



Full wwPDB NMR Structure Validation Report ⓘ

Mar 5, 2026 – 01:43 PM UTC

PDB ID : 7ELJ / pdb_00007elj
BMRB ID : 36417
Title : Prion Derived Tetrapeptide Stabilizes Thermolabile Insulin via Conformational Trapping
Authors : Banerjee, N.
Deposited on : 2021-04-11

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

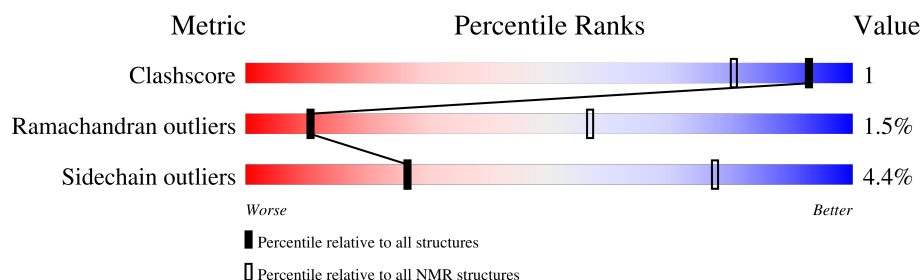
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 42%.

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	21	67% 33%
2	B	30	57% 43%
3	C	4	100%

2 Ensemble composition and analysis

This entry contains 8 models. Model 6 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:1-A:21, B:1-B:30, C:1-C:4 (55)	0.33	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 3 clusters. No single-model clusters were found.

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

3 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 866 atoms, of which 423 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Insulin A Chain.

Mol	Chain	Residues	Atoms						Trace
1	A	21	Total	C	H	N	O	S	0
			309	97	149	25	34	4	

- Molecule 2 is a protein called Insulin B chain.

Mol	Chain	Residues	Atoms						Trace
2	B	30	Total	C	H	N	O	S	0
			472	157	232	40	41	2	

- Molecule 3 is a protein called IS1.

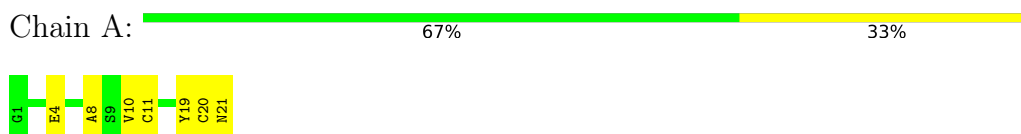
Mol	Chain	Residues	Atoms					Trace
3	C	4	Total	C	H	N	O	0
			85	29	42	7	7	

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.

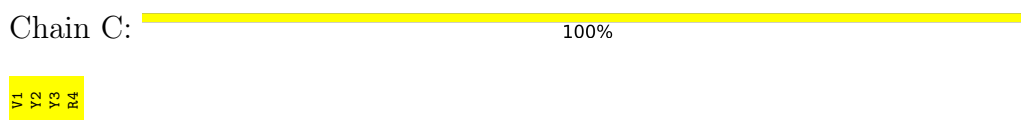
- Molecule 1: Insulin A Chain



- Molecule 2: Insulin B chain



- Molecule 3: IS1

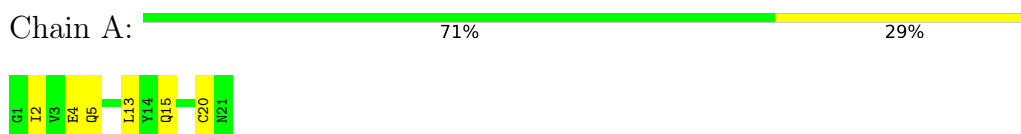


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

- Molecule 1: Insulin A Chain



- Molecule 2: Insulin B chain

Chain B:  60% 37% .



- Molecule 3: IS1

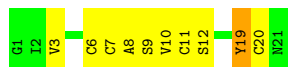
Chain C:  50% 50%



4.2.2 Score per residue for model 2

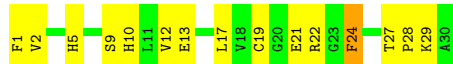
- Molecule 1: Insulin A Chain

Chain A:  52% 43% 5%

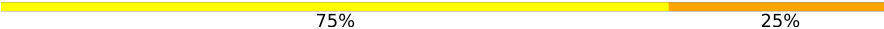


- Molecule 2: Insulin B chain

Chain B:  50% 47% .



- Molecule 3: IS1

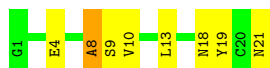
Chain C:  75% 25%



4.2.3 Score per residue for model 3

- Molecule 1: Insulin A Chain

Chain A:  62% 33% 5%



- Molecule 2: Insulin B chain

Chain B:  50% 50%



- Molecule 3: IS1

Chain C:  25% 75%



4.2.4 Score per residue for model 4

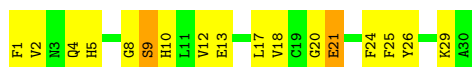
- Molecule 1: Insulin A Chain

Chain A:  62% 33% 5%



- Molecule 2: Insulin B chain

Chain B:  43% 50% 7%



- Molecule 3: IS1

Chain C:  25% 75%



4.2.5 Score per residue for model 5

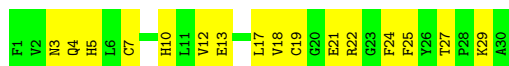
- Molecule 1: Insulin A Chain

Chain A:  43% 48% 10%

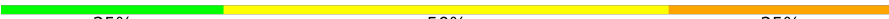


- Molecule 2: Insulin B chain

Chain B:  47% 53%



- Molecule 3: IS1

Chain C:  25% 50% 25%



4.2.6 Score per residue for model 6 (medoid)

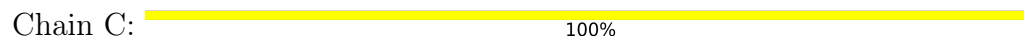
- Molecule 1: Insulin A Chain



- Molecule 2: Insulin B chain



- Molecule 3: IS1



4.2.7 Score per residue for model 7

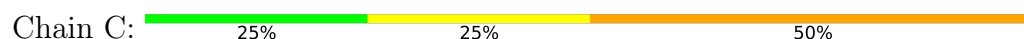
- Molecule 1: Insulin A Chain



- Molecule 2: Insulin B chain



- Molecule 3: IS1



4.2.8 Score per residue for model 8

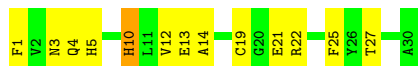
- Molecule 1: Insulin A Chain

Chain A:  67% 29% 5%



- Molecule 2: Insulin B chain

Chain B:  57% 40% 3%



- Molecule 3: IS1

Chain C:  25% 75%



5 Refinement protocol and experimental data overview

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

Of the 10 calculated structures, 8 were deposited, based on the following criterion: *all calculated structures submitted*.

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

Software name	Classification	Version
TopSpin	refinement	3.1
NMRFAM-SPARKY	structure calculation	

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	316
Number of shifts mapped to atoms	314
Number of unparsed shifts	0
Number of shifts with mapping errors	2
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	42%

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	1.90±0.12	3±1/161 (1.9± 0.7%)	2.22±0.14	6±3/216 (2.8± 1.4%)
2	B	1.99±0.08	5±2/247 (2.2± 0.7%)	2.39±0.05	14±3/332 (4.4± 0.9%)
3	C	1.88±0.20	1±1/44 (1.7± 1.5%)	2.30±0.20	3±2/57 (4.8± 3.3%)
All	All	1.95	73/3616 (2.0%)	2.32	187/4840 (3.9%)

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	1.0±1.0
2	B	0.0±0.0	0.8±0.7
3	C	0.0±0.0	0.5±0.5
All	All	0	18

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
2	B	27	THR	CA-C	9.76	1.62	1.52	2	2
2	B	27	THR	CA-CB	8.68	1.62	1.53	8	2
3	C	3	TYR	CA-C	8.14	1.63	1.52	5	1
3	C	4	ARG	CZ-NH2	-7.88	1.23	1.33	2	2
2	B	13	GLU	CA-CB	7.00	1.64	1.53	7	1
2	B	5	HIS	ND1-CE1	6.93	1.39	1.32	2	3
1	A	10	VAL	CA-CB	6.66	1.61	1.54	2	1
2	B	10	HIS	ND1-CE1	6.63	1.39	1.32	1	2
2	B	22	ARG	CZ-NH2	-6.60	1.24	1.33	8	1
2	B	26	TYR	N-CA	6.56	1.55	1.46	6	1
2	B	19	CYS	N-CA	-6.55	1.38	1.46	6	1
2	B	10	HIS	CE1-NE2	6.49	1.39	1.32	4	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	10	VAL	CA-C	6.47	1.60	1.53	6	2
1	A	17	GLU	N-CA	6.35	1.54	1.46	6	3
1	A	11	CYS	CA-C	6.33	1.60	1.52	6	2
2	B	13	GLU	C-O	-6.28	1.16	1.24	4	2
1	A	20	CYS	CA-C	6.28	1.62	1.53	5	2
3	C	2	TYR	CA-C	6.27	1.61	1.52	7	1
1	A	9	SER	CA-C	6.21	1.60	1.52	3	1
2	B	23	GLY	C-N	6.18	1.41	1.33	3	1
2	B	8	GLY	CA-C	6.11	1.58	1.52	4	1
1	A	18	ASN	CA-C	6.04	1.60	1.52	4	2
2	B	12	VAL	N-CA	6.00	1.54	1.46	5	2
1	A	14	TYR	N-CA	5.99	1.53	1.46	7	1
2	B	9	SER	N-CA	5.89	1.53	1.46	7	1
2	B	23	GLY	CA-C	5.89	1.60	1.51	7	1
1	A	3	VAL	N-CA	5.87	1.53	1.46	4	1
2	B	25	PHE	N-CA	-5.65	1.39	1.45	8	1
2	B	21	GLU	N-CA	5.63	1.53	1.46	8	1
2	B	4	GLN	N-CA	5.59	1.52	1.46	8	1
2	B	5	HIS	CE1-NE2	5.59	1.38	1.32	8	1
2	B	5	HIS	N-CA	5.58	1.53	1.46	2	2
2	B	7	CYS	CA-C	5.54	1.59	1.52	5	1
2	B	3	ASN	CA-C	5.48	1.59	1.52	5	1
3	C	4	ARG	N-CA	5.45	1.56	1.46	6	1
1	A	7	CYS	CA-C	5.43	1.60	1.52	7	1
2	B	3	ASN	CA-CB	5.42	1.60	1.53	1	1
1	A	13	LEU	N-CA	5.42	1.53	1.46	3	1
1	A	9	SER	C-N	5.41	1.40	1.33	2	1
1	A	15	GLN	CA-C	5.39	1.59	1.52	6	1
2	B	1	PHE	CG-CD2	5.39	1.50	1.38	8	1
2	B	21	GLU	CA-C	5.35	1.60	1.52	2	1
2	B	18	VAL	N-CA	5.34	1.53	1.46	4	2
2	B	22	ARG	CA-C	5.31	1.59	1.52	2	1
1	A	3	VAL	CA-C	5.29	1.59	1.52	2	1
3	C	4	ARG	CZ-NH1	-5.25	1.25	1.32	6	1
1	A	6	CYS	CA-C	5.23	1.59	1.52	2	1
2	B	22	ARG	N-CA	5.22	1.52	1.46	1	1
1	A	18	ASN	CA-CB	5.20	1.61	1.53	6	1
2	B	14	ALA	CA-CB	-5.18	1.45	1.53	6	1
1	A	19	TYR	N-CA	5.18	1.52	1.46	3	1
2	B	9	SER	CA-CB	5.14	1.61	1.53	6	1
1	A	3	VAL	C-N	5.08	1.41	1.33	8	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
2	B	10	HIS	N-CA	-5.06	1.39	1.46	1	1
2	B	11	LEU	N-CA	5.05	1.52	1.46	1	1
2	B	12	VAL	CA-C	5.02	1.59	1.52	2	1
2	B	15	LEU	CA-CB	5.01	1.61	1.53	1	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
2	B	9	SER	CA-C-N	10.06	135.61	120.31	4	1
2	B	9	SER	C-N-CA	10.06	135.61	120.31	4	1
2	B	24	PHE	CA-CB-CG	9.81	123.61	113.80	5	2
2	B	19	CYS	N-CA-C	9.49	121.39	111.14	8	1
2	B	3	ASN	OD1-CG-ND2	-9.24	113.36	122.60	6	2
2	B	5	HIS	CB-CG-CD2	-8.46	120.20	131.20	7	4
2	B	10	HIS	CA-C-N	8.40	132.06	120.63	7	2
2	B	10	HIS	C-N-CA	8.40	132.06	120.63	7	2
1	A	6	CYS	CA-C-O	-8.33	111.59	120.42	4	1
2	B	17	LEU	CA-C-N	8.12	130.92	122.97	6	3
2	B	17	LEU	C-N-CA	8.12	130.92	122.97	6	3
2	B	4	GLN	OE1-CD-NE2	-7.87	114.73	122.60	7	3
2	B	5	HIS	CB-CG-ND1	7.82	134.43	122.70	7	1
1	A	21	ASN	CA-CB-CG	7.79	120.39	112.60	3	1
2	B	13	GLU	N-CA-C	7.75	119.51	111.14	2	2
1	A	5	GLN	CA-C-N	7.73	130.98	120.54	7	1
1	A	5	GLN	C-N-CA	7.73	130.98	120.54	7	1
1	A	11	CYS	N-CA-CB	-7.71	99.03	111.22	7	2
1	A	5	GLN	OE1-CD-NE2	-7.71	114.89	122.60	1	1
2	B	1	PHE	CA-CB-CG	7.61	121.41	113.80	4	2
1	A	10	VAL	N-CA-C	7.59	118.33	110.05	5	2
1	A	2	ILE	CA-CB-CG1	7.55	123.23	110.40	6	2
2	B	22	ARG	NE-CZ-NH1	7.49	128.99	121.50	5	2
3	C	3	TYR	CA-C-N	7.27	134.79	121.70	1	2
3	C	3	TYR	C-N-CA	7.27	134.79	121.70	1	2
2	B	25	PHE	CA-CB-CG	7.26	121.06	113.80	5	4
1	A	10	VAL	CA-CB-CG2	7.24	122.70	110.40	3	1
1	A	11	CYS	CA-C-O	-7.23	113.15	121.68	8	1
2	B	27	THR	CA-C-N	7.17	127.13	120.03	6	1
2	B	27	THR	C-N-CA	7.17	127.13	120.03	6	1
2	B	10	HIS	CB-CG-CD2	-7.15	121.90	131.20	4	3
1	A	15	GLN	OE1-CD-NE2	-7.09	115.51	122.60	5	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
2	B	7	CYS	O-C-N	-7.05	114.14	122.81	3	1
2	B	18	VAL	CA-C-N	6.96	129.49	120.44	7	1
2	B	18	VAL	C-N-CA	6.96	129.49	120.44	7	1
3	C	2	TYR	CA-C-N	6.92	134.75	121.54	1	4
3	C	2	TYR	C-N-CA	6.92	134.75	121.54	1	4
1	A	11	CYS	CA-C-N	6.88	133.95	122.87	5	1
1	A	11	CYS	C-N-CA	6.88	133.95	122.87	5	1
1	A	9	SER	CA-C-O	-6.88	114.09	121.45	8	1
2	B	14	ALA	O-C-N	-6.69	114.05	122.27	3	1
1	A	2	ILE	CA-C-N	6.61	129.80	120.42	5	1
1	A	2	ILE	C-N-CA	6.61	129.80	120.42	5	1
2	B	12	VAL	CA-CB-CG2	6.58	121.58	110.40	7	1
2	B	8	GLY	O-C-N	-6.57	115.26	122.68	7	2
1	A	13	LEU	CD1-CG-CD2	-6.49	96.52	110.80	1	1
2	B	4	GLN	CA-C-O	-6.39	112.93	120.60	8	1
1	A	8	ALA	N-CA-CB	-6.33	101.91	111.15	2	1
2	B	2	VAL	CA-CB-CG2	6.33	121.15	110.40	4	3
1	A	18	ASN	OD1-CG-ND2	-6.24	116.36	122.60	3	2
2	B	24	PHE	N-CA-C	6.21	118.40	109.14	7	5
3	C	4	ARG	NE-CZ-NH2	6.18	124.77	119.20	8	2
1	A	5	GLN	CA-C-O	-6.18	114.31	120.80	1	1
1	A	12	SER	O-C-N	-6.16	116.07	123.03	2	1
3	C	2	TYR	CB-CG-CD2	6.13	130.00	120.80	2	1
2	B	12	VAL	N-CA-CB	6.11	121.30	111.23	4	1
2	B	5	HIS	CB-CA-C	6.10	119.60	109.53	5	1
3	C	2	TYR	CB-CG-CD1	-6.08	111.68	120.80	2	1
3	C	1	VAL	CA-CB-CG2	6.05	120.69	110.40	5	4
2	B	13	GLU	CA-C-N	6.04	128.69	120.54	8	2
2	B	13	GLU	C-N-CA	6.04	128.69	120.54	8	2
2	B	5	HIS	CE1-NE2-CD2	-6.03	102.97	109.00	2	1
2	B	16	TYR	CA-C-N	6.00	129.14	120.38	1	1
2	B	16	TYR	C-N-CA	6.00	129.14	120.38	1	1
2	B	10	HIS	ND1-CG-CD2	5.98	112.08	106.10	1	2
2	B	27	THR	O-C-N	5.93	126.03	121.23	3	1
2	B	11	LEU	CA-C-O	-5.91	114.62	120.82	3	1
1	A	6	CYS	N-CA-C	5.89	117.70	111.28	5	1
2	B	21	GLU	N-CA-C	5.83	120.09	113.15	1	2
2	B	12	VAL	CB-CA-C	-5.83	103.12	112.16	7	1
2	B	21	GLU	O-C-N	-5.80	114.79	122.33	4	2
2	B	14	ALA	CA-C-N	5.80	128.05	120.28	6	3
2	B	14	ALA	C-N-CA	5.80	128.05	120.28	6	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
3	C	4	ARG	NH1-CZ-NH2	-5.74	111.84	119.30	3	1
2	B	10	HIS	CA-CB-CG	-5.70	108.10	113.80	5	1
2	B	4	GLN	CA-C-N	5.69	130.58	122.72	4	1
2	B	4	GLN	C-N-CA	5.69	130.58	122.72	4	1
2	B	17	LEU	O-C-N	-5.68	114.88	122.43	5	2
2	B	7	CYS	CB-CA-C	5.67	118.57	109.61	6	1
3	C	4	ARG	CB-CA-C	5.64	120.82	110.10	4	1
2	B	22	ARG	N-CA-C	5.60	118.15	111.71	5	3
2	B	7	CYS	N-CA-CB	-5.58	101.83	110.04	3	1
2	B	5	HIS	ND1-CE1-NE2	5.58	113.98	108.40	2	1
1	A	3	VAL	N-CA-C	5.57	118.02	111.05	8	1
1	A	8	ALA	CA-C-O	-5.56	112.95	119.24	3	1
2	B	17	LEU	N-CA-C	5.56	119.16	112.38	3	2
2	B	13	GLU	CA-C-O	-5.53	115.01	120.70	2	1
2	B	18	VAL	CA-CB-CG1	5.53	119.80	110.40	5	2
2	B	5	HIS	CA-CB-CG	5.51	119.31	113.80	6	2
1	A	13	LEU	CB-CA-C	5.50	121.81	110.31	1	2
2	B	10	HIS	CE1-NE2-CD2	-5.47	103.53	109.00	8	1
2	B	25	PHE	CA-C-N	5.46	131.66	122.76	8	1
2	B	25	PHE	C-N-CA	5.46	131.66	122.76	8	1
2	B	10	HIS	ND1-CE1-NE2	5.46	113.86	108.40	8	1
1	A	8	ALA	CA-C-N	5.42	130.73	122.11	6	1
1	A	8	ALA	C-N-CA	5.42	130.73	122.11	6	1
2	B	5	HIS	CA-C-N	5.42	130.59	122.47	4	1
2	B	5	HIS	C-N-CA	5.42	130.59	122.47	4	1
2	B	18	VAL	CA-CB-CG2	-5.41	101.20	110.40	3	1
1	A	17	GLU	CA-C-O	-5.38	114.72	120.42	5	1
1	A	7	CYS	CA-CB-SG	-5.33	102.14	114.40	2	1
2	B	3	ASN	CB-CA-C	5.33	119.03	110.29	1	1
2	B	21	GLU	CA-C-N	5.30	127.82	120.29	1	1
2	B	21	GLU	C-N-CA	5.30	127.82	120.29	1	1
1	A	8	ALA	CB-CA-C	5.29	116.32	109.28	5	1
2	B	22	ARG	NH1-CZ-NH2	-5.29	112.42	119.30	5	1
1	A	20	CYS	O-C-N	-5.29	116.76	122.79	6	1
1	A	19	TYR	CG-CD2-CE2	5.29	129.13	121.20	5	1
2	B	1	PHE	CA-C-N	5.29	129.73	121.85	2	1
2	B	1	PHE	C-N-CA	5.29	129.73	121.85	2	1
1	A	7	CYS	N-CA-CB	-5.26	103.30	110.56	6	1
1	A	10	VAL	CA-CB-CG1	5.23	119.29	110.40	5	1
1	A	5	GLN	O-C-N	-5.20	116.08	122.11	5	1
2	B	20	GLY	CA-C-N	5.20	129.00	120.63	4	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
2	B	20	GLY	C-N-CA	5.20	129.00	120.63	4	1
2	B	3	ASN	CA-CB-CG	-5.15	107.45	112.60	8	1
1	A	4	GLU	CA-C-N	5.11	127.58	120.63	3	1
1	A	4	GLU	C-N-CA	5.11	127.58	120.63	3	1
2	B	4	GLN	CG-CD-NE2	5.05	123.98	116.40	5	1
1	A	19	TYR	CA-C-N	5.03	130.12	120.97	2	1
1	A	19	TYR	C-N-CA	5.03	130.12	120.97	2	1
2	B	25	PHE	N-CA-C	5.03	118.26	110.17	3	1
1	A	3	VAL	CA-C-O	5.02	125.94	120.57	8	1
1	A	10	VAL	CA-C-O	5.01	127.69	122.13	4	1
1	A	13	LEU	O-C-N	-5.01	115.72	122.43	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	20	CYS	Peptide	3
1	A	11	CYS	Peptide	2
1	A	19	TYR	Sidechain	2
2	B	28	PRO	Peptide	2
3	C	2	TYR	Sidechain	2
3	C	4	ARG	Sidechain	1
1	A	8	ALA	Peptide	1
2	B	26	TYR	Sidechain	1
3	C	3	TYR	Sidechain	1
2	B	1	PHE	Sidechain	1
2	B	10	HIS	Mainchain	1
2	B	16	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	160	149	149	1±0
2	B	240	232	232	1±1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes
3	C	43	42	42	0±0
All	All	3544	3384	3384	10

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
2:B:10:HIS:CG	3:C:1:VAL:HG11	0.53	2.39	8	1
1:A:21:ASN:N	1:A:21:ASN:HD22	0.48	2.05	8	1
2:B:19:CYS:SG	2:B:24:PHE:CG	0.47	2.99	2	1
2:B:19:CYS:SG	2:B:24:PHE:CD1	0.46	3.06	2	1
1:A:4:GLU:CD	2:B:29:LYS:H	0.44	2.20	1	3
2:B:2:VAL:CG2	2:B:4:GLN:HE21	0.43	2.26	6	1
3:C:1:VAL:HG12	3:C:2:TYR:CG	0.41	2.50	6	1
1:A:4:GLU:CD	1:A:4:GLU:N	0.40	2.80	6	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	19/21 (90%)	17±1 (91±6%)	2±1 (9±6%)	0±0 (1±2%)	20	70
2	B	28/30 (93%)	25±1 (90±3%)	3±1 (10±3%)	0±0 (0±1%)	31	76
3	C	2/4 (50%)	0±0 (0±0%)	2±0 (75±25%)	0±0 (25±25%)	0	1
All	All	392/440 (89%)	339 (86%)	47 (12%)	6 (2%)	11	57

All 4 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
3	C	3	TYR	3
2	B	29	LYS	1
1	A	8	ALA	1

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Mol	Chain	Res	Type	Models (Total)
3	C	2	TYR	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	19/19 (100%)	18±1 (96±3%)	1±1 (4±3%)	30 80
2	B	25/25 (100%)	24±1 (96±3%)	1±1 (4±3%)	26 77
3	C	4/4 (100%)	4±0 (94±11%)	0±0 (6±11%)	18 67
All	All	384/384 (100%)	367 (96%)	17 (4%)	27 77

All 8 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	21	ASN	4
2	B	9	SER	3
2	B	21	GLU	3
2	B	15	LEU	2
3	C	1	VAL	2
1	A	3	VAL	1
1	A	10	VAL	1
2	B	19	CYS	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.6 Ligand geometry

There are no ligands in this entry.

6.7 Other polymers

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

The completeness of assignment taking into account all chemical shift lists is 42% for the well-defined parts and 42% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *nmr-STAR_DATA_CHEMICAL_SHIFT.txt*

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	316
Number of shifts mapped to atoms	314
Number of unparsed shifts	0
Number of shifts with mapping errors	2
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

The following assigned chemical shifts were not mapped to the molecules present in the coordinate file.

- No matching atom found in the structure. All 2 occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	B	5	HIS	HD1	7.36	0.05	1
1	B	10	HIS	HD1	7.4	0.05	1

7.1.2 Chemical shift referencing

No chemical shift referencing corrections were calculated (not enough data).

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 42%, i.e. 313 atoms were assigned a chemical shift out of a possible 741. 0 out of 12 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	95/277 (34%)	95/113 (84%)	0/110 (0%)	0/54 (0%)
Sidechain	197/366 (54%)	197/240 (82%)	0/113 (0%)	0/13 (0%)
Aromatic	21/98 (21%)	21/47 (45%)	0/49 (0%)	0/2 (0%)
Overall	313/741 (42%)	313/400 (78%)	0/272 (0%)	0/69 (0%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 42%, i.e. 313 atoms were assigned a chemical shift out of a possible 741. 0 out of 12 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	95/277 (34%)	95/113 (84%)	0/110 (0%)	0/54 (0%)
Sidechain	197/366 (54%)	197/240 (82%)	0/113 (0%)	0/13 (0%)
Aromatic	21/98 (21%)	21/47 (45%)	0/49 (0%)	0/2 (0%)
Overall	313/741 (42%)	313/400 (78%)	0/272 (0%)	0/69 (0%)

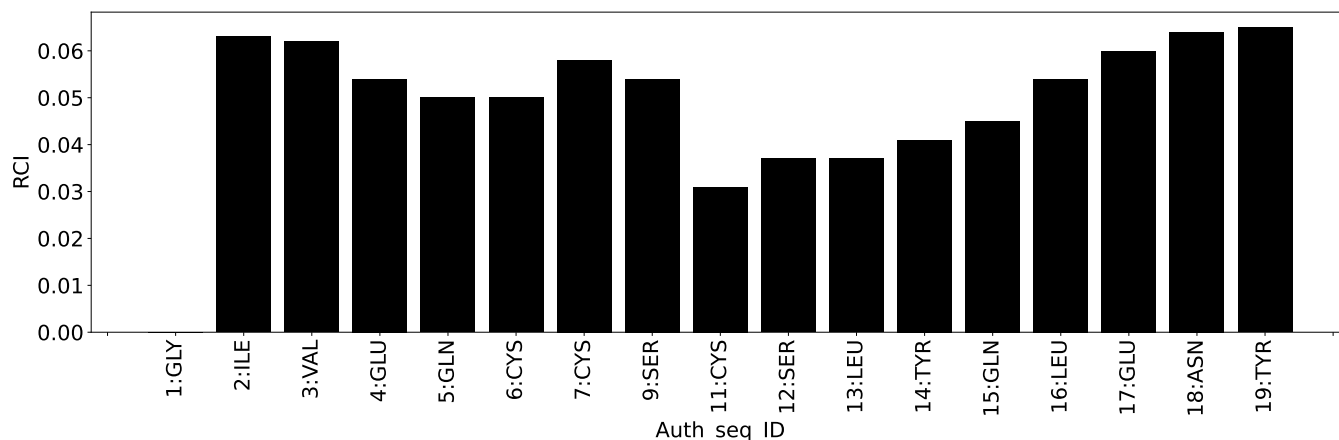
7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

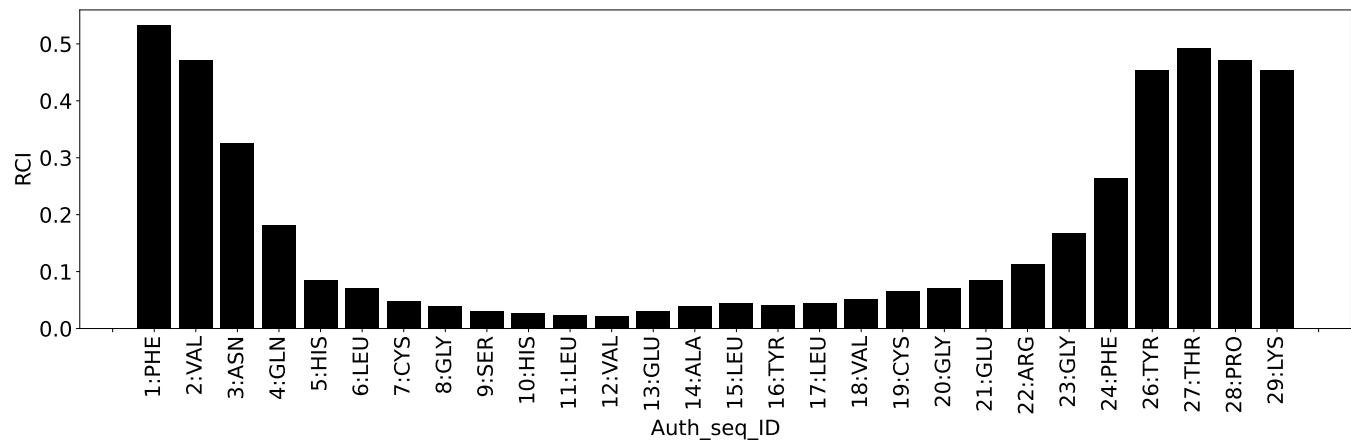
7.1.5 Random Coil Index (RCI) plots [i](#)

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:



Random coil index (RCI) for chain B:



Random coil index (RCI) for chain C:

