



wwPDB NMR Structure Validation Summary Report ⓘ

Jun 25, 2024 – 02:11 AM EDT

PDB ID : 6M78
BMRB ID : 50188
Title : Aromatic interactions drive the coupled folding and binding of the intrinsically disordered Sesbania mosaic virus VPg protein
Authors : Dixit, K.; Karanth, N.M.; Nair, S.; Kumari, K.; Chakraborti, K.S.; Savithri, H.S.; Sarma, S.P.
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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 : 4.02b-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) : 2.37.1

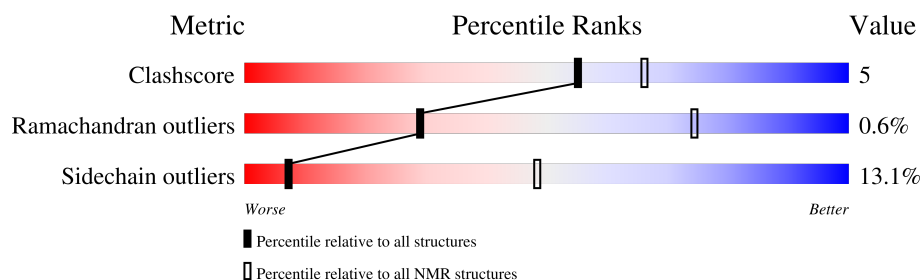
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 28%.

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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	296	
2	B	80	

2 Ensemble composition and analysis

This entry contains 4 models. Model 4 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:135-A:325, B:323-B:341, B:348-B:379 (242)	0.62	4

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 1 clusters. No single-model clusters were found.

Cluster number	Models
1	1, 2, 3, 4

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2304 atoms, of which 414 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Polyprotein.

Mol	Chain	Residues	Atoms						Trace
1	A	191	Total	C	H	N	O	S	0
			1746	899	319	241	274	13	

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	107	MET	-	initiating methionine	UNP Q9EB08
A	108	ARG	-	expression tag	UNP Q9EB08
A	109	GLY	-	expression tag	UNP Q9EB08
A	110	SER	-	expression tag	UNP Q9EB08
A	111	HIS	-	expression tag	UNP Q9EB08
A	112	HIS	-	expression tag	UNP Q9EB08
A	113	HIS	-	expression tag	UNP Q9EB08
A	114	HIS	-	expression tag	UNP Q9EB08
A	115	HIS	-	expression tag	UNP Q9EB08
A	116	HIS	-	expression tag	UNP Q9EB08
A	117	GLY	-	expression tag	UNP Q9EB08
A	118	MET	-	expression tag	UNP Q9EB08
A	119	ALA	-	expression tag	UNP Q9EB08

- Molecule 2 is a protein called Polyprotein.

Mol	Chain	Residues	Atoms						Trace
2	B	57	Total	C	H	N	O	S	0
			558	300	95	73	89	1	

There are 3 discrepancies between the modelled and reference sequences:

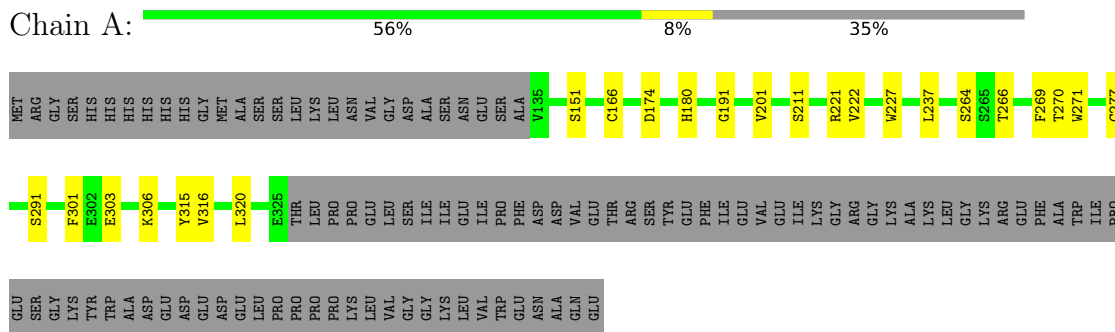
Chain	Residue	Modelled	Actual	Comment	Reference
B	323	GLY	-	expression tag	UNP Q9EB08
B	324	SER	-	expression tag	UNP Q9EB08
B	325	MET	-	expression tag	UNP Q9EB08

4 Residue-property plots

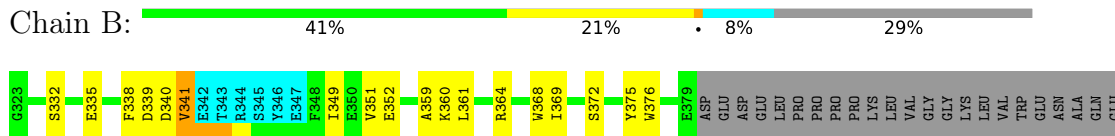
4.1 Average score per residue in the NMR ensemble

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: Polyprotein



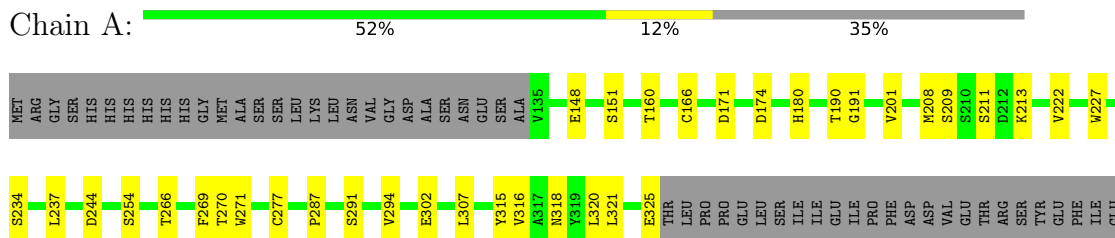
- Molecule 2: Polyprotein



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

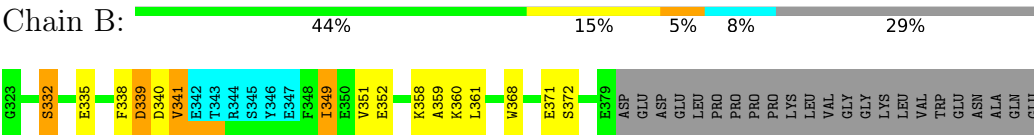
The representative model is number 4. Colouring as in section 4.1 above.

- Molecule 1: Polyprotein



VAL	GLU	ILE	LYS	GLY	ARG	GLY	LYS	ALA	LYS	LEU	GLY	LYS	ARG	GLU	PHE	ALA	TRP	ILE	PRO	GLU	SER	GLY	LYS	TYR	TRP	ALA	ASP	GLU	ASP	GLU	ASP	GLU	LEU	PRO	PRO	PRO	PRO	LYS	LEU	VAL	GLY	GLY	LYS	LEU	VAL	TRP	GLY	GLN	GLU
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

● Molecule 2: Polypeptide



5 Refinement protocol and experimental data overview

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

Of the 200 calculated structures, 4 were deposited, based on the following criterion: *structures with favorable non-bond energy*.

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

Software name	Classification	Version
HADDOCK	structure calculation	2.2
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	1
Total number of shifts	1000
Number of shifts mapped to atoms	783
Number of unparsed shifts	0
Number of shifts with mapping errors	217
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	28%

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	0.29±0.00	0±0/1461 (0.0± 0.0%)	0.42±0.00	0±0/1982 (0.0± 0.0%)
2	B	0.31±0.00	0±0/420 (0.0± 0.0%)	0.96±0.03	3±0/566 (0.5± 0.1%)
All	All	0.29	0/7524 (0.0%)	0.59	11/10192 (0.1%)

There are no bond-length outliers.

All 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
2	B	341	VAL	CB-CA-C	-18.11	77.00	111.40	4	4
2	B	341	VAL	N-CA-C	-6.88	92.43	111.00	2	4
2	B	341	VAL	N-CA-CB	6.24	125.24	111.50	4	3

There are no chirality outliers.

There are no planarity outliers.

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	1427	319	1403	12±2
2	B	409	81	406	9±2
All	All	7344	1600	7236	78

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 5.

5 of 49 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:349:ILE:HB	2:B:361:LEU:HB2	0.92	1.40	1	3
2:B:359:ALA:HB1	2:B:368:TRP:HB2	0.88	1.45	2	3
1:A:237:LEU:HG	1:A:294:VAL:HB	0.73	1.59	4	1
1:A:316:VAL:HA	1:A:320:LEU:HB2	0.69	1.65	4	3
1:A:317:ALA:HA	1:A:321:LEU:HD12	0.68	1.65	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	189/296 (64%)	176±2 (93±1%)	13±2 (7±1%)	0±0 (0±0%)	44	80
2	B	49/80 (61%)	42±1 (85±2%)	6±1 (13±2%)	1±1 (2±1%)	11	52
All	All	952/1504 (63%)	869 (91%)	77 (8%)	6 (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)
2	B	376	TRP	2
2	B	332	SER	2
1	A	181	HIS	1
1	A	182	VAL	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	161/250 (64%)	141±3 (87±2%)	20±3 (13±2%)	8	50

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	B	43/69 (62%)	36±1 (85±3%)	6±1 (15±3%)	6 44
All	All	816/1276 (64%)	709 (87%)	107 (13%)	7 48

5 of 62 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	151	SER	4
1	A	174	ASP	4
1	A	270	THR	4
1	A	271	TRP	4
1	A	291	SER	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 28% for the well-defined parts and 27% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chemical_shifts_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	1000
Number of shifts mapped to atoms	783
Number of unparsed shifts	0
Number of shifts with mapping errors	217
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	1

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 217) occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	116	HIS	CA	59.539	0.000	1
1	A	116	HIS	CB	34.359	0.000	1
1	A	117	GLY	H	8.438	0.006	1
1	A	117	GLY	CA	44.931	0.000	1
1	A	117	GLY	N	109.377	0.025	1
1	A	118	MET	CA	53.952	0.000	1
1	A	119	ALA	H	8.212	0.007	1
1	A	119	ALA	CA	52.286	0.040	1
1	A	119	ALA	N	124.97	0.042	1
1	A	120	SER	H	8.21	0.010	1
1	A	120	SER	CA	58.395	0.000	1
1	A	120	SER	N	115.191	0.041	1
1	A	125	ASN	CA	52.704	0.012	1
1	A	125	ASN	CB	38.272	0.021	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	126	VAL	H	7.991	0.007	1
1	A	126	VAL	HG11	0.761	0.000	1
1	A	126	VAL	HG12	0.761	0.000	1
1	A	126	VAL	HG13	0.761	0.000	1
1	A	126	VAL	HG21	0.761	0.000	1
1	A	126	VAL	HG22	0.761	0.000	1
1	A	126	VAL	HG23	0.761	0.000	1
1	A	126	VAL	CA	62.029	0.021	1
1	A	126	VAL	CB	31.727	0.000	1
1	A	126	VAL	N	120.2	0.069	1
1	A	127	GLY	H	8.312	0.004	1
1	A	127	GLY	CA	44.839	0.016	1
1	A	127	GLY	N	112.237	0.047	1
1	A	128	ASP	H	7.916	0.006	1
1	A	128	ASP	CA	55.287	0.000	1
1	A	128	ASP	CB	41.582	0.000	1
1	A	128	ASP	N	126.187	0.044	1
1	A	129	ALA	CA	52.028	0.000	1
1	A	129	ALA	CB	18.405	0.006	1
1	A	130	SER	H	7.781	0.007	1
1	A	130	SER	CA	59.45	0.000	1
1	A	130	SER	CB	64.234	0.000	1
1	A	130	SER	N	121.346	0.017	1
1	A	132	GLU	CA	56.73	0.000	1
1	A	133	SER	H	8.142	0.010	1
1	A	133	SER	CA	58.267	0.046	1
1	A	133	SER	CB	63.341	0.000	1
1	A	133	SER	N	116.422	0.025	1
1	A	134	ALA	H	8.058	0.003	1
1	A	134	ALA	CA	52.218	0.007	1
1	A	134	ALA	CB	18.353	0.014	1
1	A	134	ALA	N	126.118	0.043	1
1	A	135	VAL	HG11	0.761	0.000	1
1	A	135	VAL	HG12	0.761	0.000	1
1	A	135	VAL	HG13	0.761	0.000	1
1	A	135	VAL	HG21	0.761	0.000	1
1	A	135	VAL	HG22	0.761	0.000	1
1	A	135	VAL	HG23	0.761	0.000	1
1	A	136	LEU	HD11	0.803	0.000	1
1	A	136	LEU	HD12	0.803	0.000	1
1	A	136	LEU	HD13	0.803	0.000	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	136	LEU	HD21	0.803	0.000	1
1	A	136	LEU	HD22	0.803	0.000	1
1	A	136	LEU	HD23	0.803	0.000	1
1	A	143	VAL	HG11	0.796	0.000	1
1	A	143	VAL	HG12	0.796	0.000	1
1	A	143	VAL	HG13	0.796	0.000	1
1	A	152	LEU	HD11	0.868	0.000	1
1	A	152	LEU	HD12	0.868	0.000	1
1	A	152	LEU	HD13	0.868	0.000	1
1	A	152	LEU	HD21	0.868	0.000	1
1	A	152	LEU	HD22	0.868	0.000	1
1	A	152	LEU	HD23	0.868	0.000	1
1	A	182	VAL	HG11	0.669	0.008	1
1	A	182	VAL	HG12	0.669	0.008	1
1	A	182	VAL	HG13	0.669	0.008	1
1	A	182	VAL	HG21	0.669	0.008	1
1	A	182	VAL	HG22	0.669	0.008	1
1	A	182	VAL	HG23	0.669	0.008	1
1	A	199	VAL	HG11	0.651	0.000	2
1	A	199	VAL	HG12	0.651	0.000	2
1	A	199	VAL	HG13	0.651	0.000	2
1	A	199	VAL	HG21	0.862	0.000	2
1	A	199	VAL	HG22	0.862	0.000	2
1	A	199	VAL	HG23	0.862	0.000	2
1	A	201	VAL	HG11	0.26	0.000	2
1	A	201	VAL	HG12	0.26	0.000	2
1	A	201	VAL	HG13	0.26	0.000	2
1	A	201	VAL	HG21	0.463	0.000	2
1	A	201	VAL	HG22	0.463	0.000	2
1	A	201	VAL	HG23	0.463	0.000	2
1	A	215	LEU	HD11	1.111	0.000	2
1	A	215	LEU	HD12	1.111	0.000	2
1	A	215	LEU	HD13	1.111	0.000	2
1	A	215	LEU	HD21	0.595	0.000	2
1	A	215	LEU	HD22	0.595	0.000	2
1	A	215	LEU	HD23	0.595	0.000	2
1	A	232	VAL	HG11	0.3	0.000	2
1	A	232	VAL	HG12	0.3	0.000	2
1	A	232	VAL	HG13	0.3	0.000	2
1	A	232	VAL	HG21	0.839	0.000	2
1	A	232	VAL	HG22	0.839	0.000	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	232	VAL	HG23	0.839	0.000	2
1	A	257	LEU	HD11	0.825	0.004	2
1	A	257	LEU	HD12	0.825	0.004	2
1	A	257	LEU	HD13	0.825	0.004	2
1	A	257	LEU	HD21	0.821	0.000	2
1	A	257	LEU	HD22	0.821	0.000	2
1	A	257	LEU	HD23	0.821	0.000	2
1	A	261	VAL	HG11	0.804	0.009	1
1	A	261	VAL	HG12	0.804	0.009	1
1	A	261	VAL	HG13	0.804	0.009	1
1	A	273	LEU	HD11	0.663	0.000	2
1	A	273	LEU	HD12	0.663	0.000	2
1	A	273	LEU	HD13	0.663	0.000	2
1	A	273	LEU	HD21	1.138	0.000	2
1	A	273	LEU	HD22	1.138	0.000	2
1	A	273	LEU	HD23	1.138	0.000	2
1	A	284	ALA	H	8.321	0.007	1
1	A	284	ALA	CA	54.681	0.046	1
1	A	284	ALA	CB	19.392	0.015	1
1	A	284	ALA	N	123.379	0.034	1
1	A	294	VAL	HG11	0.112	0.002	2
1	A	294	VAL	HG12	0.112	0.002	2
1	A	294	VAL	HG13	0.112	0.002	2
1	A	294	VAL	HG21	0.522	0.019	2
1	A	294	VAL	HG22	0.522	0.019	2
1	A	294	VAL	HG23	0.522	0.019	2
1	A	299	VAL	HG11	0.64	0.015	2
1	A	299	VAL	HG12	0.64	0.015	2
1	A	299	VAL	HG13	0.64	0.015	2
1	A	299	VAL	HG21	1.047	0.009	2
1	A	299	VAL	HG22	1.047	0.009	2
1	A	299	VAL	HG23	1.047	0.009	2
1	A	307	LEU	HD11	0.736	0.011	1
1	A	307	LEU	HD12	0.736	0.011	1
1	A	307	LEU	HD13	0.736	0.011	1
1	B	341	VAL	HG11	-0.254	0.013	2
1	B	341	VAL	HG12	-0.254	0.013	2
1	B	341	VAL	HG13	-0.254	0.013	2
1	B	341	VAL	HG21	0.271	0.005	2
1	B	341	VAL	HG22	0.271	0.005	2
1	B	341	VAL	HG23	0.271	0.005	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	B	351	VAL	HG11	0.436	0.007	1
1	B	351	VAL	HG12	0.436	0.007	1
1	B	351	VAL	HG13	0.436	0.007	1
1	B	351	VAL	HG21	0.439	0.004	1
1	B	351	VAL	HG22	0.439	0.004	1
1	B	351	VAL	HG23	0.439	0.004	1
1	B	361	LEU	HD11	0.417	0.000	2
1	B	361	LEU	HD12	0.417	0.000	2
1	B	361	LEU	HD13	0.417	0.000	2
1	B	361	LEU	HD21	0.513	0.010	2
1	B	361	LEU	HD22	0.513	0.010	2
1	B	361	LEU	HD23	0.513	0.010	2
1	B	380	ASP	H	8.24	0.018	1
1	B	380	ASP	CA	54.097	0.021	1
1	B	380	ASP	CB	40.717	0.014	1
1	B	380	ASP	N	121.673	0.055	1
1	B	381	GLU	H	8.179	0.007	1
1	B	381	GLU	CA	56.171	0.002	1
1	B	381	GLU	CB	29.619	0.004	1
1	B	381	GLU	N	121.717	0.037	1
1	B	382	ASP	H	8.35	0.015	1
1	B	382	ASP	CA	54.142	0.024	1
1	B	382	ASP	CB	40.728	0.027	1
1	B	382	ASP	N	121.687	0.055	1
1	B	383	GLU	H	8.121	0.010	1
1	B	383	GLU	CA	55.829	0.001	1
1	B	383	GLU	CB	29.577	0.017	1
1	B	383	GLU	N	121.334	0.024	1
1	B	384	LEU	H	8.134	0.007	1
1	B	384	LEU	CA	52.539	0.000	1
1	B	384	LEU	CB	40.594	0.000	1
1	B	384	LEU	N	125.422	0.042	1
1	B	389	LYS	CA	55.209	0.000	1
1	B	389	LYS	CB	32.793	0.000	1
1	B	390	LEU	H	8.174	0.006	1
1	B	390	LEU	CA	54.677	0.031	1
1	B	390	LEU	CB	41.124	0.002	1
1	B	390	LEU	N	123.785	0.041	1
1	B	391	VAL	H	8.056	0.015	1
1	B	391	VAL	CA	61.682	0.000	1
1	B	391	VAL	CB	32.17	0.000	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	B	391	VAL	N	121.655	0.094	1
1	B	393	GLY	H	8.186	0.003	1
1	B	393	GLY	CA	44.857	0.014	1
1	B	393	GLY	N	107.632	0.240	1
1	B	394	LYS	H	7.853	0.005	1
1	B	394	LYS	CA	55.492	0.101	1
1	B	394	LYS	N	121.249	0.072	1
1	B	395	LEU	H	8.101	0.009	1
1	B	395	LEU	CA	54.334	0.034	1
1	B	395	LEU	CB	41.472	0.051	1
1	B	395	LEU	N	124.206	0.060	1
1	B	396	VAL	H	8.288	0.011	1
1	B	396	VAL	CA	61.7	0.001	1
1	B	396	VAL	CB	32.167	0.000	1
1	B	396	VAL	N	123.284	0.037	1
1	B	397	TRP	H	8.107	0.005	1
1	B	397	TRP	CA	56.648	0.020	1
1	B	397	TRP	CB	29.079	0.000	1
1	B	397	TRP	N	124.922	0.038	1
1	B	398	GLU	H	8.157	0.007	1
1	B	398	GLU	CA	56.209	0.038	1
1	B	398	GLU	CB	29.455	0.000	1
1	B	398	GLU	N	122.901	0.086	1
1	B	399	ASN	H	8.193	0.007	1
1	B	399	ASN	CA	52.793	0.016	1
1	B	399	ASN	CB	38.289	0.000	1
1	B	399	ASN	N	119.744	0.062	1
1	B	400	ALA	H	8.099	0.009	1
1	B	400	ALA	CA	52.133	0.015	1
1	B	400	ALA	CB	18.363	0.049	1
1	B	400	ALA	N	124.766	0.055	1
1	B	401	GLN	H	8.185	0.006	1
1	B	401	GLN	CA	55.273	0.004	1
1	B	401	GLN	CB	28.797	0.002	1
1	B	401	GLN	N	120.373	0.029	1
1	B	402	GLU	H	7.878	0.006	1
1	B	402	GLU	CA	57.612	0.000	1
1	B	402	GLU	CB	30.251	0.000	1
1	B	402	GLU	N	127.843	0.055	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
$^{13}\text{C}_\alpha$	250	0.39 ± 0.08	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	211	0.74 ± 0.19	Should be applied
$^{13}\text{C}'$	0	—	None (insufficient data)
^{15}N	215	0.13 ± 0.28	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 28%, i.e. 868 atoms were assigned a chemical shift out of a possible 3128. 0 out of 37 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	582/1209 (48%)	184/496 (37%)	214/484 (44%)	184/229 (80%)
Sidechain	282/1654 (17%)	99/1086 (9%)	183/522 (35%)	0/46 (0%)
Aromatic	4/265 (2%)	2/131 (2%)	0/120 (0%)	2/14 (14%)
Overall	868/3128 (28%)	285/1713 (17%)	397/1126 (35%)	186/289 (64%)

7.1.4 Statistically unusual chemical shifts ⓘ

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	268	GLU	CB	38.91	21.56 – 38.37	5.3

7.1.5 Random Coil Index (RCI) plots ⓘ

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:

