Full wwPDB NMR Structure Validation Report

Mar 6, 2022 – 11:47 AM EST

PDB ID	:	2KGF
Title	:	N-terminal domain of capsid protein from the Mason-Pfizer monkey virus
Authors	:	Macek, P.; Chmelik, J.; Zidek, L.; Kaderavek, P.; Padrta, P.; Ruml, T.; Pichova, I.; Rumlova, M.; Sklenar, V.
Deposited on	:	2009-03-10

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 (i)) were used in the production of this report:

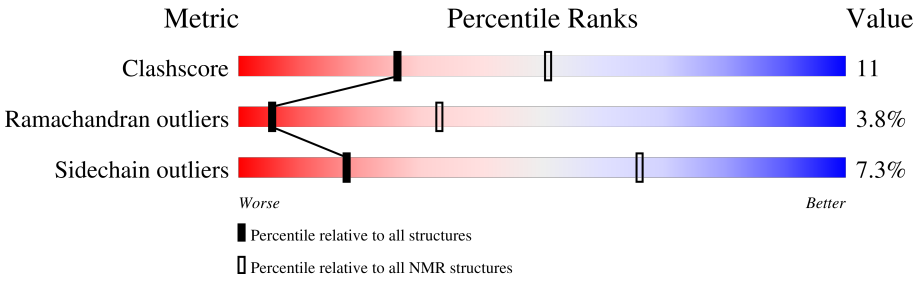
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.27
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.27

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 was not calculated.

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	140	68% 11% • 17%

2 Ensemble composition and analysis (i)

This entry contains 50 models. Model 16 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:1-A:3, A:16-A:102, A:111-A:136 (116)	0.49	16

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 8 clusters and 2 single-model clusters were found.

Cluster number	Models
1	1, 5, 11, 12, 15, 16, 17, 19, 20, 22, 26, 27, 28, 29, 30, 31, 33, 34, 40, 48
2	2, 8, 9, 10, 39, 41, 43, 45
3	3, 32, 42, 49, 50
4	6, 7, 13, 23, 38
5	21, 35, 37, 47
6	36, 44
7	4, 18
8	24, 46
Single-model clusters	14; 25

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 2126 atoms, of which 1033 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Capsid protein p27.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	140	2126	688	1033	190	212	3	0

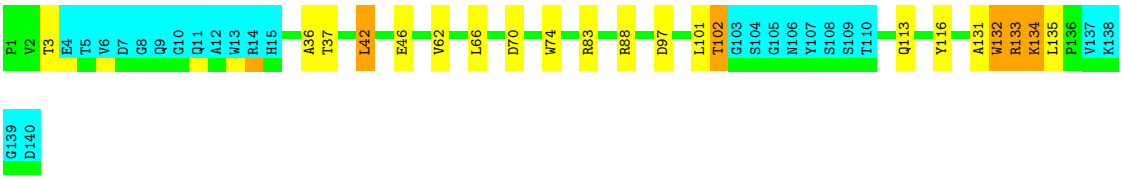
4 Residue-property plots

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: Capsid protein p27

Chain A: 



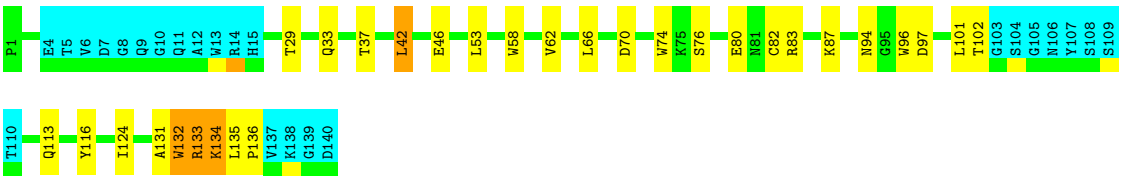
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: Capsid protein p27

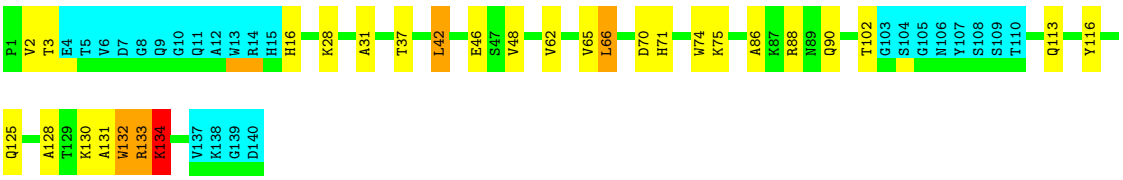
Chain A: 



4.2.2 Score per residue for model 2

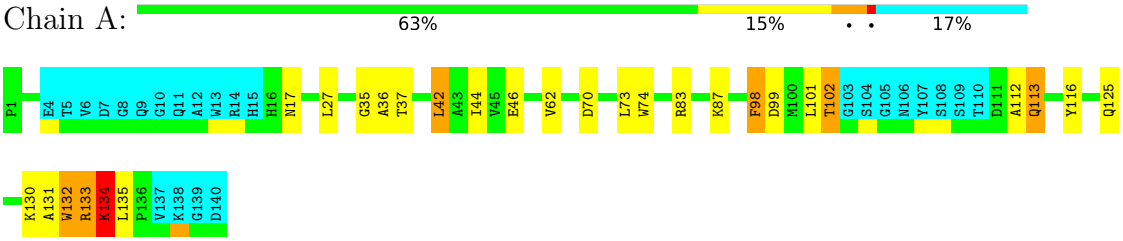
• Molecule 1: Capsid protein p27

Chain A: 



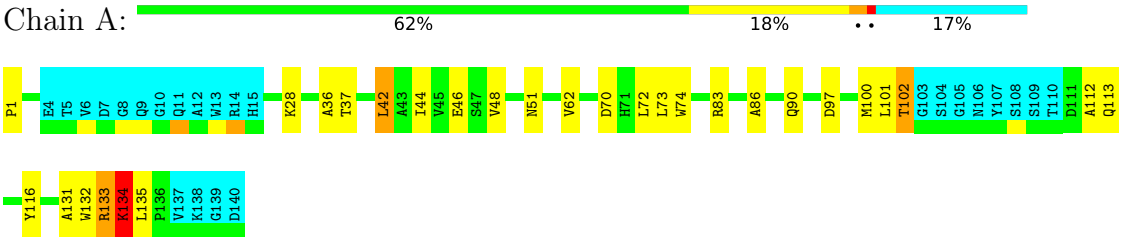
4.2.3 Score per residue for model 3

• Molecule 1: Capsid protein p27



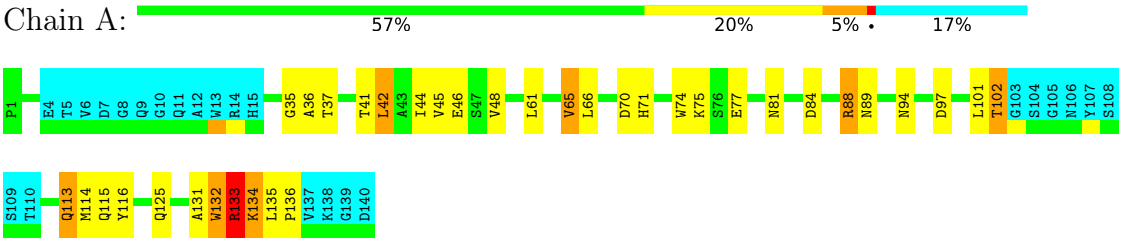
4.2.4 Score per residue for model 4

• Molecule 1: Capsid protein p27



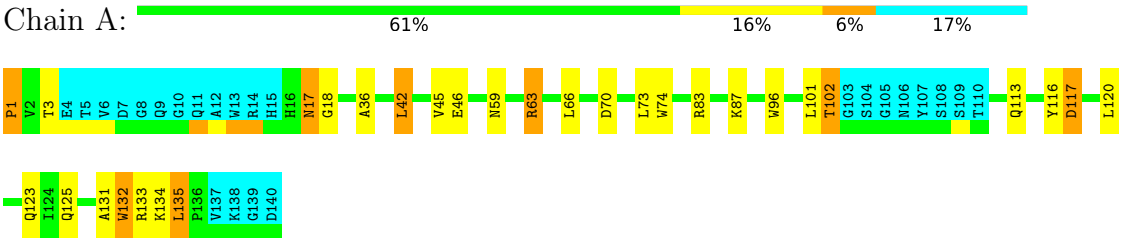
4.2.5 Score per residue for model 5

• Molecule 1: Capsid protein p27



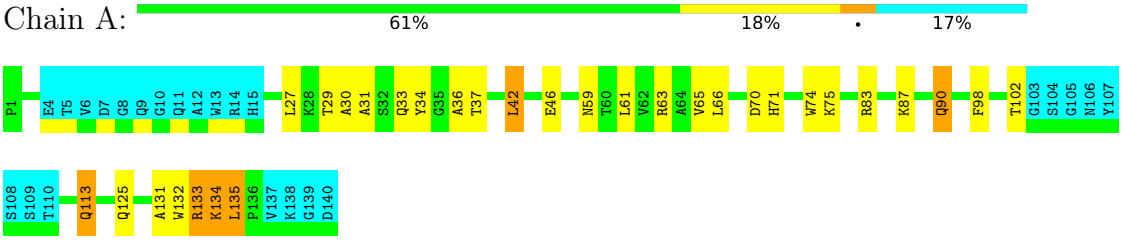
4.2.6 Score per residue for model 6

• Molecule 1: Capsid protein p27



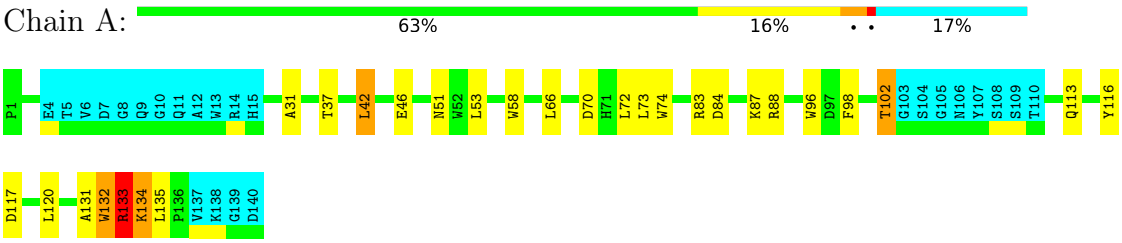
4.2.7 Score per residue for model 7

• Molecule 1: Capsid protein p27



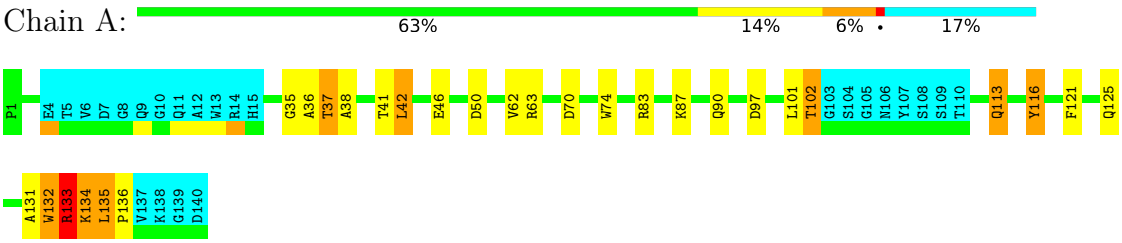
4.2.8 Score per residue for model 8

• Molecule 1: Capsid protein p27



4.2.9 Score per residue for model 9

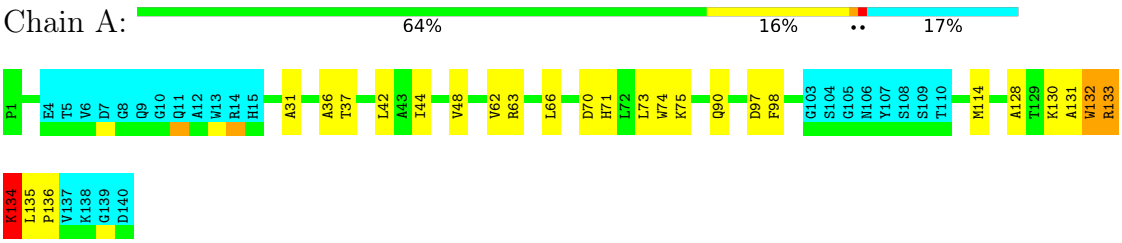
• Molecule 1: Capsid protein p27



4.2.10 Score per residue for model 10

• Molecule 1: Capsid protein p27

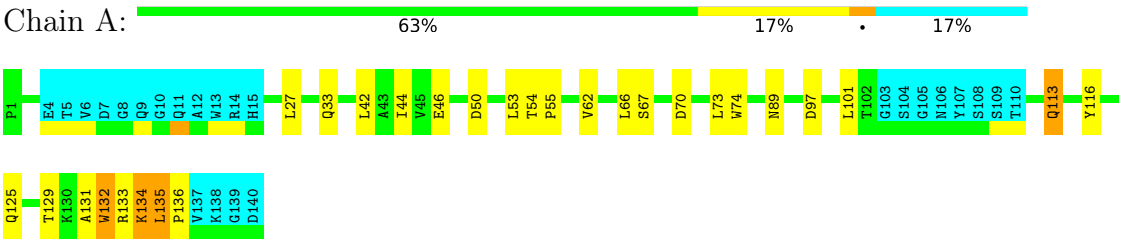
Chain A:



4.2.11 Score per residue for model 11

• Molecule 1: Capsid protein p27

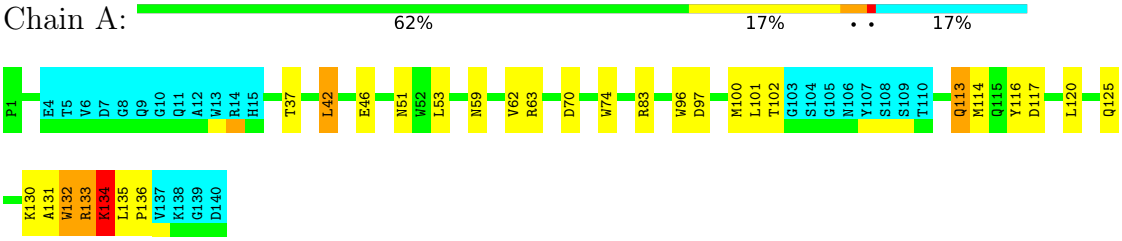
Chain A:



4.2.12 Score per residue for model 12

• Molecule 1: Capsid protein p27

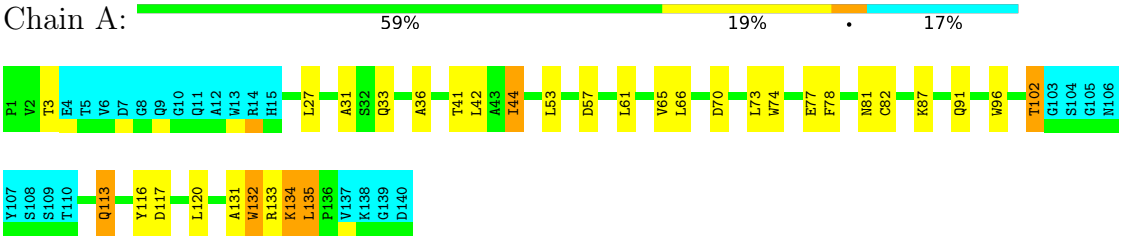
Chain A:



4.2.13 Score per residue for model 13

• Molecule 1: Capsid protein p27

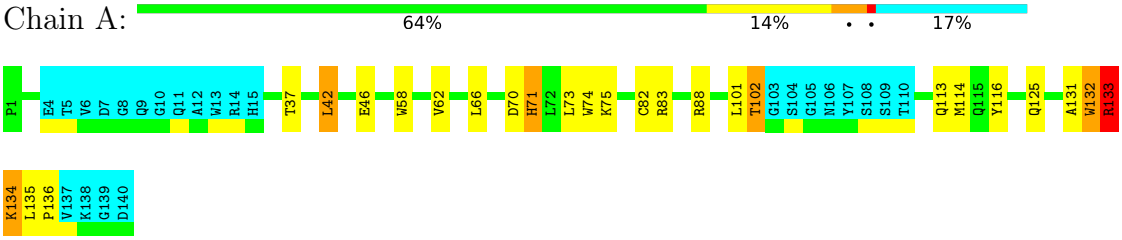
Chain A:



4.2.14 Score per residue for model 14

• Molecule 1: Capsid protein p27

Chain A:



4.2.15 Score per residue for model 15

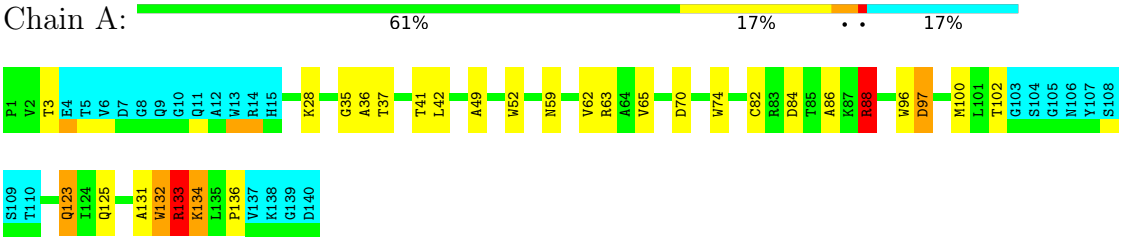
• Molecule 1: Capsid protein p27

Chain A:

4.2.16 Score per residue for model 16 (medoid)

• Molecule 1: Capsid protein p27

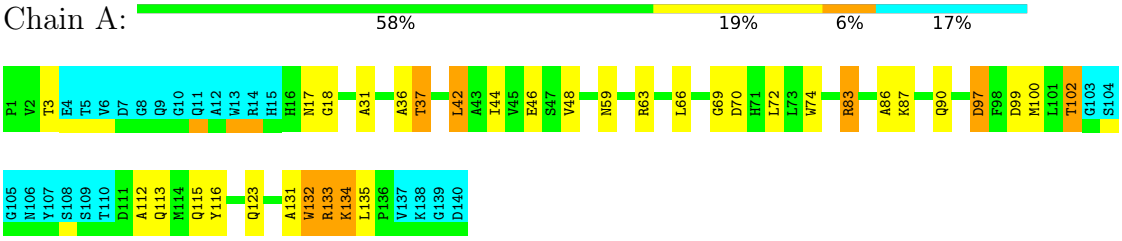
Chain A:



4.2.17 Score per residue for model 17

• Molecule 1: Capsid protein p27

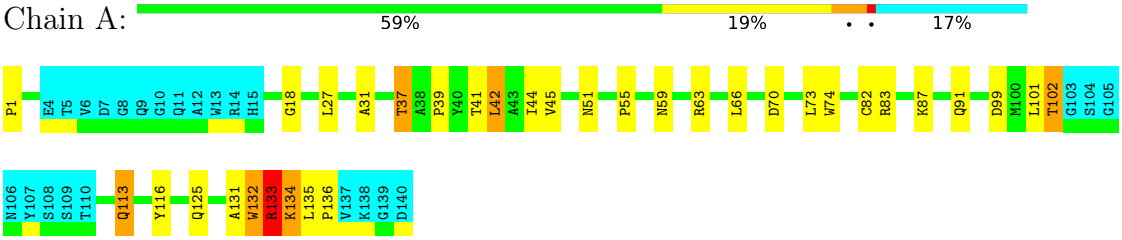
Chain A:



4.2.18 Score per residue for model 18

• Molecule 1: Capsid protein p27

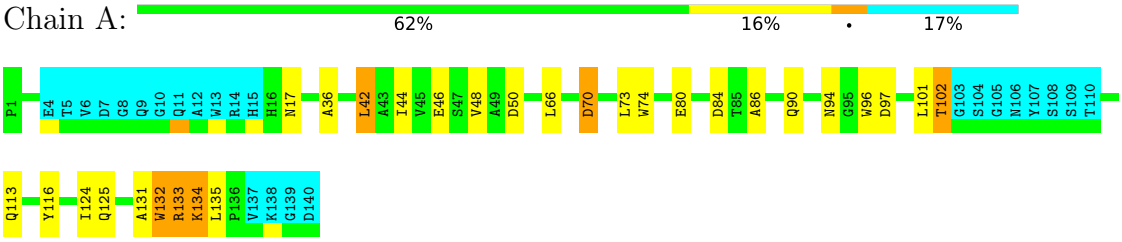
Chain A:



4.2.19 Score per residue for model 19

• Molecule 1: Capsid protein p27

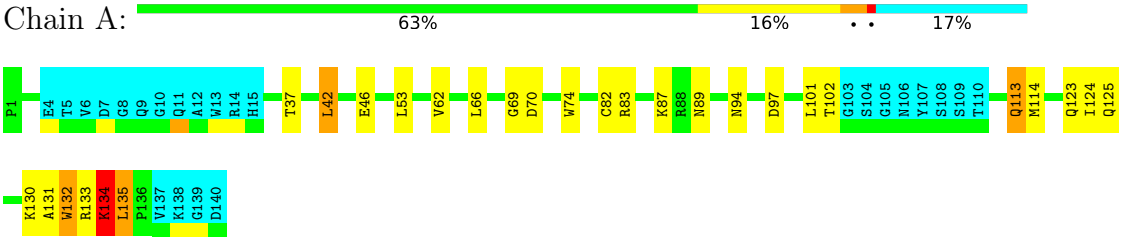
Chain A:



4.2.20 Score per residue for model 20

• Molecule 1: Capsid protein p27

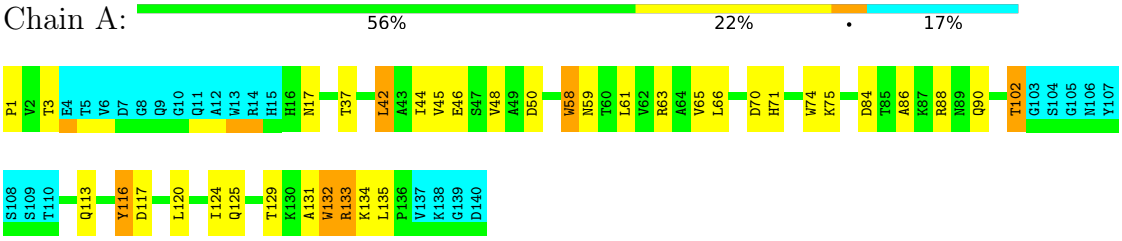
Chain A:



4.2.21 Score per residue for model 21

• Molecule 1: Capsid protein p27

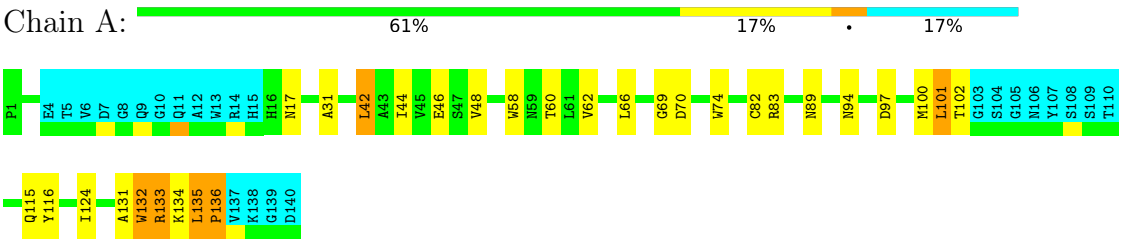
Chain A:



4.2.22 Score per residue for model 22

• Molecule 1: Capsid protein p27

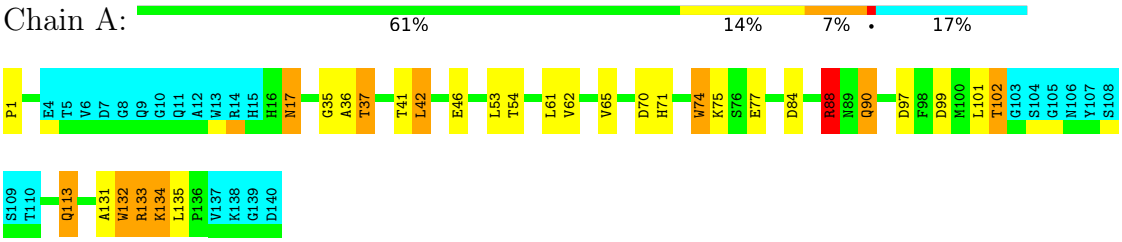
Chain A:



4.2.23 Score per residue for model 23

• Molecule 1: Capsid protein p27

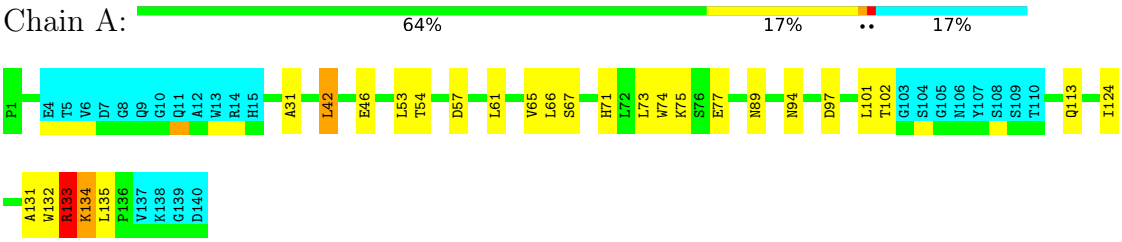
Chain A:



4.2.24 Score per residue for model 24

• Molecule 1: Capsid protein p27

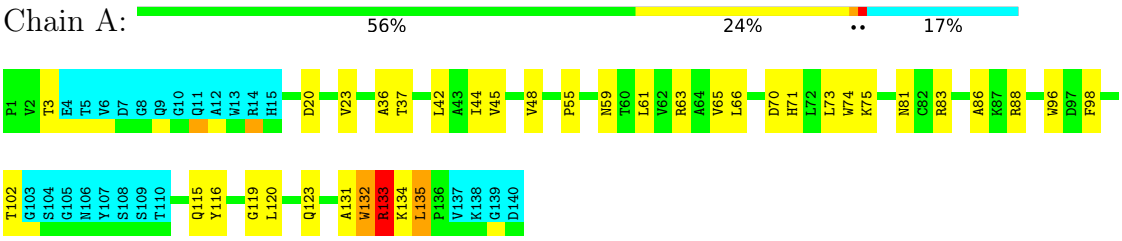
Chain A:



4.2.25 Score per residue for model 25

• Molecule 1: Capsid protein p27

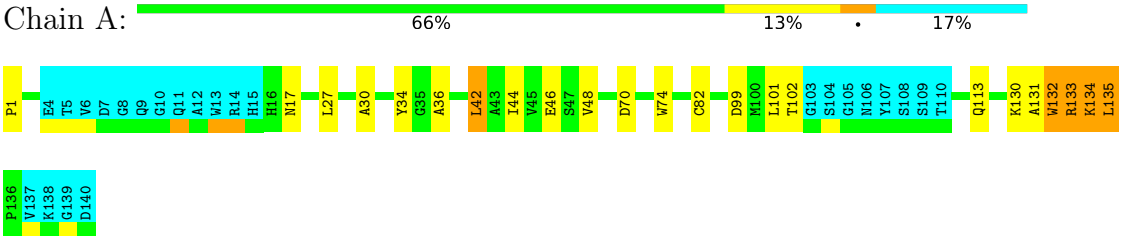
Chain A:



4.2.26 Score per residue for model 26

• Molecule 1: Capsid protein p27

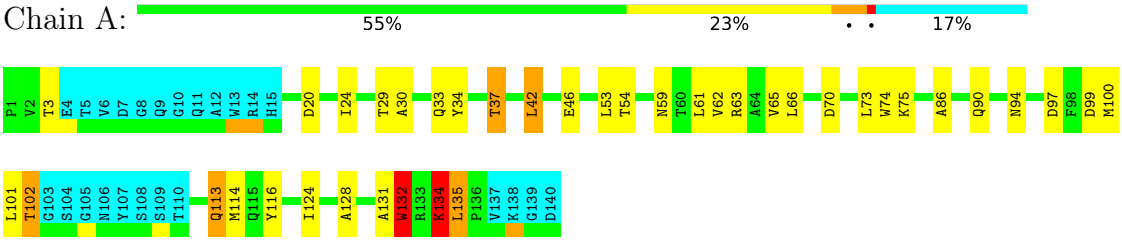
Chain A:



4.2.27 Score per residue for model 27

• Molecule 1: Capsid protein p27

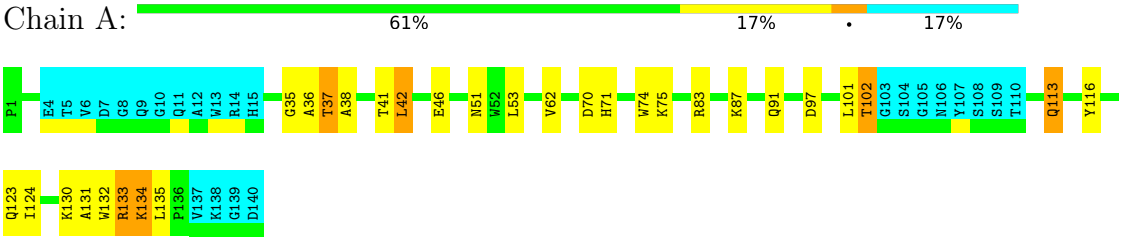
Chain A:



4.2.28 Score per residue for model 28

• Molecule 1: Capsid protein p27

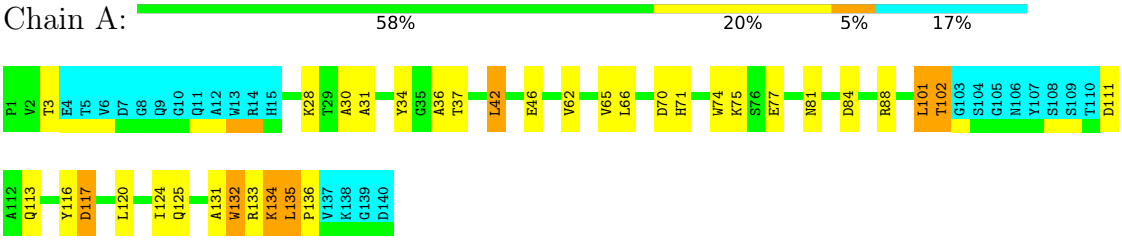
Chain A:



4.2.29 Score per residue for model 29

• Molecule 1: Capsid protein p27

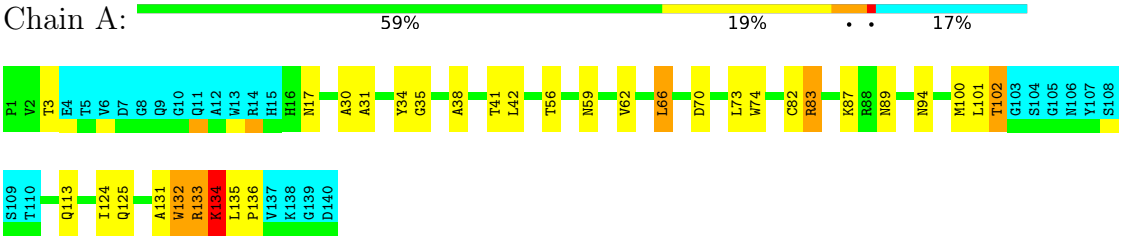
Chain A:



4.2.30 Score per residue for model 30

• Molecule 1: Capsid protein p27

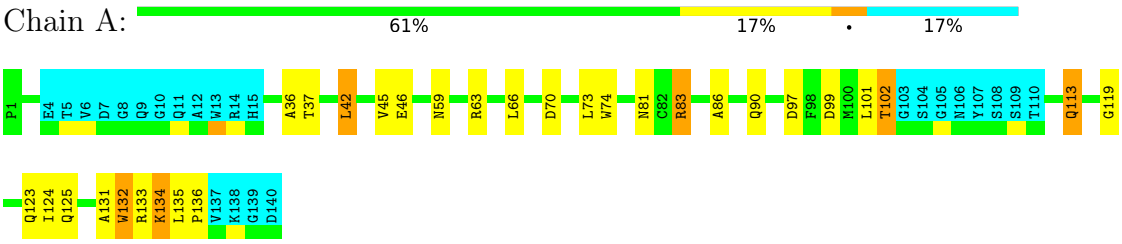
Chain A:



4.2.31 Score per residue for model 31

• Molecule 1: Capsid protein p27

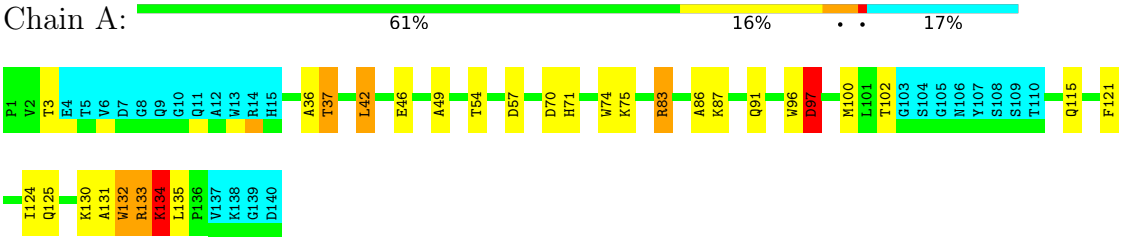
Chain A:



4.2.32 Score per residue for model 32

• Molecule 1: Capsid protein p27

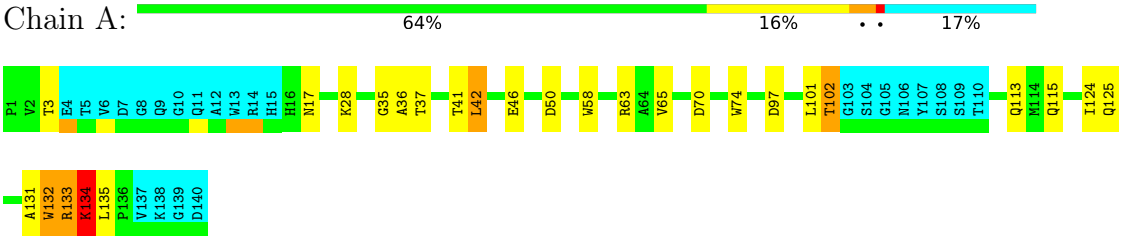
Chain A:



4.2.33 Score per residue for model 33

• Molecule 1: Capsid protein p27

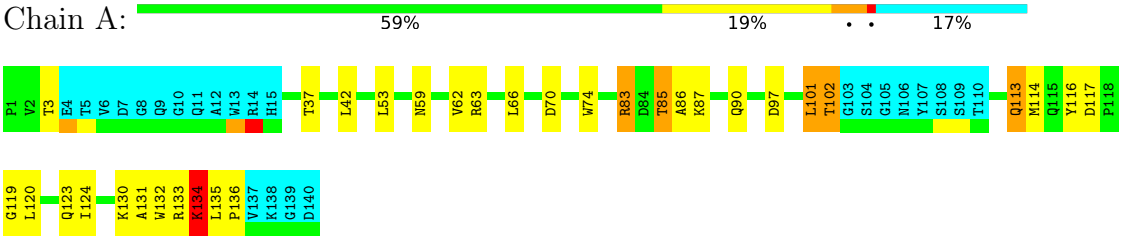
Chain A:



4.2.34 Score per residue for model 34

• Molecule 1: Capsid protein p27

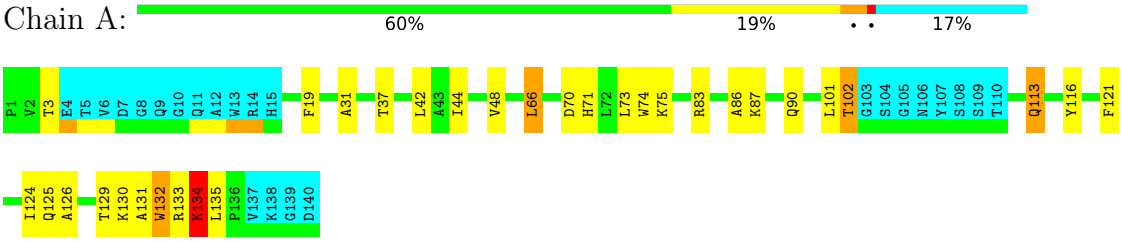
Chain A:



4.2.35 Score per residue for model 35

• Molecule 1: Capsid protein p27

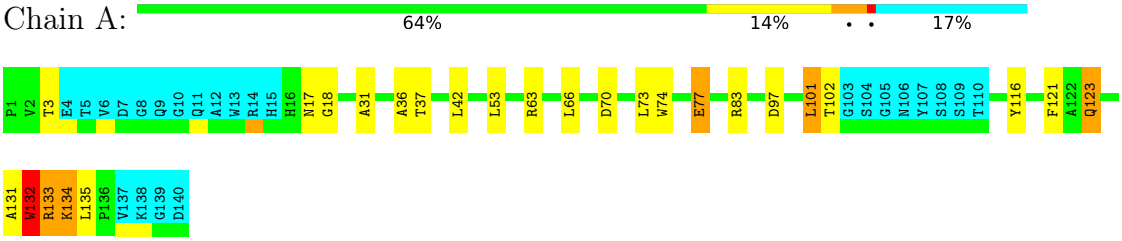
Chain A:



4.2.36 Score per residue for model 36

• Molecule 1: Capsid protein p27

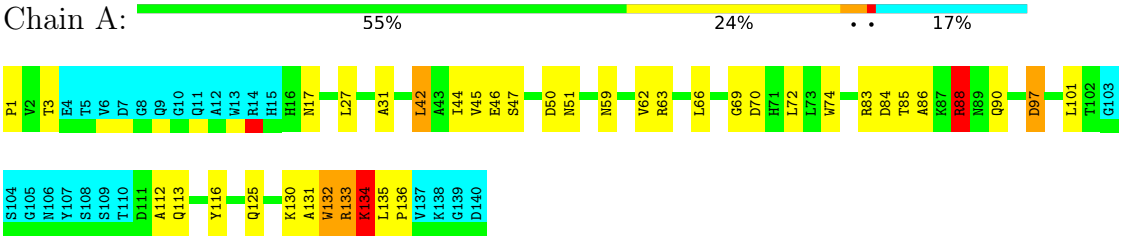
Chain A:



4.2.37 Score per residue for model 37

• Molecule 1: Capsid protein p27

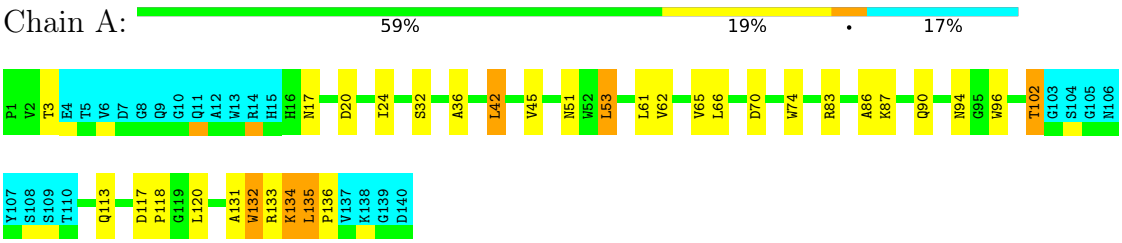
Chain A:



4.2.38 Score per residue for model 38

• Molecule 1: Capsid protein p27

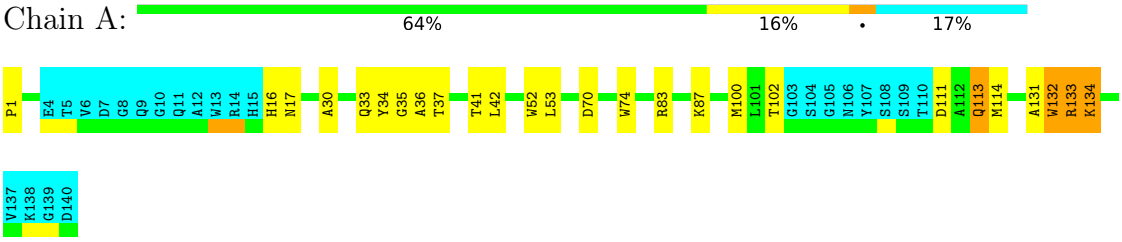
Chain A:



4.2.39 Score per residue for model 39

• Molecule 1: Capsid protein p27

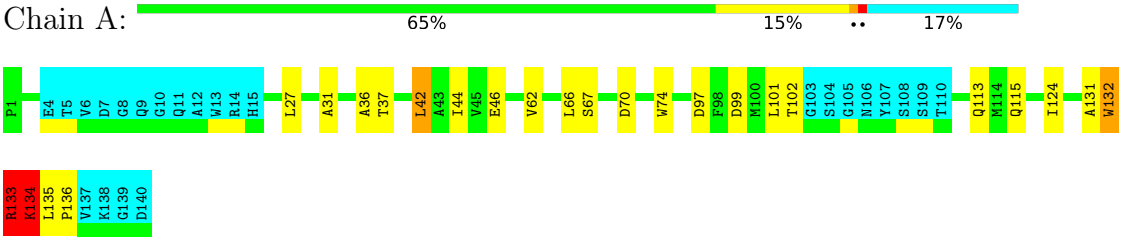
Chain A:



4.2.40 Score per residue for model 40

• Molecule 1: Capsid protein p27

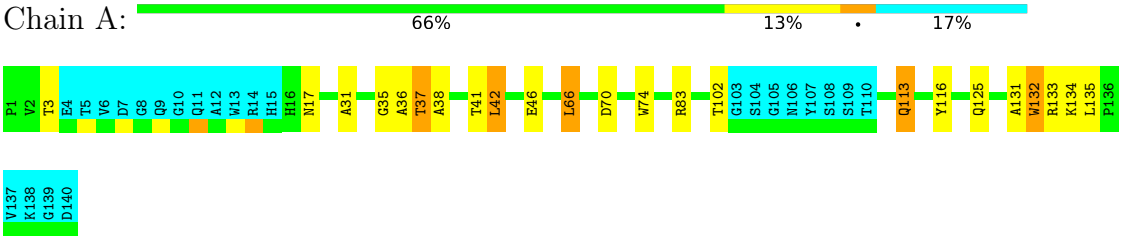
Chain A:



4.2.41 Score per residue for model 41

• Molecule 1: Capsid protein p27

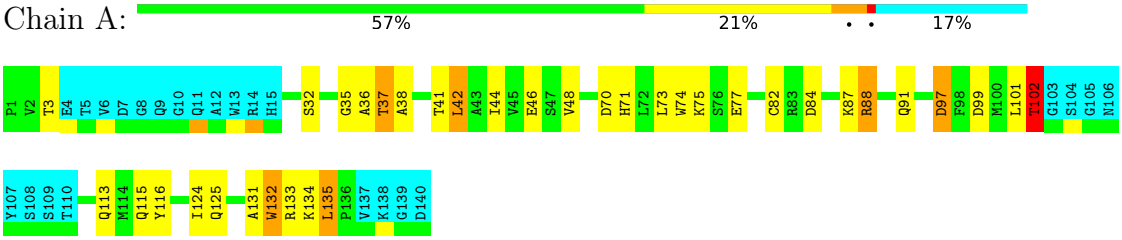
Chain A:



4.2.42 Score per residue for model 42

• Molecule 1: Capsid protein p27

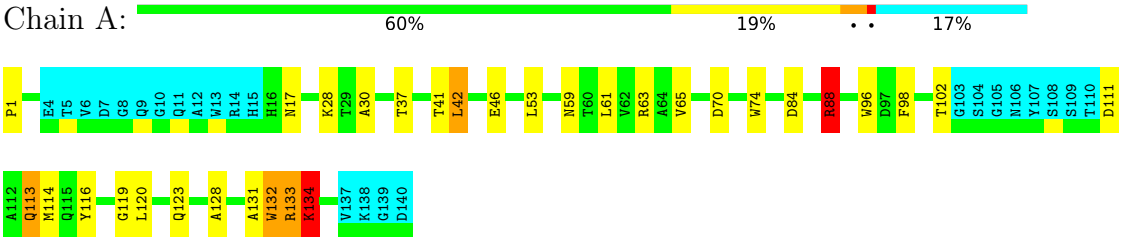
Chain A:



4.2.43 Score per residue for model 43

• Molecule 1: Capsid protein p27

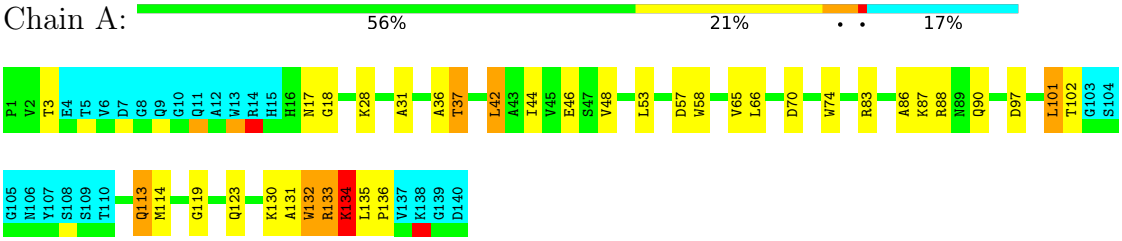
Chain A:



4.2.44 Score per residue for model 44

• Molecule 1: Capsid protein p27

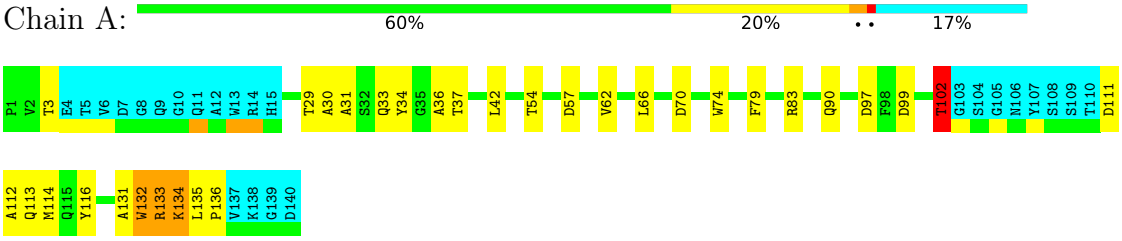
Chain A:



4.2.45 Score per residue for model 45

• Molecule 1: Capsid protein p27

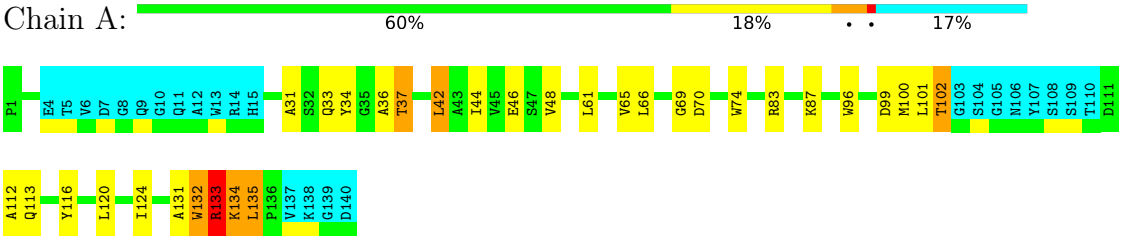
Chain A:



4.2.46 Score per residue for model 46

• Molecule 1: Capsid protein p27

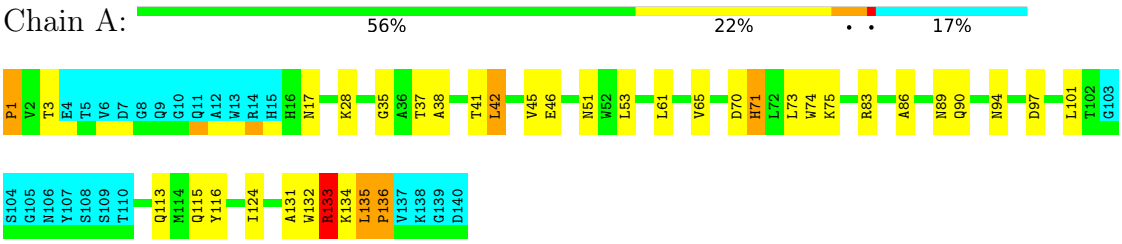
Chain A:



4.2.47 Score per residue for model 47

• Molecule 1: Capsid protein p27

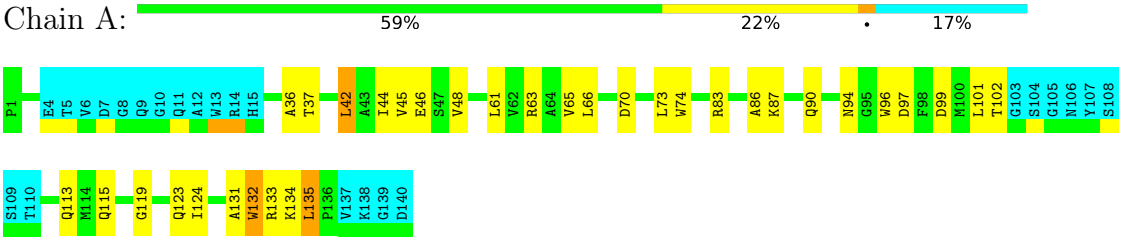
Chain A:



4.2.48 Score per residue for model 48

• Molecule 1: Capsid protein p27

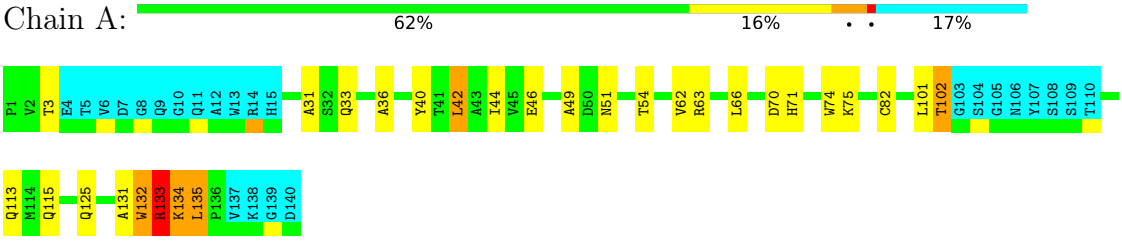
Chain A:



4.2.49 Score per residue for model 49

• Molecule 1: Capsid protein p27

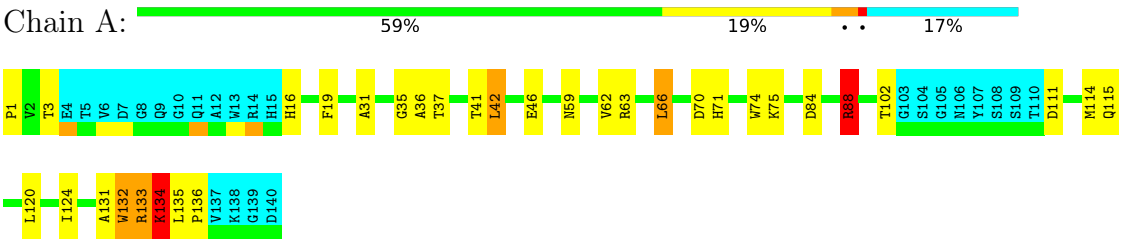
Chain A:



4.2.50 Score per residue for model 50

• Molecule 1: Capsid protein p27

Chain A:



5 Refinement protocol and experimental data overview

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

Of the 150 calculated structures, 50 were deposited, based on the following criterion: *10 structures for lowest energy.*

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

Software name	Classification	Version
CNS	refinement	

No chemical shift data was provided.

6 Model quality

6.1 Standard geometry

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	0.88±0.03	0±0/940 (0.0± 0.0%)	0.85±0.03	0±0/1283 (0.0± 0.0%)
All	All	0.88	6/47000 (0.0%)	0.85	17/64150 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	Chirality	Planarity
1	A	0.1±0.2	0.8±0.8
All	All	3	39

All unique bond 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(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	134	LYS	N-CA	6.66	1.59	1.46	50	3
1	A	132	TRP	CD1-NE1	-5.50	1.28	1.38	36	2
1	A	128	ALA	C-O	-5.20	1.13	1.23	27	1

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(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	134	LYS	N-CA-C	6.61	128.83	111.00	27	10
1	A	134	LYS	N-CA-CB	-5.89	99.99	110.60	35	2
1	A	1	PRO	N-CA-CB	5.63	110.06	103.30	47	2
1	A	16	HIS	N-CA-C	-5.20	96.95	111.00	39	1
1	A	116	TYR	CB-CA-C	-5.02	100.37	110.40	2	1
1	A	74	TRP	CA-CB-CG	5.00	123.21	113.70	23	1

All unique chiral outliers are listed below.

Mol	Chain	Res	Type	Atoms	Models (Total)
1	A	134	LYS	CA	3

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

Mol	Chain	Res	Type	Group	Models (Total)
1	A	133	ARG	Sidechain	22
1	A	88	ARG	Sidechain	9
1	A	83	ARG	Sidechain	8

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	914	877	875	20±3
All	All	45700	43850	43750	999

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 11.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:74:TRP:CG	1:A:132:TRP:HA	0.78	2.13	41	50
1:A:116:TYR:O	1:A:120:LEU:HB3	0.75	1.82	8	5
1:A:74:TRP:HA	1:A:131:ALA:O	0.70	1.85	24	50
1:A:134:LYS:HE2	1:A:134:LYS:N	0.70	2.01	30	2
1:A:69:GLY:C	1:A:135:LEU:HG	0.67	2.10	46	3
1:A:31:ALA:HB1	1:A:66:LEU:HG	0.67	1.65	2	14
1:A:74:TRP:O	1:A:131:ALA:HB1	0.67	1.90	41	50
1:A:86:ALA:HA	1:A:97:ASP:OD1	0.66	1.90	32	1
1:A:59:ASN:O	1:A:63:ARG:HG3	0.65	1.91	16	3
1:A:50:ASP:HA	1:A:125:GLN:NE2	0.65	2.06	33	5
1:A:133:ARG:NE	1:A:134:LYS:HA	0.64	2.07	14	4
1:A:62:VAL:HB	1:A:132:TRP:CZ3	0.64	2.28	14	19
1:A:73:LEU:HB2	1:A:135:LEU:HD12	0.64	1.70	24	7

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:89:ASN:OD1	1:A:94:ASN:HB2	0.63	1.94	5	6
1:A:101:LEU:HD13	1:A:124:ILE:HG12	0.63	1.71	24	1
1:A:36:ALA:HB3	1:A:135:LEU:HB2	0.62	1.69	17	8
1:A:130:LYS:O	1:A:134:LYS:HE2	0.62	1.94	15	12
1:A:61:LEU:O	1:A:65:VAL:HB	0.61	1.95	48	3
1:A:59:ASN:O	1:A:63:ARG:HG2	0.61	1.95	21	4
1:A:59:ASN:O	1:A:63:ARG:HB2	0.61	1.96	31	5
1:A:74:TRP:CD1	1:A:135:LEU:HD13	0.61	2.31	24	20
1:A:101:LEU:O	1:A:102:THR:HB	0.60	1.95	40	16
1:A:90:GLN:HE22	1:A:97:ASP:HA	0.60	1.56	9	4
1:A:84:ASP:O	1:A:88:ARG:HD3	0.60	1.96	16	9
1:A:120:LEU:O	1:A:124:ILE:HG13	0.59	1.97	50	1
1:A:113:GLN:NE2	1:A:113:GLN:HA	0.59	2.11	46	2
1:A:73:LEU:HB3	1:A:134:LYS:HG3	0.59	1.74	14	8
1:A:74:TRP:CB	1:A:132:TRP:HA	0.59	2.27	30	50
1:A:1:PRO:O	1:A:17:ASN:HB3	0.59	1.98	47	4
1:A:70:ASP:O	1:A:74:TRP:HB2	0.59	1.98	3	48
1:A:36:ALA:CB	1:A:135:LEU:HB2	0.59	2.28	49	5
1:A:42:LEU:O	1:A:46:GLU:HG3	0.58	1.98	28	19
1:A:37:THR:HG23	1:A:135:LEU:O	0.58	1.99	3	3
1:A:36:ALA:HA	1:A:41:THR:HG21	0.57	1.74	23	6
1:A:97:ASP:HA	1:A:101:LEU:HB3	0.57	1.75	4	10
1:A:38:ALA:O	1:A:41:THR:HG22	0.57	2.00	42	6
1:A:36:ALA:HB3	1:A:135:LEU:HD22	0.57	1.76	48	7
1:A:20:ASP:O	1:A:23:VAL:HB	0.56	1.99	25	1
1:A:83:ARG:O	1:A:87:LYS:HG2	0.56	2.00	38	2
1:A:58:TRP:CZ2	1:A:124:ILE:HG23	0.56	2.35	33	3
1:A:100:MET:SD	1:A:112:ALA:HB1	0.56	2.41	4	2
1:A:37:THR:HB	1:A:135:LEU:O	0.55	2.02	41	2
1:A:113:GLN:H	1:A:113:GLN:NE2	0.55	1.99	39	1
1:A:82:CYS:SG	1:A:102:THR:HG21	0.55	2.41	42	3
1:A:82:CYS:HB3	1:A:101:LEU:O	0.54	2.03	30	6
1:A:86:ALA:HA	1:A:97:ASP:HB3	0.54	1.80	34	6
1:A:101:LEU:HD13	1:A:124:ILE:HA	0.54	1.79	47	11
1:A:31:ALA:CB	1:A:66:LEU:HG	0.54	2.33	50	6
1:A:29:THR:O	1:A:33:GLN:HB3	0.54	2.03	27	4
1:A:113:GLN:NE2	1:A:113:GLN:H	0.54	2.00	43	3
1:A:85:THR:HG22	1:A:97:ASP:OD2	0.54	2.02	37	1
1:A:96:TRP:CZ2	1:A:120:LEU:HB2	0.54	2.38	46	1
1:A:83:ARG:O	1:A:87:LYS:HG3	0.54	2.03	48	16
1:A:86:ALA:O	1:A:90:GLN:HG2	0.54	2.02	35	14

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:35:GLY:O	1:A:41:THR:HG21	0.54	2.03	42	11
1:A:36:ALA:HB1	1:A:135:LEU:O	0.53	2.03	4	2
1:A:133:ARG:HD3	1:A:133:ARG:C	0.53	2.23	50	18
1:A:61:LEU:O	1:A:65:VAL:HG22	0.53	2.03	43	9
1:A:42:LEU:O	1:A:46:GLU:HG2	0.53	2.03	46	17
1:A:28:LYS:HA	1:A:65:VAL:O	0.53	2.04	43	7
1:A:86:ALA:HB1	1:A:98:PHE:HA	0.53	1.80	25	1
1:A:126:ALA:O	1:A:130:LYS:HB2	0.53	2.03	35	1
1:A:53:LEU:HB2	1:A:57:ASP:OD2	0.53	2.04	24	1
1:A:101:LEU:O	1:A:102:THR:HG22	0.52	2.03	44	9
1:A:59:ASN:O	1:A:63:ARG:HD3	0.52	2.04	50	1
1:A:42:LEU:HD13	1:A:133:ARG:HG2	0.52	1.81	25	1
1:A:27:LEU:HD13	1:A:44:ILE:HB	0.52	1.81	3	7
1:A:83:ARG:HD2	1:A:98:PHE:CE2	0.52	2.40	25	2
1:A:34:TYR:O	1:A:38:ALA:HB3	0.52	2.03	30	1
1:A:1:PRO:O	1:A:17:ASN:HB2	0.52	2.05	23	3
1:A:58:TRP:HB3	1:A:132:TRP:CH2	0.52	2.40	22	2
1:A:90:GLN:CA	1:A:90:GLN:HE21	0.52	2.17	23	2
1:A:97:ASP:O	1:A:101:LEU:HB3	0.52	2.05	47	9
1:A:66:LEU:HB2	1:A:70:ASP:HB3	0.51	1.82	38	2
1:A:96:TRP:CD1	1:A:120:LEU:HB2	0.51	2.39	25	4
1:A:83:ARG:HE	1:A:102:THR:HG21	0.51	1.66	14	2
1:A:62:VAL:HG23	1:A:74:TRP:CE3	0.51	2.40	20	13
1:A:101:LEU:O	1:A:102:THR:HG23	0.51	2.06	23	1
1:A:113:GLN:HE21	1:A:114:MET:N	0.51	2.03	20	6
1:A:74:TRP:HA	1:A:131:ALA:C	0.51	2.25	11	10
1:A:73:LEU:HG	1:A:134:LYS:O	0.51	2.06	27	8
1:A:36:ALA:O	1:A:37:THR:HB	0.50	2.05	9	6
1:A:116:TYR:CD2	1:A:121:PHE:HB2	0.50	2.41	36	3
1:A:119:GLY:O	1:A:123:GLN:HB2	0.50	2.07	34	1
1:A:96:TRP:HZ2	1:A:117:ASP:OD1	0.50	1.89	6	1
1:A:133:ARG:HD3	1:A:134:LYS:N	0.50	2.22	40	1
1:A:94:ASN:HB3	1:A:96:TRP:CE3	0.50	2.42	48	3
1:A:55:PRO:HD3	1:A:113:GLN:OE1	0.50	2.07	18	2
1:A:66:LEU:CB	1:A:70:ASP:HB3	0.49	2.37	6	13
1:A:119:GLY:O	1:A:123:GLN:HG2	0.49	2.07	25	5
1:A:113:GLN:H	1:A:113:GLN:HE21	0.49	1.50	43	2
1:A:44:ILE:O	1:A:48:VAL:HG23	0.49	2.08	42	15
1:A:45:VAL:HG11	1:A:132:TRP:O	0.49	2.07	18	10
1:A:85:THR:HG23	1:A:97:ASP:OD2	0.49	2.08	34	1
1:A:97:ASP:HA	1:A:101:LEU:CB	0.49	2.38	37	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:66:LEU:HD11	1:A:135:LEU:HD21	0.48	1.85	27	1
1:A:46:GLU:OE2	1:A:129:THR:HB	0.48	2.09	11	1
1:A:132:TRP:CD1	1:A:132:TRP:N	0.48	2.82	36	8
1:A:87:LYS:O	1:A:91:GLN:HG2	0.48	2.09	42	5
1:A:36:ALA:CB	1:A:135:LEU:HD22	0.48	2.39	42	1
1:A:59:ASN:O	1:A:63:ARG:HB3	0.47	2.10	6	1
1:A:96:TRP:HD1	1:A:100:MET:SD	0.47	2.32	32	3
1:A:49:ALA:O	1:A:125:GLN:HG3	0.47	2.09	16	3
1:A:90:GLN:NE2	1:A:97:ASP:HA	0.47	2.24	9	3
1:A:101:LEU:CD1	1:A:124:ILE:HA	0.47	2.39	46	2
1:A:82:CYS:HB2	1:A:101:LEU:HD21	0.47	1.86	22	1
1:A:31:ALA:HB1	1:A:66:LEU:HD13	0.47	1.86	37	5
1:A:132:TRP:N	1:A:132:TRP:CD1	0.46	2.83	17	34
1:A:125:GLN:O	1:A:129:THR:HG22	0.46	2.09	21	2
1:A:71:HIS:O	1:A:75:LYS:HB2	0.46	2.10	25	16
1:A:97:ASP:OD2	1:A:123:GLN:HG2	0.46	2.10	17	2
1:A:79:PHE:O	1:A:83:ARG:HG2	0.46	2.11	45	1
1:A:42:LEU:HG	1:A:133:ARG:HG3	0.46	1.88	46	1
1:A:77:GLU:HG2	1:A:134:LYS:NZ	0.46	2.26	24	1
1:A:51:ASN:O	1:A:53:LEU:HD22	0.46	2.11	38	1
1:A:77:GLU:HB3	1:A:81:ASN:ND2	0.46	2.26	29	2
1:A:120:LEU:O	1:A:124:ILE:HG23	0.46	2.11	29	1
1:A:37:THR:N	1:A:42:LEU:HD11	0.46	2.26	25	1
1:A:111:ASP:O	1:A:114:MET:HG2	0.46	2.11	45	1
1:A:90:GLN:HE21	1:A:90:GLN:N	0.45	2.08	23	1
1:A:73:LEU:O	1:A:77:GLU:HB2	0.45	2.11	42	2
1:A:80:GLU:O	1:A:84:ASP:HB2	0.45	2.11	19	1
1:A:113:GLN:O	1:A:116:TYR:HB3	0.45	2.12	35	6
1:A:2:VAL:HG22	1:A:16:HIS:CB	0.45	2.41	2	1
1:A:53:LEU:HB2	1:A:57:ASP:OD1	0.45	2.10	13	1
1:A:58:TRP:CH2	1:A:124:ILE:HB	0.45	2.47	22	1
1:A:101:LEU:HB3	1:A:124:ILE:HG22	0.45	1.87	29	1
1:A:83:ARG:NH2	1:A:102:THR:HG22	0.45	2.25	45	1
1:A:113:GLN:HE21	1:A:113:GLN:CA	0.45	2.24	7	3
1:A:37:THR:HG21	1:A:133:ARG:NH2	0.45	2.27	18	1
1:A:42:LEU:H	1:A:42:LEU:HD22	0.45	1.72	18	1
1:A:96:TRP:CH2	1:A:119:GLY:HA3	0.45	2.45	25	1
1:A:66:LEU:HB3	1:A:70:ASP:HB3	0.45	1.89	6	2
1:A:135:LEU:HB3	1:A:136:PRO:HD2	0.45	1.89	47	1
1:A:101:LEU:HG	1:A:124:ILE:HG22	0.45	1.88	42	1
1:A:86:ALA:HA	1:A:97:ASP:CB	0.44	2.42	31	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:66:LEU:HD23	1:A:74:TRP:CH2	0.44	2.47	34	1
1:A:54:THR:O	1:A:57:ASP:HB3	0.44	2.12	45	1
1:A:83:ARG:NE	1:A:102:THR:HG21	0.44	2.26	31	2
1:A:53:LEU:HG	1:A:57:ASP:OD1	0.44	2.12	44	1
1:A:73:LEU:HB3	1:A:134:LYS:CG	0.44	2.42	14	3
1:A:76:SER:O	1:A:80:GLU:HG2	0.44	2.13	1	1
1:A:30:ALA:HB1	1:A:41:THR:HB	0.44	1.90	39	2
1:A:54:THR:HA	1:A:113:GLN:OE1	0.44	2.13	27	2
1:A:73:LEU:HB2	1:A:135:LEU:CD1	0.44	2.43	13	3
1:A:47:SER:O	1:A:50:ASP:HB3	0.44	2.13	37	1
1:A:97:ASP:OD2	1:A:99:ASP:HB2	0.44	2.13	42	1
1:A:30:ALA:O	1:A:34:TYR:HB2	0.44	2.12	45	5
1:A:30:ALA:HA	1:A:34:TYR:CD2	0.44	2.47	27	1
1:A:27:LEU:HG	1:A:65:VAL:CG1	0.43	2.43	13	1
1:A:66:LEU:HD23	1:A:67:SER:N	0.43	2.28	24	3
1:A:42:LEU:H	1:A:42:LEU:HD13	0.43	1.73	20	6
1:A:20:ASP:O	1:A:24:ILE:HG12	0.43	2.14	38	2
1:A:36:ALA:HB3	1:A:135:LEU:O	0.43	2.12	9	2
1:A:61:LEU:O	1:A:65:VAL:HG12	0.43	2.14	23	1
1:A:112:ALA:O	1:A:116:TYR:HA	0.43	2.13	3	2
1:A:69:GLY:O	1:A:135:LEU:HG	0.43	2.12	46	1
1:A:27:LEU:HG	1:A:65:VAL:HG11	0.43	1.91	7	1
1:A:113:GLN:HA	1:A:113:GLN:HE21	0.43	1.73	47	1
1:A:36:ALA:CB	1:A:74:TRP:HE1	0.43	2.27	15	1
1:A:71:HIS:HA	1:A:75:LYS:HB2	0.43	1.90	21	1
1:A:66:LEU:HD23	1:A:135:LEU:HD21	0.43	1.91	48	1
1:A:111:ASP:O	1:A:114:MET:HB3	0.42	2.14	39	2
1:A:37:THR:HG22	1:A:133:ARG:HH21	0.42	1.73	47	1
1:A:96:TRP:NE1	1:A:120:LEU:HB2	0.42	2.28	25	4
1:A:98:PHE:O	1:A:102:THR:HG22	0.42	2.14	8	1
1:A:36:ALA:HB1	1:A:133:ARG:O	0.42	2.13	9	1
1:A:31:ALA:HB2	1:A:66:LEU:HD12	0.42	1.91	46	1
1:A:1:PRO:HB3	1:A:19:PHE:CD1	0.42	2.50	50	1
1:A:128:ALA:O	1:A:131:ALA:HB3	0.42	2.15	2	3
1:A:65:VAL:HG23	1:A:66:LEU:H	0.42	1.73	5	1
1:A:19:PHE:CE1	1:A:57:ASP:HA	0.42	2.50	15	1
1:A:121:PHE:HA	1:A:124:ILE:HG12	0.42	1.91	32	1
1:A:120:LEU:O	1:A:124:ILE:HG12	0.42	2.14	34	2
1:A:112:ALA:HA	1:A:115:GLN:OE1	0.42	2.14	17	1
1:A:3:THR:HB	1:A:17:ASN:OD1	0.42	2.14	30	1
1:A:36:ALA:O	1:A:37:THR:HG23	0.42	2.14	46	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:82:CYS:SG	1:A:102:THR:HA	0.41	2.55	16	1
1:A:86:ALA:HB1	1:A:98:PHE:CA	0.41	2.45	25	1
1:A:33:GLN:HB2	1:A:34:TYR:CD2	0.41	2.50	46	1
1:A:101:LEU:O	1:A:101:LEU:HG	0.41	2.15	12	2
1:A:73:LEU:HD13	1:A:134:LYS:O	0.41	2.15	4	1
1:A:77:GLU:O	1:A:81:ASN:HB3	0.41	2.15	13	1
1:A:62:VAL:HG11	1:A:75:LYS:HD3	0.41	1.91	27	1
1:A:111:ASP:O	1:A:115:GLN:HG2	0.41	2.15	50	1
1:A:1:PRO:HB3	1:A:51:ASN:OD1	0.41	2.15	4	1
1:A:90:GLN:HE21	1:A:90:GLN:HA	0.41	1.76	7	1
1:A:66:LEU:HD13	1:A:135:LEU:CD2	0.41	2.46	45	1
1:A:16:HIS:HB2	1:A:114:MET:SD	0.41	2.56	50	1
1:A:59:ASN:HB3	1:A:63:ARG:NH1	0.41	2.31	50	1
1:A:123:GLN:HE21	1:A:123:GLN:HA	0.41	1.74	36	1
1:A:84:ASP:HA	1:A:87:LYS:NZ	0.41	2.31	8	1
1:A:78:PHE:O	1:A:82:CYS:SG	0.41	2.79	13	1
1:A:42:LEU:HG	1:A:133:ARG:CG	0.41	2.46	19	1
1:A:36:ALA:HB2	1:A:66:LEU:HD21	0.41	1.93	31	1
1:A:36:ALA:HA	1:A:41:THR:CG2	0.41	2.46	5	1
1:A:30:ALA:HB1	1:A:41:THR:OG1	0.41	2.16	30	1
1:A:33:GLN:HG3	1:A:34:TYR:CD1	0.41	2.51	39	1
1:A:40:TYR:CE2	1:A:44:ILE:HD11	0.41	2.51	49	1
1:A:72:LEU:HD12	1:A:73:LEU:N	0.40	2.32	4	1
1:A:27:LEU:O	1:A:31:ALA:HB2	0.40	2.16	18	1
1:A:56:THR:HA	1:A:59:ASN:OD1	0.40	2.16	30	1
1:A:89:ASN:HD22	1:A:97:ASP:CG	0.40	2.18	11	1
1:A:69:GLY:O	1:A:72:LEU:HG	0.40	2.16	37	2
1:A:1:PRO:HD2	1:A:18:GLY:O	0.40	2.16	18	1
1:A:53:LEU:HD23	1:A:58:TRP:CD1	0.40	2.52	1	2
1:A:37:THR:CA	1:A:42:LEU:HD11	0.40	2.47	25	1
1:A:101:LEU:O	1:A:102:THR:CB	0.40	2.70	29	1
1:A:36:ALA:O	1:A:135:LEU:HB2	0.40	2.17	41	1
1:A:31:ALA:HB1	1:A:66:LEU:CG	0.40	2.44	2	1
1:A:42:LEU:HD13	1:A:42:LEU:H	0.40	1.76	6	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	115/140 (82%)	103±2 (90±2%)	7±2 (6±2%)	4±1 (4±1%)	5 33
All	All	5750/7000 (82%)	5174 (90%)	358 (6%)	218 (4%)	5 33

All 17 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	132	TRP	44
1	A	102	THR	36
1	A	134	LYS	34
1	A	37	THR	33
1	A	136	PRO	21
1	A	116	TYR	19
1	A	117	ASP	8
1	A	97	ASP	7
1	A	18	GLY	4
1	A	53	LEU	4
1	A	35	GLY	2
1	A	65	VAL	1
1	A	39	PRO	1
1	A	70	ASP	1
1	A	54	THR	1
1	A	19	PHE	1
1	A	118	PRO	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	93/111 (84%)	86±2 (93±2%)	7±2 (7±2%)	18 66
All	All	4650/5550 (84%)	4310 (93%)	340 (7%)	18 66

All 44 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	42	LEU	49
1	A	133	ARG	49
1	A	113	GLN	41
1	A	134	LYS	36
1	A	135	LEU	21
1	A	125	GLN	15
1	A	17	ASN	12
1	A	102	THR	10
1	A	53	LEU	9
1	A	88	ARG	8
1	A	63	ARG	8
1	A	115	GLN	8
1	A	51	ASN	7
1	A	66	LEU	5
1	A	123	GLN	5
1	A	83	ARG	5
1	A	101	LEU	5
1	A	98	PHE	4
1	A	33	GLN	3
1	A	37	THR	3
1	A	97	ASP	3
1	A	90	GLN	2
1	A	58	TRP	2
1	A	136	PRO	2
1	A	41	THR	2
1	A	71	HIS	2
1	A	99	ASP	2
1	A	116	TYR	2
1	A	54	THR	2
1	A	77	GLU	2
1	A	81	ASN	2
1	A	94	ASN	2
1	A	48	VAL	1
1	A	28	LYS	1
1	A	72	LEU	1
1	A	44	ILE	1
1	A	26	GLU	1
1	A	87	LYS	1
1	A	60	THR	1
1	A	1	PRO	1
1	A	117	ASP	1
1	A	57	ASP	1
1	A	85	THR	1

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Mol	Chain	Res	Type	Models (Total)
1	A	70	ASP	1

6.3.3 RNA

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates

There are no monosaccharides in this entry.

6.6 Ligand geometry

There are no ligands in this entry.

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

No chemical shift data were provided