



Full wwPDB NMR Structure Validation Report ⓘ

Mar 28, 2026 – 12:27 AM UTC

PDB ID : 1SSF / pdb_00001ssf
Title : Solution structure of the mouse 53BP1 fragment (residues 1463-1617)
Authors : Charier, G.; Couprie, J.; Alpha-Bazin, B.; Meyer, V.; Quemeneur, E.; Guerois, R.; Callebaut, I.; Gilquin, B.; Zinn-Justin, S.
Deposited on : 2004-03-24

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

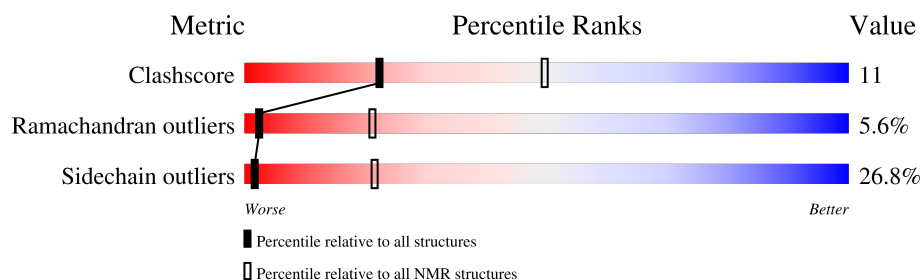
1 Overall quality at a glance

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	156	

2 Ensemble composition and analysis

This entry contains 10 models. Model 9 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 conformer*.

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:71, A:76-A:84, A:92-A:127 (106)	0.69	9

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 1 clusters and 1 single-model cluster was found.

Cluster number	Models
1	1, 2, 3, 4, 5, 6, 7, 9, 10
Single-model clusters	8

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1953 atoms, of which 966 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Transformation related protein 53 binding protein 1.

Mol	Chain	Residues	Atoms						Trace
1	A	123	Total	C	H	N	O	S	0
			1953	631	966	164	189	3	

There is a discrepancy between the modelled and reference sequences:

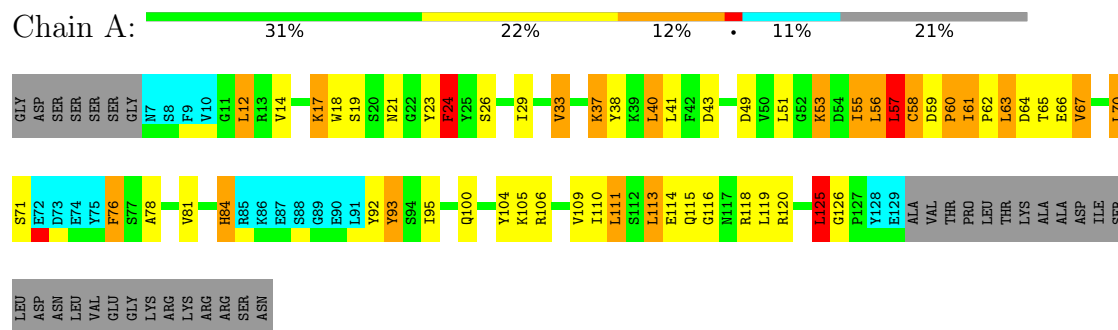
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	cloning artifact	UNP Q91YC9

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: Transformation related protein 53 binding protein 1

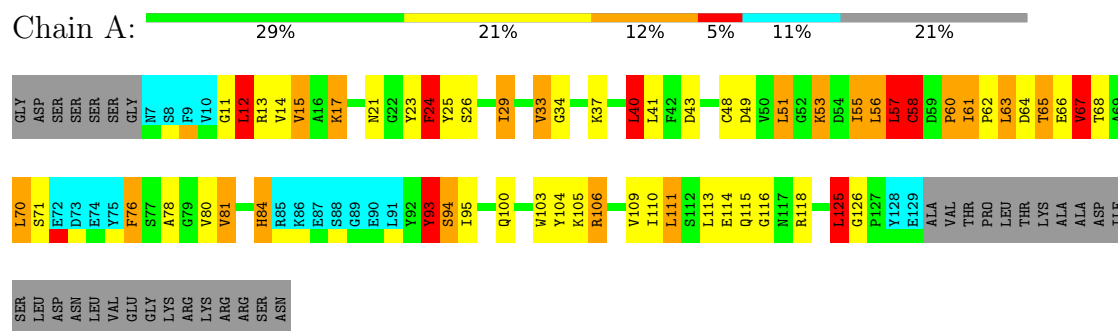


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

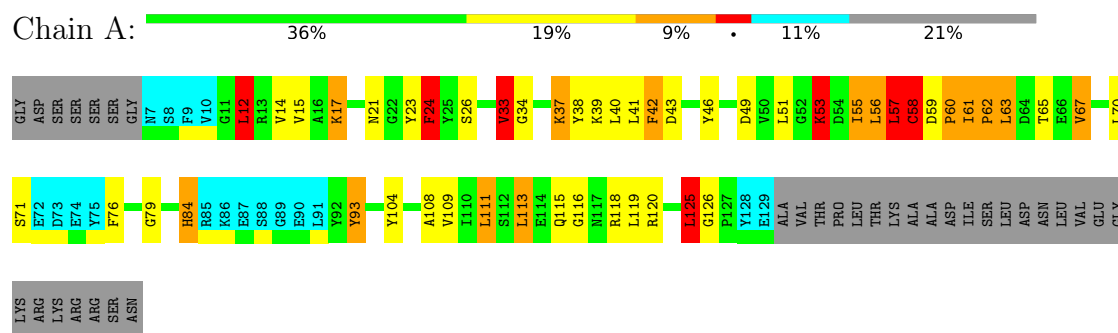
4.2.1 Score per residue for model 1

- Molecule 1: Transformation related protein 53 binding protein 1



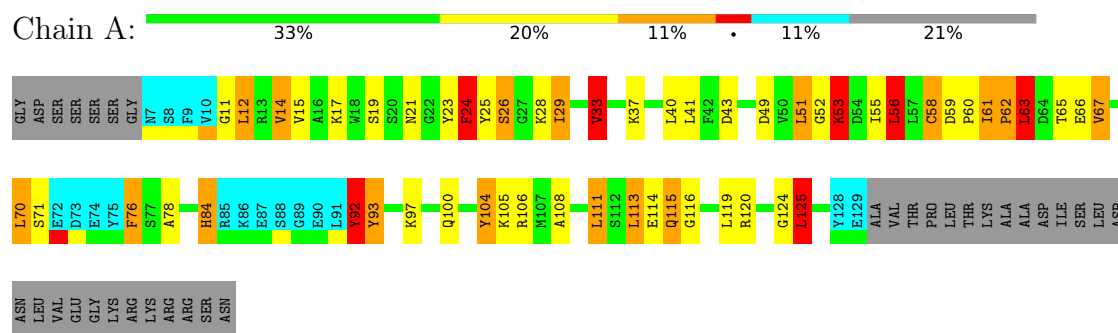
4.2.2 Score per residue for model 2

- Molecule 1: Transformation related protein 53 binding protein 1



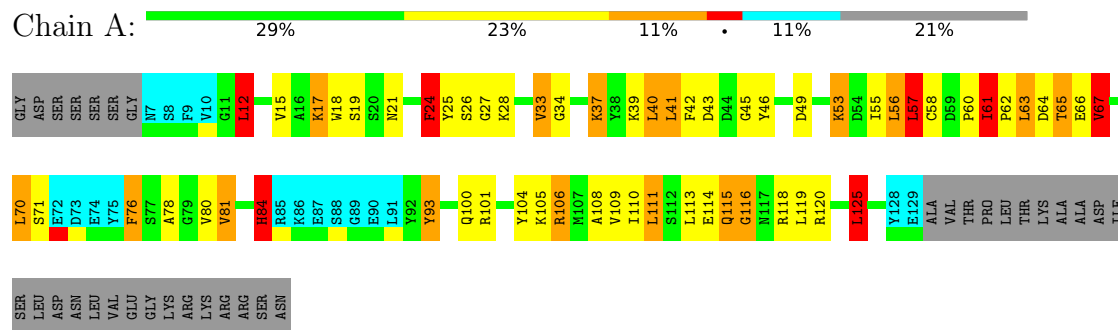
4.2.3 Score per residue for model 3

- Molecule 1: Transformation related protein 53 binding protein 1



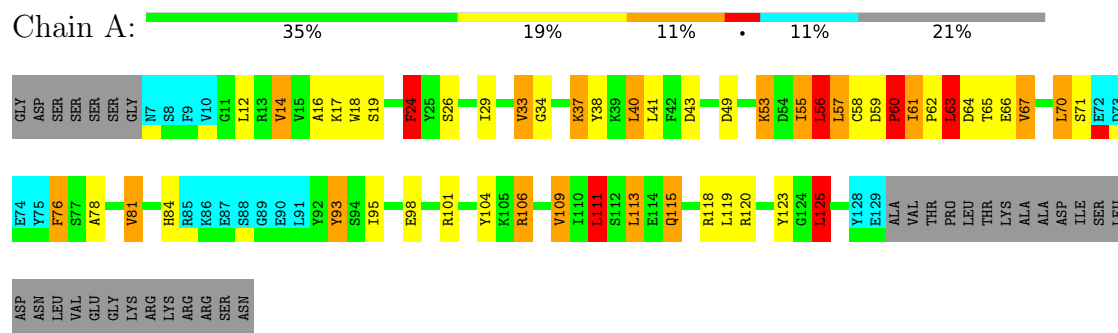
4.2.4 Score per residue for model 4

- Molecule 1: Transformation related protein 53 binding protein 1



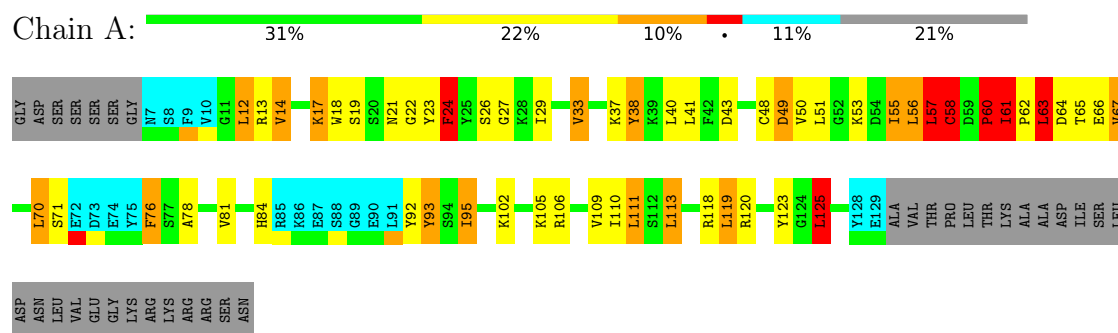
4.2.5 Score per residue for model 5

- Molecule 1: Transformation related protein 53 binding protein 1



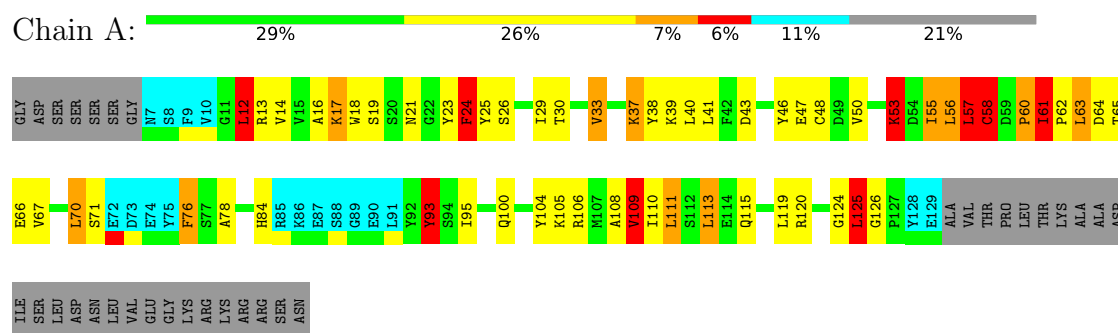
4.2.6 Score per residue for model 6

- Molecule 1: Transformation related protein 53 binding protein 1



4.2.7 Score per residue for model 7

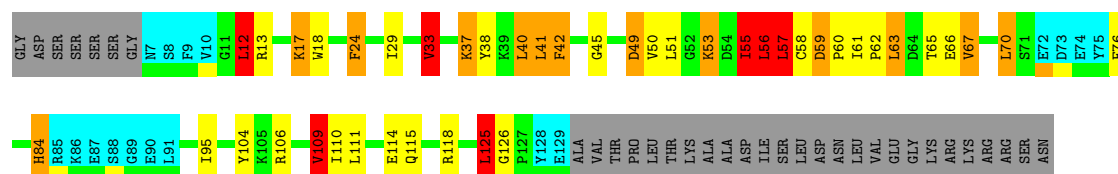
- Molecule 1: Transformation related protein 53 binding protein 1



4.2.8 Score per residue for model 8

- Molecule 1: Transformation related protein 53 binding protein 1

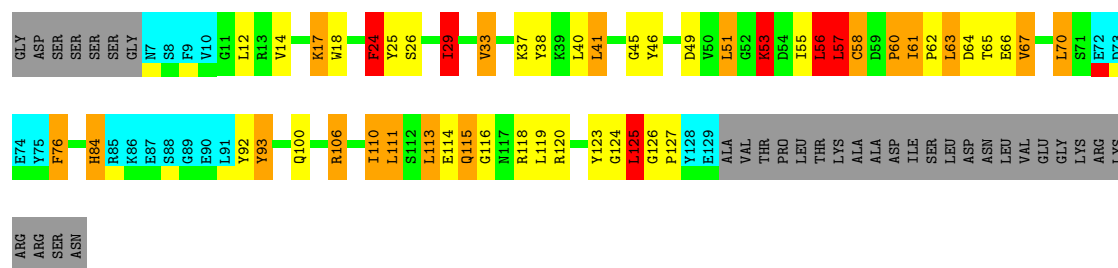




4.2.9 Score per residue for model 9 (medoid)

- Molecule 1: Transformation related protein 53 binding protein 1

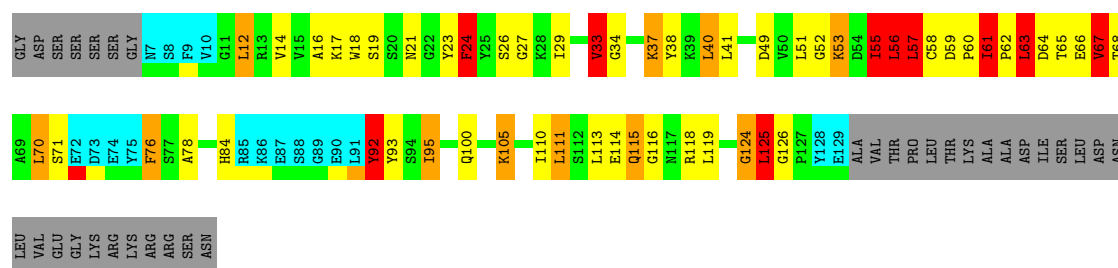
Chain A: 35% 17% 12% 11% 21%



4.2.10 Score per residue for model 10

- Molecule 1: Transformation related protein 53 binding protein 1

Chain A: 31% 23% 7% 6% 11% 21%



5 Refinement protocol and experimental data overview ⓘ

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

Of the 1000 calculated structures, 10 were deposited, based on the following criterion: *back calculated data agree with experimental NOESY spectrum, structures with acceptable covalent geometry, structures with favorable non-bond energy, structures with the least restraint violations, structures with the lowest energy*.

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

Software name	Classification	Version
CNS	refinement	1.0
CNS	structure solution	1.0

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	1.45±0.02	2±1/859 (0.2± 0.1%)	2.35±0.07	53±8/1158 (4.6± 0.7%)
All	All	1.45	17/8590 (0.2%)	2.35	527/11580 (4.6%)

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	4.5±1.1
All	All	0	45

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	65	THR	CA-C	-7.21	1.44	1.52	9	10
1	A	67	VAL	CA-C	-7.04	1.46	1.52	9	4
1	A	59	ASP	CA-C	5.11	1.59	1.52	5	1
1	A	52	GLY	CA-C	-5.07	1.46	1.52	3	1
1	A	40	LEU	CA-C	-5.02	1.46	1.52	5	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	26	SER	CA-C-N	13.24	135.51	121.48	4	6
1	A	26	SER	C-N-CA	13.24	135.51	121.48	4	6
1	A	113	LEU	N-CA-CB	12.90	129.25	110.16	6	9
1	A	66	GLU	CA-C-N	12.40	135.54	122.27	9	8
1	A	66	GLU	C-N-CA	12.40	135.54	122.27	9	8

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	61	ILE	N-CA-CB	-11.37	103.99	111.83	9	7
1	A	56	LEU	N-CA-C	9.77	124.66	109.52	8	10
1	A	58	CYS	CA-C-N	9.65	131.75	119.78	6	1
1	A	58	CYS	C-N-CA	9.65	131.75	119.78	6	1
1	A	70	LEU	CA-C-N	9.57	137.68	122.36	2	10
1	A	70	LEU	C-N-CA	9.57	137.68	122.36	2	10
1	A	53	LYS	CA-C-N	9.57	133.95	121.90	9	8
1	A	53	LYS	C-N-CA	9.57	133.95	121.90	9	8
1	A	62	PRO	CA-C-N	9.51	139.70	121.54	6	10
1	A	62	PRO	C-N-CA	9.51	139.70	121.54	6	10
1	A	115	GLN	CA-C-N	9.50	130.29	119.94	9	8
1	A	115	GLN	C-N-CA	9.50	130.29	119.94	9	8
1	A	62	PRO	N-CA-CB	-9.18	93.61	103.25	5	2
1	A	41	LEU	CB-CA-C	9.15	127.47	109.35	5	10
1	A	65	THR	CA-C-N	9.09	133.63	120.82	5	2
1	A	65	THR	C-N-CA	9.09	133.63	120.82	5	2
1	A	78	ALA	N-CA-C	9.06	122.78	110.55	10	6
1	A	71	SER	N-CA-C	-8.89	95.90	109.14	5	8
1	A	120	ARG	N-CA-C	8.87	122.06	111.33	7	6
1	A	14	VAL	CA-CB-CG2	8.68	125.16	110.40	3	5
1	A	64	ASP	N-CA-CB	-8.64	99.57	110.98	5	7
1	A	63	LEU	CA-C-N	8.56	135.22	121.18	9	7
1	A	63	LEU	C-N-CA	8.56	135.22	121.18	9	7
1	A	24	PHE	CA-C-N	8.47	137.03	122.12	5	9
1	A	24	PHE	C-N-CA	8.47	137.03	122.12	5	9
1	A	21	ASN	CA-CB-CG	8.37	120.97	112.60	2	5
1	A	58	CYS	N-CA-C	-8.34	97.69	109.69	5	2
1	A	63	LEU	N-CA-C	8.17	128.21	110.80	3	10
1	A	105	LYS	N-CA-C	-8.06	97.93	110.42	6	2
1	A	106	ARG	CA-C-N	8.02	131.82	120.28	5	2
1	A	106	ARG	C-N-CA	8.02	131.82	120.28	5	2
1	A	67	VAL	N-CA-CB	7.99	124.41	111.23	3	7
1	A	70	LEU	N-CA-C	7.98	120.64	109.15	10	5
1	A	125	LEU	CD1-CG-CD2	7.96	128.31	110.80	5	1
1	A	26	SER	N-CA-C	7.90	122.12	109.24	5	6
1	A	92	TYR	CA-CB-CG	7.73	127.82	113.90	3	2
1	A	49	ASP	N-CA-C	-7.67	95.80	108.76	5	9
1	A	61	ILE	CA-C-N	7.47	127.92	119.93	1	8
1	A	61	ILE	C-N-CA	7.47	127.92	119.93	1	8
1	A	26	SER	N-CA-CB	-7.43	98.89	110.55	6	3
1	A	11	GLY	CA-C-N	7.42	135.72	121.54	3	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	11	GLY	C-N-CA	7.42	135.72	121.54	3	2
1	A	118	ARG	CA-C-N	7.37	133.19	120.58	9	3
1	A	118	ARG	C-N-CA	7.37	133.19	120.58	9	3
1	A	61	ILE	CB-CA-C	7.30	124.66	111.36	4	4
1	A	60	PRO	N-CA-CB	7.20	110.52	102.60	5	4
1	A	94	SER	N-CA-CB	7.07	121.46	110.21	1	1
1	A	21	ASN	N-CA-CB	-7.06	101.20	110.59	7	3
1	A	109	VAL	CB-CA-C	7.04	119.11	110.73	5	1
1	A	116	GLY	CA-C-N	7.03	131.00	120.31	10	5
1	A	116	GLY	C-N-CA	7.03	131.00	120.31	10	5
1	A	58	CYS	N-CA-CB	-7.01	100.28	110.87	7	7
1	A	56	LEU	CA-C-N	6.91	134.73	121.54	4	8
1	A	56	LEU	C-N-CA	6.91	134.73	121.54	4	8
1	A	29	ILE	N-CA-C	6.88	117.55	110.05	1	2
1	A	19	SER	N-CA-C	-6.85	98.67	109.50	5	6
1	A	76	PHE	CA-CB-CG	6.85	120.65	113.80	1	9
1	A	113	LEU	N-CA-C	6.83	118.38	111.07	4	2
1	A	27	GLY	N-CA-C	6.79	121.01	111.10	4	2
1	A	114	GLU	N-CA-CB	6.78	120.74	110.30	8	1
1	A	80	VAL	N-CA-C	6.72	117.54	107.80	1	2
1	A	58	CYS	CB-CA-C	6.71	122.86	110.24	6	1
1	A	23	TYR	N-CA-C	6.70	119.36	109.24	2	2
1	A	114	GLU	CA-C-N	6.66	131.83	120.71	3	2
1	A	114	GLU	C-N-CA	6.66	131.83	120.71	3	2
1	A	70	LEU	N-CA-CB	6.56	120.24	109.88	2	1
1	A	43	ASP	CA-C-N	6.52	132.46	122.29	1	6
1	A	43	ASP	C-N-CA	6.52	132.46	122.29	1	6
1	A	12	LEU	N-CA-CB	-6.46	101.51	110.29	1	3
1	A	109	VAL	N-CA-CB	6.39	120.27	112.10	8	1
1	A	41	LEU	N-CA-CB	-6.38	99.76	111.37	3	5
1	A	12	LEU	CA-C-N	6.24	131.78	123.05	1	1
1	A	12	LEU	C-N-CA	6.24	131.78	123.05	1	1
1	A	65	THR	N-CA-CB	6.16	120.69	110.47	1	4
1	A	76	PHE	N-CA-C	6.16	118.50	110.43	4	4
1	A	108	ALA	CA-C-N	6.15	131.04	123.17	7	3
1	A	108	ALA	C-N-CA	6.15	131.04	123.17	7	3
1	A	111	LEU	N-CA-C	6.15	118.41	109.07	7	2
1	A	113	LEU	CB-CA-C	-6.12	101.27	110.88	4	3
1	A	118	ARG	N-CA-CB	6.12	118.94	110.07	8	1
1	A	81	VAL	N-CA-CB	6.10	117.18	110.53	5	3
1	A	61	ILE	N-CA-C	6.06	114.57	107.84	1	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	18	TRP	CB-CG-CD2	-6.04	118.35	126.80	5	6
1	A	49	ASP	N-CA-CB	6.02	121.21	110.80	5	2
1	A	78	ALA	CA-C-N	6.01	130.74	121.37	3	2
1	A	78	ALA	C-N-CA	6.01	130.74	121.37	3	2
1	A	12	LEU	N-CA-C	6.00	117.80	110.41	2	1
1	A	12	LEU	CB-CA-C	6.00	122.82	110.40	7	3
1	A	68	THR	CB-CA-C	6.00	119.56	109.48	1	1
1	A	125	LEU	N-CA-C	5.95	123.47	110.80	7	7
1	A	14	VAL	CA-CB-CG1	5.92	120.47	110.40	7	1
1	A	76	PHE	N-CA-CB	5.84	118.53	109.48	9	1
1	A	55	ILE	N-CA-CB	5.83	119.00	111.83	5	1
1	A	28	LYS	O-C-N	-5.83	116.28	123.33	3	1
1	A	55	ILE	CA-CB-CG1	5.76	120.19	110.40	10	2
1	A	12	LEU	CD1-CG-CD2	5.75	123.46	110.80	8	2
1	A	53	LYS	N-CA-C	-5.75	105.57	112.59	5	1
1	A	14	VAL	N-CA-C	5.75	117.13	108.96	1	3
1	A	84	HIS	N-CA-C	5.73	117.98	108.99	8	5
1	A	24	PHE	N-CA-CB	5.70	120.83	111.08	4	4
1	A	16	ALA	N-CA-CB	-5.70	102.18	110.84	5	2
1	A	57	LEU	N-CA-CB	-5.69	100.87	110.49	4	1
1	A	33	VAL	N-CA-CB	5.69	118.62	111.46	3	3
1	A	106	ARG	N-CA-CB	-5.67	100.92	110.49	8	1
1	A	57	LEU	CA-C-O	5.58	128.50	120.51	7	4
1	A	126	GLY	O-C-N	-5.58	116.19	121.77	1	3
1	A	114	GLU	N-CA-C	5.57	119.55	112.87	3	4
1	A	109	VAL	N-CA-C	5.50	116.40	106.61	7	1
1	A	127	PRO	CA-C-N	5.47	131.06	123.07	9	1
1	A	127	PRO	C-N-CA	5.47	131.06	123.07	9	1
1	A	119	LEU	CD1-CG-CD2	-5.42	98.88	110.80	6	1
1	A	84	HIS	CA-CB-CG	5.38	119.18	113.80	9	1
1	A	120	ARG	CA-C-N	5.36	131.09	121.66	2	1
1	A	120	ARG	C-N-CA	5.36	131.09	121.66	2	1
1	A	106	ARG	N-CA-C	5.33	122.15	110.80	1	2
1	A	22	GLY	N-CA-C	-5.31	107.68	114.37	6	1
1	A	40	LEU	N-CA-C	5.28	117.01	109.14	4	2
1	A	70	LEU	CA-C-O	5.28	126.90	120.62	6	3
1	A	65	THR	CA-CB-CG2	5.26	119.44	110.50	5	2
1	A	14	VAL	CA-C-N	5.23	130.28	123.06	2	1
1	A	14	VAL	C-N-CA	5.23	130.28	123.06	2	1
1	A	16	ALA	N-CA-C	5.23	117.24	107.99	10	1
1	A	29	ILE	CA-CB-CG1	5.22	119.28	110.40	9	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	105	LYS	CA-C-N	5.22	131.51	121.54	1	2
1	A	105	LYS	C-N-CA	5.22	131.51	121.54	1	2
1	A	124	GLY	CA-C-N	5.20	131.47	121.54	7	1
1	A	124	GLY	C-N-CA	5.20	131.47	121.54	7	1
1	A	41	LEU	O-C-N	-5.13	117.01	123.27	8	2
1	A	93	TYR	N-CA-CB	5.12	118.97	110.63	7	1
1	A	55	ILE	CA-C-N	5.10	130.47	122.21	2	1
1	A	55	ILE	C-N-CA	5.10	130.47	122.21	2	1
1	A	43	ASP	N-CA-C	5.09	118.96	112.34	3	1
1	A	38	TYR	CA-C-N	5.09	130.34	123.11	2	1
1	A	38	TYR	C-N-CA	5.09	130.34	123.11	2	1
1	A	79	GLY	N-CA-C	-5.07	101.17	113.18	2	1
1	A	57	LEU	CB-CA-C	-5.07	100.34	110.42	2	1
1	A	110	ILE	CA-CB-CG1	5.07	119.01	110.40	9	1
1	A	39	LYS	N-CA-C	-5.06	100.27	108.52	7	2
1	A	111	LEU	CA-C-N	5.06	131.94	121.32	2	1
1	A	111	LEU	C-N-CA	5.06	131.94	121.32	2	1
1	A	33	VAL	CA-C-N	5.05	131.31	121.41	2	2
1	A	33	VAL	C-N-CA	5.05	131.31	121.41	2	2
1	A	42	PHE	CA-CB-CG	5.05	118.85	113.80	2	1
1	A	42	PHE	O-C-N	-5.05	117.03	122.79	8	1
1	A	18	TRP	CB-CG-CD1	5.01	134.42	126.90	5	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	93	TYR	Sidechain	8
1	A	104	TYR	Sidechain	7
1	A	25	TYR	Sidechain	5
1	A	38	TYR	Sidechain	5
1	A	24	PHE	Sidechain	4
1	A	51	LEU	Peptide	4
1	A	46	TYR	Sidechain	4
1	A	92	TYR	Sidechain	4
1	A	123	TYR	Sidechain	3
1	A	23	TYR	Sidechain	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	840	840	840	19±3
All	All	8400	8400	8400	191

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 11.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:56:LEU:HD11	1:A:125:LEU:HD13	0.94	1.37	10	4
1:A:12:LEU:HD11	1:A:57:LEU:CB	0.82	2.05	6	2
1:A:12:LEU:HD11	1:A:57:LEU:HB2	0.81	1.50	2	4
1:A:12:LEU:HD22	1:A:57:LEU:HB2	0.80	1.52	7	1
1:A:24:PHE:CD2	1:A:111:LEU:HD13	0.78	2.13	10	7
1:A:12:LEU:HD22	1:A:13:ARG:H	0.76	1.39	1	2
1:A:12:LEU:HD11	1:A:57:LEU:HA	0.73	1.59	8	1
1:A:56:LEU:HD11	1:A:125:LEU:CD1	0.72	2.13	10	1
1:A:61:ILE:CG1	1:A:111:LEU:HD23	0.72	2.14	5	3
1:A:12:LEU:HD21	1:A:57:LEU:CB	0.71	2.15	9	2
1:A:24:PHE:CD2	1:A:111:LEU:HD11	0.70	2.21	8	1
1:A:56:LEU:HD21	1:A:125:LEU:HA	0.69	1.64	2	5
1:A:61:ILE:HG13	1:A:111:LEU:HD23	0.69	1.61	5	4
1:A:12:LEU:HD22	1:A:13:ARG:N	0.69	2.02	1	1
1:A:12:LEU:HD11	1:A:57:LEU:HB3	0.69	1.62	6	1
1:A:61:ILE:HD12	1:A:119:LEU:HD13	0.66	1.64	4	3
1:A:40:LEU:HD23	1:A:55:ILE:HG21	0.66	1.68	1	3
1:A:33:VAL:HG23	1:A:37:LYS:HB2	0.64	1.68	9	10
1:A:67:VAL:HA	1:A:115:GLN:HE22	0.62	1.53	10	2
1:A:12:LEU:HD23	1:A:29:ILE:HG21	0.61	1.71	9	1
1:A:40:LEU:CD2	1:A:55:ILE:HG21	0.61	2.26	8	3
1:A:104:TYR:HB3	1:A:108:ALA:HB3	0.60	1.73	3	1
1:A:12:LEU:HD21	1:A:57:LEU:HB3	0.60	1.73	5	3
1:A:56:LEU:HD22	1:A:125:LEU:HD13	0.59	1.74	9	2
1:A:84:HIS:CD2	1:A:93:TYR:CZ	0.59	2.90	5	2
1:A:12:LEU:HD21	1:A:57:LEU:HB2	0.58	1.74	9	1
1:A:12:LEU:HD13	1:A:29:ILE:HG13	0.57	1.75	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:56:LEU:CD1	1:A:125:LEU:HD13	0.57	2.24	10	1
1:A:84:HIS:CD2	1:A:93:TYR:CE2	0.56	2.92	3	4
1:A:24:PHE:CG	1:A:111:LEU:HD13	0.56	2.35	5	4
1:A:63:LEU:HA	1:A:81:VAL:HG23	0.55	1.76	5	1
1:A:61:ILE:CD1	1:A:111:LEU:HD23	0.55	2.32	3	3
1:A:52:GLY:O	1:A:56:LEU:HD12	0.55	2.02	10	1
1:A:14:VAL:HG11	1:A:29:ILE:CG2	0.55	2.32	3	1
1:A:12:LEU:HD11	1:A:57:LEU:CA	0.54	2.32	8	1
1:A:24:PHE:CD2	1:A:111:LEU:CD1	0.54	2.91	1	4
1:A:12:LEU:HD23	1:A:13:ARG:N	0.53	2.17	7	1
1:A:61:ILE:HD11	1:A:111:LEU:HD23	0.53	1.80	3	2
1:A:17:LYS:HG2	1:A:24:PHE:CG	0.51	2.40	4	7
1:A:61:ILE:HD12	1:A:115:GLN:O	0.50	2.06	5	1
1:A:24:PHE:CD2	1:A:111:LEU:HD21	0.50	2.41	7	2
1:A:41:LEU:HD21	1:A:45:GLY:HA2	0.50	1.82	4	3
1:A:24:PHE:CE2	1:A:116:GLY:HA3	0.49	2.42	2	1
1:A:61:ILE:HD13	1:A:119:LEU:CD1	0.49	2.38	3	3
1:A:95:ILE:HD12	1:A:109:VAL:HG11	0.49	1.85	1	1
1:A:12:LEU:HD22	1:A:57:LEU:CB	0.49	2.31	7	1
1:A:14:VAL:HG11	1:A:29:ILE:HG23	0.49	1.84	3	1
1:A:56:LEU:HD11	1:A:125:LEU:HA	0.48	1.84	9	2
1:A:61:ILE:HD13	1:A:119:LEU:HD13	0.48	1.85	3	3
1:A:60:PRO:HD2	1:A:93:TYR:CE2	0.48	2.44	9	1
1:A:14:VAL:HG23	1:A:27:GLY:HA3	0.48	1.86	10	1
1:A:62:PRO:CD	1:A:119:LEU:HD12	0.48	2.39	3	1
1:A:17:LYS:HG3	1:A:24:PHE:HA	0.47	1.85	8	1
1:A:41:LEU:HD23	1:A:42:PHE:O	0.47	2.08	8	2
1:A:15:VAL:HG21	1:A:125:LEU:HD21	0.47	1.85	1	1
1:A:12:LEU:HD23	1:A:29:ILE:HG13	0.47	1.87	5	1
1:A:14:VAL:HG11	1:A:29:ILE:CD1	0.47	2.39	6	1
1:A:63:LEU:H	1:A:63:LEU:CD1	0.47	2.21	6	2
1:A:12:LEU:HD21	1:A:57:LEU:HA	0.47	1.85	1	1
1:A:61:ILE:CG2	1:A:65:THR:HG21	0.47	2.40	4	1
1:A:56:LEU:HD11	1:A:125:LEU:HG	0.47	1.87	5	1
1:A:63:LEU:HD12	1:A:63:LEU:H	0.46	1.70	10	1
1:A:14:VAL:HG11	1:A:29:ILE:HG12	0.46	1.87	5	1
1:A:60:PRO:HD2	1:A:93:TYR:CE1	0.46	2.45	6	1
1:A:63:LEU:H	1:A:63:LEU:HD12	0.46	1.70	6	1
1:A:61:ILE:HD11	1:A:116:GLY:HA2	0.45	1.88	4	1
1:A:15:VAL:HG11	1:A:111:LEU:HD21	0.45	1.88	3	1
1:A:12:LEU:CD2	1:A:13:ARG:H	0.45	2.23	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:50:VAL:HG21	1:A:55:ILE:HB	0.45	1.89	8	3
1:A:95:ILE:HD13	1:A:95:ILE:N	0.45	2.26	6	1
1:A:93:TYR:HB3	1:A:109:VAL:HG11	0.45	1.89	5	1
1:A:37:LYS:HB3	1:A:51:LEU:HA	0.45	1.89	8	1
1:A:84:HIS:CG	1:A:93:TYR:CE1	0.45	3.05	6	2
1:A:95:ILE:HG13	1:A:109:VAL:HG11	0.45	1.88	7	1
1:A:61:ILE:HG12	1:A:119:LEU:HD13	0.44	1.89	6	1
1:A:93:TYR:CB	1:A:109:VAL:HG11	0.44	2.41	5	1
1:A:58:CYS:SG	1:A:125:LEU:CD2	0.44	3.06	7	1
1:A:24:PHE:CG	1:A:111:LEU:CD1	0.44	3.01	8	1
1:A:61:ILE:HD11	1:A:111:LEU:HD12	0.44	1.90	2	1
1:A:57:LEU:HD13	1:A:124:GLY:HA2	0.44	1.90	10	1
1:A:12:LEU:CD1	1:A:57:LEU:HB2	0.44	2.41	4	1
1:A:58:CYS:HB3	1:A:60:PRO:HA	0.43	1.89	6	2
1:A:58:CYS:SG	1:A:125:LEU:HD22	0.43	2.53	2	1
1:A:12:LEU:HD13	1:A:29:ILE:CG1	0.43	2.42	6	1
1:A:56:LEU:C	1:A:56:LEU:HD22	0.43	2.37	5	1
1:A:24:PHE:CG	1:A:111:LEU:HD11	0.43	2.47	8	1
1:A:24:PHE:N	1:A:24:PHE:CD1	0.43	2.87	7	4
1:A:33:VAL:HG22	1:A:38:TYR:C	0.43	2.38	7	1
1:A:65:THR:O	1:A:67:VAL:HG22	0.42	2.13	1	1
1:A:94:SER:HB3	1:A:103:TRP:CD2	0.42	2.49	1	1
1:A:60:PRO:O	1:A:119:LEU:HD13	0.42	2.15	5	1
1:A:61:ILE:CG1	1:A:111:LEU:HD13	0.42	2.44	2	1
1:A:12:LEU:HD21	1:A:57:LEU:CA	0.42	2.44	4	1
1:A:95:ILE:HG13	1:A:109:VAL:HG21	0.42	1.91	8	1
1:A:61:ILE:HD11	1:A:111:LEU:CD1	0.42	2.45	2	1
1:A:38:TYR:CE2	1:A:57:LEU:HD12	0.42	2.50	6	1
1:A:119:LEU:CD2	1:A:125:LEU:H	0.41	2.29	4	1
1:A:33:VAL:HG23	1:A:37:LYS:CB	0.41	2.44	6	1
1:A:62:PRO:HD3	1:A:119:LEU:HD12	0.41	1.91	2	1
1:A:14:VAL:HG11	1:A:29:ILE:HD11	0.41	1.92	6	1
1:A:61:ILE:HA	1:A:62:PRO:HD3	0.41	1.77	2	1
1:A:14:VAL:CG1	1:A:29:ILE:HG12	0.41	2.46	6	1
1:A:56:LEU:CD2	1:A:125:LEU:HA	0.41	2.43	2	1
1:A:61:ILE:HD11	1:A:111:LEU:CD2	0.41	2.45	3	1
1:A:17:LYS:HE3	1:A:24:PHE:CE2	0.41	2.50	8	1
1:A:24:PHE:CD1	1:A:24:PHE:N	0.41	2.89	4	1
1:A:61:ILE:HG13	1:A:111:LEU:HD13	0.40	1.91	2	1
1:A:17:LYS:HG2	1:A:24:PHE:CD1	0.40	2.51	10	1
1:A:12:LEU:H	1:A:29:ILE:CG2	0.40	2.29	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:81:VAL:HG21	1:A:93:TYR:CE2	0.40	2.51	6	1
1:A:59:ASP:O	1:A:84:HIS:CE1	0.40	2.75	8	1
1:A:95:ILE:N	1:A:95:ILE:HD13	0.40	2.31	10	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	106/156 (68%)	89±1 (84±1%)	11±1 (10±1%)	6±1 (6±1%)	2	21
All	All	1060/1560 (68%)	892 (84%)	109 (10%)	59 (6%)	2	21

All 11 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	60	PRO	10
1	A	63	LEU	10
1	A	125	LEU	9
1	A	57	LEU	7
1	A	106	ARG	6
1	A	34	GLY	5
1	A	53	LYS	4
1	A	126	GLY	3
1	A	124	GLY	3
1	A	12	LEU	1
1	A	66	GLU	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	88/131 (67%)	64±3 (73±4%)	24±3 (27±4%)	2	21
All	All	880/1310 (67%)	644 (73%)	236 (27%)	2	21

All 52 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	33	VAL	10
1	A	40	LEU	10
1	A	53	LYS	10
1	A	55	ILE	10
1	A	67	VAL	10
1	A	125	LEU	10
1	A	17	LYS	9
1	A	24	PHE	9
1	A	70	LEU	9
1	A	76	PHE	9
1	A	12	LEU	8
1	A	57	LEU	8
1	A	58	CYS	8
1	A	110	ILE	7
1	A	111	LEU	7
1	A	61	ILE	6
1	A	100	GLN	6
1	A	37	LYS	6
1	A	113	LEU	6
1	A	56	LEU	6
1	A	51	LEU	5
1	A	109	VAL	5
1	A	118	ARG	5
1	A	29	ILE	4
1	A	59	ASP	4
1	A	15	VAL	3
1	A	48	CYS	3
1	A	84	HIS	3
1	A	93	TYR	3
1	A	115	GLN	3
1	A	23	TYR	3
1	A	105	LYS	3
1	A	95	ILE	3
1	A	21	ASN	2
1	A	81	VAL	2
1	A	63	LEU	2

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Mol	Chain	Res	Type	Models (Total)
1	A	92	TYR	2
1	A	101	ARG	2
1	A	49	ASP	2
1	A	42	PHE	1
1	A	26	SER	1
1	A	97	LYS	1
1	A	28	LYS	1
1	A	39	LYS	1
1	A	120	ARG	1
1	A	98	GLU	1
1	A	102	LYS	1
1	A	30	THR	1
1	A	47	GLU	1
1	A	106	ARG	1
1	A	18	TRP	1
1	A	68	THR	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 ⓘ

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided