



Full wwPDB NMR Structure Validation Report ⓘ

Mar 9, 2026 – 03:27 AM UTC

PDB ID : 7JI1 / pdb_00007ji1
BMRB ID : 30779
Title : NMR structure of the Streptococcus pyogenes NAD⁺-glycohydrolase translocation domain
Authors : Velarde, J.J.; Piai, A.; Chou, J.J.; Wessels, M.
Deposited on : 2020-07-22

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

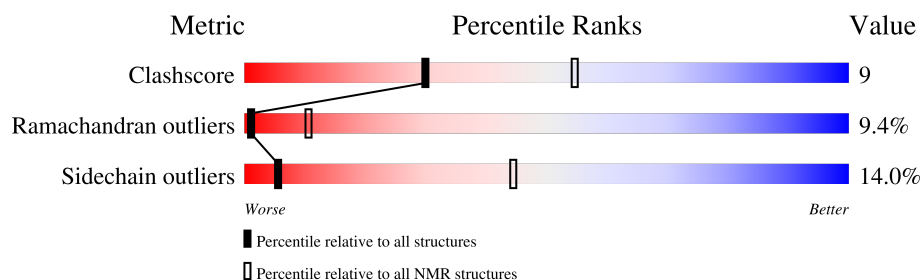
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 38%.

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	159	

2 Ensemble composition and analysis

This entry contains 15 models. Model 4 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:79-A:194 (116)	1.30	4

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 2 clusters and 2 single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1895 atoms, of which 948 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called ADP-ribosyl cyclase / cyclic ADP-ribose hydrolase.

Mol	Chain	Residues	Atoms							Trace
1	A	119	Total	C	H	N	O	S		0
			1895	599	948	161	185	2		

There are 2 discrepancies between the modelled and reference sequences:

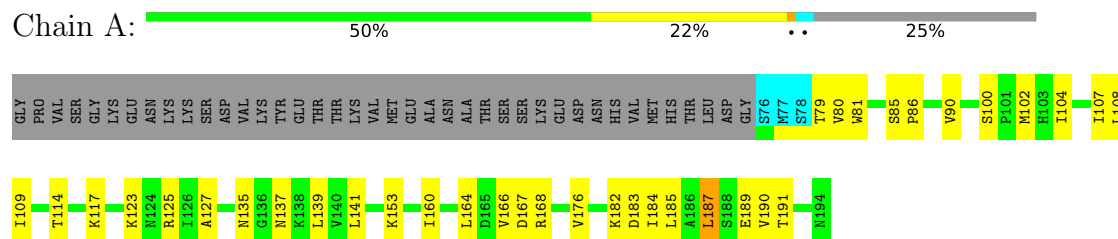
Chain	Residue	Modelled	Actual	Comment	Reference
A	36	GLY	-	expression tag	UNP Q9R2Y9
A	37	PRO	-	expression tag	UNP Q9R2Y9

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: ADP-ribosyl cyclase / cyclic ADP-ribose hydrolase

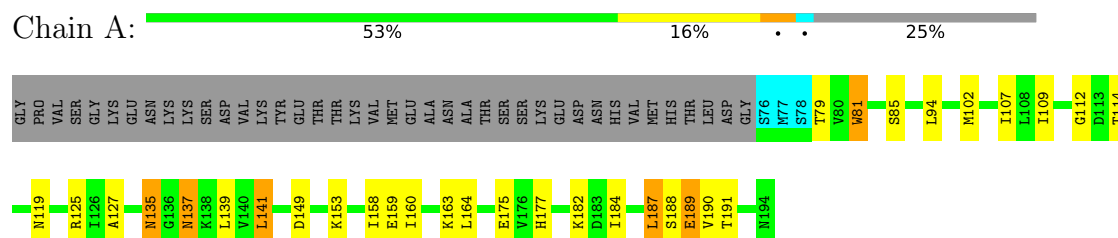


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

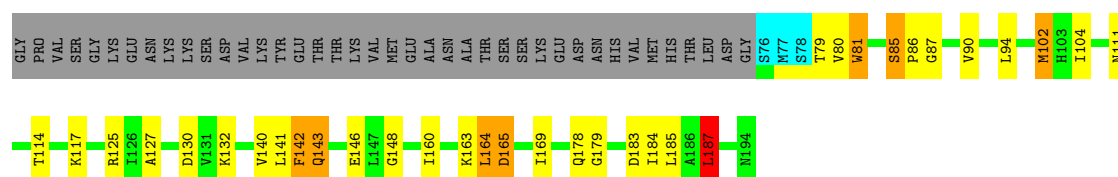
- Molecule 1: ADP-ribosyl cyclase / cyclic ADP-ribose hydrolase



4.2.2 Score per residue for model 2

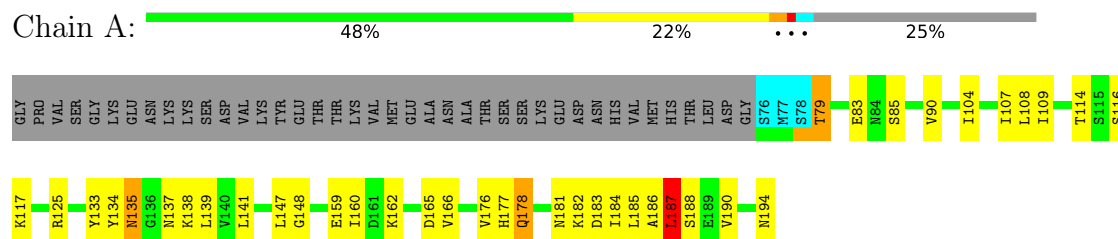
- Molecule 1: ADP-ribosyl cyclase / cyclic ADP-ribose hydrolase





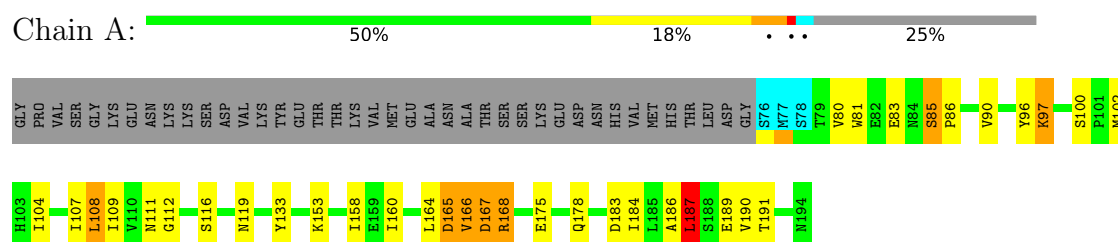
4.2.3 Score per residue for model 3

- Molecule 1: ADP-ribosyl cyclase / cyclic ADP-ribose hydrolase



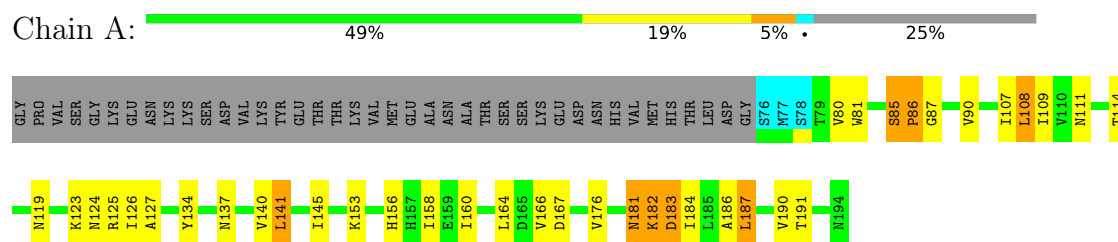
4.2.4 Score per residue for model 4 (medoid)

- Molecule 1: ADP-ribosyl cyclase / cyclic ADP-ribose hydrolase



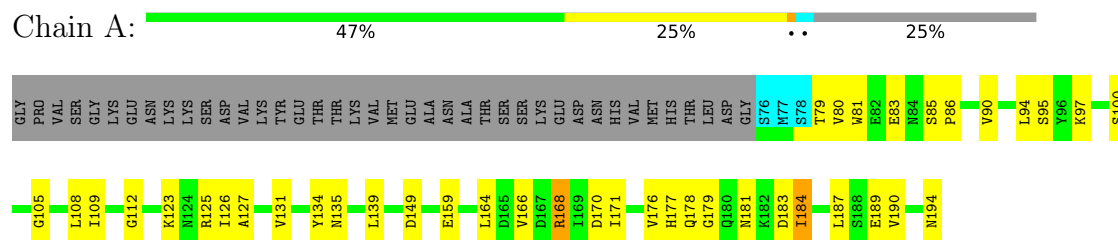
4.2.5 Score per residue for model 5

- Molecule 1: ADP-ribosyl cyclase / cyclic ADP-ribose hydrolase



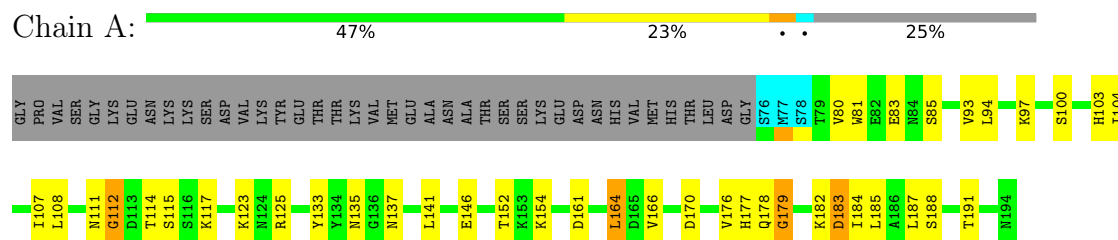
4.2.6 Score per residue for model 6

- Molecule 1: ADP-ribosyl cyclase / cyclic ADP-ribose hydrolase



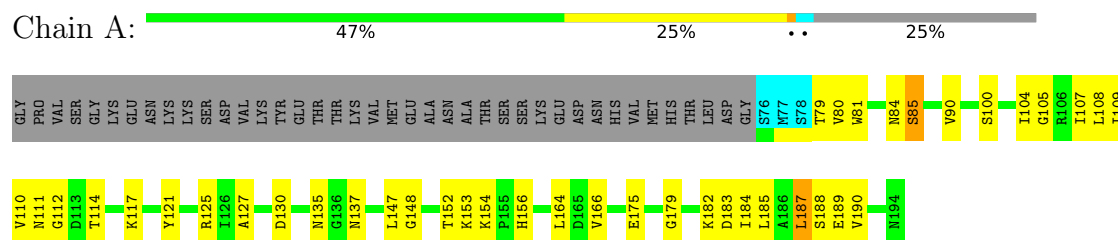
4.2.7 Score per residue for model 7

- Molecule 1: ADP-ribosyl cyclase / cyclic ADP-ribose hydrolase



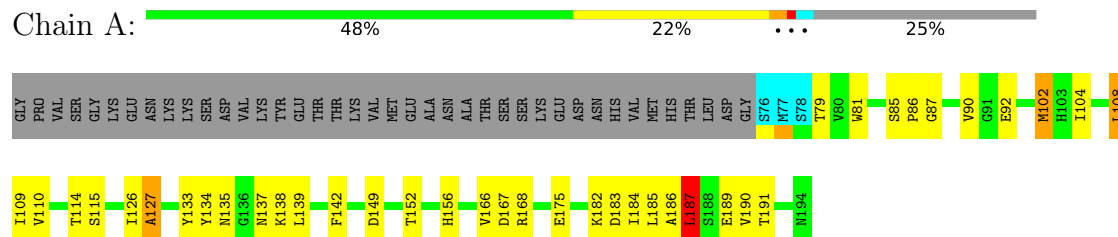
4.2.8 Score per residue for model 8

- Molecule 1: ADP-ribosyl cyclase / cyclic ADP-ribose hydrolase



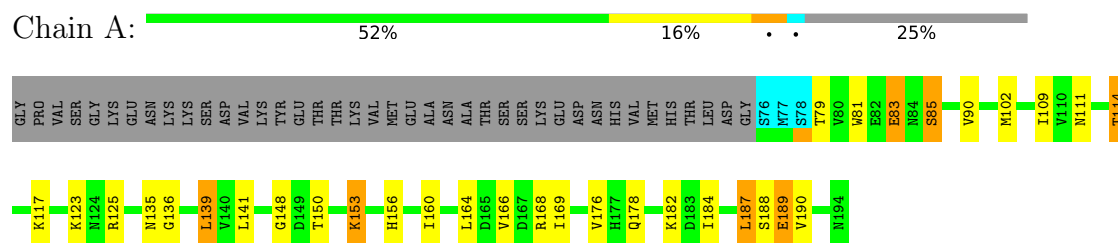
4.2.9 Score per residue for model 9

- Molecule 1: ADP-ribosyl cyclase / cyclic ADP-ribose hydrolase



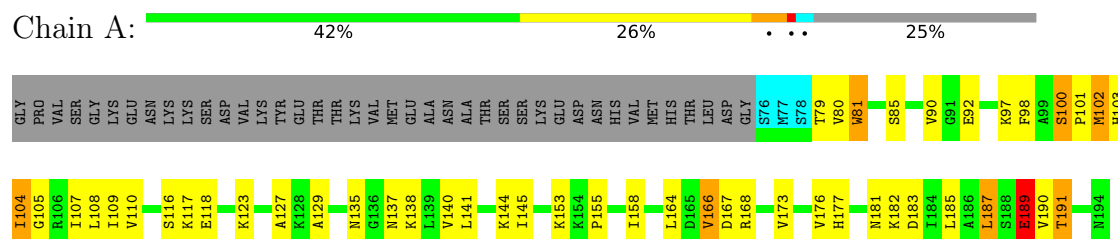
4.2.10 Score per residue for model 10

- Molecule 1: ADP-ribosyl cyclase / cyclic ADP-ribose hydrolase



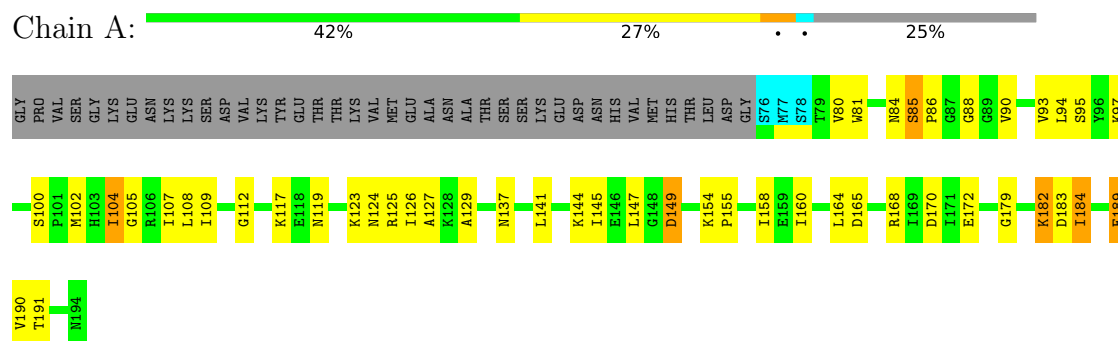
4.2.11 Score per residue for model 11

- Molecule 1: ADP-ribosyl cyclase / cyclic ADP-ribose hydrolase



4.2.12 Score per residue for model 12

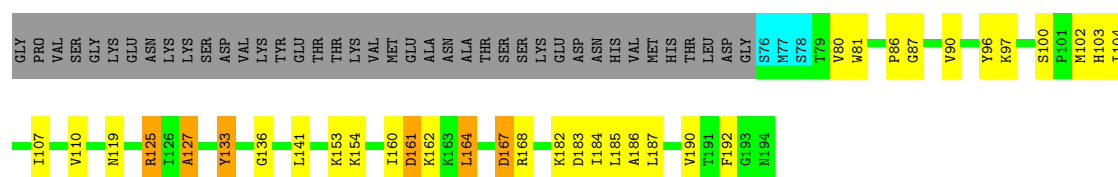
- Molecule 1: ADP-ribosyl cyclase / cyclic ADP-ribose hydrolase



4.2.13 Score per residue for model 13

- Molecule 1: ADP-ribosyl cyclase / cyclic ADP-ribose hydrolase

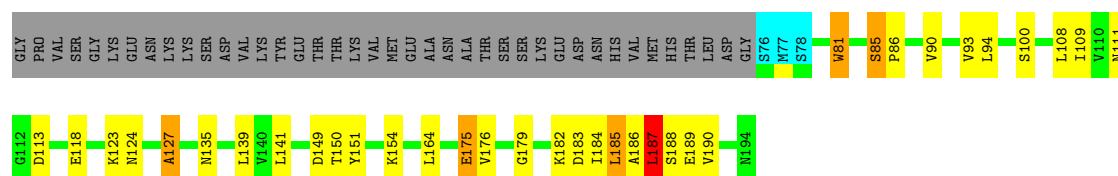




4.2.14 Score per residue for model 14

- Molecule 1: ADP-ribosyl cyclase / cyclic ADP-ribose hydrolase

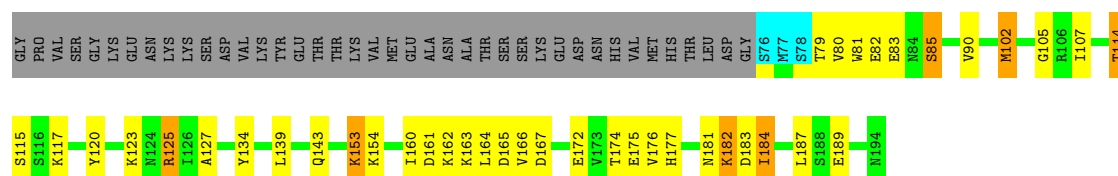
Chain A: 51% 18% ... 25%



4.2.15 Score per residue for model 15

- Molecule 1: ADP-ribosyl cyclase / cyclic ADP-ribose hydrolase

Chain A: 47% 21% . . 25%



5 Refinement protocol and experimental data overview

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

Of the 150 calculated structures, 15 were deposited, based on the following criterion: *15 structures for lowest energy*.

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

Software name	Classification	Version
X-PLOR NIH	refinement	
X-PLOR NIH	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	793
Number of shifts mapped to atoms	619
Number of unparsed shifts	0
Number of shifts with mapping errors	174
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	38%

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	0.84±0.01	0±0/944 (0.0± 0.0%)	1.11±0.02	1±1/1271 (0.1± 0.1%)
All	All	0.84	0/14160 (0.0%)	1.11	18/19065 (0.1%)

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	168	ARG	CA-C-N	-5.80	115.58	123.12	6	5
1	A	168	ARG	C-N-CA	-5.80	115.58	123.12	6	5
1	A	166	VAL	CA-C-O	-5.58	115.87	121.45	10	6
1	A	166	VAL	CA-C-N	-5.08	113.84	121.86	6	1
1	A	166	VAL	C-N-CA	-5.08	113.84	121.86	6	1

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	927	929	925	17±4
All	All	13905	13935	13875	252

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 9.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:109:ILE:HD12	1:A:190:VAL:HG23	0.90	1.43	5	1
1:A:90:VAL:HG23	1:A:176:VAL:HG22	0.79	1.52	10	6
1:A:109:ILE:HG23	1:A:190:VAL:HG12	0.78	1.54	11	5
1:A:123:LYS:HB3	1:A:184:ILE:HD13	0.78	1.54	15	5
1:A:164:LEU:O	1:A:164:LEU:HD12	0.72	1.83	10	7
1:A:145:ILE:HD13	1:A:158:ILE:HD11	0.71	1.62	5	2
1:A:81:TRP:CZ3	1:A:190:VAL:HG11	0.71	2.21	4	2
1:A:164:LEU:HD12	1:A:164:LEU:O	0.71	1.86	4	4
1:A:80:VAL:HG12	1:A:81:TRP:CE3	0.71	2.21	7	1
1:A:80:VAL:HG11	1:A:187:LEU:O	0.70	1.87	11	4
1:A:140:VAL:HG21	1:A:166:VAL:HG11	0.66	1.66	11	1
1:A:80:VAL:HG13	1:A:187:LEU:O	0.66	1.89	6	1
1:A:107:ILE:HD11	1:A:160:ILE:HD11	0.65	1.69	15	1
1:A:80:VAL:HG11	1:A:187:LEU:HB3	0.65	1.69	8	1
1:A:123:LYS:CB	1:A:184:ILE:HD13	0.65	2.21	15	2
1:A:141:LEU:CD1	1:A:160:ILE:HG23	0.65	2.23	12	3
1:A:114:THR:HG22	1:A:152:THR:HG22	0.64	1.69	7	1
1:A:102:MET:HE3	1:A:104:ILE:HD11	0.64	1.70	4	1
1:A:145:ILE:CD1	1:A:158:ILE:HD11	0.62	2.24	5	1
1:A:123:LYS:CB	1:A:184:ILE:HD12	0.61	2.25	14	1
1:A:185:LEU:HD13	1:A:186:ALA:N	0.60	2.11	13	1
1:A:109:ILE:HG23	1:A:190:VAL:CG1	0.60	2.25	10	5
1:A:186:ALA:C	1:A:187:LEU:HD22	0.60	2.22	14	4
1:A:187:LEU:HD22	1:A:187:LEU:N	0.59	2.13	3	3
1:A:81:TRP:CZ3	1:A:187:LEU:HD12	0.58	2.32	15	1
1:A:90:VAL:HG23	1:A:176:VAL:HG12	0.58	1.73	6	1
1:A:126:ILE:HD12	1:A:147:LEU:HD22	0.56	1.77	12	1
1:A:133:TYR:OH	1:A:160:ILE:HG21	0.56	2.01	13	1
1:A:102:MET:SD	1:A:104:ILE:HD11	0.55	2.41	9	2
1:A:141:LEU:HD12	1:A:160:ILE:HG23	0.55	1.79	12	1
1:A:126:ILE:HD12	1:A:187:LEU:HD13	0.55	1.78	6	1
1:A:80:VAL:HG13	1:A:190:VAL:CG1	0.55	2.31	8	1
1:A:104:ILE:HD13	1:A:133:TYR:OH	0.55	2.02	9	2
1:A:111:ASN:OD1	1:A:126:ILE:HD12	0.55	2.01	5	1
1:A:108:LEU:O	1:A:109:ILE:HD13	0.55	2.02	5	1
1:A:107:ILE:HG23	1:A:191:THR:O	0.55	2.02	5	5
1:A:126:ILE:HD11	1:A:187:LEU:CD1	0.54	2.33	9	1
1:A:81:TRP:CZ2	1:A:94:LEU:HD13	0.54	2.38	2	4
1:A:187:LEU:H	1:A:187:LEU:HD23	0.53	1.64	2	2
1:A:140:VAL:HG11	1:A:164:LEU:CD2	0.53	2.34	5	1
1:A:141:LEU:HD11	1:A:160:ILE:HG23	0.53	1.80	10	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:104:ILE:O	1:A:160:ILE:HD11	0.53	2.02	3	1
1:A:139:LEU:HD13	1:A:139:LEU:C	0.53	2.28	3	1
1:A:187:LEU:CD1	1:A:190:VAL:HG13	0.53	2.33	11	1
1:A:108:LEU:HD11	1:A:155:PRO:HG3	0.53	1.80	11	1
1:A:166:VAL:HG22	1:A:167:ASP:N	0.53	2.19	5	3
1:A:108:LEU:HD22	1:A:108:LEU:N	0.52	2.19	9	2
1:A:102:MET:HE3	1:A:167:ASP:OD1	0.52	2.05	15	2
1:A:93:VAL:HG23	1:A:172:GLU:HG2	0.51	1.83	12	1
1:A:80:VAL:HG13	1:A:190:VAL:HG12	0.51	1.80	8	2
1:A:133:TYR:OH	1:A:160:ILE:HD13	0.51	2.05	13	1
1:A:114:THR:CG2	1:A:152:THR:HG22	0.51	2.35	7	1
1:A:145:ILE:HD13	1:A:158:ILE:CD1	0.50	2.34	5	1
1:A:185:LEU:O	1:A:185:LEU:HD12	0.50	2.06	2	1
1:A:103:HIS:C	1:A:104:ILE:HD13	0.50	2.31	7	2
1:A:107:ILE:HG22	1:A:109:ILE:HD11	0.50	1.82	8	1
1:A:81:TRP:NE1	1:A:94:LEU:HD13	0.50	2.22	12	1
1:A:129:ALA:HB2	1:A:173:VAL:HG12	0.50	1.83	11	1
1:A:104:ILE:HD13	1:A:133:TYR:CZ	0.50	2.42	9	1
1:A:108:LEU:HD21	1:A:155:PRO:CB	0.50	2.37	12	1
1:A:125:ARG:NH2	1:A:127:ALA:HB2	0.50	2.21	13	1
1:A:90:VAL:HG23	1:A:176:VAL:CG2	0.49	2.33	10	2
1:A:90:VAL:HG23	1:A:176:VAL:CG1	0.49	2.37	6	1
1:A:186:ALA:C	1:A:187:LEU:HD12	0.49	2.31	5	1
1:A:81:TRP:CH2	1:A:187:LEU:HD22	0.49	2.43	8	1
1:A:109:ILE:HG23	1:A:190:VAL:HG22	0.49	1.84	12	1
1:A:104:ILE:HG22	1:A:160:ILE:CD1	0.49	2.38	4	1
1:A:141:LEU:HD23	1:A:141:LEU:N	0.48	2.23	3	1
1:A:108:LEU:HD13	1:A:109:ILE:N	0.48	2.23	4	2
1:A:104:ILE:HG22	1:A:160:ILE:HD12	0.48	1.83	2	2
1:A:107:ILE:HB	1:A:158:ILE:HG22	0.48	1.86	12	2
1:A:109:ILE:HG12	1:A:190:VAL:HG23	0.48	1.85	14	2
1:A:109:ILE:CG1	1:A:190:VAL:HG23	0.47	2.39	3	1
1:A:81:TRP:CZ2	1:A:187:LEU:HD22	0.47	2.44	8	1
1:A:108:LEU:C	1:A:108:LEU:HD13	0.47	2.34	14	1
1:A:109:ILE:HG13	1:A:190:VAL:HG23	0.47	1.86	3	1
1:A:103:HIS:O	1:A:104:ILE:HD13	0.47	2.09	7	1
1:A:187:LEU:N	1:A:187:LEU:HD23	0.47	2.24	11	1
1:A:81:TRP:CZ2	1:A:94:LEU:HD23	0.47	2.44	7	1
1:A:125:ARG:HH22	1:A:127:ALA:HB2	0.47	1.70	13	1
1:A:107:ILE:CD1	1:A:160:ILE:HD11	0.47	2.39	15	1
1:A:185:LEU:HD12	1:A:185:LEU:C	0.47	2.35	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:90:VAL:O	1:A:90:VAL:HG13	0.47	2.10	12	10
1:A:107:ILE:HD11	1:A:133:TYR:OH	0.47	2.10	3	1
1:A:81:TRP:CD2	1:A:187:LEU:HD13	0.47	2.44	13	1
1:A:80:VAL:HG22	1:A:188:SER:HA	0.46	1.87	7	1
1:A:127:ALA:HB3	1:A:175:GLU:O	0.46	2.10	9	2
1:A:108:LEU:C	1:A:108:LEU:HD23	0.46	2.36	12	1
1:A:123:LYS:HB3	1:A:184:ILE:HD12	0.46	1.86	14	1
1:A:80:VAL:HG12	1:A:81:TRP:HE3	0.46	1.70	11	2
1:A:187:LEU:HD23	1:A:190:VAL:HB	0.46	1.88	8	1
1:A:111:ASN:O	1:A:112:GLY:C	0.46	2.58	7	1
1:A:164:LEU:HD13	1:A:166:VAL:HG12	0.46	1.86	4	1
1:A:107:ILE:HD13	1:A:192:PHE:CE2	0.46	2.45	13	1
1:A:79:THR:HG21	1:A:82:GLU:OE1	0.46	2.11	15	1
1:A:114:THR:HG23	1:A:120:TYR:OH	0.45	2.11	15	1
1:A:90:VAL:CG2	1:A:176:VAL:HG22	0.45	2.40	5	1
1:A:80:VAL:HG11	1:A:187:LEU:HB2	0.45	1.87	4	1
1:A:80:VAL:HG13	1:A:189:GLU:HG2	0.45	1.88	11	1
1:A:81:TRP:CE3	1:A:187:LEU:HD13	0.45	2.46	13	1
1:A:125:ARG:CZ	1:A:125:ARG:H	0.45	2.24	13	1
1:A:160:ILE:HG22	1:A:161:ASP:N	0.45	2.27	15	1
1:A:79:THR:HG21	1:A:82:GLU:CD	0.45	2.37	15	1
1:A:108:LEU:HD12	1:A:108:LEU:N	0.44	2.26	7	2
1:A:134:TYR:O	1:A:168:ARG:CB	0.44	2.65	6	1
1:A:126:ILE:CD1	1:A:187:LEU:HD13	0.44	2.42	6	1
1:A:108:LEU:HD11	1:A:155:PRO:CG	0.44	2.42	11	1
1:A:158:ILE:HD12	1:A:158:ILE:N	0.44	2.27	4	1
1:A:182:LYS:O	1:A:183:ASP:CB	0.44	2.65	5	1
1:A:80:VAL:HG11	1:A:187:LEU:CB	0.44	2.41	8	1
1:A:186:ALA:HB1	1:A:187:LEU:HD22	0.44	1.90	14	1
1:A:187:LEU:HD23	1:A:187:LEU:N	0.44	2.27	1	1
1:A:134:TYR:O	1:A:135:ASN:CB	0.44	2.66	3	1
1:A:86:PRO:HB2	1:A:90:VAL:HG12	0.44	1.89	5	1
1:A:104:ILE:HB	1:A:160:ILE:HD13	0.44	1.90	12	1
1:A:185:LEU:N	1:A:185:LEU:HD12	0.43	2.28	7	1
1:A:134:TYR:CZ	1:A:139:LEU:HD12	0.43	2.48	15	1
1:A:87:GLY:O	1:A:90:VAL:HG23	0.43	2.13	2	1
1:A:102:MET:HE2	1:A:167:ASP:HB3	0.43	1.89	4	1
1:A:114:THR:HG23	1:A:152:THR:OG1	0.43	2.13	9	1
1:A:187:LEU:HD11	1:A:190:VAL:HG13	0.43	1.89	11	1
1:A:80:VAL:O	1:A:81:TRP:CE3	0.43	2.71	15	4
1:A:133:TYR:CZ	1:A:160:ILE:HD13	0.43	2.48	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:141:LEU:CD2	1:A:164:LEU:HD11	0.43	2.44	2	1
1:A:111:ASN:O	1:A:114:THR:HG23	0.43	2.14	10	1
1:A:141:LEU:C	1:A:141:LEU:HD23	0.43	2.38	12	1
1:A:141:LEU:HD23	1:A:141:LEU:C	0.43	2.39	10	1
1:A:141:LEU:HD21	1:A:160:ILE:HG23	0.43	1.90	1	1
1:A:80:VAL:CG1	1:A:190:VAL:HG12	0.43	2.44	4	1
1:A:187:LEU:H	1:A:187:LEU:HD12	0.43	1.73	13	1
1:A:131:VAL:HG12	1:A:171:ILE:HG23	0.43	1.91	6	1
1:A:147:LEU:HD23	1:A:156:HIS:CE1	0.42	2.49	8	1
1:A:141:LEU:C	1:A:141:LEU:HD12	0.42	2.38	2	1
1:A:104:ILE:HG21	1:A:133:TYR:OH	0.42	2.14	3	2
1:A:98:PHE:CD1	1:A:102:MET:HE3	0.42	2.49	11	1
1:A:110:VAL:HG22	1:A:155:PRO:HB3	0.42	1.91	11	1
1:A:104:ILE:CG2	1:A:160:ILE:HD11	0.42	2.45	13	1
1:A:84:ASN:O	1:A:85:SER:C	0.42	2.63	12	2
1:A:125:ARG:CZ	1:A:177:HIS:O	0.42	2.67	15	1
1:A:139:LEU:H	1:A:139:LEU:HD13	0.42	1.75	10	1
1:A:165:ASP:OD2	1:A:165:ASP:C	0.42	2.63	3	2
1:A:100:SER:CB	1:A:101:PRO:CD	0.42	2.98	11	1
1:A:129:ALA:O	1:A:145:ILE:HG22	0.42	2.15	12	1
1:A:100:SER:O	1:A:167:ASP:OD1	0.42	2.38	13	1
1:A:150:THR:HG22	1:A:151:TYR:N	0.42	2.30	14	1
1:A:109:ILE:CD1	1:A:190:VAL:HG23	0.41	2.31	5	1
1:A:80:VAL:HG12	1:A:81:TRP:CZ3	0.41	2.50	7	1
1:A:126:ILE:HD11	1:A:187:LEU:HD11	0.41	1.90	9	1
1:A:109:ILE:N	1:A:109:ILE:HD12	0.41	2.31	10	1
1:A:187:LEU:HD23	1:A:187:LEU:H	0.41	1.75	11	1
1:A:177:HIS:O	1:A:178:GLN:C	0.41	2.63	3	1
1:A:96:TYR:CZ	1:A:97:LYS:O	0.41	2.73	13	1
1:A:188:SER:O	1:A:189:GLU:HB2	0.41	2.15	1	1
1:A:177:HIS:O	1:A:179:GLY:N	0.41	2.54	7	1
1:A:147:LEU:HD12	1:A:147:LEU:N	0.41	2.31	8	1
1:A:93:VAL:O	1:A:93:VAL:HG13	0.41	2.16	7	1
1:A:135:ASN:C	1:A:137:ASN:H	0.41	2.24	1	1
1:A:134:TYR:O	1:A:166:VAL:HG21	0.41	2.16	5	1
1:A:181:ASN:O	1:A:182:LYS:C	0.41	2.64	5	2
1:A:185:LEU:HD12	1:A:185:LEU:O	0.41	2.16	8	2
1:A:133:TYR:CE1	1:A:160:ILE:HD13	0.41	2.51	13	1
1:A:141:LEU:HD12	1:A:142:PHE:HB2	0.41	1.91	2	1
1:A:187:LEU:N	1:A:187:LEU:CD2	0.41	2.84	3	1
1:A:96:TYR:CE1	1:A:97:LYS:O	0.41	2.74	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:109:ILE:HD12	1:A:190:VAL:CG2	0.41	2.32	5	1
1:A:110:VAL:HG13	1:A:110:VAL:O	0.41	2.16	13	1
1:A:161:ASP:O	1:A:162:LYS:C	0.40	2.64	13	1
1:A:184:ILE:CG1	1:A:185:LEU:N	0.40	2.85	14	1
1:A:102:MET:HE3	1:A:167:ASP:CG	0.40	2.40	15	1
1:A:165:ASP:OD1	1:A:165:ASP:N	0.40	2.55	2	1
1:A:81:TRP:CH2	1:A:94:LEU:HD23	0.40	2.51	7	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	115/159 (72%)	91±2 (79±2%)	13±2 (11±2%)	11±2 (9±2%)	1	10
All	All	1725/2385 (72%)	1364 (79%)	198 (11%)	163 (9%)	1	10

All 32 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	85	SER	13
1	A	183	ASP	13
1	A	127	ALA	11
1	A	182	LYS	11
1	A	184	ILE	9
1	A	187	LEU	9
1	A	189	GLU	9
1	A	79	THR	8
1	A	153	LYS	8
1	A	86	PRO	8
1	A	137	ASN	7
1	A	112	GLY	6
1	A	135	ASN	6
1	A	179	GLY	6
1	A	105	GLY	5

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Mol	Chain	Res	Type	Models (Total)
1	A	149	ASP	4
1	A	148	GLY	4
1	A	83	GLU	3
1	A	138	LYS	3
1	A	178	GLN	3
1	A	87	GLY	3
1	A	163	LYS	2
1	A	156	HIS	2
1	A	136	GLY	2
1	A	143	GLN	1
1	A	162	LYS	1
1	A	111	ASN	1
1	A	114	THR	1
1	A	150	THR	1
1	A	100	SER	1
1	A	88	GLY	1
1	A	124	ASN	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	102/140 (73%)	88±3 (86±3%)	14±3 (14±3%)	5	44
All	All	1530/2100 (73%)	1316 (86%)	214 (14%)	5	44

All 72 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	125	ARG	11
1	A	102	MET	8
1	A	117	LYS	8
1	A	187	LEU	8
1	A	85	SER	7
1	A	81	TRP	6
1	A	114	THR	6
1	A	141	LEU	6

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Mol	Chain	Res	Type	Models (Total)
1	A	100	SER	6
1	A	154	LYS	6
1	A	119	ASN	5
1	A	139	LEU	5
1	A	175	GLU	5
1	A	164	LEU	5
1	A	97	LYS	5
1	A	165	ASP	4
1	A	181	ASN	4
1	A	185	LEU	4
1	A	188	SER	4
1	A	83	GLU	4
1	A	108	LEU	4
1	A	159	GLU	3
1	A	177	HIS	3
1	A	111	ASN	3
1	A	178	GLN	3
1	A	116	SER	3
1	A	168	ARG	3
1	A	170	ASP	3
1	A	115	SER	3
1	A	104	ILE	3
1	A	135	ASN	3
1	A	189	GLU	3
1	A	130	ASP	2
1	A	142	PHE	2
1	A	143	GLN	2
1	A	146	GLU	2
1	A	169	ILE	2
1	A	194	ASN	2
1	A	167	ASP	2
1	A	124	ASN	2
1	A	95	SER	2
1	A	123	LYS	2
1	A	161	ASP	2
1	A	110	VAL	2
1	A	184	ILE	2
1	A	92	GLU	2
1	A	149	ASP	2
1	A	191	THR	2
1	A	153	LYS	2
1	A	118	GLU	2

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Mol	Chain	Res	Type	Models (Total)
1	A	144	LYS	2
1	A	182	LYS	2
1	A	132	LYS	1
1	A	140	VAL	1
1	A	163	LYS	1
1	A	79	THR	1
1	A	147	LEU	1
1	A	156	HIS	1
1	A	176	VAL	1
1	A	183	ASP	1
1	A	121	TYR	1
1	A	152	THR	1
1	A	166	VAL	1
1	A	134	TYR	1
1	A	137	ASN	1
1	A	103	HIS	1
1	A	133	TYR	1
1	A	93	VAL	1
1	A	113	ASP	1
1	A	162	LYS	1
1	A	172	GLU	1
1	A	174	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 [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 38% for the well-defined parts and 38% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *BMRB_final.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	793
Number of shifts mapped to atoms	619
Number of unparsed shifts	0
Number of shifts with mapping errors	174
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 174 occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	38	VAL	H	8.512	0.01	1
1	A	38	VAL	C	176.128	0.05	1
1	A	38	VAL	CA	61.987	0.05	1
1	A	38	VAL	CB	31.706	0.05	1
1	A	38	VAL	N	120.745	0.03	1
1	A	39	SER	H	8.56	0.01	1
1	A	39	SER	C	174.97	0.05	1
1	A	39	SER	CA	57.928	0.05	1
1	A	39	SER	CB	63.555	0.05	1
1	A	39	SER	N	119.913	0.03	1
1	A	40	GLY	H	8.509	0.01	1
1	A	40	GLY	HA2	3.999	0.01	1
1	A	40	GLY	C	174.128	0.05	1
1	A	40	GLY	CA	44.883	0.05	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	40	GLY	N	111.211	0.03	1
1	A	41	LYS	H	8.199	0.01	1
1	A	41	LYS	HA	4.74	0.01	1
1	A	41	LYS	C	176.654	0.05	1
1	A	41	LYS	CA	55.833	0.05	1
1	A	41	LYS	CB	32.205	0.05	1
1	A	41	LYS	N	120.565	0.03	1
1	A	42	GLU	H	8.541	0.01	1
1	A	42	GLU	C	176.141	0.05	1
1	A	42	GLU	CA	56.11	0.05	1
1	A	42	GLU	CB	29.254	0.05	1
1	A	42	GLU	N	121.422	0.03	1
1	A	43	ASN	H	8.48	0.01	1
1	A	43	ASN	C	174.97	0.05	1
1	A	43	ASN	CA	52.82	0.05	1
1	A	43	ASN	CB	38.106	0.05	1
1	A	43	ASN	N	120.238	0.03	1
1	A	44	LYS	H	8.405	0.01	1
1	A	44	LYS	HA	4.649	0.01	1
1	A	44	LYS	C	174.247	0.05	1
1	A	44	LYS	CA	54.93	0.05	1
1	A	44	LYS	CB	37.809	0.05	1
1	A	44	LYS	N	118.572	0.03	1
1	A	45	LYS	H	8.337	0.01	1
1	A	45	LYS	HA	4.295	0.01	1
1	A	45	LYS	C	176.436	0.05	1
1	A	45	LYS	CA	55.813	0.05	1
1	A	45	LYS	CB	32.039	0.05	1
1	A	45	LYS	N	118.235	0.03	1
1	A	46	SER	H	8.33	0.01	1
1	A	46	SER	HA	4.322	0.01	1
1	A	46	SER	C	174.128	0.05	1
1	A	46	SER	CA	57.808	0.05	1
1	A	46	SER	CB	63.79	0.05	1
1	A	46	SER	N	116.757	0.03	1
1	A	47	ASP	H	8.417	0.01	1
1	A	47	ASP	C	176.009	0.05	1
1	A	47	ASP	CA	53.886	0.05	1
1	A	47	ASP	N	122.8	0.03	1
1	A	48	VAL	H	8.001	0.01	1
1	A	48	VAL	HA	4.02	0.01	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	48	VAL	C	175.859	0.05	1
1	A	48	VAL	CA	61.94	0.05	1
1	A	48	VAL	CB	31.626	0.05	1
1	A	48	VAL	N	120.378	0.03	1
1	A	49	LYS	H	8.404	0.01	1
1	A	49	LYS	CA	54.825	0.05	1
1	A	49	LYS	N	123.656	0.03	1
1	A	50	TYR	C	177.021	0.05	1
1	A	50	TYR	CA	62.5	0.05	1
1	A	51	GLU	H	8.4	0.01	1
1	A	51	GLU	C	176.308	0.05	1
1	A	51	GLU	CA	61.866	0.05	1
1	A	51	GLU	N	120.463	0.03	1
1	A	52	THR	H	8.484	0.01	1
1	A	52	THR	HA	4.736	0.01	1
1	A	52	THR	C	175.049	0.05	1
1	A	52	THR	CA	58.002	0.05	1
1	A	52	THR	CB	63.54	0.05	1
1	A	52	THR	N	119.607	0.03	1
1	A	55	VAL	H	8.14	0.01	1
1	A	55	VAL	C	174.551	0.05	1
1	A	55	VAL	CA	61.923	0.05	1
1	A	55	VAL	N	121.975	0.03	1
1	A	56	MET	H	8.457	0.01	1
1	A	56	MET	C	176.136	0.05	1
1	A	56	MET	CA	54.856	0.05	1
1	A	56	MET	N	123.976	0.03	1
1	A	57	GLU	H	8.423	0.01	1
1	A	57	GLU	C	176.176	0.05	1
1	A	57	GLU	CA	56.01	0.05	1
1	A	57	GLU	CB	29.414	0.05	1
1	A	57	GLU	N	122.457	0.03	1
1	A	58	ALA	H	8.378	0.01	1
1	A	58	ALA	HA	4.259	0.01	1
1	A	58	ALA	C	177.439	0.05	1
1	A	58	ALA	CA	52.251	0.05	1
1	A	58	ALA	CB	18.527	0.05	1
1	A	58	ALA	N	124.973	0.03	1
1	A	59	ASN	H	8.468	0.01	1
1	A	59	ASN	C	174.996	0.05	1
1	A	59	ASN	CA	52.71	0.05	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	59	ASN	CB	38.047	0.05	1
1	A	59	ASN	N	117.518	0.03	1
1	A	60	ALA	H	8.286	0.01	1
1	A	60	ALA	HA	4.359	0.01	1
1	A	60	ALA	C	177.996	0.05	1
1	A	60	ALA	CA	52.416	0.05	1
1	A	60	ALA	CB	18.491	0.05	1
1	A	60	ALA	N	124.115	0.03	1
1	A	61	THR	H	8.164	0.01	1
1	A	61	THR	C	174.656	0.05	1
1	A	61	THR	CA	61.423	0.05	1
1	A	61	THR	CB	69.192	0.05	1
1	A	61	THR	N	112.711	0.03	1
1	A	62	SER	H	8.273	0.01	1
1	A	62	SER	C	174.498	0.05	1
1	A	62	SER	CA	57.955	0.05	1
1	A	62	SER	CB	63.707	0.05	1
1	A	62	SER	N	117.635	0.03	1
1	A	63	SER	H	8.384	0.01	1
1	A	63	SER	HA	4.519	0.01	1
1	A	63	SER	C	174.496	0.05	1
1	A	63	SER	CA	57.918	0.05	1
1	A	63	SER	CB	63.457	0.05	1
1	A	63	SER	N	117.926	0.03	1
1	A	64	LYS	H	8.368	0.01	1
1	A	64	LYS	HA	4.481	0.01	1
1	A	64	LYS	C	176.496	0.05	1
1	A	64	LYS	CA	56.017	0.05	1
1	A	64	LYS	CB	32.096	0.05	1
1	A	64	LYS	N	123.252	0.03	1
1	A	65	GLU	H	8.381	0.01	1
1	A	65	GLU	HA	4.336	0.01	1
1	A	65	GLU	C	175.996	0.05	1
1	A	65	GLU	CA	55.98	0.05	1
1	A	65	GLU	CB	29.296	0.05	1
1	A	65	GLU	N	121.483	0.03	1
1	A	66	ASP	H	8.296	0.01	1
1	A	66	ASP	HA	4.256	0.01	1
1	A	66	ASP	C	175.667	0.05	1
1	A	66	ASP	CA	53.739	0.05	1
1	A	66	ASP	CB	40.434	0.05	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	66	ASP	N	121.36	0.03	1
1	A	67	ASN	H	8.334	0.01	1
1	A	67	ASN	HA	4.573	0.01	1
1	A	67	ASN	C	174.947	0.05	1
1	A	67	ASN	CA	52.864	0.05	1
1	A	67	ASN	CB	37.94	0.05	1
1	A	67	ASN	N	118.909	0.03	1
1	A	68	HIS	H	8.313	0.01	1
1	A	68	HIS	HA	4.705	0.01	1
1	A	68	HIS	C	176.523	0.05	1
1	A	68	HIS	CA	55.833	0.05	1
1	A	68	HIS	CB	32.122	0.05	1
1	A	68	HIS	N	122.032	0.03	1
1	A	69	VAL	H	8.403	0.01	1
1	A	69	VAL	HA	4.322	0.01	1
1	A	69	VAL	C	174.894	0.05	1
1	A	69	VAL	N	122.884	0.03	1
1	A	70	MET	H	8.323	0.01	1
1	A	70	MET	C	175.43	0.05	1
1	A	70	MET	CA	54.168	0.05	1
1	A	70	MET	N	124.453	0.03	1
1	A	71	HIS	H	8.687	0.01	1
1	A	71	HIS	CA	53.965	0.05	1
1	A	71	HIS	N	121.764	0.03	1
1	A	73	LEU	C	175.902	0.05	1
1	A	73	LEU	CA	54.1	0.05	1
1	A	74	ASP	H	8.364	0.01	1
1	A	74	ASP	HA	4.552	0.01	1
1	A	74	ASP	C	176.902	0.05	1
1	A	74	ASP	CA	53.233	0.05	1
1	A	74	ASP	CB	40.217	0.05	1
1	A	74	ASP	N	120.674	0.03	1
1	A	75	GLY	H	8.432	0.01	1
1	A	75	GLY	HA2	4.066	0.01	1
1	A	75	GLY	C	173.914	0.05	1
1	A	75	GLY	CA	45.577	0.05	1
1	A	75	GLY	N	110.502	0.03	1

7.1.2 Chemical shift referencing ⓘ

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	148	0.22 ± 0.13	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	113	1.19 ± 0.13	Should be checked
$^{13}\text{C}'$	141	0.13 ± 0.11	None needed (< 0.5 ppm)
^{15}N	140	0.07 ± 0.42	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 38%, i.e. 605 atoms were assigned a chemical shift out of a possible 1599. 0 out of 18 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	516/584 (88%)	195/239 (82%)	217/232 (94%)	104/113 (92%)
Sidechain	89/887 (10%)	0/572 (0%)	89/282 (32%)	0/33 (0%)
Aromatic	0/128 (0%)	0/61 (0%)	0/58 (0%)	0/9 (0%)
Overall	605/1599 (38%)	195/872 (22%)	306/572 (53%)	104/155 (67%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 38%, i.e. 619 atoms were assigned a chemical shift out of a possible 1630. 0 out of 18 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	529/599 (88%)	200/245 (82%)	222/238 (93%)	107/116 (92%)
Sidechain	90/903 (10%)	0/583 (0%)	90/287 (31%)	0/33 (0%)
Aromatic	0/128 (0%)	0/61 (0%)	0/58 (0%)	0/9 (0%)
Overall	619/1630 (38%)	200/889 (22%)	312/583 (54%)	107/158 (68%)

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:

