



Full wwPDB NMR Structure Validation Report ⓘ

Apr 26, 2016 – 10:48 PM BST

PDB ID : 2K4I
Title : Solution structure of HIV-2 myrMA bound to di-C4-PI(4,5)P2
Authors : Saad, J.S.; Ablan, S.D.; Ghanam, R.H.; Kim, A.; Andrews, K.; Nagashima, K.; Freed, E.O.; Summers, M.F.
Deposited on : 2008-06-08

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 ⓘ symbol.

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

Cyrange : Kirchner and Güntert (2011)
NmrClust : Kelley et al. (1996)
MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : rb-20027457
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027457

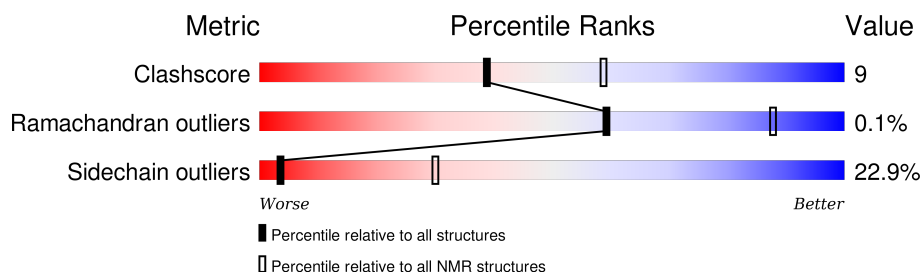
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 79%.

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	114402	11133
Ramachandran outliers	111179	9975
Sidechain outliers	111093	9958

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	134	

2 Ensemble composition and analysis

This entry contains 20 models. Model 3 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *fewest violations*.

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:13-A:108 (96)	0.43	3

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

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

The models can be grouped into 4 clusters and 5 single-model clusters were found.

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

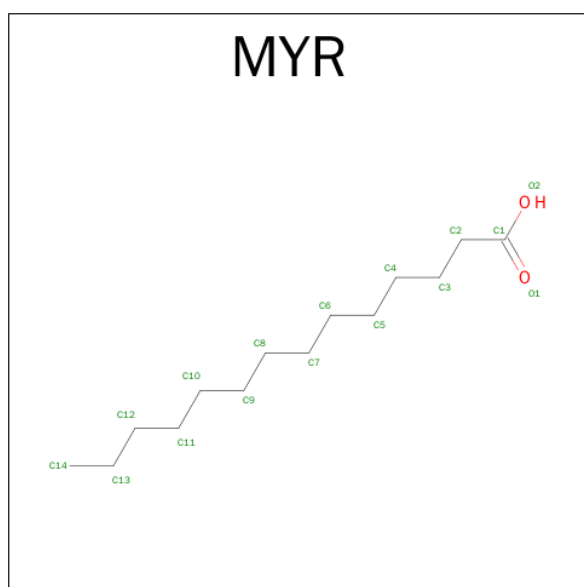
3 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 2236 atoms, of which 1140 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called HIV-2 myristoylated matrix protein.

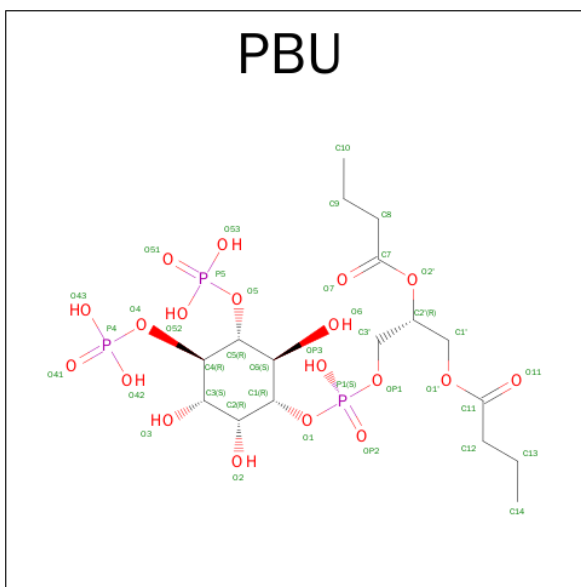
Mol	Chain	Residues	Atoms						Trace
1	A	134	Total	C	H	N	O	S	0
			2127	651	1085	194	192	5	

- Molecule 2 is MYRISTIC ACID (three-letter code: MYR) (formula: $C_{14}H_{28}O_2$).



Mol	Chain	Residues	Atoms			
2	A	1	Total	C	H	O
			42	14	27	1

- Molecule 3 is (2R)-3-[[[(R)-HYDROXY{[(1R,2R,3S,4R,5R,6S)-2,3,6-TRIHYDROXY-4,5-BIS(PHOSPHONOOXY)CYCLOHEXYL]OXY}PHOSPHORYL]OXY}PROPANE-1,2-DIYL DIBUTANOATE (three-letter code: PBU) (formula: $C_{17}H_{33}O_{19}P_3$).



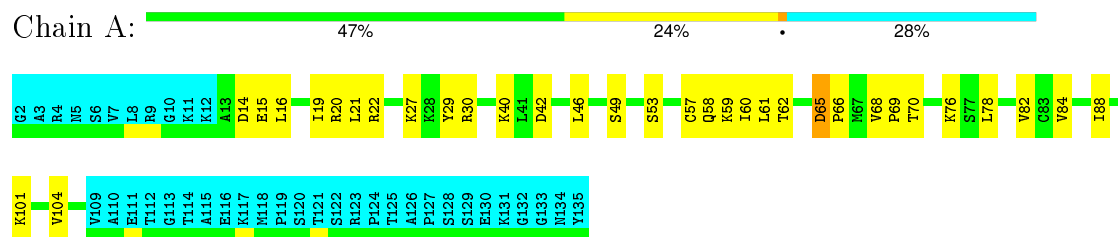
Mol	Chain	Residues	Atoms				
3	A	1	Total	C	H	O	P
			67	17	28	19	3

4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

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: HIV-2 myristoylated matrix protein

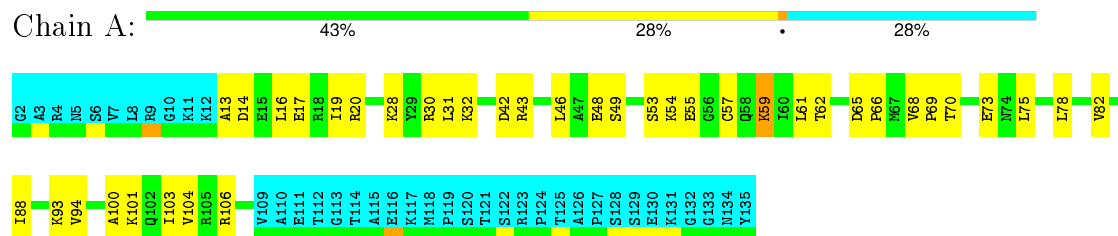


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

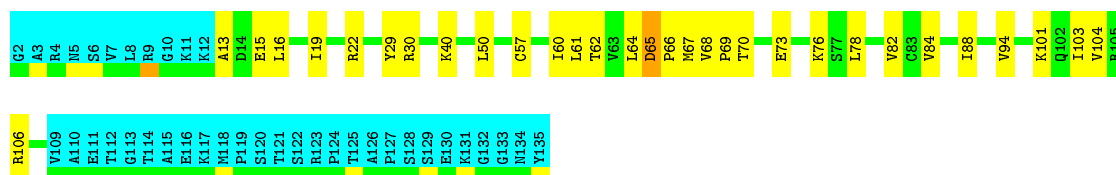
- Molecule 1: HIV-2 myristoylated matrix protein



4.2.2 Score per residue for model 2

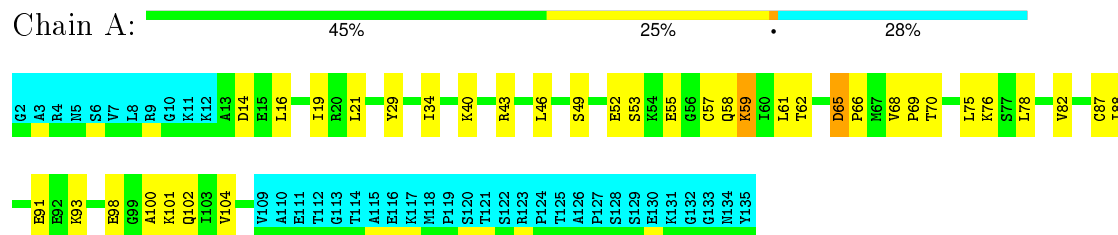
- Molecule 1: HIV-2 myristoylated matrix protein





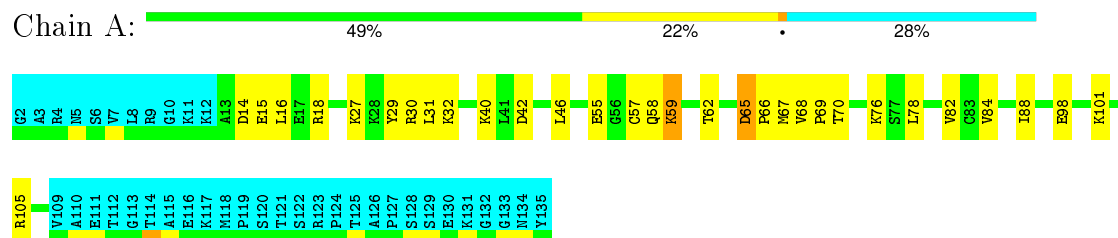
4.2.3 Score per residue for model 3 (medoid)

- Molecule 1: HIV-2 myristoylated matrix protein



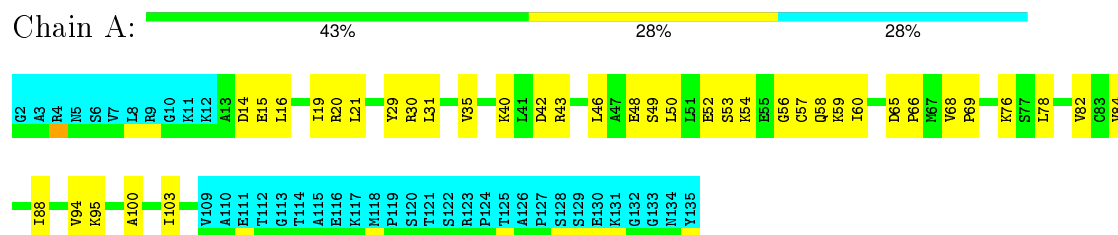
4.2.4 Score per residue for model 4

- Molecule 1: HIV-2 myristoylated matrix protein



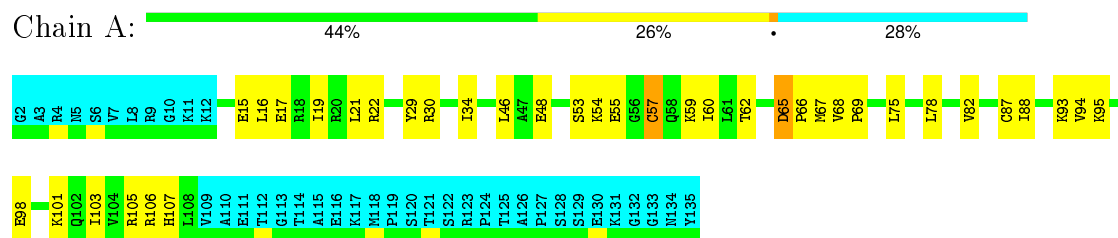
4.2.5 Score per residue for model 5

- Molecule 1: HIV-2 myristoylated matrix protein



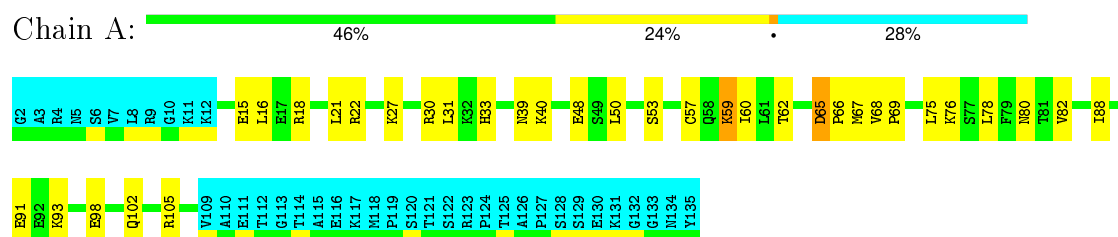
4.2.6 Score per residue for model 6

- Molecule 1: HIV-2 myristoylated matrix protein



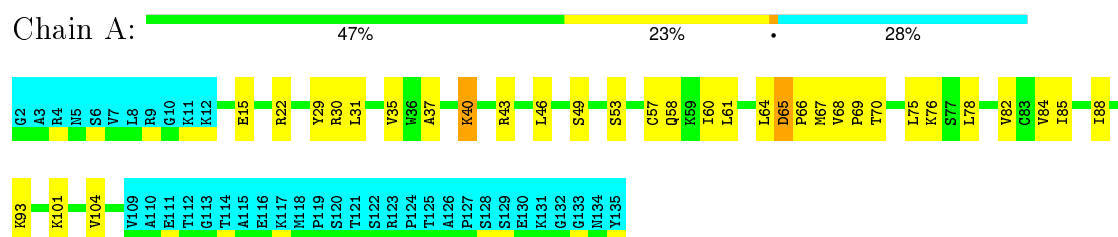
4.2.7 Score per residue for model 7

- Molecule 1: HIV-2 myristoylated matrix protein



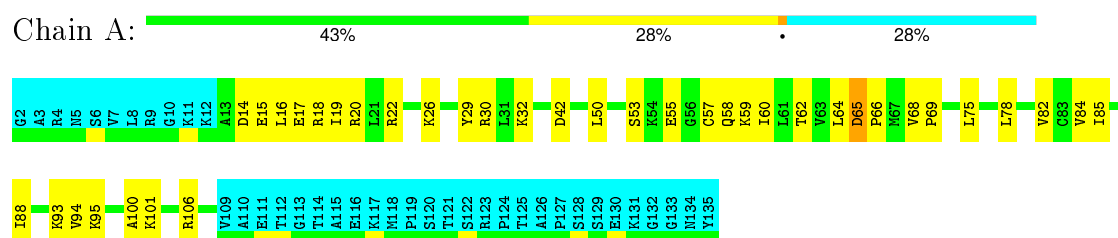
4.2.8 Score per residue for model 8

- Molecule 1: HIV-2 myristoylated matrix protein



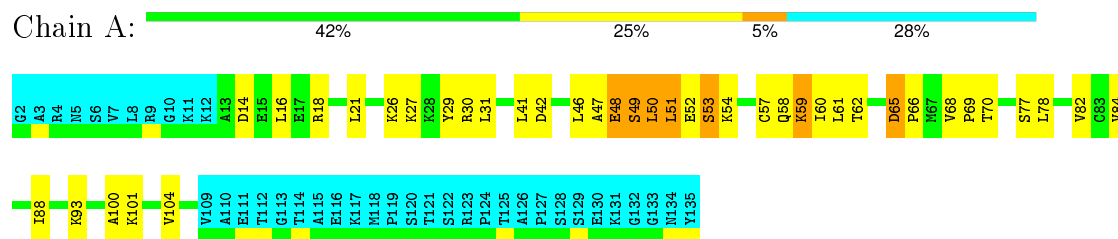
4.2.9 Score per residue for model 9

- Molecule 1: HIV-2 myristoylated matrix protein



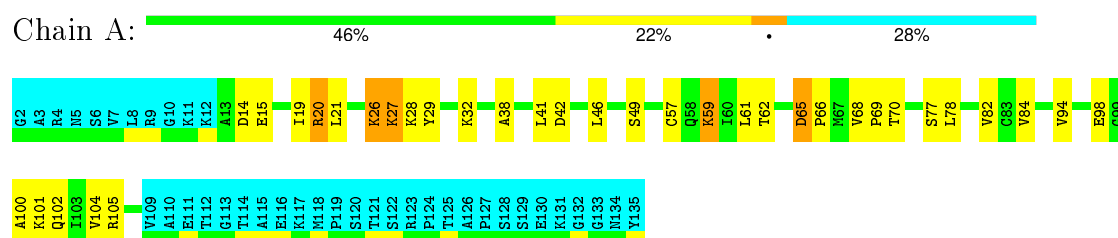
4.2.14 Score per residue for model 14

- Molecule 1: HIV-2 myristoylated matrix protein



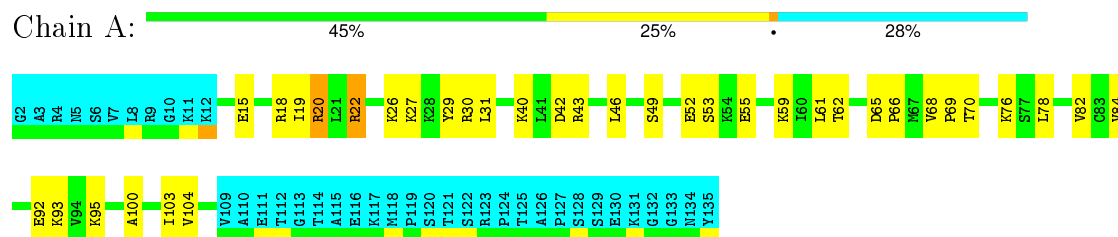
4.2.15 Score per residue for model 15

- Molecule 1: HIV-2 myristoylated matrix protein



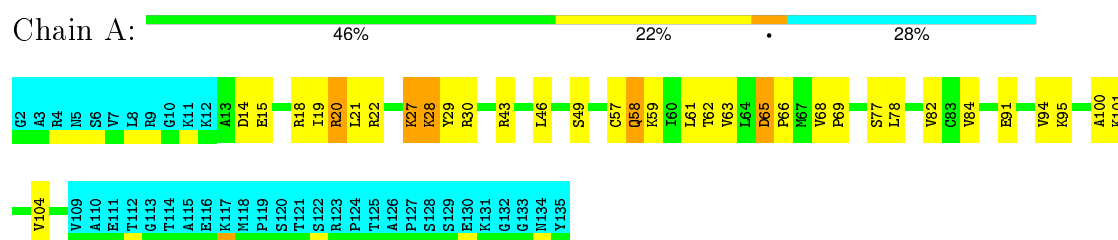
4.2.16 Score per residue for model 16

- Molecule 1: HIV-2 myristoylated matrix protein



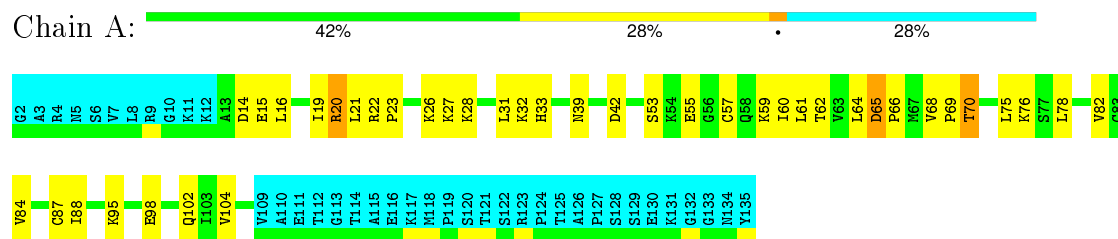
4.2.17 Score per residue for model 17

- Molecule 1: HIV-2 myristoylated matrix protein



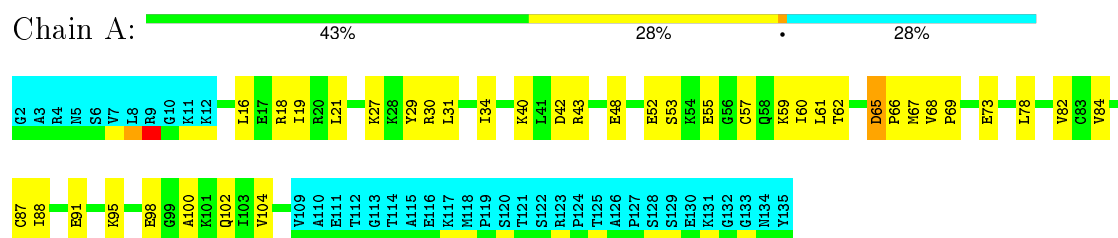
4.2.18 Score per residue for model 18

- Molecule 1: HIV-2 myristoylated matrix protein



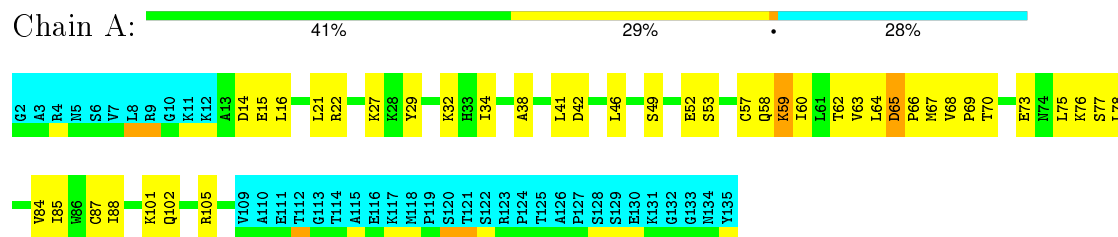
4.2.19 Score per residue for model 19

- Molecule 1: HIV-2 myristoylated matrix protein



4.2.20 Score per residue for model 20

- Molecule 1: HIV-2 myristoylated matrix protein



5 Refinement protocol and experimental data overview

The models were refined using the following method: *distance geometry*.

Of the 50 calculated structures, 20 were deposited, based on the following criterion: *target function*.

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

Software name	Classification	Version
CYANA	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)	BMRB entry 16889
Number of chemical shift lists	1
Total number of shifts	1319
Number of shifts mapped to atoms	1278
Number of unparsed shifts	0
Number of shifts with mapping errors	41
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	79%

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

6 Model quality ⓘ

6.1 Standard geometry ⓘ

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

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	769	808	808	16±3
2	A	15	27	27	1±1
All	All	16460	17260	17260	320

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.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:19:ILE:HD13	1:A:84:VAL:HG13	0.83	1.47	17	6
1:A:64:LEU:HD21	1:A:78:LEU:HD23	0.81	1.52	20	1
1:A:16:LEU:HD23	1:A:88:ILE:HD11	0.79	1.54	2	13
1:A:94:VAL:HG21	1:A:100:ALA:HB2	0.76	1.58	17	2
1:A:41:LEU:HD12	1:A:51:LEU:HD12	0.74	1.60	14	1
1:A:61:LEU:HD12	1:A:104:VAL:HG11	0.71	1.62	12	1
1:A:61:LEU:HD13	1:A:104:VAL:HG11	0.69	1.63	17	13
1:A:20:ARG:HD3	1:A:22:ARG:O	0.69	1.87	16	1
1:A:29:TYR:CE2	1:A:84:VAL:HG21	0.69	2.23	2	10
1:A:78:LEU:O	1:A:82:VAL:HG23	0.63	1.94	4	19
1:A:61:LEU:CD1	1:A:104:VAL:HG11	0.63	2.24	13	7

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:21:LEU:HD11	1:A:33:HIS:CE1	0.63	2.28	18	2
1:A:21:LEU:HD12	1:A:27:LYS:HB3	0.63	1.68	7	4
1:A:16:LEU:CD1	1:A:34:ILE:HD11	0.63	2.23	19	1
1:A:50:LEU:HB2	1:A:60:ILE:HD11	0.61	1.72	12	6
1:A:16:LEU:HG	2:A:1:MYR:H141	0.61	1.72	14	3
1:A:19:ILE:HG12	1:A:94:VAL:HG23	0.59	1.73	15	4
1:A:19:ILE:HD13	1:A:84:VAL:CG1	0.59	2.26	13	5
1:A:31:LEU:O	1:A:35:VAL:HG23	0.57	1.99	5	2
1:A:34:ILE:CD1	2:A:1:MYR:H142	0.57	2.29	20	2
1:A:59:LYS:O	1:A:63:VAL:HG23	0.56	2.00	17	2
1:A:57:CYS:HA	1:A:60:ILE:HD12	0.56	1.77	19	6
1:A:94:VAL:HG11	1:A:100:ALA:HA	0.56	1.76	12	3
1:A:85:ILE:HA	1:A:88:ILE:HD12	0.56	1.76	11	4
1:A:34:ILE:HD11	2:A:1:MYR:H142	0.56	1.76	6	1
1:A:21:LEU:HD12	1:A:27:LYS:CB	0.56	2.30	7	4
1:A:84:VAL:O	1:A:88:ILE:HD12	0.56	2.01	19	1
1:A:29:TYR:CZ	1:A:84:VAL:HG21	0.56	2.35	4	2
1:A:38:ALA:HA	1:A:41:LEU:HD12	0.55	1.76	20	3
1:A:100:ALA:O	1:A:104:VAL:HG23	0.55	2.01	17	7
1:A:16:LEU:HA	1:A:19:ILE:HD12	0.55	1.78	3	4
1:A:29:TYR:OH	1:A:84:VAL:HG21	0.55	2.00	4	2
1:A:40:LYS:HB3	1:A:78:LEU:HD22	0.55	1.78	2	3
1:A:16:LEU:HD23	1:A:88:ILE:CD1	0.55	2.32	3	6
1:A:21:LEU:HD23	1:A:29:TYR:CZ	0.55	2.36	13	8
1:A:34:ILE:HD13	2:A:1:MYR:H142	0.54	1.79	20	1
1:A:29:TYR:CE1	1:A:84:VAL:HG21	0.53	2.39	17	1
1:A:88:ILE:HD13	2:A:1:MYR:H143	0.53	1.81	9	2
1:A:94:VAL:CG1	1:A:103:ILE:HD12	0.53	2.34	1	3
1:A:19:ILE:CD1	1:A:88:ILE:HD11	0.52	2.35	19	1
1:A:50:LEU:CB	1:A:60:ILE:HD11	0.52	2.35	7	3
1:A:50:LEU:HD22	1:A:56:GLY:O	0.51	2.06	5	1
1:A:65:ASP:CB	1:A:66:PRO:CD	0.50	2.89	10	20
1:A:88:ILE:HD13	2:A:1:MYR:C14	0.50	2.36	9	1
1:A:16:LEU:CD2	1:A:88:ILE:HD11	0.50	2.36	9	2
1:A:34:ILE:HG21	2:A:1:MYR:C9	0.49	2.38	6	1
1:A:67:MET:HB3	1:A:75:LEU:HD11	0.49	1.83	7	2
1:A:50:LEU:O	1:A:53:SER:N	0.49	2.46	14	1
1:A:20:ARG:HG3	1:A:22:ARG:H	0.48	1.68	18	1
1:A:30:ARG:O	1:A:31:LEU:CB	0.48	2.60	11	1
1:A:41:LEU:CD1	1:A:51:LEU:HD12	0.48	2.36	14	1
1:A:19:ILE:HD12	1:A:88:ILE:HD11	0.48	1.86	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:34:ILE:HG21	2:A:1:MYR:H101	0.48	1.85	3	1
1:A:92:GLU:CD	1:A:103:ILE:HG21	0.48	2.29	16	1
1:A:68:VAL:N	1:A:69:PRO:HD2	0.48	2.24	9	20
1:A:59:LYS:O	1:A:62:THR:HG22	0.48	2.09	13	13
1:A:61:LEU:HD13	1:A:104:VAL:CG1	0.47	2.37	17	2
1:A:41:LEU:HD22	1:A:46:LEU:HB2	0.47	1.86	14	1
1:A:21:LEU:HD12	1:A:27:LYS:HD3	0.47	1.85	19	1
1:A:20:ARG:HG2	1:A:27:LYS:C	0.47	2.30	15	3
1:A:64:LEU:O	1:A:68:VAL:HG23	0.47	2.09	10	3
1:A:85:ILE:CD1	2:A:1:MYR:H143	0.47	2.39	20	1
1:A:80:ASN:OD1	1:A:97:THR:HG21	0.46	2.10	13	1
1:A:50:LEU:HB3	1:A:60:ILE:HD11	0.46	1.88	7	1
1:A:22:ARG:CB	1:A:23:PRO:HD2	0.46	2.41	18	1
1:A:69:PRO:O	1:A:70:THR:HG23	0.46	2.10	18	1
1:A:47:ALA:O	1:A:48:GLU:CG	0.45	2.64	14	1
1:A:68:VAL:CB	1:A:69:PRO:CD	0.45	2.95	10	19
1:A:94:VAL:HG12	1:A:103:ILE:HD12	0.45	1.89	5	2
1:A:20:ARG:HE	1:A:21:LEU:N	0.44	2.09	18	1
1:A:16:LEU:HD22	1:A:16:LEU:O	0.44	2.12	11	1
1:A:65:ASP:N	1:A:66:PRO:HD2	0.44	2.28	7	10
1:A:34:ILE:HG21	2:A:1:MYR:H91	0.44	1.90	6	1
1:A:40:LYS:CB	1:A:78:LEU:HD22	0.44	2.43	8	2
1:A:20:ARG:NE	1:A:22:ARG:H	0.43	2.11	17	3
1:A:103:ILE:HG22	1:A:107:HIS:CD2	0.43	2.49	11	2
1:A:60:ILE:HG22	1:A:64:LEU:HD12	0.43	1.91	18	1
1:A:64:LEU:CD1	1:A:82:VAL:HG21	0.43	2.44	11	1
1:A:60:ILE:HG22	1:A:64:LEU:CD1	0.42	2.44	18	1
1:A:67:MET:CB	1:A:75:LEU:HD21	0.42	2.44	20	1
1:A:16:LEU:O	1:A:16:LEU:HD13	0.42	2.15	10	1
1:A:68:VAL:HB	1:A:69:PRO:HD3	0.42	1.91	10	7
1:A:58:GLN:HA	1:A:61:LEU:HD12	0.42	1.91	17	1
1:A:94:VAL:HG11	1:A:100:ALA:CA	0.42	2.44	12	1
1:A:47:ALA:C	1:A:49:SER:N	0.41	2.73	14	1
1:A:20:ARG:HA	1:A:28:LYS:HA	0.41	1.92	17	1
1:A:37:ALA:HB2	1:A:81:THR:HG21	0.41	1.92	12	1
1:A:37:ALA:HB1	1:A:78:LEU:CD1	0.41	2.45	8	1
1:A:62:THR:O	1:A:66:PRO:CD	0.41	2.69	2	1
1:A:20:ARG:CD	1:A:22:ARG:O	0.41	2.65	16	1
1:A:68:VAL:HB	1:A:69:PRO:CD	0.40	2.46	10	1
1:A:67:MET:HB3	1:A:75:LEU:HD21	0.40	1.91	6	1
1:A:94:VAL:HG11	1:A:100:ALA:HB2	0.40	1.92	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:51:LEU:N	1:A:60:ILE:HD11	0.40	2.30	14	1
1:A:20:ARG:HD2	1:A:26:LYS:N	0.40	2.31	15	1
1:A:67:MET:O	1:A:75:LEU:HD22	0.40	2.17	8	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	96/134 (72%)	92±2 (95±2%)	4±2 (4±2%)	0±0 (0±0%)	59	88
All	All	1920/2680 (72%)	1833 (95%)	86 (4%)	1 (0%)	59	88

All 1 unique Ramachandran outliers are listed below.

Mol	Chain	Res	Type	Models (Total)
1	A	26	LYS	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	84/113 (74%)	65±3 (77±3%)	19±3 (23±3%)	3	30
All	All	1680/2260 (74%)	1296 (77%)	384 (23%)	3	30

All 48 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	65	ASP	17
1	A	53	SER	15

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Mol	Chain	Res	Type	Models (Total)
1	A	30	ARG	15
1	A	46	LEU	14
1	A	57	CYS	14
1	A	101	LYS	14
1	A	76	LYS	13
1	A	15	GLU	13
1	A	58	GLN	12
1	A	59	LYS	12
1	A	14	ASP	12
1	A	42	ASP	11
1	A	70	THR	11
1	A	49	SER	11
1	A	22	ARG	10
1	A	98	GLU	10
1	A	55	GLU	10
1	A	95	LYS	9
1	A	43	ARG	9
1	A	20	ARG	9
1	A	93	LYS	9
1	A	40	LYS	9
1	A	32	LYS	9
1	A	18	ARG	8
1	A	102	GLN	8
1	A	52	GLU	8
1	A	48	GLU	7
1	A	106	ARG	7
1	A	27	LYS	6
1	A	73	GLU	6
1	A	87	CYS	6
1	A	54	LYS	6
1	A	77	SER	5
1	A	28	LYS	5
1	A	91	GLU	5
1	A	105	ARG	5
1	A	75	LEU	5
1	A	26	LYS	5
1	A	31	LEU	5
1	A	39	ASN	4
1	A	67	MET	3
1	A	17	GLU	3
1	A	62	THR	3
1	A	80	ASN	2

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Mol	Chain	Res	Type	Models (Total)
1	A	64	LEU	1
1	A	74	ASN	1
1	A	51	LEU	1
1	A	50	LEU	1

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 ⓘ

2 ligands are 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	MYR	A	1	1	14,14,15	1.05±0.00	0±0 (0±0%)
3	PBU	A	300	-	37,39,39	1.50±0.00	0±0 (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	MYR	A	1	1	13,13,15	0.44±0.00	0±0 (0±0%)
3	PBU	A	300	-	53,57,57	1.58±0.00	0±0 (0±0%)

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	MYR	A	1	1	-	0±0,12,12,13	0±0,0,0,0
3	PBU	A	300	-	-	0±0,36,60,60	0±0,1,1,1

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

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

Mol	Chain	Res	Type	Atoms	Models (Total)
3	A	300	PBU	P1-O1-C1-C2	8
3	A	300	PBU	C2'-O2'-C7-C8	2

There are no ring outliers.

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 79% for the well-defined parts and 68% for the entire structure.

7.1 Chemical shift list 1

File name: BMRB entry 16889

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	1319
Number of shifts mapped to atoms	1278
Number of unparsed shifts	0
Number of shifts with mapping errors	41
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.

- Chain not found in structure. All 41 occurrences are reported below.

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	1	PBU	H4	4.322	0.02	1
UNMAPPED	1	PBU	H92	1.565	0.02	1
UNMAPPED	1	PBU	H12	0.865	0.02	1
UNMAPPED	1	PBU	C1	75.792	0.05	1
UNMAPPED	1	PBU	H91	1.565	0.02	1
UNMAPPED	1	PBU	H131	1.582	0.02	1
UNMAPPED	1	PBU	H141	0.851	0.02	1
UNMAPPED	1	PBU	H13	0.865	0.02	1
UNMAPPED	1	PBU	H3'1	4.089	0.02	1
UNMAPPED	1	PBU	C1'	62.945	0.05	1
UNMAPPED	1	PBU	H1'1	4.277	0.02	1
UNMAPPED	1	PBU	H11	0.865	0.02	1
UNMAPPED	1	PBU	H132	1.582	0.02	1
UNMAPPED	1	PBU	H142	0.851	0.02	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	1	PBU	C9	18.002	0.05	1
UNMAPPED	1	PBU	H121	2.386	0.02	1
UNMAPPED	1	PBU	C13	18.002	0.05	1
UNMAPPED	1	PBU	C7	176.135	0.05	1
UNMAPPED	1	PBU	H3	3.661	0.02	1
UNMAPPED	1	PBU	C3'	63.872	0.05	1
UNMAPPED	1	PBU	H143	0.851	0.02	1
UNMAPPED	1	PBU	H2	4.22	0.02	1
UNMAPPED	1	PBU	C6	70.932	0.05	1
UNMAPPED	1	PBU	C3	70.33	0.05	1
UNMAPPED	1	PBU	H1	3.991	0.02	1
UNMAPPED	1	PBU	H6	3.92	0.02	1
UNMAPPED	1	PBU	H1'2	4.394	0.02	1
UNMAPPED	1	PBU	C5	78.318	0.05	1
UNMAPPED	1	PBU	H2'	5.216	0.02	1
UNMAPPED	1	PBU	H122	2.386	0.02	1
UNMAPPED	1	PBU	H3'2	4.114	0.02	1
UNMAPPED	1	PBU	H5	4.044	0.02	1
UNMAPPED	1	PBU	H81	2.349	0.02	1
UNMAPPED	1	PBU	C2'	70.889	0.05	1
UNMAPPED	1	PBU	C12	33.99	0.05	1
UNMAPPED	1	PBU	C14	13.462	0.05	1
UNMAPPED	1	PBU	H82	2.349	0.02	1
UNMAPPED	1	PBU	C8	34.199	0.05	1
UNMAPPED	1	PBU	C2	70.759	0.05	1
UNMAPPED	1	PBU	C4	76.887	0.05	1
UNMAPPED	1	PBU	C10	13.54	0.05	1

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	113	2.23 ± 0.18	Should be applied
$^{13}\text{C}_\beta$	100	2.92 ± 0.05	Should be applied
$^{13}\text{C}'$	0	—	—
^{15}N	123	0.90 ± 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 79%, i.e. 980 atoms were assigned a chemical shift out of a possible 1246. 3 out of 19 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	370/474 (78%)	185/189 (98%)	94/192 (49%)	91/93 (98%)
Sidechain	571/701 (81%)	353/411 (86%)	215/253 (85%)	3/37 (8%)
Aromatic	39/71 (55%)	20/38 (53%)	17/28 (61%)	2/5 (40%)
Overall	980/1246 (79%)	558/638 (87%)	326/473 (69%)	96/135 (71%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 68%, i.e. 1143 atoms were assigned a chemical shift out of a possible 1677. 3 out of 22 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	474/658 (72%)	238/262 (91%)	113/268 (42%)	123/128 (96%)
Sidechain	630/940 (67%)	390/554 (70%)	237/334 (71%)	3/52 (6%)
Aromatic	39/79 (49%)	20/42 (48%)	17/32 (53%)	2/5 (40%)
Overall	1143/1677 (68%)	648/858 (76%)	367/634 (58%)	128/185 (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.

Random coil index (RCI) for chain A:

