



Full wwPDB NMR Structure Validation Report ⓘ

Jun 14, 2021 – 12:07 PM BST

PDB ID : 7A05
Title : NMR structure of D3-D4 domains of *Vibrio vulnificus* ribosomal protein S1
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Deposited on : 2020-08-06

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.

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A user guide is available at

<https://www.wwpdb.org/validation/2017/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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	:	2.20
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.20

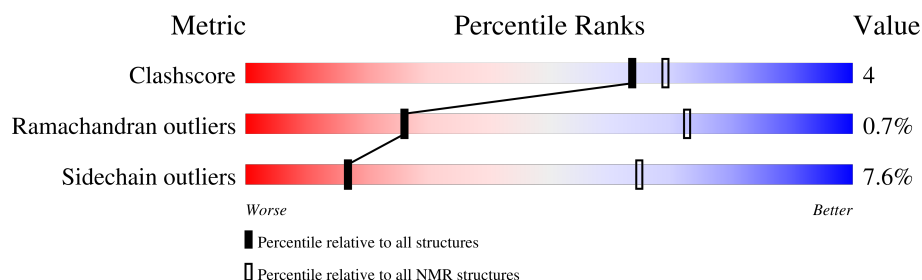
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 87%.

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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	173	

2 Ensemble composition and analysis

This entry contains 20 models. Model 11 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:185-A:310, A:314-A:348 (161)	0.26	11

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 4 clusters and 5 single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2731 atoms, of which 1370 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called 30S ribosomal protein S1.

Mol	Chain	Residues	Atoms						Trace
1	A	173	Total	C	H	N	O	S	0
			2731	856	1370	238	261	6	

There are 3 discrepancies between the modelled and reference sequences:

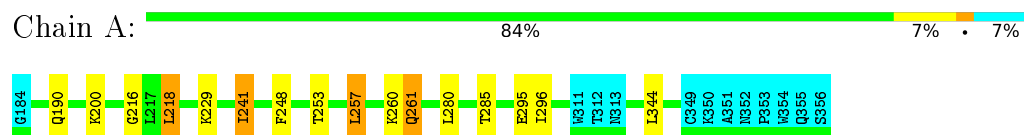
Chain	Residue	Modelled	Actual	Comment	Reference
A	184	GLY	-	expression tag	UNP A0A087IKW3
A	185	ALA	-	expression tag	UNP A0A087IKW3
A	186	MET	-	expression tag	UNP A0A087IKW3

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: 30S ribosomal protein S1

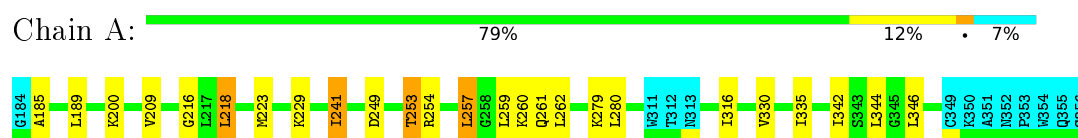


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

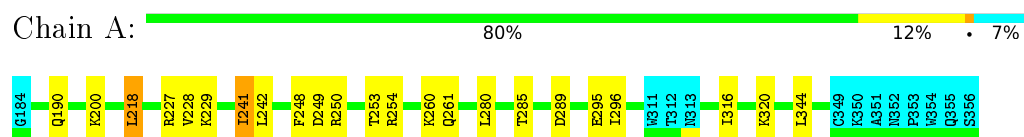
4.2.1 Score per residue for model 1

- Molecule 1: 30S ribosomal protein S1



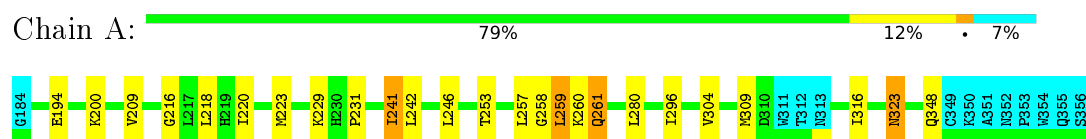
4.2.2 Score per residue for model 2

- Molecule 1: 30S ribosomal protein S1



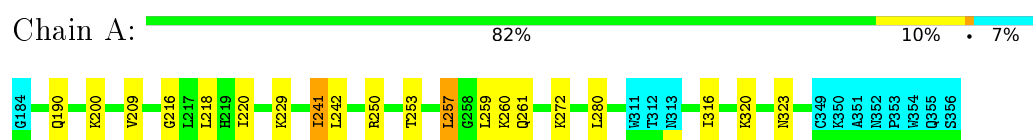
4.2.3 Score per residue for model 3

- Molecule 1: 30S ribosomal protein S1



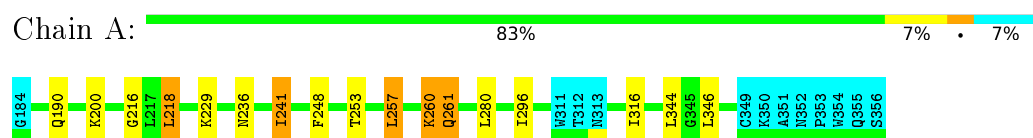
4.2.4 Score per residue for model 4

- Molecule 1: 30S ribosomal protein S1



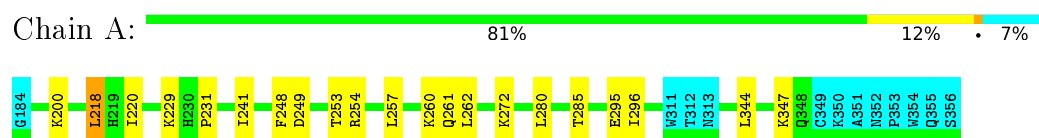
4.2.5 Score per residue for model 5

- Molecule 1: 30S ribosomal protein S1



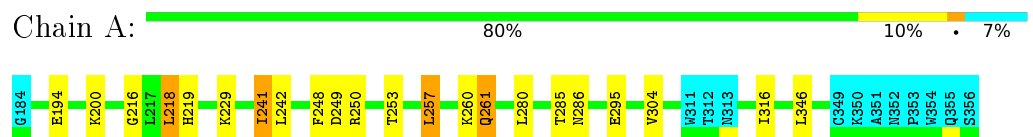
4.2.6 Score per residue for model 6

- Molecule 1: 30S ribosomal protein S1



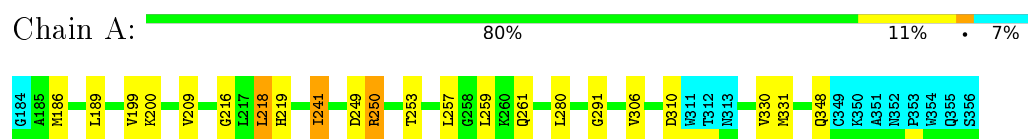
4.2.7 Score per residue for model 7

- Molecule 1: 30S ribosomal protein S1



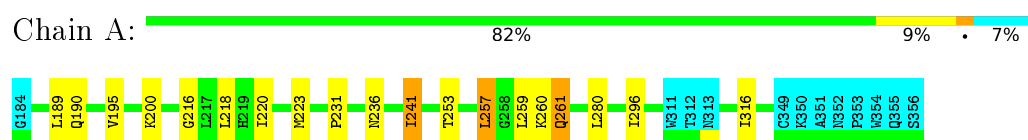
4.2.8 Score per residue for model 8

- Molecule 1: 30S ribosomal protein S1



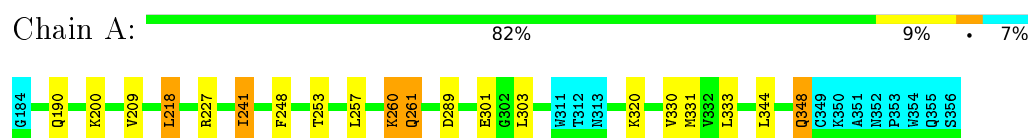
4.2.9 Score per residue for model 9

- Molecule 1: 30S ribosomal protein S1



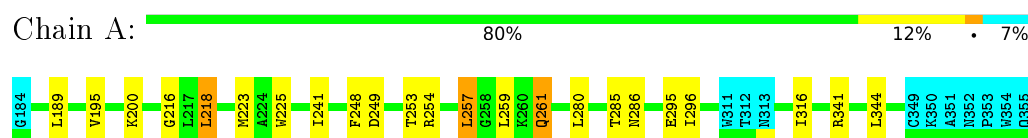
4.2.10 Score per residue for model 10

- Molecule 1: 30S ribosomal protein S1



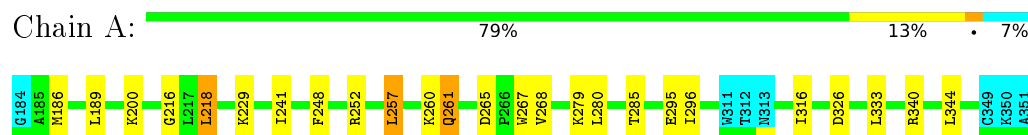
4.2.11 Score per residue for model 11 (medoid)

- Molecule 1: 30S ribosomal protein S1



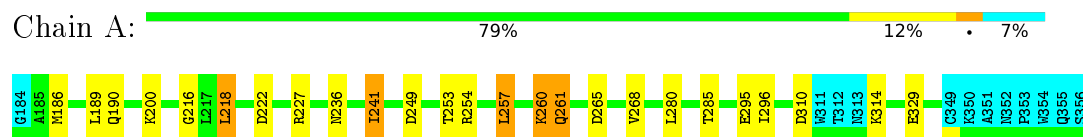
4.2.12 Score per residue for model 12

- Molecule 1: 30S ribosomal protein S1



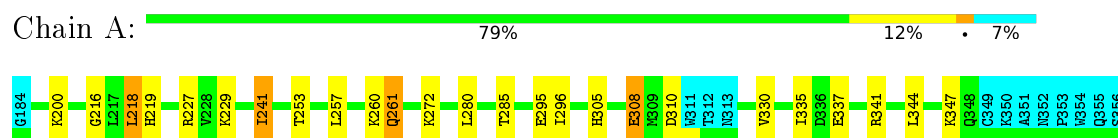
4.2.13 Score per residue for model 13

- Molecule 1: 30S ribosomal protein S1



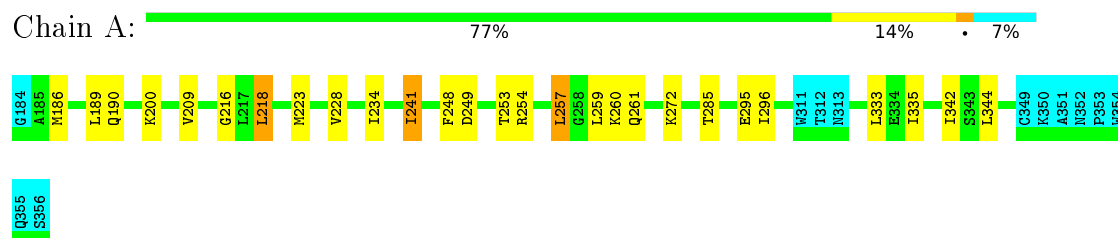
4.2.14 Score per residue for model 14

- Molecule 1: 30S ribosomal protein S1



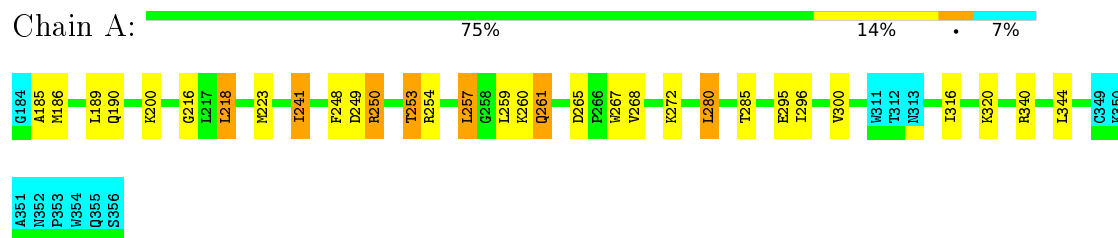
4.2.15 Score per residue for model 15

- Molecule 1: 30S ribosomal protein S1



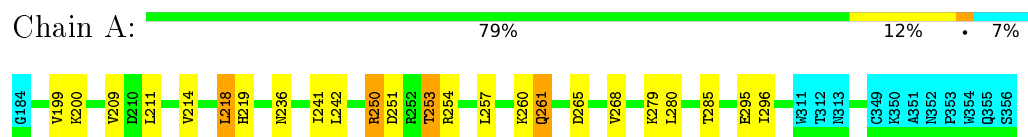
4.2.16 Score per residue for model 16

- Molecule 1: 30S ribosomal protein S1



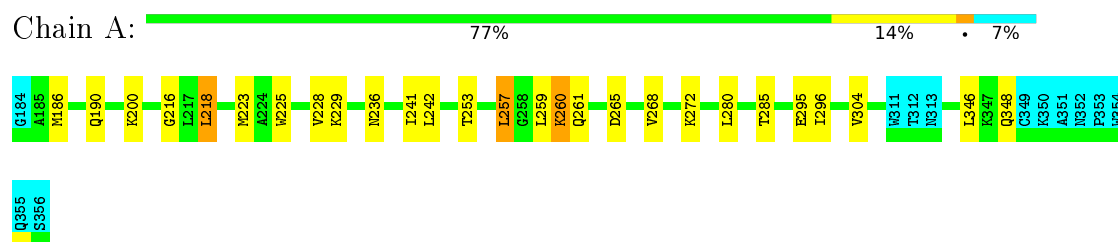
4.2.17 Score per residue for model 17

- Molecule 1: 30S ribosomal protein S1



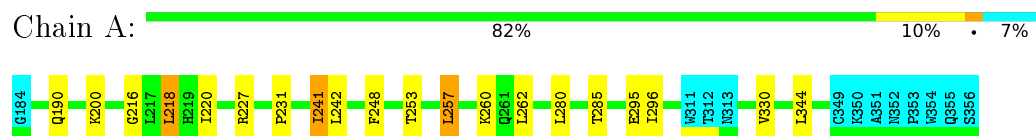
4.2.18 Score per residue for model 18

- Molecule 1: 30S ribosomal protein S1



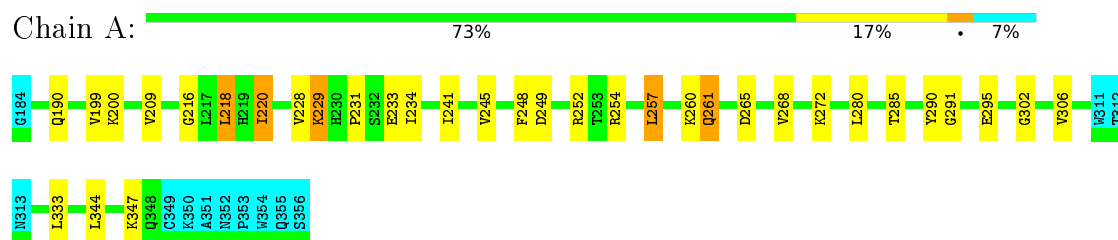
4.2.19 Score per residue for model 19

- Molecule 1: 30S ribosomal protein S1



4.2.20 Score per residue for model 20

- Molecule 1: 30S ribosomal protein S1



5 Refinement protocol and experimental data overview

The models were refined using the following method: *simulated annealing with torsion angle dynamics, cartesian angle dynamics, molecular dynamics*.

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *target function*.

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

Software name	Classification	Version
CYANA	structure calculation	3.x
CNS	structure calculation	1.1
ARIA	refinement	1.2 HJ

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	4058
Number of shifts mapped to atoms	4058
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	87%

6 Model quality ⓘ

6.1 Standard geometry ⓘ

There are no covalent bond-length or bond-angle outliers.

There are no bond-length outliers.

There are no bond-angle outliers.

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	1263	1283	1278	11±3
All	All	25260	25660	25560	218

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 4.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:280:LEU:HD13	1:A:296:ILE:HG23	0.62	1.71	18	12
1:A:261:GLN:CD	1:A:261:GLN:H	0.62	1.97	15	8
1:A:323:ASN:HD22	1:A:323:ASN:N	0.62	1.92	3	1
1:A:296:ILE:HD11	1:A:344:LEU:HD11	0.58	1.74	11	7
1:A:216:GLY:HA3	1:A:257:LEU:HD21	0.58	1.73	14	16
1:A:218:LEU:HG	1:A:257:LEU:HD23	0.58	1.75	16	15
1:A:290:TYR:C	1:A:306:VAL:HG13	0.57	2.19	20	1
1:A:223:MET:SD	1:A:259:LEU:HD12	0.57	2.39	15	3
1:A:261:GLN:H	1:A:261:GLN:NE2	0.57	1.98	5	6
1:A:220:ILE:HD11	1:A:231:PRO:HD3	0.55	1.76	19	5
1:A:249:ASP:HB2	1:A:254:ARG:HB3	0.54	1.80	2	2
1:A:257:LEU:HD22	1:A:257:LEU:N	0.52	2.20	16	16
1:A:330:VAL:HG21	1:A:344:LEU:HD23	0.51	1.82	19	2
1:A:223:MET:HA	1:A:259:LEU:HB2	0.51	1.83	9	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:209:VAL:HG23	1:A:218:LEU:HD11	0.50	1.82	1	6
1:A:262:LEU:H	1:A:262:LEU:HD22	0.49	1.67	6	1
1:A:189:LEU:HG	1:A:190:GLN:H	0.48	1.67	16	1
1:A:189:LEU:HD11	1:A:195:VAL:HG11	0.47	1.85	9	2
1:A:285:THR:HG21	1:A:295:GLU:HB2	0.47	1.84	17	13
1:A:246:LEU:HD11	1:A:261:GLN:HG3	0.47	1.86	3	1
1:A:218:LEU:HG	1:A:257:LEU:HB2	0.47	1.86	3	3
1:A:304:VAL:HG23	1:A:309:MET:SD	0.47	2.50	3	1
1:A:218:LEU:HG	1:A:257:LEU:HD12	0.47	1.87	17	3
1:A:218:LEU:HD12	1:A:218:LEU:H	0.46	1.70	6	3
1:A:262:LEU:HD22	1:A:262:LEU:N	0.45	2.26	6	3
1:A:218:LEU:HD12	1:A:218:LEU:N	0.45	2.27	6	5
1:A:304:VAL:HG11	1:A:346:LEU:HB2	0.45	1.88	18	2
1:A:249:ASP:HB2	1:A:254:ARG:HB2	0.45	1.89	11	4
1:A:262:LEU:H	1:A:262:LEU:CD2	0.44	2.25	6	1
1:A:291:GLY:N	1:A:306:VAL:HG13	0.44	2.28	20	2
1:A:241:ILE:HD13	1:A:241:ILE:H	0.44	1.73	15	11
1:A:260:LYS:HG2	1:A:261:GLN:N	0.44	2.28	10	2
1:A:199:VAL:HG22	1:A:209:VAL:CG2	0.43	2.44	17	3
1:A:265:ASP:O	1:A:268:VAL:HG22	0.43	2.13	18	4
1:A:335:ILE:HG12	1:A:342:ILE:HG23	0.42	1.91	1	2
1:A:305:HIS:HB3	1:A:308:GLU:OE1	0.42	2.14	14	1
1:A:330:VAL:HB	1:A:344:LEU:HB3	0.42	1.92	1	1
1:A:330:VAL:HA	1:A:348:GLN:NE2	0.42	2.28	8	1
1:A:280:LEU:HD13	1:A:280:LEU:N	0.42	2.29	16	1
1:A:258:GLY:HA3	1:A:261:GLN:HE21	0.42	1.74	3	1
1:A:335:ILE:HG23	1:A:337:GLU:OE2	0.42	2.14	14	1
1:A:346:LEU:O	1:A:346:LEU:HD23	0.42	2.15	1	2
1:A:267:TRP:CZ3	1:A:340:ARG:HA	0.42	2.50	16	2
1:A:185:ALA:O	1:A:189:LEU:HD13	0.41	2.16	1	1
1:A:194:GLU:HG2	1:A:242:LEU:HD11	0.41	1.92	7	2
1:A:265:ASP:HB3	1:A:268:VAL:HG13	0.41	1.93	16	2
1:A:186:MET:HA	1:A:189:LEU:HB2	0.41	1.91	12	2
1:A:228:VAL:HG21	1:A:234:ILE:HD13	0.41	1.91	15	1
1:A:249:ASP:HB3	1:A:254:ARG:H	0.41	1.75	16	1
1:A:211:LEU:HD12	1:A:214:VAL:HG13	0.41	1.92	17	1
1:A:296:ILE:HD12	1:A:300:VAL:HG12	0.41	1.92	16	1
1:A:330:VAL:CG2	1:A:344:LEU:HD23	0.41	2.45	19	1
1:A:302:GLY:HA3	1:A:344:LEU:CD2	0.41	2.44	20	1
1:A:261:GLN:CD	1:A:261:GLN:N	0.41	2.73	1	2
1:A:253:THR:HG23	1:A:254:ARG:H	0.41	1.75	1	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:249:ASP:O	1:A:250:ARG:C	0.41	2.59	8	2
1:A:222:ASP:HA	1:A:260:LYS:CD	0.41	2.46	13	1
1:A:249:ASP:HB3	1:A:253:THR:HG23	0.41	1.93	1	1
1:A:218:LEU:N	1:A:218:LEU:HD12	0.41	2.31	19	3
1:A:241:ILE:H	1:A:241:ILE:HD13	0.41	1.75	4	3
1:A:186:MET:HA	1:A:189:LEU:HB3	0.41	1.92	15	2
1:A:331:MET:HB3	1:A:348:GLN:HG2	0.41	1.92	8	2
1:A:330:VAL:HG21	1:A:344:LEU:HD13	0.41	1.93	10	1
1:A:228:VAL:CG2	1:A:229:LYS:N	0.41	2.84	20	1
1:A:250:ARG:HD3	1:A:251:ASP:H	0.40	1.76	17	1
1:A:225:TRP:CD1	1:A:260:LYS:HB2	0.40	2.52	18	1
1:A:233:GLU:C	1:A:234:ILE:HD12	0.40	2.37	20	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	161/173 (93%)	147±2 (91±1%)	13±2 (8±1%)	1±1 (1±0%)	26	73
All	All	3220/3460 (93%)	2940 (91%)	257 (8%)	23 (1%)	26	73

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

Mol	Chain	Res	Type	Models (Total)
1	A	253	THR	18
1	A	250	ARG	2
1	A	186	MET	2
1	A	185	ALA	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	140/150 (93%)	129±3 (92±2%)	11±3 (8±2%)	17 65
All	All	2800/3000 (93%)	2586 (92%)	214 (8%)	17 65

All 38 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	200	LYS	20
1	A	241	ILE	20
1	A	260	LYS	18
1	A	218	LEU	17
1	A	261	GLN	16
1	A	257	LEU	13
1	A	229	LYS	11
1	A	248	PHE	11
1	A	190	GLN	10
1	A	272	LYS	7
1	A	280	LEU	6
1	A	227	ARG	5
1	A	242	LEU	5
1	A	236	ASN	5
1	A	320	LYS	4
1	A	250	ARG	4
1	A	219	HIS	4
1	A	333	LEU	4
1	A	259	LEU	3
1	A	348	GLN	3
1	A	347	LYS	3
1	A	228	VAL	2
1	A	289	ASP	2
1	A	323	ASN	2
1	A	220	ILE	2
1	A	286	ASN	2
1	A	341	ARG	2
1	A	252	ARG	2
1	A	279	LYS	2
1	A	301	GLU	1
1	A	303	LEU	1
1	A	225	TRP	1
1	A	326	ASP	1
1	A	310	ASP	1

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Mol	Chain	Res	Type	Models (Total)
1	A	314	LYS	1
1	A	308	GLU	1
1	A	253	THR	1
1	A	245	VAL	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 monosaccharides 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 87% for the well-defined parts and 87% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *D_1292110584_cs_P1.str.V1*

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	1947
Number of shifts mapped to atoms	1947
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	3

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	170	-0.03 ± 0.11	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	147	-0.17 ± 0.07	None needed (< 0.5 ppm)
$^{13}\text{C}'$	0	—	None (insufficient data)
^{15}N	160	0.30 ± 0.22	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 79%, i.e. 1569 atoms were assigned a chemical shift out of a possible 1984. 38 out of 38 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	620/797 (78%)	311/318 (98%)	158/322 (49%)	151/157 (96%)
Sidechain	859/1072 (80%)	525/619 (85%)	327/406 (81%)	7/47 (15%)

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	Total	¹H	¹³C	¹⁵N
Aromatic	90/115 (78%)	47/59 (80%)	41/44 (93%)	2/12 (17%)
Overall	1569/1984 (79%)	883/996 (89%)	526/772 (68%)	160/216 (74%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 79%, i.e. 1691 atoms were assigned a chemical shift out of a possible 2130. 38 out of 38 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	662/855 (77%)	332/341 (97%)	170/346 (49%)	160/168 (95%)
Sidechain	917/1136 (81%)	563/658 (86%)	344/427 (81%)	10/51 (20%)
Aromatic	112/139 (81%)	58/71 (82%)	50/54 (93%)	4/14 (29%)
Overall	1691/2130 (79%)	953/1070 (89%)	564/827 (68%)	174/233 (75%)

7.1.4 Statistically unusual chemical shifts ⓘ

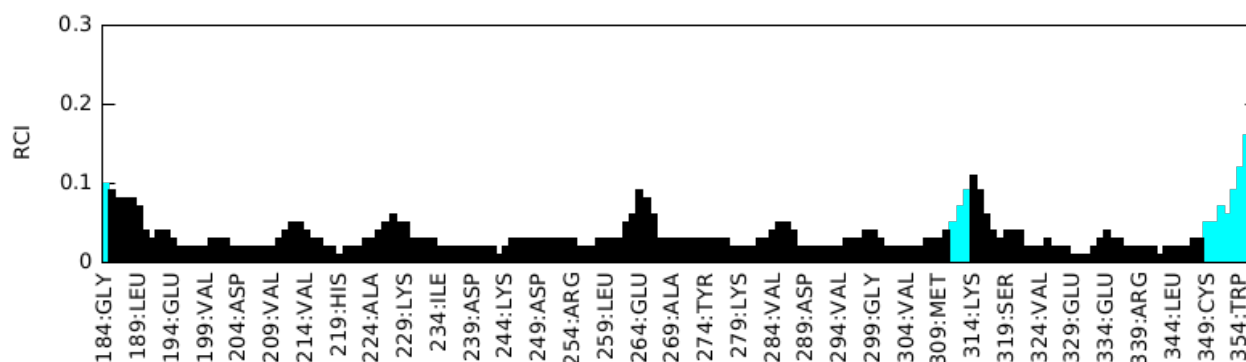
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

Mol	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	260	LYS	HD3	0.24	2.75 – 0.45	-5.9
1	A	260	LYS	HG3	-0.20	2.76 – -0.04	-5.6
1	A	260	LYS	HD2	0.37	2.76 – 0.46	-5.4

7.1.5 Random Coil Index (RCI) plots ⓘ

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:



7.2 Chemical shift list 2

File name: working_cs.cif

Chemical shift list name: *S134-bmr-b-c.tbl*

7.2.1 Bookkeeping [i](#)

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	2111
Number of shifts mapped to atoms	2111
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	3

7.2.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	170	-0.00 ± 0.17	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	147	-0.21 ± 0.10	None needed (< 0.5 ppm)
$^{13}\text{C}'$	164	0.35 ± 0.17	None needed (< 0.5 ppm)
^{15}N	160	0.12 ± 0.42	None needed (< 0.5 ppm)

7.2.3 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 87%, i.e. 1725 atoms were assigned a chemical shift out of a possible 1984. 38 out of 38 assigned methyl groups (LEU and VAL) were assigned

stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	776/797 (97%)	311/318 (98%)	314/322 (98%)	151/157 (96%)
Sidechain	859/1072 (80%)	525/619 (85%)	327/406 (81%)	7/47 (15%)
Aromatic	90/115 (78%)	47/59 (80%)	41/44 (93%)	2/12 (17%)
Overall	1725/1984 (87%)	883/996 (89%)	682/772 (88%)	160/216 (74%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 87%, i.e. 1855 atoms were assigned a chemical shift out of a possible 2130. 38 out of 38 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	826/855 (97%)	332/341 (97%)	334/346 (97%)	160/168 (95%)
Sidechain	917/1136 (81%)	563/658 (86%)	344/427 (81%)	10/51 (20%)
Aromatic	112/139 (81%)	58/71 (82%)	50/54 (93%)	4/14 (29%)
Overall	1855/2130 (87%)	953/1070 (89%)	728/827 (88%)	174/233 (75%)

7.2.4 Statistically unusual chemical shifts [i](#)

The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

Mol	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	260	LYS	HD3	0.24	2.75 – 0.45	-5.9
1	A	260	LYS	HG3	-0.20	2.76 – -0.04	-5.6
1	A	260	LYS	HD2	0.37	2.76 – 0.46	-5.4

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.

Random coil index (RCI) for chain A:

