



wwPDB NMR Structure Validation Summary Report ⓘ

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PDB ID : 2J5D / pdb_00002j5d
BMRB ID : 7288
Title : NMR structure of BNIP3 transmembrane domain in lipid bicelles
Authors : Bocharov, E.V.; Pustovalova, Y.E.; Volynsky, P.E.; Maslennikov, I.V.; Goncharuk, M.V.; Ermolyuk, Y.S.; Arseniev, A.S.
Deposited on : 2006-09-14

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A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

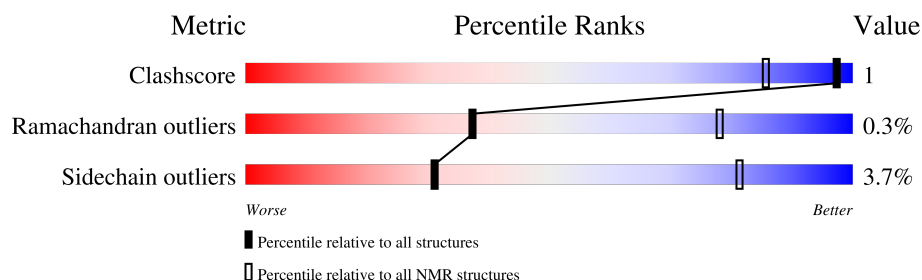
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 75%.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	45	
1	B	45	

2 Ensemble composition and analysis

This entry contains 16 models. Model 7 is the overall representative, medoid model (most similar to other models).

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:166-A:185, B:165-B:183 (39)	0.75	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 2 clusters and 3 single-model clusters were found.

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

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 1114 atoms, of which 420 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called BCL2/ADENOVIRUS E1B 19 KDA PROTEIN-INTERACTING PROTEIN 3.

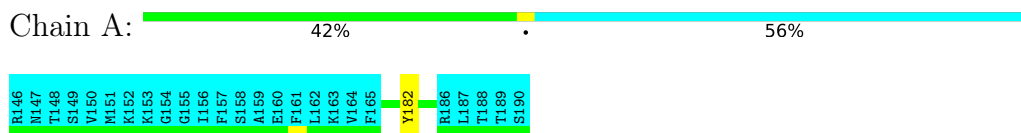
Mol	Chain	Residues	Atoms						Trace
1	A	45	Total	C	H	N	O	S	0
			557	228	210	60	58	1	
1	B	45	Total	C	H	N	O	S	0
			557	228	210	60	58	1	

4 Residue-property plots [i](#)

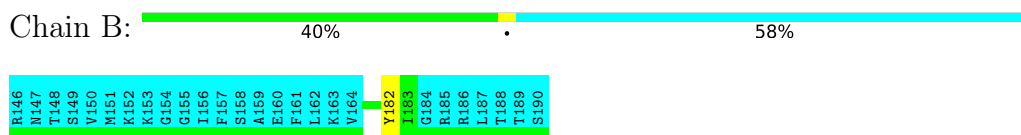
4.1 Average score per residue in the NMR ensemble

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: BCL2/ADENOVIRUS E1B 19 KDA PROTEIN-INTERACTING PROTEIN 3



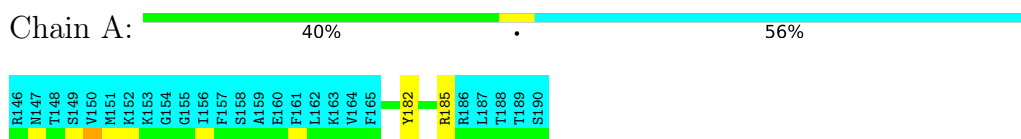
- Molecule 1: BCL2/ADENOVIRUS E1B 19 KDA PROTEIN-INTERACTING PROTEIN 3



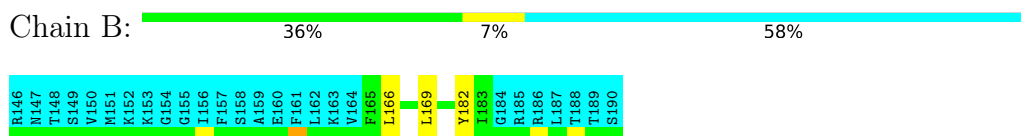
4.2 Residue scores for the representative (medoid) model from the NMR ensemble

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

- Molecule 1: BCL2/ADENOVIRUS E1B 19 KDA PROTEIN-INTERACTING PROTEIN 3



- Molecule 1: BCL2/ADENOVIRUS E1B 19 KDA PROTEIN-INTERACTING PROTEIN 3



5 Refinement protocol and experimental data overview

The models were refined using the following method: *TAD*.

Of the 200 calculated structures, 16 were deposited, based on the following criterion: *THE BEST TARGET FUNCTION*.

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

Software name	Classification	Version
GROMACS	refinement	
CYANA	structure solution	

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	964
Number of shifts mapped to atoms	696
Number of unparsed shifts	0
Number of shifts with mapping errors	268
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	75%

6 Model quality i

6.1 Standard geometry i

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the (average) root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	1.12±0.04	0±0/152 (0.0± 0.0%)	1.58±0.09	0±0/207 (0.1± 0.2%)
1	B	1.14±0.04	0±0/149 (0.0± 0.2%)	1.61±0.10	1±1/204 (0.3± 0.4%)
All	All	1.13	1/4816 (0.0%)	1.60	11/6576 (0.2%)

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

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	1.0±0.7
1	B	0.0±0.0	1.4±0.7
All	All	0	38

All unique bond outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	B	173	HIS	CG-ND1	-5.04	1.32	1.38	4	1

5 of 7 unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	B	165	PHE	CA-CB-CG	6.83	120.62	113.80	5	1
1	B	183	ILE	CA-C-N	5.21	125.88	119.99	16	3
1	B	183	ILE	C-N-CA	5.21	125.88	119.99	16	3
1	B	177	ILE	CA-C-N	5.03	125.67	119.99	13	1
1	B	177	ILE	C-N-CA	5.03	125.67	119.99	13	1

There are no chirality outliers.

5 of 6 unique planar outliers are listed below. They are sorted by the frequency of occurrence in

the ensemble.

Mol	Chain	Res	Type	Group	Models (Total)
1	B	182	TYR	Sidechain	14
1	A	182	TYR	Sidechain	10
1	A	185	ARG	Sidechain	5
1	B	169	LEU	Mainchain	5
1	B	165	PHE	Sidechain	3

6.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	149	87	170	0±0
1	B	145	83	163	0±0
All	All	4704	2720	5328	6

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 1.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:179:LEU:O	1:B:182:TYR:HB3	0.44	2.13	3	2
1:A:177:ILE:O	1:A:181:ILE:HD12	0.44	2.13	14	1
1:A:179:LEU:O	1:A:183:ILE:HG12	0.42	2.14	16	1
1:A:177:ILE:HG13	1:B:176:ALA:HB1	0.42	1.91	12	1
1:B:180:GLY:HA2	1:B:183:ILE:HD12	0.41	1.92	2	1

6.3 Torsion angles [i](#)

6.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the backbone conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	20/45 (44%)	18±1 (92±5%)	2±1 (8±5%)	0±0 (0±1%)	37	78
1	B	19/45 (42%)	18±1 (94±6%)	1±1 (6±6%)	0±0 (0±1%)	37	78
All	All	624/1440 (43%)	580 (93%)	42 (7%)	2 (0%)	37	78

All 2 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	167	PRO	1
1	B	167	PRO	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	16/38 (42%)	15±1 (96±4%)	1±1 (4±4%)	30	80
1	B	16/38 (42%)	15±0 (96±3%)	1±0 (4±3%)	32	82
All	All	512/1216 (42%)	493 (96%)	19 (4%)	31	81

5 of 15 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	175	LEU	2
1	B	174	LEU	2
1	B	166	LEU	2
1	A	166	LEU	2
1	A	170	LEU	1

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 oligosaccharides 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 75% for the well-defined parts and 75% 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	964
Number of shifts mapped to atoms	696
Number of unparsed shifts	0
Number of shifts with mapping errors	268
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 268) occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	146	ARG	HD2	3.23	0.02	2
1	A	146	ARG	HD3	3.23	0.02	2
1	A	147	ASN	HD21	6.95	0.02	2
1	A	147	ASN	HD22	7.61	0.02	2
1	A	148	THR	HG21	1.18	0.02	1
1	A	148	THR	HG22	1.18	0.02	1
1	A	148	THR	HG23	1.18	0.02	1
1	A	150	VAL	HG11	0.92	0.02	2
1	A	150	VAL	HG12	0.92	0.02	2
1	A	150	VAL	HG13	0.92	0.02	2
1	A	150	VAL	HG21	0.92	0.02	2
1	A	150	VAL	HG22	0.92	0.02	2
1	A	150	VAL	HG23	0.92	0.02	2
1	A	152	LYS	HD2	1.45	0.02	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	152	LYS	HD3	1.45	0.02	1
1	A	153	LYS	HD2	1.41	0.02	1
1	A	153	LYS	HD3	1.41	0.02	1
1	A	153	LYS	HE2	2.97	0.02	1
1	A	153	LYS	HE3	2.97	0.02	1
1	A	156	ILE	HD11	0.61	0.02	1
1	A	156	ILE	HD12	0.61	0.02	1
1	A	156	ILE	HD13	0.61	0.02	1
1	A	156	ILE	HG12	0.89	0.02	2
1	A	156	ILE	HG13	1.02	0.02	2
1	A	156	ILE	HG21	0.44	0.02	1
1	A	156	ILE	HG22	0.44	0.02	1
1	A	156	ILE	HG23	0.44	0.02	1
1	A	157	PHE	HD1	7.19	0.02	1
1	A	157	PHE	HD2	7.19	0.02	1
1	A	157	PHE	HE1	7.13	0.02	1
1	A	157	PHE	HE2	7.13	0.02	1
1	A	161	PHE	HD1	7.18	0.02	1
1	A	161	PHE	HD2	7.18	0.02	1
1	A	161	PHE	HE1	6.88	0.02	1
1	A	161	PHE	HE2	6.88	0.02	1
1	A	162	LEU	HD11	0.78	0.02	2
1	A	162	LEU	HD12	0.78	0.02	2
1	A	162	LEU	HD13	0.78	0.02	2
1	A	162	LEU	HD21	0.98	0.02	2
1	A	162	LEU	HD22	0.98	0.02	2
1	A	162	LEU	HD23	0.98	0.02	2
1	A	163	LYS	HD2	1.63	0.02	1
1	A	163	LYS	HD3	1.63	0.02	1
1	A	163	LYS	HE2	2.95	0.02	1
1	A	163	LYS	HE3	2.95	0.02	1
1	A	164	VAL	HG11	0.8	0.02	2
1	A	164	VAL	HG12	0.8	0.02	2
1	A	164	VAL	HG13	0.8	0.02	2
1	A	164	VAL	HG21	0.99	0.02	2
1	A	164	VAL	HG22	0.99	0.02	2
1	A	164	VAL	HG23	0.99	0.02	2
1	A	165	PHE	HD1	7.08	0.02	1
1	A	165	PHE	HD2	7.08	0.02	1
1	A	165	PHE	HE1	7.22	0.02	1
1	A	165	PHE	HE2	7.22	0.02	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	166	LEU	HD11	0.88	0.02	2
1	A	166	LEU	HD12	0.88	0.02	2
1	A	166	LEU	HD13	0.88	0.02	2
1	A	166	LEU	HD21	0.96	0.02	2
1	A	166	LEU	HD22	0.96	0.02	2
1	A	166	LEU	HD23	0.96	0.02	2
1	A	167	PRO	HD2	3.53	0.02	2
1	A	167	PRO	HD3	3.62	0.02	2
1	A	169	LEU	HD11	0.81	0.02	2
1	A	169	LEU	HD12	0.81	0.02	2
1	A	169	LEU	HD13	0.81	0.02	2
1	A	169	LEU	HD21	0.88	0.02	2
1	A	169	LEU	HD22	0.88	0.02	2
1	A	169	LEU	HD23	0.88	0.02	2
1	A	171	LEU	HD11	0.8	0.02	2
1	A	171	LEU	HD12	0.8	0.02	2
1	A	171	LEU	HD13	0.8	0.02	2
1	A	171	LEU	HD21	0.92	0.02	2
1	A	171	LEU	HD22	0.92	0.02	2
1	A	171	LEU	HD23	0.92	0.02	2
1	A	173	HIS	HD2	6.21	0.02	1
1	A	173	HIS	HE1	6.88	0.02	1
1	A	174	LEU	HD11	0.83	0.02	2
1	A	174	LEU	HD12	0.83	0.02	2
1	A	174	LEU	HD13	0.83	0.02	2
1	A	175	LEU	HD11	0.81	0.02	2
1	A	175	LEU	HD12	0.81	0.02	2
1	A	175	LEU	HD13	0.81	0.02	2
1	A	175	LEU	HD21	0.98	0.02	2
1	A	175	LEU	HD22	0.98	0.02	2
1	A	175	LEU	HD23	0.98	0.02	2
1	A	177	ILE	HD11	0.86	0.02	1
1	A	177	ILE	HD12	0.86	0.02	1
1	A	177	ILE	HD13	0.86	0.02	1
1	A	177	ILE	HG12	1.27	0.02	2
1	A	177	ILE	HG13	2.21	0.02	2
1	A	177	ILE	HG21	0.85	0.02	1
1	A	177	ILE	HG22	0.85	0.02	1
1	A	177	ILE	HG23	0.85	0.02	1
1	A	179	LEU	HD11	0.87	0.02	2
1	A	179	LEU	HD12	0.87	0.02	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	179	LEU	HD13	0.87	0.02	2
1	A	181	ILE	HD11	1.04	0.02	1
1	A	181	ILE	HD12	1.04	0.02	1
1	A	181	ILE	HD13	1.04	0.02	1
1	A	181	ILE	HG12	1.86	0.02	2
1	A	181	ILE	HG21	0.86	0.02	1
1	A	181	ILE	HG22	0.86	0.02	1
1	A	181	ILE	HG23	0.86	0.02	1
1	A	182	TYR	HD1	7.03	0.02	1
1	A	182	TYR	HD2	7.03	0.02	1
1	A	182	TYR	HE1	6.78	0.02	1
1	A	182	TYR	HE2	6.78	0.02	1
1	A	183	ILE	HD11	0.88	0.02	1
1	A	183	ILE	HD12	0.88	0.02	1
1	A	183	ILE	HD13	0.88	0.02	1
1	A	183	ILE	HG12	1.11	0.02	2
1	A	183	ILE	HG13	2.17	0.02	2
1	A	183	ILE	HG21	0.86	0.02	1
1	A	183	ILE	HG22	0.86	0.02	1
1	A	183	ILE	HG23	0.86	0.02	1
1	A	185	ARG	HD2	3.11	0.02	2
1	A	185	ARG	HD3	3.18	0.02	2
1	A	185	ARG	HE	7.5	0.02	1
1	A	186	ARG	HD2	2.93	0.02	1
1	A	186	ARG	HD3	2.93	0.02	1
1	A	186	ARG	HE	7.37	0.02	1
1	A	187	LEU	HD11	0.87	0.02	2
1	A	187	LEU	HD12	0.87	0.02	2
1	A	187	LEU	HD13	0.87	0.02	2
1	A	187	LEU	HD21	0.87	0.02	2
1	A	187	LEU	HD22	0.87	0.02	2
1	A	187	LEU	HD23	0.87	0.02	2
1	A	188	THR	HG21	1.28	0.02	1
1	A	188	THR	HG22	1.28	0.02	1
1	A	188	THR	HG23	1.28	0.02	1
1	A	189	THR	HG21	1.24	0.02	1
1	A	189	THR	HG22	1.24	0.02	1
1	A	189	THR	HG23	1.24	0.02	1
1	B	146	ARG	HD2	3.23	0.02	2
1	B	146	ARG	HD3	3.23	0.02	2
1	B	147	ASN	HD21	6.95	0.02	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	B	147	ASN	HD22	7.61	0.02	2
1	B	148	THR	HG21	1.18	0.02	1
1	B	148	THR	HG22	1.18	0.02	1
1	B	148	THR	HG23	1.18	0.02	1
1	B	150	VAL	HG11	0.92	0.02	2
1	B	150	VAL	HG12	0.92	0.02	2
1	B	150	VAL	HG13	0.92	0.02	2
1	B	150	VAL	HG21	0.92	0.02	2
1	B	150	VAL	HG22	0.92	0.02	2
1	B	150	VAL	HG23	0.92	0.02	2
1	B	152	LYS	HD2	1.45	0.02	1
1	B	152	LYS	HD3	1.45	0.02	1
1	B	153	LYS	HD2	1.41	0.02	1
1	B	153	LYS	HD3	1.41	0.02	1
1	B	153	LYS	HE2	2.97	0.02	1
1	B	153	LYS	HE3	2.97	0.02	1
1	B	156	ILE	HD11	0.61	0.02	1
1	B	156	ILE	HD12	0.61	0.02	1
1	B	156	ILE	HD13	0.61	0.02	1
1	B	156	ILE	HG12	0.89	0.02	2
1	B	156	ILE	HG13	1.02	0.02	2
1	B	156	ILE	HG21	0.44	0.02	1
1	B	156	ILE	HG22	0.44	0.02	1
1	B	156	ILE	HG23	0.44	0.02	1
1	B	157	PHE	HD1	7.19	0.02	1
1	B	157	PHE	HD2	7.19	0.02	1
1	B	157	PHE	HE1	7.13	0.02	1
1	B	157	PHE	HE2	7.13	0.02	1
1	B	161	PHE	HD1	7.18	0.02	1
1	B	161	PHE	HD2	7.18	0.02	1
1	B	161	PHE	HE1	6.88	0.02	1
1	B	161	PHE	HE2	6.88	0.02	1
1	B	162	LEU	HD11	0.78	0.02	2
1	B	162	LEU	HD12	0.78	0.02	2
1	B	162	LEU	HD13	0.78	0.02	2
1	B	162	LEU	HD21	0.98	0.02	2
1	B	162	LEU	HD22	0.98	0.02	2
1	B	162	LEU	HD23	0.98	0.02	2
1	B	163	LYS	HD2	1.63	0.02	1
1	B	163	LYS	HD3	1.63	0.02	1
1	B	163	LYS	HE2	2.95	0.02	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	B	163	LYS	HE3	2.95	0.02	1
1	B	164	VAL	HG11	0.8	0.02	2
1	B	164	VAL	HG12	0.8	0.02	2
1	B	164	VAL	HG13	0.8	0.02	2
1	B	164	VAL	HG21	0.99	0.02	2
1	B	164	VAL	HG22	0.99	0.02	2
1	B	164	VAL	HG23	0.99	0.02	2
1	B	165	PHE	HD1	7.08	0.02	1
1	B	165	PHE	HD2	7.08	0.02	1
1	B	165	PHE	HE1	7.22	0.02	1
1	B	165	PHE	HE2	7.22	0.02	1
1	B	166	LEU	HD11	0.88	0.02	2
1	B	166	LEU	HD12	0.88	0.02	2
1	B	166	LEU	HD13	0.88	0.02	2
1	B	166	LEU	HD21	0.96	0.02	2
1	B	166	LEU	HD22	0.96	0.02	2
1	B	166	LEU	HD23	0.96	0.02	2
1	B	167	PRO	HD2	3.53	0.02	2
1	B	167	PRO	HD3	3.62	0.02	2
1	B	169	LEU	HD11	0.81	0.02	2
1	B	169	LEU	HD12	0.81	0.02	2
1	B	169	LEU	HD13	0.81	0.02	2
1	B	169	LEU	HD21	0.88	0.02	2
1	B	169	LEU	HD22	0.88	0.02	2
1	B	169	LEU	HD23	0.88	0.02	2
1	B	171	LEU	HD11	0.8	0.02	2
1	B	171	LEU	HD12	0.8	0.02	2
1	B	171	LEU	HD13	0.8	0.02	2
1	B	171	LEU	HD21	0.92	0.02	2
1	B	171	LEU	HD22	0.92	0.02	2
1	B	171	LEU	HD23	0.92	0.02	2
1	B	173	HIS	HD2	6.21	0.02	1
1	B	173	HIS	HE1	6.88	0.02	1
1	B	174	LEU	HD11	0.83	0.02	2
1	B	174	LEU	HD12	0.83	0.02	2
1	B	174	LEU	HD13	0.83	0.02	2
1	B	175	LEU	HD11	0.81	0.02	2
1	B	175	LEU	HD12	0.81	0.02	2
1	B	175	LEU	HD13	0.81	0.02	2
1	B	175	LEU	HD21	0.98	0.02	2
1	B	175	LEU	HD22	0.98	0.02	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	B	175	LEU	HD23	0.98	0.02	2
1	B	177	ILE	HD11	0.86	0.02	1
1	B	177	ILE	HD12	0.86	0.02	1
1	B	177	ILE	HD13	0.86	0.02	1
1	B	177	ILE	HG12	1.27	0.02	2
1	B	177	ILE	HG13	2.21	0.02	2
1	B	177	ILE	HG21	0.85	0.02	1
1	B	177	ILE	HG22	0.85	0.02	1
1	B	177	ILE	HG23	0.85	0.02	1
1	B	179	LEU	HD11	0.87	0.02	2
1	B	179	LEU	HD12	0.87	0.02	2
1	B	179	LEU	HD13	0.87	0.02	2
1	B	181	ILE	HD11	1.04	0.02	1
1	B	181	ILE	HD12	1.04	0.02	1
1	B	181	ILE	HD13	1.04	0.02	1
1	B	181	ILE	HG12	1.86	0.02	2
1	B	181	ILE	HG21	0.86	0.02	1
1	B	181	ILE	HG22	0.86	0.02	1
1	B	181	ILE	HG23	0.86	0.02	1
1	B	182	TYR	HD1	7.03	0.02	1
1	B	182	TYR	HD2	7.03	0.02	1
1	B	182	TYR	HE1	6.78	0.02	1
1	B	182	TYR	HE2	6.78	0.02	1
1	B	183	ILE	HD11	0.88	0.02	1
1	B	183	ILE	HD12	0.88	0.02	1
1	B	183	ILE	HD13	0.88	0.02	1
1	B	183	ILE	HG12	1.11	0.02	2
1	B	183	ILE	HG13	2.17	0.02	2
1	B	183	ILE	HG21	0.86	0.02	1
1	B	183	ILE	HG22	0.86	0.02	1
1	B	183	ILE	HG23	0.86	0.02	1
1	B	185	ARG	HD2	3.11	0.02	2
1	B	185	ARG	HD3	3.18	0.02	2
1	B	185	ARG	HE	7.5	0.02	1
1	B	186	ARG	HD2	2.93	0.02	1
1	B	186	ARG	HD3	2.93	0.02	1
1	B	186	ARG	HE	7.37	0.02	1
1	B	187	LEU	HD11	0.87	0.02	2
1	B	187	LEU	HD12	0.87	0.02	2
1	B	187	LEU	HD13	0.87	0.02	2
1	B	187	LEU	HD21	0.87	0.02	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	B	187	LEU	HD22	0.87	0.02	2
1	B	187	LEU	HD23	0.87	0.02	2
1	B	188	THR	HG21	1.28	0.02	1
1	B	188	THR	HG22	1.28	0.02	1
1	B	188	THR	HG23	1.28	0.02	1
1	B	189	THR	HG21	1.24	0.02	1
1	B	189	THR	HG22	1.24	0.02	1
1	B	189	THR	HG23	1.24	0.02	1

7.1.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	88	1.14 ± 0.09	Should be checked
$^{13}\text{C}_\beta$	70	1.93 ± 0.08	Should be checked
$^{13}\text{C}'$	0	—	None (insufficient data)
^{15}N	84	2.69 ± 0.20	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 75%, i.e. 424 atoms were assigned a chemical shift out of a possible 567. 0 out of 14 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	157/196 (80%)	81/81 (100%)	39/78 (50%)	37/37 (100%)
Sidechain	246/331 (74%)	189/227 (83%)	56/101 (55%)	1/3 (33%)
Aromatic	21/40 (52%)	17/21 (81%)	4/19 (21%)	0/0 (—%)
Overall	424/567 (75%)	287/329 (87%)	99/198 (50%)	38/40 (95%)

7.1.4 Statistically unusual chemical shifts [i](#)

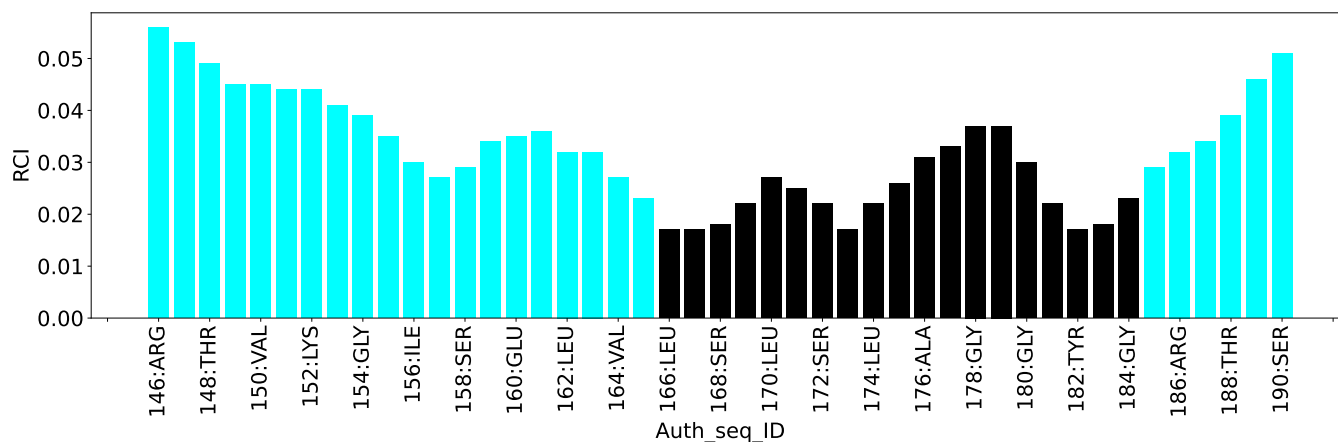
There are no statistically unusual chemical shifts.

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:



Random coil index (RCI) for chain B:

