



Full wwPDB NMR Structure Validation Report ⓘ

Jun 24, 2024 – 04:06 PM EDT

PDB ID : 7KRB
BMRB ID : 30814
Title : Solution Structure of the Dysferlin C2A Domain in its Calcium-bound State
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Deposited on : 2020-11-19

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 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 : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
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) : 2.37.1

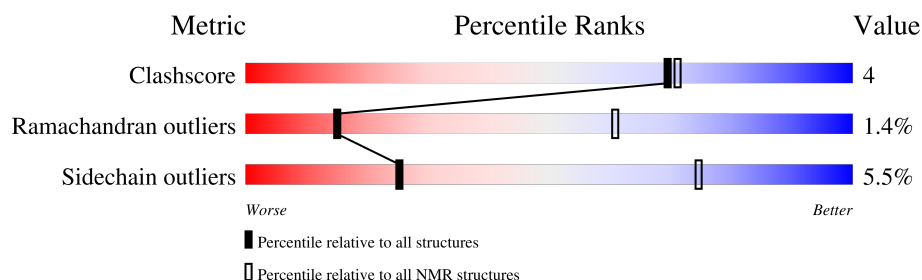
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 76%.

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	138	

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)	0.60	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

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:

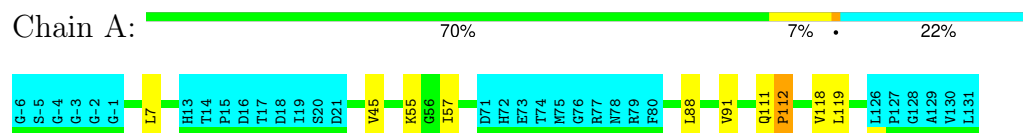
Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	GLY	-	expression tag	UNP O75923
A	-5	SER	-	expression tag	UNP O75923
A	-4	GLY	-	expression tag	UNP O75923
A	-3	GLY	-	expression tag	UNP O75923
A	-2	GLY	-	expression tag	UNP O75923
A	-1	GLY	-	expression tag	UNP O75923
A	0	GLY	-	expression tag	UNP O75923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

4 Residue-property plots [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: Isoform 15 of Dysferlin

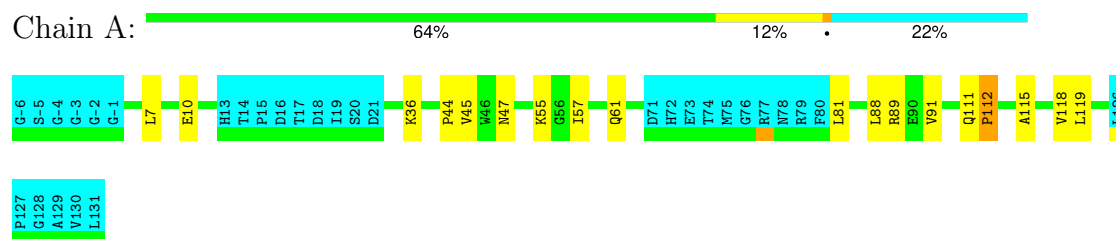


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

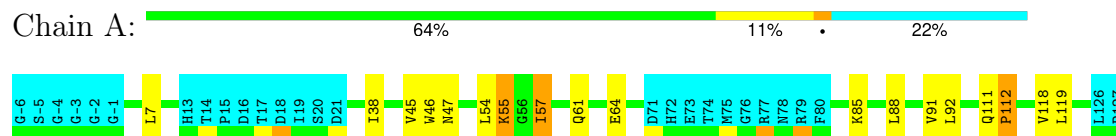
4.2.1 Score per residue for model 1

- Molecule 1: Isoform 15 of Dysferlin



4.2.2 Score per residue for model 2

- Molecule 1: Isoform 15 of Dysferlin



G128
A129
V130
L131

4.2.3 Score per residue for model 3

- Molecule 1: Isoform 15 of Dysferlin

Chain A: 

G-6 S-5 G-4 G-3 G-2 G-1 G0 H1 H13 T14 T15 P15 D16 T17 D18 D19 D20 D21 K39 N40 N52 K55 G56 I57 D71 H72 E73 T74 M75 G76 R77 N78 R79 F80 L88 V91 K110 Q111 P112 L117 V118 L119 L126 P127 G128 A129 V130 L131

4.2.4 Score per residue for model 4 (medoid)

- Molecule 1: Isoform 15 of Dysferlin

Chain A: 

G-6 S-5 G-4 G-3 G-2 G-1 H13 T14 T15 P15 D16 T17 D18 D19 D20 D21 K33 V45 V46 N47 E51 L54 K55 G56 I57 E64 V69 R70 D71 H72 E73 T74 M75 G76 R77 N78 R79 F80 E83 L88 R89 E90 V91 L105 K109 K110 Q111 P112 L126

P127
G128
A129
V130
L131

4.2.5 Score per residue for model 5

- Molecule 1: Isoform 15 of Dysferlin

Chain A: 

G-6 S-5 G-4 G-3 G-2 G-1 L2 L7 H13 T14 T15 P15 D16 T17 D18 D19 D20 D21 A26 V27 F28 K33 T38 P44 V45 E51 L54 K55 G56 I57 L65 D71 H72 E73 T74 M75 G76 R77 N78 R79 F80 K85 D107 T108 V118 L119

L126
P127
G128
A129
V130
L131

4.2.6 Score per residue for model 6

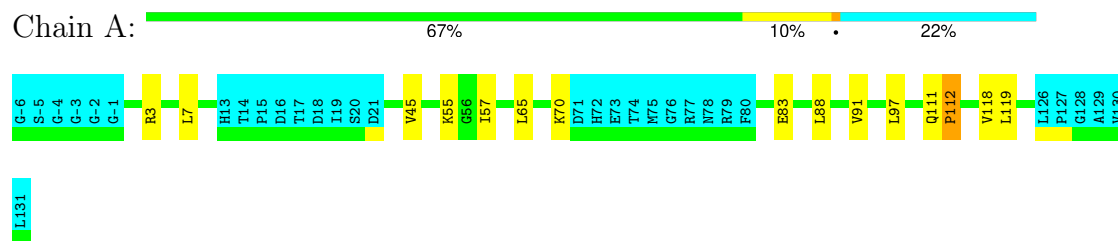
- Molecule 1: Isoform 15 of Dysferlin

Chain A: 

G-6 S-5 G-4 G-3 G-2 G-1 L7 H13 T14 T15 P15 D16 T17 D18 D19 D20 D21 V45 K55 G56 I57 Q61 D71 H72 E73 T74 M75 G76 R77 N78 R79 F80 E83 L88 R89 E90 V91 L119 L126 P127 G128 A129 V130 L131

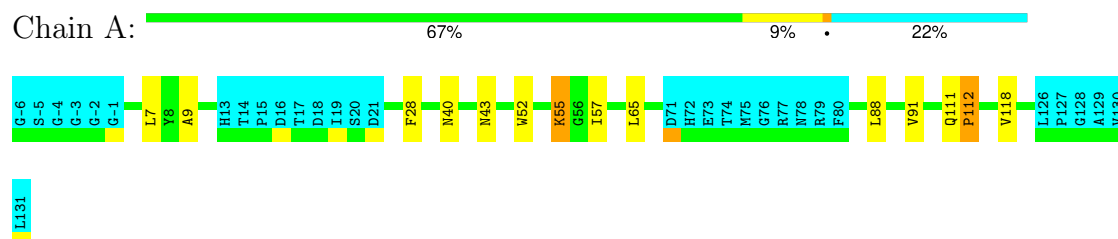
4.2.7 Score per residue for model 7

- Molecule 1: Isoform 15 of Dysferlin



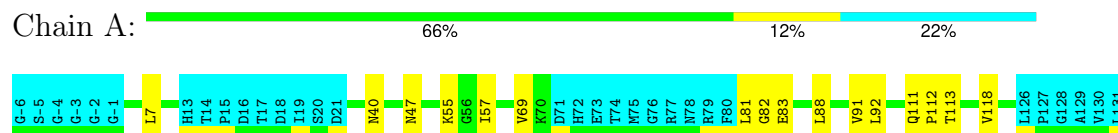
4.2.8 Score per residue for model 8

- Molecule 1: Isoform 15 of Dysferlin



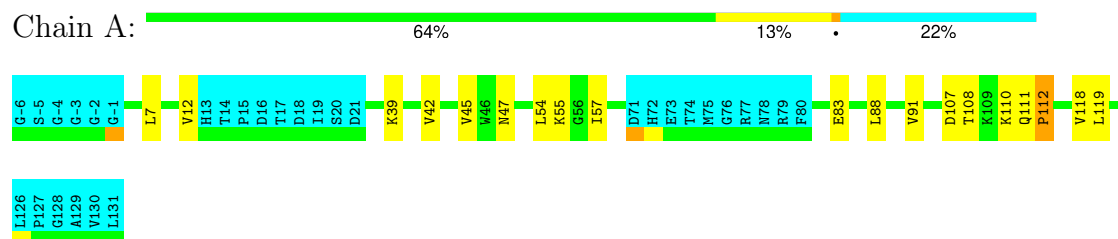
4.2.9 Score per residue for model 9

- Molecule 1: Isoform 15 of Dysferlin



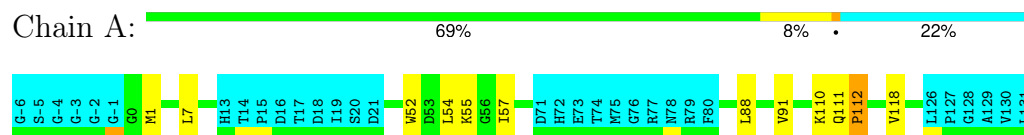
4.2.10 Score per residue for model 10

- Molecule 1: Isoform 15 of Dysferlin



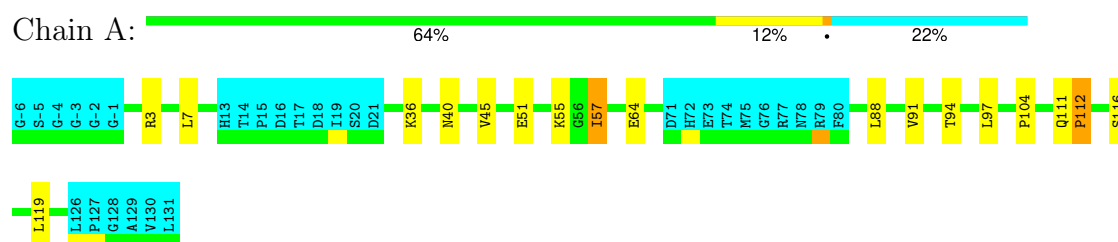
4.2.11 Score per residue for model 11

- Molecule 1: Isoform 15 of Dysferlin



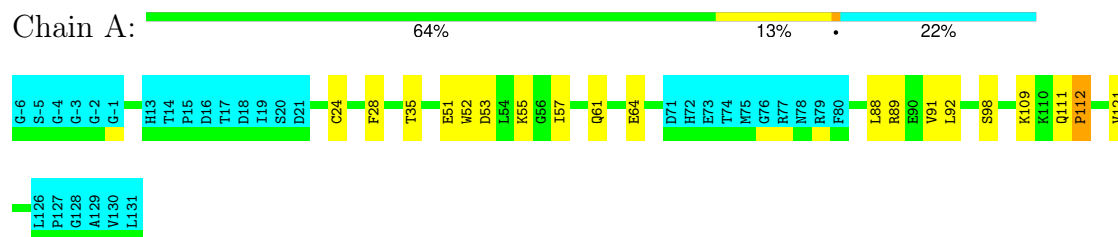
4.2.12 Score per residue for model 12

- Molecule 1: Isoform 15 of Dysferlin



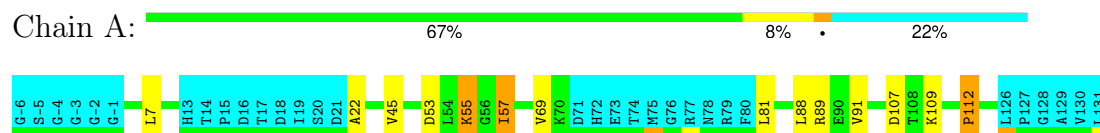
4.2.13 Score per residue for model 13

- Molecule 1: Isoform 15 of Dysferlin



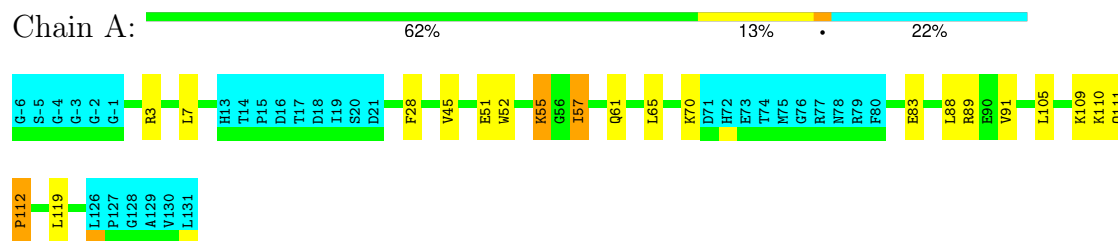
4.2.14 Score per residue for model 14

- Molecule 1: Isoform 15 of Dysferlin



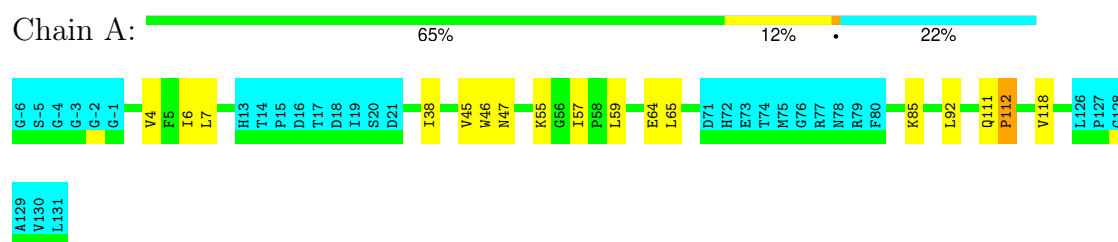
4.2.15 Score per residue for model 15

- Molecule 1: Isoform 15 of Dysferlin



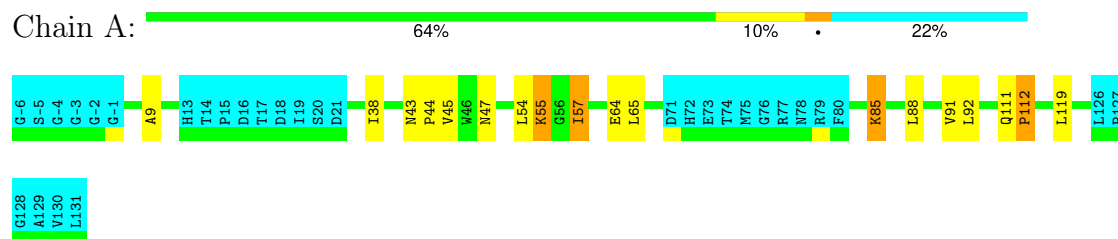
4.2.16 Score per residue for model 16

- Molecule 1: Isoform 15 of Dysferlin



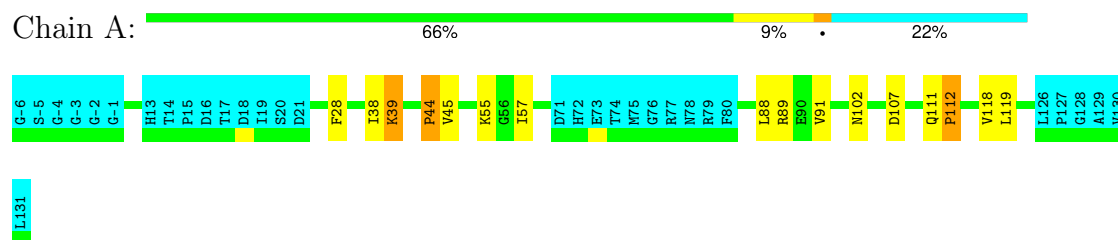
4.2.17 Score per residue for model 17

- Molecule 1: Isoform 15 of Dysferlin



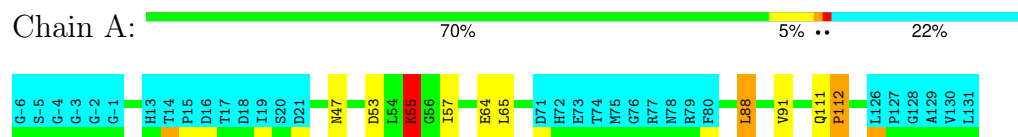
4.2.18 Score per residue for model 18

- Molecule 1: Isoform 15 of Dysferlin



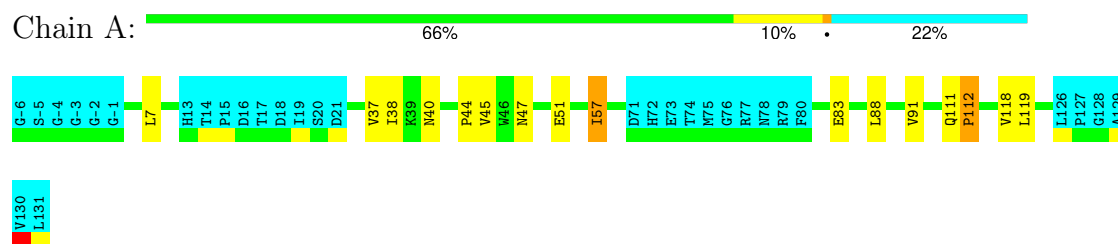
4.2.19 Score per residue for model 19

- Molecule 1: Isoform 15 of Dysferlin



4.2.20 Score per residue for model 20

- Molecule 1: Isoform 15 of Dysferlin



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	1464
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	76%

6 Model quality [i](#)

6.1 Standard geometry [i](#)

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 [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	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:HD3	1:A:55:LYS:H	0.47	1.69	19	2

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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:H	1:A:55:LYS:HD2	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: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	5
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:55:LYS:HD2	1:A:55:LYS:H	0.41	1.75	3	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	40	ASN	1
1	A	22	ALA	1
1	A	88	LEU	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

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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	39	LYS	3
1	A	89	ARG	3
1	A	65	LEU	3
1	A	92	LEU	3
1	A	36	LYS	2
1	A	109	LYS	2
1	A	51	GLU	2
1	A	81	LEU	1
1	A	117	LEU	1
1	A	3	ARG	1
1	A	70	LYS	1
1	A	111	GLN	1
1	A	53	ASP	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 ⓘ

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 76% for the well-defined parts and 74% 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	1464
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	1

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

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

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	-1	GLY	HA3	4.1200	0.0000	2
1	A	0	GLY	HA3	4.3790	0.0000	2
1	A	1	MET	HB3	1.9790	0.0000	2
1	A	1	MET	HG3	2.4010	0.0000	2
1	A	2	LEU	HB3	1.1140	0.0000	2
1	A	3	ARG	HB3	1.8660	0.0000	2
1	A	3	ARG	HG3	1.5320	0.0000	2
1	A	5	PHE	HB3	2.8880	0.0000	2
1	A	6	ILE	HG13	1.0140	0.0000	2
1	A	7	LEU	HB3	1.9500	0.0000	2
1	A	8	TYR	HB3	3.3140	0.0000	2
1	A	10	GLU	HB3	1.9290	0.0000	2
1	A	10	GLU	HG3	2.1690	0.0000	2
1	A	11	ASN	HB3	3.2100	0.0000	2
1	A	13	HIS	HB3	3.2520	0.0000	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	15	PRO	HB3	2.4510	0.0000	2
1	A	15	PRO	HG3	1.9590	0.0000	2
1	A	15	PRO	HD3	3.4370	0.0000	2
1	A	16	ASP	HB3	2.6480	0.0000	2
1	A	18	ASP	HB3	2.7980	0.0000	2
1	A	19	ILE	HG13	1.6030	0.0000	2
1	A	20	SER	HB3	3.3860	0.0000	2
1	A	21	ASP	HB3	2.4490	0.0000	2
1	A	28	PHE	HB3	0.7600	0.0000	2
1	A	30	GLY	HA3	4.0720	0.0000	2
1	A	32	LYS	HB3	1.7780	0.0000	2
1	A	32	LYS	HG3	1.2560	0.0000	2
1	A	33	LYS	HB3	0.6220	0.0000	2
1	A	33	LYS	HG3	0.4390	0.0000	2
1	A	33	LYS	HD3	0.4330	0.0000	2
1	A	34	ARG	HB3	1.7620	0.0000	2
1	A	34	ARG	HG3	1.7850	0.0000	2
1	A	34	ARG	HD3	3.1030	0.0000	2
1	A	36	LYS	HB3	2.0450	0.0000	2
1	A	36	LYS	HG3	1.6700	0.0000	2
1	A	38	ILE	HG13	0.5000	0.0000	2
1	A	39	LYS	HB3	1.7260	0.0000	2
1	A	39	LYS	HG3	1.5120	0.0000	2
1	A	40	ASN	HB3	2.9170	0.0000	2
1	A	41	SER	HB3	3.6080	0.0000	2
1	A	43	ASN	HB3	2.7730	0.0000	2
1	A	44	PRO	HB3	0.0960	0.0000	2
1	A	44	PRO	HG3	2.0800	0.0000	2
1	A	46	TRP	HB3	3.2570	0.0000	2
1	A	47	ASN	HB3	3.0710	0.0000	2
1	A	48	GLU	HB3	1.5620	0.0000	2
1	A	48	GLU	HG3	2.2350	0.0000	2
1	A	49	GLY	HA3	3.3700	0.0000	2
1	A	50	PHE	HB3	2.5290	0.0000	2
1	A	51	GLU	HB3	1.9970	0.0000	2
1	A	53	ASP	HB3	2.9260	0.0000	2
1	A	54	LEU	HB3	2.2000	0.0000	2
1	A	55	LYS	HB3	1.9200	0.0000	2
1	A	55	LYS	HG3	1.3610	0.0000	2
1	A	56	GLY	HA3	4.1330	0.0000	2
1	A	57	ILE	HG13	1.1850	0.0000	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	58	PRO	HB3	2.2890	0.0000	2
1	A	58	PRO	HG3	2.0110	0.0000	2
1	A	58	PRO	HD3	3.9200	0.0000	2
1	A	59	LEU	HB3	1.1010	0.0000	2
1	A	60	ASP	HB3	2.6000	0.0000	2
1	A	61	GLN	HB3	2.1300	0.0000	2
1	A	62	GLY	HA3	4.2730	0.0000	2
1	A	63	SER	HB3	3.9650	0.0000	2
1	A	64	GLU	HB3	1.6900	0.0000	2
1	A	64	GLU	HG3	2.1340	0.0000	2
1	A	65	LEU	HB3	0.9910	0.0000	2
1	A	66	HIS	HB3	3.2630	0.0000	2
1	A	70	LYS	HB3	0.6070	0.0000	2
1	A	70	LYS	HD3	1.6010	0.0000	2
1	A	72	HIS	HB3	3.2300	0.0000	2
1	A	75	MET	HB3	2.0640	0.0000	2
1	A	75	MET	HG3	2.5990	0.0000	2
1	A	76	GLY	HA3	3.8890	0.0000	2
1	A	77	ARG	HB3	1.8660	0.0000	2
1	A	78	ASN	HB3	2.7630	0.0000	2
1	A	80	PHE	HB3	3.1790	0.0000	2
1	A	81	LEU	HB3	1.0890	0.0000	2
1	A	82	GLY	HA3	3.9120	0.0000	2
1	A	83	GLU	HB3	2.3100	0.0000	2
1	A	83	GLU	HG3	2.2650	0.0000	2
1	A	85	LYS	HB3	1.5880	0.0000	2
1	A	85	LYS	HG3	1.2010	0.0000	2
1	A	85	LYS	HD3	1.3630	0.0000	2
1	A	85	LYS	HE3	2.2990	0.0000	2
1	A	87	PRO	HD3	3.6390	0.0000	2
1	A	88	LEU	HB3	1.5780	0.0000	2
1	A	90	GLU	HG3	2.3340	0.0000	2
1	A	92	LEU	HB3	1.6050	0.0000	2
1	A	95	PRO	HB3	2.4230	0.0000	2
1	A	96	SER	HB3	3.8800	0.0000	2
1	A	97	LEU	HB3	2.2380	0.0000	2
1	A	98	SER	HB3	3.7270	0.0000	2
1	A	100	SER	HB3	3.6500	0.0000	2
1	A	101	PHE	HB3	2.9740	0.0000	2
1	A	102	ASN	HB3	2.5660	0.0000	2
1	A	104	PRO	HB3	1.8760	0.0000	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	104	PRO	HD3	4.1950	0.0000	2
1	A	105	LEU	HB3	0.8970	0.0000	2
1	A	106	LEU	HB3	1.2850	0.0000	2
1	A	107	ASP	HB3	2.7510	0.0000	2
1	A	109	LYS	HB3	1.8840	0.0000	2
1	A	110	LYS	HB3	2.2450	0.0000	2
1	A	110	LYS	HG3	0.9410	0.0000	2
1	A	111	GLN	HB3	2.2620	0.0000	2
1	A	111	GLN	HG3	2.2810	0.0000	2
1	A	112	PRO	HB3	2.0010	0.0000	2
1	A	112	PRO	HG3	2.2320	0.0000	2
1	A	114	GLY	HA3	4.6600	0.0000	2
1	A	116	SER	HB3	3.7370	0.0000	2
1	A	117	LEU	HB3	1.7110	0.0000	2
1	A	119	LEU	HB3	1.5840	0.0000	2
1	A	120	GLN	HB3	2.1160	0.0000	2
1	A	120	GLN	HG3	2.2900	0.0000	2
1	A	123	TYR	HB3	2.7610	0.0000	2
1	A	125	PRO	HB3	1.8870	0.0000	2
1	A	125	PRO	HG3	1.7460	0.0000	2
1	A	125	PRO	HD3	3.1600	0.0000	2
1	A	126	LEU	HB3	1.5490	0.0000	2
1	A	127	PRO	HB3	1.9070	0.0000	2
1	A	127	PRO	HG3	2.0710	0.0000	2
1	A	127	PRO	HD3	3.6220	0.0000	2

7.1.2 Chemical shift referencing ⓘ

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	133	0.07 ± 0.10	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	123	-0.06 ± 0.11	None needed (< 0.5 ppm)
$^{13}\text{C}'$	0	—	None (insufficient data)
^{15}N	126	-0.16 ± 0.18	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 76%, i.e. 1109 atoms were assigned a chemical shift out of a possible 1460. 0 out of 27 assigned methyl groups (LEU and VAL) were assigned

stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	414/528 (78%)	207/214 (97%)	107/214 (50%)	100/100 (100%)
Sidechain	640/834 (77%)	398/549 (72%)	235/259 (91%)	7/26 (27%)
Aromatic	55/98 (56%)	28/48 (58%)	25/47 (53%)	2/3 (67%)
Overall	1109/1460 (76%)	633/811 (78%)	367/520 (71%)	109/129 (84%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 74%, i.e. 1341 atoms were assigned a chemical shift out of a possible 1822. 0 out of 30 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	518/686 (76%)	259/281 (92%)	133/276 (48%)	126/129 (98%)
Sidechain	756/1014 (75%)	470/665 (71%)	278/316 (88%)	8/33 (24%)
Aromatic	67/122 (55%)	34/61 (56%)	31/56 (55%)	2/5 (40%)
Overall	1341/1822 (74%)	763/1007 (76%)	442/648 (68%)	136/167 (81%)

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.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	113	THR	HG1	5.88	0.08 – 2.19	22.5

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. 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:

