wwPDB NMR Structure Validation Summary Report

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PDB ID	:	2MTN
BMRB ID	:	25171
Title	:	Solution structure of MLL-IBD complex
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Deposited on	:	2014-08-23

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:

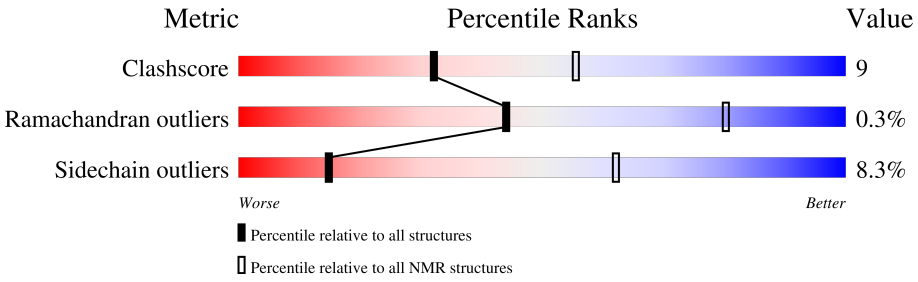
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
SOLUTION NMR

The overall completeness of chemical shifts assignment is 74%.

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	164	41% 9% • 26% 24%

2 Ensemble composition and analysis

This entry contains 20 models. Model 3 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative.

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:148-A:151, A:350-A:428 (83)	0.58	3

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 4 clusters and 2 single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1969 atoms, of which 989 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Histone-lysine N-methyltransferase 2A, PC4 and SFRS1-interacting protein fusion.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	125	1969	608	989	175	190	7	0

There are 7 discrepancies between the modelled and reference sequences:

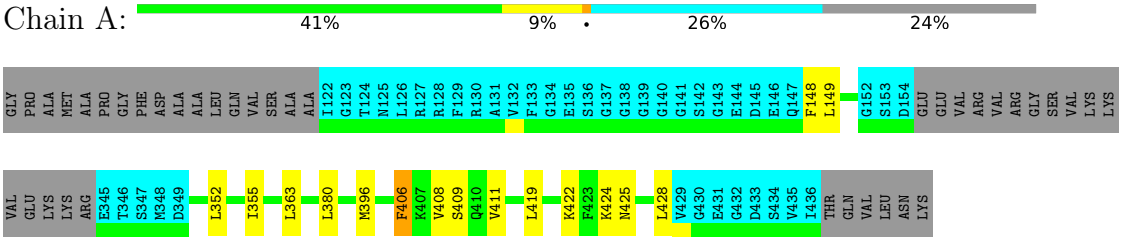
Chain	Residue	Modelled	Actual	Comment	Reference
A	105	GLY	-	expression tag	UNP Q03164
A	106	PRO	-	expression tag	UNP Q03164
A	107	ALA	-	expression tag	UNP Q03164
A	108	MET	-	expression tag	UNP Q03164
A	109	ALA	-	expression tag	UNP Q03164
A	335	GLY	-	linker	UNP Q03164
A	336	SER	-	linker	UNP Q03164

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.

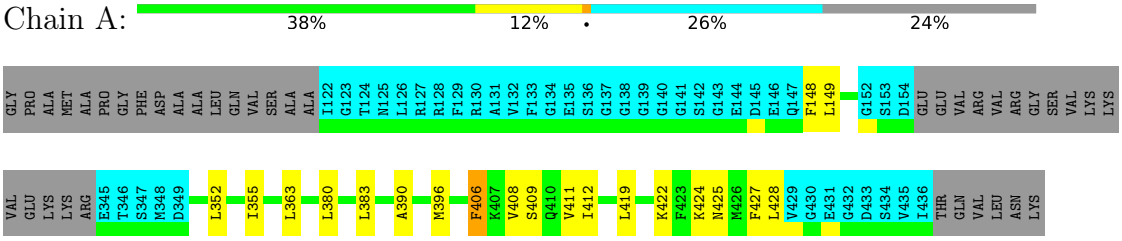
• Molecule 1: Histone-lysine N-methyltransferase 2A, PC4 and SFRS1-interacting protein fusion



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

The representative model is number 3. Colouring as in section 4.1 above.

• Molecule 1: Histone-lysine N-methyltransferase 2A, PC4 and SFRS1-interacting protein fusion



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 solution	2.1
CYANA	refinement	2.1

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	1425
Number of shifts mapped to atoms	1198
Number of unparsed shifts	0
Number of shifts with mapping errors	227
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	74%

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	685	726	726	13±2
All	All	13700	14520	14520	266

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 9.

5 of 91 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:400:LEU:HD21	1:A:419:LEU:HD23	0.91	1.40	11	1
1:A:352:LEU:HD22	1:A:396:MET:HE1	0.69	1.64	19	4
1:A:149:LEU:HD12	1:A:408:VAL:HG13	0.69	1.64	8	5
1:A:370:VAL:HG23	1:A:412:ILE:HD11	0.69	1.64	13	1
1:A:149:LEU:HD22	1:A:408:VAL:HG13	0.67	1.64	16	7

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	83/164 (51%)	76±2 (92±2%)	7±2 (8±2%)	0±0 (0±1%)	44 80
All	All	1660/3280 (51%)	1522 (92%)	133 (8%)	5 (0%)	44 80

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

Mol	Chain	Res	Type	Models (Total)
1	A	365	ILE	2
1	A	367	ASN	1
1	A	368	LEU	1
1	A	366	ASP	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	78/138 (57%)	72±2 (92±2%)	6±2 (8±2%)	15 62
All	All	1560/2760 (57%)	1431 (92%)	129 (8%)	15 62

5 of 39 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	406	PHE	20
1	A	355	ILE	14
1	A	422	LYS	13
1	A	368	LEU	6
1	A	424	LYS	5

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 74% for the well-defined parts and 70% 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	1425
Number of shifts mapped to atoms	1198
Number of unparsed shifts	0
Number of shifts with mapping errors	227
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 227) occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	106	PRO	HA	4.469	0.000	.
1	A	106	PRO	C	176.462	0.000	.
1	A	106	PRO	CA	62.991	0.000	.
1	A	106	PRO	CB	32.313	0.000	.
1	A	107	ALA	H	8.486	0.002	.
1	A	107	ALA	HA	4.317	0.004	.
1	A	107	ALA	HB1	1.419	0.000	.
1	A	107	ALA	HB2	1.419	0.000	.
1	A	107	ALA	HB3	1.419	0.000	.
1	A	107	ALA	C	177.614	0.003	.
1	A	107	ALA	CA	52.562	0.016	.
1	A	107	ALA	CB	19.149	0.013	.
1	A	107	ALA	N	124.559	0.039	.
1	A	108	MET	H	8.323	0.001	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	108	MET	HA	4.456	0.000	.
1	A	108	MET	C	175.518	0.001	.
1	A	108	MET	CA	54.975	0.013	.
1	A	108	MET	CB	33.298	0.025	.
1	A	108	MET	N	119.871	0.012	.
1	A	109	ALA	H	8.338	0.001	.
1	A	109	ALA	HA	4.633	0.000	.
1	A	109	ALA	HB1	1.398	0.001	.
1	A	109	ALA	HB2	1.398	0.001	.
1	A	109	ALA	HB3	1.398	0.001	.
1	A	109	ALA	C	175.415	0.000	.
1	A	109	ALA	CA	50.56	0.049	.
1	A	109	ALA	CB	18.256	0.067	.
1	A	109	ALA	N	126.837	0.039	.
1	A	110	PRO	C	177.6	0.000	.
1	A	110	PRO	CA	63.535	0.000	.
1	A	110	PRO	CB	31.984	0.000	.
1	A	111	GLY	H	8.489	0.001	.
1	A	111	GLY	HA2	3.929	0.000	.
1	A	111	GLY	HA3	3.929	0.000	.
1	A	111	GLY	C	174.2	0.007	.
1	A	111	GLY	CA	45.239	0.009	.
1	A	111	GLY	N	109.242	0.021	.
1	A	112	PHE	H	8.09	0.003	.
1	A	112	PHE	HA	4.583	0.007	.
1	A	112	PHE	HB2	3.15	0.013	.
1	A	112	PHE	HB3	3.15	0.013	.
1	A	112	PHE	HD1	7.288	0.000	.
1	A	112	PHE	HD2	7.288	0.000	.
1	A	112	PHE	C	175.345	0.002	.
1	A	112	PHE	CA	58.316	0.053	.
1	A	112	PHE	CB	39.749	0.027	.
1	A	112	PHE	N	120.31	0.040	.
1	A	113	ASP	H	8.256	0.005	.
1	A	113	ASP	HA	4.55	0.014	.
1	A	113	ASP	HB2	2.611	0.008	.
1	A	113	ASP	HB3	2.611	0.008	.
1	A	113	ASP	C	176.263	0.002	.
1	A	113	ASP	CA	54.135	0.010	.
1	A	113	ASP	CB	41.271	0.002	.
1	A	113	ASP	N	122.406	0.030	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	114	ALA	H	8.235	0.003	.
1	A	114	ALA	HA	4.18	0.002	.
1	A	114	ALA	HB1	1.455	0.000	.
1	A	114	ALA	HB2	1.455	0.000	.
1	A	114	ALA	HB3	1.455	0.000	.
1	A	114	ALA	C	178.165	0.004	.
1	A	114	ALA	CA	53.512	0.041	.
1	A	114	ALA	CB	18.98	0.007	.
1	A	114	ALA	N	125.612	0.035	.
1	A	115	ALA	H	8.229	0.002	.
1	A	115	ALA	HA	4.262	0.012	.
1	A	115	ALA	HB1	1.432	0.000	.
1	A	115	ALA	HB2	1.432	0.000	.
1	A	115	ALA	HB3	1.432	0.000	.
1	A	115	ALA	C	178.356	0.022	.
1	A	115	ALA	CA	53.231	0.026	.
1	A	115	ALA	CB	18.806	0.013	.
1	A	115	ALA	N	121.211	0.010	.
1	A	116	LEU	H	7.851	0.001	.
1	A	116	LEU	HA	4.308	0.011	.
1	A	116	LEU	HD11	0.897	0.007	.
1	A	116	LEU	HD12	0.897	0.007	.
1	A	116	LEU	HD13	0.897	0.007	.
1	A	116	LEU	HD21	0.961	0.002	.
1	A	116	LEU	HD22	0.961	0.002	.
1	A	116	LEU	HD23	0.961	0.002	.
1	A	116	LEU	C	177.661	0.000	.
1	A	116	LEU	CA	55.476	0.011	.
1	A	116	LEU	CB	42.304	0.016	.
1	A	116	LEU	CD1	23.492	0.098	.
1	A	116	LEU	CD2	24.829	0.027	.
1	A	116	LEU	N	119.57	0.025	.
1	A	117	GLN	H	8.117	0.002	.
1	A	117	GLN	HA	4.333	0.000	.
1	A	117	GLN	C	176.32	0.006	.
1	A	117	GLN	CA	56.221	0.032	.
1	A	117	GLN	CB	29.22	0.002	.
1	A	117	GLN	N	120.32	0.009	.
1	A	118	VAL	H	8.064	0.001	.
1	A	118	VAL	HA	4.136	0.000	.
1	A	118	VAL	HB	2.127	0.000	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	118	VAL	C	176.438	0.014	.
1	A	118	VAL	CA	62.859	0.015	.
1	A	118	VAL	CB	32.743	0.029	.
1	A	118	VAL	N	120.441	0.022	.
1	A	119	SER	H	8.303	0.002	.
1	A	119	SER	HA	4.427	0.000	.
1	A	119	SER	C	174.711	0.005	.
1	A	119	SER	CA	58.716	0.052	.
1	A	119	SER	CB	63.915	0.077	.
1	A	119	SER	N	118.488	0.035	.
1	A	120	ALA	H	8.334	0.001	.
1	A	120	ALA	C	177.717	0.015	.
1	A	120	ALA	CA	52.932	0.086	.
1	A	120	ALA	CB	19.159	0.015	.
1	A	120	ALA	N	125.919	0.021	.
1	A	121	ALA	H	8.167	0.005	.
1	A	121	ALA	HA	4.345	0.012	.
1	A	121	ALA	HB1	1.442	0.003	.
1	A	121	ALA	HB2	1.442	0.003	.
1	A	121	ALA	HB3	1.442	0.003	.
1	A	121	ALA	C	178.069	0.012	.
1	A	121	ALA	CA	52.85	0.033	.
1	A	121	ALA	CB	19.031	0.032	.
1	A	121	ALA	N	122.61	0.007	.
1	A	329	GLU	H	8.16	0.003	.
1	A	329	GLU	CA	57.113	0.000	.
1	A	329	GLU	N	120.255	0.031	.
1	A	333	VAL	H	8.189	0.002	.
1	A	333	VAL	C	176.29	0.016	.
1	A	333	VAL	CA	62.463	0.044	.
1	A	333	VAL	CB	32.713	0.000	.
1	A	333	VAL	N	121.376	0.048	.
1	A	334	ARG	H	8.485	0.003	.
1	A	334	ARG	C	176.875	0.017	.
1	A	334	ARG	CA	56.564	0.012	.
1	A	334	ARG	CB	30.677	0.079	.
1	A	334	ARG	N	125.191	0.007	.
1	A	335	GLY	H	8.469	0.001	.
1	A	335	GLY	HA2	3.997	0.000	.
1	A	335	GLY	HA3	3.997	0.000	.
1	A	335	GLY	C	174.065	0.001	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	335	GLY	CA	45.392	0.009	.
1	A	335	GLY	N	110.077	0.087	.
1	A	336	SER	H	8.221	0.003	.
1	A	336	SER	C	174.654	0.008	.
1	A	336	SER	CA	58.322	0.025	.
1	A	336	SER	CB	64.075	0.006	.
1	A	336	SER	N	115.584	0.024	.
1	A	337	VAL	H	8.194	0.003	.
1	A	337	VAL	HA	4.153	0.000	.
1	A	337	VAL	C	176.079	0.012	.
1	A	337	VAL	CA	62.378	0.035	.
1	A	337	VAL	CB	32.668	0.000	.
1	A	337	VAL	N	121.889	0.004	.
1	A	338	LYS	H	8.367	0.002	.
1	A	338	LYS	HA	4.318	0.000	.
1	A	338	LYS	C	176.3	0.013	.
1	A	338	LYS	CA	56.281	0.055	.
1	A	338	LYS	CB	33.093	0.009	.
1	A	338	LYS	N	125.359	0.002	.
1	A	339	LYS	H	8.375	0.001	.
1	A	339	LYS	C	176.344	0.006	.
1	A	339	LYS	CA	56.462	0.070	.
1	A	339	LYS	CB	33.069	0.082	.
1	A	339	LYS	N	123.696	0.008	.
1	A	340	VAL	H	8.239	0.001	.
1	A	340	VAL	C	175.943	0.008	.
1	A	340	VAL	CA	62.325	0.021	.
1	A	340	VAL	CB	32.812	0.000	.
1	A	340	VAL	N	122.356	0.017	.
1	A	341	GLU	H	8.497	0.003	.
1	A	341	GLU	C	176.292	0.003	.
1	A	341	GLU	CA	56.332	0.055	.
1	A	341	GLU	CB	30.583	0.023	.
1	A	341	GLU	N	125.454	0.031	.
1	A	342	LYS	H	8.454	0.001	.
1	A	342	LYS	C	176.644	0.000	.
1	A	342	LYS	CA	56.647	0.000	.
1	A	342	LYS	CB	32.914	0.000	.
1	A	342	LYS	N	123.485	0.010	.
1	A	437	THR	H	8.166	0.012	.
1	A	437	THR	HA	4.296	0.054	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	437	THR	HB	4.218	0.003	.
1	A	437	THR	HG21	1.228	0.009	.
1	A	437	THR	HG22	1.228	0.009	.
1	A	437	THR	HG23	1.228	0.009	.
1	A	437	THR	C	174.413	0.005	.
1	A	437	THR	CA	62.217	0.042	.
1	A	437	THR	CB	69.757	0.051	.
1	A	437	THR	CG2	21.792	0.049	.
1	A	437	THR	N	118.148	0.033	.
1	A	438	GLN	H	8.302	0.002	.
1	A	438	GLN	HA	4.381	0.000	.
1	A	438	GLN	C	175.683	0.000	.
1	A	438	GLN	CA	55.999	0.044	.
1	A	438	GLN	CB	29.698	0.022	.
1	A	438	GLN	N	122.953	0.017	.
1	A	439	VAL	H	8.212	0.002	.
1	A	439	VAL	HA	4.088	0.000	.
1	A	439	VAL	C	175.947	0.002	.
1	A	439	VAL	CA	62.652	0.003	.
1	A	439	VAL	CB	32.664	0.033	.
1	A	439	VAL	N	121.816	0.019	.
1	A	440	LEU	H	8.33	0.001	.
1	A	440	LEU	HA	4.431	0.004	.
1	A	440	LEU	HB2	1.623	0.000	.
1	A	440	LEU	HB3	1.69	0.000	.
1	A	440	LEU	HG	1.651	0.000	.
1	A	440	LEU	HD11	0.898	0.005	.
1	A	440	LEU	HD12	0.898	0.005	.
1	A	440	LEU	HD13	0.898	0.005	.
1	A	440	LEU	HD21	0.954	0.000	.
1	A	440	LEU	HD22	0.954	0.000	.
1	A	440	LEU	HD23	0.954	0.000	.
1	A	440	LEU	C	176.823	0.003	.
1	A	440	LEU	CA	55.082	0.020	.
1	A	440	LEU	CB	42.596	0.054	.
1	A	440	LEU	CG	26.907	0.000	.
1	A	440	LEU	CD1	23.499	0.112	.
1	A	440	LEU	CD2	24.928	0.148	.
1	A	440	LEU	N	125.709	0.014	.
1	A	441	ASN	H	8.388	0.001	.
1	A	441	ASN	C	173.964	0.003	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	441	ASN	CA	53.416	0.009	.
1	A	441	ASN	CB	39.051	0.000	.
1	A	441	ASN	N	120.03	0.027	.
1	A	442	LYS	H	7.855	0.002	.
1	A	442	LYS	C	181.151	0.000	.
1	A	442	LYS	CA	57.93	0.000	.
1	A	442	LYS	CB	33.823	0.000	.
1	A	442	LYS	N	126.465	0.003	.

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	150	-0.65 ± 0.10	Should be checked
$^{13}C_{\beta}$	135	0.16 ± 0.11	None needed (< 0.5 ppm)
$^{13}C'$	145	-0.37 ± 0.09	None needed (< 0.5 ppm)
^{15}N	142	-0.16 ± 0.27	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 74%, i.e. 912 atoms were assigned a chemical shift out of a possible 1237. 0 out of 14 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	392/416 (94%)	154/167 (92%)	160/166 (96%)	78/83 (94%)
Sidechain	488/748 (65%)	323/485 (67%)	160/228 (70%)	5/35 (14%)
Aromatic	32/73 (44%)	32/37 (86%)	0/34 (0%)	0/2 (0%)
Overall	912/1237 (74%)	509/689 (74%)	320/428 (75%)	83/120 (69%)

7.1.4 Statistically unusual chemical shifts

There are no statistically unusual chemical shifts.

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: