



wwPDB NMR Structure Validation Summary Report ⓘ

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PDB ID : 2L8R / pdb_00002l8r
BMRB ID : 17421
Title : Solution structure of human protein C6orf130 in complex with ADP-ribose
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Deposited on : 2011-01-22

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
wwPDB-ShiftChecker : v1.2
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

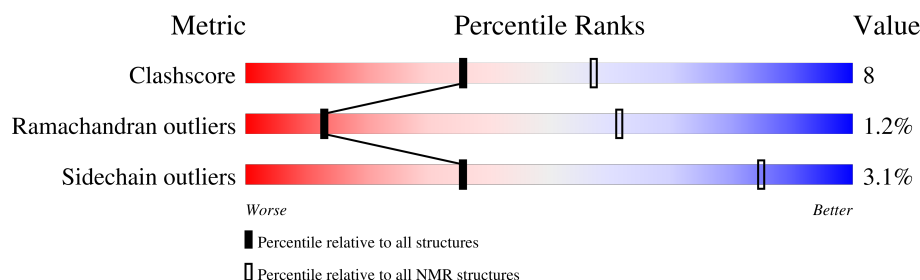
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 89%.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and a grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	151	 81% 11% 7% .

2 Ensemble composition and analysis

This entry contains 20 models. Model 9 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:13-A:152 (140)	0.73	9

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 5 clusters and 4 single-model clusters were found.

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

3 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 2256 atoms, of which 1043 are hydrogens and 0 are deuteriums.

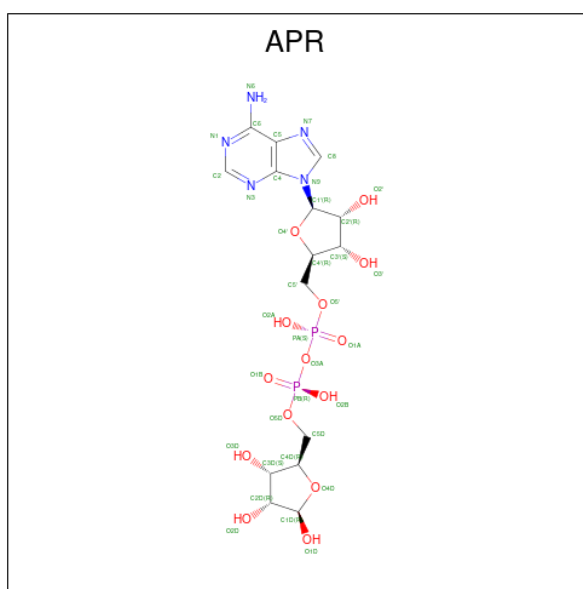
- Molecule 1 is a protein called Uncharacterized protein C6orf130.

Mol	Chain	Residues	Atoms						Trace
1	A	150	Total	C	H	N	O	S	0
			2197	741	1020	203	224	9	

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	GLY	-	expression tag	UNP Q9Y530

- Molecule 2 is ADENOSINE-5-DIPHOSPHORIBOSE (CCD ID: APR) (formula: $C_{15}H_{23}N_5O_{14}P_2$).



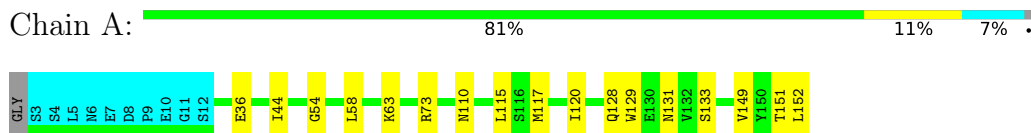
Mol	Chain	Residues	Atoms					
2	A	1	Total	C	H	N	O	P
			59	15	23	5	14	2

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.

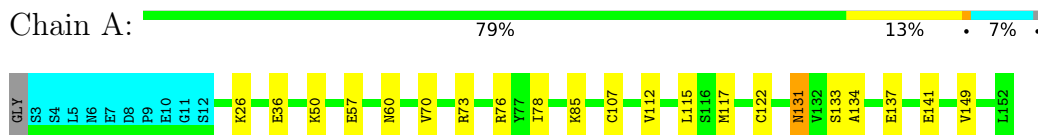
- Molecule 1: Uncharacterized protein C6orf130



4.2 Residue scores for the representative (medoid) model from the NMR ensemble

The representative model is number 9. Colouring as in section 4.1 above.

- Molecule 1: Uncharacterized protein C6orf130



5 Refinement protocol and experimental data overview

The models were refined using the following method: *AUTOMATED METHODS WERE USED FOR BACKBONE CHEMICAL SHIFT ASSIGNMENT AND ITERATIVE NOE REFINEMENT. FINAL STRUCTURES WERE OBTAINED BY MOLECULAR DYNAMICS IN EXPLICIT SOLVENT., torsion angle dynamics, AUTOMATED METHODS WERE USED FOR BACKBONE CHEMICAL SHIFT ASSIGNMENT AND ITERATIVE NOE REFINEMENT. FINAL STRUCTURES WERE OBTAINED BY MOLECULAR DYNAMICS IN EXPLICIT SOLVENT.*

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
Xplor-NIH	refinement	2.9.3
CYANA	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	1854
Number of shifts mapped to atoms	1691
Number of unparsed shifts	0
Number of shifts with mapping errors	163
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	89%

6 Model quality i

6.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: APR

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	1.03±0.02	1±1/1123 (0.1± 0.1%)	0.93±0.02	0±0/1505 (0.0± 0.0%)
All	All	1.03	12/22460 (0.1%)	0.93	3/30100 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	0.1±0.3
All	All	0	2

All unique bond 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(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	92	THR	N-CA	-6.41	1.38	1.45	7	4
1	A	121	GLY	N-CA	-5.81	1.40	1.45	17	2
1	A	120	ILE	CA-CB	5.52	1.60	1.53	14	1
1	A	72	LYS	C-N	-5.31	1.26	1.33	17	2
1	A	151	THR	N-CA	-5.28	1.39	1.46	17	3

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	24	CYS	CA-C-N	6.34	127.77	119.84	8	1
1	A	24	CYS	C-N-CA	6.34	127.77	119.84	8	1
1	A	13	ARG	N-CA-C	-6.15	103.90	112.45	19	1

There are no chirality outliers.

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

Mol	Chain	Res	Type	Group	Models (Total)
1	A	13	ARG	Sidechain	1
1	A	39	ARG	Sidechain	1

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	1106	967	1140	18±3
2	A	36	23	21	4±2
All	All	22840	19800	23220	360

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.

5 of 163 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:152:LEU:HD11	2:A:186:APR:C2	0.81	2.04	5	12
1:A:152:LEU:HD21	2:A:186:APR:C2	0.80	2.06	12	3
1:A:152:LEU:HD21	2:A:186:APR:N3	0.80	1.92	12	1
1:A:124:LEU:HB2	2:A:186:APR:HR'4	0.72	1.61	6	1
1:A:57:GLU:HA	1:A:60:ASN:ND2	0.68	2.02	13	5

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	139/151 (92%)	130±1 (94±1%)	7±1 (5±1%)	2±1 (1±1%)	13	61
All	All	2780/3020 (92%)	2605 (94%)	143 (5%)	32 (1%)	13	61

5 of 13 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	53	GLY	7
1	A	122	CYS	5
1	A	62	GLN	3
1	A	118	PRO	3
1	A	123	GLY	3

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	121/130 (93%)	117±1 (97±1%)	4±1 (3±1%)	36	85
All	All	2420/2600 (93%)	2346 (97%)	74 (3%)	36	85

5 of 22 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	110	ASN	16
1	A	115	LEU	10
1	A	63	LYS	8
1	A	152	LEU	5
1	A	146	LYS	4

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds for which Mogul statistics could be retrieved, the number of bonds that are observed in the model and the number of bonds that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length is the number of standard deviations the observed value is removed from the expected value. A bond length with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond lengths.

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
2	APR	A	186	-	39,39,39	1.54±0.06	6±1 (15±2%)

In the following table, the Counts columns list the number of angles for which Mogul statistics could be retrieved, the number of angles that are observed in the model and the number of angles that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond angle is the number of standard deviations the observed value is removed from the expected value. A bond angle with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond angles.

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
2	APR	A	186	-	56,60,60	1.59±0.02	9±1 (16±1%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	APR	A	186	-	-	0±0,22,54,54	0±0,4,4,4

5 of 11 unique bond 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(Å)	Ideal(Å)	Models	
								Worst	Total
2	A	186	APR	C1D-C2D	5.37	1.58	1.52	6	20
2	A	186	APR	C4-N9	3.61	1.30	1.37	14	20
2	A	186	APR	C5-N7	3.56	1.32	1.39	6	20
2	A	186	APR	C3'-C4'	2.57	1.59	1.53	12	13
2	A	186	APR	PB-O3A	2.55	1.62	1.59	10	5

5 of 11 unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

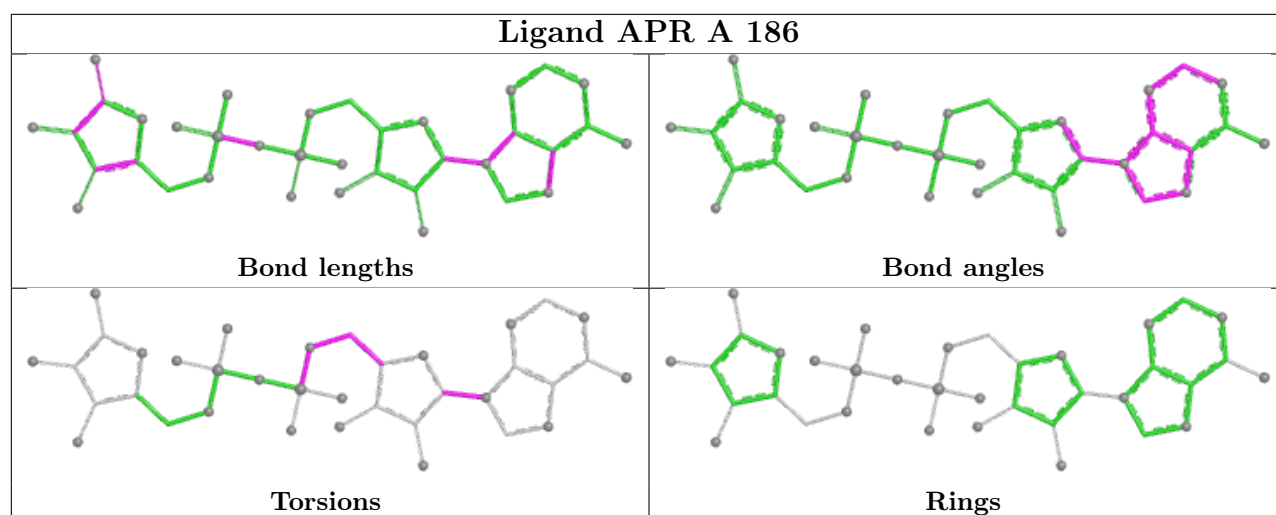
Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
2	A	186	APR	N3-C2-N1	5.25	120.64	128.58	9	20
2	A	186	APR	C5-C4-N3	5.13	119.65	126.72	16	20
2	A	186	APR	N9-C8-N7	4.17	108.02	113.94	11	20
2	A	186	APR	C2-N3-C4	3.82	121.16	111.83	12	20
2	A	186	APR	N3-C4-N9	3.21	132.63	127.17	16	20

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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 89% for the well-defined parts and 89% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

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	1854
Number of shifts mapped to atoms	1691
Number of unparsed shifts	0
Number of shifts with mapping errors	163
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	6

The following assigned chemical shifts were not mapped to the molecules present in the coordinate file.

- No matching atom found in the structure. First 5 (of 163) occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	5	LEU	HD11	0.9	0.02	1
1	A	5	LEU	HD12	0.9	0.02	1
1	A	5	LEU	HD22	0.85	0.016	1
1	A	5	LEU	HD23	0.85	0.016	1
1	A	6	ASN	HD22	7.617	0.008	2
1	A	14	ILE	HD12	0.896	0.013	1
1	A	14	ILE	HD13	0.896	0.013	1
1	A	14	ILE	HG13	1.532	0.02	2
1	A	14	ILE	HG21	0.199	0.002	1
1	A	14	ILE	HG22	0.199	0.002	1
1	A	15	THR	HG22	1.132	0.001	1
1	A	15	THR	HG23	1.132	0.001	1
1	A	17	VAL	HG11	0.658	0.005	1
1	A	17	VAL	HG12	0.658	0.005	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	17	VAL	HG22	0.401	0.02	1
1	A	17	VAL	HG23	0.401	0.02	1
1	A	21	LEU	HD11	0.291	0.007	1
1	A	21	LEU	HD12	0.291	0.007	1
1	A	21	LEU	HD22	0.425	0.008	1
1	A	21	LEU	HD23	0.425	0.008	1
1	A	27	THR	HG22	1.239	0.007	1
1	A	27	THR	HG23	1.239	0.007	1
1	A	30	LEU	HD11	0.69	0.02	1
1	A	30	LEU	HD12	0.69	0.02	1
1	A	30	LEU	HD22	0.722	0.010	1
1	A	30	LEU	HD23	0.722	0.010	1
1	A	34	ILE	HD12	0.988	0.02	1
1	A	34	ILE	HD13	0.988	0.02	1
1	A	34	ILE	HG13	1.273	0.02	2
1	A	34	ILE	HG21	0.718	0.002	1
1	A	34	ILE	HG22	0.718	0.002	1
1	A	44	ILE	HD12	-0.12	0.007	1
1	A	44	ILE	HD13	-0.12	0.007	1
1	A	44	ILE	HG13	1.6	0.014	2
1	A	44	ILE	HG21	1.097	0.006	1
1	A	44	ILE	HG22	1.097	0.006	1
1	A	46	VAL	HG22	0.976	0.008	1
1	A	46	VAL	HG23	0.976	0.008	1
1	A	47	LEU	HD11	0.785	0.005	1
1	A	47	LEU	HD12	0.785	0.005	1
1	A	47	LEU	HD22	1.127	0.02	1
1	A	47	LEU	HD23	1.127	0.02	1
1	A	55	VAL	HG11	1.012	0.003	1
1	A	55	VAL	HG12	1.012	0.003	1
1	A	55	VAL	HG22	0.954	0.008	1
1	A	55	VAL	HG23	0.954	0.008	1
1	A	56	GLN	HE22	7.51	0.003	2
1	A	58	LEU	HD11	0.1	0.02	1
1	A	58	LEU	HD12	0.1	0.02	1
1	A	58	LEU	HD22	-0.037	0.003	1
1	A	58	LEU	HD23	-0.037	0.003	1
1	A	59	LEU	HD11	0.915	0.011	1
1	A	59	LEU	HD12	0.915	0.011	1
1	A	59	LEU	HD22	0.854	0.011	1
1	A	59	LEU	HD23	0.854	0.011	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	60	ASN	HD22	7.672	0.02	2
1	A	61	GLN	HE22	7.716	0.005	2
1	A	62	GLN	HE22	7.464	0.02	2
1	A	68	VAL	HG11	0.818	0.001	1
1	A	68	VAL	HG12	0.818	0.001	1
1	A	68	VAL	HG22	1.11	0.02	1
1	A	68	VAL	HG23	1.11	0.02	1
1	A	70	VAL	HG22	0.522	0.002	1
1	A	70	VAL	HG23	0.522	0.002	1
1	A	71	LEU	HD11	0.848	0.02	1
1	A	71	LEU	HD12	0.848	0.02	1
1	A	71	LEU	HD22	0.896	0.005	1
1	A	71	LEU	HD23	0.896	0.005	1
1	A	78	ILE	HD12	0.053	0.005	1
1	A	78	ILE	HD13	0.053	0.005	1
1	A	78	ILE	HG13	0.763	0.006	2
1	A	78	ILE	HG21	0.627	0.02	1
1	A	78	ILE	HG22	0.627	0.02	1
1	A	81	LEU	HD11	0.799	0.004	1
1	A	81	LEU	HD12	0.799	0.004	1
1	A	81	LEU	HD22	0.706	0.002	1
1	A	81	LEU	HD23	0.706	0.002	1
1	A	82	ILE	HD12	0.516	0.004	1
1	A	82	ILE	HD13	0.516	0.004	1
1	A	82	ILE	HG13	1.018	0.008	2
1	A	82	ILE	HG21	0.562	0.02	1
1	A	82	ILE	HG22	0.562	0.02	1
1	A	83	THR	HG22	1.219	0.007	1
1	A	83	THR	HG23	1.219	0.007	1
1	A	92	THR	HG22	1.344	0.006	1
1	A	92	THR	HG23	1.344	0.006	1
1	A	95	ASN	HD22	8.217	0.02	2
1	A	96	LEU	HD11	0.841	0.013	1
1	A	96	LEU	HD12	0.841	0.013	1
1	A	96	LEU	HD22	0.926	0.002	1
1	A	96	LEU	HD23	0.926	0.002	1
1	A	97	GLN	HE22	7.448	0.005	2
1	A	100	LEU	HD11	0.735	0.02	1
1	A	100	LEU	HD12	0.735	0.02	1
1	A	100	LEU	HD22	0.763	0.007	1
1	A	100	LEU	HD23	0.763	0.007	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	108	LEU	HD11	0.897	0.02	1
1	A	108	LEU	HD12	0.897	0.02	1
1	A	108	LEU	HD22	1.002	0.006	1
1	A	108	LEU	HD23	1.002	0.006	1
1	A	110	ASN	HD22	6.708	0.009	2
1	A	112	VAL	HG11	1.276	0.009	1
1	A	112	VAL	HG12	1.276	0.009	1
1	A	112	VAL	HG22	1.419	0.002	1
1	A	112	VAL	HG23	1.419	0.002	1
1	A	113	THR	HG22	1.133	0.004	1
1	A	113	THR	HG23	1.133	0.004	1
1	A	115	LEU	HD11	0.656	0.006	1
1	A	115	LEU	HD12	0.656	0.006	1
1	A	115	LEU	HD22	0.686	0.009	1
1	A	115	LEU	HD23	0.686	0.009	1
1	A	120	ILE	HD12	0.767	0.006	1
1	A	120	ILE	HD13	0.767	0.006	1
1	A	120	ILE	HG13	2.374	0.008	2
1	A	120	ILE	HG21	1.224	0.005	1
1	A	120	ILE	HG22	1.224	0.005	1
1	A	124	LEU	HD11	1.127	0.008	1
1	A	124	LEU	HD12	1.127	0.008	1
1	A	124	LEU	HD22	0.995	0.015	1
1	A	124	LEU	HD23	0.995	0.015	1
1	A	127	LEU	HD11	0.231	0.004	1
1	A	127	LEU	HD12	0.231	0.004	1
1	A	127	LEU	HD22	0.474	0.02	1
1	A	127	LEU	HD23	0.474	0.02	1
1	A	128	GLN	HE22	7.726	0.009	2
1	A	131	ASN	HD22	6.862	0.02	2
1	A	132	VAL	HG11	1.098	0.006	1
1	A	132	VAL	HG12	1.098	0.006	1
1	A	132	VAL	HG22	0.985	0.005	1
1	A	132	VAL	HG23	0.985	0.005	1
1	A	136	ILE	HD12	0.847	0.004	1
1	A	136	ILE	HD13	0.847	0.004	1
1	A	136	ILE	HG13	1.887	0.02	2
1	A	136	ILE	HG21	0.738	0.02	1
1	A	136	ILE	HG22	0.738	0.02	1
1	A	139	VAL	HG11	0.146	0.008	1
1	A	139	VAL	HG12	0.146	0.008	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	139	VAL	HG22	1.097	0.003	1
1	A	139	VAL	HG23	1.097	0.003	1
1	A	143	THR	HG22	1.245	0.007	1
1	A	143	THR	HG23	1.245	0.007	1
1	A	145	ILE	HD12	1.1	0.004	1
1	A	145	ILE	HD13	1.1	0.004	1
1	A	145	ILE	HG13	1.749	0.02	2
1	A	145	ILE	HG21	0.5	0.006	1
1	A	145	ILE	HG22	0.5	0.006	1
1	A	147	ILE	HD12	-0.175	0.007	1
1	A	147	ILE	HD13	-0.175	0.007	1
1	A	147	ILE	HG13	1.031	0.002	2
1	A	147	ILE	HG21	0.64	0.012	1
1	A	147	ILE	HG22	0.64	0.012	1
1	A	148	THR	HG22	0.687	0.02	1
1	A	148	THR	HG23	0.687	0.02	1
1	A	149	VAL	HG11	0.86	0.005	1
1	A	149	VAL	HG12	0.86	0.005	1
1	A	149	VAL	HG22	0.503	0.003	1
1	A	149	VAL	HG23	0.503	0.003	1
1	A	151	THR	HG22	1.206	0.001	1
1	A	151	THR	HG23	1.206	0.001	1
1	A	152	LEU	HD11	0.391	0.004	1
1	A	152	LEU	HD12	0.391	0.004	1
1	A	152	LEU	HD22	0.265	0.006	1
1	A	152	LEU	HD23	0.265	0.006	1

7.1.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	150	-0.85 ± 0.15	Should be checked
$^{13}\text{C}_\beta$	138	-0.14 ± 0.17	None needed (< 0.5 ppm)
$^{13}\text{C}'$	147	-0.21 ± 0.12	None needed (< 0.5 ppm)
^{15}N	145	0.40 ± 0.25	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 89%, i.e. 1736 atoms were assigned a chemical

shift out of a possible 1945. 0 out of 23 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	699/704 (99%)	285/287 (99%)	278/280 (99%)	136/137 (99%)
Sidechain	943/1111 (85%)	629/722 (87%)	301/344 (88%)	13/45 (29%)
Aromatic	94/130 (72%)	57/62 (92%)	35/61 (57%)	2/7 (29%)
Overall	1736/1945 (89%)	971/1071 (91%)	614/685 (90%)	151/189 (80%)

7.1.4 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.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	143	THR	HG1	5.46	0.08 – 2.19	20.5
1	A	92	THR	HG1	5.34	0.08 – 2.19	19.9
1	A	83	THR	HG1	5.07	0.08 – 2.19	18.6
1	A	119	ARG	HG3	-0.12	0.15 – 2.94	-6.0
1	A	51	LYS	HB2	0.41	0.58 – 2.97	-5.7
1	A	51	LYS	HD2	0.47	0.58 – 2.64	-5.5

7.1.5 Random Coil Index (RCI) plots [i](#)

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition. If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain A:

