wwPDB NMR Structure Validation Summary Report

Apr 21, 2024 – 02:49 AM EDT

PDB ID	:	2LY4
BMRB ID	:	18709
Title	:	HMGB1-facilitated p53 DNA binding occurs via HMG-box/p53 transactivation domain interaction and is regulated by the acidic tail
Authors	:	Rowell, J.P.; Simpson, K.L.; Stott, K.; Watson, M.; Thomas, J.O.
Deposited on	:	2012-09-12

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:

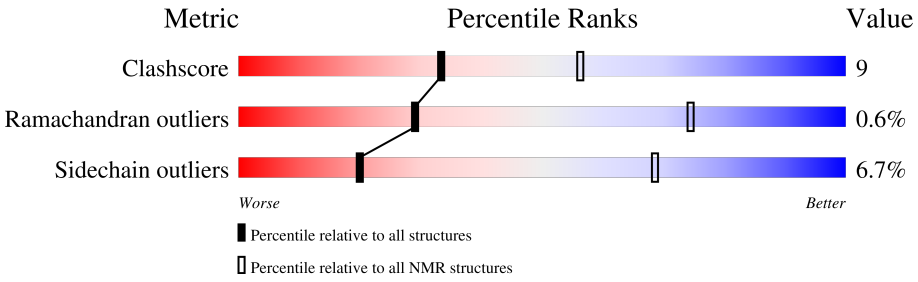
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson 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 93%.

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	83	69% 8% 23%
2	B	93	20% 6% 24% 49%

2 Ensemble composition and analysis

This entry contains 10 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:8-A:71, B:43-B:54 (76)	0.98	9
2	B:16-B:28 (13)	0.97	2

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 2 clusters. No single-model clusters were found.

Cluster number	Models
1	2, 3, 4, 6, 9
2	1, 5, 7, 8, 10

3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 2084 atoms, of which 1031 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called High mobility group protein B1.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	83	1358	425	681	122	124	6	0

- Molecule 2 is a protein called Cellular tumor antigen p53.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
2	B	47	726	240	350	55	79	2	0

4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

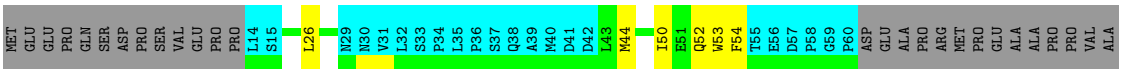
These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for 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: High mobility group protein B1

Chain A:

• Molecule 2: Cellular tumor antigen p53

Chain B:



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

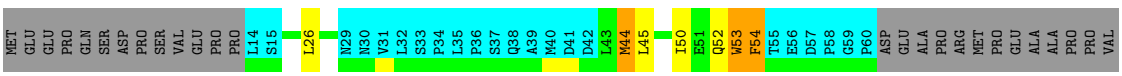
The representative model is number 9. Colouring as in section 4.1 above.

• Molecule 1: High mobility group protein B1

Chain A:

• Molecule 2: Cellular tumor antigen p53

Chain B:



ALA
PRO
ALA
PRO
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ALA
PRO
THR
PRO
ALA
ALA
PRO
ALA
PRO
ALA
PRO
SER
TRP
PRO
LEU

5 Refinement protocol and experimental data overview

The models were refined using the following method: *DGSA-distance geometry simulated annealing.*

Of the 100 calculated structures, 10 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
ARIA	structure solution	
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	2
Total number of shifts	2080
Number of shifts mapped to atoms	1624
Number of unparsed shifts	0
Number of shifts with mapping errors	456
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	93%

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	527	519	517	9±2
2	B	217	203	203	6±2
All	All	7440	7220	7200	133

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 93 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:16:ALA:HA	2:B:44:MET:HB3	0.84	1.49	5	3
1:A:10:GLY:HA3	1:A:70:TYR:HB2	0.83	1.49	4	1
2:B:50:ILE:HB	2:B:54:PHE:HB3	0.83	1.51	2	2
1:A:9:ARG:HG3	2:B:53:TRP:HB2	0.73	1.59	6	1
1:A:23:ARG:HD3	2:B:54:PHE:HA	0.72	1.59	3	1

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	64/83 (77%)	62±1 (97±1%)	2±1 (3±2%)	0±0 (0±1%)	32 76
2	B	25/93 (27%)	20±1 (80±4%)	5±1 (19±4%)	0±0 (1±2%)	24 71
All	All	890/1760 (51%)	819 (92%)	66 (7%)	5 (1%)	29 74

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	12	MET	2
1	A	11	LYS	1
2	B	28	GLU	1
2	B	43	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	56/72 (78%)	53±1 (94±2%)	3±1 (6±2%)	25 74
2	B	25/80 (31%)	23±1 (91±6%)	2±1 (9±6%)	13 59
All	All	810/1520 (53%)	756 (93%)	54 (7%)	20 68

5 of 23 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	17	PHE	6
1	A	15	TYR	5
1	A	23	ARG	5
2	B	54	PHE	5
2	B	26	LEU	4

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 93% for the well-defined parts and 92% 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	1031
Number of shifts mapped to atoms	1031
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	2

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	82	-0.33 ± 0.21	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	78	0.09 ± 0.14	None needed (< 0.5 ppm)
$^{13}C'$	76	-1.63 ± 0.13	Should be applied
^{15}N	77	-0.45 ± 0.24	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 65%, i.e. 804 atoms were assigned a chemical shift out of a possible 1242. 0 out of 7 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	317/439 (72%)	128/176 (73%)	127/178 (71%)	62/85 (73%)
Sidechain	401/663 (60%)	270/422 (64%)	129/212 (61%)	2/29 (7%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	86/140 (61%)	43/69 (62%)	42/64 (66%)	1/7 (14%)
Overall	804/1242 (65%)	441/667 (66%)	298/454 (66%)	65/121 (54%)

7.1.4 Statistically unusual chemical shifts (i)

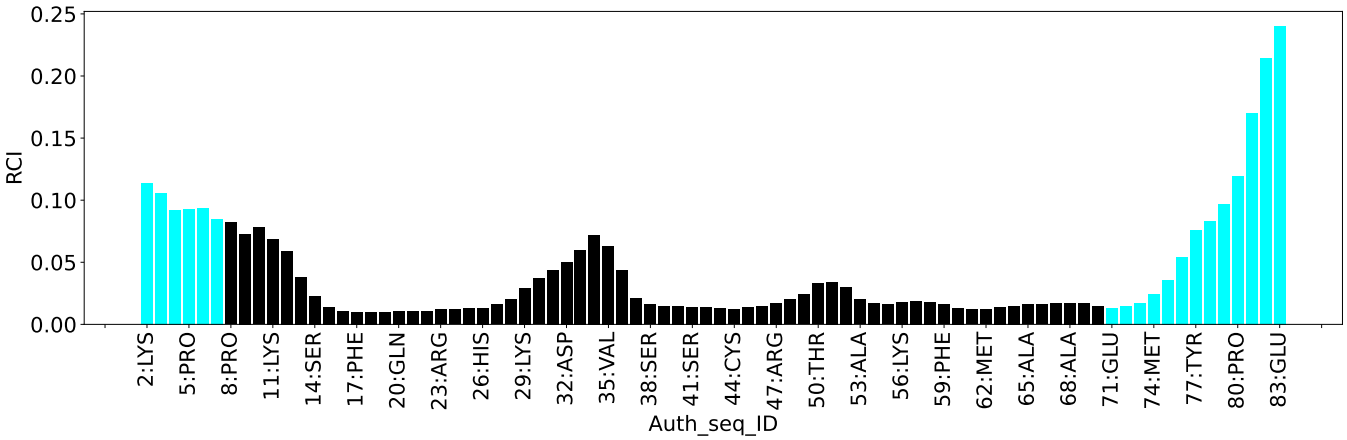
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	56	LYS	HE2	1.25	1.95 – 3.88	-8.6
1	A	56	LYS	HG2	-0.01	0.13 – 2.61	-5.6

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:



7.2 Chemical shift list 2

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_2*

7.2.1 Bookkeeping (i)

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	1049
Number of shifts mapped to atoms	593
Number of unparsed shifts	0
Number of shifts with mapping errors	456
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 456) occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
2	B	1	MET	C	175.517	0.000	1
2	B	1	MET	CA	55.54	0.066	1
2	B	1	MET	CB	32.043	0.184	1
2	B	1	MET	HA	4.442	0.013	1
2	B	1	MET	HB2	2.013	0.013	2
2	B	1	MET	HB3	2.516	0.002	2
2	B	1	MET	HG2	2.507	0.000	1
2	B	2	GLU	C	176.141	0.000	1
2	B	2	GLU	CA	56.472	0.041	1
2	B	2	GLU	CB	30.302	0.109	1
2	B	2	GLU	CG	36.304	0.023	1
2	B	2	GLU	H	8.652	0.011	1
2	B	2	GLU	HA	4.293	0.003	1
2	B	2	GLU	HB2	1.954	0.027	2
2	B	2	GLU	HB3	2.039	0.002	2
2	B	2	GLU	HG2	2.246	0.021	2
2	B	2	GLU	HG3	2.277	0.000	2
2	B	2	GLU	N	122.378	0.024	1
2	B	3	GLU	CA	54.349	0.024	1
2	B	3	GLU	CB	29.93	0.024	1
2	B	3	GLU	CG	36.285	0.000	1
2	B	3	GLU	H	8.462	0.005	1
2	B	3	GLU	HA	4.576	0.005	1
2	B	3	GLU	HB2	1.891	0.011	2
2	B	3	GLU	HB3	2.028	0.005	2
2	B	3	GLU	HG2	2.29	0.000	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
2	B	3	GLU	N	123.125	0.016	1
2	B	4	PRO	C	177.015	0.000	1
2	B	4	PRO	CA	63.015	0.078	1
2	B	4	PRO	CB	32.077	0.016	1
2	B	4	PRO	CD	50.685	0.013	1
2	B	4	PRO	CG	27.292	0.016	1
2	B	4	PRO	HA	4.414	0.011	1
2	B	4	PRO	HB2	1.902	0.002	2
2	B	4	PRO	HB3	2.29	0.007	2
2	B	4	PRO	HD2	3.672	0.000	2
2	B	4	PRO	HD3	3.79	0.027	2
2	B	4	PRO	HG2	2.003	0.032	1
2	B	5	GLN	C	175.982	0.000	1
2	B	5	GLN	CA	55.581	0.002	1
2	B	5	GLN	CB	29.622	0.106	1
2	B	5	GLN	CG	33.902	0.022	1
2	B	5	GLN	H	8.566	0.006	1
2	B	5	GLN	HA	4.351	0.009	1
2	B	5	GLN	HB2	2.05	0.044	2
2	B	5	GLN	HB3	2.119	0.004	2
2	B	5	GLN	HE21	6.896	0.000	1
2	B	5	GLN	HE22	7.612	0.000	1
2	B	5	GLN	HG2	2.385	0.025	1
2	B	5	GLN	N	120.568	0.027	1
2	B	5	GLN	NE2	112.661	0.001	1
2	B	6	SER	C	173.295	0.000	1
2	B	6	SER	CA	58.268	0.090	1
2	B	6	SER	CB	64.022	0.003	1
2	B	6	SER	H	8.393	0.005	1
2	B	6	SER	HA	4.434	0.005	1
2	B	6	SER	HB2	3.826	0.002	2
2	B	6	SER	HB3	3.867	0.001	2
2	B	6	SER	N	117.321	0.010	1
2	B	7	ASP	CA	52.187	0.042	1
2	B	7	ASP	CB	41.286	0.021	1
2	B	7	ASP	H	8.446	0.005	1
2	B	7	ASP	HA	4.912	0.010	1
2	B	7	ASP	HB2	2.543	0.010	2
2	B	7	ASP	HB3	2.786	0.005	2
2	B	7	ASP	N	123.218	0.033	1
2	B	8	PRO	C	177.287	0.000	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
2	B	8	PRO	CA	63.379	0.091	1
2	B	8	PRO	CB	32.062	0.064	1
2	B	8	PRO	CD	50.815	0.001	1
2	B	8	PRO	CG	27.004	0.000	1
2	B	8	PRO	HA	4.448	0.013	1
2	B	8	PRO	HB2	1.902	0.003	2
2	B	8	PRO	HB3	2.28	0.011	2
2	B	8	PRO	HD2	3.677	0.000	2
2	B	8	PRO	HD3	3.834	0.012	2
2	B	8	PRO	HG2	2.01	0.000	1
2	B	9	SER	C	174.237	0.000	1
2	B	9	SER	CA	58.94	0.000	1
2	B	9	SER	CB	63.72	0.073	1
2	B	9	SER	H	8.533	0.004	1
2	B	9	SER	HA	4.397	0.004	1
2	B	9	SER	HB2	3.89	0.005	1
2	B	9	SER	N	115.588	0.012	1
2	B	10	VAL	C	175.758	0.000	1
2	B	10	VAL	CA	61.842	0.002	1
2	B	10	VAL	CB	32.897	0.023	1
2	B	10	VAL	CG1	20.795	0.015	2
2	B	10	VAL	CG2	20.81	0.006	2
2	B	10	VAL	H	7.871	0.004	1
2	B	10	VAL	HA	4.184	0.003	1
2	B	10	VAL	HB	2.114	0.004	1
2	B	10	VAL	HG11	0.922	0.002	2
2	B	10	VAL	HG12	0.922	0.002	2
2	B	10	VAL	HG13	0.922	0.002	2
2	B	10	VAL	HG21	0.924	0.001	2
2	B	10	VAL	HG22	0.924	0.001	2
2	B	10	VAL	HG23	0.924	0.001	2
2	B	10	VAL	N	120.621	0.015	1
2	B	11	GLU	CA	54.259	0.048	1
2	B	11	GLU	CB	29.914	0.028	1
2	B	11	GLU	CG	35.952	0.000	1
2	B	11	GLU	H	8.341	0.006	1
2	B	11	GLU	HA	4.575	0.000	1
2	B	11	GLU	HB2	1.89	0.000	2
2	B	11	GLU	HB3	2.035	0.000	2
2	B	11	GLU	HG2	2.288	0.000	1
2	B	11	GLU	N	125.69	0.031	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
2	B	12	PRO	HD2	3.866	0.000	1
2	B	12	PRO	HD3	3.866	0.000	1
2	B	13	PRO	C	177.111	0.000	1
2	B	13	PRO	CA	62.744	0.000	1
2	B	13	PRO	CB	31.976	0.013	1
2	B	13	PRO	CD	50.382	0.000	1
2	B	13	PRO	CG	27.287	0.000	1
2	B	13	PRO	HA	4.445	0.000	1
2	B	13	PRO	HB2	1.902	0.000	2
2	B	13	PRO	HB3	2.289	0.000	2
2	B	13	PRO	HD2	3.628	0.000	2
2	B	13	PRO	HD3	3.797	0.000	2
2	B	13	PRO	HG2	1.981	0.000	1
2	B	61	ASP	C	176.154	0.000	1
2	B	61	ASP	CA	54.554	0.047	1
2	B	61	ASP	CB	41.099	0.059	1
2	B	61	ASP	H	8.454	0.004	1
2	B	61	ASP	HA	4.579	0.004	1
2	B	61	ASP	HB2	2.589	0.009	2
2	B	61	ASP	HB3	2.711	0.014	2
2	B	61	ASP	N	119.57	0.014	1
2	B	62	GLU	C	175.731	0.000	1
2	B	62	GLU	CA	56.1	0.002	1
2	B	62	GLU	CB	30.77	0.001	1
2	B	62	GLU	CG	36.282	0.000	1
2	B	62	GLU	H	8.143	0.005	1
2	B	62	GLU	HA	4.275	0.005	1
2	B	62	GLU	HB2	1.908	0.003	2
2	B	62	GLU	HB3	2.029	0.002	2
2	B	62	GLU	HG2	2.215	0.011	2
2	B	62	GLU	HG3	2.276	0.002	2
2	B	62	GLU	N	120.545	0.016	1
2	B	63	ALA	CA	50.531	0.170	1
2	B	63	ALA	CB	18.149	0.015	1
2	B	63	ALA	H	8.282	0.005	1
2	B	63	ALA	HA	4.58	0.004	1
2	B	63	ALA	HB1	1.36	0.006	1
2	B	63	ALA	HB2	1.36	0.006	1
2	B	63	ALA	HB3	1.36	0.006	1
2	B	63	ALA	N	126.231	0.014	1
2	B	64	PRO	C	176.915	0.000	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
2	B	64	PRO	CA	62.91	0.001	1
2	B	64	PRO	CB	32.074	0.000	1
2	B	64	PRO	CD	50.439	0.000	1
2	B	64	PRO	CG	27.398	0.000	1
2	B	64	PRO	HA	4.382	0.010	1
2	B	64	PRO	HB2	1.911	0.000	2
2	B	64	PRO	HB3	2.298	0.013	2
2	B	64	PRO	HD2	3.632	0.008	2
2	B	64	PRO	HD3	3.791	0.008	2
2	B	64	PRO	HG2	2.01	0.007	1
2	B	64	PRO	HG3	2.01	0.007	1
2	B	65	ARG	C	176.315	0.000	1
2	B	65	ARG	CA	55.709	0.054	1
2	B	65	ARG	CB	30.976	0.019	1
2	B	65	ARG	CD	43.341	0.022	1
2	B	65	ARG	CG	27.13	0.008	1
2	B	65	ARG	H	8.469	0.005	1
2	B	65	ARG	HA	4.322	0.005	1
2	B	65	ARG	HB2	1.739	0.006	2
2	B	65	ARG	HB3	1.813	0.001	2
2	B	65	ARG	HD2	3.193	0.000	1
2	B	65	ARG	HD3	3.193	0.001	1
2	B	65	ARG	HG2	1.638	0.000	2
2	B	65	ARG	HG3	1.667	0.015	2
2	B	65	ARG	N	121.536	0.024	1
2	B	66	MET	CA	53.177	0.016	1
2	B	66	MET	CB	32.233	0.007	1
2	B	66	MET	CE	14.852	0.000	1
2	B	66	MET	H	8.505	0.005	1
2	B	66	MET	HA	4.798	0.002	1
2	B	66	MET	HB2	1.963	0.001	2
2	B	66	MET	HB3	2.083	0.003	2
2	B	66	MET	HE1	2.02	0.000	1
2	B	66	MET	HE2	2.02	0.000	1
2	B	66	MET	HE3	2.02	0.000	1
2	B	66	MET	HG2	2.622	0.000	1
2	B	66	MET	HG3	2.622	0.000	1
2	B	66	MET	N	122.996	0.013	1
2	B	67	PRO	C	176.969	0.000	1
2	B	67	PRO	CA	63.152	0.025	1
2	B	67	PRO	CB	32.098	0.019	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
2	B	67	PRO	CD	50.713	0.020	1
2	B	67	PRO	CG	27.349	0.010	1
2	B	67	PRO	HA	4.413	0.007	1
2	B	67	PRO	HB2	1.922	0.000	2
2	B	67	PRO	HB3	2.293	0.006	2
2	B	67	PRO	HD2	3.705	0.004	2
2	B	67	PRO	HD3	3.813	0.000	2
2	B	67	PRO	HG2	1.991	0.008	1
2	B	67	PRO	HG3	2.0	0.000	1
2	B	68	GLU	C	176.224	0.000	1
2	B	68	GLU	CA	56.46	0.004	1
2	B	68	GLU	CB	29.964	0.000	1
2	B	68	GLU	CG	31.825	0.000	1
2	B	68	GLU	H	8.539	0.004	1
2	B	68	GLU	HA	4.24	0.012	1
2	B	68	GLU	HB2	1.966	0.000	1
2	B	68	GLU	HG2	2.292	0.000	1
2	B	68	GLU	N	120.89	0.026	1
2	B	69	ALA	C	177.064	0.000	1
2	B	69	ALA	CA	52.138	0.033	1
2	B	69	ALA	CB	19.331	0.000	1
2	B	69	ALA	H	8.329	0.008	1
2	B	69	ALA	HA	4.301	0.000	1
2	B	69	ALA	HB1	1.39	0.000	1
2	B	69	ALA	HB2	1.39	0.000	1
2	B	69	ALA	HB3	1.39	0.000	1
2	B	69	ALA	N	125.243	0.031	1
2	B	70	ALA	CA	50.294	0.019	1
2	B	70	ALA	CB	18.321	0.000	1
2	B	70	ALA	H	8.279	0.006	1
2	B	70	ALA	HA	4.572	0.019	1
2	B	70	ALA	HB1	1.352	0.002	1
2	B	70	ALA	HB2	1.352	0.002	1
2	B	70	ALA	HB3	1.352	0.002	1
2	B	70	ALA	N	124.753	0.021	1
2	B	72	PRO	C	176.986	0.000	1
2	B	72	PRO	CA	62.789	0.000	1
2	B	72	PRO	CB	31.999	0.021	1
2	B	72	PRO	CD	50.423	0.000	1
2	B	72	PRO	CG	27.245	0.000	1
2	B	72	PRO	HA	4.454	0.000	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
2	B	72	PRO	HB2	1.917	0.000	2
2	B	72	PRO	HB3	2.284	0.000	2
2	B	72	PRO	HD2	3.659	0.000	2
2	B	72	PRO	HD3	3.807	0.000	2
2	B	72	PRO	HG2	1.988	0.000	1
2	B	73	VAL	C	175.526	0.000	1
2	B	73	VAL	CA	61.928	0.018	1
2	B	73	VAL	CB	32.826	0.009	1
2	B	73	VAL	CG1	20.999	0.012	2
2	B	73	VAL	CG2	20.93	0.070	2
2	B	73	VAL	H	8.17	0.006	1
2	B	73	VAL	HA	4.062	0.003	1
2	B	73	VAL	HB	2.012	0.007	1
2	B	73	VAL	HG11	0.94	0.000	1
2	B	73	VAL	HG12	0.94	0.000	1
2	B	73	VAL	HG13	0.94	0.000	1
2	B	73	VAL	HG21	0.94	0.000	1
2	B	73	VAL	HG22	0.94	0.000	1
2	B	73	VAL	HG23	0.94	0.000	1
2	B	73	VAL	N	120.048	0.018	1
2	B	74	ALA	CA	50.322	0.017	1
2	B	74	ALA	CB	18.391	0.015	1
2	B	74	ALA	H	8.403	0.006	1
2	B	74	ALA	HA	4.591	0.015	1
2	B	74	ALA	HB1	1.361	0.007	1
2	B	74	ALA	HB2	1.361	0.007	1
2	B	74	ALA	HB3	1.361	0.007	1
2	B	74	ALA	N	129.229	0.029	1
2	B	75	PRO	C	176.326	0.000	1
2	B	75	PRO	CA	62.661	0.000	1
2	B	75	PRO	CB	32.029	0.000	1
2	B	75	PRO	CD	50.32	0.000	1
2	B	75	PRO	CG	27.195	0.000	1
2	B	75	PRO	HA	4.401	0.000	1
2	B	75	PRO	HB2	1.881	0.000	2
2	B	75	PRO	HB3	2.275	0.000	2
2	B	75	PRO	HD2	3.649	0.000	2
2	B	75	PRO	HD3	3.78	0.000	2
2	B	75	PRO	HG2	1.966	0.000	1
2	B	76	ALA	CA	50.37	0.027	1
2	B	76	ALA	CB	18.227	0.023	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
2	B	76	ALA	H	8.378	0.008	1
2	B	76	ALA	HA	4.602	0.000	1
2	B	76	ALA	HB1	1.364	0.000	1
2	B	76	ALA	HB2	1.364	0.000	1
2	B	76	ALA	HB3	1.364	0.000	1
2	B	76	ALA	N	125.383	0.010	1
2	B	77	PRO	C	176.59	0.000	1
2	B	77	PRO	CA	62.705	0.000	1
2	B	77	PRO	CB	31.893	0.000	1
2	B	77	PRO	CD	50.388	0.014	1
2	B	77	PRO	CG	27.272	0.000	1
2	B	77	PRO	HA	4.393	0.000	1
2	B	77	PRO	HB2	1.919	0.000	2
2	B	77	PRO	HB3	2.298	0.000	2
2	B	77	PRO	HD2	3.684	0.008	2
2	B	77	PRO	HD3	3.816	0.001	2
2	B	77	PRO	HG2	2.029	0.000	1
2	B	78	ALA	C	177.168	0.000	1
2	B	78	ALA	CA	52.102	0.000	1
2	B	78	ALA	CB	19.473	0.000	1
2	B	78	ALA	H	8.367	0.002	1
2	B	78	ALA	HA	4.28	0.000	1
2	B	78	ALA	HB1	1.383	0.000	1
2	B	78	ALA	HB2	1.383	0.000	1
2	B	78	ALA	HB3	1.383	0.000	1
2	B	78	ALA	N	124.237	0.008	1
2	B	79	ALA	CA	50.309	0.014	1
2	B	79	ALA	CB	18.101	0.000	1
2	B	79	ALA	H	8.29	0.012	1
2	B	79	ALA	HA	4.581	0.000	1
2	B	79	ALA	HB1	1.38	0.000	1
2	B	79	ALA	HB2	1.38	0.000	1
2	B	79	ALA	HB3	1.38	0.000	1
2	B	79	ALA	N	124.518	0.036	1
2	B	80	PRO	C	176.97	0.000	1
2	B	80	PRO	CA	62.855	0.016	1
2	B	80	PRO	CB	32.082	0.019	1
2	B	80	PRO	CD	50.46	0.000	1
2	B	80	PRO	CG	27.276	0.000	1
2	B	80	PRO	HA	4.469	0.014	1
2	B	80	PRO	HB2	1.908	0.000	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
2	B	80	PRO	HB3	2.3	0.008	2
2	B	80	PRO	HD2	3.678	0.000	2
2	B	80	PRO	HD3	3.792	0.000	2
2	B	80	PRO	HG2	1.984	0.000	1
2	B	81	THR	CA	59.805	0.004	1
2	B	81	THR	CB	69.715	0.019	1
2	B	81	THR	CG2	21.455	0.000	1
2	B	81	THR	H	8.322	0.006	1
2	B	81	THR	HA	4.571	0.000	1
2	B	81	THR	HB	4.142	0.000	1
2	B	81	THR	HG21	1.27	0.000	1
2	B	81	THR	HG22	1.27	0.000	1
2	B	81	THR	HG23	1.27	0.000	1
2	B	81	THR	N	117.018	0.023	1
2	B	82	PRO	C	176.602	0.000	1
2	B	82	PRO	CA	62.976	0.000	1
2	B	82	PRO	CB	32.119	0.023	1
2	B	82	PRO	CD	50.835	0.028	1
2	B	82	PRO	CG	27.304	0.000	1
2	B	82	PRO	HA	4.393	0.000	1
2	B	82	PRO	HB2	1.927	0.000	2
2	B	82	PRO	HB3	2.306	0.008	2
2	B	82	PRO	HD2	3.703	0.000	2
2	B	82	PRO	HD3	3.86	0.000	2
2	B	82	PRO	HG2	1.975	0.000	1
2	B	83	ALA	C	177.334	0.000	1
2	B	83	ALA	CA	52.161	0.025	1
2	B	83	ALA	CB	19.298	0.021	1
2	B	83	ALA	H	8.367	0.005	1
2	B	83	ALA	HA	4.287	0.000	1
2	B	83	ALA	HB1	1.379	0.003	1
2	B	83	ALA	HB2	1.379	0.003	1
2	B	83	ALA	HB3	1.379	0.003	1
2	B	83	ALA	N	124.221	0.010	1
2	B	84	ALA	CA	50.344	0.023	1
2	B	84	ALA	CB	18.037	0.000	1
2	B	84	ALA	H	8.27	0.005	1
2	B	84	ALA	HA	4.59	0.000	1
2	B	84	ALA	HB1	1.361	0.000	1
2	B	84	ALA	HB2	1.361	0.000	1
2	B	84	ALA	HB3	1.361	0.000	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
2	B	84	ALA	N	124.531	0.049	1
2	B	85	PRO	C	176.332	0.000	1
2	B	85	PRO	CA	62.683	0.000	1
2	B	85	PRO	CB	32.043	0.000	1
2	B	85	PRO	CD	50.313	0.000	1
2	B	85	PRO	CG	27.248	0.000	1
2	B	85	PRO	HA	4.398	0.000	1
2	B	85	PRO	HB2	1.884	0.000	2
2	B	85	PRO	HB3	2.274	0.000	2
2	B	85	PRO	HD2	3.65	0.000	2
2	B	85	PRO	HD3	3.781	0.000	2
2	B	85	PRO	HG2	1.965	0.000	1
2	B	86	ALA	CA	50.339	0.035	1
2	B	86	ALA	CB	18.224	0.019	1
2	B	86	ALA	H	8.384	0.006	1
2	B	86	ALA	HA	4.594	0.000	1
2	B	86	ALA	HB1	1.36	0.000	1
2	B	86	ALA	HB2	1.36	0.000	1
2	B	86	ALA	HB3	1.36	0.000	1
2	B	86	ALA	N	125.388	0.009	1
2	B	87	PRO	C	176.001	0.000	1
2	B	87	PRO	CA	62.664	0.000	1
2	B	87	PRO	HA	4.401	0.000	1
2	B	87	PRO	HB2	1.887	0.000	2
2	B	87	PRO	HB3	2.281	0.000	2
2	B	87	PRO	HD2	3.655	0.000	2
2	B	87	PRO	HD3	3.782	0.000	2
2	B	87	PRO	HG2	2.008	0.000	1
2	B	88	ALA	CA	50.373	0.022	1
2	B	88	ALA	CB	18.23	0.000	1
2	B	88	ALA	H	8.323	0.009	1
2	B	88	ALA	HA	4.581	0.000	1
2	B	88	ALA	HB1	1.363	0.000	1
2	B	88	ALA	HB2	1.363	0.000	1
2	B	88	ALA	HB3	1.363	0.000	1
2	B	88	ALA	N	125.205	0.031	1
2	B	89	PRO	C	176.705	0.000	1
2	B	89	PRO	CA	62.953	0.000	1
2	B	89	PRO	CB	31.933	0.000	1
2	B	89	PRO	CG	27.261	0.000	1
2	B	89	PRO	HA	4.312	0.000	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
2	B	89	PRO	HB2	2.017	0.000	1
2	B	89	PRO	HB3	2.017	0.000	1
2	B	89	PRO	HD2	3.773	0.000	2
2	B	89	PRO	HD3	3.65	0.000	2
2	B	89	PRO	HG2	1.647	0.000	1
2	B	89	PRO	HG3	1.647	0.000	1
2	B	90	SER	C	173.113	0.000	1
2	B	90	SER	CB	63.899	0.001	1
2	B	90	SER	H	8.139	0.005	1
2	B	90	SER	HA	4.364	0.000	1
2	B	90	SER	HB2	3.747	0.000	1
2	B	90	SER	HB3	3.747	0.000	1
2	B	90	SER	N	115.323	0.015	1
2	B	91	TRP	CA	54.725	0.000	1
2	B	91	TRP	CB	29.314	0.060	1
2	B	91	TRP	CD1	127.477	0.000	1
2	B	91	TRP	CE3	120.902	0.000	1
2	B	91	TRP	CH2	124.62	0.000	1
2	B	91	TRP	CZ2	114.644	0.000	1
2	B	91	TRP	CZ3	122.116	0.000	1
2	B	91	TRP	H	8.037	0.004	1
2	B	91	TRP	HA	5.011	0.000	1
2	B	91	TRP	HB2	3.347	0.001	2
2	B	91	TRP	HB3	3.14	0.003	2
2	B	91	TRP	HD1	7.261	0.000	1
2	B	91	TRP	HE1	10.148	0.000	1
2	B	91	TRP	HE3	7.713	0.000	1
2	B	91	TRP	HH2	7.251	0.000	1
2	B	91	TRP	HZ2	7.513	0.000	1
2	B	91	TRP	HZ3	7.18	0.000	1
2	B	91	TRP	N	123.45	0.020	1
2	B	91	TRP	NE1	128.823	0.001	1
2	B	92	PRO	C	175.851	0.000	1
2	B	92	PRO	CA	63.334	0.019	1
2	B	92	PRO	CB	31.844	0.000	1
2	B	92	PRO	CD	50.72	0.000	1
2	B	92	PRO	CG	27.237	0.000	1
2	B	92	PRO	HA	4.446	0.000	1
2	B	92	PRO	HB2	2.24	0.000	2
2	B	92	PRO	HB3	1.977	0.000	2
2	B	92	PRO	HD2	3.781	0.000	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
2	B	92	PRO	HD3	3.502	0.000	2
2	B	92	PRO	HG2	1.977	0.000	1
2	B	92	PRO	HG3	1.977	0.000	1
2	B	93	LEU	CA	56.748	0.021	1
2	B	93	LEU	CB	43.517	0.025	1
2	B	93	LEU	CD1	25.184	0.016	1
2	B	93	LEU	CD2	23.598	0.002	1
2	B	93	LEU	CG	27.206	0.038	1
2	B	93	LEU	H	7.824	0.006	1
2	B	93	LEU	HA	4.218	0.004	1
2	B	93	LEU	HB2	1.601	0.003	1
2	B	93	LEU	HB3	1.601	0.003	1
2	B	93	LEU	HD11	0.921	0.005	1
2	B	93	LEU	HD12	0.921	0.005	1
2	B	93	LEU	HD13	0.921	0.005	1
2	B	93	LEU	HD21	0.902	0.027	1
2	B	93	LEU	HD22	0.902	0.027	1
2	B	93	LEU	HD23	0.902	0.027	1
2	B	93	LEU	HG	1.65	0.007	1
2	B	93	LEU	N	127.919	0.011	1

7.2.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	90	-0.02 ± 0.22	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	88	0.21 ± 0.10	None needed (< 0.5 ppm)
$^{13}C'$	69	-0.14 ± 0.15	None needed (< 0.5 ppm)
^{15}N	70	-0.02 ± 0.16	None needed (< 0.5 ppm)

7.2.3 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 28%, i.e. 347 atoms were assigned a chemical shift out of a possible 1242. 0 out of 7 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	118/439 (27%)	48/176 (27%)	47/178 (26%)	23/85 (27%)

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	Total	^{1}H	^{13}C	^{15}N
Sidechain	185/663 (28%)	125/422 (30%)	58/212 (27%)	2/29 (7%)
Aromatic	44/140 (31%)	22/69 (32%)	20/64 (31%)	2/7 (29%)
Overall	347/1242 (28%)	195/667 (29%)	125/454 (28%)	27/121 (22%)

7.2.4 Statistically unusual chemical shifts (i)

There are no statistically unusual chemical shifts.

7.2.5 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 B: