Full wwPDB NMR Structure Validation Report (i)

Jan 19, 2021 – 12:07 PM EST

PDB ID	:	7KRB
Title	:	Solution Structure of the Dysferlin C2A Domain in its Calcium-bound State
Authors	:	Wang, Y.; Mercier, P.; Santamaria, L.; Shaw, G.S.
Deposited on	:	2020-11-19

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:

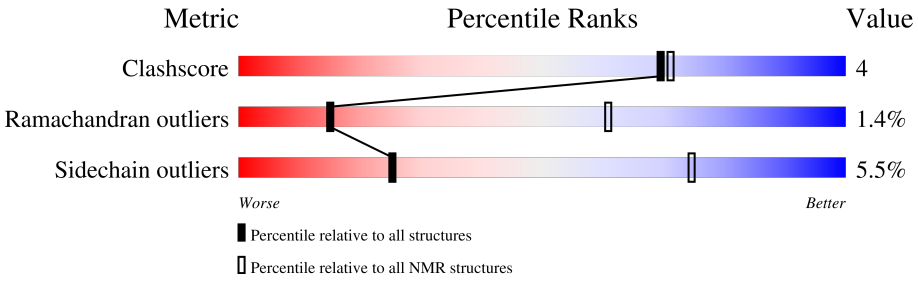
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.16
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.16

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 85%.

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	138	70% 7% • 22%

2 Ensemble composition and analysis

This entry contains 20 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:0-A:12, A:22-A:70, A:81-A:125 (107)	0.35	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 3 clusters and 5 single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 2099 atoms, of which 1055 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Isoform 15 of Dysferlin.

Mol	Chain	Residues	Atoms						Trace
1	A	138	Total	C	H	N	O	S	0
			2099	665	1055	179	197	3	

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	GLY	-	expression tag	UNP O75923
A	-5	SER	-	expression tag	UNP O75923
A	-4	GLY	-	expression tag	UNP O75923
A	-3	GLY	-	expression tag	UNP O75923
A	-2	GLY	-	expression tag	UNP O75923
A	-1	GLY	-	expression tag	UNP O75923
A	0	GLY	-	expression tag	UNP O75923
A	131	LEU	-	expression tag	UNP O75923

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: Isoform 15 of Dysferlin

Chain A:

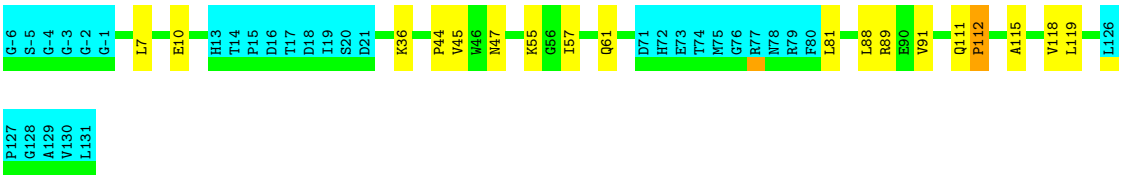
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: Isoform 15 of Dysferlin

Chain A:



4.2.2 Score per residue for model 2

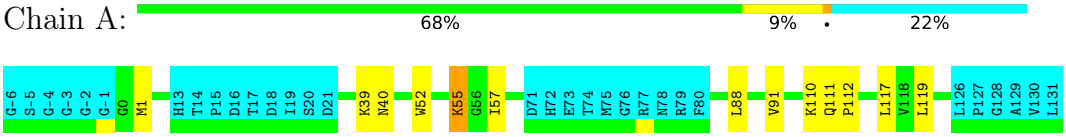
• Molecule 1: Isoform 15 of Dysferlin

Chain A:

4.2.3 Score per residue for model 3

• Molecule 1: Isoform 15 of Dysferlin

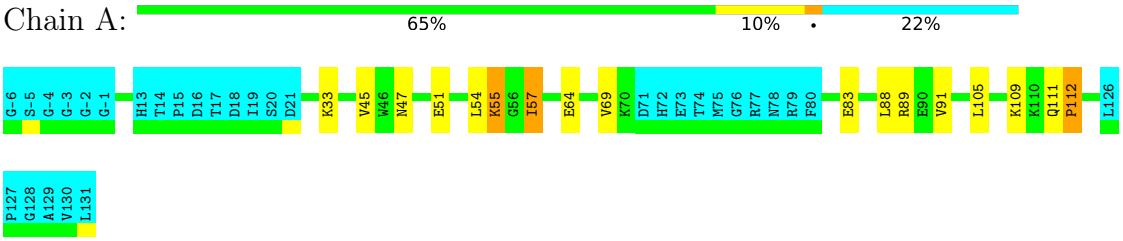
Chain A:



4.2.4 Score per residue for model 4 (medoid)

• Molecule 1: Isoform 15 of Dysferlin

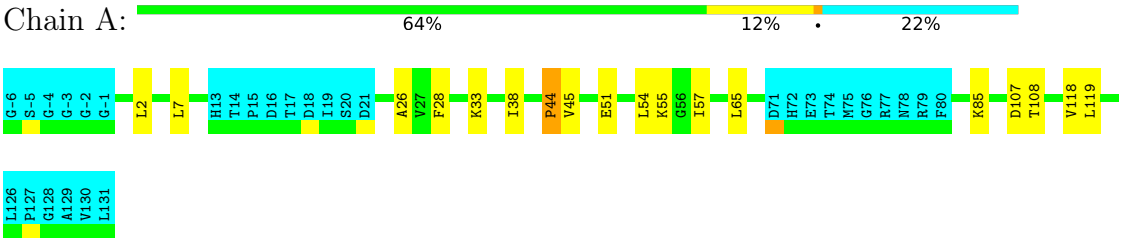
Chain A:



4.2.5 Score per residue for model 5

• Molecule 1: Isoform 15 of Dysferlin

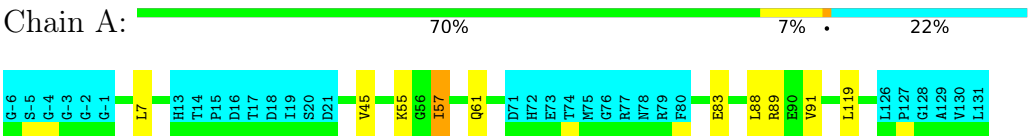
Chain A:



4.2.6 Score per residue for model 6

• Molecule 1: Isoform 15 of Dysferlin

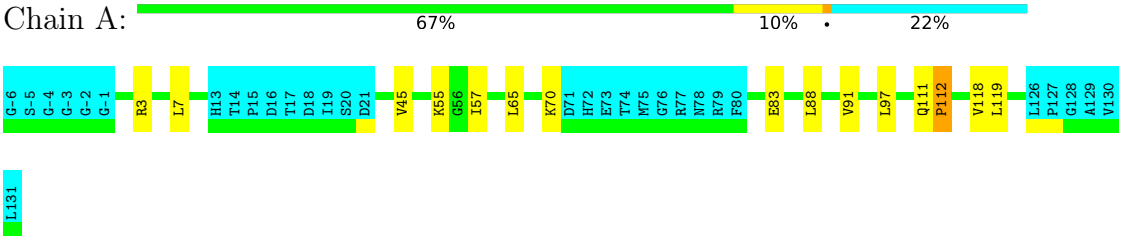
Chain A:



4.2.7 Score per residue for model 7

• Molecule 1: Isoform 15 of Dysferlin

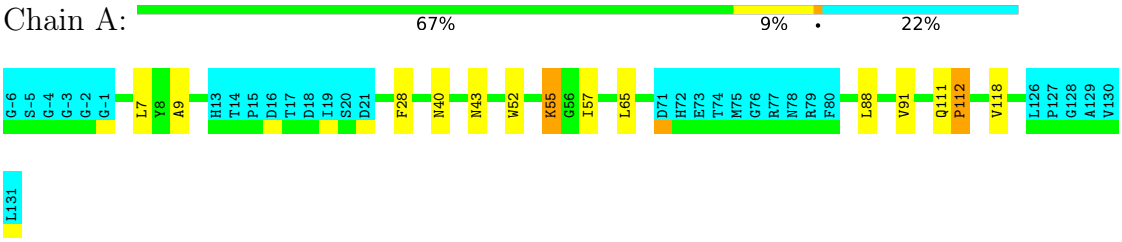
Chain A:



4.2.8 Score per residue for model 8

• Molecule 1: Isoform 15 of Dysferlin

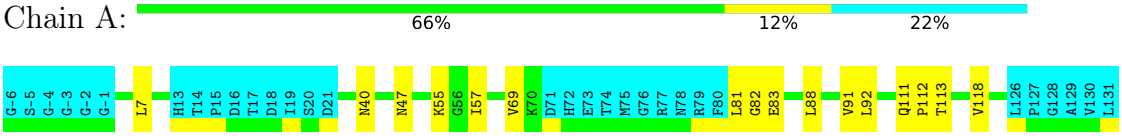
Chain A:



4.2.9 Score per residue for model 9

• Molecule 1: Isoform 15 of Dysferlin

Chain A:



4.2.10 Score per residue for model 10

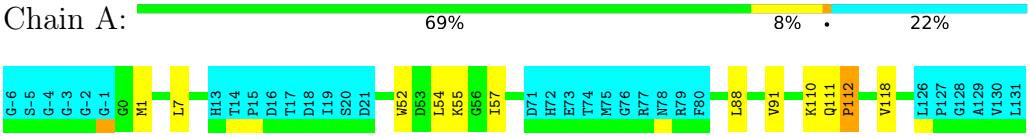
• Molecule 1: Isoform 15 of Dysferlin

Chain A:

4.2.11 Score per residue for model 11

• Molecule 1: Isoform 15 of Dysferlin

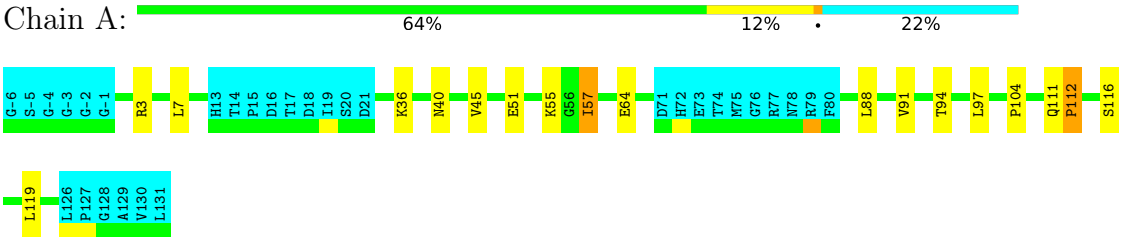
Chain A:



4.2.12 Score per residue for model 12

• Molecule 1: Isoform 15 of Dysferlin

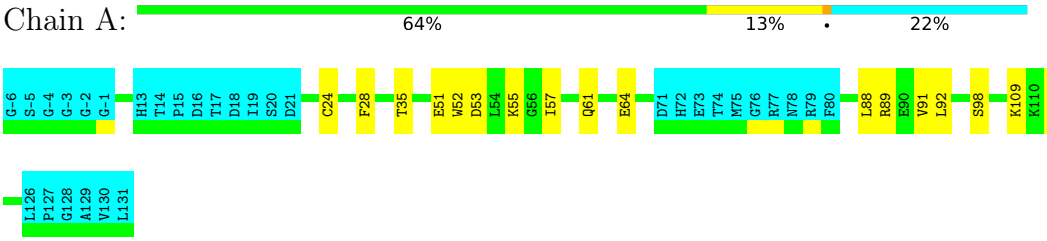
Chain A:



4.2.13 Score per residue for model 13

• Molecule 1: Isoform 15 of Dysferlin

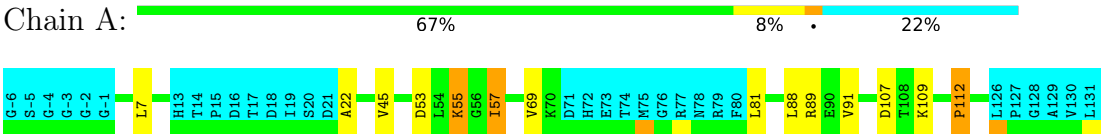
Chain A:



4.2.14 Score per residue for model 14

• Molecule 1: Isoform 15 of Dysferlin

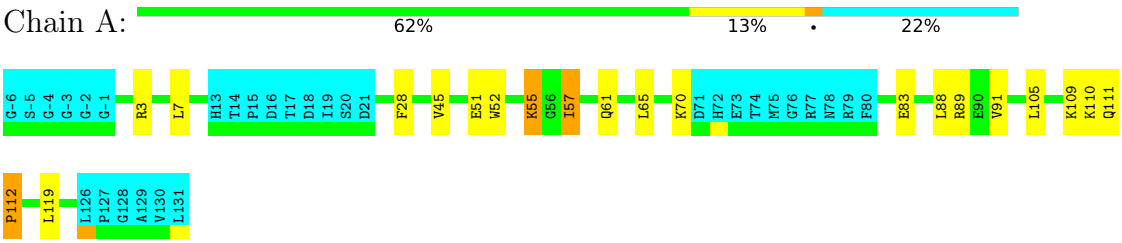
Chain A:



4.2.15 Score per residue for model 15

• Molecule 1: Isoform 15 of Dysferlin

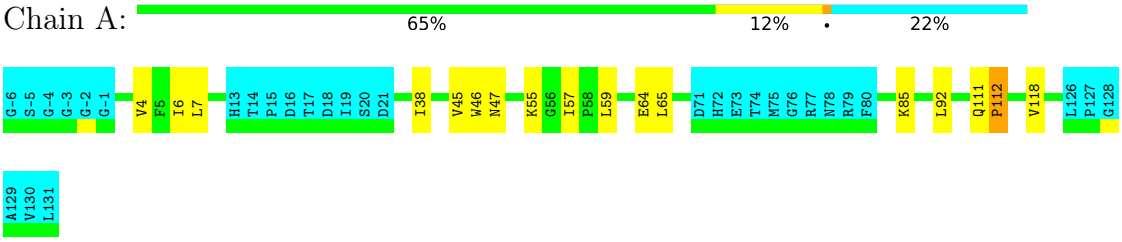
Chain A:



4.2.16 Score per residue for model 16

• Molecule 1: Isoform 15 of Dysferlin

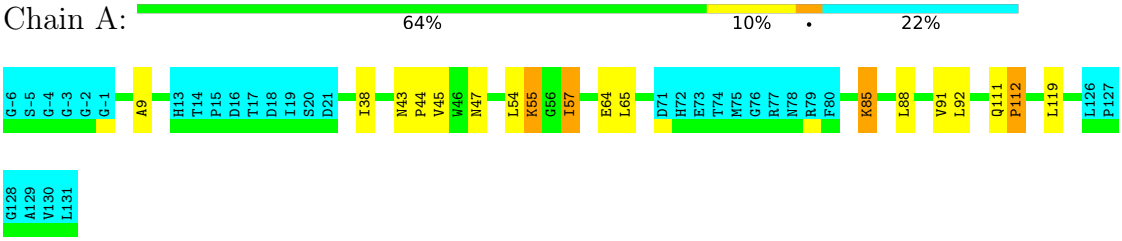
Chain A:



4.2.17 Score per residue for model 17

• Molecule 1: Isoform 15 of Dysferlin

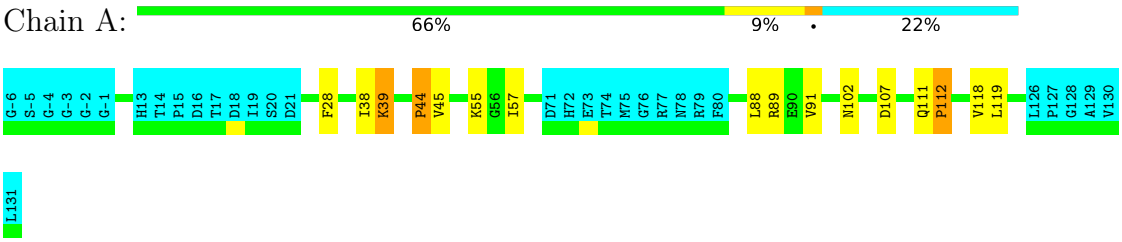
Chain A:



4.2.18 Score per residue for model 18

• Molecule 1: Isoform 15 of Dysferlin

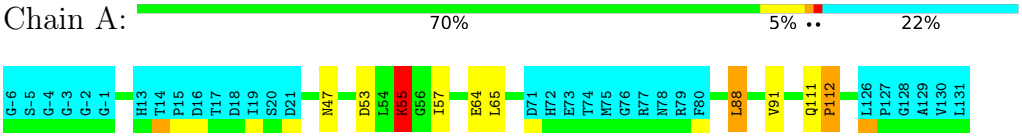
Chain A:



4.2.19 Score per residue for model 19

• Molecule 1: Isoform 15 of Dysferlin

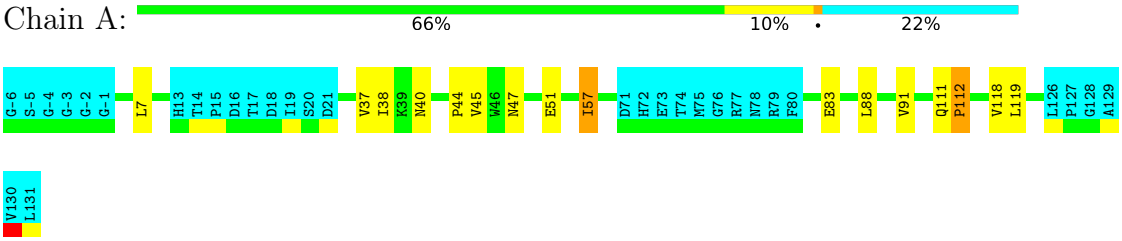
Chain A:



4.2.20 Score per residue for model 20

• Molecule 1: Isoform 15 of Dysferlin

Chain A:



5 Refinement protocol and experimental data overview

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

Of the 100 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
CYANA	structure calculation	2.1
X-PLOR 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	1
Total number of shifts	1464
Number of shifts mapped to atoms	1342
Number of unparsed shifts	122
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	85%

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	822	854	854	6±2
All	All	16440	17080	17080	124

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:7:LEU:HB2	1:A:118:VAL:HG23	0.61	1.73	9	10
1:A:88:LEU:O	1:A:91:VAL:HG12	0.61	1.96	20	18
1:A:111:GLN:N	1:A:112:PRO:HD3	0.60	2.11	7	16
1:A:28:PHE:HB2	1:A:65:LEU:HD13	0.57	1.75	5	1
1:A:7:LEU:O	1:A:45:VAL:HG23	0.55	2.01	2	7
1:A:26:ALA:HB1	1:A:65:LEU:HD11	0.54	1.80	5	1
1:A:54:LEU:HB3	1:A:57:ILE:O	0.53	2.04	2	3
1:A:12:VAL:O	1:A:42:VAL:HA	0.49	2.06	10	1
1:A:69:VAL:HG23	1:A:81:LEU:HB2	0.48	1.86	14	1
1:A:69:VAL:HG21	1:A:105:LEU:HD13	0.47	1.86	4	1
1:A:69:VAL:HG22	1:A:82:GLY:O	0.47	2.08	9	1
1:A:81:LEU:O	1:A:112:PRO:HB2	0.47	2.09	9	1
1:A:91:VAL:O	1:A:97:LEU:HA	0.47	2.10	7	2
1:A:55:LYS:H	1:A:55:LYS:HD3	0.47	1.69	19	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:6:ILE:O	1:A:47:ASN:HA	0.47	2.10	16	1
1:A:61:GLN:O	1:A:89:ARG:HD3	0.46	2.10	13	3
1:A:38:ILE:HG21	1:A:44:PRO:CA	0.46	2.41	18	3
1:A:94:THR:O	1:A:97:LEU:HD12	0.45	2.10	12	1
1:A:38:ILE:HG12	1:A:46:TRP:CD1	0.45	2.45	16	1
1:A:39:LYS:HD3	1:A:39:LYS:H	0.45	1.71	18	1
1:A:33:LYS:HE3	1:A:51:GLU:O	0.44	2.11	5	2
1:A:55:LYS:HD2	1:A:55:LYS:H	0.44	1.71	2	2
1:A:28:PHE:CE1	1:A:88:LEU:HD12	0.44	2.48	18	1
1:A:1:MET:HG3	1:A:52:TRP:O	0.44	2.12	3	2
1:A:55:LYS:H	1:A:55:LYS:HD2	0.44	1.73	4	1
1:A:55:LYS:HD3	1:A:55:LYS:H	0.43	1.74	15	1
1:A:65:LEU:HB2	1:A:88:LEU:HD11	0.43	1.89	19	1
1:A:107:ASP:CG	1:A:108:THR:H	0.43	2.17	5	2
1:A:107:ASP:CB	1:A:112:PRO:HG3	0.43	2.44	18	2
1:A:57:ILE:HD13	1:A:57:ILE:N	0.43	2.28	12	2
1:A:57:ILE:N	1:A:57:ILE:HD13	0.43	2.27	15	3
1:A:61:GLN:O	1:A:89:ARG:HD2	0.43	2.13	1	1
1:A:28:PHE:HB3	1:A:52:TRP:CE2	0.43	2.49	15	3
1:A:61:GLN:NE2	1:A:92:LEU:HD11	0.43	2.29	2	1
1:A:109:LYS:O	1:A:111:GLN:HG2	0.43	2.14	13	2
1:A:38:ILE:HD13	1:A:46:TRP:CD1	0.42	2.49	2	1
1:A:111:GLN:N	1:A:112:PRO:CD	0.42	2.81	12	2
1:A:38:ILE:HG21	1:A:44:PRO:HA	0.42	1.91	18	1
1:A:45:VAL:HG12	1:A:47:ASN:ND2	0.42	2.30	4	2
1:A:38:ILE:HG21	1:A:44:PRO:CB	0.42	2.45	5	1
1:A:59:LEU:HB3	1:A:92:LEU:CD2	0.42	2.44	16	1
1:A:3:ARG:HG3	1:A:51:GLU:HG2	0.41	1.92	12	2
1:A:2:LEU:HB2	1:A:54:LEU:HD11	0.41	1.93	5	1
1:A:24:CYS:SG	1:A:35:THR:HG21	0.41	2.55	13	1
1:A:53:ASP:HB2	1:A:55:LYS:CD	0.41	2.45	19	2
1:A:9:ALA:O	1:A:43:ASN:HA	0.41	2.15	17	2
1:A:83:GLU:O	1:A:105:LEU:HA	0.41	2.16	15	1
1:A:53:ASP:OD1	1:A:55:LYS:HE2	0.41	2.15	19	1
1:A:65:LEU:O	1:A:85:LYS:HA	0.41	2.15	17	1
1:A:102:ASN:HD22	1:A:118:VAL:HG22	0.41	1.76	18	1
1:A:10:GLU:O	1:A:115:ALA:HA	0.40	2.15	1	1
1:A:104:PRO:HA	1:A:116:SER:HA	0.40	1.94	12	1
1:A:4:VAL:HG21	1:A:65:LEU:CD1	0.40	2.47	16	1
1:A:98:SER:HA	1:A:121:VAL:O	0.40	2.17	13	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	107/138 (78%)	98±2 (92±2%)	7±1 (7±1%)	1±1 (1±1%)	15 61
All	All	2140/2760 (78%)	1962 (92%)	149 (7%)	29 (1%)	15 61

All 7 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	112	PRO	16
1	A	45	VAL	5
1	A	44	PRO	3
1	A	55	LYS	2
1	A	88	LEU	1
1	A	22	ALA	1
1	A	40	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	91/114 (80%)	86±1 (94±1%)	5±1 (6±1%)	25 74
All	All	1820/2280 (80%)	1719 (94%)	101 (6%)	25 74

All 21 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	57	ILE	20
1	A	55	LYS	19
1	A	119	LEU	12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	64	GLU	7
1	A	47	ASN	6
1	A	83	GLU	5
1	A	85	LYS	4
1	A	110	LYS	4
1	A	92	LEU	3
1	A	89	ARG	3
1	A	39	LYS	3
1	A	65	LEU	3
1	A	36	LYS	2
1	A	51	GLU	2
1	A	109	LYS	2
1	A	117	LEU	1
1	A	81	LEU	1
1	A	53	ASP	1
1	A	70	LYS	1
1	A	111	GLN	1
1	A	3	ARG	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 (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 85% for the well-defined parts and 83% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_0*

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	1464
Number of shifts mapped to atoms	1342
Number of unparsed shifts	122
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

The following errors were found when reading this chemical shift list.

- Chemical shift has been reported more than once. All 122 occurences are reported below.

Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
16	A	-1	GLY	HA3	4.1200	0.0000	2
21	A	0	GLY	HA3	4.3790	0.0000	2
28	A	1	MET	HB3	1.9790	0.0000	2
31	A	1	MET	HG3	2.4010	0.0000	2
42	A	2	LEU	HB3	1.1140	0.0000	2
59	A	3	ARG	HB3	1.8660	0.0000	2
62	A	3	ARG	HG3	1.5320	0.0000	2
85	A	5	PHE	HB3	2.8880	0.0000	2
98	A	6	ILE	HG13	1.0140	0.0000	2
113	A	7	LEU	HB3	1.9500	0.0000	2
130	A	8	TYR	HB3	3.3140	0.0000	2
149	A	10	GLU	HB3	1.9290	0.0000	2
152	A	10	GLU	HG3	2.1690	0.0000	2
159	A	11	ASN	HB3	3.2100	0.0000	2
183	A	13	HIS	HB3	3.2520	0.0000	2

Continued on next page...

Continued from previous page...

Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
202	A	15	PRO	HB3	2.4510	0.0000	2
205	A	15	PRO	HG3	1.9590	0.0000	2
208	A	15	PRO	HD3	3.4370	0.0000	2
214	A	16	ASP	HB3	2.6480	0.0000	2
231	A	18	ASP	HB3	2.7980	0.0000	2
240	A	19	ILE	HG13	1.6030	0.0000	2
255	A	20	SER	HB3	3.3860	0.0000	2
262	A	21	ASP	HB3	2.4490	0.0000	2
317	A	28	PHE	HB3	0.7600	0.0000	2
334	A	30	GLY	HA3	4.0720	0.0000	2
355	A	32	LYS	HB3	1.7780	0.0000	2
358	A	32	LYS	HG3	1.2560	0.0000	2
369	A	33	LYS	HB3	0.6220	0.0000	2
372	A	33	LYS	HG3	0.4390	0.0000	2
375	A	33	LYS	HD3	0.4330	0.0000	2
384	A	34	ARG	HB3	1.7620	0.0000	2
387	A	34	ARG	HG3	1.7850	0.0000	2
390	A	34	ARG	HD3	3.1030	0.0000	2
407	A	36	LYS	HB3	2.0450	0.0000	2
410	A	36	LYS	HG3	1.6700	0.0000	2
437	A	38	ILE	HG13	0.5000	0.0000	2
452	A	39	LYS	HB3	1.7260	0.0000	2
455	A	39	LYS	HG3	1.5120	0.0000	2
466	A	40	ASN	HB3	2.9170	0.0000	2
476	A	41	SER	HB3	3.6080	0.0000	2
497	A	43	ASN	HB3	2.7730	0.0000	2
502	A	44	PRO	HB3	0.0960	0.0000	2
505	A	44	PRO	HG3	2.0800	0.0000	2
528	A	46	TRP	HB3	3.2570	0.0000	2
546	A	47	ASN	HB3	3.0710	0.0000	2
556	A	48	GLU	HB3	1.5620	0.0000	2
559	A	48	GLU	HG3	2.2350	0.0000	2
564	A	49	GLY	HA3	3.3700	0.0000	2
571	A	50	PHE	HB3	2.5290	0.0000	2
582	A	51	GLU	HB3	1.9970	0.0000	2
609	A	53	ASP	HB3	2.9260	0.0000	2
616	A	54	LEU	HB3	2.2000	0.0000	2
633	A	55	LYS	HB3	1.9200	0.0000	2
636	A	55	LYS	HG3	1.3610	0.0000	2
645	A	56	GLY	HA3	4.1330	0.0000	2
654	A	57	ILE	HG13	1.1850	0.0000	2

Continued on next page...

Continued from previous page...

Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
667	A	58	PRO	HB3	2.2890	0.0000	2
670	A	58	PRO	HG3	2.0110	0.0000	2
673	A	58	PRO	HD3	3.9200	0.0000	2
680	A	59	LEU	HB3	1.1010	0.0000	2
697	A	60	ASP	HB3	2.6000	0.0000	2
704	A	61	GLN	HB3	2.1300	0.0000	2
714	A	62	GLY	HA3	4.2730	0.0000	2
721	A	63	SER	HB3	3.9650	0.0000	2
728	A	64	GLU	HB3	1.6900	0.0000	2
731	A	64	GLU	HG3	2.1340	0.0000	2
738	A	65	LEU	HB3	0.9910	0.0000	2
755	A	66	HIS	HB3	3.2630	0.0000	2
808	A	70	LYS	HB3	0.6070	0.0000	2
811	A	70	LYS	HD3	1.6010	0.0000	2
825	A	72	HIS	HB3	3.2300	0.0000	2
848	A	75	MET	HB3	2.0640	0.0000	2
851	A	75	MET	HG3	2.5990	0.0000	2
860	A	76	GLY	HA3	3.8890	0.0000	2
867	A	77	ARG	HB3	1.8660	0.0000	2
878	A	78	ASN	HB3	2.7630	0.0000	2
896	A	80	PHE	HB3	3.1790	0.0000	2
907	A	81	LEU	HB3	1.0890	0.0000	2
922	A	82	GLY	HA3	3.9120	0.0000	2
929	A	83	GLU	HB3	2.3100	0.0000	2
932	A	83	GLU	HG3	2.2650	0.0000	2
947	A	85	LYS	HB3	1.5880	0.0000	2
950	A	85	LYS	HG3	1.2010	0.0000	2
953	A	85	LYS	HD3	1.3630	0.0000	2
956	A	85	LYS	HE3	2.2990	0.0000	2
979	A	87	PRO	HD3	3.6390	0.0000	2
986	A	88	LEU	HB3	1.5780	0.0000	2
1015	A	90	GLU	HG3	2.3340	0.0000	2
1036	A	92	LEU	HB3	1.6050	0.0000	2
1069	A	95	PRO	HB3	2.4230	0.0000	2
1080	A	96	SER	HB3	3.8800	0.0000	2
1087	A	97	LEU	HB3	2.2380	0.0000	2
1103	A	98	SER	HB3	3.7270	0.0000	2
1118	A	100	SER	HB3	3.6500	0.0000	2
1125	A	101	PHE	HB3	2.9740	0.0000	2
1136	A	102	ASN	HB3	2.5660	0.0000	2
1152	A	104	PRO	HB3	1.8760	0.0000	2

Continued on next page...

Continued from previous page...

Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1157	A	104	PRO	HD3	4.1950	0.0000	2
1164	A	105	LEU	HB3	0.8970	0.0000	2
1179	A	106	LEU	HB3	1.2850	0.0000	2
1196	A	107	ASP	HB3	2.7510	0.0000	2
1213	A	109	LYS	HB3	1.8840	0.0000	2
1226	A	110	LYS	HB3	2.2450	0.0000	2
1229	A	110	LYS	HG3	0.9410	0.0000	2
1240	A	111	GLN	HB3	2.2620	0.0000	2
1243	A	111	GLN	HG3	2.2810	0.0000	2
1251	A	112	PRO	HB3	2.0010	0.0000	2
1254	A	112	PRO	HG3	2.2320	0.0000	2
1272	A	114	GLY	HA3	4.6600	0.0000	2
1287	A	116	SER	HB3	3.7370	0.0000	2
1294	A	117	LEU	HB3	1.7110	0.0000	2
1325	A	119	LEU	HB3	1.5840	0.0000	2
1342	A	120	GLN	HB3	2.1160	0.0000	2
1345	A	120	GLN	HG3	2.2900	0.0000	2
1375	A	123	TYR	HB3	2.7610	0.0000	2
1394	A	125	PRO	HB3	1.8870	0.0000	2
1397	A	125	PRO	HG3	1.7460	0.0000	2
1400	A	125	PRO	HD3	3.1600	0.0000	2
1407	A	126	LEU	HB3	1.5490	0.0000	2
1420	A	127	PRO	HB3	1.9070	0.0000	2
1423	A	127	PRO	HG3	2.0710	0.0000	2
1426	A	127	PRO	HD3	3.6220	0.0000	2

7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	133	0.06 ± 0.13	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	123	-0.07 ± 0.13	None needed (< 0.5 ppm)
$^{13}C'$	0	—	None (insufficient data)
^{15}N	126	-0.16 ± 0.51	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 85%, i.e. 1108 atoms were assigned a chemical shift out of a possible 1296. 0 out of 27 assigned methyl groups (LEU and VAL) were assigned

stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	414/521 (79%)	207/207 (100%)	107/214 (50%)	100/100 (100%)
Sidechain	611/684 (89%)	373/399 (93%)	231/259 (89%)	7/26 (27%)
Aromatic	83/91 (91%)	42/48 (88%)	39/40 (98%)	2/3 (67%)
Overall	1108/1296 (85%)	622/654 (95%)	377/513 (73%)	109/129 (84%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 83%, i.e. 1343 atoms were assigned a chemical shift out of a possible 1624. 0 out of 30 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	518/672 (77%)	259/267 (97%)	133/276 (48%)	126/129 (98%)
Sidechain	726/838 (87%)	446/489 (91%)	272/316 (86%)	8/33 (24%)
Aromatic	99/114 (87%)	50/61 (82%)	47/48 (98%)	2/5 (40%)
Overall	1343/1624 (83%)	755/817 (92%)	452/640 (71%)	136/167 (81%)

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: