wwPDB NMR Structure Validation Summary Report

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PDB ID	:	2LU1
BMRB ID	:	18504
Title	:	pfsub2 solution NMR structure
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Deposited on	:	2012-06-06

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:

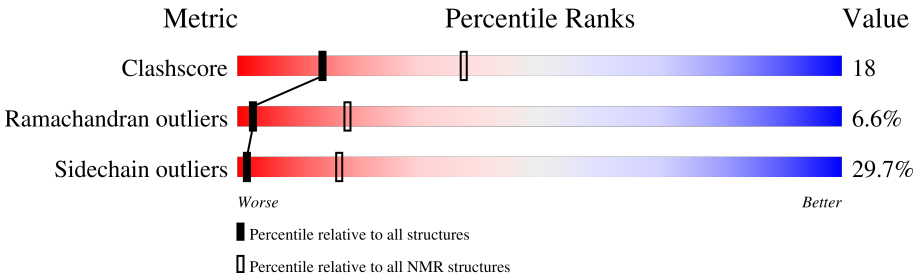
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson 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 61%.

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	149	25% 30% • 5% 40%

2 Ensemble composition and analysis

This entry contains 20 models. Model 7 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:27-A:39, A:43-A:111 (82)	1.71	7

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 2 single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1502 atoms, of which 760 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Subtilase.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	89	1502	483	760	119	136	4	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	THR	-	expression tag	UNP O97364
A	2	SER	-	expression tag	UNP O97364

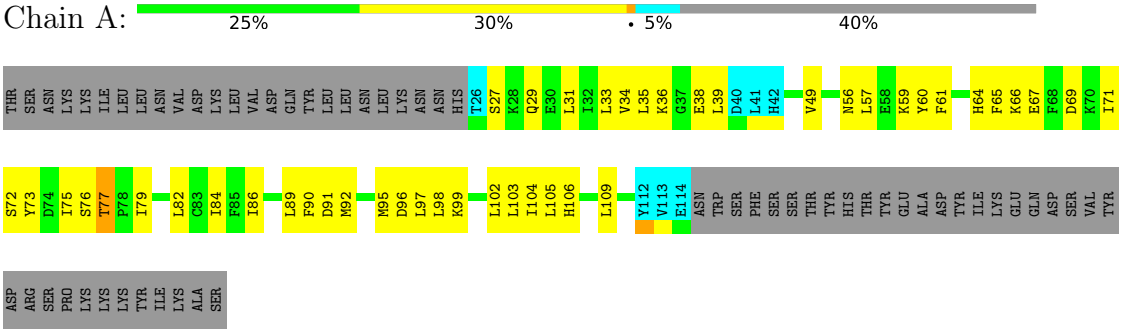
4 Residue-property plots

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: Subtilase

Chain A:

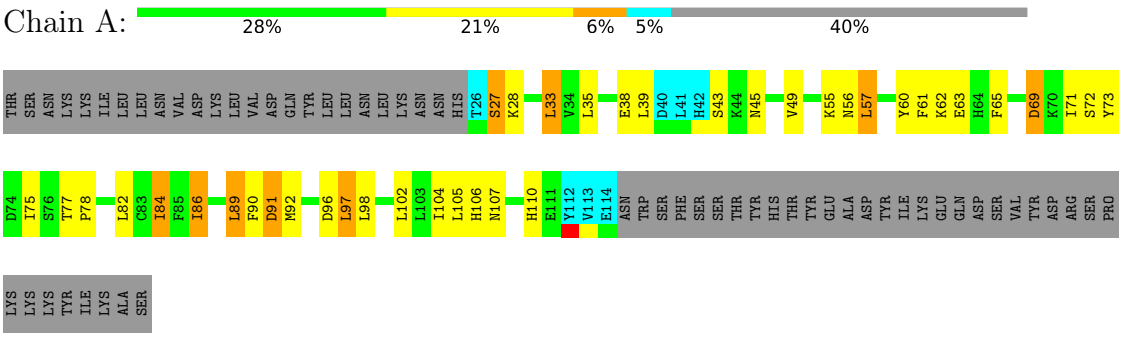


4.2 Residue scores for the representative (medoid) model from the NMR ensemble

The representative model is number 7. Colouring as in section 4.1 above.

• Molecule 1: Subtilase

Chain A:



5 Refinement protocol and experimental data overview

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

Of the 500 calculated structures, 20 were deposited, based on the following criterion: *structures with acceptable covalent geometry*.

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

Software name	Classification	Version
CNS	refinement	1.21

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	1150
Number of shifts mapped to atoms	795
Number of unparsed shifts	0
Number of shifts with mapping errors	355
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	61%

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	681	706	704	24±4
All	All	13620	14120	14080	485

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 18.

5 of 282 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:48:ASN:ND2	1:A:104:ILE:HD11	0.80	1.91	10	1
1:A:73:TYR:HB2	1:A:84:ILE:HD12	0.80	1.54	15	3
1:A:49:VAL:HG11	1:A:73:TYR:HB3	0.79	1.53	17	12
1:A:33:LEU:HD23	1:A:105:LEU:HD22	0.79	1.53	17	1
1:A:105:LEU:HD12	1:A:106:HIS:N	0.78	1.94	16	11

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	82/149 (55%)	66±2 (81±3%)	10±2 (12±3%)	5±2 (7±2%)	2 18
All	All	1640/2980 (55%)	1327 (81%)	205 (12%)	108 (7%)	2 18

5 of 19 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	90	PHE	17
1	A	91	ASP	15
1	A	77	THR	12
1	A	95	MET	9
1	A	65	PHE	7

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	79/144 (55%)	56±4 (70±5%)	23±4 (30±5%)	1 17
All	All	1580/2880 (55%)	1111 (70%)	469 (30%)	1 17

5 of 73 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	92	MET	17
1	A	35	LEU	16
1	A	66	LYS	15
1	A	59	LYS	14
1	A	72	SER	12

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 61% for the well-defined parts and 61% 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	1150
Number of shifts mapped to atoms	795
Number of unparsed shifts	0
Number of shifts with mapping errors	355
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 355) occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	4	LYS	C	176.016	0	1
1	A	4	LYS	CA	56.809	0	1
1	A	4	LYS	CB	32.045	0	1
1	A	5	LYS	H	7.829	0.003	1
1	A	5	LYS	HA	4.253	0.007	1
1	A	5	LYS	HB3	2.195	0	2
1	A	5	LYS	C	177.862	0	1
1	A	5	LYS	CA	57.862	0	1
1	A	5	LYS	CB	31.6	0	1
1	A	5	LYS	N	126.4	0	1
1	A	6	ILE	H	9.012	0.013	1
1	A	6	ILE	HA	4.255	0.015	1
1	A	6	ILE	HB	2.63	0.013	1
1	A	6	ILE	C	178.826	0	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	6	ILE	CA	57.81	0	1
1	A	6	ILE	CB	39.896	0	1
1	A	6	ILE	N	119.896	0.009	1
1	A	7	LEU	H	8.104	0.011	1
1	A	7	LEU	HA	4.226	0.045	1
1	A	7	LEU	HB2	2.341	0.022	2
1	A	7	LEU	HB3	1.54	0.014	2
1	A	7	LEU	HG	1.786	0	1
1	A	7	LEU	C	179.872	0	1
1	A	7	LEU	CA	57.02	0	1
1	A	7	LEU	CB	41.632	0	1
1	A	7	LEU	N	117.909	0.006	1
1	A	8	LEU	H	6.781	0.028	1
1	A	8	LEU	HA	3.329	0	1
1	A	8	LEU	HB2	1.448	0	1
1	A	8	LEU	HB3	1.448	0	1
1	A	8	LEU	CA	56.945	0	1
1	A	8	LEU	CB	38.951	0	1
1	A	8	LEU	N	121.284	0.018	1
1	A	9	ASN	HA	4.266	0.005	1
1	A	9	ASN	HB2	3.176	0	1
1	A	9	ASN	HB3	3.176	0	1
1	A	9	ASN	C	179.215	0	1
1	A	9	ASN	CA	58.507	0	1
1	A	9	ASN	CB	42.115	0	1
1	A	10	VAL	H	8.014	0.005	1
1	A	10	VAL	HA	4.041	0	1
1	A	10	VAL	C	177.523	0	1
1	A	10	VAL	CA	67.407	0.241	1
1	A	10	VAL	CB	30.875	0	1
1	A	10	VAL	N	119.438	0	1
1	A	11	ASP	H	7.738	0.007	1
1	A	11	ASP	C	178.742	0	1
1	A	11	ASP	CA	58.228	0.072	1
1	A	11	ASP	CB	40.226	0.336	1
1	A	11	ASP	N	118.82	0.215	1
1	A	12	LYS	H	7.62	0.003	1
1	A	12	LYS	HA	4.133	0	1
1	A	12	LYS	HB2	1.942	0	1
1	A	12	LYS	HB3	1.942	0	1
1	A	12	LYS	CA	58.504	0	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	12	LYS	CB	31.871	0	1
1	A	12	LYS	N	118.846	0.21	1
1	A	14	VAL	HA	4.059	0.051	1
1	A	14	VAL	HB	1.843	0.063	1
1	A	14	VAL	C	175.786	0	1
1	A	14	VAL	CA	62.956	0	1
1	A	14	VAL	CB	31.928	0	1
1	A	15	ASP	H	8.817	0.014	1
1	A	15	ASP	HA	4.089	0	1
1	A	15	ASP	C	174.704	0	1
1	A	15	ASP	CA	54.261	0	1
1	A	15	ASP	CB	42.402	0	1
1	A	15	ASP	N	129.019	0.03	1
1	A	16	GLN	H	8.698	0.024	1
1	A	16	GLN	HA	4.266	0.004	1
1	A	16	GLN	HB2	2.059	0	1
1	A	16	GLN	HB3	2.059	0	1
1	A	16	GLN	C	176.596	0.02	1
1	A	16	GLN	CA	57.335	0.029	1
1	A	16	GLN	CB	28.684	0.045	1
1	A	16	GLN	N	116.557	0.096	1
1	A	17	TYR	H	7.336	0.03	1
1	A	17	TYR	HA	4.274	0.001	1
1	A	17	TYR	HB2	1.728	0.011	1
1	A	17	TYR	HB3	1.728	0.011	1
1	A	17	TYR	CA	54.415	0	1
1	A	17	TYR	CB	42.964	0	1
1	A	17	TYR	N	119.909	0	1
1	A	20	ASN	HA	4.025	0.067	1
1	A	20	ASN	HB2	2.861	0.009	2
1	A	20	ASN	HB3	2.558	0.024	2
1	A	20	ASN	C	177.974	0	1
1	A	20	ASN	CA	55.345	0	1
1	A	20	ASN	CB	38.017	0	1
1	A	21	LEU	H	7.664	0.039	1
1	A	21	LEU	HA	3.856	0.005	1
1	A	21	LEU	HB2	1.629	0.02	2
1	A	21	LEU	HB3	1.353	0.001	2
1	A	21	LEU	HD11	0.82	0.02	2
1	A	21	LEU	HD12	0.82	0.02	2
1	A	21	LEU	HD13	0.82	0.02	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	21	LEU	C	178.296	0.014	1
1	A	21	LEU	CA	56.794	0.294	1
1	A	21	LEU	CB	42.665	0.133	1
1	A	21	LEU	CG	30.33	0	1
1	A	21	LEU	CD1	24.534	0	1
1	A	21	LEU	N	120.035	0.165	1
1	A	22	LYS	H	7.521	0.024	1
1	A	22	LYS	HA	4.279	0.026	1
1	A	22	LYS	HB2	1.897	0.015	1
1	A	22	LYS	HB3	1.897	0.015	1
1	A	22	LYS	C	176.886	0.031	1
1	A	22	LYS	CA	57.979	0.05	1
1	A	22	LYS	CB	32.526	0.04	1
1	A	22	LYS	CG	25.003	0	1
1	A	22	LYS	CD	29.979	0	1
1	A	22	LYS	CE	41.922	0	1
1	A	22	LYS	N	116.504	0.108	1
1	A	23	ASN	H	7.622	0.009	1
1	A	23	ASN	HA	4.824	0.028	1
1	A	23	ASN	HB2	2.89	0.018	2
1	A	23	ASN	HB3	2.659	0.01	2
1	A	23	ASN	C	173.946	0.076	1
1	A	23	ASN	CA	53.633	0.24	1
1	A	23	ASN	CB	39.308	0.077	1
1	A	23	ASN	N	116.609	0.306	1
1	A	24	ASN	H	7.581	0.044	1
1	A	24	ASN	HA	4.373	0.092	1
1	A	24	ASN	HB2	2.713	0.067	1
1	A	24	ASN	HB3	2.713	0.067	1
1	A	24	ASN	C	179.456	0	1
1	A	24	ASN	CA	55.525	0.047	1
1	A	24	ASN	CB	40.811	0.06	1
1	A	24	ASN	N	123.849	0.047	1
1	A	25	HIS	H	8.401	0.029	1
1	A	25	HIS	HA	4.413	0.044	1
1	A	25	HIS	HB2	1.897	0.027	2
1	A	25	HIS	HB3	1.727	0	2
1	A	25	HIS	C	175.574	0.242	1
1	A	25	HIS	CA	57.687	0	1
1	A	25	HIS	CB	29.879	0	1
1	A	25	HIS	N	123.95	0.151	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	122	TYR	HA	4.07	0.032	1
1	A	122	TYR	HB2	2.233	0.003	2
1	A	122	TYR	HB3	1.779	0.014	2
1	A	122	TYR	HD1	7.189	0.043	1
1	A	122	TYR	HD2	7.189	0.043	1
1	A	122	TYR	HE1	6.782	0.051	1
1	A	122	TYR	HE2	6.782	0.051	1
1	A	122	TYR	C	175.991	0	1
1	A	122	TYR	CA	62.195	0	1
1	A	122	TYR	CB	38.307	0.005	1
1	A	123	HIS	H	8.075	0.007	1
1	A	123	HIS	HA	4.203	0.024	1
1	A	123	HIS	HB2	1.77	0	2
1	A	123	HIS	HB3	1.448	0.069	2
1	A	123	HIS	CA	56.715	0	1
1	A	123	HIS	CB	32.74	0	1
1	A	123	HIS	N	124.549	0.026	1
1	A	124	THR	HA	4.274	0	1
1	A	124	THR	C	180.323	0	1
1	A	124	THR	CA	62.254	0	1
1	A	124	THR	CB	70.157	0	1
1	A	125	TYR	H	8.112	0.004	1
1	A	125	TYR	HA	4.132	0.018	1
1	A	125	TYR	HB2	1.835	0.01	1
1	A	125	TYR	HB3	1.835	0.01	1
1	A	125	TYR	HD1	7.258	0	1
1	A	125	TYR	HD2	7.258	0	1
1	A	125	TYR	HE1	6.91	0	1
1	A	125	TYR	HE2	6.91	0	1
1	A	125	TYR	C	175.172	0	1
1	A	125	TYR	CA	61.575	0.025	1
1	A	125	TYR	CB	38.86	0.026	1
1	A	125	TYR	N	121.992	0.149	1
1	A	126	GLU	H	7.835	0.015	1
1	A	126	GLU	C	179.388	0	1
1	A	126	GLU	CA	57.106	0.171	1
1	A	126	GLU	CB	30.624	0.227	1
1	A	126	GLU	CG	36.477	0	1
1	A	126	GLU	N	127.245	0.054	1
1	A	127	ALA	H	8.091	0.016	1
1	A	127	ALA	HA	4.215	0.019	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	127	ALA	HB1	1.35	0.022	1
1	A	127	ALA	HB2	1.35	0.022	1
1	A	127	ALA	HB3	1.35	0.022	1
1	A	127	ALA	C	177.573	0.016	1
1	A	127	ALA	CA	53.203	0.081	1
1	A	127	ALA	CB	19.267	0.014	1
1	A	127	ALA	N	123.948	0.04	1
1	A	128	ASP	H	8.15	0.007	1
1	A	128	ASP	HA	4.531	0.003	1
1	A	128	ASP	HB2	2.628	0.018	1
1	A	128	ASP	HB3	2.628	0.018	1
1	A	128	ASP	C	176.104	0.034	1
1	A	128	ASP	CA	55.037	0.015	1
1	A	128	ASP	CB	41.123	0.045	1
1	A	128	ASP	N	118.462	0.006	1
1	A	129	TYR	H	7.813	0.005	1
1	A	129	TYR	HA	4.508	0.001	1
1	A	129	TYR	HB2	2.993	0	1
1	A	129	TYR	HB3	2.993	0	1
1	A	129	TYR	HD1	7.023	0	1
1	A	129	TYR	HD2	7.023	0	1
1	A	129	TYR	HE1	6.764	0	1
1	A	129	TYR	HE2	6.764	0	1
1	A	129	TYR	C	175.625	0.074	1
1	A	129	TYR	CA	58.296	0.019	1
1	A	129	TYR	CB	38.684	0.02	1
1	A	129	TYR	N	119.646	0.026	1
1	A	130	ILE	H	7.802	0.004	1
1	A	130	ILE	HA	4.215	0	1
1	A	130	ILE	C	176.159	0	1
1	A	130	ILE	CA	61.477	0.081	1
1	A	130	ILE	CB	38.528	0.105	1
1	A	130	ILE	CG1	27.461	0	1
1	A	130	ILE	CG2	17.216	0	1
1	A	130	ILE	N	122.284	0.006	1
1	A	131	LYS	H	8.053	0.056	1
1	A	131	LYS	HA	4.222	0	1
1	A	131	LYS	HB2	1.807	0	1
1	A	131	LYS	HB3	1.807	0	1
1	A	131	LYS	C	176.825	0	1
1	A	131	LYS	CA	56.93	0.003	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	131	LYS	CB	33.161	0.215	1
1	A	131	LYS	CG	24.768	0	1
1	A	131	LYS	CD	29.628	0	1
1	A	131	LYS	CE	42.097	0	1
1	A	131	LYS	N	123.816	0.414	1
1	A	132	GLU	H	8.296	0.005	1
1	A	132	GLU	HA	4.252	0	1
1	A	132	GLU	C	175.827	0.045	1
1	A	132	GLU	CA	56.962	0.059	1
1	A	132	GLU	CB	29.768	0.123	1
1	A	132	GLU	N	121.558	0.02	1
1	A	133	GLN	H	8.259	0.064	1
1	A	133	GLN	HA	4.249	0.003	1
1	A	133	GLN	C	176.708	0	1
1	A	133	GLN	CA	56.592	0.041	1
1	A	133	GLN	CB	29.645	0.165	1
1	A	133	GLN	CG	34.194	0	1
1	A	133	GLN	N	121.031	0.018	1
1	A	134	ASP	H	8.253	0.034	1
1	A	134	ASP	HA	4.632	0	1
1	A	134	ASP	HB2	2.698	0.01	1
1	A	134	ASP	HB3	2.698	0.01	1
1	A	134	ASP	C	176.386	0	1
1	A	134	ASP	CA	54.97	0.027	1
1	A	134	ASP	CB	41.436	0.081	1
1	A	134	ASP	N	120.377	0.028	1
1	A	135	SER	H	8.163	0.03	1
1	A	135	SER	HA	4.6	0.047	1
1	A	135	SER	HB2	3.908	0	1
1	A	135	SER	HB3	3.908	0	1
1	A	135	SER	C	173.577	0	1
1	A	135	SER	CA	58.608	0.04	1
1	A	135	SER	CB	64.19	0.077	1
1	A	135	SER	N	115.471	0.162	1
1	A	136	VAL	H	7.66	0.015	1
1	A	136	VAL	HA	3.99	0.042	1
1	A	136	VAL	HB	2.04	0.021	1
1	A	136	VAL	HG11	0.941	0	2
1	A	136	VAL	HG12	0.941	0	2
1	A	136	VAL	HG13	0.941	0	2
1	A	136	VAL	C	176.182	0	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	136	VAL	CA	63.507	0.026	1
1	A	136	VAL	CB	32.693	0.105	1
1	A	136	VAL	CG1	20.67	0	1
1	A	136	VAL	N	125.328	0.002	1
1	A	137	TYR	H	7.966	0.033	1
1	A	137	TYR	HA	4.565	0.002	1
1	A	137	TYR	HB2	2.646	0.009	1
1	A	137	TYR	HB3	2.646	0.009	1
1	A	137	TYR	HD1	7.05	0	1
1	A	137	TYR	HD2	7.05	0	1
1	A	137	TYR	HE1	6.702	0	1
1	A	137	TYR	HE2	6.702	0	1
1	A	137	TYR	C	175.508	0	1
1	A	137	TYR	CA	58.238	0.086	1
1	A	137	TYR	CB	38.782	0.06	1
1	A	137	TYR	N	121.579	0.204	1
1	A	138	ASP	H	8.053	0.01	1
1	A	138	ASP	CA	54.538	0	1
1	A	138	ASP	CB	41.307	0	1
1	A	138	ASP	N	121.53	0.163	1
1	A	139	ARG	HA	4.344	0.016	1
1	A	139	ARG	HB2	1.873	0.053	1
1	A	139	ARG	HB3	1.873	0.053	1
1	A	139	ARG	C	176.255	0	1
1	A	139	ARG	CA	56.048	0	1
1	A	139	ARG	CB	30.581	0	1
1	A	139	ARG	CG	27.052	0	1
1	A	139	ARG	CD	43.444	0	1
1	A	140	SER	H	8.202	0.006	1
1	A	140	SER	HA	4.305	0	1
1	A	140	SER	CA	56.763	0	1
1	A	140	SER	CB	63.437	0	1
1	A	140	SER	N	117.321	0.213	1
1	A	142	LYS	C	175.86	0	1
1	A	142	LYS	CA	56.575	0	1
1	A	142	LYS	CB	33.099	0	1
1	A	142	LYS	CG	24.768	0	1
1	A	142	LYS	CD	29.569	0	1
1	A	142	LYS	CE	41.805	0	1
1	A	143	LYS	H	8.15	0.017	1
1	A	143	LYS	HA	4.317	0	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	143	LYS	HB2	1.822	0	1
1	A	143	LYS	HB3	1.822	0	1
1	A	143	LYS	C	175.552	0	1
1	A	143	LYS	CA	56.833	0.02	1
1	A	143	LYS	CB	33.142	0.069	1
1	A	143	LYS	CG	24.768	0	1
1	A	143	LYS	CD	29.101	0	1
1	A	143	LYS	CE	42.273	0	1
1	A	143	LYS	N	121.435	0.036	1
1	A	144	LYS	H	7.887	0.007	1
1	A	144	LYS	C	181.245	0	1
1	A	144	LYS	CA	57.788	0	1
1	A	144	LYS	CB	33.609	0	1
1	A	144	LYS	N	128.243	0.124	1
1	A	145	TYR	HA	4.561	0.032	1
1	A	145	TYR	HB2	2.987	0.007	1
1	A	145	TYR	HB3	2.987	0.007	1
1	A	145	TYR	HD1	7.023	0	1
1	A	145	TYR	HD2	7.023	0	1
1	A	145	TYR	HE1	6.743	0	1
1	A	145	TYR	HE2	6.743	0	1
1	A	145	TYR	C	175.201	0	1
1	A	145	TYR	CA	57.804	0	1
1	A	145	TYR	CB	38.778	0	1
1	A	146	ILE	H	7.914	0.015	1
1	A	146	ILE	HA	4.061	0.033	1
1	A	146	ILE	HB	1.779	0.006	1
1	A	146	ILE	C	175.43	0.025	1
1	A	146	ILE	CA	60.853	0.098	1
1	A	146	ILE	CB	39.016	0.047	1
1	A	146	ILE	CG1	27.227	0	1
1	A	146	ILE	CD1	17.216	0	1
1	A	146	ILE	N	123.473	0.015	1
1	A	147	LYS	H	8.186	0.064	1
1	A	147	LYS	HA	4.274	0.013	1
1	A	147	LYS	HB2	1.785	0.008	1
1	A	147	LYS	HB3	1.785	0.008	1
1	A	147	LYS	C	175.743	0	1
1	A	147	LYS	CA	56.403	0.003	1
1	A	147	LYS	CB	33.161	0.047	1
1	A	147	LYS	CG	24.768	0	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	147	LYS	CD	29.335	0	1
1	A	147	LYS	CE	41.922	0	1
1	A	147	LYS	N	126.191	0.09	1
1	A	148	ALA	H	8.321	0.014	1
1	A	148	ALA	HA	4.354	0	1
1	A	148	ALA	C	176.738	0	1
1	A	148	ALA	CA	52.754	0.081	1
1	A	148	ALA	CB	19.501	0.061	1
1	A	148	ALA	N	127.131	0.16	1
1	A	149	SER	H	7.836	0.003	1
1	A	149	SER	CA	59.866	0	1
1	A	149	SER	CB	64.959	0	1
1	A	149	SER	N	120.767	0.03	1

7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	134	-0.61 ± 0.30	Should be checked
$^{13}C_{\beta}$	133	0.37 ± 0.08	None needed (< 0.5 ppm)
$^{13}C'$	125	-0.28 ± 0.19	None needed (< 0.5 ppm)
^{15}N	118	0.79 ± 0.29	Should be applied

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 61%, i.e. 731 atoms were assigned a chemical shift out of a possible 1206. 0 out of 15 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	386/407 (95%)	151/163 (93%)	161/164 (98%)	74/80 (92%)
Sidechain	329/697 (47%)	201/452 (44%)	128/223 (57%)	0/22 (0%)
Aromatic	16/102 (16%)	14/50 (28%)	2/46 (4%)	0/6 (0%)
Overall	731/1206 (61%)	366/665 (55%)	291/433 (67%)	74/108 (69%)

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.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: