



Full wwPDB NMR Structure Validation Report ⓘ

Mar 27, 2026 – 05:37 AM UTC

PDB ID : 2N77 / pdb_00002n77
BMRB ID : 25796
Title : NMR solution structure of a complex of PEP-19 bound to the C-domain of apo calmodulin
Authors : Wang, X.; Putkey, J.A.
Deposited on : 2015-09-04

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

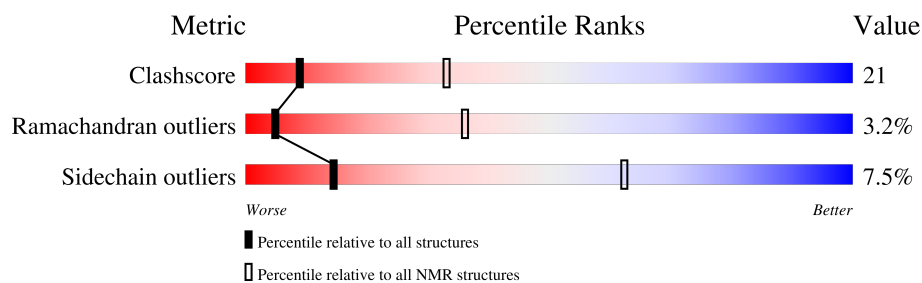
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 89%.

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	73	
2	B	62	

2 Ensemble composition and analysis

This entry contains 20 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: *closest to the average*.

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:81-A:130, A:134-A:145, B:35-B:55 (83)	0.35	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 8 single-model clusters were found.

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

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 1652 atoms, of which 804 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Calmodulin.

Mol	Chain	Residues	Atoms						Trace
1	A	73	Total	C	H	N	O	S	0
			1132	356	546	96	129	5	

- Molecule 2 is a protein called Purkinje cell protein 4.

Mol	Chain	Residues	Atoms						Trace
2	B	33	Total	C	H	N	O	S	0
			520	162	258	47	52	1	

There are 2 discrepancies between the modelled and reference sequences:

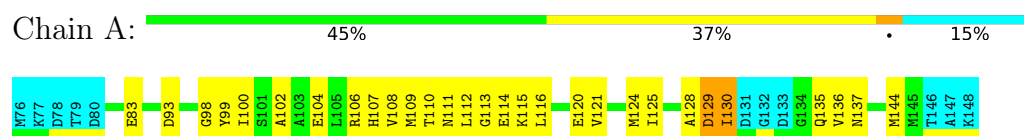
Chain	Residue	Modelled	Actual	Comment	Reference
B	1	MET	-	expression tag	UNP P48539
B	2	ALA	-	expression tag	UNP P48539

4 Residue-property plots [i](#)

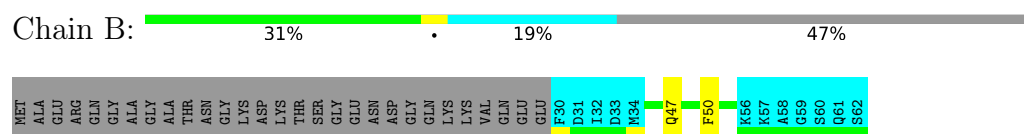
4.1 Average score per residue in the NMR ensemble

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: Calmodulin



• Molecule 2: Purkinje cell protein 4

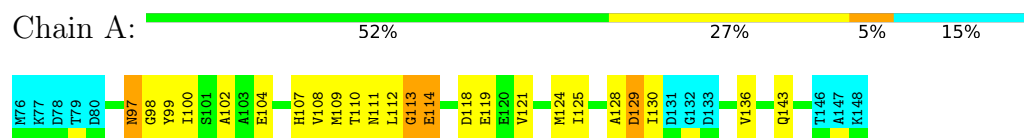


4.2 Scores per residue for each member of the ensemble

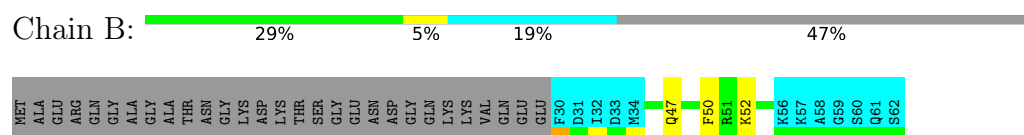
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: Calmodulin

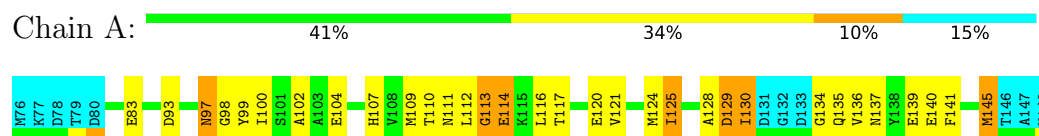


• Molecule 2: Purkinje cell protein 4

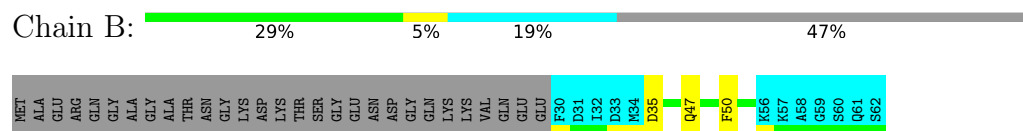


4.2.2 Score per residue for model 2

• Molecule 1: Calmodulin

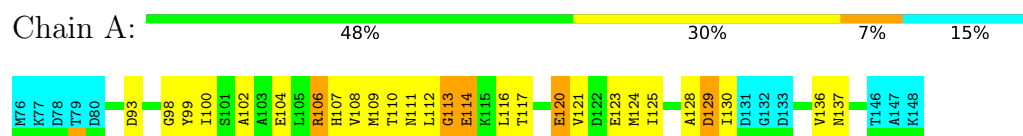


• Molecule 2: Purkinje cell protein 4

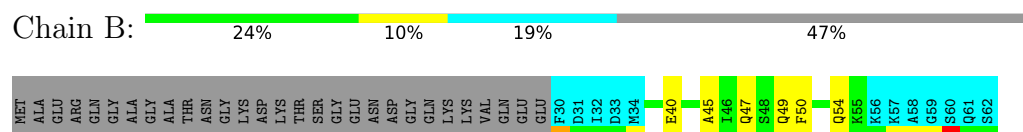


4.2.3 Score per residue for model 3 (medoid)

• Molecule 1: Calmodulin

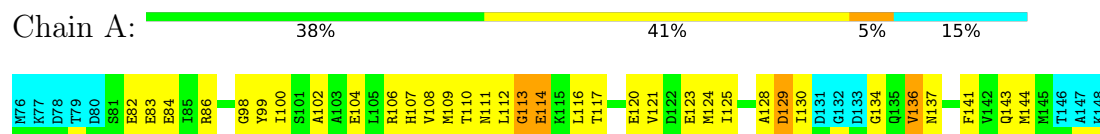


• Molecule 2: Purkinje cell protein 4

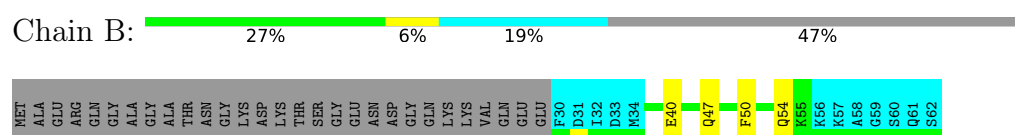


4.2.4 Score per residue for model 4

• Molecule 1: Calmodulin

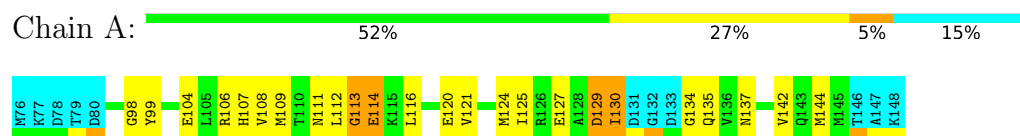


• Molecule 2: Purkinje cell protein 4

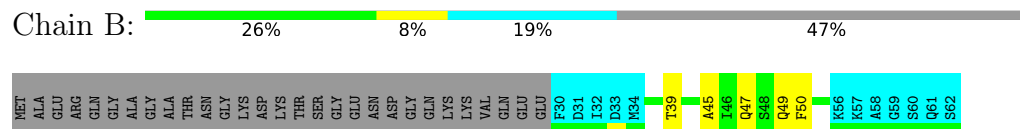


4.2.5 Score per residue for model 5

• Molecule 1: Calmodulin



• Molecule 2: Purkinje cell protein 4

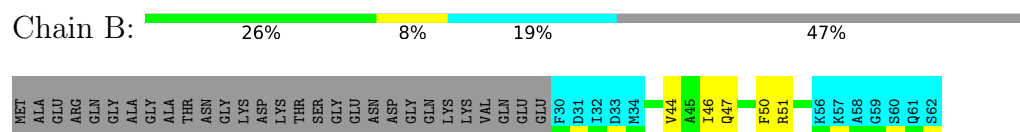


4.2.6 Score per residue for model 6

• Molecule 1: Calmodulin

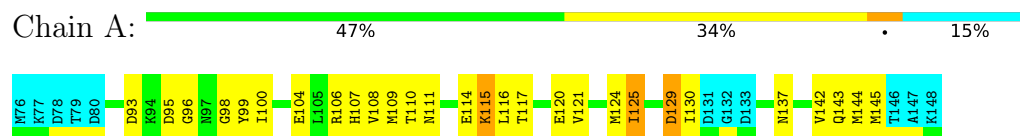


• Molecule 2: Purkinje cell protein 4

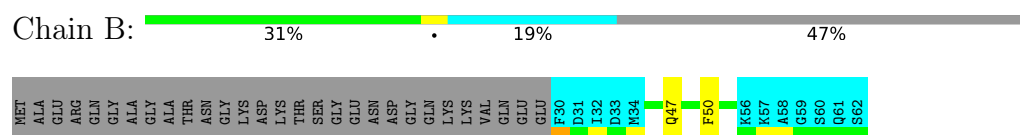


4.2.7 Score per residue for model 7

• Molecule 1: Calmodulin

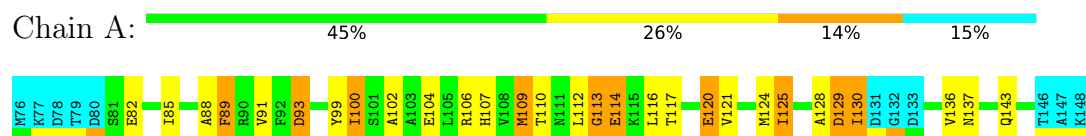


• Molecule 2: Purkinje cell protein 4

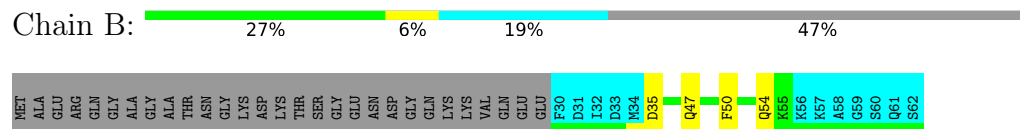


4.2.8 Score per residue for model 8

• Molecule 1: Calmodulin

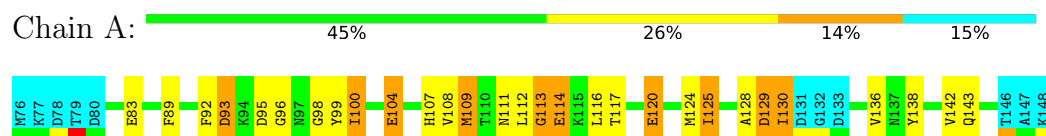


• Molecule 2: Purkinje cell protein 4

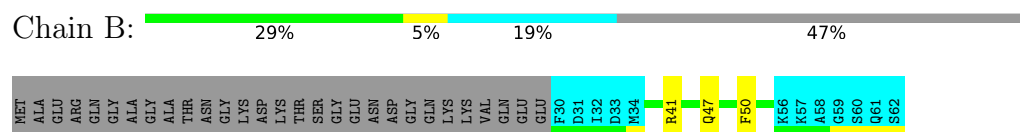


4.2.9 Score per residue for model 9

• Molecule 1: Calmodulin

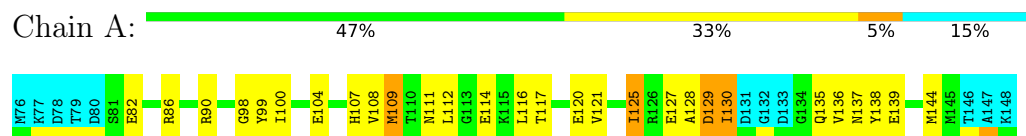


• Molecule 2: Purkinje cell protein 4

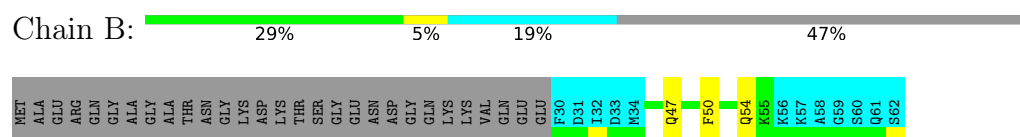


4.2.10 Score per residue for model 10

• Molecule 1: Calmodulin

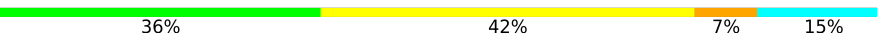


• Molecule 2: Purkinje cell protein 4



4.2.11 Score per residue for model 11

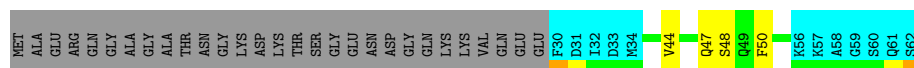
• Molecule 1: Calmodulin

Chain A: 



• Molecule 2: Purkinje cell protein 4

Chain B: 



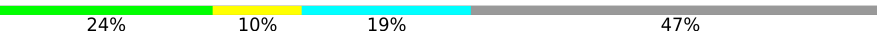
4.2.12 Score per residue for model 12

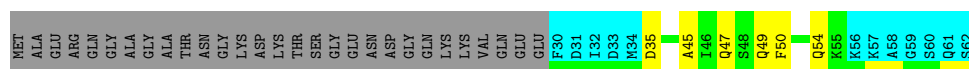
• Molecule 1: Calmodulin

Chain A: 



• Molecule 2: Purkinje cell protein 4

Chain B: 



4.2.13 Score per residue for model 13

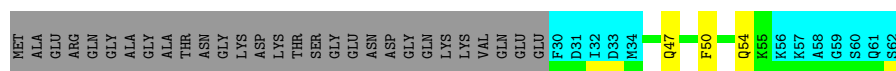
• Molecule 1: Calmodulin

Chain A: 



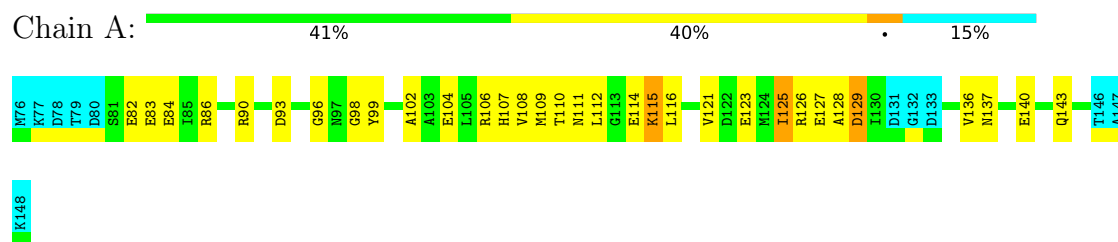
• Molecule 2: Purkinje cell protein 4

Chain B: 

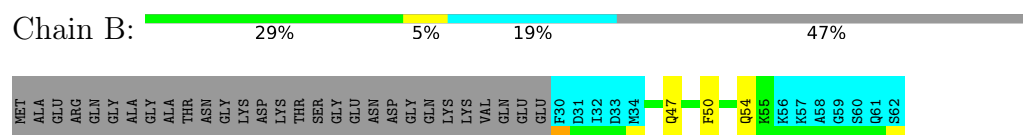


4.2.14 Score per residue for model 14

- Molecule 1: Calmodulin

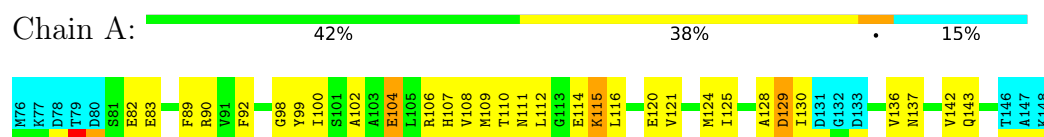


- Molecule 2: Purkinje cell protein 4

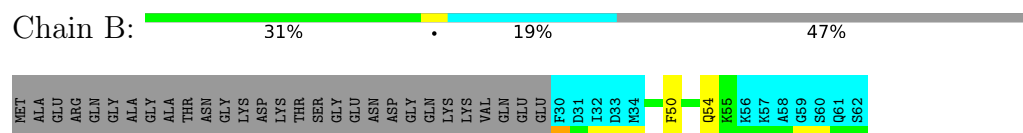


4.2.15 Score per residue for model 15

- Molecule 1: Calmodulin

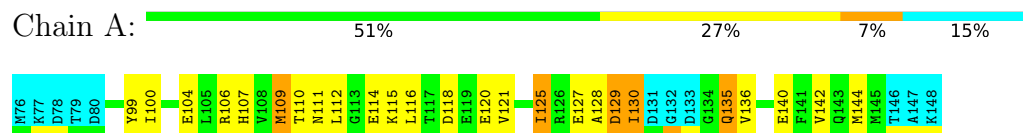


- Molecule 2: Purkinje cell protein 4

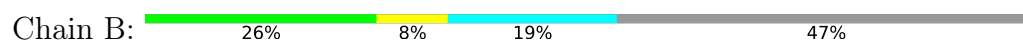


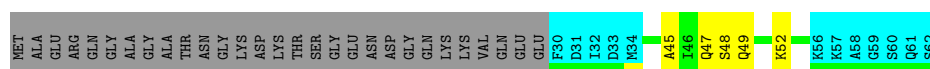
4.2.16 Score per residue for model 16

- Molecule 1: Calmodulin



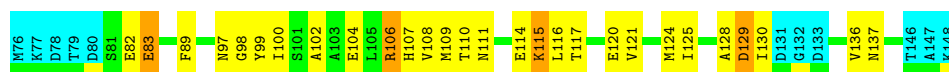
- Molecule 2: Purkinje cell protein 4



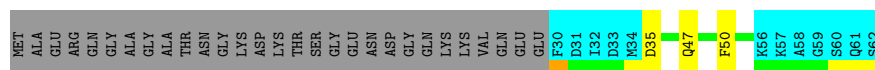
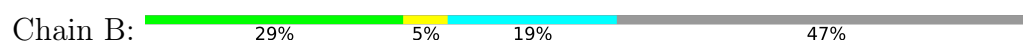


4.2.17 Score per residue for model 17

- Molecule 1: Calmodulin

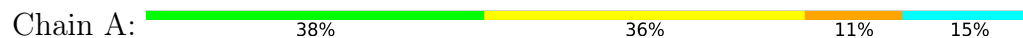


- Molecule 2: Purkinje cell protein 4

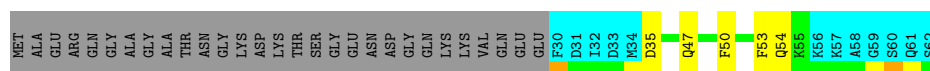
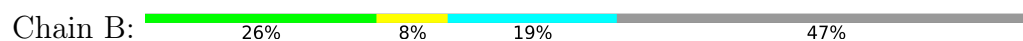


4.2.18 Score per residue for model 18

- Molecule 1: Calmodulin



- Molecule 2: Purkinje cell protein 4

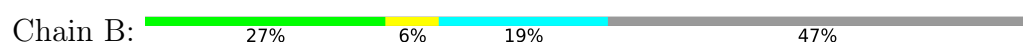


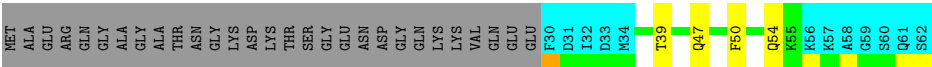
4.2.19 Score per residue for model 19

- Molecule 1: Calmodulin



- Molecule 2: Purkinje cell protein 4



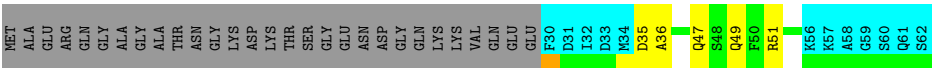
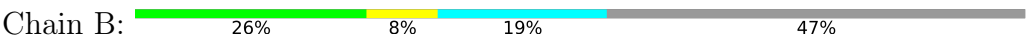


4.2.20 Score per residue for model 20

- Molecule 1: Calmodulin



- Molecule 2: Purkinje cell protein 4



5 Refinement protocol and experimental data overview

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

Of the 300 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
XPLOR-NIH	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	2
Total number of shifts	1258
Number of shifts mapped to atoms	1225
Number of unparsed shifts	0
Number of shifts with mapping errors	33
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	89%

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±0.00	0±0/510 (0.0± 0.0%)	1.03±0.01	0±0/684 (0.0± 0.1%)
2	B	0.59±0.01	0±0/173 (0.0± 0.0%)	1.00±0.01	0±0/232 (0.0± 0.0%)
All	All	0.63	0/13660 (0.0%)	1.02	5/18320 (0.0%)

There are no bond-length outliers.

All unique angle outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	89	PHE	CA-CB-CG	-5.31	108.49	113.80	18	5

There are no chirality outliers.

There are no planarity outliers.

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	504	471	470	26±6
2	B	170	169	169	5±2
All	All	13480	12800	12780	546

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 21.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:106:ARG:CZ	1:A:121:VAL:HG11	0.71	2.15	5	2
1:A:116:LEU:HD23	2:B:47:GLN:NE2	0.68	2.03	11	1
1:A:130:ILE:HG22	1:A:130:ILE:O	0.67	1.90	17	8
1:A:88:ALA:O	1:A:91:VAL:HG12	0.66	1.90	8	1
1:A:104:GLU:O	1:A:108:VAL:HG23	0.65	1.93	12	17
1:A:116:LEU:HD23	2:B:47:GLN:HE21	0.64	1.53	11	1
1:A:106:ARG:NE	1:A:121:VAL:HG11	0.63	2.09	5	2
2:B:50:PHE:CE2	2:B:54:GLN:NE2	0.63	2.67	3	5
1:A:113:GLY:O	1:A:114:GLU:C	0.62	2.42	1	8
1:A:106:ARG:NH1	1:A:110:THR:HG21	0.62	2.10	16	2
1:A:107:HIS:CE1	1:A:111:ASN:ND2	0.62	2.67	18	8
1:A:124:MET:SD	2:B:50:PHE:CD1	0.61	2.93	15	12
1:A:86:ARG:NH2	1:A:90:ARG:NH2	0.61	2.49	13	2
1:A:85:ILE:HD12	2:B:49:GLN:CD	0.60	2.21	20	1
1:A:124:MET:SD	2:B:50:PHE:CE1	0.60	2.94	2	8
1:A:124:MET:SD	2:B:50:PHE:CG	0.60	2.95	6	5
1:A:107:HIS:NE2	1:A:111:ASN:ND2	0.58	2.50	16	7
1:A:129:ASP:CG	1:A:130:ILE:N	0.57	2.61	20	10
1:A:86:ARG:CZ	1:A:90:ARG:NH2	0.57	2.67	10	3
1:A:102:ALA:HB2	1:A:136:VAL:HG23	0.57	1.76	14	11
1:A:97:ASN:HD22	1:A:99:TYR:H	0.57	1.42	2	2
1:A:93:ASP:OD1	1:A:93:ASP:N	0.57	2.34	9	3
1:A:110:THR:CG2	1:A:121:VAL:HG21	0.57	2.30	11	10
1:A:113:GLY:O	2:B:47:GLN:NE2	0.56	2.38	9	8
1:A:128:ALA:HB1	1:A:136:VAL:CG2	0.56	2.31	14	9
1:A:86:ARG:CZ	1:A:90:ARG:HH21	0.56	2.14	13	1
1:A:121:VAL:HG12	1:A:125:ILE:HD13	0.55	1.78	10	7
2:B:45:ALA:O	2:B:49:GLN:NE2	0.55	2.40	5	2
1:A:107:HIS:ND1	1:A:111:ASN:OD1	0.55	2.40	9	1
1:A:114:GLU:O	2:B:47:GLN:NE2	0.55	2.40	3	4
1:A:141:PHE:O	1:A:145:MET:SD	0.54	2.66	2	3
1:A:114:GLU:O	1:A:116:LEU:HD22	0.54	2.03	19	2
1:A:107:HIS:ND1	1:A:111:ASN:ND2	0.54	2.55	14	1
1:A:107:HIS:O	1:A:111:ASN:N	0.54	2.41	1	16
1:A:123:GLU:OE1	1:A:126:ARG:NH2	0.54	2.41	14	1
1:A:118:ASP:OD1	1:A:119:GLU:N	0.54	2.41	1	3
1:A:116:LEU:CD2	2:B:47:GLN:NE2	0.54	2.71	11	2
2:B:35:ASP:OD1	2:B:36:ALA:N	0.53	2.41	20	1
1:A:120:GLU:N	1:A:120:GLU:OE1	0.53	2.41	2	6
1:A:128:ALA:O	1:A:129:ASP:CG	0.53	2.52	8	10
1:A:95:ASP:OD1	1:A:96:GLY:N	0.53	2.42	9	1
1:A:128:ALA:O	1:A:129:ASP:CB	0.53	2.56	1	10

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:128:ALA:HB1	1:A:136:VAL:HG21	0.53	1.80	13	8
1:A:95:ASP:OD2	1:A:97:ASN:ND2	0.53	2.42	19	1
1:A:117:THR:O	1:A:121:VAL:HG23	0.53	2.03	17	4
1:A:122:ASP:OD1	1:A:126:ARG:NH1	0.53	2.42	18	1
2:B:48:SER:OG	2:B:52:LYS:NZ	0.52	2.42	16	1
1:A:129:ASP:OD2	1:A:137:ASN:ND2	0.52	2.42	6	3
1:A:82:GLU:CD	1:A:83:GLU:N	0.52	2.68	17	2
1:A:98:GLY:O	1:A:137:ASN:ND2	0.52	2.42	2	1
1:A:109:MET:SD	1:A:109:MET:N	0.52	2.82	10	5
1:A:106:ARG:NH2	1:A:118:ASP:OD1	0.52	2.42	16	1
1:A:97:ASN:ND2	1:A:99:TYR:H	0.52	2.02	2	2
1:A:116:LEU:HD12	1:A:120:GLU:HB3	0.52	1.81	3	15
1:A:82:GLU:OE2	1:A:86:ARG:NH2	0.52	2.42	4	1
1:A:116:LEU:N	1:A:116:LEU:HD22	0.51	2.20	10	2
1:A:122:ASP:CG	1:A:126:ARG:NH1	0.51	2.68	18	1
1:A:114:GLU:OE1	2:B:51:ARG:NH1	0.51	2.43	20	1
1:A:99:TYR:CD1	1:A:99:TYR:N	0.51	2.78	10	20
1:A:109:MET:HE3	2:B:47:GLN:OE1	0.51	2.06	11	1
1:A:113:GLY:C	2:B:47:GLN:HE22	0.51	2.14	3	2
1:A:120:GLU:N	1:A:120:GLU:CD	0.51	2.69	2	6
1:A:113:GLY:O	1:A:114:GLU:O	0.50	2.30	9	1
1:A:106:ARG:CD	1:A:121:VAL:HG11	0.50	2.36	20	4
1:A:114:GLU:N	2:B:47:GLN:OE1	0.50	2.45	17	5
1:A:143:GLN:O	1:A:143:GLN:NE2	0.50	2.44	9	1
1:A:127:GLU:CD	1:A:144:MET:SD	0.49	2.95	5	2
1:A:145:MET:SD	2:B:49:GLN:OE1	0.49	2.71	20	1
1:A:112:LEU:O	1:A:113:GLY:O	0.49	2.31	9	9
1:A:93:ASP:OD2	1:A:138:TYR:CE2	0.48	2.66	9	1
1:A:117:THR:OG1	1:A:120:GLU:OE1	0.48	2.31	10	7
1:A:129:ASP:OD2	1:A:130:ILE:N	0.48	2.47	11	6
1:A:106:ARG:CD	1:A:106:ARG:C	0.48	2.87	3	3
1:A:113:GLY:O	2:B:47:GLN:OE1	0.47	2.31	4	7
2:B:50:PHE:CZ	2:B:54:GLN:NE2	0.47	2.82	18	3
1:A:107:HIS:CE1	1:A:111:ASN:CB	0.47	2.97	20	1
1:A:114:GLU:O	1:A:115:LYS:O	0.47	2.32	7	6
1:A:116:LEU:HD12	1:A:120:GLU:CB	0.47	2.39	2	6
1:A:98:GLY:C	1:A:99:TYR:CD1	0.47	2.92	11	16
1:A:83:GLU:CD	1:A:84:GLU:N	0.47	2.72	11	2
1:A:93:ASP:OD1	1:A:100:ILE:HG22	0.47	2.10	8	3
1:A:114:GLU:H	2:B:47:GLN:CD	0.47	2.18	10	1
1:A:116:LEU:N	1:A:116:LEU:CD2	0.47	2.78	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:91:VAL:HG11	2:B:39:THR:HG23	0.47	1.85	19	1
1:A:144:MET:O	2:B:53:PHE:CE1	0.47	2.68	18	1
1:A:95:ASP:CG	1:A:97:ASN:ND2	0.47	2.73	19	1
1:A:102:ALA:HB3	1:A:134:GLY:O	0.46	2.10	4	1
1:A:107:HIS:CE1	1:A:111:ASN:CG	0.46	2.93	9	2
1:A:128:ALA:O	1:A:140:GLU:OE2	0.46	2.34	14	3
1:A:137:ASN:OD1	1:A:137:ASN:O	0.46	2.34	15	11
1:A:120:GLU:CD	1:A:120:GLU:N	0.46	2.73	10	1
1:A:145:MET:HE1	2:B:46:ILE:HG23	0.46	1.87	6	1
1:A:129:ASP:OD1	1:A:130:ILE:N	0.46	2.49	5	1
2:B:45:ALA:O	2:B:49:GLN:OE1	0.46	2.34	16	2
1:A:121:VAL:CG1	1:A:125:ILE:HD13	0.45	2.41	14	1
1:A:129:ASP:CG	1:A:130:ILE:H	0.45	2.18	5	2
1:A:125:ILE:HG13	1:A:130:ILE:HD11	0.45	1.89	2	2
1:A:116:LEU:CD2	2:B:47:GLN:OE1	0.45	2.65	10	2
1:A:118:ASP:OD1	1:A:118:ASP:N	0.45	2.50	13	1
1:A:93:ASP:OD1	1:A:95:ASP:OD1	0.45	2.34	7	2
1:A:112:LEU:O	2:B:47:GLN:NE2	0.45	2.50	1	4
1:A:93:ASP:OD1	1:A:99:TYR:O	0.45	2.35	2	3
1:A:107:HIS:O	1:A:111:ASN:CB	0.45	2.65	18	7
1:A:106:ARG:O	1:A:110:THR:HG23	0.45	2.12	14	3
1:A:114:GLU:O	2:B:47:GLN:OE1	0.45	2.35	8	4
1:A:120:GLU:OE1	1:A:120:GLU:N	0.45	2.49	10	1
1:A:106:ARG:CZ	1:A:121:VAL:CG1	0.45	2.95	19	1
1:A:130:ILE:O	1:A:130:ILE:CG2	0.44	2.62	3	4
1:A:138:TYR:CE1	1:A:139:GLU:OE2	0.44	2.70	10	1
1:A:114:GLU:O	1:A:115:LYS:C	0.44	2.60	13	2
1:A:89:PHE:O	1:A:93:ASP:OD1	0.44	2.35	8	3
2:B:50:PHE:CE2	2:B:54:GLN:CD	0.44	2.95	10	1
1:A:104:GLU:O	1:A:108:VAL:CG2	0.44	2.66	9	4
1:A:123:GLU:OE2	2:B:54:GLN:NE2	0.44	2.51	4	1
1:A:129:ASP:OD1	1:A:129:ASP:C	0.44	2.60	12	3
1:A:128:ALA:O	1:A:129:ASP:OD1	0.44	2.35	15	1
1:A:124:MET:O	1:A:128:ALA:N	0.44	2.51	1	1
1:A:104:GLU:CD	1:A:104:GLU:C	0.44	2.85	2	3
1:A:93:ASP:OD1	1:A:96:GLY:N	0.44	2.51	14	1
1:A:95:ASP:O	1:A:95:ASP:OD1	0.44	2.36	20	2
1:A:127:GLU:O	1:A:140:GLU:OE2	0.44	2.35	16	2
1:A:141:PHE:CE1	1:A:144:MET:CE	0.43	3.00	4	1
1:A:129:ASP:OD2	1:A:135:GLN:O	0.43	2.36	11	4
1:A:118:ASP:OD1	1:A:119:GLU:OE1	0.43	2.36	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:129:ASP:O	1:A:130:ILE:C	0.43	2.60	10	4
1:A:137:ASN:OD1	1:A:139:GLU:OE1	0.43	2.36	10	1
1:A:83:GLU:CD	1:A:83:GLU:C	0.43	2.87	2	3
1:A:113:GLY:C	2:B:47:GLN:OE1	0.43	2.61	5	3
2:B:35:ASP:C	2:B:35:ASP:OD1	0.43	2.62	2	1
1:A:137:ASN:O	1:A:137:ASN:CG	0.43	2.62	8	3
1:A:97:ASN:OD1	1:A:97:ASN:O	0.43	2.37	11	1
1:A:123:GLU:CD	1:A:123:GLU:C	0.43	2.87	3	1
2:B:40:GLU:N	2:B:40:GLU:CD	0.43	2.77	3	1
1:A:92:PHE:CD1	1:A:104:GLU:OE1	0.43	2.72	15	2
1:A:114:GLU:C	2:B:47:GLN:OE1	0.43	2.62	10	1
1:A:83:GLU:OE1	1:A:83:GLU:C	0.42	2.62	19	1
1:A:118:ASP:OD1	1:A:122:ASP:CG	0.42	2.62	20	1
1:A:114:GLU:N	1:A:114:GLU:OE1	0.42	2.52	8	1
1:A:124:MET:CG	2:B:50:PHE:CZ	0.42	3.02	8	1
2:B:35:ASP:OD1	2:B:35:ASP:C	0.42	2.62	18	4
1:A:97:ASN:OD1	1:A:99:TYR:N	0.42	2.50	17	1
2:B:50:PHE:CE2	2:B:54:GLN:OE1	0.42	2.72	8	1
1:A:107:HIS:CG	1:A:111:ASN:OD1	0.42	2.73	9	1
1:A:86:ARG:NE	1:A:90:ARG:NH2	0.42	2.67	13	2
1:A:118:ASP:OD1	1:A:122:ASP:OD2	0.42	2.38	20	1
1:A:106:ARG:HD3	1:A:121:VAL:HG11	0.42	1.92	15	2
1:A:127:GLU:OE2	1:A:144:MET:SD	0.42	2.77	10	1
1:A:83:GLU:C	1:A:83:GLU:CD	0.42	2.88	14	1
1:A:84:GLU:CD	1:A:84:GLU:C	0.42	2.88	14	1
1:A:134:GLY:C	1:A:135:GLN:NE2	0.42	2.78	5	1
1:A:135:GLN:OE1	1:A:135:GLN:O	0.42	2.37	12	1
1:A:97:ASN:OD1	1:A:97:ASN:C	0.42	2.63	17	2
1:A:89:PHE:O	1:A:93:ASP:CG	0.42	2.63	18	1
1:A:134:GLY:C	1:A:135:GLN:OE1	0.42	2.62	2	1
2:B:40:GLU:CD	2:B:40:GLU:C	0.42	2.88	4	1
1:A:82:GLU:CD	1:A:82:GLU:C	0.42	2.88	19	3
1:A:143:GLN:CD	1:A:143:GLN:C	0.41	2.87	9	1
1:A:139:GLU:CD	1:A:139:GLU:C	0.41	2.88	19	2
1:A:83:GLU:OE2	1:A:84:GLU:OE2	0.41	2.38	19	1
1:A:102:ALA:HB2	1:A:136:VAL:CG2	0.41	2.45	4	1
1:A:116:LEU:CD2	2:B:47:GLN:HE21	0.41	2.28	9	1
1:A:113:GLY:O	2:B:47:GLN:CD	0.41	2.63	9	1
2:B:44:VAL:O	2:B:48:SER:CB	0.41	2.69	11	1
1:A:83:GLU:CG	1:A:84:GLU:N	0.41	2.84	18	1
1:A:114:GLU:CB	2:B:51:ARG:HH22	0.41	2.29	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:95:ASP:O	1:A:96:GLY:C	0.41	2.64	7	1
1:A:127:GLU:OE1	1:A:144:MET:SD	0.41	2.79	10	1
1:A:109:MET:N	1:A:109:MET:SD	0.41	2.94	16	1
1:A:98:GLY:O	1:A:138:TYR:CE2	0.40	2.74	10	1
1:A:106:ARG:NH1	1:A:110:THR:CG2	0.40	2.83	16	1
1:A:113:GLY:C	1:A:114:GLU:O	0.40	2.63	9	1
1:A:89:PHE:O	1:A:90:ARG:C	0.40	2.63	15	1
1:A:89:PHE:O	1:A:92:PHE:N	0.40	2.50	15	1
1:A:87:GLU:CD	1:A:87:GLU:C	0.40	2.89	20	1
1:A:110:THR:HG22	1:A:116:LEU:O	0.40	2.17	7	1
1:A:120:GLU:OE1	2:B:54:GLN:NE2	0.40	2.50	15	1
1:A:118:ASP:OD1	1:A:118:ASP:C	0.40	2.64	18	1

6.3 Torsion angles ⓘ

6.3.1 Protein backbone ⓘ

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	62/73 (85%)	57±1 (92±1%)	3±1 (4±2%)	3±1 (4±2%)	3	28
2	B	21/62 (34%)	21±0 (100±0%)	0±0 (0±0%)	0±0 (0±0%)	100	100
All	All	1660/2700 (61%)	1556 (94%)	51 (3%)	53 (3%)	5	36

All 5 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	129	ASP	20
1	A	113	GLY	9
1	A	114	GLU	9
1	A	130	ILE	8
1	A	115	LYS	7

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	54/63 (86%)	49±2 (90±3%)	5±2 (10±3%)	10	55
2	B	17/48 (35%)	17±0 (99±2%)	0±0 (1±2%)	68	95
All	All	1420/2220 (64%)	1314 (93%)	106 (7%)	14	62

All 20 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	109	MET	20
1	A	125	ILE	20
1	A	100	ILE	18
1	A	144	MET	7
1	A	135	GLN	5
1	A	130	ILE	5
1	A	120	GLU	4
1	A	137	ASN	4
1	A	145	MET	3
1	A	106	ARG	3
1	A	93	ASP	3
1	A	83	GLU	3
1	A	97	ASN	2
1	A	85	ILE	2
1	A	104	GLU	2
2	B	52	LYS	1
1	A	136	VAL	1
2	B	44	VAL	1
2	B	41	ARG	1
1	A	94	LYS	1

6.3.3 RNA ⓘ

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 89% for the well-defined parts and 86% 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	848
Number of shifts mapped to atoms	848
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
$^{13}\text{C}_\alpha$	71	-0.34 ± 0.19	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	66	-0.03 ± 0.25	None needed (< 0.5 ppm)
$^{13}\text{C}'$	69	-0.25 ± 0.08	None needed (< 0.5 ppm)
^{15}N	70	0.21 ± 0.40	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 67%, i.e. 763 atoms were assigned a chemical shift out of a possible 1142. 0 out of 9 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	311/417 (75%)	127/169 (75%)	123/166 (74%)	61/82 (74%)
Sidechain	416/649 (64%)	284/414 (69%)	127/205 (62%)	5/30 (17%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	36/76 (47%)	23/37 (62%)	13/37 (35%)	0/2 (0%)
Overall	763/1142 (67%)	434/620 (70%)	263/408 (64%)	66/114 (58%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 60%, i.e. 848 atoms were assigned a chemical shift out of a possible 1417. 0 out of 9 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	356/534 (67%)	146/217 (67%)	140/212 (66%)	70/105 (67%)
Sidechain	456/797 (57%)	311/507 (61%)	140/255 (55%)	5/35 (14%)
Aromatic	36/86 (42%)	23/42 (55%)	13/42 (31%)	0/2 (0%)
Overall	848/1417 (60%)	480/766 (63%)	293/509 (58%)	75/142 (53%)

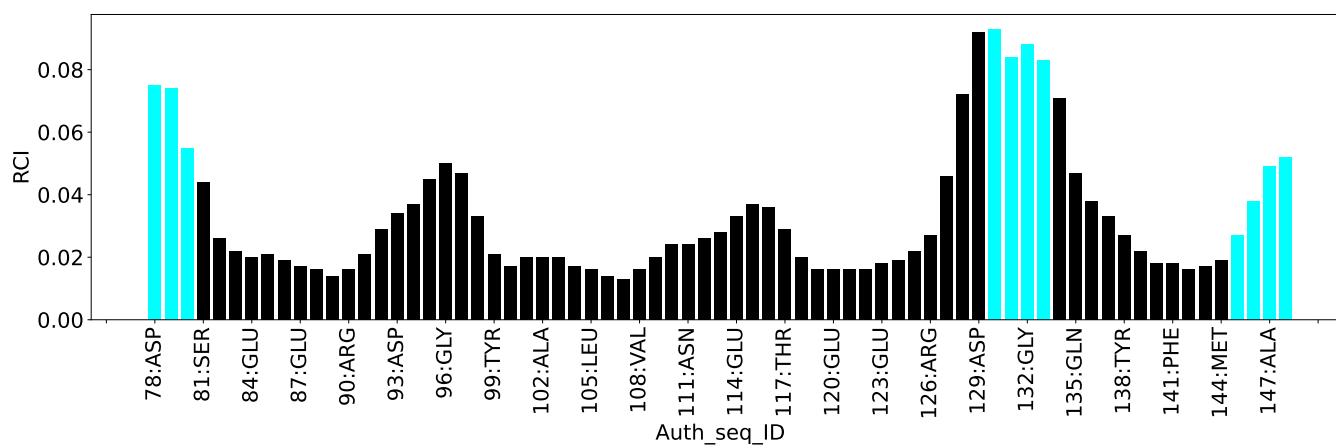
7.1.4 Statistically unusual chemical shifts [i](#)

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:



7.2 Chemical shift list 2

File name: working_cs.cif

Chemical shift list name: *Assigned_chem_shift_list_2*

7.2.1 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	410
Number of shifts mapped to atoms	377
Number of unparsed shifts	0
Number of shifts with mapping errors	33
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 33 occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
2	B	27	GLN	H	8.439	0.02	1
2	B	27	GLN	HA	4.2659	0.02	1
2	B	27	GLN	HB2	1.986	0.02	2
2	B	27	GLN	HB3	2.09	0.02	2
2	B	27	GLN	HG2	2.3253	0.02	2
2	B	27	GLN	HG3	2.384	0.02	2
2	B	27	GLN	C	175.56	0.3	1
2	B	27	GLN	CA	55.95	0.3	1
2	B	27	GLN	CB	29.47	0.3	1
2	B	27	GLN	CG	33.69	0.3	1
2	B	27	GLN	N	124.23	0.1	1
2	B	28	GLU	H	8.398	0.02	1
2	B	28	GLU	HA	4.172	0.02	1
2	B	28	GLU	HB2	1.8574	0.02	2
2	B	28	GLU	HB3	1.8574	0.02	2
2	B	28	GLU	HG2	2.185	0.02	2
2	B	28	GLU	HG3	2.185	0.02	2
2	B	28	GLU	C	175.78	0.3	1
2	B	28	GLU	CA	56.94	0.3	1
2	B	28	GLU	CB	30.52	0.3	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
2	B	28	GLU	CG	36.266	0.3	1
2	B	28	GLU	N	122.92	0.1	1
2	B	29	GLU	H	8.159	0.02	1
2	B	29	GLU	HA	4.172	0.02	1
2	B	29	GLU	HB2	1.787	0.02	2
2	B	29	GLU	HB3	1.787	0.02	2
2	B	29	GLU	HG2	2.021	0.02	2
2	B	29	GLU	HG3	2.115	0.02	2
2	B	29	GLU	C	175.67	0.3	1
2	B	29	GLU	CA	56.31	0.3	1
2	B	29	GLU	CB	30.64	0.3	1
2	B	29	GLU	CG	36.03	0.3	1
2	B	29	GLU	N	121.37	0.1	1

7.2.2 Chemical shift referencing ⓘ

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	36	-0.52 ± 0.08	Should be checked
$^{13}\text{C}_\beta$	35	0.34 ± 0.17	None needed (< 0.5 ppm)
$^{13}\text{C}'$	33	-0.37 ± 0.19	None needed (< 0.5 ppm)
^{15}N	34	0.15 ± 0.27	None needed (< 0.5 ppm)

7.2.3 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 22%, i.e. 248 atoms were assigned a chemical shift out of a possible 1142. 0 out of 9 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	102/417 (24%)	41/169 (24%)	41/166 (25%)	20/82 (24%)
Sidechain	136/649 (21%)	94/414 (23%)	39/205 (19%)	3/30 (10%)
Aromatic	10/76 (13%)	10/37 (27%)	0/37 (0%)	0/2 (0%)
Overall	248/1142 (22%)	145/620 (23%)	80/408 (20%)	23/114 (20%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 27%, i.e. 377 atoms were assigned a chemical shift out of a possible 1417. 0 out of 9 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	160/534 (30%)	66/217 (30%)	63/212 (30%)	31/105 (30%)
Sidechain	198/797 (25%)	137/507 (27%)	58/255 (23%)	3/35 (9%)
Aromatic	19/86 (22%)	15/42 (36%)	4/42 (10%)	0/2 (0%)
Overall	377/1417 (27%)	218/766 (28%)	125/509 (25%)	34/142 (24%)

7.2.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

7.2.5 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 B:

