wwPDB NMR Structure Validation Summary Report

Jun 12, 2024 – 08:28 AM EDT

PDB ID	:	2BN8
BMRB ID	:	5950
Title	:	Solution Structure and interactions of the E .coli Cell Division Activator Protein CedA
Authors	:	Chen, H.A.; Simpson, P.; Huyton, T.; Roper, D.; Matthews, S.
Deposited on	:	2005-03-22

This is a wwPDB NMR Structure Validation Summary 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

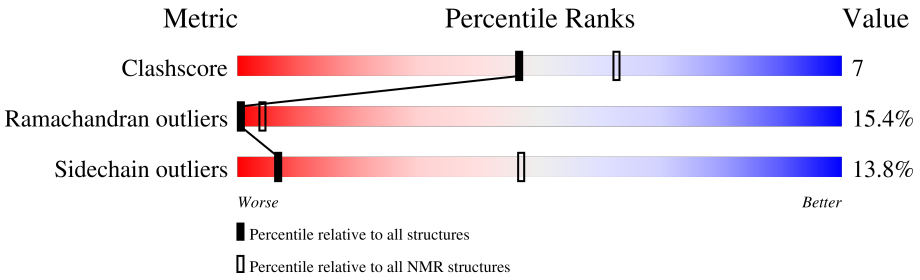
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 90%.

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	87	53% 15% 9% 23%

2 Ensemble composition and analysis (i)

This entry contains 1 models. Identification of well-defined residues and clustering analysis are not possible.

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1075 atoms, of which 529 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called CELL DIVISION ACTIVATOR CEDA.

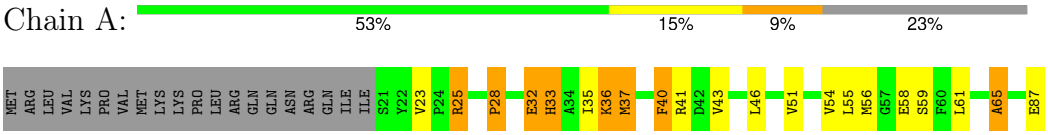
Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	67	1075	348	529	95	100	3	0

4 Residue-property plots (i)

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: CELL DIVISION ACTIVATOR CEDA

Chain A:



5 Refinement protocol and experimental data overview

Of the ? calculated structures, 1 were deposited, based on the following criterion: *?*.

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

Software name	Classification	Version
CNS	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	1123
Number of shifts mapped to atoms	851
Number of unparsed shifts	0
Number of shifts with mapping errors	272
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	90%

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	546	529	527	7
All	All	546	529	527	7

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 7.

5 of 7 clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:55:LEU:HD13	1:A:59:SER:HB2	0.63	1.69
1:A:35:ILE:HG22	1:A:37:MET:H	0.50	1.65
1:A:28:PRO:HB3	1:A:33:HIS:HB3	0.48	1.85
1:A:36:LYS:H	1:A:36:LYS:HD2	0.48	1.68
1:A:55:LEU:HD22	1:A:59:SER:H	0.47	1.70

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	65/87 (75%)	40 (62%)	15 (23%)	10 (15%)	0 4
All	All	65/87 (75%)	40 (62%)	15 (23%)	10 (15%)	0 4

5 of 10 Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type
1	A	23	VAL
1	A	25	ARG
1	A	28	PRO
1	A	32	GLU
1	A	33	HIS

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	58/78 (74%)	50 (86%)	8 (14%)	7 47
All	All	58/78 (74%)	50 (86%)	8 (14%)	7 47

5 of 8 residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type
1	A	25	ARG
1	A	32	GLU
1	A	36	LYS
1	A	40	PHE
1	A	46	LEU

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 90% for the well-defined parts and 90% 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	1123
Number of shifts mapped to atoms	851
Number of unparsed shifts	0
Number of shifts with mapping errors	272
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

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 272) occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	1	MET	CA	54.907	0.500	1
1	A	1	MET	HA	4.123	0.020	1
1	A	1	MET	CB	32.938	0.500	1
1	A	1	MET	HB2	2.15	0.020	1
1	A	1	MET	HB3	2.15	0.020	1
1	A	2	ARG	H	8.705	0.020	1
1	A	2	ARG	N	124.723	0.200	1
1	A	2	ARG	CA	56.065	0.500	1
1	A	2	ARG	HA	4.362	0.020	1
1	A	2	ARG	CB	35.984	0.500	1
1	A	2	ARG	HB2	1.742	0.020	1
1	A	2	ARG	HB3	1.742	0.020	1
1	A	2	ARG	CG	27.13	0.500	1
1	A	2	ARG	HG2	1.577	0.020	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	2	ARG	HG3	1.577	0.020	1
1	A	2	ARG	CD	43.543	0.500	1
1	A	2	ARG	HD2	3.173	0.020	1
1	A	2	ARG	HD3	3.173	0.020	1
1	A	3	LEU	H	8.429	0.020	1
1	A	3	LEU	N	125.567	0.200	1
1	A	3	LEU	CA	55.221	0.500	1
1	A	3	LEU	HA	4.379	0.020	1
1	A	3	LEU	C	176.849	0.500	1
1	A	3	LEU	CB	42.875	0.500	1
1	A	3	LEU	HB2	1.565	0.020	1
1	A	3	LEU	HB3	1.565	0.020	1
1	A	3	LEU	CG	27.13	0.500	1
1	A	3	LEU	CD1	24.857	0.500	1
1	A	3	LEU	HD11	0.906	0.020	1
1	A	3	LEU	HD12	0.906	0.020	1
1	A	3	LEU	HD13	0.906	0.020	1
1	A	3	LEU	CD2	23.847	0.500	1
1	A	3	LEU	HD21	0.861	0.020	1
1	A	3	LEU	HD22	0.861	0.020	1
1	A	3	LEU	HD23	0.861	0.020	1
1	A	3	LEU	HG	1.586	0.020	1
1	A	4	VAL	H	8.196	0.020	1
1	A	4	VAL	N	122.83	0.200	1
1	A	4	VAL	CA	61.978	0.500	1
1	A	4	VAL	HA	4.085	0.020	1
1	A	4	VAL	CB	32.685	0.500	1
1	A	4	VAL	HB	1.998	0.020	1
1	A	4	VAL	CG1	20.816	0.500	1
1	A	4	VAL	HG11	0.884	0.020	1
1	A	4	VAL	HG12	0.884	0.020	1
1	A	4	VAL	HG13	0.884	0.020	1
1	A	4	VAL	CG2	20.816	0.500	1
1	A	4	VAL	HG21	0.884	0.020	1
1	A	4	VAL	HG22	0.884	0.020	1
1	A	4	VAL	HG23	0.884	0.020	1
1	A	5	LYS	H	8.315	0.020	1
1	A	5	LYS	N	126.815	0.200	1
1	A	5	LYS	CA	54.119	0.500	1
1	A	5	LYS	HA	4.587	0.020	1
1	A	5	LYS	CB	39.465	0.500	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	5	LYS	HB2	1.805	0.020	1
1	A	5	LYS	HB3	1.805	0.020	1
1	A	5	LYS	CG	24.857	0.500	1
1	A	5	LYS	HG2	1.452	0.020	1
1	A	5	LYS	HG3	1.452	0.020	1
1	A	5	LYS	CD	29.15	0.500	1
1	A	5	LYS	HD2	1.673	0.020	1
1	A	5	LYS	HD3	1.673	0.020	1
1	A	5	LYS	CE	41.523	0.500	1
1	A	5	LYS	HE2	2.978	0.020	1
1	A	5	LYS	HE3	2.978	0.020	1
1	A	6	PRO	CA	62.988	0.500	1
1	A	6	PRO	HA	4.401	0.020	1
1	A	6	PRO	CB	31.971	0.500	1
1	A	6	PRO	HB2	2.257	0.020	1
1	A	6	PRO	HB3	1.85	0.020	1
1	A	6	PRO	CG	27.382	0.500	1
1	A	6	PRO	HG2	1.977	0.020	1
1	A	6	PRO	HG3	1.977	0.020	1
1	A	6	PRO	CD	50.614	0.500	1
1	A	6	PRO	HD2	3.792	0.020	1
1	A	6	PRO	HD3	3.606	0.020	1
1	A	7	VAL	H	8.205	0.020	1
1	A	7	VAL	N	120.95	0.200	1
1	A	7	VAL	CA	62.202	0.500	1
1	A	7	VAL	HA	4.035	0.020	1
1	A	7	VAL	CB	32.981	0.500	1
1	A	7	VAL	HB	1.994	0.020	1
1	A	7	VAL	CG1	20.816	0.500	1
1	A	7	VAL	HG11	0.91	0.020	1
1	A	7	VAL	HG12	0.91	0.020	1
1	A	7	VAL	HG13	0.91	0.020	1
1	A	7	VAL	CG2	20.816	0.500	1
1	A	7	VAL	HG21	0.91	0.020	1
1	A	7	VAL	HG22	0.91	0.020	1
1	A	7	VAL	HG23	0.91	0.020	1
1	A	8	MET	H	8.422	0.020	1
1	A	8	MET	N	125.165	0.200	1
1	A	8	MET	CA	60.967	0.500	1
1	A	8	MET	HA	4.469	0.020	1
1	A	8	MET	C	175.869	0.500	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	8	MET	CB	32.881	0.500	1
1	A	8	MET	HB2	1.993	0.020	1
1	A	8	MET	HB3	1.951	0.020	1
1	A	8	MET	CG	31.927	0.500	1
1	A	8	MET	HG2	2.556	0.020	1
1	A	8	MET	HG3	2.492	0.020	1
1	A	9	LYS	H	8.331	0.020	1
1	A	9	LYS	N	123.938	0.200	1
1	A	9	LYS	CA	56.123	0.500	1
1	A	9	LYS	HA	4.294	0.020	1
1	A	9	LYS	CB	32.938	0.500	1
1	A	9	LYS	HB2	1.763	0.020	1
1	A	9	LYS	HB3	1.693	0.020	1
1	A	9	LYS	CG	24.604	0.500	1
1	A	9	LYS	HG2	1.414	0.020	1
1	A	9	LYS	HG3	1.414	0.020	1
1	A	9	LYS	CD	29.15	0.500	1
1	A	9	LYS	HD2	1.655	0.020	1
1	A	9	LYS	HD3	1.655	0.020	1
1	A	9	LYS	CE	41.523	0.500	1
1	A	9	LYS	HE2	2.981	0.020	1
1	A	9	LYS	HE3	2.981	0.020	1
1	A	10	LYS	H	8.301	0.020	1
1	A	10	LYS	N	124.201	0.200	1
1	A	10	LYS	CA	54.212	0.500	1
1	A	10	LYS	HA	4.568	0.020	1
1	A	10	LYS	CB	33.23	0.500	1
1	A	10	LYS	HB2	1.79	0.020	1
1	A	10	LYS	HB3	1.79	0.020	1
1	A	10	LYS	CG	24.857	0.500	1
1	A	10	LYS	HG2	1.438	0.020	1
1	A	10	LYS	HG3	1.438	0.020	1
1	A	10	LYS	CD	29.15	0.500	1
1	A	10	LYS	HD2	1.683	0.020	1
1	A	10	LYS	HD3	1.683	0.020	1
1	A	10	LYS	CE	41.523	0.500	1
1	A	10	LYS	HE2	2.979	0.020	1
1	A	10	LYS	HE3	2.979	0.020	1
1	A	11	PRO	CA	62.735	0.500	1
1	A	11	PRO	HA	4.41	0.020	1
1	A	11	PRO	CB	32.225	0.500	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	11	PRO	HB2	2.24	0.020	1
1	A	11	PRO	HB3	1.824	0.020	1
1	A	11	PRO	CG	27.382	0.500	1
1	A	11	PRO	HG3	1.952	0.020	1
1	A	11	PRO	CD	50.614	0.500	1
1	A	11	PRO	HD2	3.801	0.020	1
1	A	11	PRO	HD3	3.625	0.020	1
1	A	12	LEU	H	8.301	0.020	1
1	A	12	LEU	N	122.884	0.200	1
1	A	12	LEU	CA	55.289	0.500	1
1	A	12	LEU	HA	4.292	0.020	1
1	A	12	LEU	C	177.531	0.500	1
1	A	12	LEU	CB	42.625	0.500	1
1	A	12	LEU	HB2	1.591	0.020	1
1	A	12	LEU	HB3	1.591	0.020	1
1	A	12	LEU	CG	27.13	0.500	1
1	A	12	LEU	CD1	24.857	0.500	1
1	A	12	LEU	HD11	0.897	0.020	1
1	A	12	LEU	HD12	0.897	0.020	1
1	A	12	LEU	HD13	0.897	0.020	1
1	A	12	LEU	CD2	23.594	0.500	1
1	A	12	LEU	HD21	0.862	0.020	1
1	A	12	LEU	HD22	0.862	0.020	1
1	A	12	LEU	HD23	0.862	0.020	1
1	A	12	LEU	HG	1.565	0.020	1
1	A	13	ARG	H	8.303	0.020	1
1	A	13	ARG	N	121.856	0.200	1
1	A	13	ARG	CA	56.174	0.500	1
1	A	13	ARG	HA	4.302	0.020	1
1	A	13	ARG	CB	30.902	0.500	1
1	A	13	ARG	HB2	1.746	0.020	1
1	A	13	ARG	HB3	1.746	0.020	1
1	A	13	ARG	CG	27.13	0.500	1
1	A	13	ARG	HG2	1.608	0.020	1
1	A	13	ARG	HG3	1.608	0.020	1
1	A	13	ARG	CD	43.543	0.500	1
1	A	13	ARG	HD2	3.175	0.020	1
1	A	13	ARG	HD3	3.175	0.020	1
1	A	14	GLN	H	8.403	0.020	1
1	A	14	GLN	N	121.829	0.200	1
1	A	14	GLN	CA	55.993	0.500	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	14	GLN	HA	4.309	0.020	1
1	A	14	GLN	CB	29.394	0.500	1
1	A	14	GLN	HB2	2.049	0.020	1
1	A	14	GLN	HB3	1.942	0.020	1
1	A	14	GLN	CG	33.66	0.500	1
1	A	14	GLN	HG2	2.297	0.020	1
1	A	14	GLN	HG3	2.297	0.020	1
1	A	14	GLN	NE2	112.213	0.200	1
1	A	14	GLN	HE21	7.499	0.020	1
1	A	14	GLN	HE22	6.826	0.020	1
1	A	15	GLN	H	8.461	0.020	1
1	A	15	GLN	N	121.78	0.200	1
1	A	15	GLN	CA	56.168	0.500	1
1	A	15	GLN	HA	4.299	0.020	1
1	A	15	GLN	CB	29.735	0.500	1
1	A	15	GLN	HB2	2.06	0.020	1
1	A	15	GLN	HB3	1.965	0.020	1
1	A	15	GLN	CG	33.832	0.500	1
1	A	15	GLN	HG2	2.319	0.020	1
1	A	15	GLN	HG3	2.319	0.020	1
1	A	15	GLN	NE2	112.135	0.200	1
1	A	15	GLN	HE21	7.512	0.020	1
1	A	15	GLN	HE22	6.849	0.020	1
1	A	16	ASN	H	8.485	0.020	1
1	A	16	ASN	N	120.167	0.200	1
1	A	16	ASN	CA	53.585	0.500	1
1	A	16	ASN	HA	4.669	0.020	1
1	A	16	ASN	C	175.145	0.500	1
1	A	16	ASN	CB	38.837	0.500	1
1	A	16	ASN	HB2	2.81	0.020	1
1	A	16	ASN	HB3	2.74	0.020	1
1	A	17	ARG	H	8.485	0.020	1
1	A	17	ARG	N	120.167	0.200	1
1	A	17	ARG	CA	56.331	0.500	1
1	A	17	ARG	HA	4.302	0.020	1
1	A	17	ARG	C	176.187	0.500	1
1	A	17	ARG	CB	30.624	0.500	1
1	A	17	ARG	HB2	1.795	0.020	1
1	A	17	ARG	HB3	1.723	0.020	1
1	A	17	ARG	CG	27.635	0.500	1
1	A	17	ARG	HG2	1.587	0.020	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	17	ARG	HG3	1.587	0.020	1
1	A	17	ARG	CD	43.543	0.500	1
1	A	17	ARG	HD2	3.166	0.020	1
1	A	17	ARG	HD3	3.166	0.020	1
1	A	18	GLN	H	8.436	0.020	1
1	A	18	GLN	N	121.588	0.200	1
1	A	18	GLN	CA	61.262	0.500	1
1	A	18	GLN	HA	4.315	0.020	1
1	A	18	GLN	C	175.741	0.500	1
1	A	18	GLN	CB	29.566	0.500	1
1	A	18	GLN	HB2	2.023	0.020	1
1	A	18	GLN	HB3	2.023	0.020	1
1	A	18	GLN	HG2	2.389	0.020	1
1	A	18	GLN	HG3	2.389	0.020	1
1	A	18	GLN	NE2	112.079	0.200	1
1	A	18	GLN	HE21	7.559	0.020	1
1	A	18	GLN	HE22	6.907	0.020	1
1	A	19	ILE	H	8.415	0.020	1
1	A	19	ILE	N	126.286	0.200	1
1	A	19	ILE	CA	60.968	0.500	1
1	A	19	ILE	HA	4.185	0.020	1
1	A	19	ILE	C	176.125	0.500	1
1	A	19	ILE	CB	38.746	0.500	1
1	A	19	ILE	HB	1.793	0.020	1
1	A	19	ILE	CG2	17.534	0.500	1
1	A	19	ILE	HG21	0.826	0.020	1
1	A	19	ILE	HG22	0.826	0.020	1
1	A	19	ILE	HG23	0.826	0.020	1
1	A	19	ILE	CG1	27.382	0.500	1
1	A	19	ILE	HG12	1.436	0.020	1
1	A	19	ILE	HG13	1.13	0.020	1
1	A	19	ILE	CD1	13.038	0.500	1
1	A	19	ILE	HD11	0.814	0.020	1
1	A	19	ILE	HD12	0.814	0.020	1
1	A	19	ILE	HD13	0.814	0.020	1
1	A	20	ILE	H	8.342	0.020	1
1	A	20	ILE	N	126.142	0.200	1
1	A	20	ILE	CA	60.859	0.500	1
1	A	20	ILE	HA	4.154	0.020	1
1	A	20	ILE	C	175.898	0.500	1
1	A	20	ILE	CB	38.677	0.500	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	20	ILE	HB	1.766	0.020	1
1	A	20	ILE	CG2	17.582	0.500	1
1	A	20	ILE	HG21	0.772	0.020	1
1	A	20	ILE	HG22	0.772	0.020	1
1	A	20	ILE	HG23	0.772	0.020	1
1	A	20	ILE	CG1	27.177	0.500	1
1	A	20	ILE	HG12	1.401	0.020	1
1	A	20	ILE	HG13	1.115	0.020	1
1	A	20	ILE	CD1	12.785	0.500	1
1	A	20	ILE	HD11	0.785	0.020	1
1	A	20	ILE	HD12	0.785	0.020	1
1	A	20	ILE	HD13	0.785	0.020	1

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	87	-0.16 ± 0.13	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	84	0.30 ± 0.16	None needed (< 0.5 ppm)
$^{13}C'$	67	0.03 ± 0.13	None needed (< 0.5 ppm)
^{15}N	78	-0.51 ± 0.38	None needed (imprecise)

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 90%, i.e. 844 atoms were assigned a chemical shift out of a possible 937. 0 out of 9 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	318/326 (98%)	131/131 (100%)	126/134 (94%)	61/61 (100%)
Sidechain	460/521 (88%)	309/338 (91%)	138/159 (87%)	13/24 (54%)
Aromatic	66/90 (73%)	33/44 (75%)	31/42 (74%)	2/4 (50%)
Overall	844/937 (90%)	473/513 (92%)	295/335 (88%)	76/89 (85%)

7.1.4 Statistically unusual chemical shifts

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.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: