



Full wwPDB NMR Structure Validation Report ⓘ

Mar 7, 2026 – 02:42 AM UTC

PDB ID : 6TL0 / pdb_00006tl0
BMRB ID : 34461
Title : Solution structure and ¹H, ¹³C and ¹⁵N chemical shift assignments for the complex of VPS29 with VARP 687-747
Authors : Owen, D.J.; Neuhaus, D.; Yang, J.-C.; Crawley-Snowdon, H.
Deposited on : 2019-11-29

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

<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

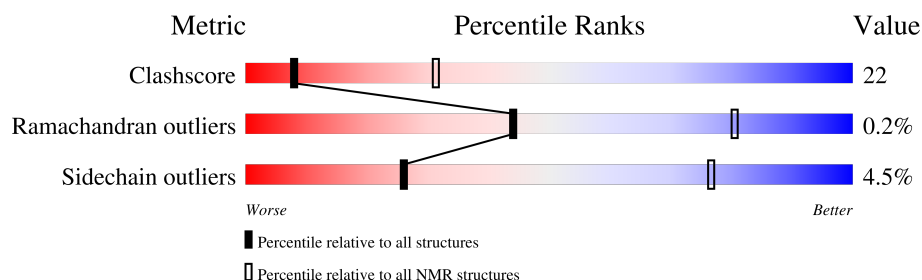
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 73%.

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	192	
2	B	61	

2 Ensemble composition and analysis

This entry contains 25 models. Model 11 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:0-A:181, B:712-B:714 (185)	0.11	11

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 4 single-model clusters were found.

Cluster number	Models
1	2, 6, 7, 13, 15, 19, 20, 23, 24, 25
2	3, 8, 11, 14, 16, 17, 21
3	5, 12
4	1, 4
Single-model clusters	9; 10; 18; 22

3 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 3902 atoms, of which 1937 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Vacuolar protein sorting-associated protein 29.

Mol	Chain	Residues	Atoms						Trace
1	A	192	Total	C	H	N	O	S	0
			3051	980	1527	258	280	6	

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-9	GLY	-	expression tag	UNP Q9QZ88
A	-8	SER	-	expression tag	UNP Q9QZ88
A	-7	PRO	-	expression tag	UNP Q9QZ88
A	-6	GLU	-	expression tag	UNP Q9QZ88
A	-5	PHE	-	expression tag	UNP Q9QZ88
A	-4	GLY	-	expression tag	UNP Q9QZ88
A	-3	THR	-	expression tag	UNP Q9QZ88
A	-2	ARG	-	expression tag	UNP Q9QZ88
A	-1	ASP	-	expression tag	UNP Q9QZ88
A	0	ARG	-	expression tag	UNP Q9QZ88

- Molecule 2 is a protein called Ankyrin repeat domain-containing protein 27.

Mol	Chain	Residues	Atoms						Trace
2	B	61	Total	C	H	N	O	S	0
			850	267	410	74	95	4	

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	687	GLY	-	expression tag	UNP Q96NW4
B	688	PRO	-	expression tag	UNP Q96NW4
B	689	LEU	-	expression tag	UNP Q96NW4
B	690	GLY	-	expression tag	UNP Q96NW4
B	691	SER	-	expression tag	UNP Q96NW4
B	747	TRP	-	expression tag	UNP Q96NW4

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

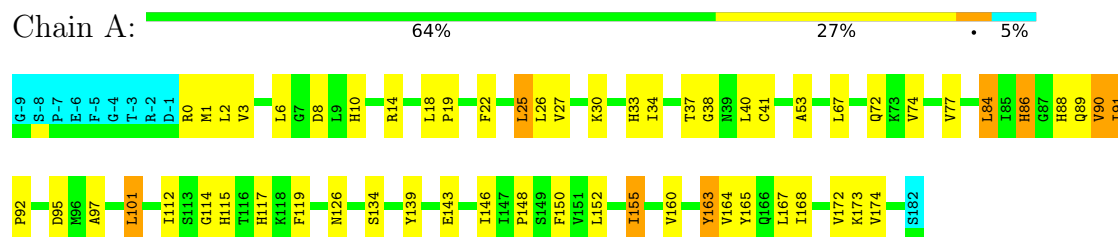
Mol	Chain	Residues	Atoms	
3	B	1	Total	Zn
			1	1

4 Residue-property plots

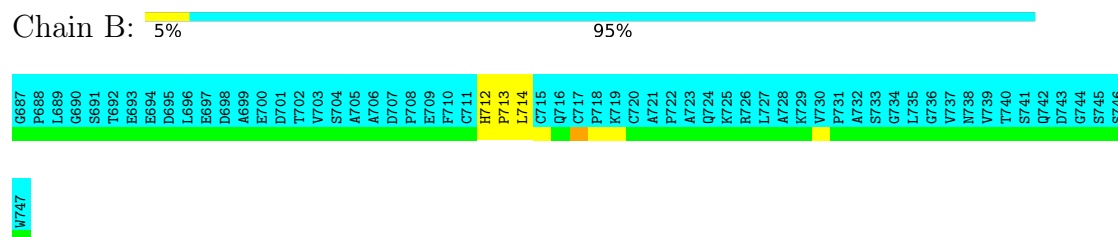
4.1 Average score per residue in the NMR ensemble

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: Vacuolar protein sorting-associated protein 29



- Molecule 2: Ankyrin repeat domain-containing protein 27

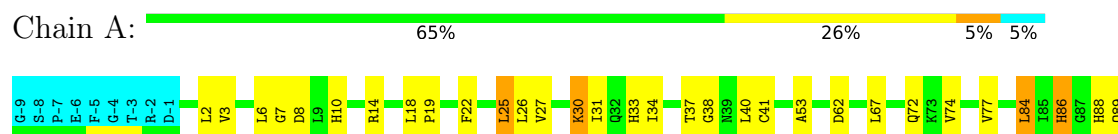


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

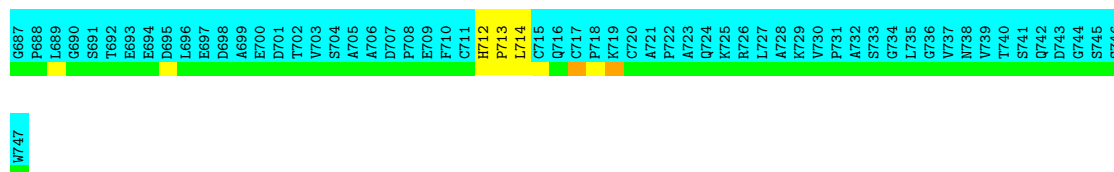
- Molecule 1: Vacuolar protein sorting-associated protein 29





- Molecule 2: Ankyrin repeat domain-containing protein 27

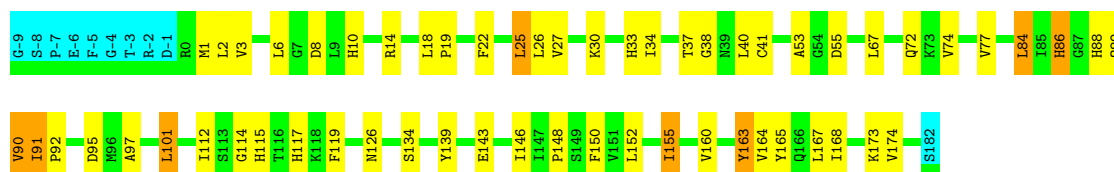
Chain B: 5% 95%



4.2.2 Score per residue for model 2

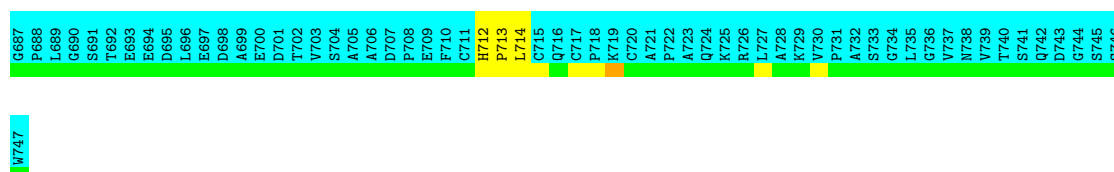
- Molecule 1: Vacuolar protein sorting-associated protein 29

Chain A: 65% 26% 5%



- Molecule 2: Ankyrin repeat domain-containing protein 27

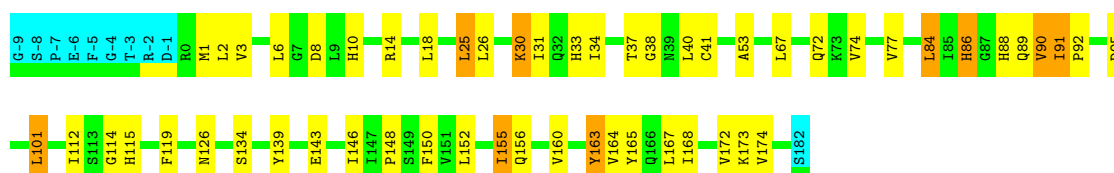
Chain B: 5% 95%



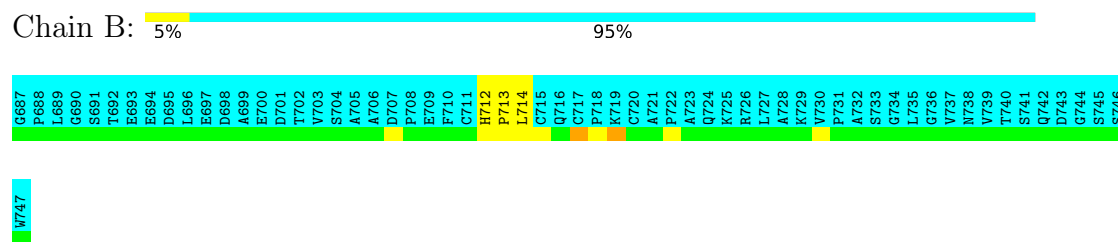
4.2.3 Score per residue for model 3

- Molecule 1: Vacuolar protein sorting-associated protein 29

Chain A: 66% 24% 5% 5%

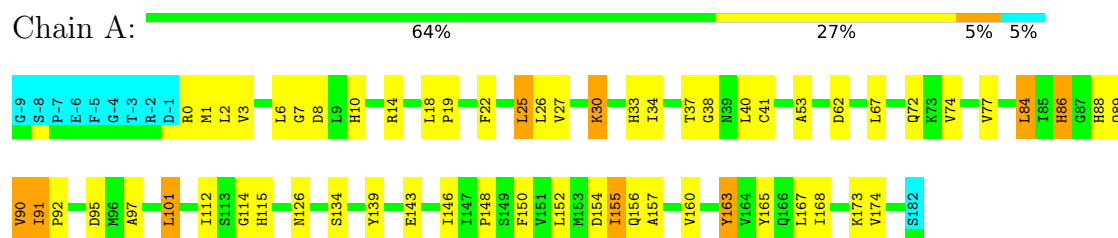


- Molecule 2: Ankyrin repeat domain-containing protein 27

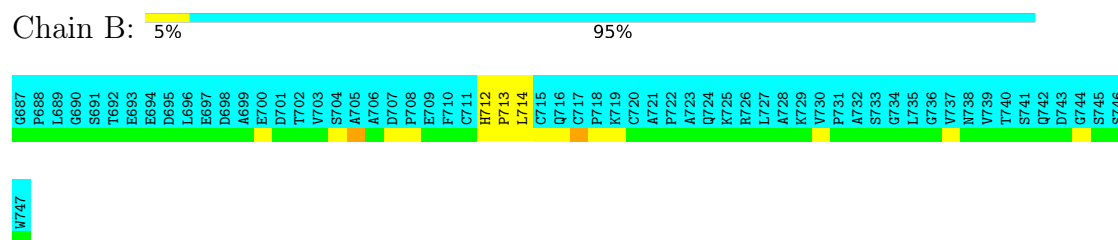


4.2.4 Score per residue for model 4

- Molecule 1: Vacuolar protein sorting-associated protein 29

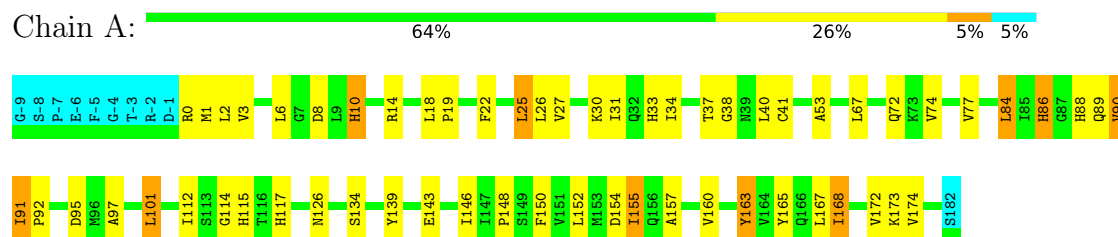


- Molecule 2: Ankyrin repeat domain-containing protein 27

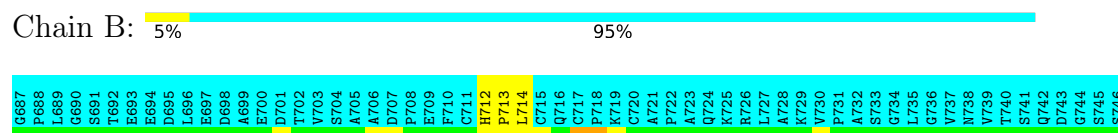


4.2.5 Score per residue for model 5

- Molecule 1: Vacuolar protein sorting-associated protein 29



- Molecule 2: Ankyrin repeat domain-containing protein 27

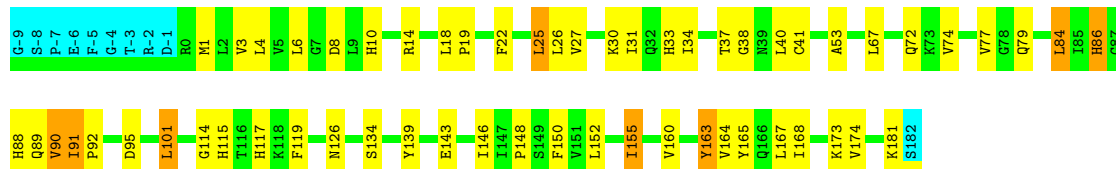


W747

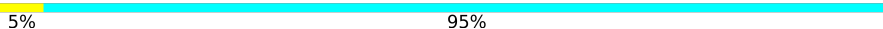
4.2.6 Score per residue for model 6

- Molecule 1: Vacuolar protein sorting-associated protein 29

Chain A:  65% 26% 5%



- Molecule 2: Ankyrin repeat domain-containing protein 27

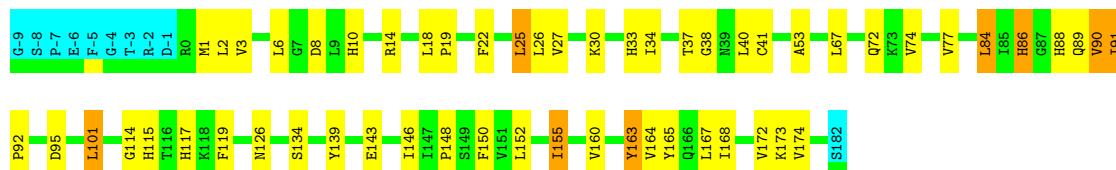
Chain B:  5% 95%



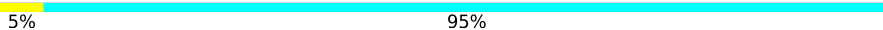
4.2.7 Score per residue for model 7

- Molecule 1: Vacuolar protein sorting-associated protein 29

Chain A:  66% 25% 5%



- Molecule 2: Ankyrin repeat domain-containing protein 27

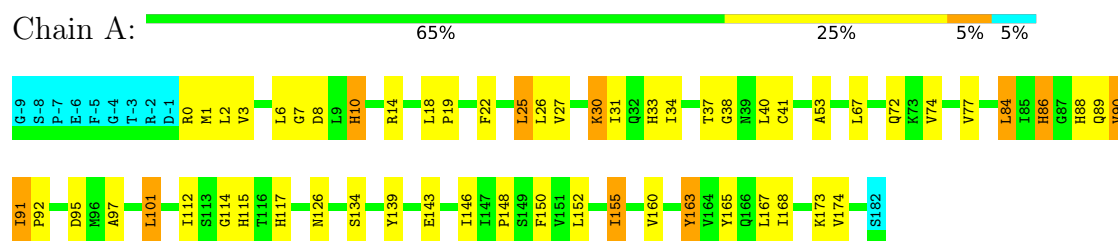
Chain B:  5% 95%



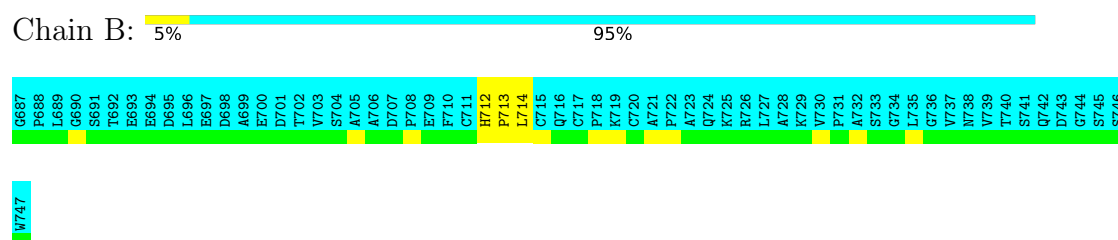
W747

4.2.8 Score per residue for model 8

- Molecule 1: Vacuolar protein sorting-associated protein 29

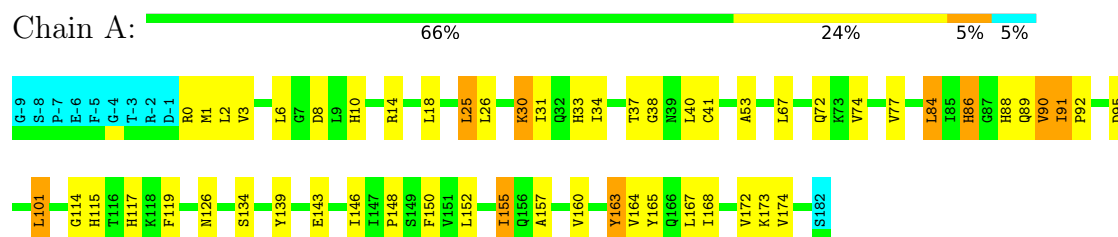


- Molecule 2: Ankyrin repeat domain-containing protein 27

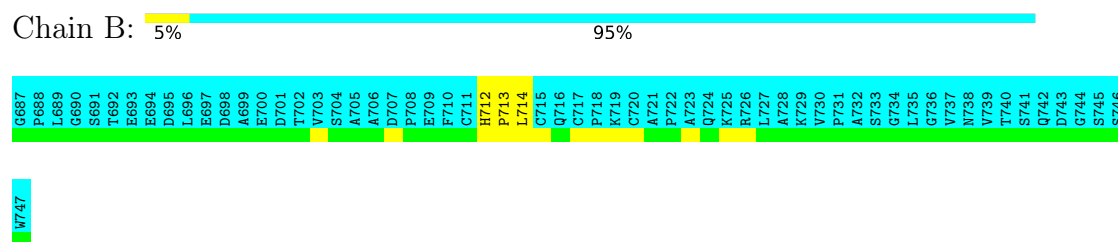


4.2.9 Score per residue for model 9

- Molecule 1: Vacuolar protein sorting-associated protein 29

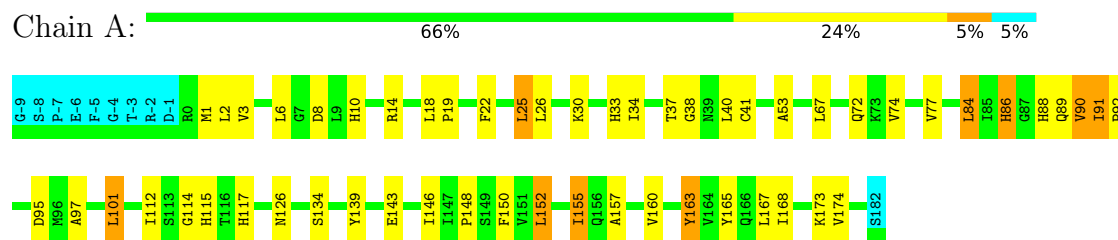


- Molecule 2: Ankyrin repeat domain-containing protein 27

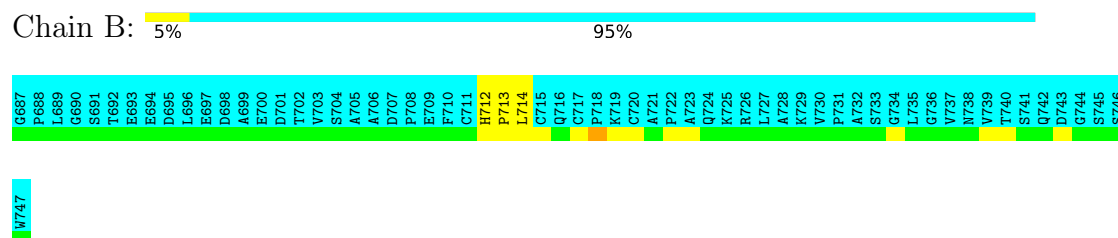


4.2.10 Score per residue for model 10

- Molecule 1: Vacuolar protein sorting-associated protein 29

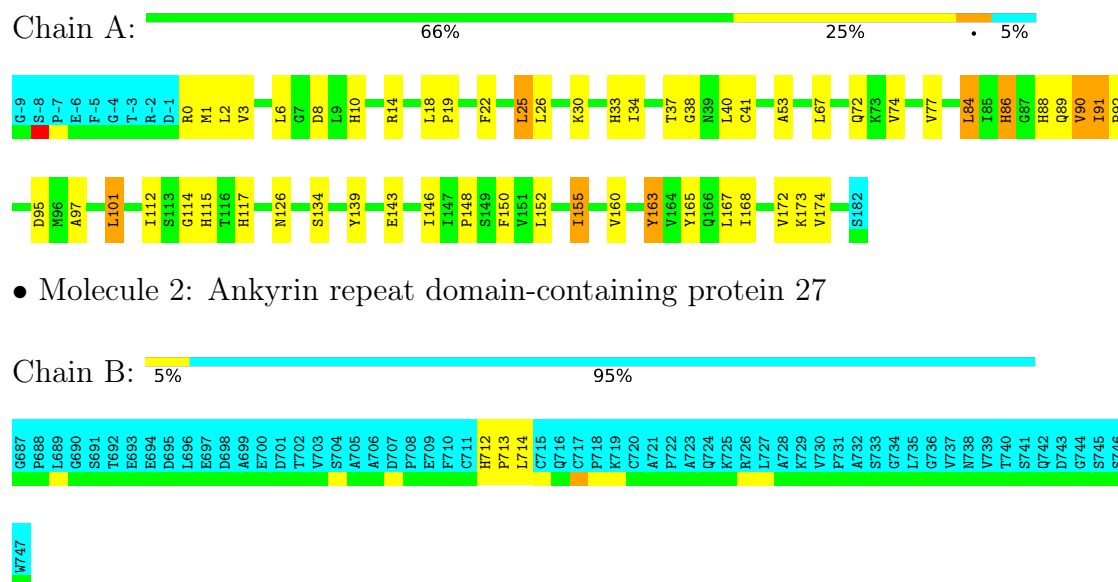


- Molecule 2: Ankyrin repeat domain-containing protein 27



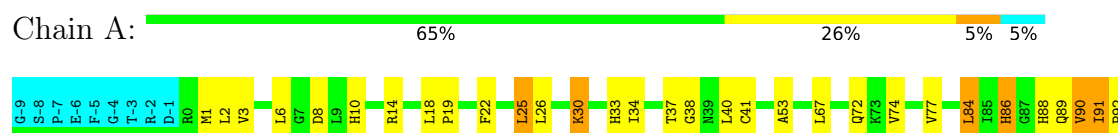
4.2.11 Score per residue for model 11 (medoid)

- Molecule 1: Vacuolar protein sorting-associated protein 29



4.2.12 Score per residue for model 12

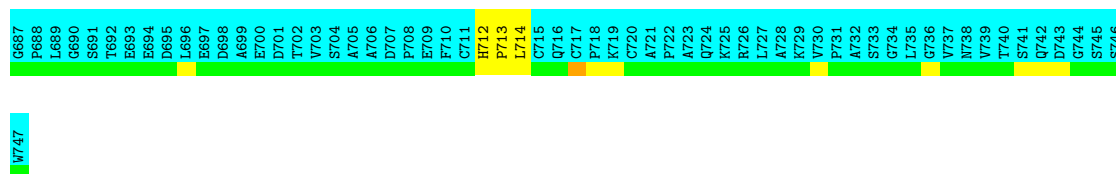
- Molecule 1: Vacuolar protein sorting-associated protein 29





- Molecule 2: Ankyrin repeat domain-containing protein 27

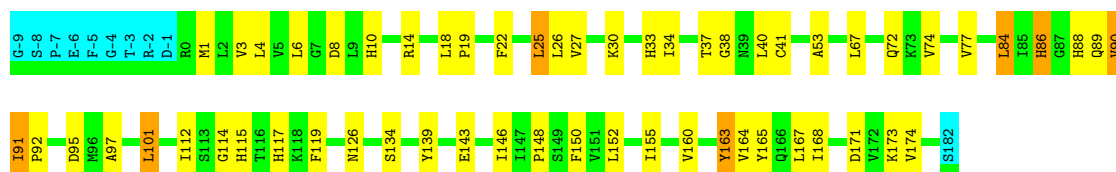
Chain B: 5% 95%



4.2.13 Score per residue for model 13

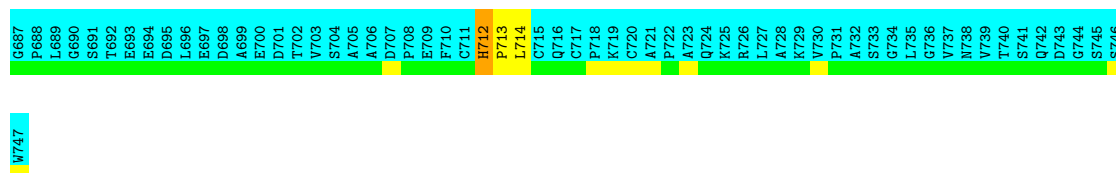
- Molecule 1: Vacuolar protein sorting-associated protein 29

Chain A: 65% 27% 5%



- Molecule 2: Ankyrin repeat domain-containing protein 27

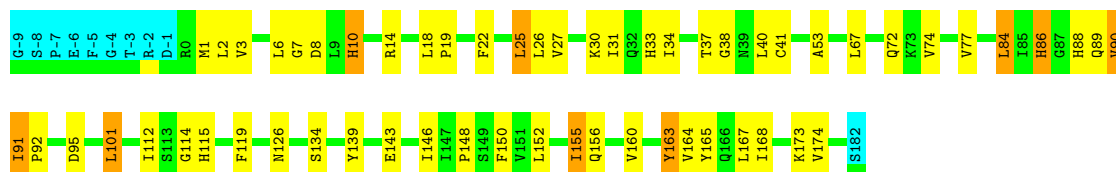
Chain B: 95%



4.2.14 Score per residue for model 14

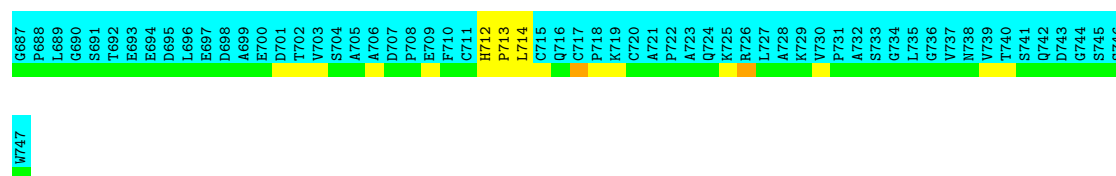
- Molecule 1: Vacuolar protein sorting-associated protein 29

Chain A: 65% 26% 5% 5%



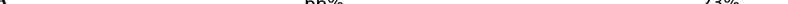
- Molecule 2: Ankyrin repeat domain-containing protein 27

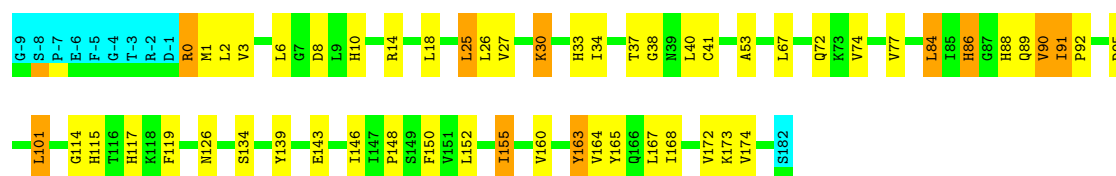
Chain B:  5% 95%



4.2.15 Score per residue for model 15

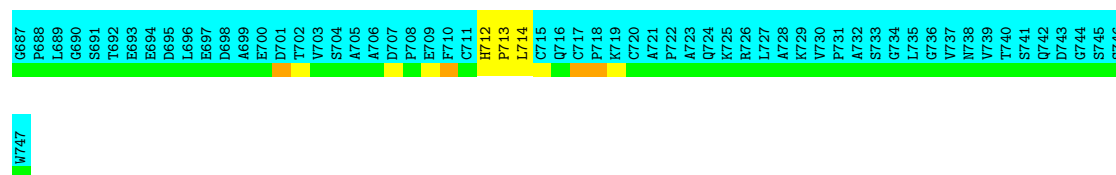
- Molecule 1: Vacuolar protein sorting-associated protein 29

Chain A:  66% 23% 5% 5%



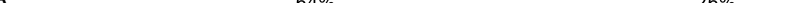
- Molecule 2: Ankyrin repeat domain-containing protein 27

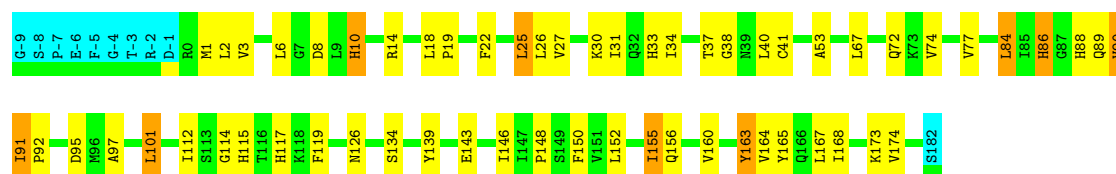
Chain B: 5% 95%



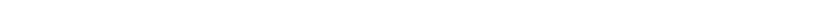
4.2.16 Score per residue for model 16

- Molecule 1: Vacuolar protein sorting-associated protein 29

Chain A: 



- Molecule 2: Ankyrin repeat domain-containing protein 27

Chain B:  5% 95%

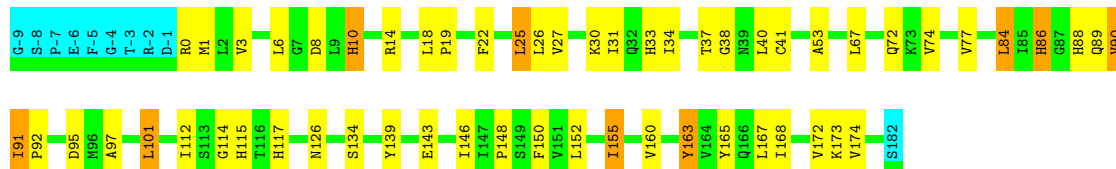


W747

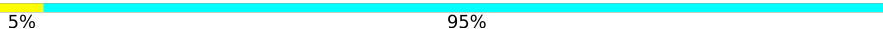
4.2.17 Score per residue for model 17

- Molecule 1: Vacuolar protein sorting-associated protein 29

Chain A: 



- Molecule 2: Ankyrin repeat domain-containing protein 27

Chain B: 

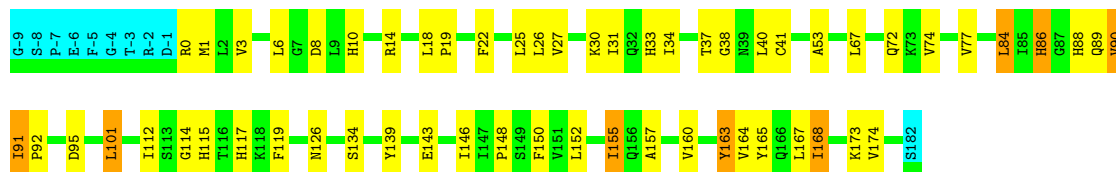


W747

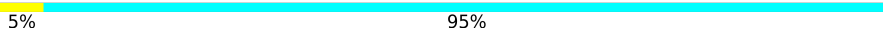
4.2.18 Score per residue for model 18

- Molecule 1: Vacuolar protein sorting-associated protein 29

Chain A: 



- Molecule 2: Ankyrin repeat domain-containing protein 27

Chain B: 

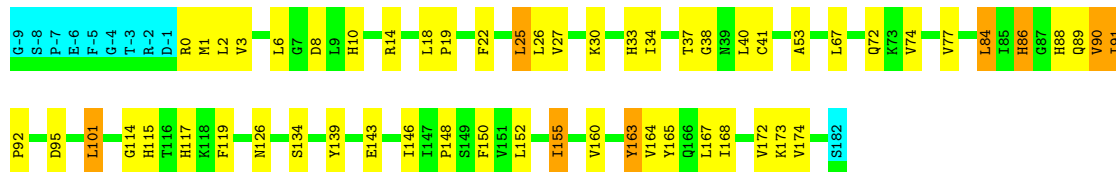


W747

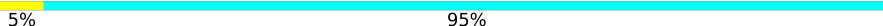
4.2.19 Score per residue for model 19

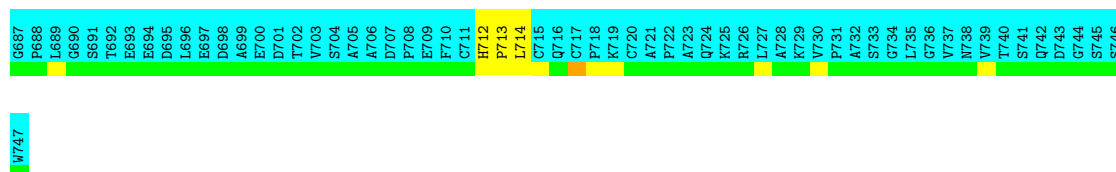
- Molecule 1: Vacuolar protein sorting-associated protein 29

Chain A: 



- Molecule 2: Ankyrin repeat domain-containing protein 27

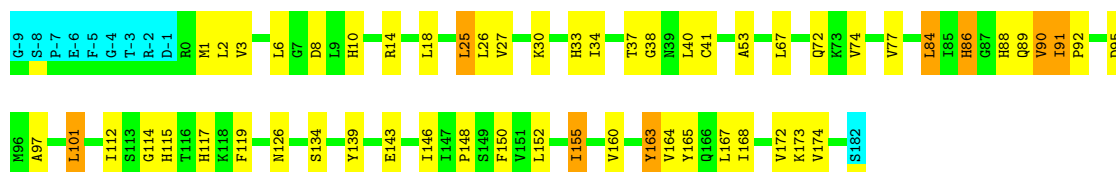
Chain B: 



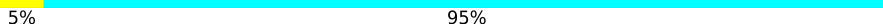
4.2.20 Score per residue for model 20

- Molecule 1: Vacuolar protein sorting-associated protein 29

Chain A: 



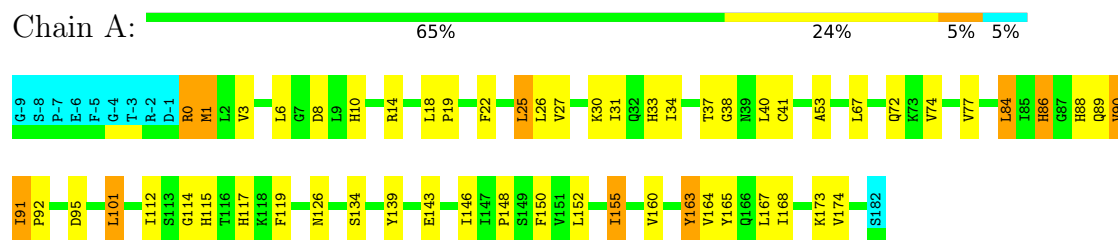
- Molecule 2: Ankyrin repeat domain-containing protein 27

Chain B: 

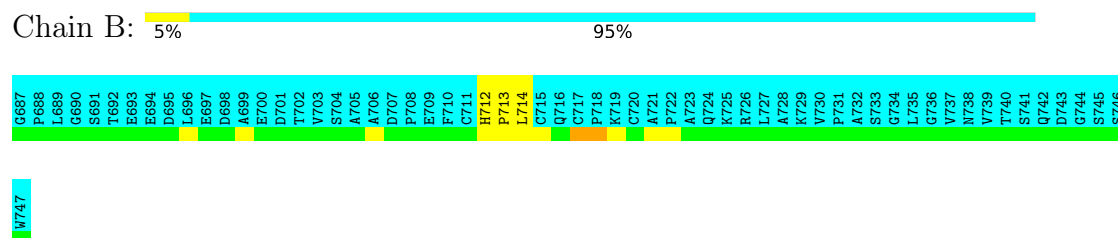


4.2.21 Score per residue for model 21

- Molecule 1: Vacuolar protein sorting-associated protein 29

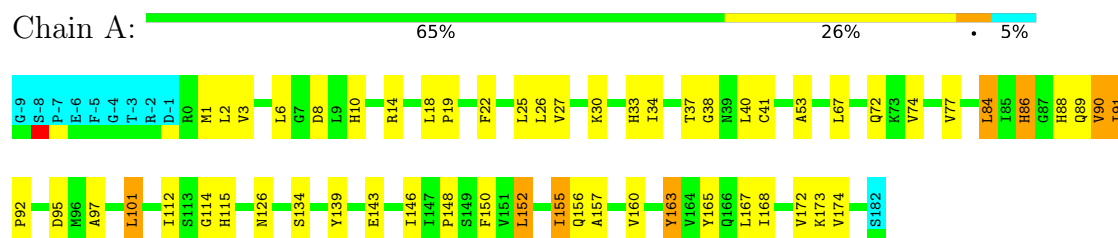


- Molecule 2: Ankyrin repeat domain-containing protein 27

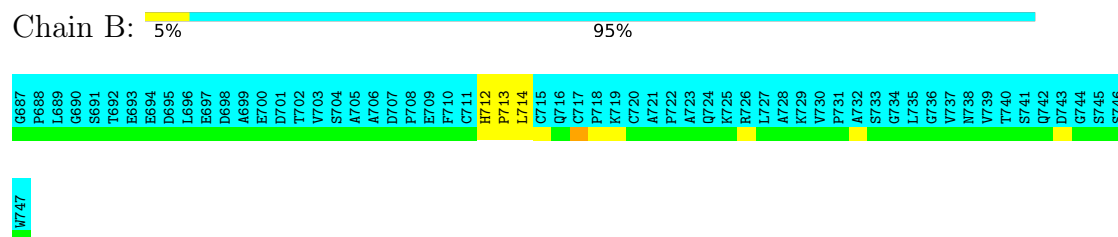


4.2.22 Score per residue for model 22

- Molecule 1: Vacuolar protein sorting-associated protein 29

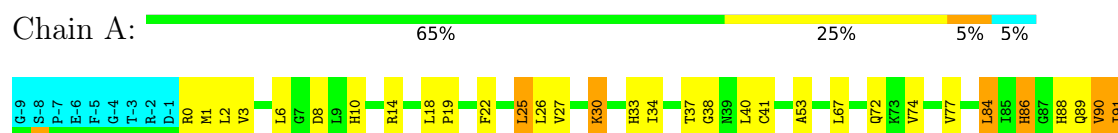


- Molecule 2: Ankyrin repeat domain-containing protein 27



4.2.23 Score per residue for model 23

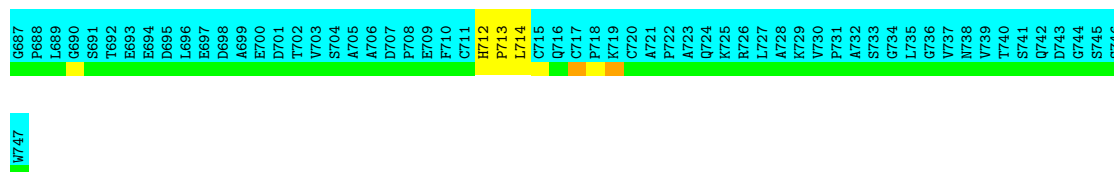
- Molecule 1: Vacuolar protein sorting-associated protein 29





- Molecule 2: Ankyrin repeat domain-containing protein 27

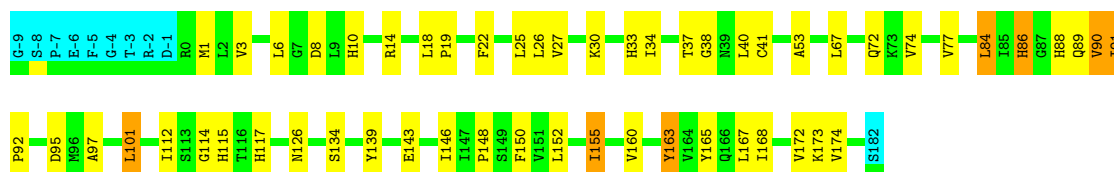
Chain B: 5% 95%



4.2.24 Score per residue for model 24

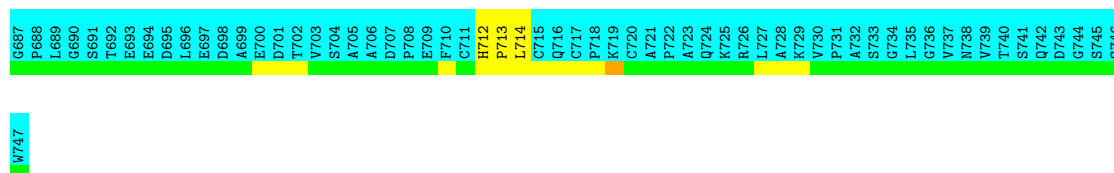
- Molecule 1: Vacuolar protein sorting-associated protein 29

Chain A: 66% 25% 5%



- Molecule 2: Ankyrin repeat domain-containing protein 27

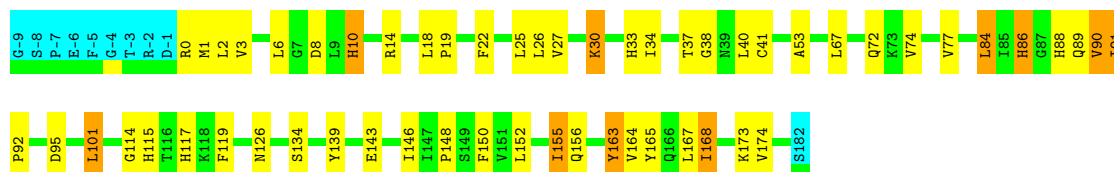
Chain B: 5% 95%



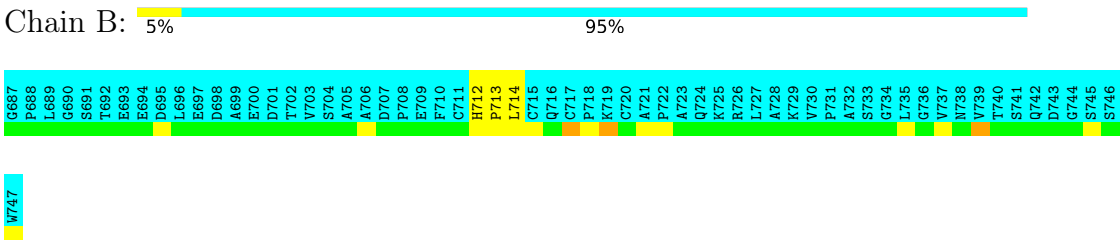
4.2.25 Score per residue for model 25

- Molecule 1: Vacuolar protein sorting-associated protein 29

Chain A: 66% 24% 5% 5%



- Molecule 2: Ankyrin repeat domain-containing protein 27



5 Refinement protocol and experimental data overview

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

Of the 50 calculated structures, 25 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
X-PLOR NIH	structure calculation	2.28

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	2436
Number of shifts mapped to atoms	2436
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	73%

6 Model quality [i](#)

6.1 Standard geometry [i](#)

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

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	1.46±0.00	0±0/1484 (0.0± 0.0%)	1.64±0.00	6±1/2013 (0.3± 0.0%)
2	B	1.28±0.03	0±0/27 (0.0± 0.0%)	1.60±0.05	0±0/38 (0.0± 0.0%)
All	All	1.46	0/37775 (0.0%)	1.64	161/51275 (0.3%)

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
1	A	77	VAL	N-CA-CB	-6.41	104.90	112.40	18	25
1	A	91	ILE	N-CA-CB	-6.33	104.83	111.61	15	25
1	A	86	HIS	CA-CB-CG	-6.22	107.58	113.80	9	25
1	A	155	ILE	N-CA-CB	-5.84	104.54	111.90	4	24
1	A	31	ILE	N-CA-CB	-5.66	104.55	110.72	18	2
1	A	74	VAL	N-CA-CB	-5.42	104.83	111.67	5	25
1	A	90	VAL	N-CA-CB	-5.30	104.78	111.41	17	25
1	A	168	ILE	N-CA-CB	-5.10	105.24	111.21	18	3
1	A	172	VAL	N-CA-CB	-5.08	104.90	110.99	3	1
1	A	10	HIS	CA-CB-CG	-5.05	108.75	113.80	25	6

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	1450	1463	1463	63±3
2	B	25	25	25	15±2
All	All	36900	37200	37200	1642

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 22.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:152:LEU:HD11	2:B:714:LEU:HD22	1.08	1.14	1	11
1:A:30:LYS:HE2	2:B:714:LEU:HD23	0.83	1.50	7	13
1:A:152:LEU:HD11	2:B:714:LEU:HD12	0.81	1.50	12	9
1:A:37:THR:HG22	1:A:84:LEU:HD21	0.81	1.50	2	25
1:A:152:LEU:CD1	2:B:714:LEU:HD22	0.81	2.03	1	10
1:A:152:LEU:HD11	2:B:714:LEU:CD2	0.80	2.06	24	9
1:A:26:LEU:HD23	2:B:714:LEU:HD23	0.80	1.53	16	10
1:A:26:LEU:HD23	2:B:714:LEU:HD13	0.79	1.53	21	12
1:A:163:TYR:CE1	2:B:712:HIS:HB3	0.79	2.13	7	25
1:A:25:LEU:HD23	2:B:714:LEU:HB3	0.78	1.55	5	9
1:A:152:LEU:HD11	2:B:714:LEU:CD1	0.77	2.09	21	11
1:A:25:LEU:O	2:B:714:LEU:HB3	0.75	1.82	15	22
1:A:37:THR:HG22	1:A:84:LEU:CD2	0.74	2.12	20	25
2:B:712:HIS:HB2	2:B:713:PRO:HD2	0.74	1.57	10	25
1:A:152:LEU:HD21	2:B:714:LEU:CD1	0.74	2.13	10	2
1:A:92:PRO:HG2	1:A:95:ASP:HB2	0.72	1.60	14	25
1:A:67:LEU:HD23	1:A:67:LEU:O	0.71	1.85	9	25
1:A:26:LEU:HD23	2:B:714:LEU:CD1	0.70	2.15	20	13
1:A:38:GLY:HA2	1:A:86:HIS:CD2	0.70	2.22	24	25
1:A:31:ILE:HD11	2:B:714:LEU:HD21	0.70	1.63	5	9
1:A:152:LEU:HD12	1:A:165:TYR:CE2	0.69	2.23	9	17
1:A:150:PHE:CZ	1:A:165:TYR:CD2	0.69	2.81	10	21
1:A:26:LEU:HD23	2:B:714:LEU:CD2	0.68	2.18	13	10
1:A:152:LEU:HD12	1:A:165:TYR:CE1	0.68	2.23	1	4
1:A:25:LEU:HD22	1:A:150:PHE:HZ	0.68	1.49	5	17
1:A:0:ARG:HA	1:A:155:ILE:O	0.66	1.91	21	10
1:A:101:LEU:HD12	1:A:101:LEU:O	0.66	1.90	12	25
1:A:25:LEU:HD12	1:A:25:LEU:O	0.66	1.90	25	2
1:A:26:LEU:HD23	2:B:714:LEU:HD21	0.64	1.69	24	2
1:A:167:LEU:CD1	1:A:172:VAL:HG12	0.63	2.22	19	3
1:A:26:LEU:CD2	2:B:714:LEU:HD23	0.63	2.23	8	8

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:713:PRO:O	2:B:714:LEU:HB2	0.63	1.92	24	17
1:A:167:LEU:HD12	1:A:172:VAL:HG12	0.63	1.70	5	3
1:A:163:TYR:CE1	2:B:712:HIS:CB	0.62	2.83	13	25
1:A:150:PHE:CZ	1:A:165:TYR:CD1	0.61	2.88	13	4
1:A:168:ILE:HD12	1:A:173:LYS:HD2	0.61	1.72	2	25
1:A:150:PHE:CE1	1:A:165:TYR:CD2	0.61	2.88	20	21
1:A:30:LYS:HG2	2:B:714:LEU:CD2	0.61	2.25	21	2
1:A:167:LEU:HD12	1:A:172:VAL:HG22	0.60	1.72	20	6
1:A:167:LEU:CD1	1:A:172:VAL:HG22	0.60	2.26	20	10
1:A:25:LEU:HD23	2:B:714:LEU:CB	0.60	2.26	3	14
1:A:91:ILE:N	1:A:91:ILE:HD12	0.60	2.12	13	25
1:A:148:PRO:HG2	1:A:167:LEU:HB3	0.60	1.74	20	24
1:A:90:VAL:C	1:A:91:ILE:HD12	0.59	2.22	22	25
1:A:25:LEU:HD23	2:B:714:LEU:HB2	0.59	1.74	15	8
1:A:25:LEU:HD22	1:A:150:PHE:CZ	0.59	2.32	5	4
1:A:152:LEU:HD21	2:B:714:LEU:HD11	0.59	1.72	10	2
1:A:6:LEU:HD23	1:A:6:LEU:N	0.58	2.14	11	25
1:A:8:ASP:N	1:A:38:GLY:HA3	0.57	2.15	4	21
1:A:3:VAL:HG22	1:A:33:HIS:HB2	0.56	1.78	11	25
1:A:0:ARG:HG2	1:A:156:GLN:HG2	0.56	1.78	23	1
1:A:37:THR:HG21	1:A:112:ILE:HG22	0.55	1.78	1	18
1:A:0:ARG:HG2	1:A:156:GLN:OE1	0.55	2.01	23	1
1:A:30:LYS:CE	2:B:714:LEU:HD23	0.55	2.30	18	8
1:A:2:LEU:HD21	2:B:713:PRO:HB2	0.55	1.76	10	19
1:A:8:ASP:H	1:A:38:GLY:HA3	0.55	1.62	2	25
1:A:30:LYS:HE2	2:B:714:LEU:HD12	0.55	1.78	13	10
1:A:150:PHE:CE1	1:A:165:TYR:CD1	0.54	2.95	1	3
1:A:114:GLY:O	1:A:115:HIS:HB3	0.54	2.02	2	25
1:A:0:ARG:CA	1:A:155:ILE:O	0.53	2.57	25	1
1:A:152:LEU:HD12	1:A:165:TYR:HE2	0.53	1.63	2	11
1:A:152:LEU:HD12	1:A:165:TYR:OH	0.53	2.04	6	3
1:A:25:LEU:HD23	2:B:714:LEU:O	0.53	2.04	19	7
1:A:26:LEU:CD2	2:B:714:LEU:HD13	0.52	2.33	4	2
1:A:18:LEU:HD12	1:A:18:LEU:H	0.52	1.64	10	25
1:A:152:LEU:HD12	1:A:165:TYR:HE1	0.52	1.62	1	3
1:A:34:ILE:CD1	1:A:53:ALA:HB3	0.52	2.35	6	25
1:A:163:TYR:CD1	1:A:174:VAL:CG2	0.52	2.93	20	25
1:A:163:TYR:CD1	2:B:712:HIS:CB	0.51	2.93	20	3
1:A:2:LEU:HD11	1:A:152:LEU:HD12	0.51	1.82	23	2
2:B:714:LEU:CD1	2:B:714:LEU:N	0.51	2.74	3	10
1:A:30:LYS:HG2	2:B:714:LEU:HD23	0.51	1.82	21	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:155:ILE:HG12	1:A:160:VAL:HG23	0.50	1.83	5	22
1:A:152:LEU:HD13	2:B:713:PRO:HB2	0.50	1.83	13	4
1:A:0:ARG:HG3	1:A:155:ILE:C	0.50	2.31	5	1
1:A:40:LEU:HB2	1:A:41:CYS:HA	0.50	1.84	2	25
1:A:155:ILE:CG1	1:A:160:VAL:HG23	0.50	2.36	4	24
1:A:40:LEU:CB	1:A:41:CYS:CA	0.49	2.90	1	25
1:A:152:LEU:HD13	2:B:713:PRO:HG2	0.49	1.84	20	3
1:A:25:LEU:HD12	2:B:714:LEU:O	0.48	2.07	24	2
1:A:150:PHE:CE1	1:A:165:TYR:CE2	0.48	3.01	22	11
1:A:25:LEU:CD1	2:B:714:LEU:HB3	0.48	2.38	24	1
1:A:88:HIS:CE1	1:A:89:GLN:CD	0.48	2.90	11	25
2:B:713:PRO:O	2:B:714:LEU:CB	0.48	2.61	18	10
1:A:101:LEU:HD12	1:A:101:LEU:C	0.48	2.33	6	25
1:A:18:LEU:HD12	1:A:18:LEU:N	0.47	2.23	10	25
1:A:91:ILE:HA	1:A:92:PRO:C	0.47	2.34	1	25
1:A:37:THR:CG2	1:A:84:LEU:HD21	0.47	2.37	6	15
1:A:119:PHE:CE2	1:A:164:VAL:CG2	0.47	2.98	6	16
1:A:37:THR:CG2	1:A:112:ILE:HG22	0.47	2.39	1	5
1:A:152:LEU:HD13	2:B:714:LEU:HD13	0.46	1.86	13	1
1:A:26:LEU:C	1:A:27:VAL:HG13	0.46	2.35	1	19
1:A:25:LEU:HD23	1:A:150:PHE:CE2	0.46	2.45	18	2
1:A:38:GLY:HA2	1:A:86:HIS:NE2	0.46	2.24	4	11
1:A:119:PHE:CD2	1:A:164:VAL:HG21	0.46	2.46	6	4
1:A:92:PRO:CG	1:A:95:ASP:HB2	0.46	2.37	14	25
2:B:713:PRO:C	2:B:714:LEU:HG	0.46	2.36	18	10
1:A:4:LEU:HD13	1:A:152:LEU:HD21	0.46	1.87	13	1
1:A:114:GLY:O	1:A:115:HIS:CB	0.46	2.64	1	25
1:A:6:LEU:N	1:A:6:LEU:CD2	0.45	2.79	11	25
1:A:150:PHE:HE1	1:A:152:LEU:CD2	0.45	2.24	23	3
1:A:19:PRO:HG2	1:A:22:PHE:HB2	0.45	1.87	2	20
1:A:143:GLU:HB3	1:A:146:ILE:HD11	0.45	1.89	8	25
1:A:91:ILE:N	1:A:91:ILE:CD1	0.45	2.80	25	25
1:A:134:SER:O	1:A:148:PRO:HA	0.44	2.12	13	25
1:A:150:PHE:CD1	1:A:150:PHE:C	0.44	2.96	18	9
1:A:0:ARG:NH1	1:A:154:ASP:OD2	0.44	2.51	4	1
1:A:163:TYR:CD1	2:B:712:HIS:HB3	0.44	2.48	7	2
1:A:40:LEU:CB	1:A:41:CYS:HA	0.43	2.43	1	25
2:B:714:LEU:HD12	2:B:714:LEU:N	0.43	2.28	13	1
1:A:4:LEU:CD1	1:A:152:LEU:CD2	0.43	2.97	6	1
1:A:25:LEU:CD2	2:B:714:LEU:HB2	0.43	2.44	19	1
1:A:2:LEU:CD1	1:A:152:LEU:HD12	0.43	2.42	23	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:152:LEU:HD12	1:A:165:TYR:CZ	0.43	2.48	9	2
1:A:150:PHE:HE1	1:A:152:LEU:HD23	0.43	1.74	22	2
1:A:0:ARG:CG	1:A:156:GLN:OE1	0.43	2.67	23	1
1:A:150:PHE:CE1	1:A:165:TYR:CE1	0.42	3.06	13	2
1:A:33:HIS:CE1	1:A:55:ASP:OD2	0.42	2.72	2	1
1:A:119:PHE:CE2	1:A:164:VAL:HG21	0.42	2.49	6	1
1:A:67:LEU:O	1:A:67:LEU:CD2	0.42	2.64	1	25
1:A:174:VAL:HG21	2:B:712:HIS:CD2	0.42	2.49	5	2
1:A:126:ASN:OD1	1:A:126:ASN:N	0.42	2.53	1	25
1:A:152:LEU:HD21	2:B:714:LEU:HD12	0.42	1.87	10	1
1:A:25:LEU:CD1	2:B:714:LEU:O	0.42	2.68	18	1
1:A:4:LEU:CD1	1:A:152:LEU:HD21	0.42	2.45	6	1
1:A:4:LEU:HD12	1:A:152:LEU:CD2	0.42	2.44	6	1
1:A:10:HIS:CD2	1:A:14:ARG:CZ	0.42	3.03	7	25
1:A:2:LEU:HG	1:A:152:LEU:HD12	0.42	1.90	10	1
1:A:30:LYS:CE	2:B:714:LEU:HD12	0.42	2.44	13	1
1:A:40:LEU:HB2	1:A:41:CYS:CA	0.42	2.44	15	8
1:A:119:PHE:CD2	1:A:164:VAL:CG2	0.41	3.03	6	5
1:A:25:LEU:CD2	2:B:714:LEU:HB3	0.41	2.44	13	1
1:A:25:LEU:CD2	2:B:714:LEU:O	0.41	2.68	16	1
1:A:152:LEU:HD11	2:B:714:LEU:CG	0.41	2.45	21	1
1:A:25:LEU:HD12	2:B:714:LEU:HB3	0.41	1.91	24	1
1:A:119:PHE:CE2	1:A:164:VAL:HB	0.41	2.50	25	2
1:A:2:LEU:CG	1:A:152:LEU:HD12	0.41	2.45	10	1
1:A:40:LEU:N	1:A:41:CYS:HA	0.41	2.29	15	4
1:A:0:ARG:HG2	1:A:156:GLN:CG	0.41	2.44	23	1
1:A:0:ARG:CB	1:A:156:GLN:HA	0.41	2.46	25	1
1:A:30:LYS:HB3	2:B:714:LEU:CD2	0.41	2.46	25	1
1:A:19:PRO:HG2	1:A:22:PHE:CG	0.41	2.51	22	2
1:A:7:GLY:O	1:A:8:ASP:HB2	0.40	2.16	1	4
1:A:117:HIS:CD2	1:A:117:HIS:N	0.40	2.88	25	21
1:A:152:LEU:HD23	1:A:165:TYR:HE2	0.40	1.76	10	1
1:A:2:LEU:HD21	2:B:713:PRO:CB	0.40	2.46	23	1
1:A:0:ARG:CG	1:A:154:ASP:OD1	0.40	2.69	5	1
1:A:79:GLN:O	1:A:181:LYS:HE3	0.40	2.16	6	1
1:A:25:LEU:HD12	1:A:25:LEU:C	0.40	2.38	25	1
1:A:62:ASP:OD1	1:A:86:HIS:CE1	0.40	2.75	1	2
1:A:95:ASP:OD1	1:A:97:ALA:HB3	0.40	2.17	2	13
2:B:714:LEU:N	2:B:714:LEU:CD1	0.40	2.84	13	1

6.3 Torsion angles

6.3.1 Protein backbone

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	182/192 (95%)	175±1 (96±0%)	7±1 (4±0%)	0±0 (0±0%)	44	80
2	B	3/61 (5%)	1±0 (37±11%)	2±0 (63±11%)	0±0 (0±0%)	100	100
All	All	4625/6325 (73%)	4399 (95%)	216 (5%)	10 (0%)	44	80

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	157	ALA	8
1	A	0	ARG	2

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	160/168 (95%)	153±1 (95±0%)	7±1 (5±0%)	25	76
2	B	3/49 (6%)	3±0 (99±7%)	0±0 (1±7%)	59	94
All	All	4075/5425 (75%)	3891 (95%)	184 (5%)	26	77

All 10 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	72	GLN	25
1	A	84	LEU	25
1	A	101	LEU	25
1	A	139	TYR	25
1	A	163	TYR	25

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Mol	Chain	Res	Type	Models (Total)
1	A	1	MET	24
1	A	25	LEU	21
1	A	30	LYS	10
1	A	152	LEU	3
2	B	712	HIS	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](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

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 [i](#)

The completeness of assignment taking into account all chemical shift lists is 73% for the well-defined parts and 72% for the entire structure.

7.1 Chemical shift list 1

File name: `working_cs.cif`

Chemical shift list name: `starch_output`

7.1.1 Bookkeeping [i](#)

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	2436
Number of shifts mapped to atoms	2436
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 [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	245	-0.38 ± 0.05	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	212	0.04 ± 0.14	None needed (< 0.5 ppm)
$^{13}\text{C}'$	0	—	None (insufficient data)
^{15}N	227	-0.19 ± 0.14	None needed (< 0.5 ppm)

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 73%, i.e. 1896 atoms were assigned a chemical shift out of a possible 2589. 0 out of 37 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	707/922 (77%)	357/375 (95%)	180/370 (49%)	170/177 (96%)
Sidechain	1081/1433 (75%)	709/939 (76%)	366/450 (81%)	6/44 (14%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	108/234 (46%)	68/118 (58%)	39/105 (37%)	1/11 (9%)
Overall	1896/2589 (73%)	1134/1432 (79%)	585/925 (63%)	177/232 (76%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 72%, i.e. 2436 atoms were assigned a chemical shift out of a possible 3377. 0 out of 45 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	950/1257 (76%)	478/512 (93%)	245/506 (48%)	227/239 (95%)
Sidechain	1370/1854 (74%)	897/1210 (74%)	463/587 (79%)	10/57 (18%)
Aromatic	116/266 (44%)	73/134 (54%)	41/120 (34%)	2/12 (17%)
Overall	2436/3377 (72%)	1448/1856 (78%)	749/1213 (62%)	239/308 (78%)

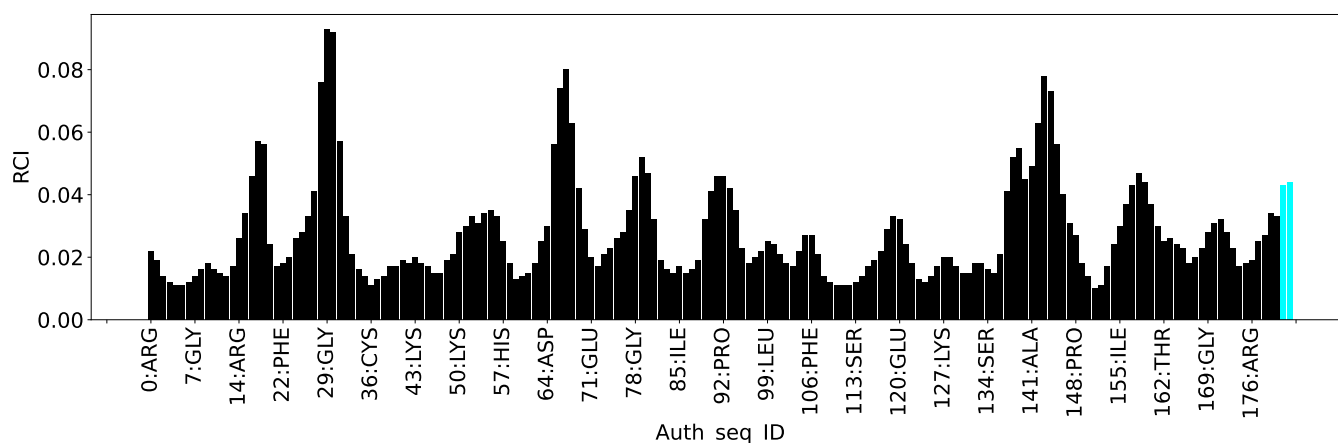
7.1.4 Statistically unusual chemical shifts ⓘ

There are no statistically unusual chemical shifts.

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:

