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P R O T E I N   D A T A   B A N K

Full wwPDB NMR Structure Validation Report (i)

Feb 13, 2017 – 03:11 pm GMT

PDB ID	:	2KAD
Title	:	Magic-Angle-Spinning Solid-State NMR Structure of Influenza A M2 Transmembrane Domain
Authors	:	Hong, M.; Cady, S.D.; Mishanina, T.V.
Deposited on	:	2008-11-04

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
http://wwpdb.org/validation/2016/NMRValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

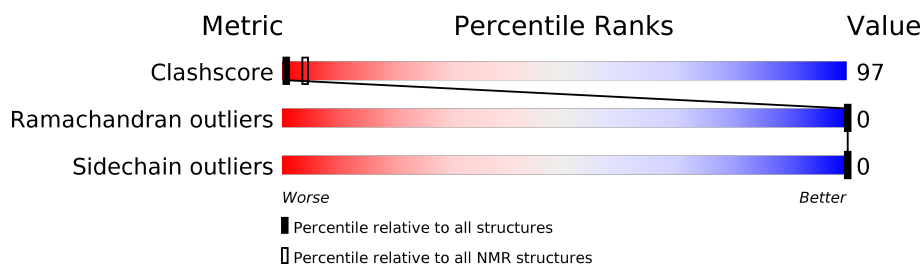|		
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	trunk28760
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
SOLID-STATE NMR

The overall completeness of chemical shifts assignment is 21%.

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	Percentile Ranks	Value
Clashscore		97
Ramachandran outliers		0
Sidechain outliers		0

Worse — *Better*

■ Percentile relative to all structures
▯ Percentile relative to all NMR structures

Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	125131	11601
Ramachandran outliers	121729	10391
Sidechain outliers	121581	10367

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	25	60% 40%
1	B	25	60% 40%
1	C	25	60% 40%
1	D	25	60% 40%

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2 Ensemble composition and analysis ⓘ

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

3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 1620 atoms, of which 849 are hydrogens and 0 are deuteriums.
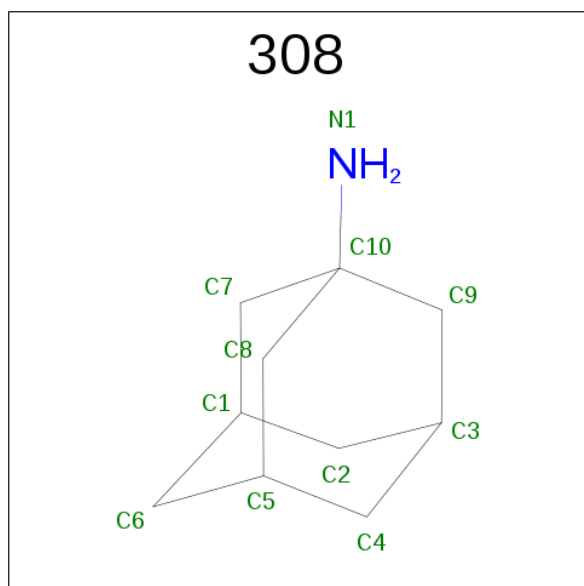
- Molecule 1 is a protein called Transmembrane peptide of Matrix protein 2.

Mol	Chain	Residues	Atoms					Trace
1	A	25	Total	C	H	N	O	0
			398	126	208	31	33	
1	B	25	Total	C	H	N	O	0
			398	126	208	31	33	
1	C	25	Total	C	H	N	O	0
			398	126	208	31	33	
1	D	25	Total	C	H	N	O	0
			398	126	208	31	33	

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	40	ALA	LEU	ENGINEERED	UNP O70632
B	40	ALA	LEU	ENGINEERED	UNP O70632
C	40	ALA	LEU	ENGINEERED	UNP O70632
D	40	ALA	LEU	ENGINEERED	UNP O70632

- Molecule 2 is (3S,5S,7S)-TRICYCLO[3.3.1.1 3,7]DECAN-1-AMINE (three-letter code: 308) (formula: $C_{10}H_{17}N$).

Mol	Chain	Residues	Atoms			
			Total	C	H	N
2	A	1	28	10	17	1

4 Residue-property plots ⓘ

These plots are provided for all protein, RNA and DNA 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: Transmembrane peptide of Matrix protein 2

Chain A:

• Molecule 1: Transmembrane peptide of Matrix protein 2

Chain B:

• Molecule 1: Transmembrane peptide of Matrix protein 2

Chain C:

• Molecule 1: Transmembrane peptide of Matrix protein 2

Chain D:

5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *torsion angle dynamics.*

Of the 1 calculated structures, 1 were deposited, based on the following criterion: *structures with the least restraint violations.*

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

Software name	Classification	Version
InsightII	structure solution	2005
InsightII	refinement	2005

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)	BMRB entry 16020
Number of chemical shift lists	1
Total number of shifts	248
Number of shifts mapped to atoms	248
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	21%

Note: This is a solid-state NMR structure, where hydrogen atoms are typically not assigned a chemical shift value, which may lead to lower completeness of assignment measure.

No validations of the models with respect to experimental NMR restraints is performed at this time.

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6 Model quality ⓘ

6.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 308

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	1.02	2/193 (1.0%)	1.31	5/263 (1.9%)
1	B	1.02	2/193 (1.0%)	1.31	5/263 (1.9%)
1	C	1.01	2/193 (1.0%)	1.31	5/263 (1.9%)
1	D	1.02	2/193 (1.0%)	1.31	5/263 (1.9%)
All	All	1.02	8/772 (1.0%)	1.31	20/1052 (1.9%)

All bond outliers are listed below. They are sorted according to the Z-score.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	46	LEU	C-OXT	-7.36	1.09	1.23
1	B	46	LEU	C-OXT	-7.32	1.09	1.23
1	A	46	LEU	C-OXT	-7.30	1.09	1.23
1	C	46	LEU	C-OXT	-7.22	1.09	1.23
1	B	44	ASP	CG-OD2	5.71	1.38	1.25
1	D	44	ASP	CG-OD2	5.67	1.38	1.25
1	C	44	ASP	CG-OD2	5.67	1.38	1.25
1	A	44	ASP	CG-OD2	5.63	1.38	1.25

All angle outliers are listed below. They are sorted according to the Z-score.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	44	ASP	CB-CG-OD1	8.46	125.91	118.30
1	B	44	ASP	CB-CG-OD1	8.44	125.89	118.30
1	C	44	ASP	CB-CG-OD1	8.39	125.85	118.30
1	D	44	ASP	CB-CG-OD1	8.36	125.83	118.30
1	A	24	ASP	CB-CG-OD1	7.51	125.06	118.30
1	C	24	ASP	CB-CG-OD1	7.49	125.04	118.30
1	D	24	ASP	CB-CG-OD1	7.43	124.99	118.30
1	B	24	ASP	CB-CG-OD1	7.42	124.98	118.30
1	B	44	ASP	CB-CG-OD2	-7.34	111.69	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	44	ASP	CB-CG-OD2	-7.33	111.70	118.30
1	D	44	ASP	CB-CG-OD2	-7.28	111.74	118.30
1	C	44	ASP	CB-CG-OD2	-7.26	111.77	118.30
1	C	45	ARG	NE-CZ-NH2	-6.62	116.99	120.30
1	D	45	ARG	NE-CZ-NH2	-6.47	117.06	120.30
1	B	45	ARG	NE-CZ-NH2	-6.41	117.10	120.30
1	A	45	ARG	NE-CZ-NH2	-6.32	117.14	120.30
1	B	24	ASP	CB-CG-OD2	-5.35	113.48	118.30
1	A	24	ASP	CB-CG-OD2	-5.26	113.56	118.30
1	D	24	ASP	CB-CG-OD2	-5.23	113.59	118.30
1	C	24	ASP	CB-CG-OD2	-5.23	113.59	118.30

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	190	208	205	77
1	B	190	208	205	77
1	C	190	208	205	77
1	D	190	208	205	77
All	All	771	849	837	156

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 97.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:35:ILE:CD1	1:D:30:ALA:O	1.38	1.72
1:A:30:ALA:O	1:C:35:ILE:CD1	1.37	1.73
1:A:37:HIS:CD2	1:C:41:TRP:CZ3	1.36	2.11
1:B:41:TRP:CZ3	1:C:37:HIS:CD2	1.34	2.15
1:B:30:ALA:O	1:D:35:ILE:CD1	1.34	1.73
1:B:41:TRP:CD2	1:C:37:HIS:NE2	1.33	1.95

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:B:35:ILE:CD1	1:C:30:ALA:O	1.33	1.74
1:A:37:HIS:NE2	1:C:41:TRP:CD2	1.32	1.96
1:B:41:TRP:CE3	1:C:37:HIS:CD2	1.28	2.22
1:A:41:TRP:CZ3	1:D:37:HIS:CD2	1.28	2.19
1:A:37:HIS:CD2	1:C:41:TRP:CE3	1.26	2.21
1:B:37:HIS:CD2	1:D:41:TRP:CZ3	1.25	2.23
1:B:37:HIS:NE2	1:D:41:TRP:CD2	1.25	2.04
1:A:41:TRP:CD2	1:D:37:HIS:NE2	1.24	2.05
1:A:41:TRP:CE3	1:D:37:HIS:CD2	1.24	2.26
1:B:37:HIS:CD2	1:D:41:TRP:CE3	1.21	2.27
1:A:30:ALA:O	1:C:35:ILE:HD12	1.08	1.42
1:B:30:ALA:HB1	1:D:35:ILE:CG1	1.08	1.77
1:A:30:ALA:HB1	1:C:35:ILE:HG13	1.07	1.13
1:A:35:ILE:HD12	1:D:30:ALA:O	1.07	1.42
1:B:35:ILE:HD11	1:C:30:ALA:O	1.06	1.49
1:B:30:ALA:O	1:D:35:ILE:HD12	1.05	1.49
1:B:35:ILE:CD1	1:C:30:ALA:C	1.05	2.25
1:B:35:ILE:HG13	1:C:30:ALA:HB1	1.05	1.10
1:B:35:ILE:CG1	1:C:30:ALA:HB1	1.05	1.80
1:B:30:ALA:HB1	1:D:35:ILE:HG13	1.04	1.05
1:B:30:ALA:C	1:D:35:ILE:CD1	1.04	2.24
1:A:35:ILE:CG1	1:D:30:ALA:HB1	1.04	1.81
1:B:35:ILE:HD12	1:C:30:ALA:O	1.04	1.49
1:A:35:ILE:HD11	1:D:30:ALA:O	1.03	1.48
1:A:30:ALA:C	1:C:35:ILE:CD1	1.03	2.26
1:A:35:ILE:CD1	1:D:30:ALA:C	1.02	2.26
1:A:30:ALA:O	1:C:35:ILE:HD11	1.02	1.51
1:A:35:ILE:HG13	1:D:30:ALA:HB1	1.01	1.08
1:B:41:TRP:CE2	1:C:37:HIS:NE2	1.01	2.25
1:A:30:ALA:HB1	1:C:35:ILE:CG1	1.00	1.84
1:B:30:ALA:C	1:D:35:ILE:HD11	1.00	1.75
1:A:37:HIS:CD2	1:C:41:TRP:CH2	1.00	2.48
1:A:38:LEU:HD23	1:D:37:HIS:ND1	0.99	1.70
1:B:30:ALA:O	1:D:35:ILE:HD11	0.99	1.46
1:B:41:TRP:CH2	1:C:37:HIS:CD2	0.99	2.50
1:B:37:HIS:ND1	1:D:38:LEU:HD23	0.99	1.72
1:B:35:ILE:HD11	1:C:30:ALA:C	0.99	1.76
1:A:37:HIS:NE2	1:C:41:TRP:CE3	0.98	2.30
1:B:30:ALA:CB	1:D:35:ILE:HG13	0.98	1.88
1:B:37:HIS:NE2	1:D:41:TRP:CE2	0.97	2.32
1:A:35:ILE:HG13	1:D:30:ALA:CB	0.96	1.90
1:A:37:HIS:NE2	1:C:41:TRP:CE2	0.96	2.28

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:37:HIS:ND1	1:C:38:LEU:HD23	0.95	1.77
1:B:35:ILE:HG13	1:C:30:ALA:CB	0.95	1.91
1:A:35:ILE:HD11	1:D:30:ALA:C	0.94	1.80
1:A:41:TRP:CH2	1:D:37:HIS:CD2	0.94	2.55
1:A:30:ALA:C	1:C:35:ILE:HD11	0.94	1.82
1:A:41:TRP:CE2	1:D:37:HIS:NE2	0.94	2.34
1:B:38:LEU:HD23	1:C:37:HIS:ND1	0.93	1.78
1:B:37:HIS:CD2	1:D:41:TRP:CH2	0.92	2.56
1:A:30:ALA:CB	1:C:35:ILE:HG13	0.92	1.94
1:B:41:TRP:CH2	1:C:37:HIS:HD2	0.92	1.81
1:A:37:HIS:HD2	1:C:41:TRP:CZ3	0.90	1.79
1:A:41:TRP:CZ3	1:D:37:HIS:HD2	0.89	1.84
1:B:41:TRP:CE3	1:C:37:HIS:NE2	0.86	2.34
1:A:37:HIS:HD2	1:C:41:TRP:CH2	0.85	1.81
1:B:37:HIS:HD2	1:D:41:TRP:CH2	0.85	1.86
1:A:41:TRP:CE3	1:D:37:HIS:NE2	0.84	2.40
1:B:37:HIS:HD2	1:D:41:TRP:CZ3	0.84	1.89
1:A:41:TRP:CH2	1:D:37:HIS:HD2	0.83	1.86
1:B:41:TRP:CD2	1:C:37:HIS:CE1	0.82	2.67
1:B:37:HIS:CD2	1:D:41:TRP:CD2	0.82	2.60
1:A:37:HIS:CE1	1:C:41:TRP:CD2	0.81	2.67
1:A:37:HIS:CD2	1:C:41:TRP:CD2	0.78	2.63
1:B:41:TRP:CZ3	1:C:37:HIS:HD2	0.76	1.83
1:B:41:TRP:CD2	1:C:37:HIS:CD2	0.74	2.58
1:A:30:ALA:C	1:C:35:ILE:HD12	0.73	1.96
1:A:35:ILE:HD12	1:D:30:ALA:C	0.72	1.96
1:A:41:TRP:CD2	1:D:37:HIS:CE1	0.72	2.77
1:B:41:TRP:CE3	1:C:37:HIS:CG	0.72	2.77
1:B:37:HIS:CE1	1:D:41:TRP:CD2	0.72	2.77
1:A:41:TRP:CD2	1:D:37:HIS:CD2	0.71	2.65
1:B:41:TRP:CG	1:C:37:HIS:CE1	0.70	2.79
1:B:30:ALA:C	1:D:35:ILE:HD12	0.70	1.99
1:A:37:HIS:CG	1:C:41:TRP:CE3	0.70	2.78
1:B:35:ILE:HD12	1:C:30:ALA:C	0.68	1.98
1:B:34:GLY:CA	1:D:38:LEU:HD13	0.68	2.19
1:B:38:LEU:HD13	1:C:34:GLY:CA	0.68	2.18
1:A:34:GLY:CA	1:C:38:LEU:HD13	0.68	2.19
1:B:37:HIS:CG	1:D:41:TRP:CE3	0.67	2.82
1:A:38:LEU:HD13	1:D:34:GLY:HA2	0.67	1.67
1:B:34:GLY:HA2	1:D:38:LEU:HD13	0.67	1.67
1:B:41:TRP:CG	1:C:37:HIS:NE2	0.66	2.61
1:A:38:LEU:HD13	1:D:34:GLY:CA	0.66	2.20

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:41:TRP:CE3	1:D:37:HIS:CG	0.66	2.83
1:A:34:GLY:HA2	1:C:38:LEU:HD13	0.66	1.68
1:A:37:HIS:CE1	1:C:41:TRP:CG	0.66	2.83
1:B:38:LEU:HD13	1:C:34:GLY:HA2	0.65	1.69
1:B:41:TRP:CZ2	1:C:37:HIS:CD2	0.65	2.85
1:B:37:HIS:NE2	1:D:41:TRP:CG	0.64	2.65
1:B:37:HIS:CE1	1:D:41:TRP:CG	0.63	2.86
1:A:37:HIS:NE2	1:C:41:TRP:CG	0.61	2.67
1:B:41:TRP:CE2	1:C:37:HIS:CD2	0.61	2.88
1:B:37:HIS:CD2	1:D:41:TRP:CZ2	0.61	2.88
1:A:37:HIS:CE1	1:C:41:TRP:CE3	0.60	2.88
1:A:37:HIS:CD2	1:C:41:TRP:CZ2	0.60	2.89
1:A:41:TRP:CG	1:D:37:HIS:CE1	0.59	2.90
1:A:41:TRP:CG	1:D:37:HIS:NE2	0.58	2.70
1:A:41:TRP:CZ2	1:D:37:HIS:CD2	0.57	2.92
1:B:37:HIS:CD2	1:D:41:TRP:CE2	0.57	2.89
1:B:41:TRP:CE3	1:C:37:HIS:CE1	0.56	2.92
1:B:30:ALA:CA	1:D:35:ILE:HD12	0.56	2.30
1:B:30:ALA:HB1	1:D:35:ILE:CD1	0.55	2.31
1:A:38:LEU:HD22	1:D:37:HIS:HB3	0.55	1.78
1:B:30:ALA:CB	1:D:35:ILE:CG1	0.55	2.68
1:B:37:HIS:HB3	1:D:38:LEU:HD22	0.55	1.77
1:B:37:HIS:NE2	1:D:41:TRP:CE3	0.54	2.44
1:B:35:ILE:HD12	1:C:30:ALA:CA	0.54	2.31
1:B:35:ILE:CG1	1:C:30:ALA:CB	0.53	2.70
1:A:35:ILE:HD12	1:D:30:ALA:CA	0.53	2.34
1:B:38:LEU:HD22	1:C:37:HIS:HB3	0.53	1.81
1:B:30:ALA:CA	1:D:35:ILE:CD1	0.52	2.87
1:A:37:HIS:HB3	1:C:38:LEU:HD22	0.51	1.81
1:A:41:TRP:CE2	1:D:37:HIS:CD2	0.51	2.96
1:B:35:ILE:CD1	1:C:30:ALA:CA	0.51	2.89
1:B:35:ILE:CD1	1:C:30:ALA:HB1	0.50	2.33
1:A:30:ALA:CA	1:C:35:ILE:HD12	0.50	2.37
1:A:41:TRP:CE3	1:D:37:HIS:CE1	0.49	2.99
1:A:38:LEU:CD2	1:D:37:HIS:ND1	0.49	2.62
1:B:34:GLY:HA2	1:D:38:LEU:CD1	0.48	2.37
1:A:37:HIS:CD2	1:C:41:TRP:CE2	0.48	2.95
1:B:37:HIS:HB3	1:D:38:LEU:CD2	0.47	2.39
1:B:41:TRP:CZ3	1:C:37:HIS:CG	0.47	2.91
1:B:38:LEU:CD1	1:C:34:GLY:HA2	0.47	2.39
1:B:37:HIS:CE1	1:D:41:TRP:CE3	0.46	3.03
1:A:35:ILE:CD1	1:D:30:ALA:CA	0.46	2.93

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:37:HIS:CG	1:C:41:TRP:CZ3	0.46	2.90
1:A:35:ILE:CD1	1:D:30:ALA:HB1	0.46	2.39
1:A:38:LEU:CD1	1:D:34:GLY:HA2	0.45	2.40
1:A:30:ALA:CA	1:C:35:ILE:CD1	0.45	2.95
1:C:34:GLY:O	1:C:38:LEU:HD12	0.44	2.13
1:B:30:ALA:CB	1:D:35:ILE:CD1	0.44	2.95
1:B:34:GLY:O	1:B:38:LEU:HD12	0.44	2.12
1:B:38:LEU:HD22	1:C:34:GLY:HA2	0.44	1.88
1:A:30:ALA:HB1	1:C:35:ILE:CG2	0.44	2.42
1:D:34:GLY:O	1:D:38:LEU:HD12	0.44	2.13
1:B:38:LEU:CD2	1:C:37:HIS:HB3	0.43	2.43
1:A:30:ALA:HB1	1:C:35:ILE:HG21	0.43	1.90
1:A:34:GLY:O	1:A:38:LEU:HD12	0.43	2.12
1:A:30:ALA:HB1	1:C:35:ILE:CD1	0.43	2.41
1:A:41:TRP:CZ3	1:D:37:HIS:CG	0.43	2.97
1:A:38:LEU:CD2	1:D:37:HIS:HB3	0.42	2.43
1:B:35:ILE:CD1	1:C:30:ALA:CB	0.42	2.96
1:A:35:ILE:CG1	1:D:30:ALA:CB	0.42	2.71
1:A:37:HIS:ND1	1:C:38:LEU:CD2	0.42	2.67
1:B:34:GLY:HA2	1:D:38:LEU:HD22	0.42	1.91
1:A:37:HIS:NE2	1:C:41:TRP:CZ2	0.41	2.82
1:B:37:HIS:ND1	1:D:38:LEU:CD2	0.41	2.64
1:A:35:ILE:CG2	1:D:30:ALA:HB1	0.41	2.45
1:A:34:GLY:HA2	1:C:38:LEU:CD1	0.41	2.41

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	23/25 (92%)	22 (96%)	1 (4%)	0 (0%)	100	100
1	B	23/25 (92%)	22 (96%)	1 (4%)	0 (0%)	100	100
1	C	23/25 (92%)	22 (96%)	1 (4%)	0 (0%)	100	100
1	D	23/25 (92%)	22 (96%)	1 (4%)	0 (0%)	100	100
All	All	92/100 (92%)	88 (96%)	4 (4%)	0 (0%)	100	100

There are no Ramachandran outliers.

6.3.2 Protein sidechains ⓘ

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	21/21 (100%)	21 (100%)	0 (0%)	100	100
1	B	21/21 (100%)	21 (100%)	0 (0%)	100	100
1	C	21/21 (100%)	21 (100%)	0 (0%)	100	100
1	D	21/21 (100%)	21 (100%)	0 (0%)	100	100
All	All	84/84 (100%)	84 (100%)	0 (0%)	100	100

There are no protein residues with a non-rotameric sidechain to report.

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.6 Ligand geometry ⓘ

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds for which Mogul statistics could be retrieved, the number of bonds that are observed in the model and the number of bonds that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length is the number of standard deviations the observed value is removed from the expected value. A bond length with $|Z| > 2$ is

considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond lengths.

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
2	308	A	1	-	13,13,13	1.45	0 (0%)

In the following table, the Counts columns list the number of angles for which Mogul statistics could be retrieved, the number of angles that are observed in the model and the number of angles that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond angle is the number of standard deviations the observed value is removed from the expected value. A bond angle with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond angles.

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
2	308	A	1	-	18,21,21	1.57	1 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	308	A	1	-	-	0,0,27,27	0,0,3,3

There are no bond-length outliers.

All angle outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1	308	C10-C9-C3	5.08	104.29	109.91

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6.7 Other polymers ⓘ

There are no such molecules in this entry.

6.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

7 Chemical shift validation ⓘ

The completeness of assignment taking into account all chemical shift lists is 21% for the well-defined parts and 21% for the entire structure.

7.1 Chemical shift list 1

File name: BMRB entry 16020

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	248
Number of shifts mapped to atoms	248
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.1.2 Chemical shift referencing ⓘ

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_\alpha$	44	-0.15 ± 0.09	None needed (< 0.5 ppm)
$^{13}C_\beta$	40	0.40 ± 0.06	None needed (< 0.5 ppm)
$^{13}C'$	44	-0.01 ± 0.16	None needed (< 0.5 ppm)
^{15}N	44	-1.06 ± 0.75	None needed (imprecise)

7.1.3 Completeness of resonance assignments ⓘ

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 21%, i.e. 248 atoms were assigned a chemical shift out of a possible 1200. 0 out of 28 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	132/492 (27%)	0/196 (0%)	88/200 (44%)	44/96 (46%)
Sidechain	116/632 (18%)	0/360 (0%)	116/260 (45%)	0/12 (0%)

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	Total	**¹H**	**¹³C**	**¹⁵N**
Aromatic	0/76 (0%)	0/40 (0%)	0/28 (0%)	0/8 (0%)
Overall	248/1200 (21%)	0/596 (0%)	204/488 (42%)	44/116 (38%)

Note: This is a solid-state NMR structure, where hydrogen atoms are typically not assigned a chemical shift value, which may lead to lower completeness of assignment measure.
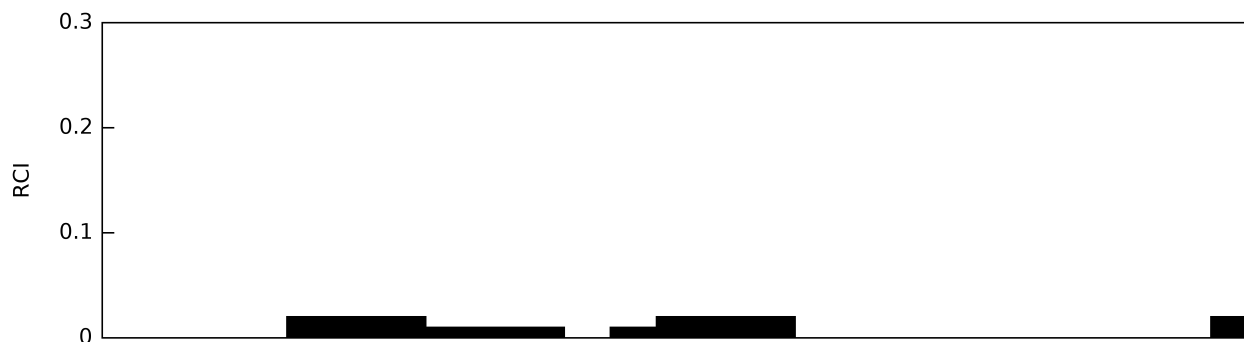
The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 21%, i.e. 248 atoms were assigned a chemical shift out of a possible 1200. 0 out of 28 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	**¹H**	**¹³C**	**¹⁵N**
Backbone	132/492 (27%)	0/196 (0%)	88/200 (44%)	44/96 (46%)
Sidechain	116/632 (18%)	0/360 (0%)	116/260 (45%)	0/12 (0%)
Aromatic	0/76 (0%)	0/40 (0%)	0/28 (0%)	0/8 (0%)
Overall	248/1200 (21%)	0/596 (0%)	204/488 (42%)	44/116 (38%)

Note: This is a solid-state NMR structure, where hydrogen atoms are typically not assigned a chemical shift value, which may lead to lower completeness of assignment measure.

7.1.4 Statistically unusual chemical shifts ⓘ
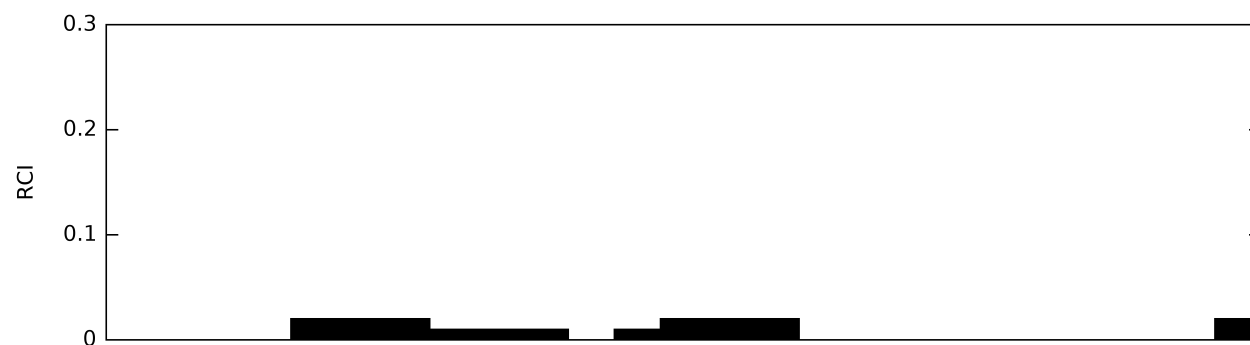
There are no statistically unusual chemical shifts.

7.1.5 Random Coil Index (RCI) plots ⓘ

The images below report *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.
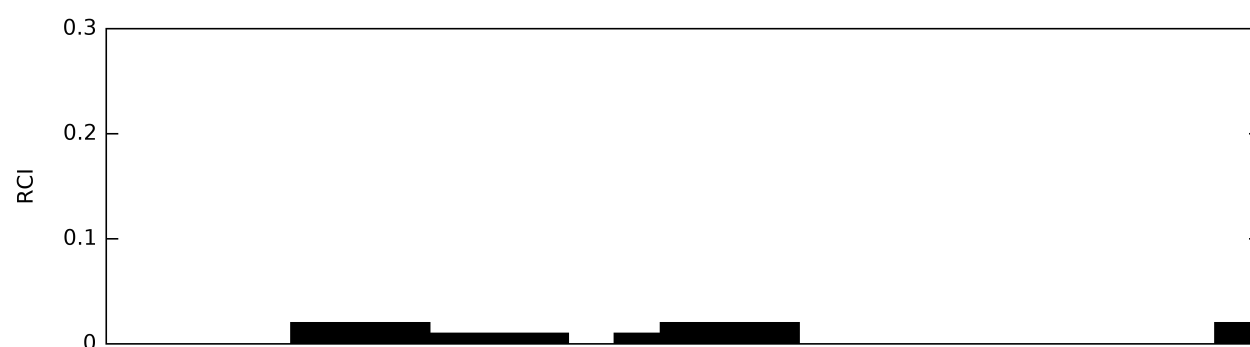
Random coil index (RCI) for chain A:

Random coil index (RCI) for chain B:

Random coil index (RCI) for chain C:

Random coil index (RCI) for chain D: