Full wwPDB NMR Structure Validation Report (i)

Oct 14, 2020 – 02:20 PM BST

PDB ID	:	6TL0
Title	:	Solution structure and 1H, 13C and 15N chemical shift assignments for the complex of VPS29 with VARP 687-747
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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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

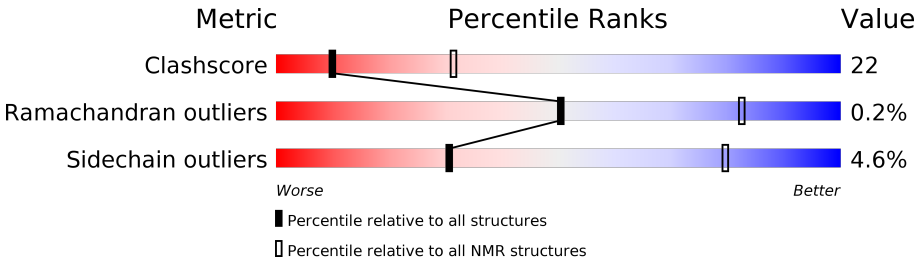
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.14.6
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.14.6

1 Overall quality at a glance (i)

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	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 <=5%

Mol	Chain	Length	Quality of chain
1	A	192	65% 28% • 5%
2	B	61	5% 95%

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)	0.06	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

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 (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	
3	B	1	Total	Zn
			1	1

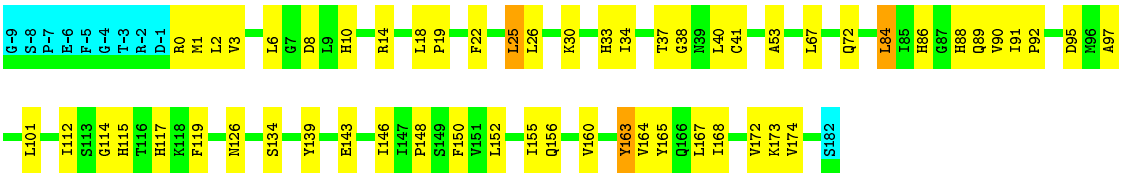
4 Residue-property plots

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.

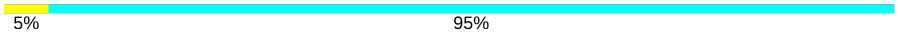
• Molecule 1: Vacuolar protein sorting-associated protein 29

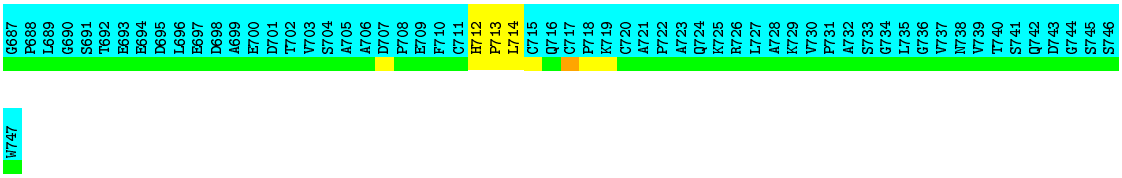
Chain A:



• Molecule 2: Ankyrin repeat domain-containing protein 27

Chain B:





4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

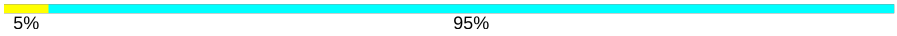
4.2.1 Score per residue for model 1

• Molecule 1: Vacuolar protein sorting-associated protein 29

Chain A:

- Molecule 2: Ankyrin repeat domain-containing protein 27

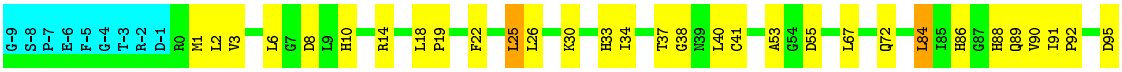
Chain B:

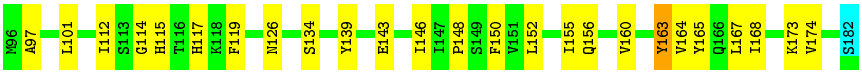


4.2.2 Score per residue for model 2

- Molecule 1: Vacuolar protein sorting-associated protein 29

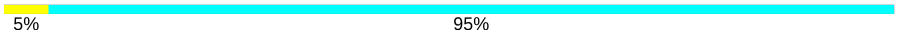
Chain A:





- Molecule 2: Ankyrin repeat domain-containing protein 27

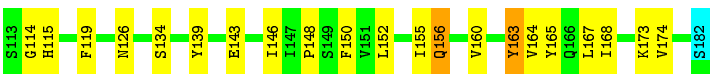
Chain B:



4.2.3 Score per residue for model 3

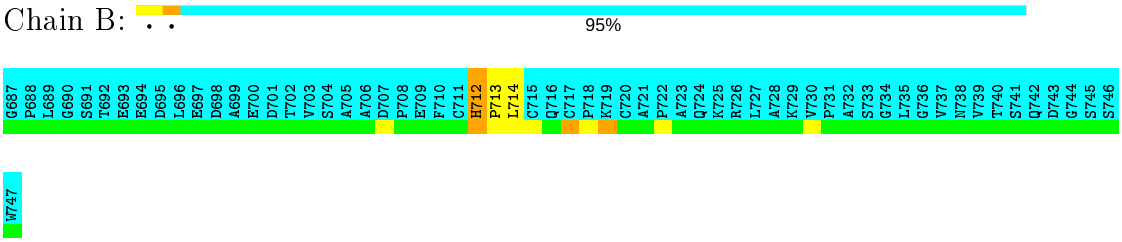
- Molecule 1: Vacuolar protein sorting-associated protein 29

Chain A:



- Molecule 2: Ankyrin repeat domain-containing protein 27

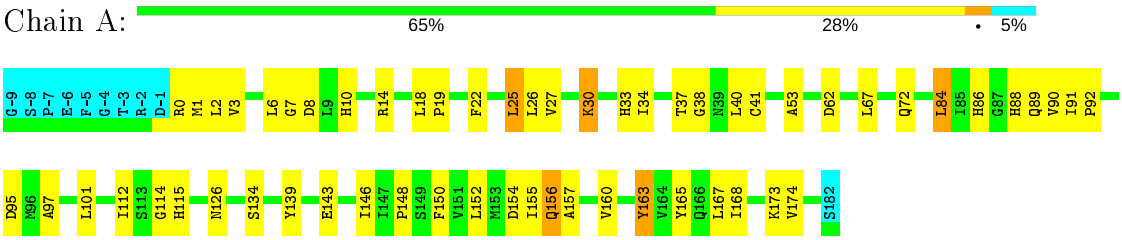
Chain B:



4.2.4 Score per residue for model 4

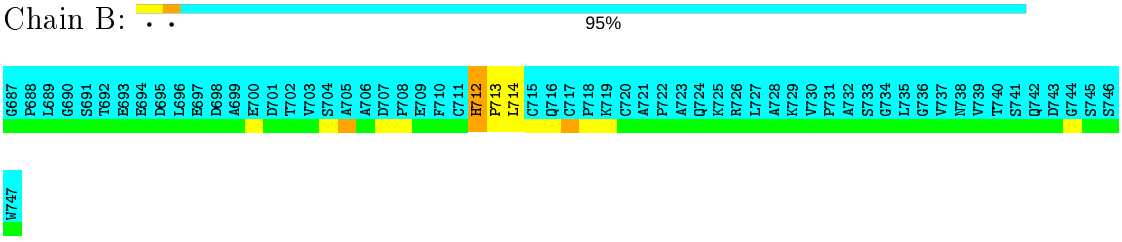
- Molecule 1: Vacuolar protein sorting-associated protein 29

Chain A:



- Molecule 2: Ankyrin repeat domain-containing protein 27

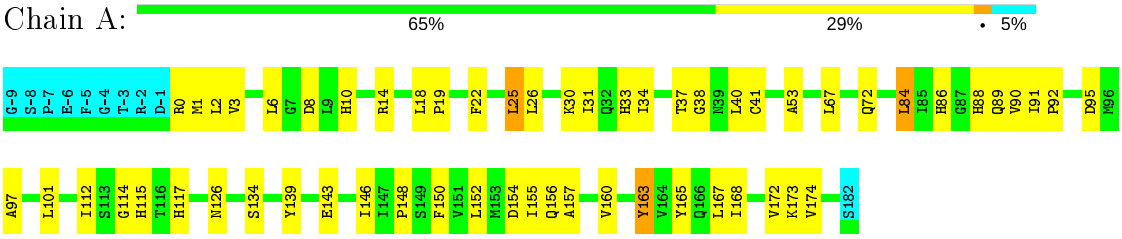
Chain B:



4.2.5 Score per residue for model 5

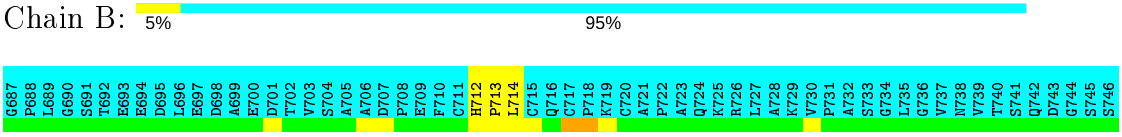
- Molecule 1: Vacuolar protein sorting-associated protein 29

Chain A:



- Molecule 2: Ankyrin repeat domain-containing protein 27

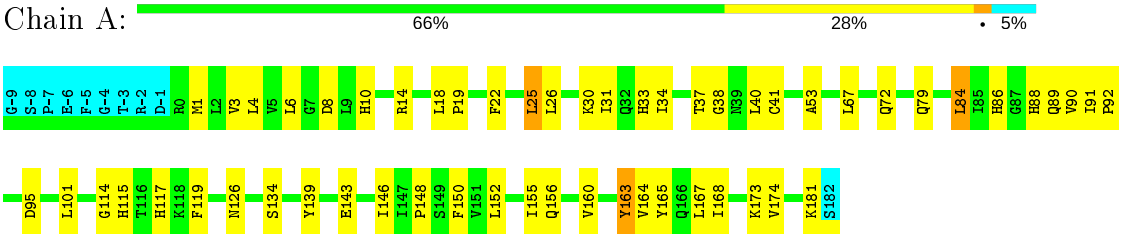
Chain B:



4.2.6 Score per residue for model 6

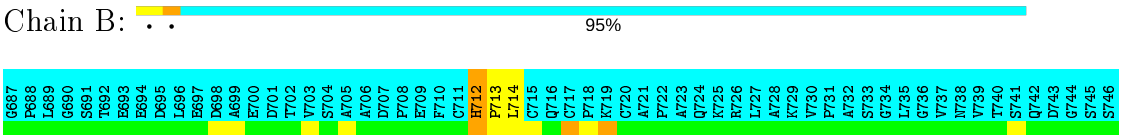
• Molecule 1: Vacuolar protein sorting-associated protein 29

Chain A:



• Molecule 2: Ankyrin repeat domain-containing protein 27

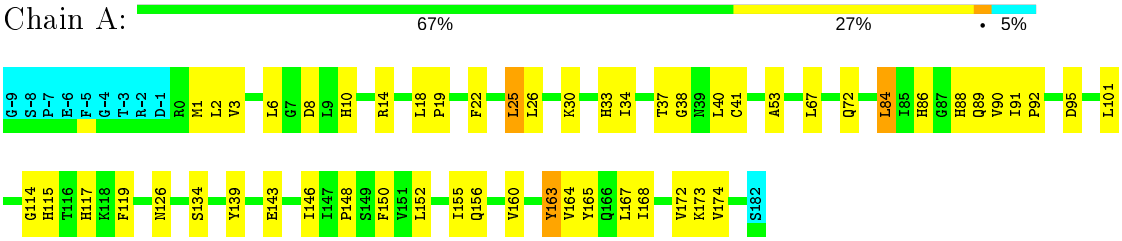
Chain B:



4.2.7 Score per residue for model 7

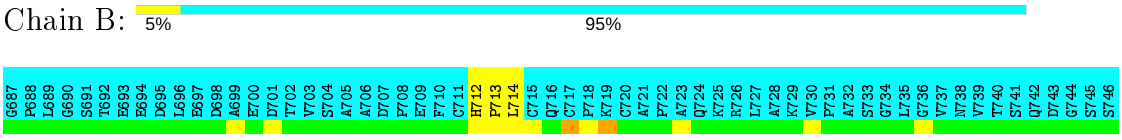
• Molecule 1: Vacuolar protein sorting-associated protein 29

Chain A:



• Molecule 2: Ankyrin repeat domain-containing protein 27

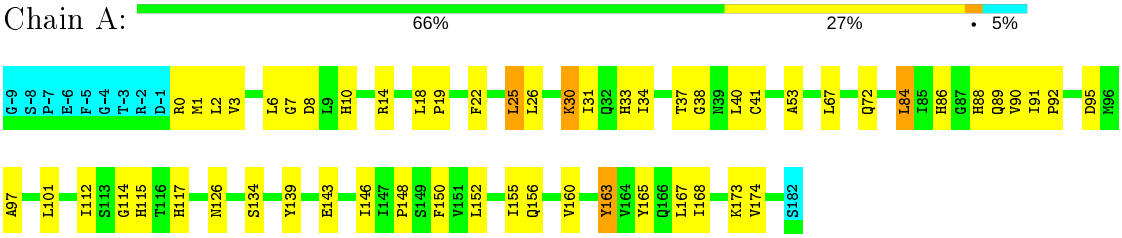
Chain B:



4.2.8 Score per residue for model 8

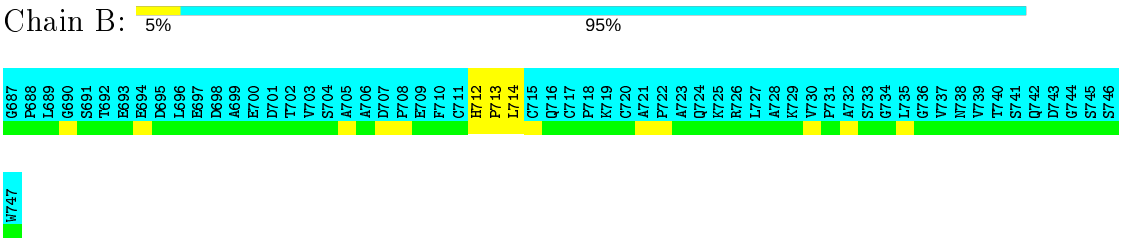
• Molecule 1: Vacuolar protein sorting-associated protein 29

Chain A:



• Molecule 2: Ankyrin repeat domain-containing protein 27

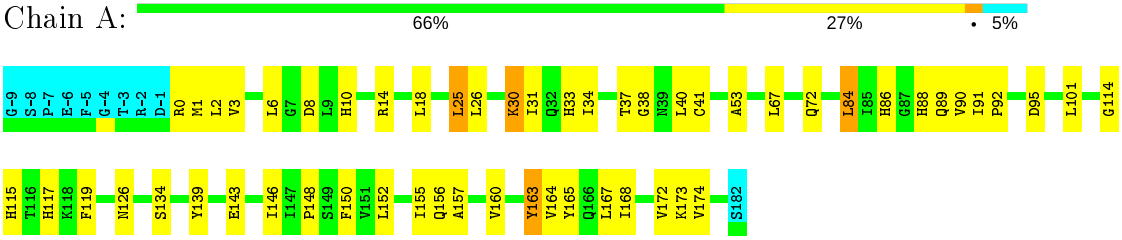
Chain B:



4.2.9 Score per residue for model 9

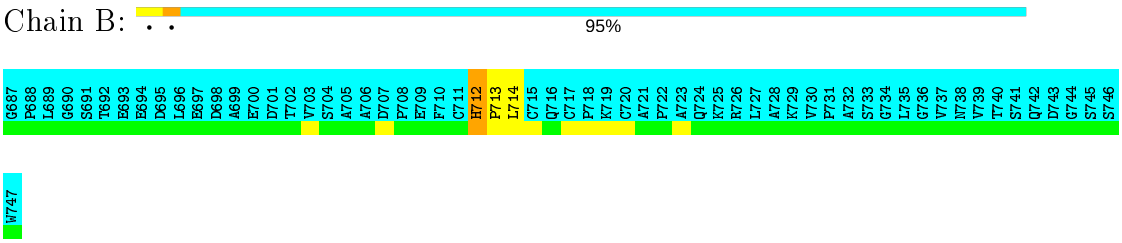
• Molecule 1: Vacuolar protein sorting-associated protein 29

Chain A:



• Molecule 2: Ankyrin repeat domain-containing protein 27

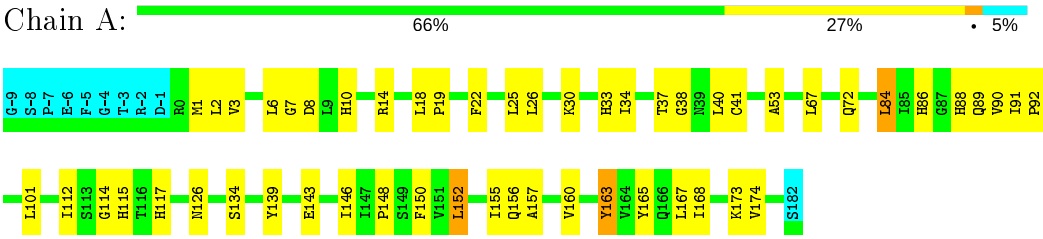
Chain B:



4.2.10 Score per residue for model 10

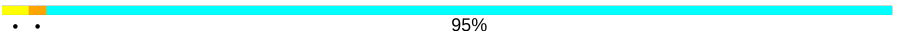
• Molecule 1: Vacuolar protein sorting-associated protein 29

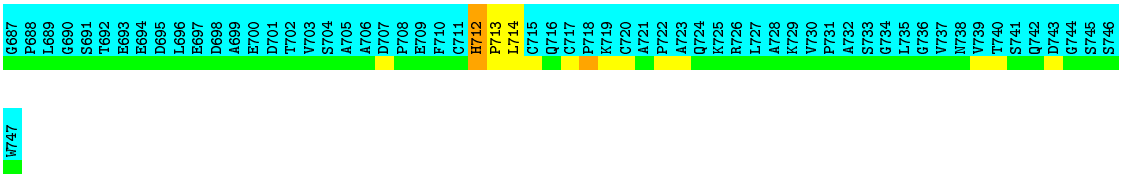
Chain A:



• Molecule 2: Ankyrin repeat domain-containing protein 27

Chain B:

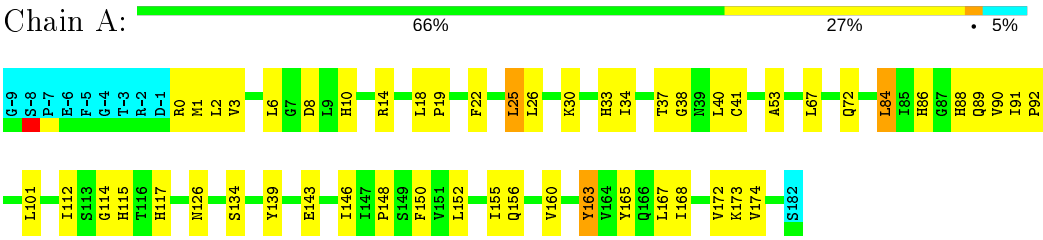




4.2.11 Score per residue for model 11 (medoid)

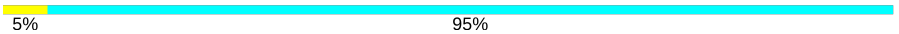
• Molecule 1: Vacuolar protein sorting-associated protein 29

Chain A:



• Molecule 2: Ankyrin repeat domain-containing protein 27

Chain B:



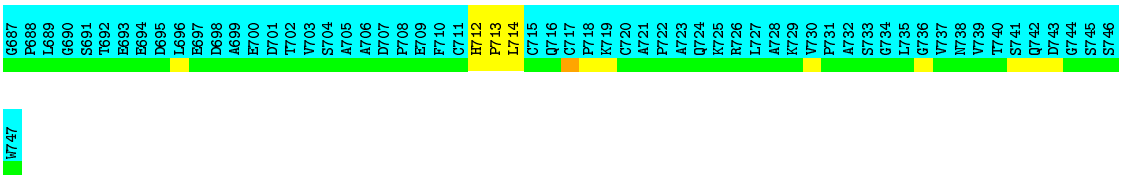
4.2.12 Score per residue for model 12

• Molecule 1: Vacuolar protein sorting-associated protein 29

Chain A:

• Molecule 2: Ankyrin repeat domain-containing protein 27

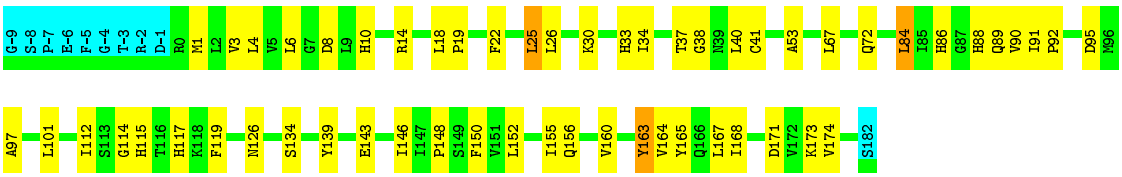
Chain B: 5% 95%



4.2.13 Score per residue for model 13

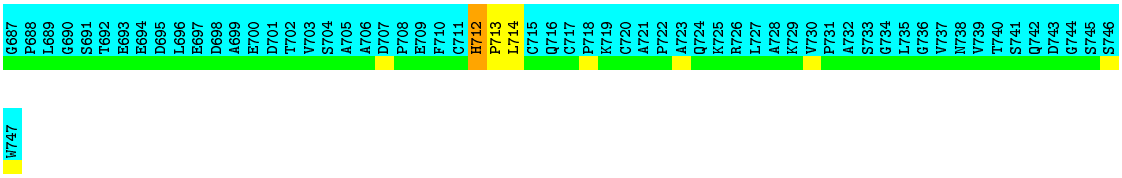
• Molecule 1: Vacuolar protein sorting-associated protein 29

Chain A: 66% 28% • 5%



• Molecule 2: Ankyrin repeat domain-containing protein 27

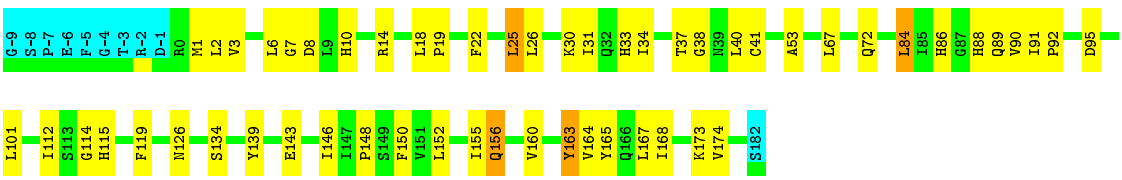
Chain B: • • 95%



4.2.14 Score per residue for model 14

• Molecule 1: Vacuolar protein sorting-associated protein 29

Chain A: 66% 27% • 5%



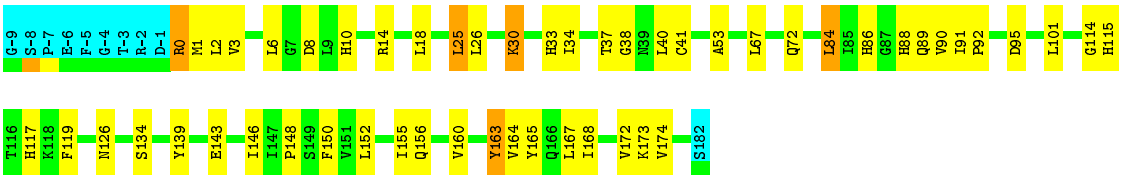
• Molecule 2: Ankyrin repeat domain-containing protein 27

Chain B: 5% 95%

4.2.15 Score per residue for model 15

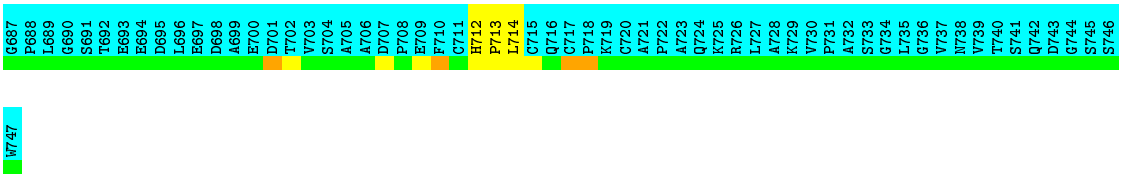
- Molecule 1: Vacuolar protein sorting-associated protein 29

Chain A: 67% 25% 5%



- Molecule 2: Ankyrin repeat domain-containing protein 27

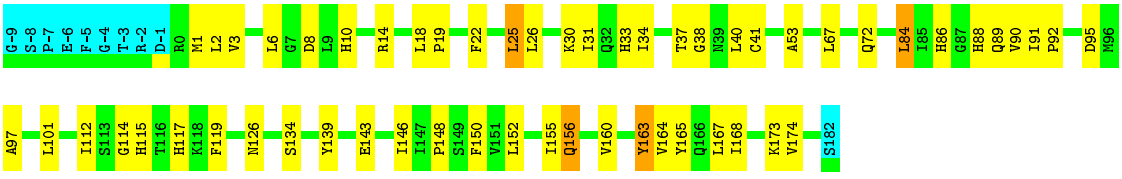
Chain B: 5% 95%



4.2.16 Score per residue for model 16

- Molecule 1: Vacuolar protein sorting-associated protein 29

Chain A: 66% 27% 5%



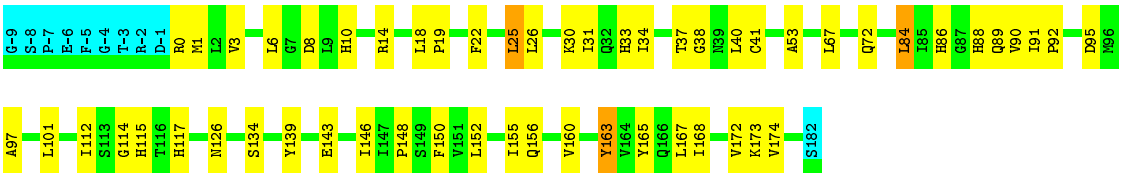
- Molecule 2: Ankyrin repeat domain-containing protein 27

Chain B: 5% 95%

4.2.17 Score per residue for model 17

• Molecule 1: Vacuolar protein sorting-associated protein 29

Chain A:



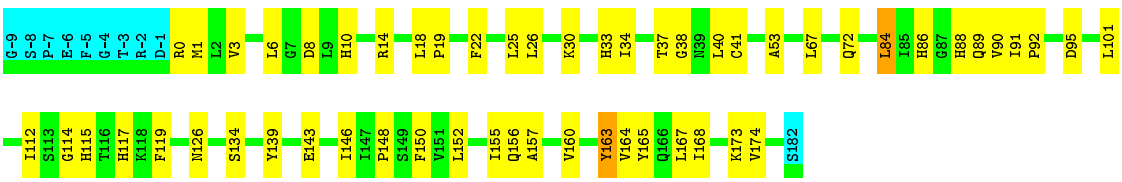
• Molecule 2: Ankyrin repeat domain-containing protein 27

Chain B:

4.2.18 Score per residue for model 18

• Molecule 1: Vacuolar protein sorting-associated protein 29

Chain A:



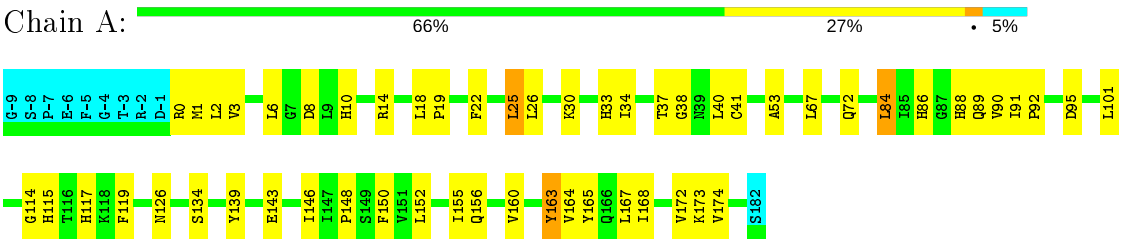
• Molecule 2: Ankyrin repeat domain-containing protein 27

Chain B:

4.2.19 Score per residue for model 19

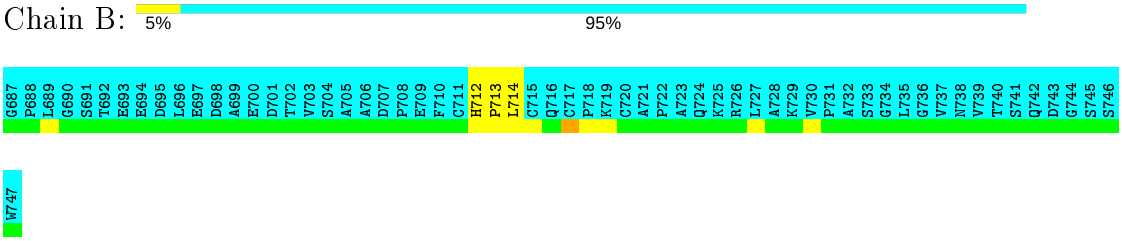
• Molecule 1: Vacuolar protein sorting-associated protein 29

Chain A:



• Molecule 2: Ankyrin repeat domain-containing protein 27

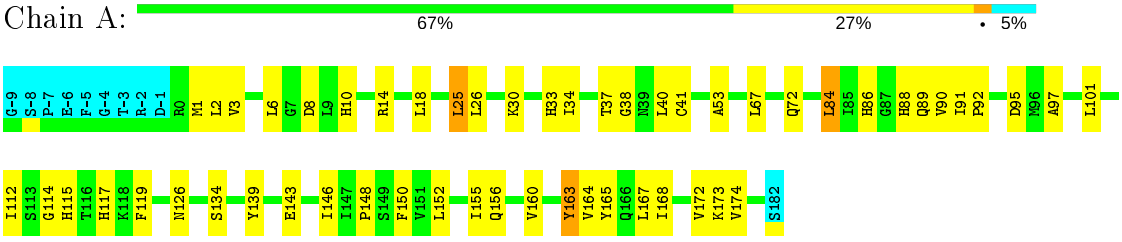
Chain B:



4.2.20 Score per residue for model 20

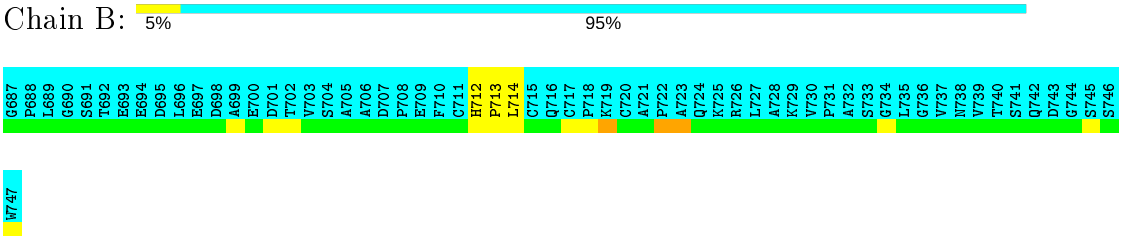
• Molecule 1: Vacuolar protein sorting-associated protein 29

Chain A:



• Molecule 2: Ankyrin repeat domain-containing protein 27

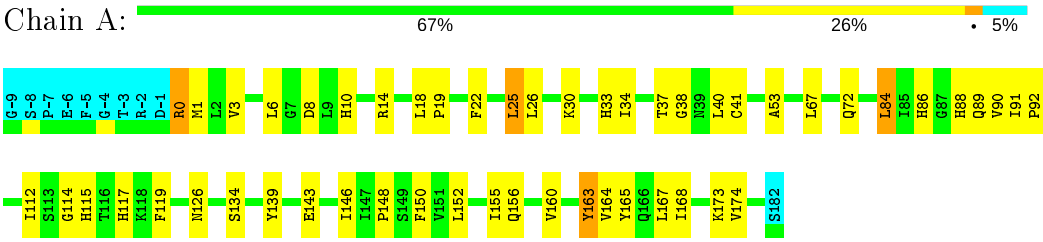
Chain B:



4.2.21 Score per residue for model 21

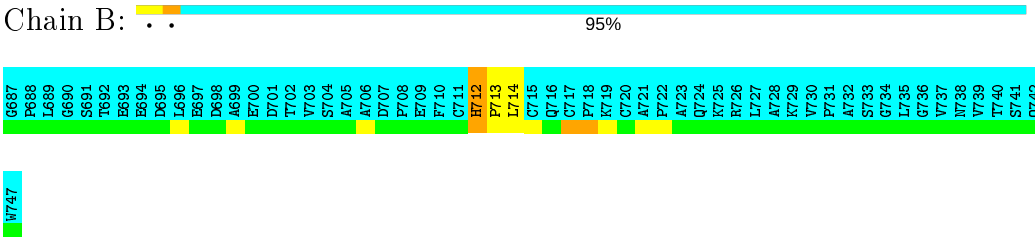
• Molecule 1: Vacuolar protein sorting-associated protein 29

Chain A:



• Molecule 2: Ankyrin repeat domain-containing protein 27

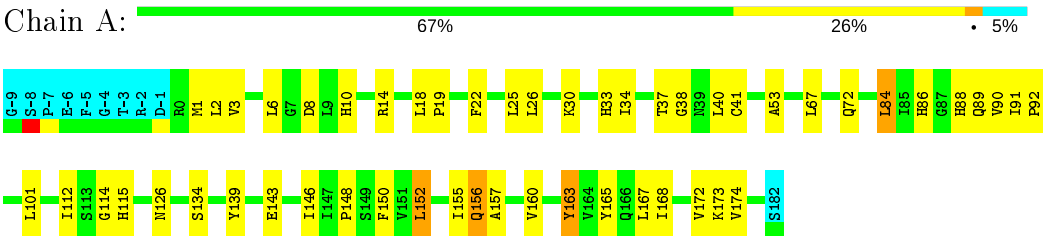
Chain B:



4.2.22 Score per residue for model 22

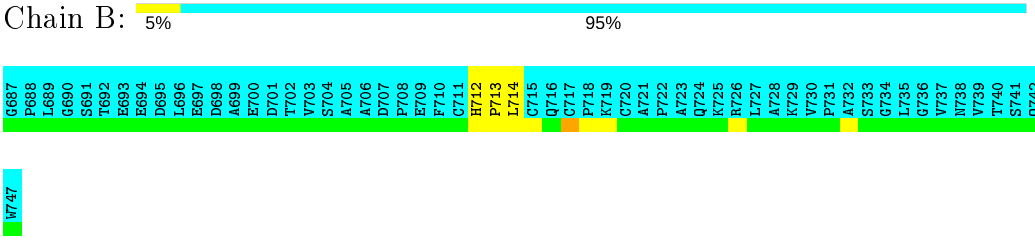
• Molecule 1: Vacuolar protein sorting-associated protein 29

Chain A:



• Molecule 2: Ankyrin repeat domain-containing protein 27

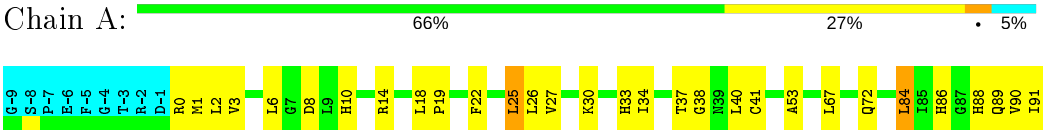
Chain B:



4.2.23 Score per residue for model 23

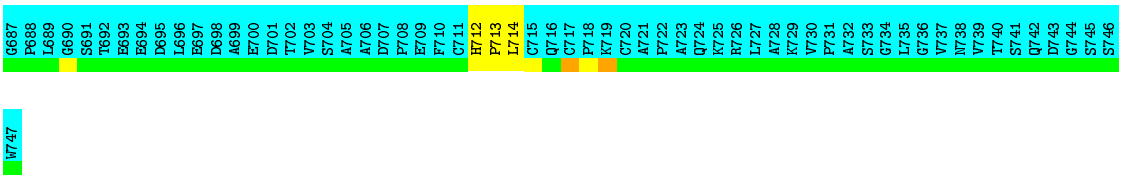
• Molecule 1: Vacuolar protein sorting-associated protein 29

Chain A:



• Molecule 2: Ankyrin repeat domain-containing protein 27

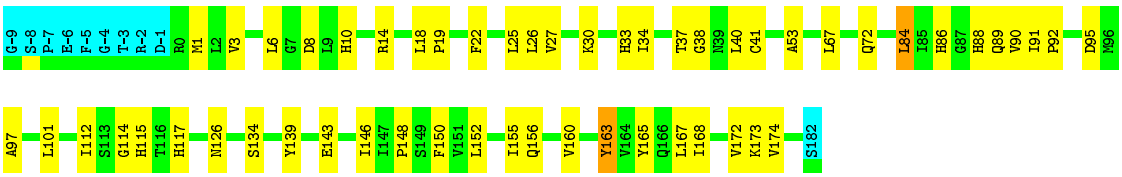
Chain B: 5% 95%



4.2.24 Score per residue for model 24

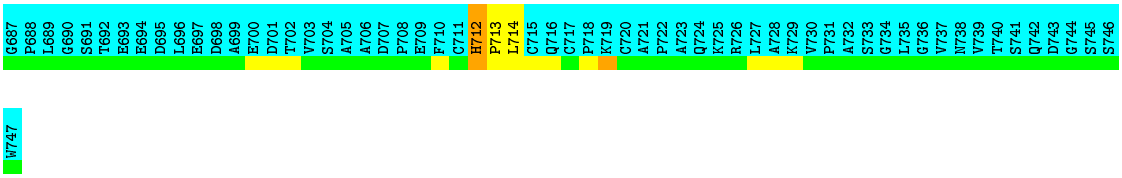
• Molecule 1: Vacuolar protein sorting-associated protein 29

Chain A: 67% 27% • 5%



• Molecule 2: Ankyrin repeat domain-containing protein 27

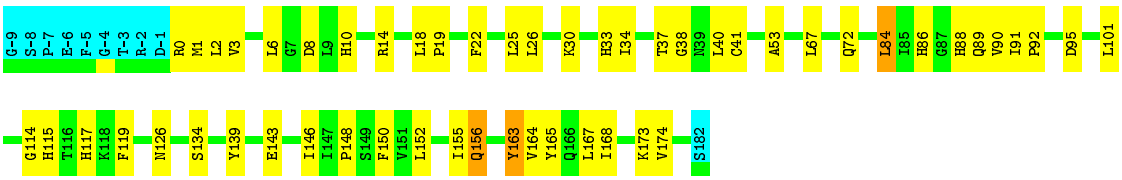
Chain B: • • 95%



4.2.25 Score per residue for model 25

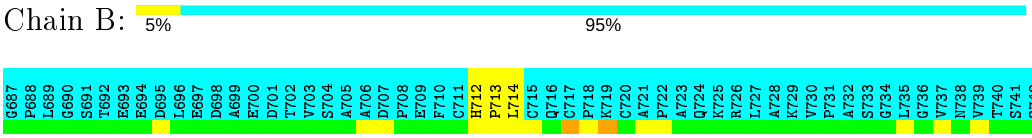
• Molecule 1: Vacuolar protein sorting-associated protein 29

Chain A: 67% 26% • 5%



• Molecule 2: Ankyrin repeat domain-containing protein 27

Chain B:


5%
95%
G687 P688 L689 G690 S691 T692 E693 E694 D695 L696 E697 D698 A699 E700 D701 T702 V703 S704 A705 A706 D707 P708 E709 F710 C711 H712 P713 L714 C715 Q716 C717 P718 K719 C720 A721 P722 A723 Q724 K725 R726 L727 A728 K729 V730 P731 A732 S733 G734 L735 G736 V737 N738 V739 T740 S741 Q742 D743 G744 S745 S746
W747

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%

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: ZN

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	1450	1463	1463	62±3
2	B	25	25	25	15±2
All	All	36900	37200	37200	1612

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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:25:LEU:O	2:B:714:LEU:HB3	0.75	1.82	15	22
2:B:712:HIS:HB2	2:B:713:PRO:HD2	0.74	1.57	10	25
1:A:37:THR:HG22	1:A:84:LEU:CD2	0.74	2.12	20	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:O	1:A:67:LEU:HD23	0.71	1.85	9	15
1:A:67:LEU:HD23	1:A:67:LEU:O	0.71	1.85	2	10
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:O	1:A:101:LEU:HD12	0.66	1.90	12	12
1:A:101:LEU:HD12	1:A:101:LEU:O	0.66	1.90	11	13
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
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:168:ILE:HD12	1:A:173:LYS:HD2	0.61	1.72	2	25
1:A:150:PHE:CZ	1:A:165:TYR:CD1	0.61	2.88	13	4
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:148:PRO:HG2	1:A:167:LEU:HB3	0.60	1.74	20	24
1:A:91:ILE:HD12	1:A:91:ILE:N	0.60	2.12	13	14
1:A:91:ILE:N	1:A:91:ILE:HD12	0.60	2.12	3	11
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:N	1:A:6:LEU:HD23	0.58	2.14	11	17
1:A:8:ASP:N	1:A:38:GLY:HA3	0.57	2.15	4	21
1:A:6:LEU:HD23	1:A:6:LEU:N	0.56	2.15	13	8

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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:90:VAL:C	1:A:91:ILE:HD12	0.55	2.22	22	25
1:A:8:ASP:H	1:A:38:GLY:HA3	0.55	1.62	2	25
1:A:2:LEU:HD21	2:B:713:PRO:HB2	0.55	1.76	10	19
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	4	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	15
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	24	25
1:A:18:LEU:H	1:A:18:LEU:HD12	0.52	1.64	25	10
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	7
1:A:30:LYS:HG2	2:B:714:LEU:HD23	0.51	1.82	21	1
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:155:ILE:CG1	1:A:160:VAL:HG23	0.50	2.36	4	24
1:A:40:LEU:HB2	1:A:41:CYS:HA	0.50	1.84	4	25
2:B:714:LEU:N	2:B:714:LEU:CD1	0.50	2.75	9	4
1:A:40:LEU:CB	1:A:41:CYS:CA	0.49	2.89	4	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
2:B:713:PRO:O	2:B:714:LEU:CB	0.48	2.61	18	10
1:A:18:LEU:HD12	1:A:18:LEU:N	0.47	2.23	10	14
1:A:18:LEU:N	1:A:18:LEU:HD12	0.47	2.23	11	11
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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:152:LEU:HD13	2:B:714:LEU:HD13	0.46	1.86	13	1
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
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	4	25
1:A:0:ARG:HG3	1:A:155:ILE:C	0.45	2.31	5	1
1:A:6:LEU:N	1:A:6:LEU:CD2	0.45	2.79	11	18
1:A:150:PHE:HE1	1:A:152:LEU:CD2	0.45	2.24	23	3
1:A:143:GLU:HB3	1:A:146:ILE:HD11	0.45	1.89	11	25
1:A:19:PRO:HG2	1:A:22:PHE:HB2	0.45	1.87	2	20
1:A:91:ILE:CD1	1:A:91:ILE:N	0.45	2.80	25	11
1:A:6:LEU:CD2	1:A:6:LEU:N	0.45	2.79	13	7
1:A:91:ILE:N	1:A:91:ILE:CD1	0.44	2.80	9	14
1:A:134:SER:O	1:A:148:PRO:HA	0.44	2.12	13	25
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:88:HIS:CE1	1:A:89:GLN:CD	0.43	2.90	11	25
1:A:40:LEU:CB	1:A:41:CYS:HA	0.43	2.43	1	25
2:B:714:LEU:N	2:B:714:LEU:HD12	0.43	2.28	13	1
1:A:4:LEU:CD1	1:A:152:LEU:CD2	0.43	2.97	6	1
1:A:101:LEU:HD12	1:A:101:LEU:C	0.43	2.33	21	14
1:A:25:LEU:CD2	2:B:714:LEU:HB2	0.43	2.44	19	1
1:A:101:LEU:C	1:A:101:LEU:HD12	0.43	2.33	11	11
1:A:2:LEU:CD1	1:A:152:LEU:HD12	0.43	2.42	23	2
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:91:ILE:HA	1:A:92:PRO:C	0.42	2.34	1	25
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:CD2	1:A:67:LEU:O	0.42	2.64	1	8
1:A:174:VAL:HG21	2:B:712:HIS:CD2	0.42	2.49	5	2
1:A:126:ASN:N	1:A:126:ASN:OD1	0.42	2.53	4	10
1:A:126:ASN:OD1	1:A:126:ASN:N	0.42	2.53	5	15
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:67:LEU:O	1:A:67:LEU:CD2	0.42	2.64	5	17
1:A:4:LEU:HD12	1:A:152:LEU:CD2	0.42	2.44	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:4:LEU:CD1	1:A:152:LEU:HD21	0.42	2.45	6	1
1:A:10:HIS:CD2	1:A:14:ARG:CZ	0.42	3.03	22	25
1:A:2:LEU:HG	1:A:152:LEU:HD12	0.42	1.90	10	1
1:A:26:LEU:C	1:A:27:VAL:HG13	0.42	2.35	1	3
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:O	0.41	2.68	16	1
1:A:25:LEU:CD2	2:B:714:LEU:HB3	0.41	2.44	13	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
2:B:713:PRO:C	2:B:714:LEU:HG	0.41	2.36	19	4
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	5
1:A:117:HIS:N	1:A:117:HIS:CD2	0.40	2.88	25	11
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:172:VAL:HG23	1:A:172:VAL:O	0.40	2.16	7	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:117:HIS:CD2	1:A:117:HIS:N	0.40	2.88	10	10
1:A:62:ASP:OD1	1:A:86:HIS:CE1	0.40	2.75	4	2
1:A:95:ASP:OD1	1:A:97:ALA:HB3	0.40	2.17	4	13

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	182/192 (95%)	175±1 (96±0%)	7±1 (4±0%)	0±0 (0±0%)	50 82

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
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%)	50 82

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 (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	160/168 (95%)	153±1 (96±0%)	7±1 (4±0%)	31 80
2	B	3/49 (6%)	3±0 (87±16%)	0±0 (13±16%)	7 48
All	All	4075/5425 (75%)	3886 (95%)	189 (5%)	31 79

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	163	TYR	25
1	A	139	TYR	25
1	A	156	GLN	25
1	A	1	MET	24
1	A	25	LEU	20
2	B	712	HIS	10
1	A	30	LYS	7
1	A	152	LEU	3

6.3.3 RNA (i)

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 monosaccharides in this entry.

6.6 Ligand geometry

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

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 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

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

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	245	-0.38 ± 0.09	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	212	0.05 ± 0.12	None needed (< 0.5 ppm)
$^{13}C'$	0	—	None (insufficient data)
^{15}N	227	-0.20 ± 0.32	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 73%, i.e. 1681 atoms were assigned a chemical shift out of a possible 2310. 0 out of 37 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	696/909 (77%)	346/362 (96%)	180/370 (49%)	170/177 (96%)
Sidechain	880/1183 (74%)	515/689 (75%)	359/450 (80%)	6/44 (14%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	105/218 (48%)	68/118 (58%)	36/89 (40%)	1/11 (9%)
Overall	1681/2310 (73%)	929/1169 (79%)	575/909 (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. 2184 atoms were assigned a chemical shift out of a possible 3035. 0 out of 45 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	936/1237 (76%)	464/492 (94%)	245/506 (48%)	227/239 (95%)
Sidechain	1135/1550 (73%)	673/906 (74%)	452/587 (77%)	10/57 (18%)
Aromatic	113/248 (46%)	73/134 (54%)	38/102 (37%)	2/12 (17%)
Overall	2184/3035 (72%)	1210/1532 (79%)	735/1195 (62%)	239/308 (78%)

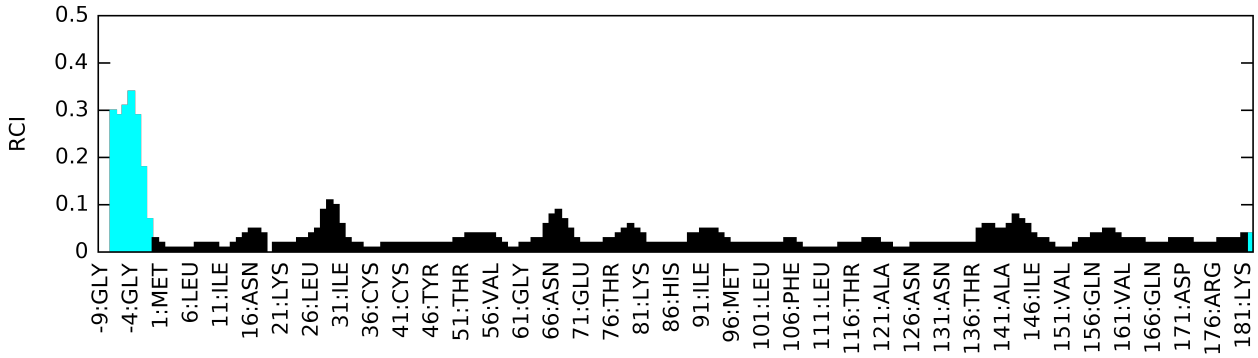
7.1.4 Statistically unusual chemical shifts (i)

There are no statistically unusual chemical shifts.

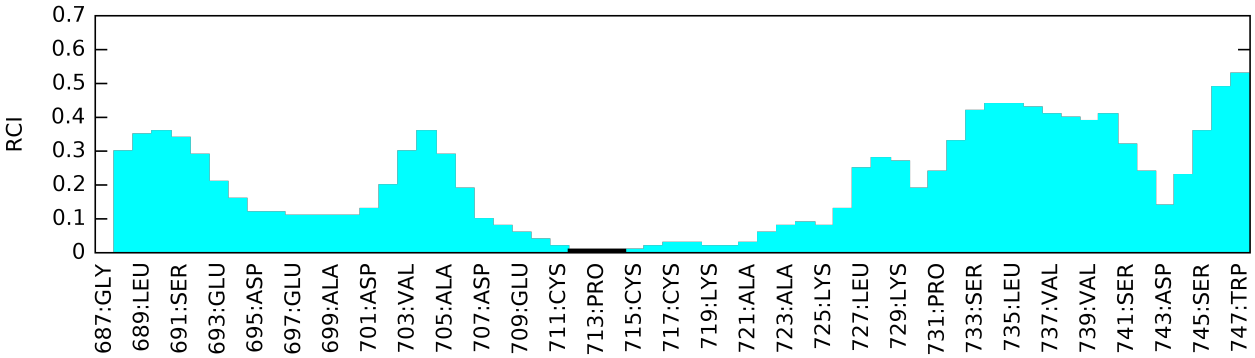
7.1.5 Random Coil Index (RCI) plots (i)

The 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:


RCI
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
687:GLY
689:LEU
691:SER
693:GLU
695:ASP
697:GLU
699:ALA
701:ASP
703:VAL
705:ALA
707:ASP
709:GLU
711:CYS
713:PRO
715:CYS
717:CYS
719:LYS
721:ALA
723:ALA
725:LYS
727:LEU
729:LYS
731:PRO
733:SER
735:LEU
737:VAL
739:VAL
741:SER
743:ASP
745:SER
747:TRP