Full wwPDB NMR Structure Validation Report (i)

Jan 31, 2022 – 10:49 AM EST

PDB ID	:	7JI1
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 (i) symbol.

The following versions of software and data (see references (i)) were used in the production of this report:

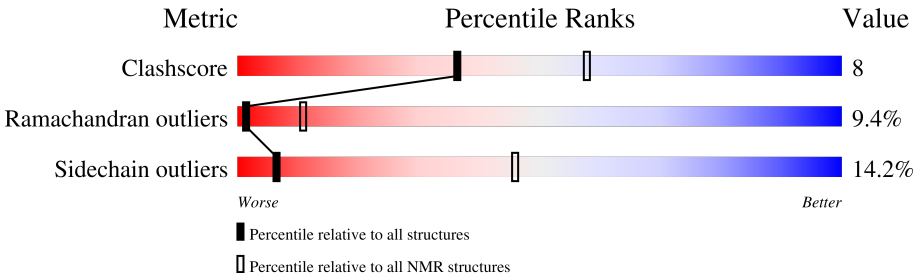
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.26
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.26

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 41%.

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	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	159	54% 18% • • 25%

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)	0.75	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
			Total	C	H	N	O	S	
1	A	119	1895	599	948	161	185	2	0

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

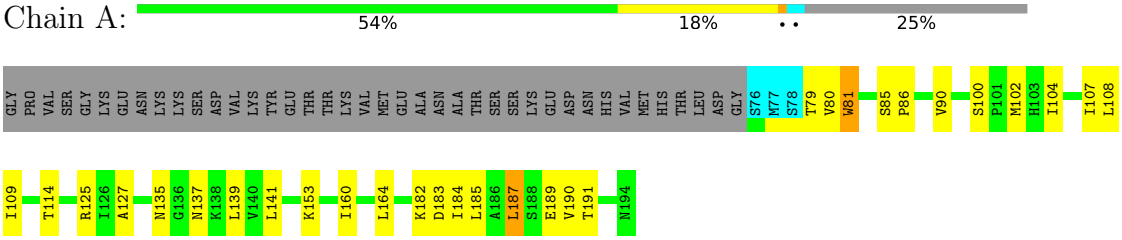
4 Residue-property plots

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

Chain A:



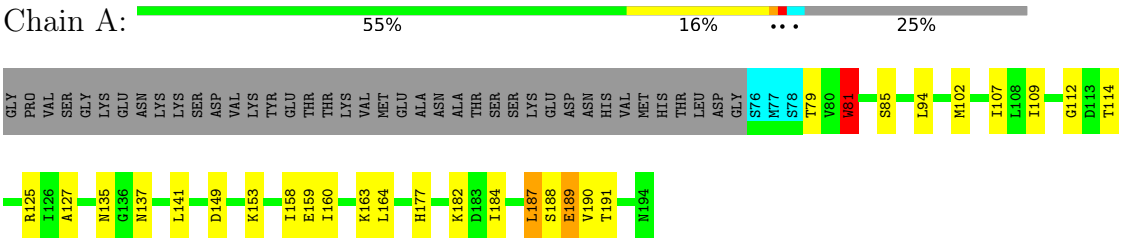
4.2 Scores per residue for each member of the ensemble

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

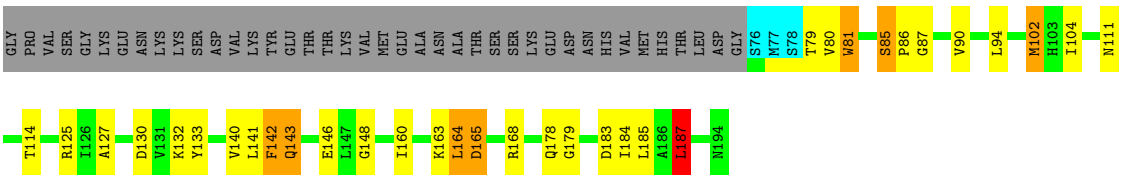
Chain A:



4.2.2 Score per residue for model 2

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

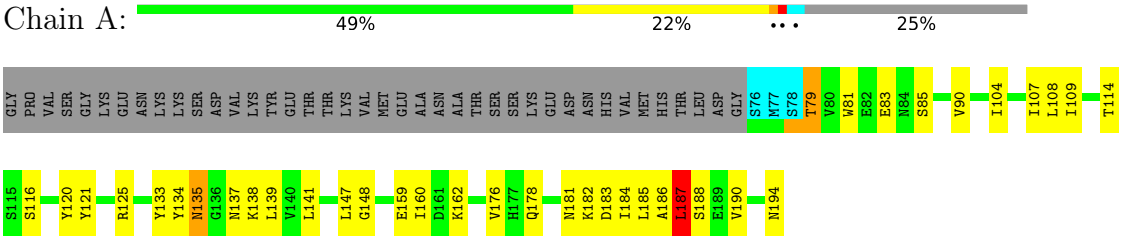
Chain A:



4.2.3 Score per residue for model 3

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

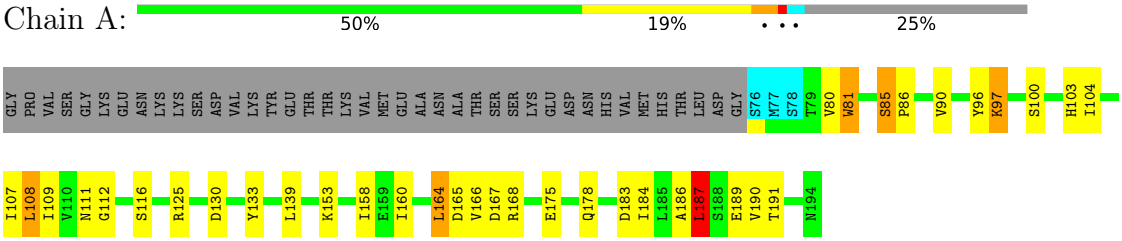
Chain A:



4.2.4 Score per residue for model 4 (medoid)

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

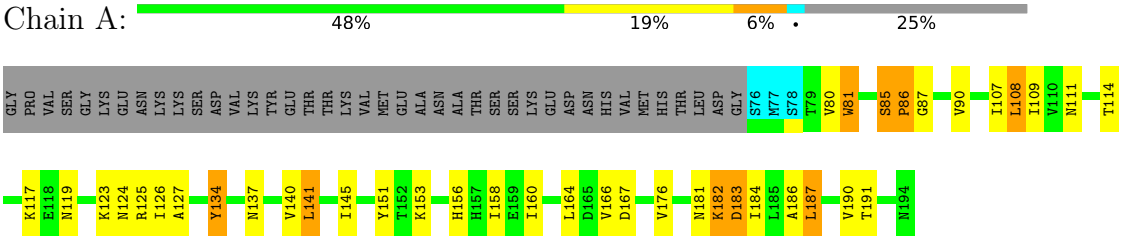
Chain A:



4.2.5 Score per residue for model 5

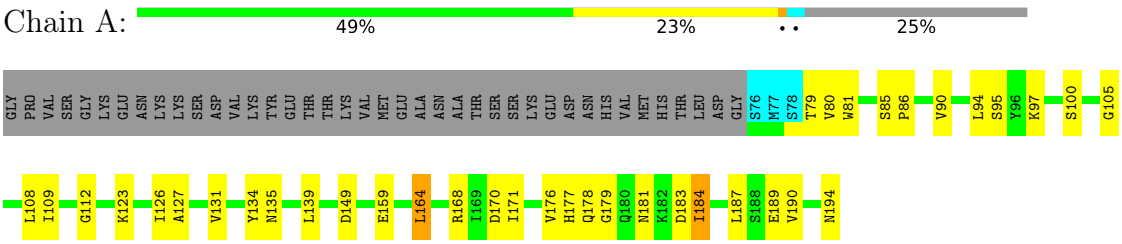
• Molecule 1: ADP-ribosyl cyclase / cyclic ADP-ribose hydrolase

Chain A:



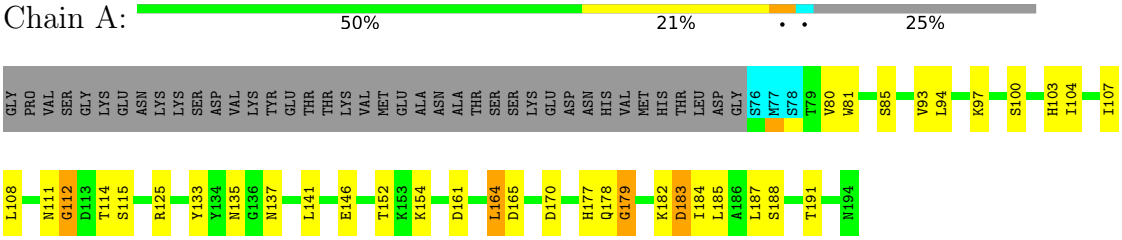
4.2.6 Score per residue for model 6

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



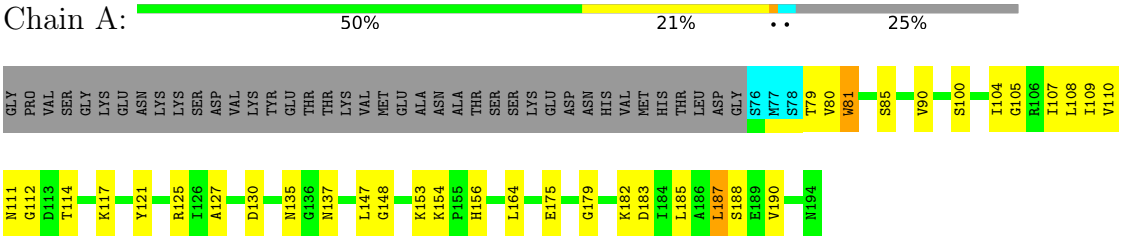
4.2.7 Score per residue for model 7

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



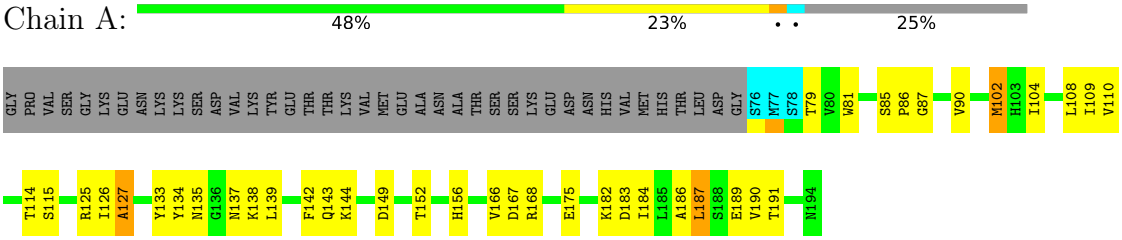
4.2.8 Score per residue for model 8

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



4.2.9 Score per residue for model 9

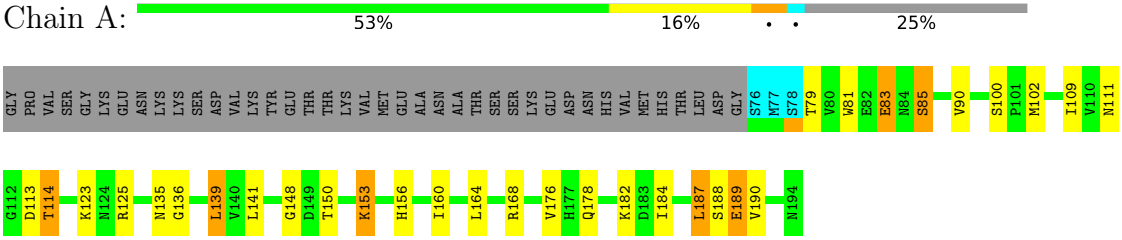
• Molecule 1: ADP-ribosyl cyclase / cyclic ADP-ribose hydrolase



4.2.10 Score per residue for model 10

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

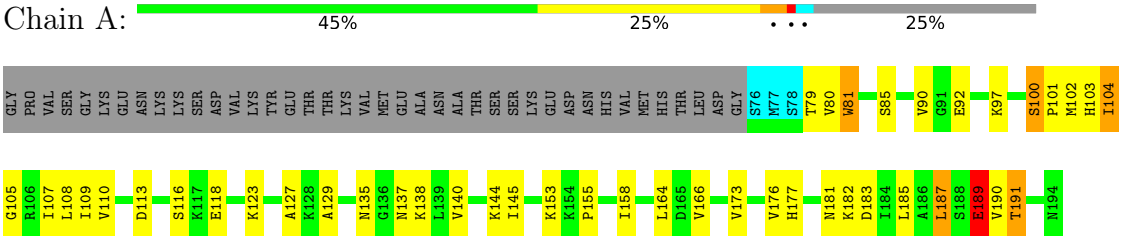
Chain A:



4.2.11 Score per residue for model 11

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

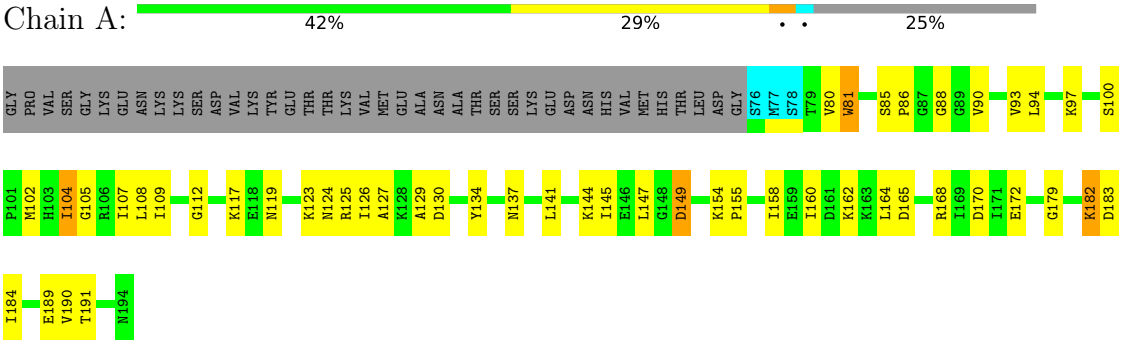
Chain A:



4.2.12 Score per residue for model 12

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

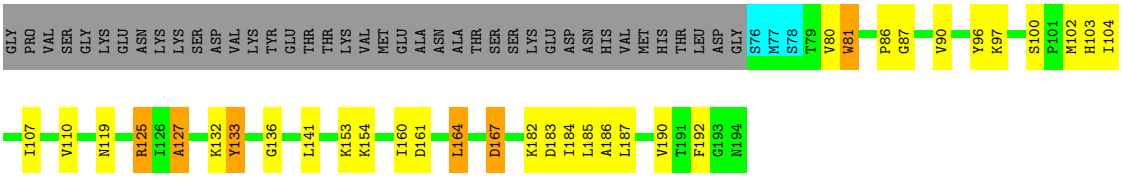
Chain A:



4.2.13 Score per residue for model 13

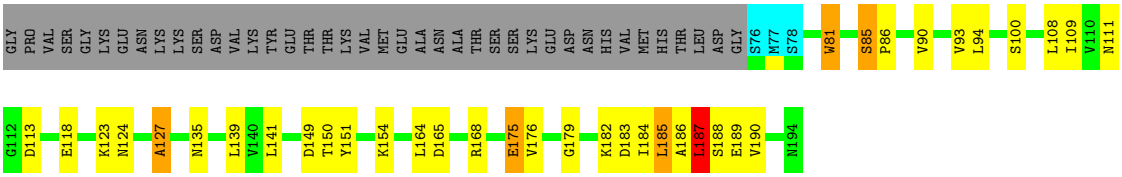
• Molecule 1: ADP-ribosyl cyclase / cyclic ADP-ribose hydrolase

Chain A:



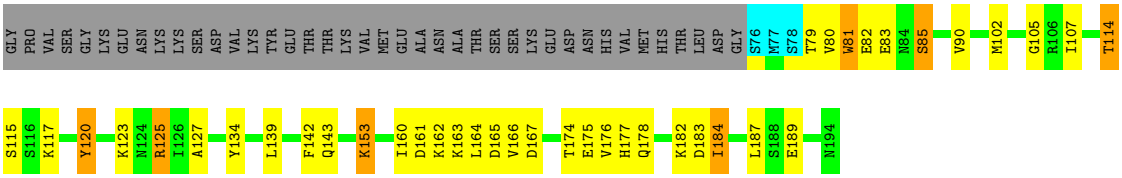
4.2.14 Score per residue for model 14

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



4.2.15 Score per residue for model 15

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



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	793
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	41%

6 Model quality

6.1 Standard geometry

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	0.76±0.01	0±0/944 (0.0± 0.0%)	0.82±0.01	0±0/1271 (0.0± 0.0%)
All	All	0.76	0/14160 (0.0%)	0.82	4/19065 (0.0%)

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(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	120	TYR	CB-CG-CD2	-5.71	117.57	121.00	3	2
1	A	81	TRP	CB-CG-CD2	5.30	133.49	126.60	1	1
1	A	133	TYR	CB-CG-CD2	-5.23	117.86	121.00	2	1

There are no chirality outliers.

There are no planarity outliers.

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	927	929	925	16±3
All	All	13905	13935	13875	233

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 8.

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	9
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: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:164:LEU:HD12	1:A:164:LEU:O	0.69	1.87	5	2
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: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: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:186:ALA:C	1:A:187:LEU:HD22	0.55	2.22	14	4
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
1:A:104:ILE:O	1:A:160:ILE:HD11	0.53	2.02	3	1
1:A:187:LEU:CD1	1:A:190:VAL:HG13	0.53	2.33	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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: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: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: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:139:LEU:HD13	1:A:139:LEU:C	0.48	2.28	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:109:ILE:HG13	1:A:190:VAL:HG23	0.47	1.86	3	1
1:A:187:LEU:HD23	1:A:187:LEU:N	0.47	2.24	11	2
1:A:103:HIS:O	1:A:104:ILE:HD13	0.47	2.09	7	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: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: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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:187:LEU:HD23	1:A:190:VAL:HB	0.46	1.88	8	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:103:HIS:C	1:A:104:ILE:HD13	0.45	2.31	7	2
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:186:ALA:C	1:A:187:LEU:HD12	0.45	2.31	5	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: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: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
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: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:108:LEU:C	1:A:108:LEU:HD13	0.43	2.34	14	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:104:ILE:HG21	1:A:133:TYR:OH	0.42	2.14	3	2
1:A:110:VAL:HG22	1:A:155:PRO:HB3	0.42	1.91	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:104:ILE:CG2	1:A:160:ILE:HD11	0.42	2.45	13	1
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:100:SER:CB	1:A:101:PRO:CD	0.42	2.98	11	1
1:A:108:LEU:HD23	1:A:108:LEU:C	0.42	2.36	12	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:96:TYR:CZ	1:A:97:LYS:O	0.41	2.73	13	1
1:A:185:LEU:HD12	1:A:185:LEU:C	0.41	2.35	2	1
1:A:111:ASN:O	1:A:112:GLY:C	0.41	2.58	7	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:134:TYR:O	1:A:166:VAL:HG21	0.41	2.16	5	1
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
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:184:ILE:CG1	1:A:185:LEU:N	0.40	2.85	14	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 11
All	All	1725/2385 (72%)	1364 (79%)	198 (11%)	163 (9%)	1 11

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
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 (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the sidechain conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	102/140 (73%)	88±3 (86±3%)	14±3 (14±3%)	6 46
All	All	1530/2100 (73%)	1313 (86%)	217 (14%)	6 46

All 67 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	81	TRP	13
1	A	125	ARG	12
1	A	102	MET	8
1	A	85	SER	7
1	A	164	LEU	7
1	A	187	LEU	7
1	A	100	SER	7
1	A	114	THR	6
1	A	165	ASP	6
1	A	168	ARG	6
1	A	97	LYS	5
1	A	139	LEU	5
1	A	154	LYS	5
1	A	130	ASP	4
1	A	178	GLN	4
1	A	181	ASN	4
1	A	188	SER	4
1	A	175	GLU	4
1	A	117	LYS	4
1	A	141	LEU	4
1	A	159	GLU	3
1	A	177	HIS	3
1	A	111	ASN	3
1	A	142	PHE	3
1	A	143	GLN	3
1	A	116	SER	3
1	A	185	LEU	3
1	A	108	LEU	3
1	A	119	ASN	3

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Mol	Chain	Res	Type	Models (Total)
1	A	134	TYR	3
1	A	170	ASP	3
1	A	115	SER	3
1	A	104	ILE	3
1	A	135	ASN	3
1	A	144	LYS	3
1	A	113	ASP	3
1	A	132	LYS	2
1	A	146	GLU	2
1	A	121	TYR	2
1	A	194	ASN	2
1	A	103	HIS	2
1	A	167	ASP	2
1	A	124	ASN	2
1	A	161	ASP	2
1	A	110	VAL	2
1	A	149	ASP	2
1	A	191	THR	2
1	A	153	LYS	2
1	A	189	GLU	2
1	A	118	GLU	2
1	A	162	LYS	2
1	A	182	LYS	2
1	A	140	VAL	1
1	A	163	LYS	1
1	A	79	THR	1
1	A	147	LEU	1
1	A	151	TYR	1
1	A	156	HIS	1
1	A	95	SER	1
1	A	183	ASP	1
1	A	83	GLU	1
1	A	92	GLU	1
1	A	123	LYS	1
1	A	137	ASN	1
1	A	133	TYR	1
1	A	93	VAL	1
1	A	174	THR	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 monosaccharides 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 41% for the well-defined parts and 41% 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	793
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 ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	148	0.22 ± 0.10	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	113	1.18 ± 0.20	Should be applied
$^{13}C'$	141	0.13 ± 0.13	None needed (< 0.5 ppm)
^{15}N	140	0.07 ± 0.42	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 41%, i.e. 595 atoms were assigned a chemical shift out of a possible 1446. 0 out of 18 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	506/574 (88%)	185/229 (81%)	217/232 (94%)	104/113 (92%)
Sidechain	89/753 (12%)	0/438 (0%)	89/282 (32%)	0/33 (0%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	0/119 (0%)	0/61 (0%)	0/49 (0%)	0/9 (0%)
Overall	595/1446 (41%)	185/728 (25%)	306/563 (54%)	104/155 (67%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 41%, i.e. 609 atoms were assigned a chemical shift out of a possible 1475. 0 out of 18 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	519/589 (88%)	190/235 (81%)	222/238 (93%)	107/116 (92%)
Sidechain	90/767 (12%)	0/447 (0%)	90/287 (31%)	0/33 (0%)
Aromatic	0/119 (0%)	0/61 (0%)	0/49 (0%)	0/9 (0%)
Overall	609/1475 (41%)	190/743 (26%)	312/574 (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.

Random coil index (RCI) for chain A: