	5.93	129.03	120.38	7	2
1	A	70	LEU	C-N-CA	5.93	129.03	120.38	7	2
1	A	72	LYS	CB-CA-C	5.92	120.25	110.90	16	1
1	A	31	ARG	CA-C-O	-5.91	114.62	120.82	2	1
1	A	47	VAL	N-CA-C	5.90	115.73	108.53	15	1
1	A	68	ARG	O-C-N	-5.89	115.78	122.08	5	2
1	A	71	GLU	N-CA-C	5.89	117.70	111.28	13	1
1	A	52	VAL	N-CA-C	5.88	118.44	111.09	11	3
1	A	70	LEU	N-CA-C	-5.86	104.48	111.69	11	1
1	A	42	ALA	N-CA-CB	-5.85	101.51	110.12	7	2
1	A	25	LYS	CA-C-O	-5.85	113.00	120.31	16	1
1	A	23	TYR	N-CA-CB	-5.85	101.90	110.26	7	1
1	A	63	THR	CA-CB-CG2	5.83	120.42	110.50	11	1
1	A	76	ILE	N-CA-C	5.81	117.80	108.85	15	2
1	A	25	LYS	O-C-N	-5.79	114.53	122.46	6	3
1	A	40	GLN	O-C-N	5.78	129.75	122.23	13	1
1	A	38	GLN	O-C-N	-5.78	115.99	122.12	6	2
1	A	72	LYS	O-C-N	-5.78	114.39	122.37	1	1
1	A	59	LYS	N-CA-CB	-5.74	101.62	110.46	6	2
1	A	29	THR	O-C-N	5.74	128.06	122.09	8	1
1	A	57	SER	CA-C-O	5.74	126.31	119.60	10	1
1	A	45	LEU	O-C-N	-5.73	115.44	122.20	3	1
1	A	46	LYS	CA-C-O	-5.73	113.70	120.81	6	1
1	A	32	GLU	N-CA-C	5.73	117.20	111.07	4	1
1	A	72	LYS	N-CA-C	5.73	119.45	112.23	15	2
1	A	74	LEU	CA-C-O	5.72	126.54	119.79	3	1
1	A	30	ALA	N-CA-CB	-5.70	101.52	110.06	8	2
1	A	56	GLU	O-C-N	5.68	128.67	122.20	5	1
1	A	51	ILE	N-CA-C	5.67	116.45	110.72	6	1
1	A	61	LYS	CB-CA-C	5.67	115.54	110.44	13	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	60	LEU	N-CA-C	5.66	118.43	108.75	2	2
1	A	27	ILE	CA-C-O	-5.64	115.25	121.29	15	1
1	A	37	SER	CA-C-N	5.64	128.15	120.54	12	1
1	A	37	SER	C-N-CA	5.64	128.15	120.54	12	1
1	A	38	GLN	N-CA-C	-5.63	105.14	111.28	3	2
1	A	64	ILE	CA-C-N	5.63	127.76	120.44	13	1
1	A	64	ILE	C-N-CA	5.63	127.76	120.44	13	1
1	A	68	ARG	CA-C-O	-5.63	114.90	120.70	4	2
1	A	48	SER	N-CA-CB	-5.62	103.56	110.98	16	2
1	A	23	TYR	N-CA-C	5.62	118.38	110.23	11	1
1	A	69	GLN	O-C-N	-5.60	114.73	122.46	16	1
1	A	24	TYR	N-CA-CB	-5.59	102.40	110.45	1	1
1	A	25	LYS	N-CA-C	5.59	119.20	112.38	9	2
1	A	63	THR	N-CA-C	5.58	117.73	110.53	16	1
1	A	39	GLN	CB-CA-C	5.58	120.04	110.79	10	1
1	A	76	ILE	CB-CG1-CD1	-5.57	102.11	113.80	3	1
1	A	50	ASN	N-CA-CB	-5.57	101.65	110.28	13	1
1	A	58	GLY	O-C-N	-5.56	115.42	122.32	13	1
1	A	54	ARG	CA-C-O	-5.55	114.99	120.70	14	1
1	A	32	GLU	CA-CB-CG	-5.54	103.02	114.10	15	1
1	A	47	VAL	O-C-N	-5.52	117.09	123.00	16	2
1	A	36	ILE	CA-C-O	-5.50	116.02	122.13	14	1
1	A	32	GLU	CA-C-N	5.48	128.64	120.31	8	1
1	A	32	GLU	C-N-CA	5.48	128.64	120.31	8	1
1	A	71	GLU	CA-C-O	5.47	126.07	119.61	14	1
1	A	41	LEU	CA-C-O	5.47	126.31	120.24	8	1
1	A	62	PRO	CA-C-N	5.47	130.84	121.87	12	1
1	A	62	PRO	C-N-CA	5.47	130.84	121.87	12	1
1	A	28	LYS	CB-CA-C	5.46	119.41	110.95	3	1
1	A	60	LEU	CD1-CG-CD2	-5.44	98.83	110.80	16	2
1	A	36	ILE	O-C-N	-5.42	116.77	122.57	12	3
1	A	76	ILE	CA-C-O	-5.42	114.00	120.78	10	3
1	A	61	LYS	CA-C-O	-5.42	114.94	119.76	7	1
1	A	64	ILE	N-CA-C	5.42	115.86	110.23	10	1
1	A	67	ALA	CA-C-N	5.41	127.47	120.44	8	1
1	A	67	ALA	C-N-CA	5.41	127.47	120.44	8	1
1	A	56	GLU	CB-CG-CD	-5.41	103.41	112.60	5	1
1	A	48	SER	O-C-N	5.40	127.65	121.93	2	3
1	A	78	LEU	N-CA-C	5.39	117.46	108.99	2	2
1	A	54	ARG	CA-C-N	5.39	129.80	120.58	13	1
1	A	54	ARG	C-N-CA	5.39	129.80	120.58	13	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	63	THR	N-CA-CB	-5.37	102.73	111.22	9	1
1	A	76	ILE	CB-CA-C	-5.35	103.20	110.90	7	1
1	A	57	SER	O-C-N	5.31	128.66	122.24	8	1
1	A	52	VAL	CA-C-O	-5.29	115.17	121.05	12	2
1	A	33	GLN	CB-CA-C	5.28	120.40	110.63	7	1
1	A	39	GLN	CG-CD-NE2	5.28	124.32	116.40	15	1
1	A	71	GLU	CB-CA-C	5.27	119.25	110.81	12	1
1	A	49	GLU	CB-CG-CD	5.27	121.56	112.60	2	1
1	A	57	SER	N-CA-CB	-5.27	101.64	110.39	15	1
1	A	74	LEU	N-CA-C	5.27	117.10	111.36	15	1
1	A	33	GLN	CG-CD-NE2	5.26	124.29	116.40	3	1
1	A	34	LEU	N-CA-C	-5.25	107.05	113.50	4	1
1	A	36	ILE	CA-CB-CG1	5.24	119.31	110.40	11	2
1	A	26	ILE	CA-CB-CG1	5.23	119.28	110.40	11	1
1	A	69	GLN	N-CA-CB	-5.22	102.44	110.12	9	1
1	A	33	GLN	CA-CB-CG	5.21	124.53	114.10	11	1
1	A	31	ARG	CB-CA-C	5.21	119.38	110.74	5	1
1	A	58	GLY	CA-C-N	5.20	131.50	122.56	8	2
1	A	58	GLY	C-N-CA	5.20	131.50	122.56	8	2
1	A	72	LYS	CA-CB-CG	-5.20	103.71	114.10	13	1
1	A	53	LYS	CG-CD-CE	5.19	123.25	111.30	12	1
1	A	49	GLU	N-CA-C	5.19	118.88	112.54	14	1
1	A	31	ARG	NH1-CZ-NH2	-5.19	112.56	119.30	14	1
1	A	42	ALA	CB-CA-C	5.18	119.39	110.79	10	1
1	A	31	ARG	NE-CZ-NH2	-5.16	114.55	119.20	5	1
1	A	59	LYS	CA-CB-CG	-5.16	103.78	114.10	2	1
1	A	61	LYS	N-CA-CB	-5.16	101.64	110.72	1	1
1	A	67	ALA	N-CA-CB	-5.16	101.78	110.49	6	1
1	A	34	LEU	CA-C-O	5.15	125.70	119.11	13	1
1	A	78	LEU	CA-C-O	5.15	126.48	120.20	15	1
1	A	59	LYS	N-CA-C	5.14	121.31	113.61	2	1
1	A	71	GLU	CB-CG-CD	-5.13	103.88	112.60	4	1
1	A	37	SER	CA-CB-OG	-5.13	100.84	111.10	14	1
1	A	73	ILE	N-CA-CB	5.12	116.19	110.51	10	1
1	A	34	LEU	CA-C-N	5.12	131.44	121.41	5	1
1	A	34	LEU	C-N-CA	5.12	131.44	121.41	5	1
1	A	40	GLN	N-CA-CB	-5.12	102.35	110.28	8	1
1	A	54	ARG	CD-NE-CZ	5.11	131.56	124.40	11	1
1	A	23	TYR	O-C-N	-5.10	116.60	122.87	6	2
1	A	24	TYR	CA-C-O	5.10	126.87	121.16	16	1
1	A	26	ILE	N-CA-C	5.08	119.91	109.34	9	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	47	VAL	CA-CB-CG2	5.07	119.02	110.40	11	1
1	A	72	LYS	CA-C-O	-5.06	113.82	120.00	7	1
1	A	59	LYS	CA-C-N	5.06	130.84	122.33	11	2
1	A	59	LYS	C-N-CA	5.06	130.84	122.33	11	2
1	A	27	ILE	N-CA-CB	5.05	116.12	110.62	15	1
1	A	43	GLN	CB-CA-C	5.04	119.16	110.79	14	1
1	A	52	VAL	CB-CA-C	5.04	118.64	112.04	6	1
1	A	33	GLN	O-C-N	5.03	127.45	122.12	13	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	24	TYR	Sidechain,Peptide	8
1	A	23	TYR	Sidechain	5
1	A	68	ARG	Sidechain	4
1	A	56	GLU	Peptide	3
1	A	31	ARG	Sidechain	2
1	A	60	LEU	Peptide	2
1	A	77	LYS	Peptide	1
1	A	44	LYS	Peptide	1
1	A	47	VAL	Peptide	1
1	A	52	VAL	Peptide	1
1	A	70	LEU	Peptide	1
1	A	55	PHE	Sidechain	1
1	A	78	LEU	Peptide	1
1	A	34	LEU	Mainchain	1
1	A	25	LYS	Peptide	1
1	A	66	GLN	Peptide	1
1	A	54	ARG	Sidechain	1
1	A	73	ILE	Mainchain	1
1	A	48	SER	Mainchain	1

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	454	506	506	1±2
All	All	7264	8096	8096	20

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:48:SER:C	1:A:52:VAL:H	0.82	1.82	16	2
1:A:50:ASN:H	1:A:51:ILE:C	0.54	2.11	2	1
1:A:69:GLN:C	1:A:72:LYS:H	0.53	2.12	2	2
1:A:61:LYS:HB2	1:A:62:PRO:HD2	0.52	1.81	4	1
1:A:64:ILE:C	1:A:66:GLN:N	0.48	2.69	4	1
1:A:48:SER:CA	1:A:52:VAL:H	0.46	2.23	2	1
1:A:63:THR:H	1:A:66:GLN:HB2	0.45	1.72	10	1
1:A:61:LYS:HB2	1:A:62:PRO:CD	0.45	2.41	4	1
1:A:64:ILE:HD12	1:A:64:ILE:H	0.44	1.73	14	1
1:A:74:LEU:C	1:A:76:ILE:H	0.44	2.21	5	2
1:A:64:ILE:C	1:A:66:GLN:H	0.43	2.21	4	1
1:A:23:TYR:HD1	1:A:60:LEU:H	0.43	1.54	2	1
1:A:75:GLY:O	1:A:76:ILE:HG23	0.43	2.14	16	1
1:A:61:LYS:CB	1:A:62:PRO:HD2	0.42	2.45	4	1
1:A:70:LEU:C	1:A:72:LYS:H	0.42	2.23	14	1
1:A:61:LYS:CB	1:A:62:PRO:CD	0.41	2.97	4	1
1:A:48:SER:C	1:A:52:VAL:N	0.40	2.67	2	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	56/106 (53%)	49±3 (87±5%)	5±2 (10±4%)	2±1 (4±2%)	4	32
All	All	896/1696 (53%)	777 (87%)	87 (10%)	32 (4%)	4	32

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	46	LYS	7
1	A	75	GLY	3
1	A	28	LYS	3
1	A	74	LEU	2
1	A	76	ILE	2
1	A	35	GLY	2
1	A	67	ALA	2
1	A	25	LYS	1
1	A	78	LEU	1
1	A	61	LYS	1
1	A	64	ILE	1
1	A	24	TYR	1
1	A	53	LYS	1
1	A	77	LYS	1
1	A	70	LEU	1
1	A	26	ILE	1
1	A	38	GLN	1
1	A	54	ARG	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	50/96 (52%)	48±1 (97±3%)	2±1 (3±3%)	33	83
All	All	800/1536 (52%)	773 (97%)	27 (3%)	33	83

All 17 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	26	ILE	4
1	A	52	VAL	3
1	A	51	ILE	2
1	A	46	LYS	2
1	A	39	GLN	2
1	A	60	LEU	2
1	A	24	TYR	2
1	A	33	GLN	1

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Mol	Chain	Res	Type	Models (Total)
1	A	71	GLU	1
1	A	29	THR	1
1	A	76	ILE	1
1	A	38	GLN	1
1	A	68	ARG	1
1	A	64	ILE	1
1	A	77	LYS	1
1	A	49	GLU	1
1	A	53	LYS	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 30% for the well-defined parts and 27% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

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	392
Number of shifts mapped to atoms	392
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	2

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	82	-0.23 ± 0.15	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	76	-0.12 ± 0.19	None needed (< 0.5 ppm)
$^{13}\text{C}'$	80	-0.31 ± 0.13	None needed (< 0.5 ppm)
^{15}N	77	1.74 ± 0.30	Should be applied

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 30%, i.e. 255 atoms were assigned a chemical shift out of a possible 841. 0 out of 9 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	206/281 (73%)	50/114 (44%)	106/112 (95%)	50/55 (91%)
Sidechain	49/532 (9%)	0/344 (0%)	49/162 (30%)	0/26 (0%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	0/28 (0%)	0/13 (0%)	0/15 (0%)	0/0 (—%)
Overall	255/841 (30%)	50/471 (11%)	155/289 (54%)	50/81 (62%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 27%, i.e. 392 atoms were assigned a chemical shift out of a possible 1442. 0 out of 18 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	316/512 (62%)	77/208 (37%)	162/204 (79%)	77/100 (77%)
Sidechain	76/878 (9%)	0/564 (0%)	76/280 (27%)	0/34 (0%)
Aromatic	0/52 (0%)	0/26 (0%)	0/24 (0%)	0/2 (0%)
Overall	392/1442 (27%)	77/798 (10%)	238/508 (47%)	77/136 (57%)

7.1.4 Statistically unusual chemical shifts ⓘ

The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	25	LYS	CB	58.06	24.03 – 41.47	14.5
1	A	25	LYS	CA	32.76	46.18 – 67.77	-11.2

7.1.5 Random Coil Index (RCI) plots ⓘ

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:

