Full wwPDB NMR Structure Validation Report (i)

Jun 5, 2023 – 11:19 AM EDT

PDB ID	:	2M8P
BMRB ID	:	19264
Title	:	The structure of the W184AM185A mutant of the HIV-1 capsid protein
Authors	:	Deshmukh, L.; Schwieters, C.D.; Grishaev, A.; Clore, G.; Ghirlando, R.
Deposited on	:	2013-05-24

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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

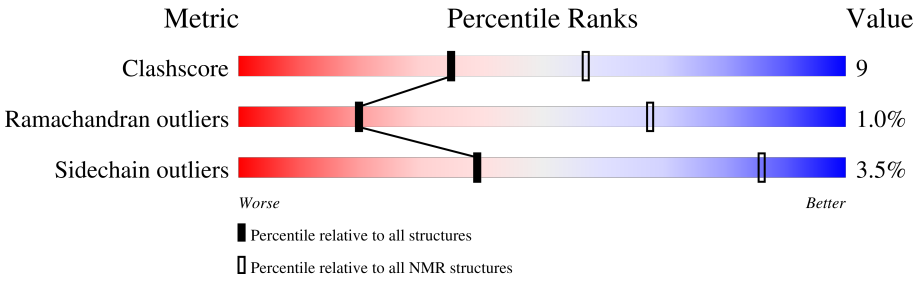
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.33

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
SOLUTION NMR, SOLUTION SCATTERING

The overall completeness of chemical shifts assignment is 34%.

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	231	81% 13%

2 Ensemble composition and analysis (i)

This entry contains 100 models. Model 35 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:145 (145)	0.05	35
2	A:150-A:221 (72)	0.04	51

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 15 clusters and 4 single-model clusters were found.

Cluster number	Models
1	3, 5, 8, 10, 15, 20, 21, 28, 30, 35, 40, 45, 50, 51, 60, 63, 70, 73, 76, 85, 90, 93, 98, 100
2	1, 6, 11, 25, 26, 36, 46, 49, 55, 65, 66, 75, 80, 81, 95, 96
3	7, 12, 27, 37, 47, 67, 82, 97
4	19, 23, 34, 44, 53, 59, 78
5	24, 54, 64, 74, 79, 94
6	4, 9, 14, 29, 39, 99
7	17, 32, 42, 57, 87
8	16, 31, 41, 56
9	18, 43, 58, 88
10	13, 38, 48, 72
11	61, 71, 91
12	22, 52, 77
13	62, 92
14	2, 33
15	69, 84
Single-model clusters	68; 83; 86; 89

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 3436 atoms, of which 1723 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Capsid protein p24.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	221	3436	1078	1723	300	323	12	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	184	ALA	TRP	engineered mutation	UNP P12497
A	185	ALA	MET	engineered mutation	UNP P12497

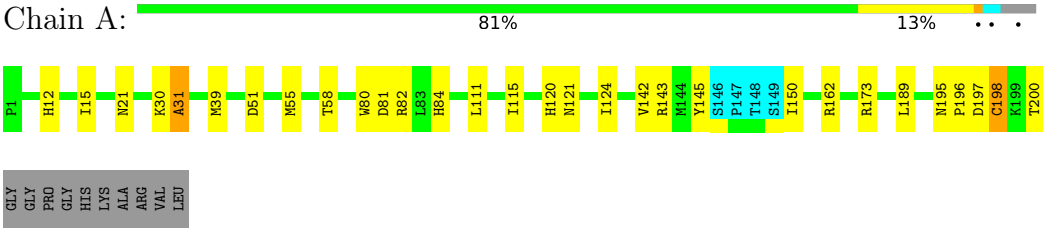
4 Residue-property plots

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 p24

Chain A:



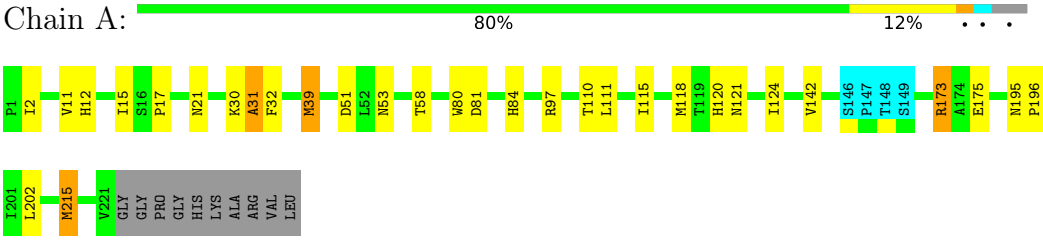
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: Capsid protein p24

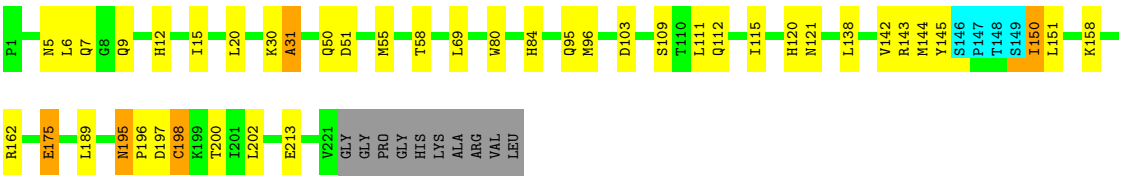
Chain A:



4.2.2 Score per residue for model 2

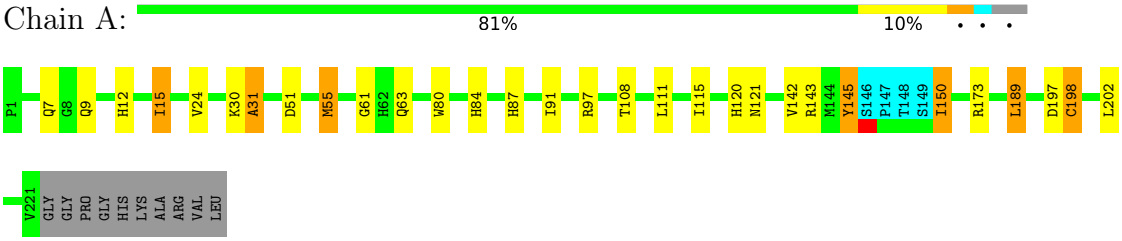
• Molecule 1: Capsid protein p24

Chain A:



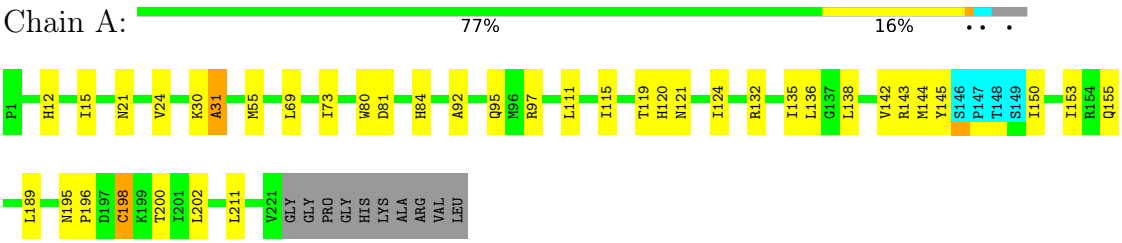
4.2.3 Score per residue for model 3

• Molecule 1: Capsid protein p24



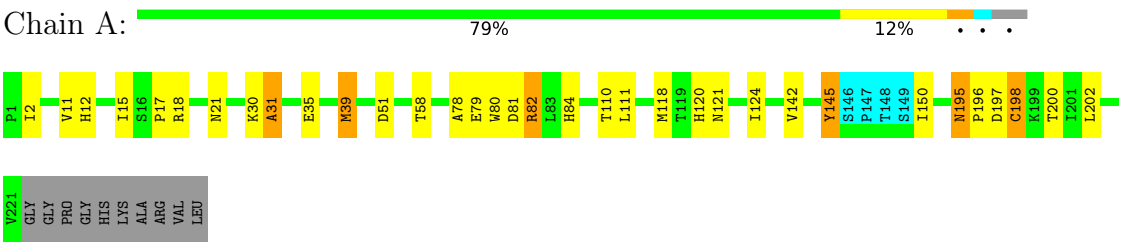
4.2.4 Score per residue for model 4

• Molecule 1: Capsid protein p24



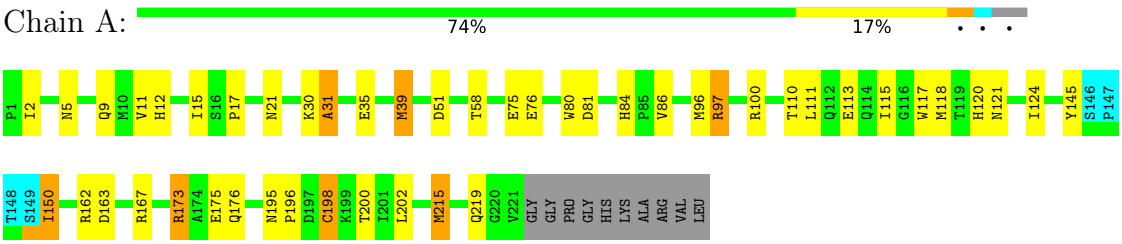
4.2.5 Score per residue for model 5

• Molecule 1: Capsid protein p24



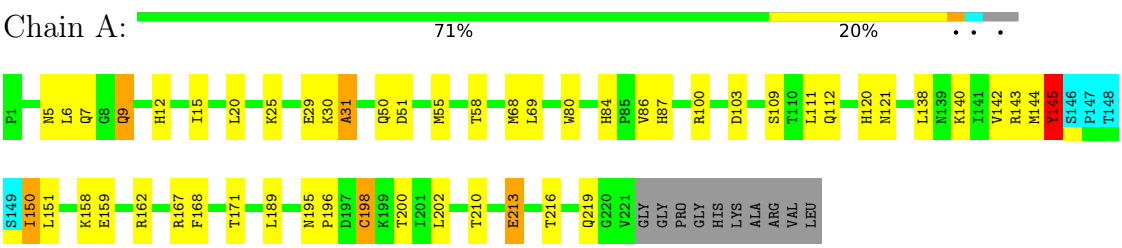
4.2.6 Score per residue for model 6

• Molecule 1: Capsid protein p24



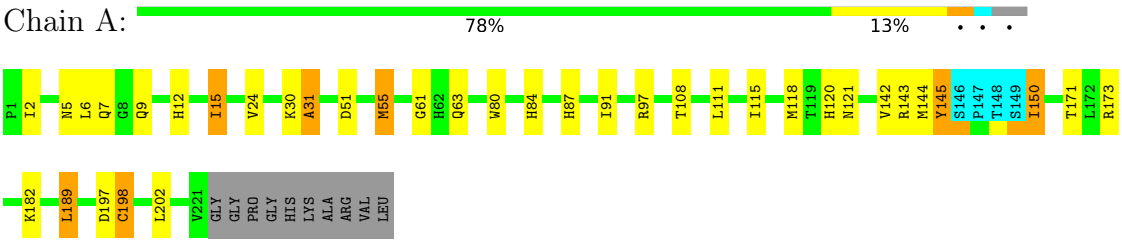
4.2.7 Score per residue for model 7

- Molecule 1: Capsid protein p24



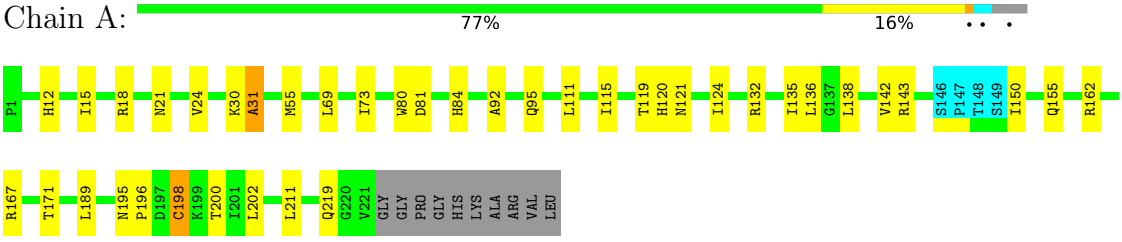
4.2.8 Score per residue for model 8

- Molecule 1: Capsid protein p24



4.2.9 Score per residue for model 9

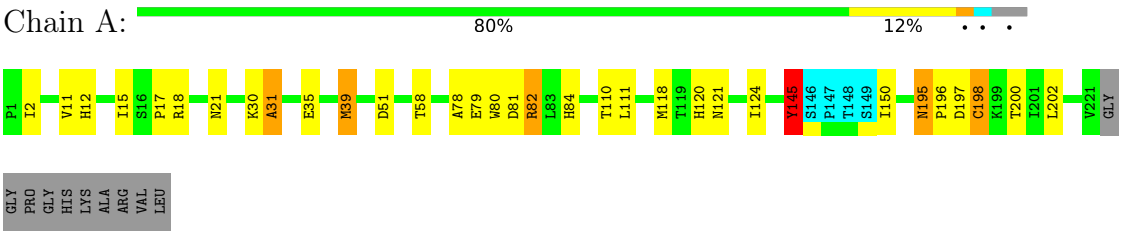
- Molecule 1: Capsid protein p24



4.2.10 Score per residue for model 10

• Molecule 1: Capsid protein p24

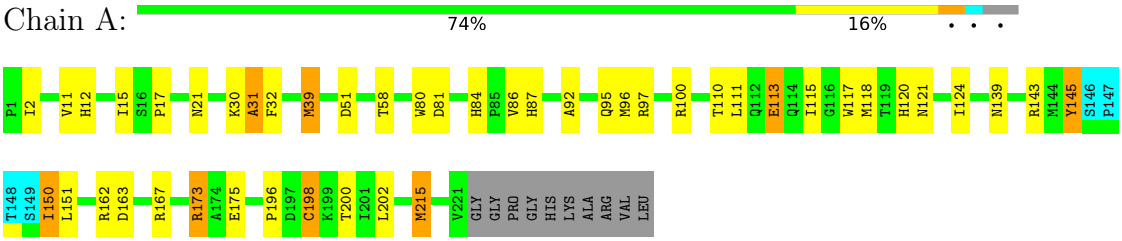
Chain A:



4.2.11 Score per residue for model 11

• Molecule 1: Capsid protein p24

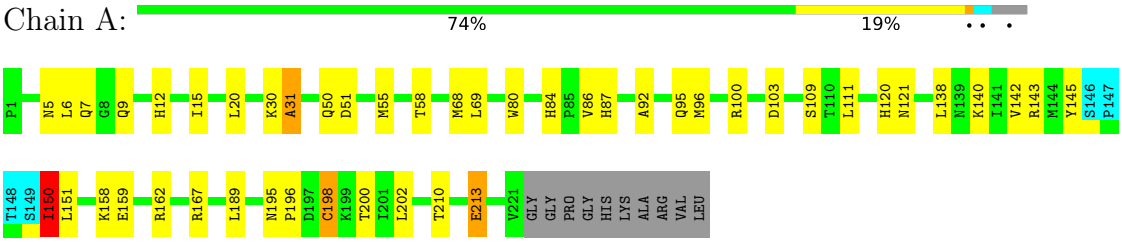
Chain A:



4.2.12 Score per residue for model 12

• Molecule 1: Capsid protein p24

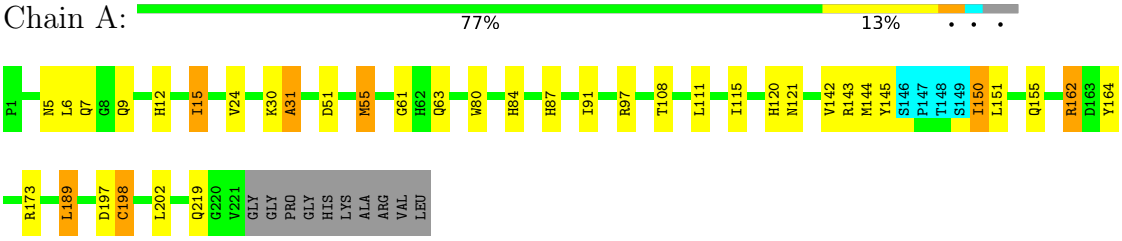
Chain A:



4.2.13 Score per residue for model 13

• Molecule 1: Capsid protein p24

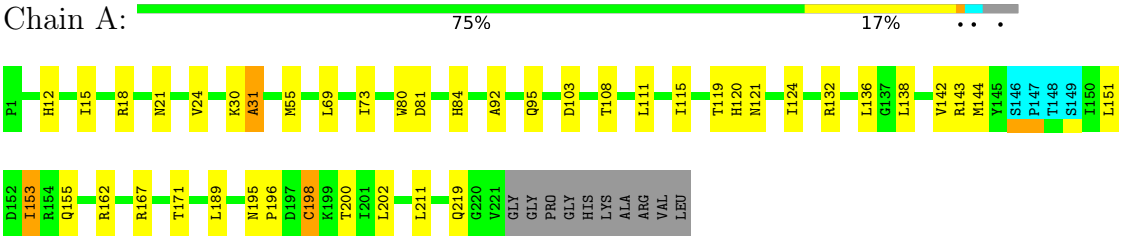
Chain A:



4.2.14 Score per residue for model 14

• Molecule 1: Capsid protein p24

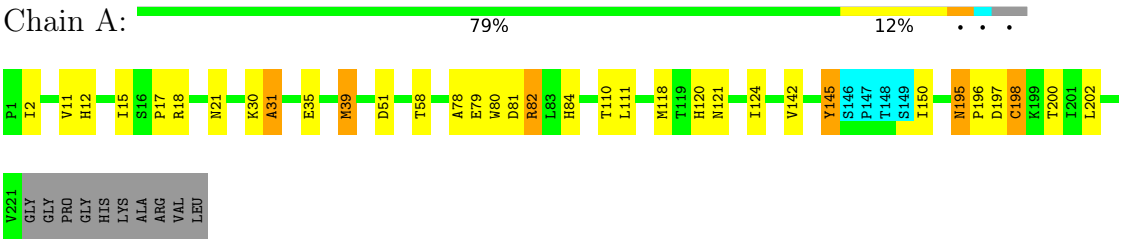
Chain A:



4.2.15 Score per residue for model 15

• Molecule 1: Capsid protein p24

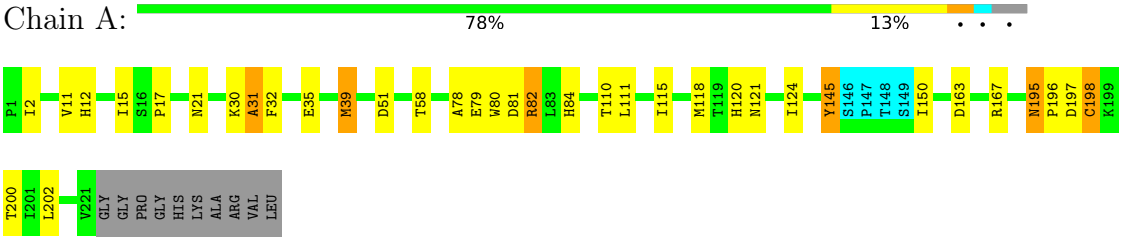
Chain A:



4.2.16 Score per residue for model 16

• Molecule 1: Capsid protein p24

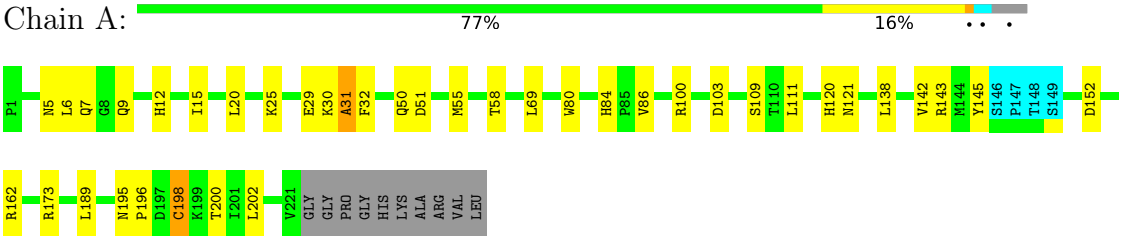
Chain A:



4.2.17 Score per residue for model 17

• Molecule 1: Capsid protein p24

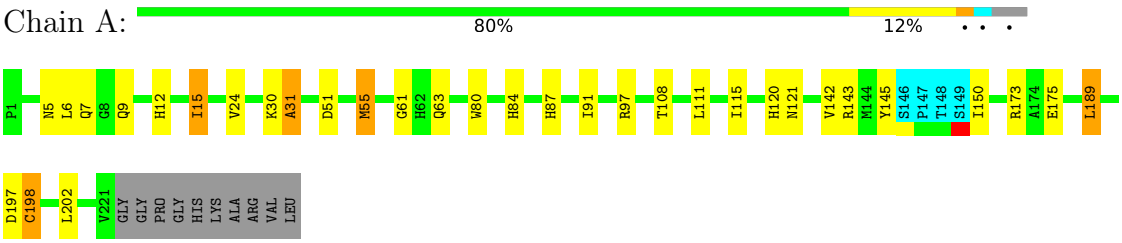
Chain A:



4.2.18 Score per residue for model 18

• Molecule 1: Capsid protein p24

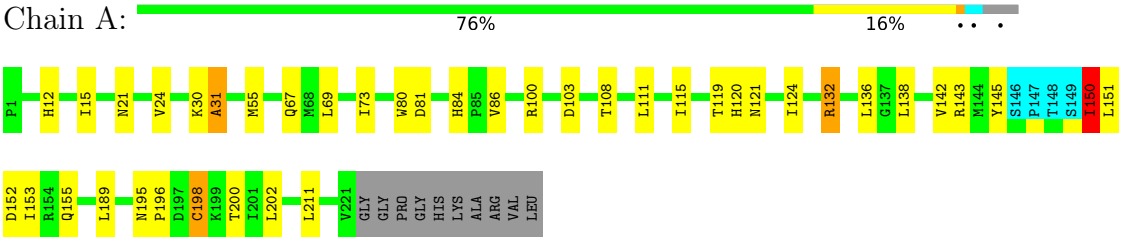
Chain A:



4.2.19 Score per residue for model 19

• Molecule 1: Capsid protein p24

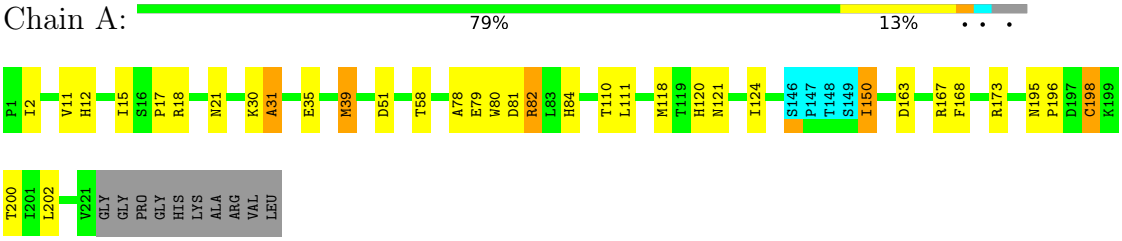
Chain A:



4.2.20 Score per residue for model 20

• Molecule 1: Capsid protein p24

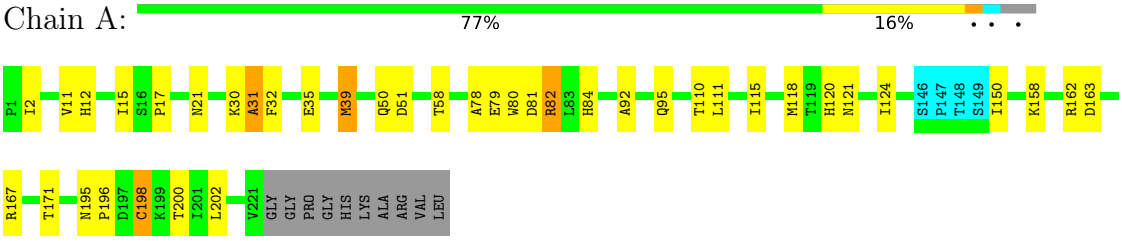
Chain A:



4.2.21 Score per residue for model 21

• Molecule 1: Capsid protein p24

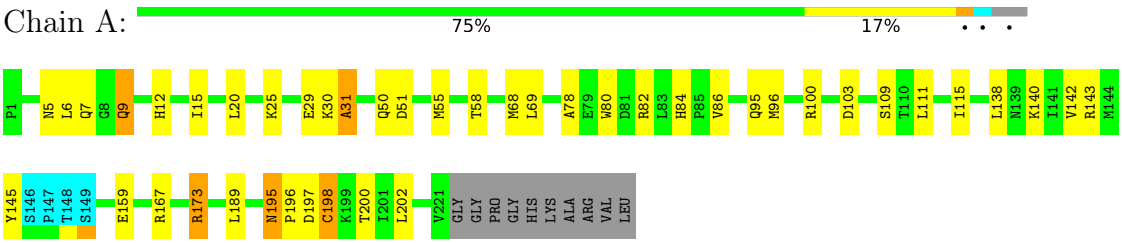
Chain A:



4.2.22 Score per residue for model 22

• Molecule 1: Capsid protein p24

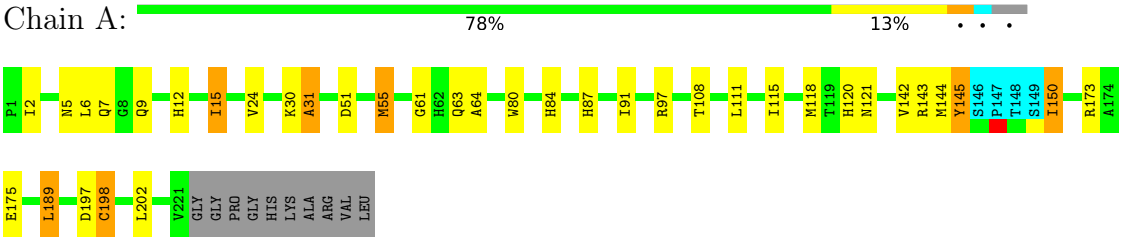
Chain A:



4.2.23 Score per residue for model 23

• Molecule 1: Capsid protein p24

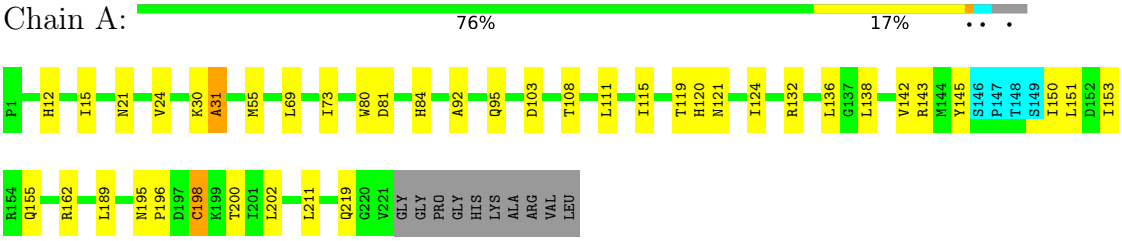
Chain A:



4.2.24 Score per residue for model 24

• Molecule 1: Capsid protein p24

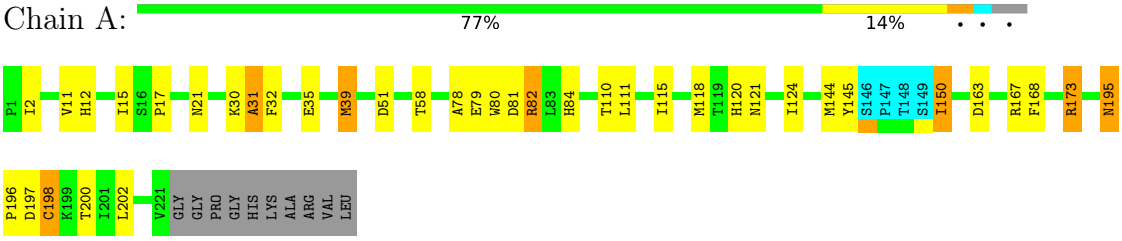
Chain A:



4.2.25 Score per residue for model 25

• Molecule 1: Capsid protein p24

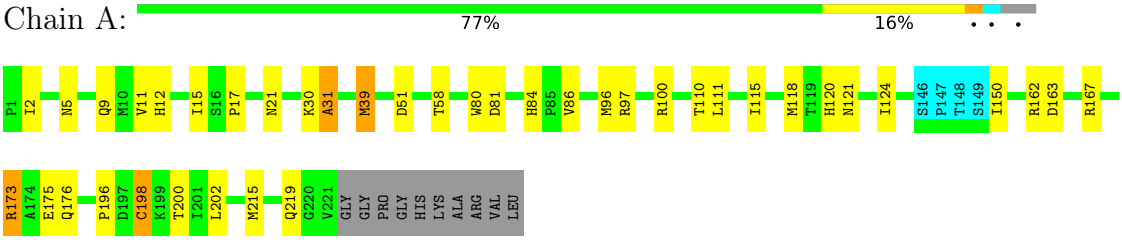
Chain A:



4.2.26 Score per residue for model 26

• Molecule 1: Capsid protein p24

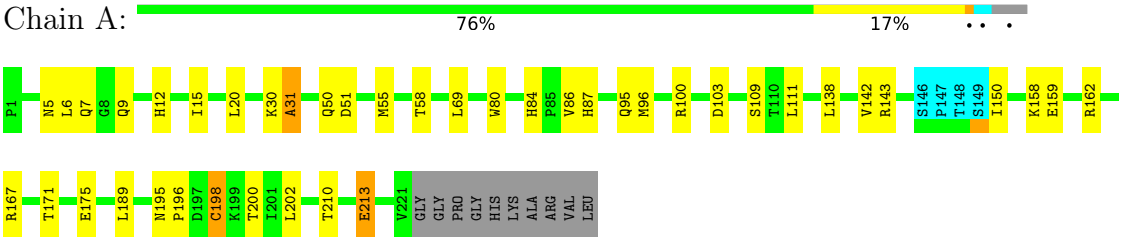
Chain A:



4.2.27 Score per residue for model 27

• Molecule 1: Capsid protein p24

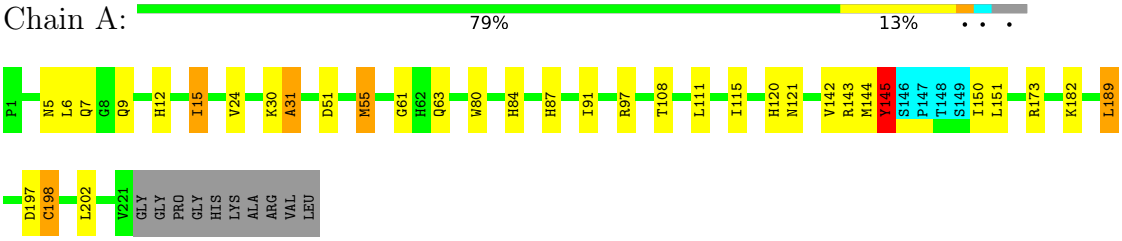
Chain A:



4.2.28 Score per residue for model 28

• Molecule 1: Capsid protein p24

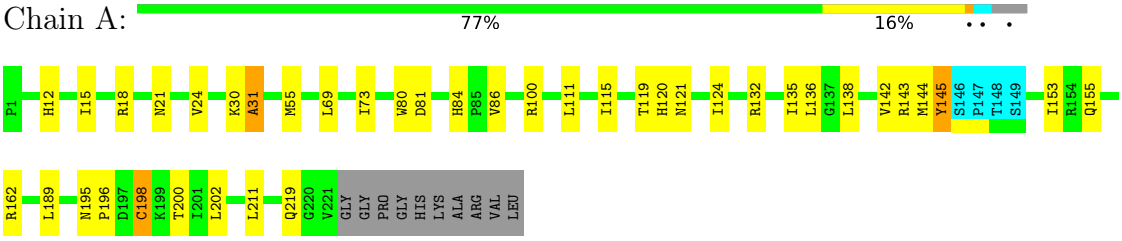
Chain A:



4.2.29 Score per residue for model 29

• Molecule 1: Capsid protein p24

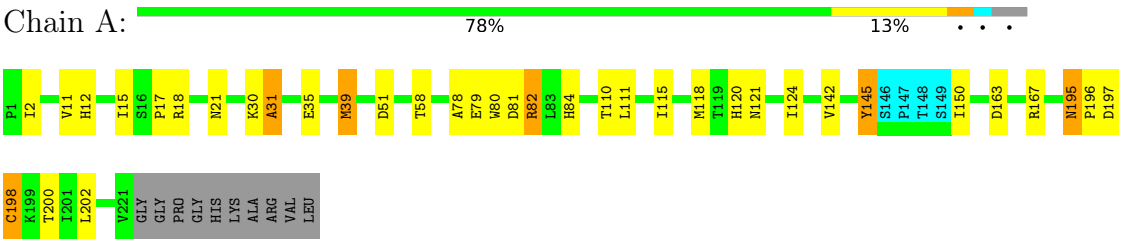
Chain A:



4.2.30 Score per residue for model 30

• Molecule 1: Capsid protein p24

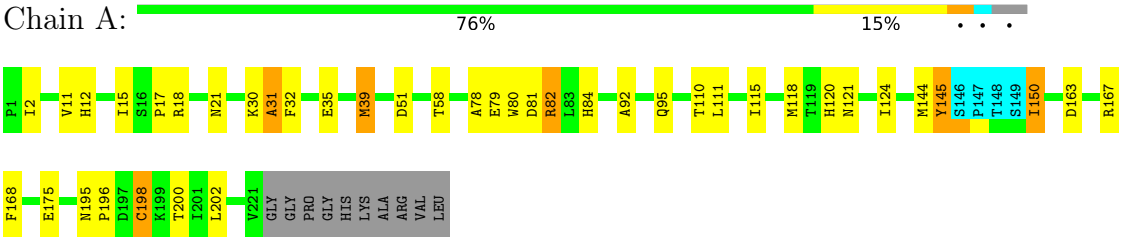
Chain A:



4.2.31 Score per residue for model 31

• Molecule 1: Capsid protein p24

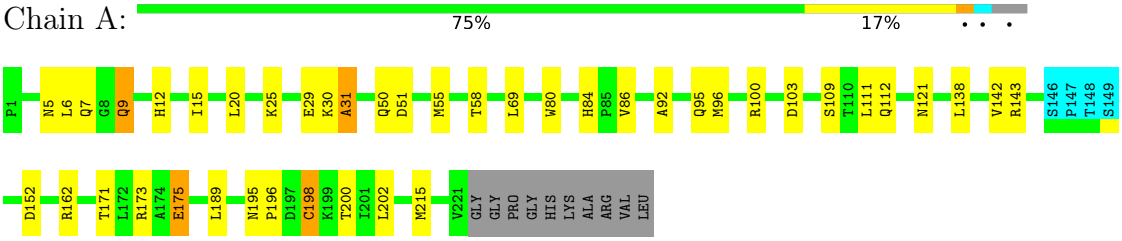
Chain A:



4.2.32 Score per residue for model 32

• Molecule 1: Capsid protein p24

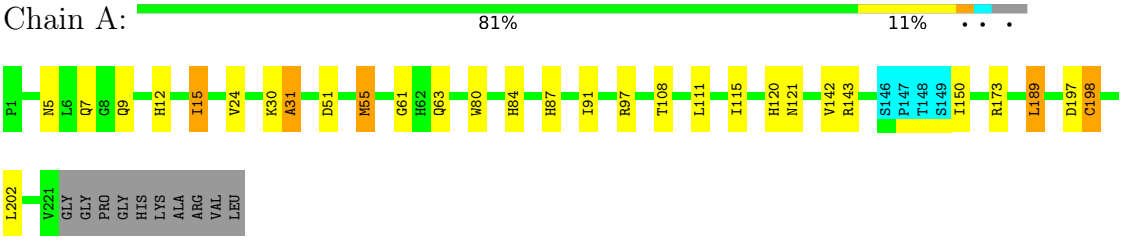
Chain A:



4.2.33 Score per residue for model 33

• Molecule 1: Capsid protein p24

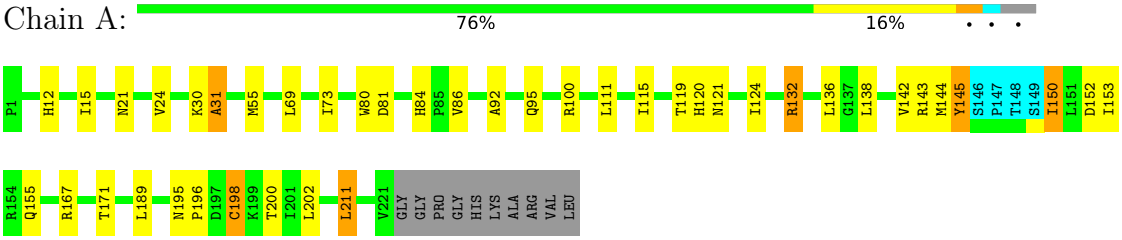
Chain A:



4.2.34 Score per residue for model 34

• Molecule 1: Capsid protein p24

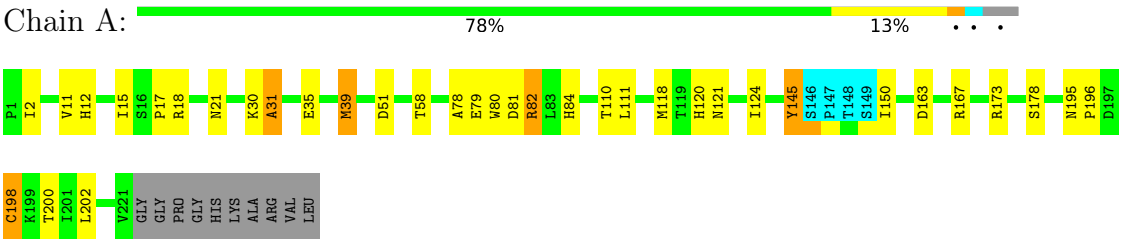
Chain A:



4.2.35 Score per residue for model 35 (medoid)

• Molecule 1: Capsid protein p24

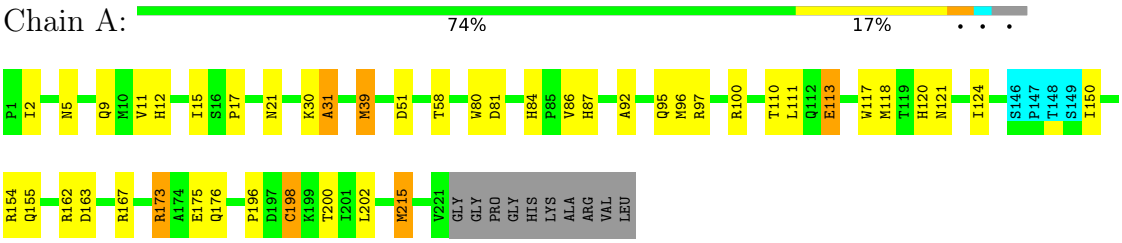
Chain A:



4.2.36 Score per residue for model 36

• Molecule 1: Capsid protein p24

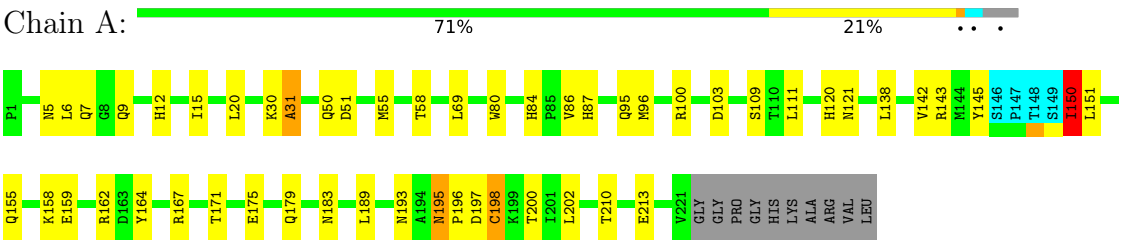
Chain A:



4.2.37 Score per residue for model 37

• Molecule 1: Capsid protein p24

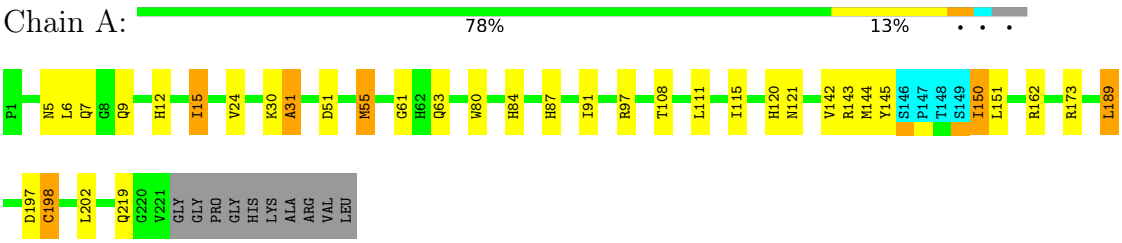
Chain A:



4.2.38 Score per residue for model 38

• Molecule 1: Capsid protein p24

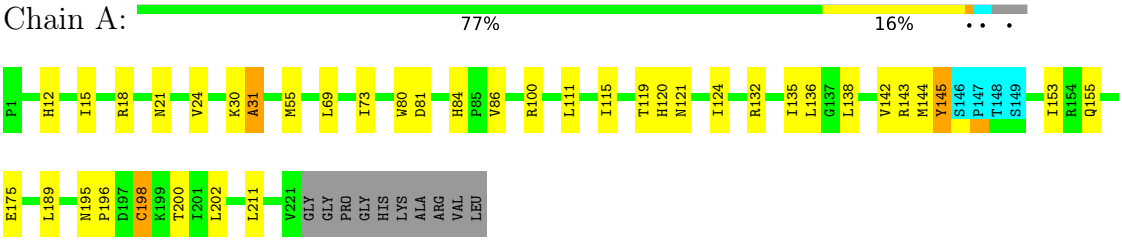
Chain A:



4.2.39 Score per residue for model 39

• Molecule 1: Capsid protein p24

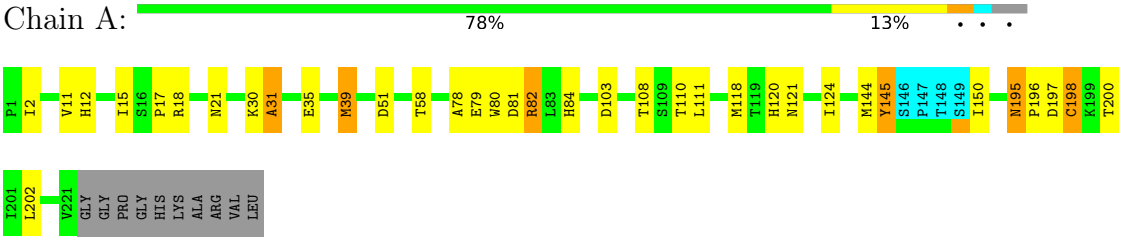
Chain A:



4.2.40 Score per residue for model 40

• Molecule 1: Capsid protein p24

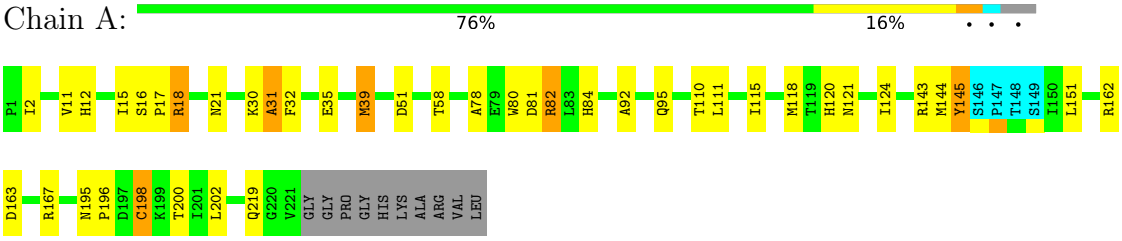
Chain A:



4.2.41 Score per residue for model 41

• Molecule 1: Capsid protein p24

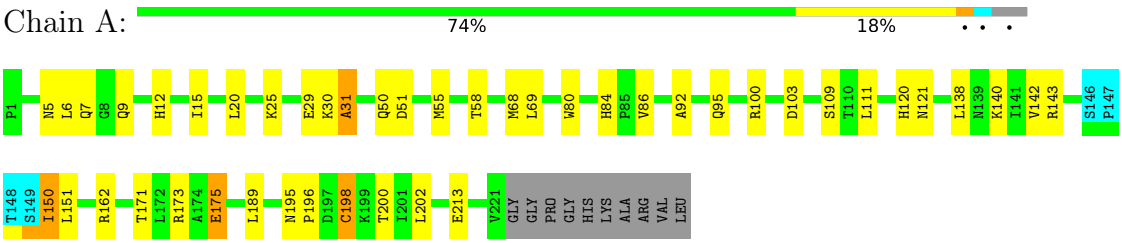
Chain A:



4.2.42 Score per residue for model 42

• Molecule 1: Capsid protein p24

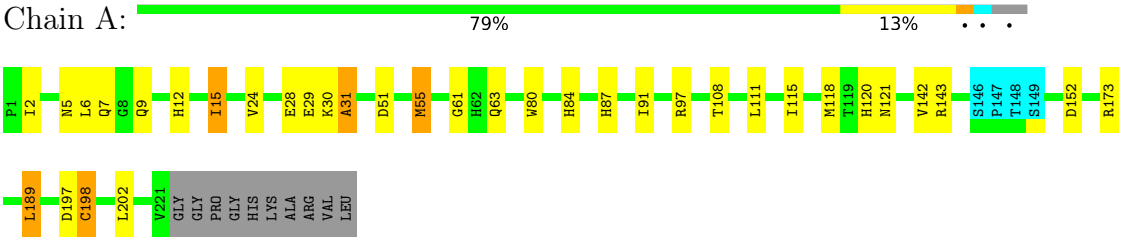
Chain A:



4.2.43 Score per residue for model 43

• Molecule 1: Capsid protein p24

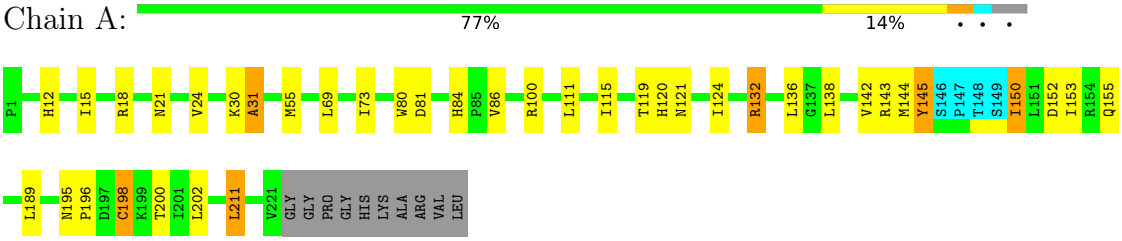
Chain A:



4.2.44 Score per residue for model 44

• Molecule 1: Capsid protein p24

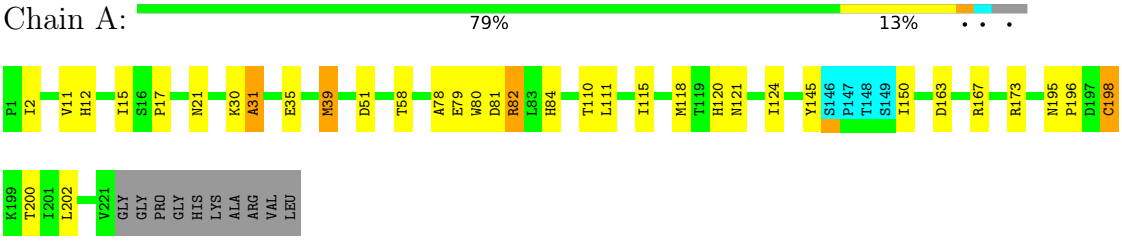
Chain A:



4.2.45 Score per residue for model 45

• Molecule 1: Capsid protein p24

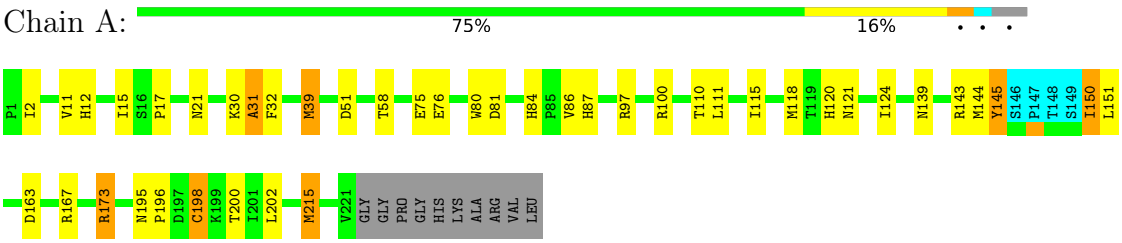
Chain A:



4.2.46 Score per residue for model 46

• Molecule 1: Capsid protein p24

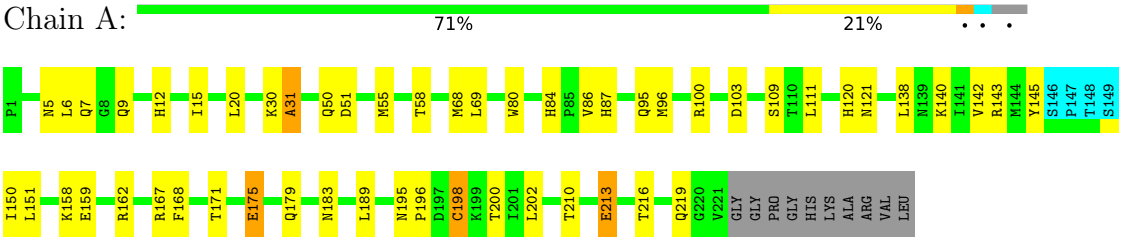
Chain A:



4.2.47 Score per residue for model 47

• Molecule 1: Capsid protein p24

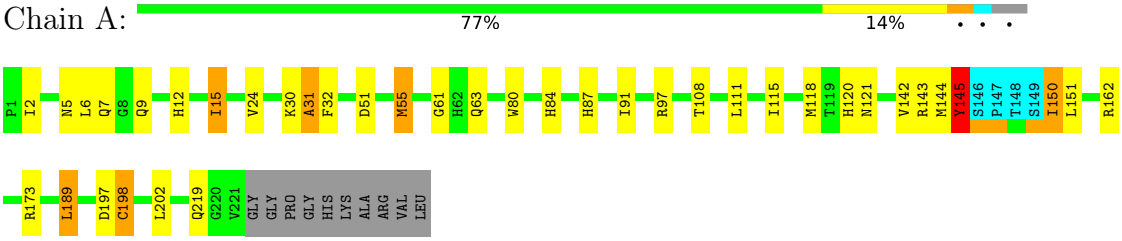
Chain A:



4.2.48 Score per residue for model 48

• Molecule 1: Capsid protein p24

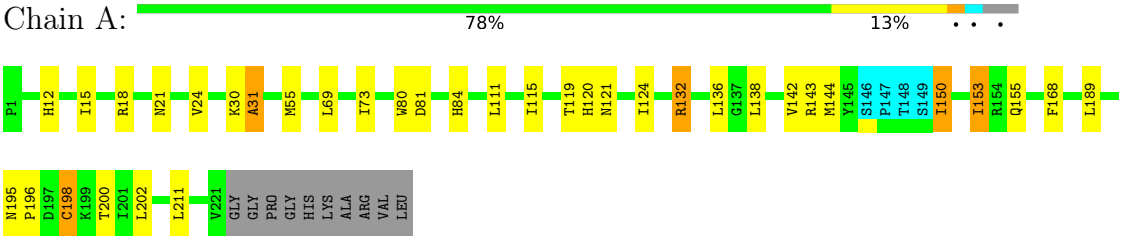
Chain A:



4.2.49 Score per residue for model 49

• Molecule 1: Capsid protein p24

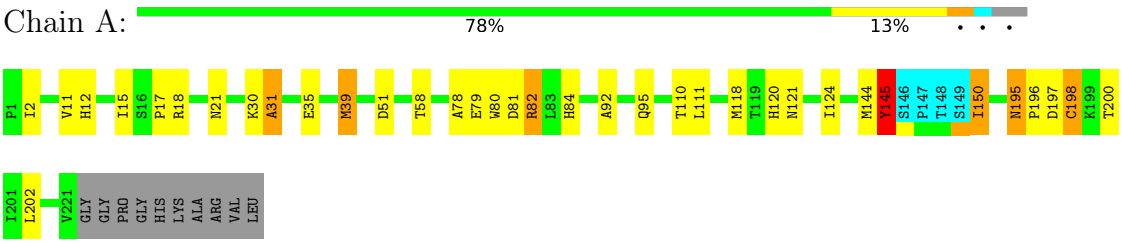
Chain A:



4.2.50 Score per residue for model 50

• Molecule 1: Capsid protein p24

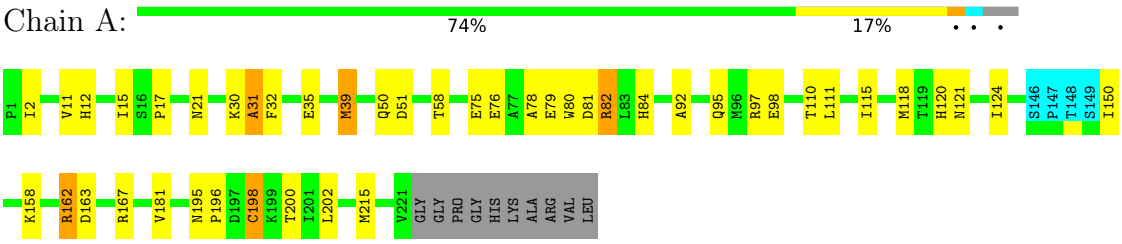
Chain A:



4.2.51 Score per residue for model 51

• Molecule 1: Capsid protein p24

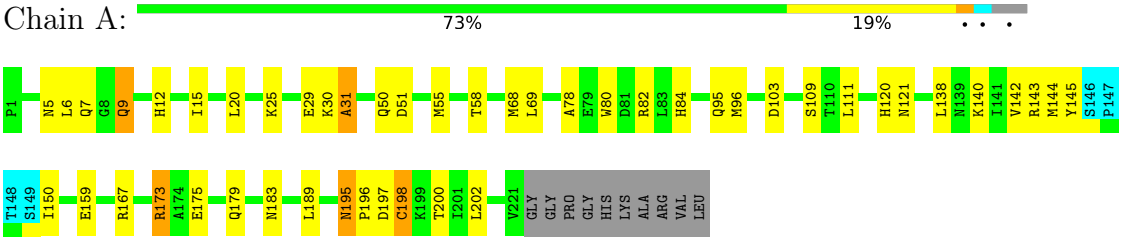
Chain A:



4.2.52 Score per residue for model 52

• Molecule 1: Capsid protein p24

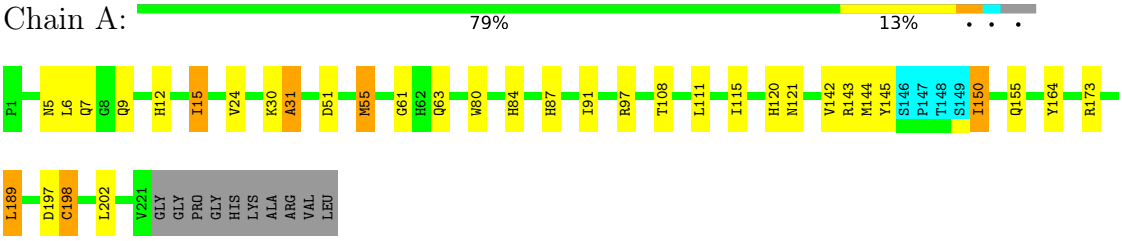
Chain A:



4.2.53 Score per residue for model 53

• Molecule 1: Capsid protein p24

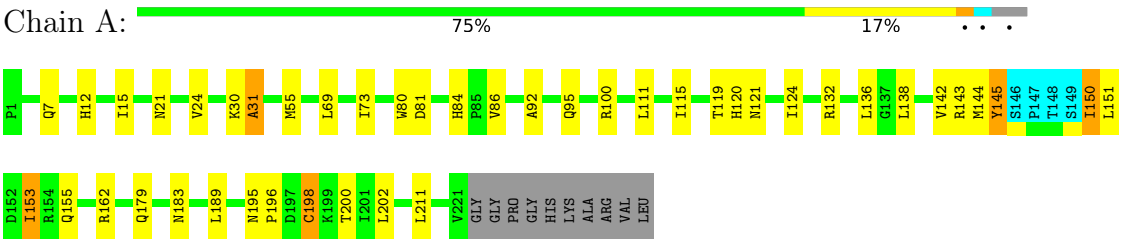
Chain A:



4.2.54 Score per residue for model 54

• Molecule 1: Capsid protein p24

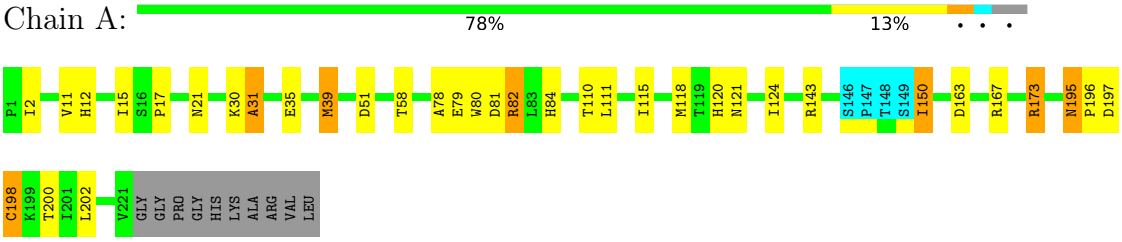
Chain A:



4.2.55 Score per residue for model 55

• Molecule 1: Capsid protein p24

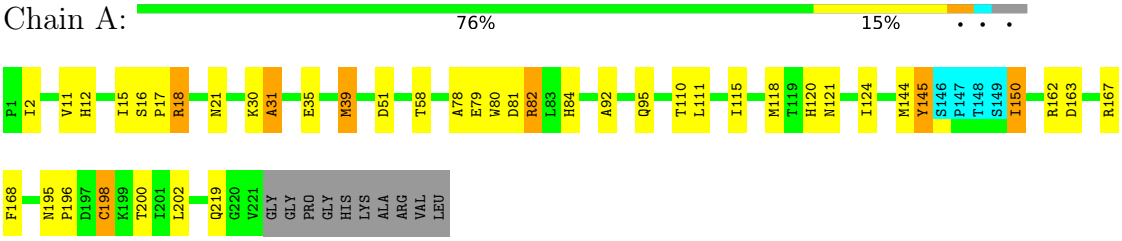
Chain A:



4.2.56 Score per residue for model 56

• Molecule 1: Capsid protein p24

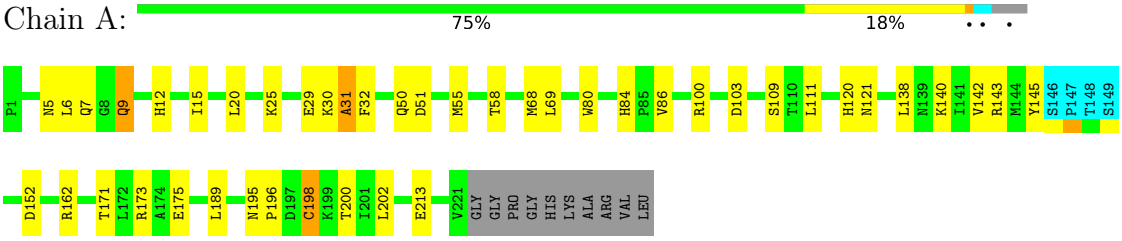
Chain A:



4.2.57 Score per residue for model 57

• Molecule 1: Capsid protein p24

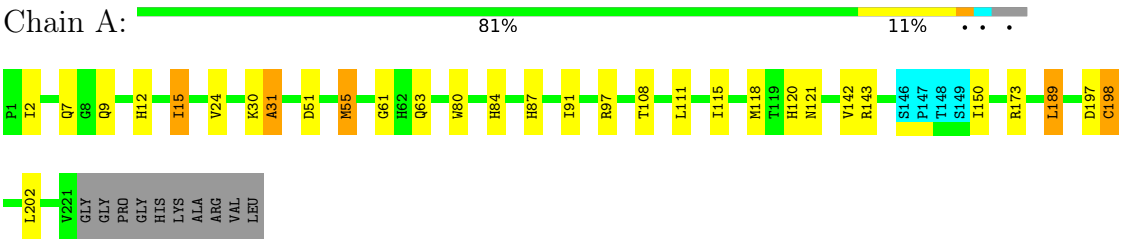
Chain A:



4.2.58 Score per residue for model 58

• Molecule 1: Capsid protein p24

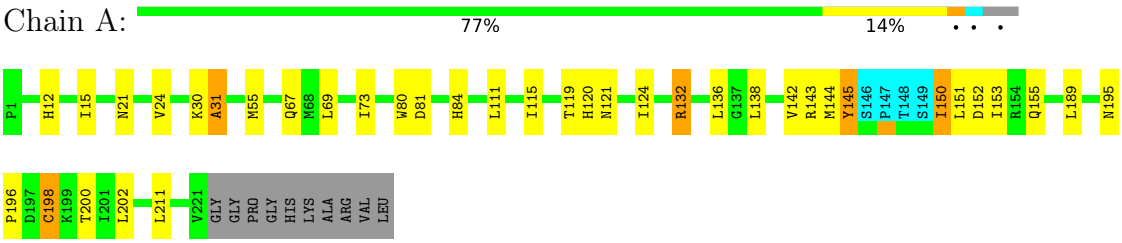
Chain A:



4.2.59 Score per residue for model 59

• Molecule 1: Capsid protein p24

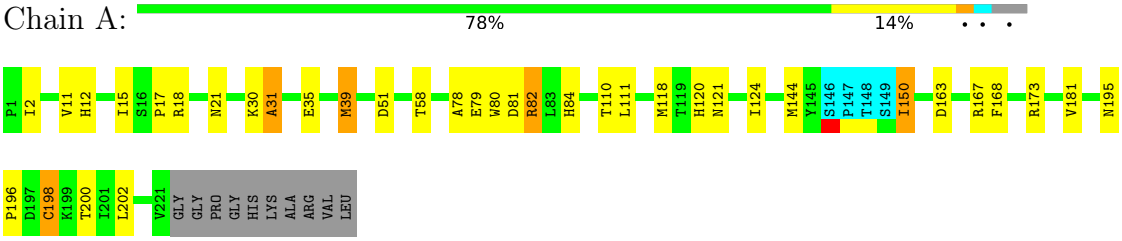
Chain A:



4.2.60 Score per residue for model 60

• Molecule 1: Capsid protein p24

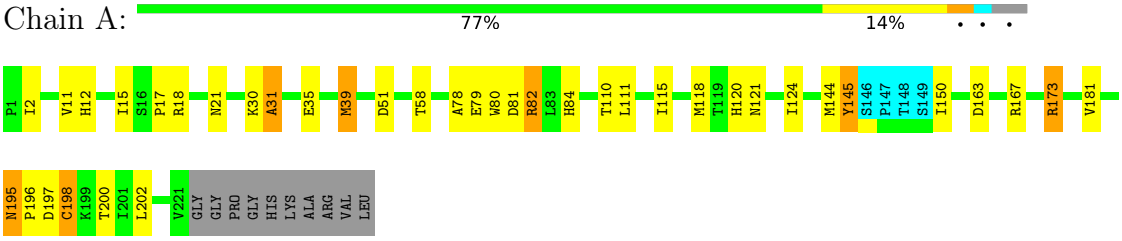
Chain A:



4.2.61 Score per residue for model 61

• Molecule 1: Capsid protein p24

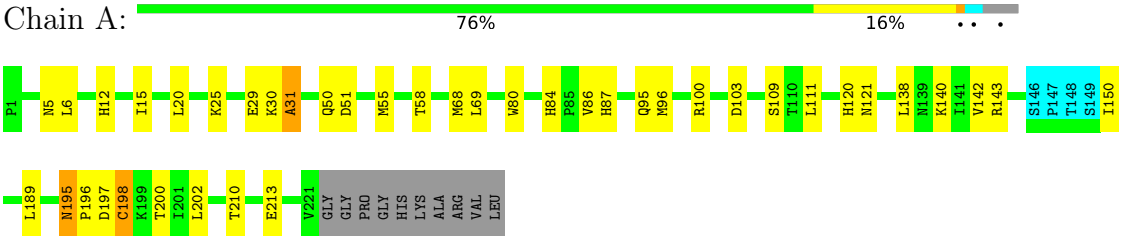
Chain A:



4.2.62 Score per residue for model 62

• Molecule 1: Capsid protein p24

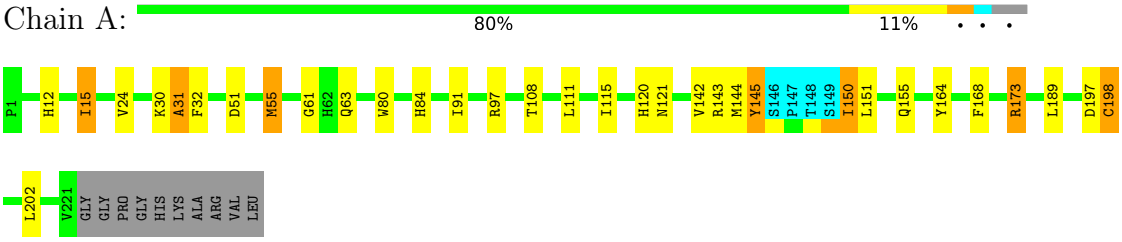
Chain A:



4.2.63 Score per residue for model 63

• Molecule 1: Capsid protein p24

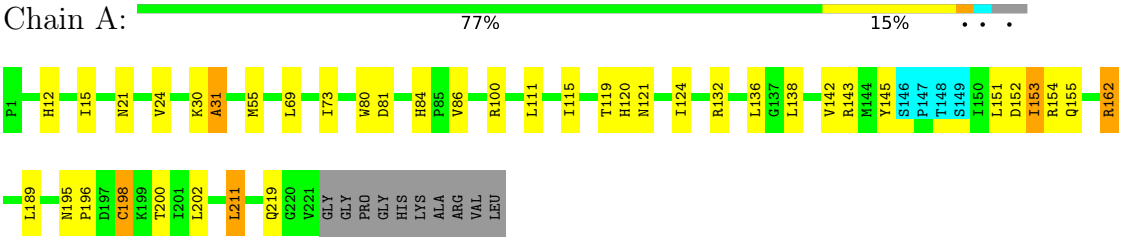
Chain A:



4.2.64 Score per residue for model 64

• Molecule 1: Capsid protein p24

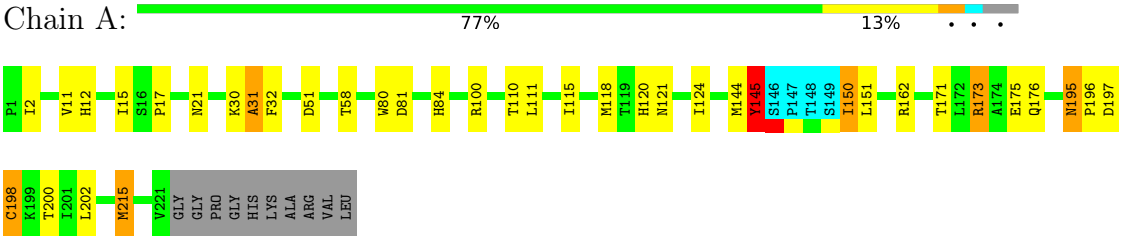
Chain A:



4.2.65 Score per residue for model 65

• Molecule 1: Capsid protein p24

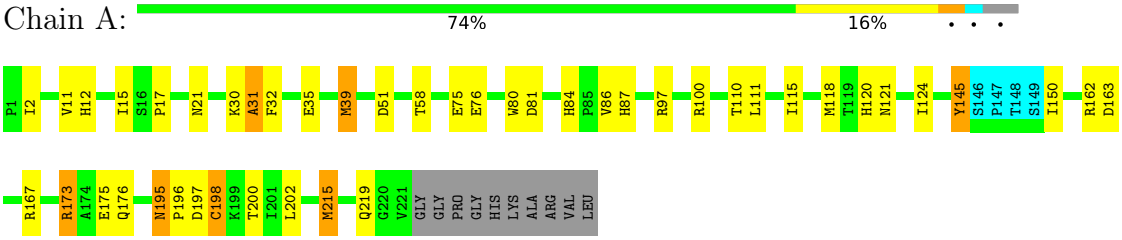
Chain A:



4.2.66 Score per residue for model 66

• Molecule 1: Capsid protein p24

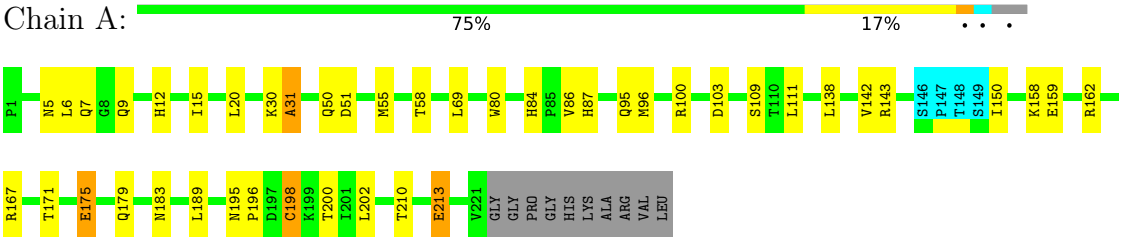
Chain A:



4.2.67 Score per residue for model 67

• Molecule 1: Capsid protein p24

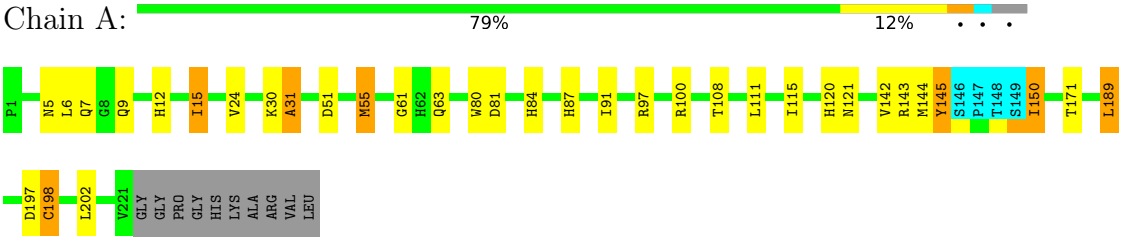
Chain A:



4.2.68 Score per residue for model 68

• Molecule 1: Capsid protein p24

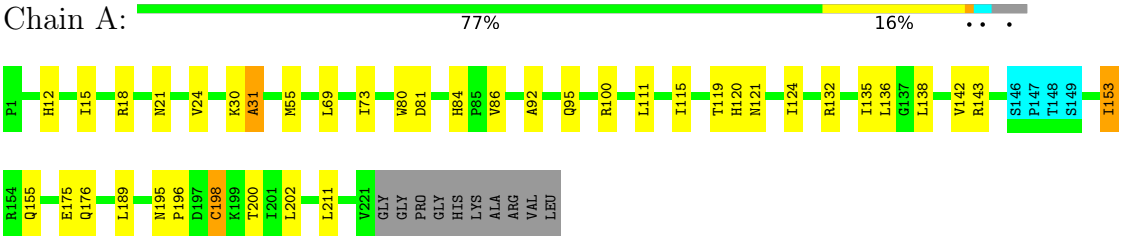
Chain A:



4.2.69 Score per residue for model 69

• Molecule 1: Capsid protein p24

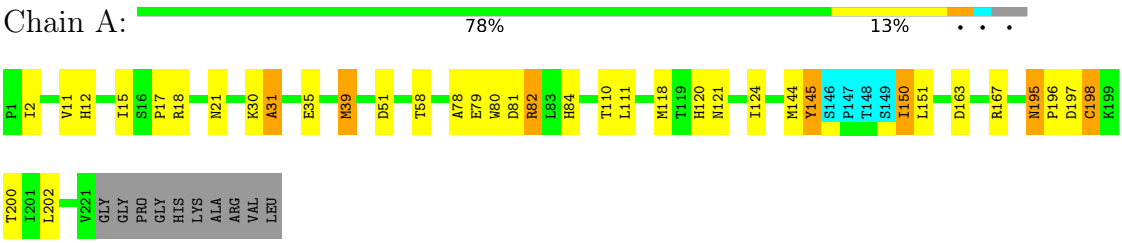
Chain A:



4.2.70 Score per residue for model 70

• Molecule 1: Capsid protein p24

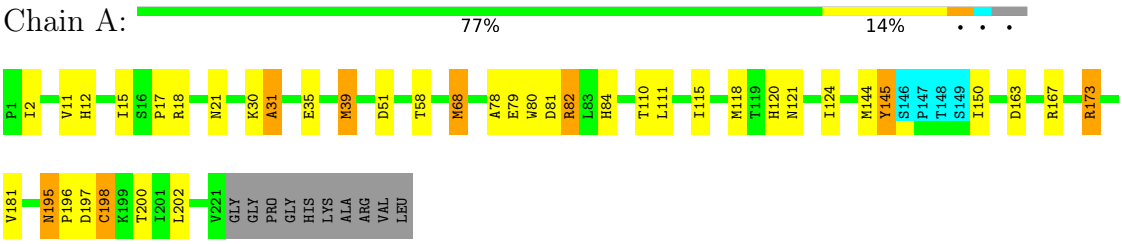
Chain A:



4.2.71 Score per residue for model 71

• Molecule 1: Capsid protein p24

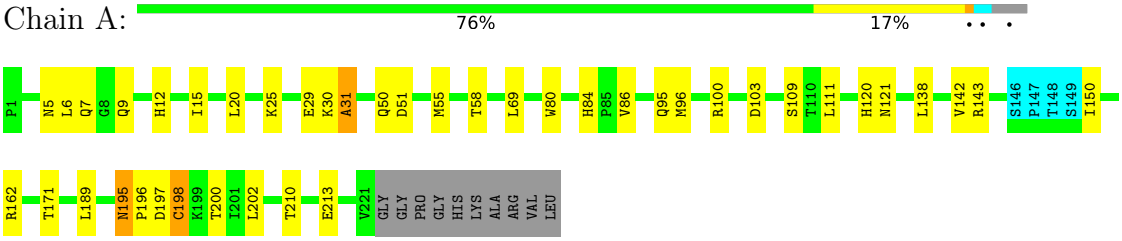
Chain A:



4.2.72 Score per residue for model 72

• Molecule 1: Capsid protein p24

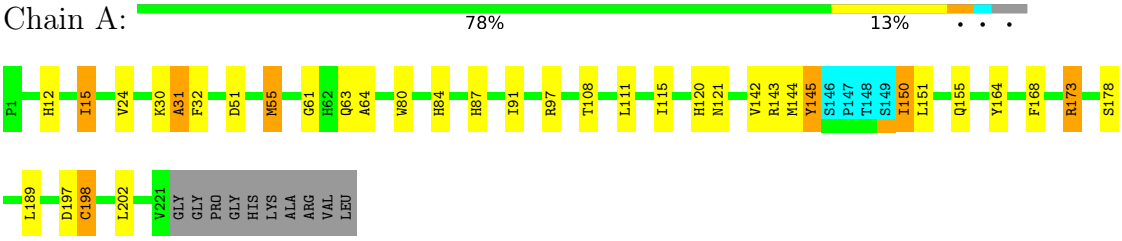
Chain A:



4.2.73 Score per residue for model 73

• Molecule 1: Capsid protein p24

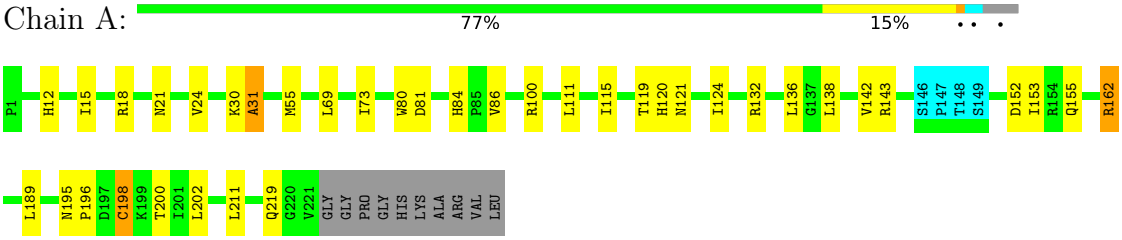
Chain A:



4.2.74 Score per residue for model 74

• Molecule 1: Capsid protein p24

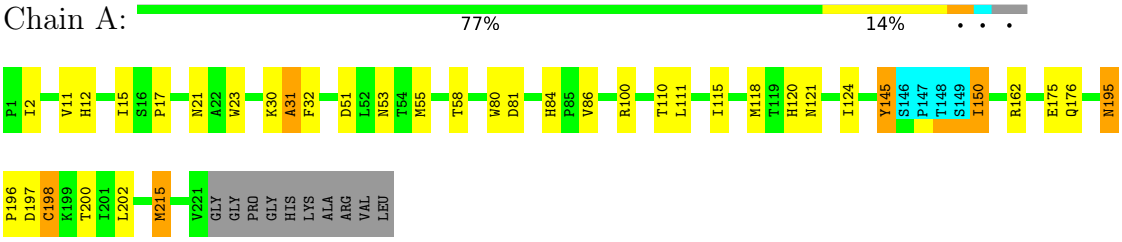
Chain A:



4.2.75 Score per residue for model 75

• Molecule 1: Capsid protein p24

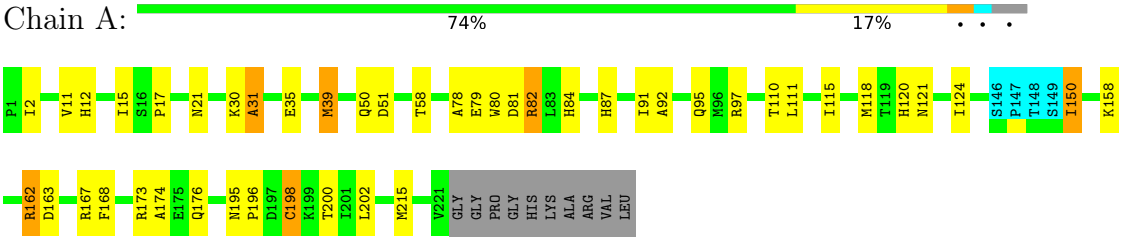
Chain A:



4.2.76 Score per residue for model 76

• Molecule 1: Capsid protein p24

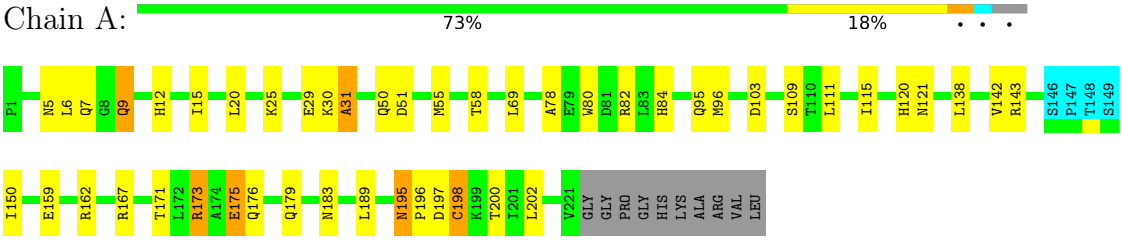
Chain A:



4.2.77 Score per residue for model 77

• Molecule 1: Capsid protein p24

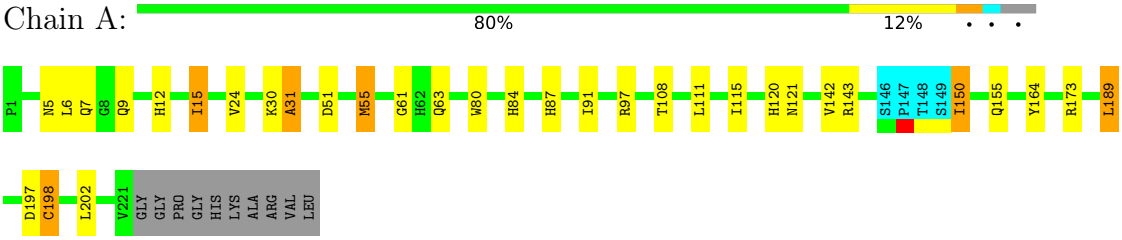
Chain A:



4.2.78 Score per residue for model 78

• Molecule 1: Capsid protein p24

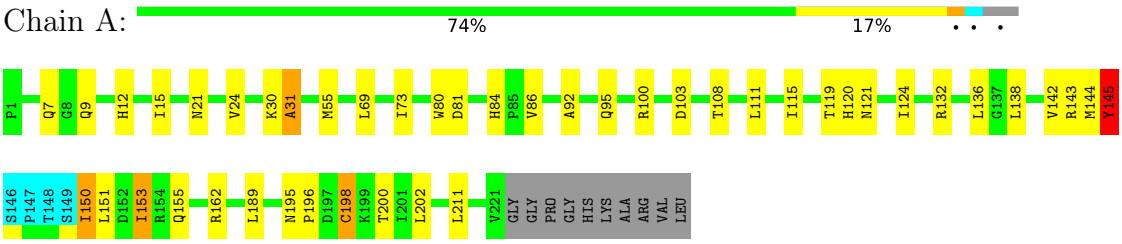
Chain A:



4.2.79 Score per residue for model 79

• Molecule 1: Capsid protein p24

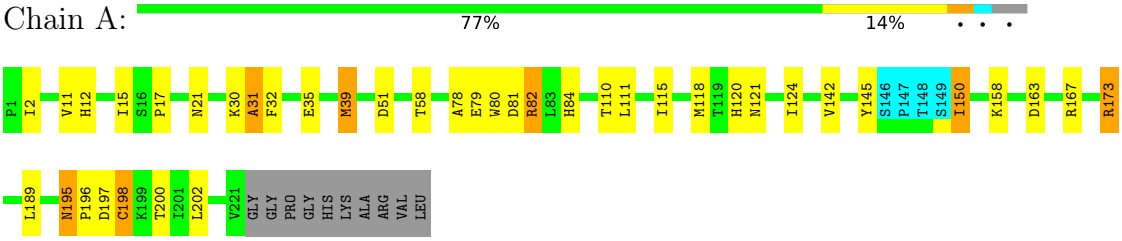
Chain A:



4.2.80 Score per residue for model 80

• Molecule 1: Capsid protein p24

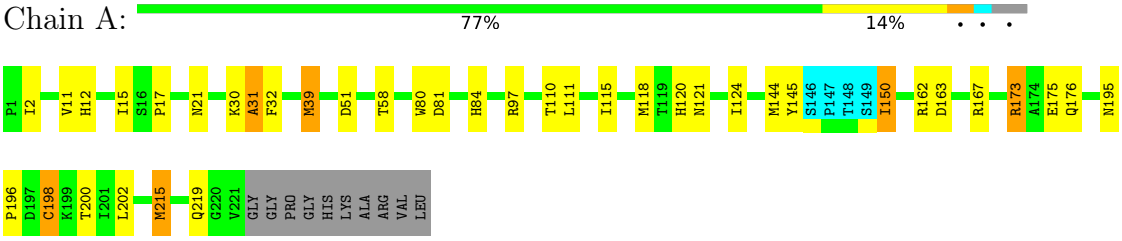
Chain A:



4.2.81 Score per residue for model 81

• Molecule 1: Capsid protein p24

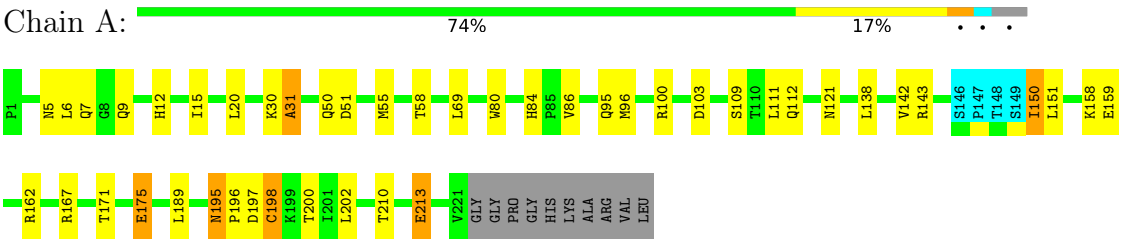
Chain A:



4.2.82 Score per residue for model 82

• Molecule 1: Capsid protein p24

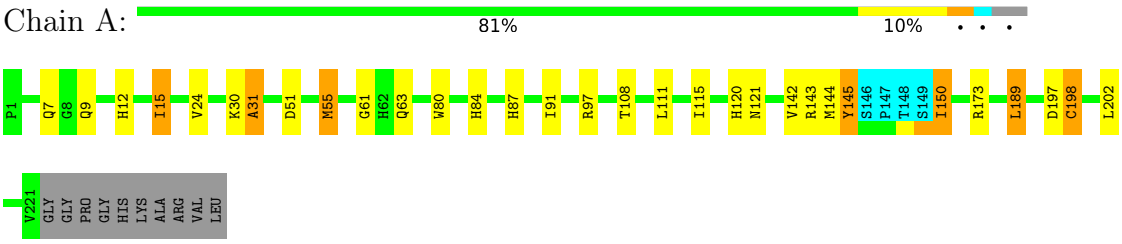
Chain A:



4.2.83 Score per residue for model 83

• Molecule 1: Capsid protein p24

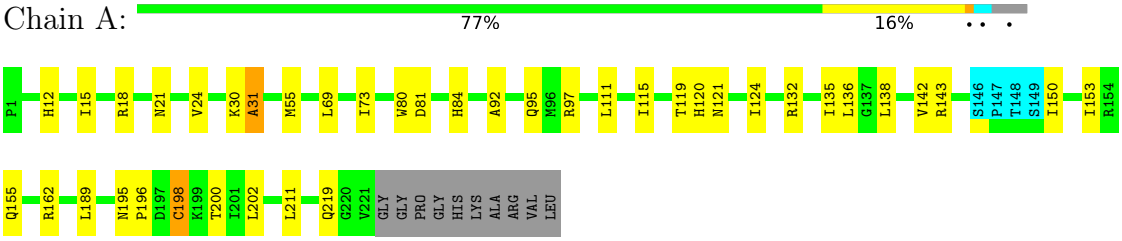
Chain A:



4.2.84 Score per residue for model 84

• Molecule 1: Capsid protein p24

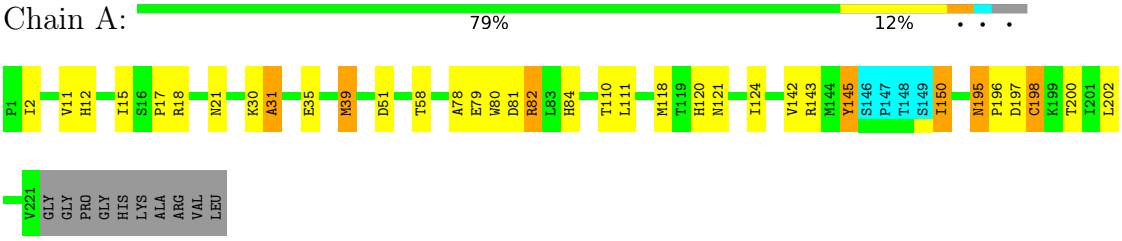
Chain A:



4.2.85 Score per residue for model 85

• Molecule 1: Capsid protein p24

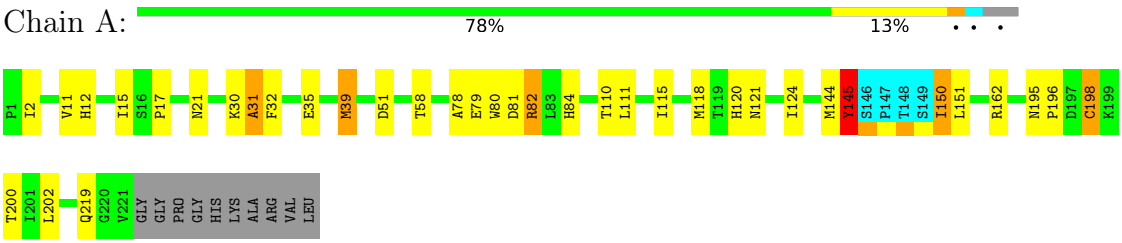
Chain A:



4.2.86 Score per residue for model 86

• Molecule 1: Capsid protein p24

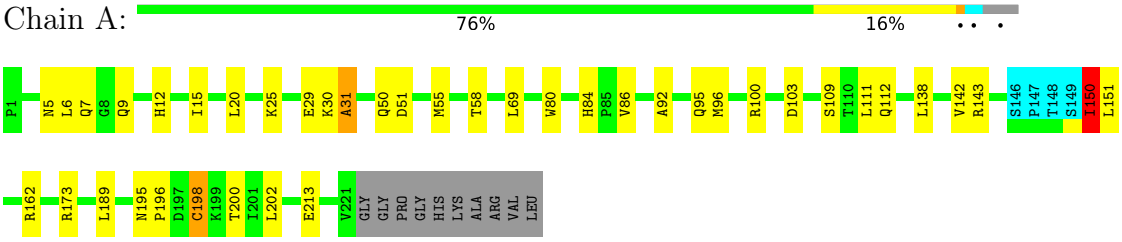
Chain A:



4.2.87 Score per residue for model 87

• Molecule 1: Capsid protein p24

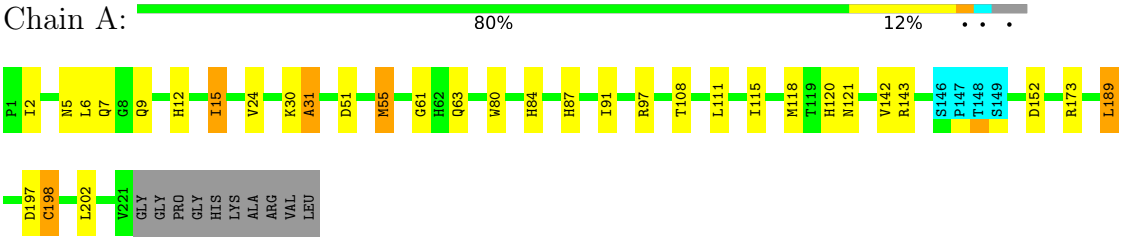
Chain A:



4.2.88 Score per residue for model 88

• Molecule 1: Capsid protein p24

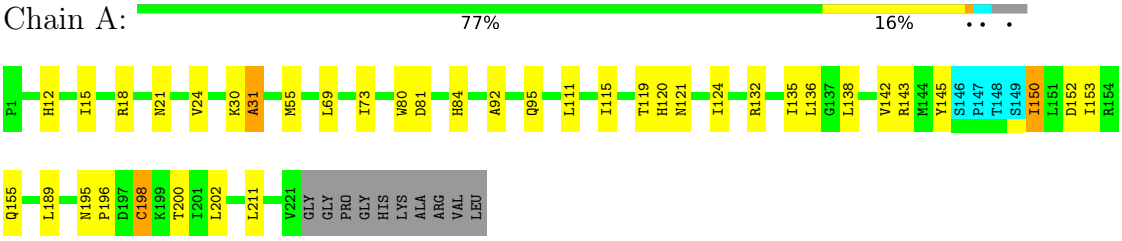
Chain A:



4.2.89 Score per residue for model 89

• Molecule 1: Capsid protein p24

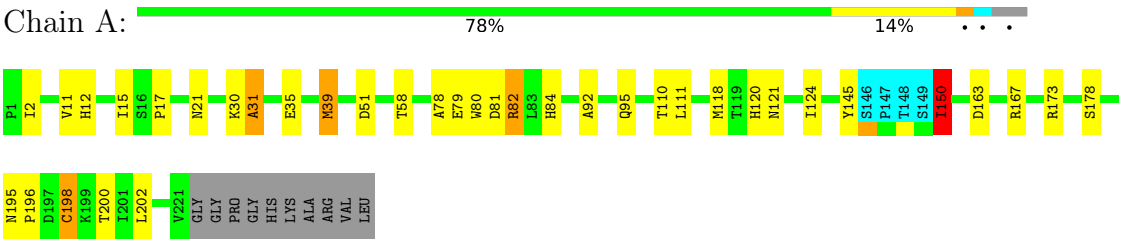
Chain A:



4.2.90 Score per residue for model 90

• Molecule 1: Capsid protein p24

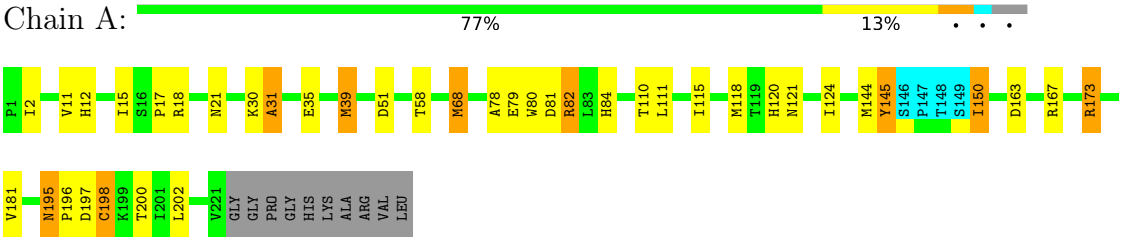
Chain A:



4.2.91 Score per residue for model 91

• Molecule 1: Capsid protein p24

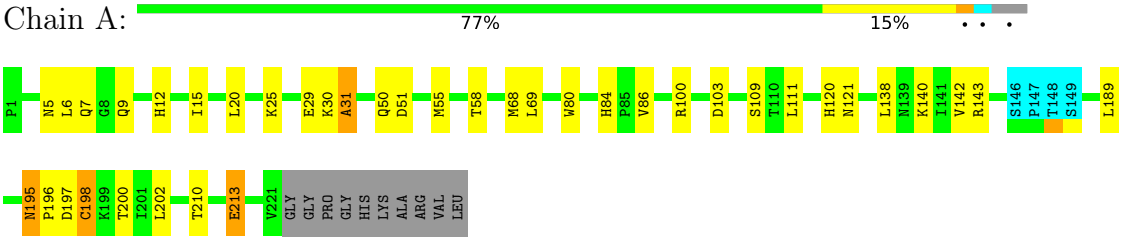
Chain A:



4.2.92 Score per residue for model 92

• Molecule 1: Capsid protein p24

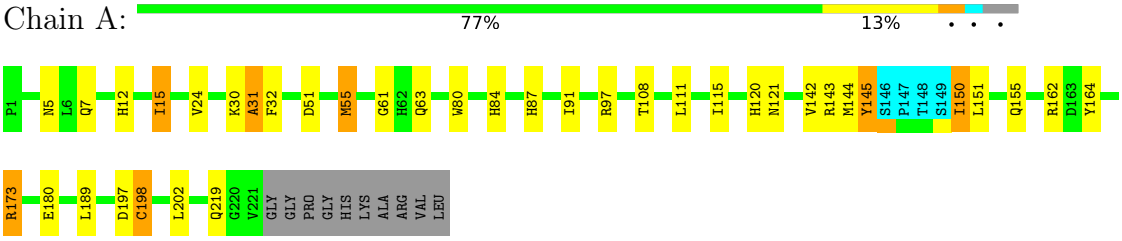
Chain A:



4.2.93 Score per residue for model 93

• Molecule 1: Capsid protein p24

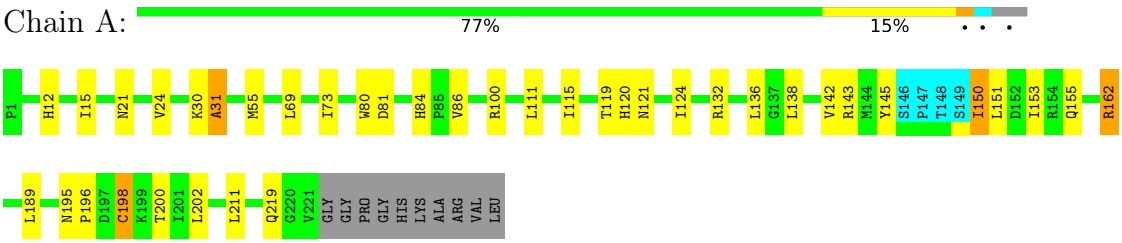
Chain A:



4.2.94 Score per residue for model 94

• Molecule 1: Capsid protein p24

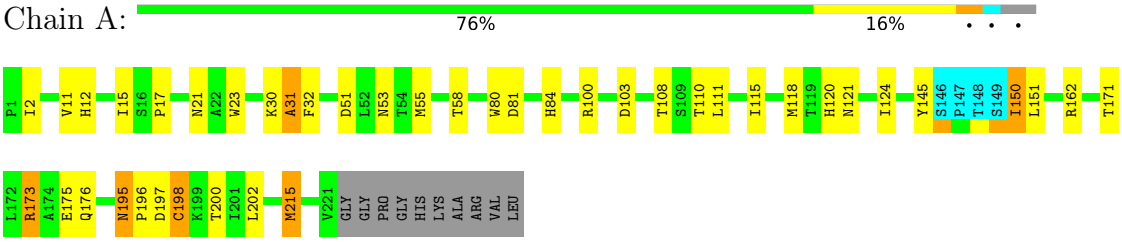
Chain A:



4.2.95 Score per residue for model 95

• Molecule 1: Capsid protein p24

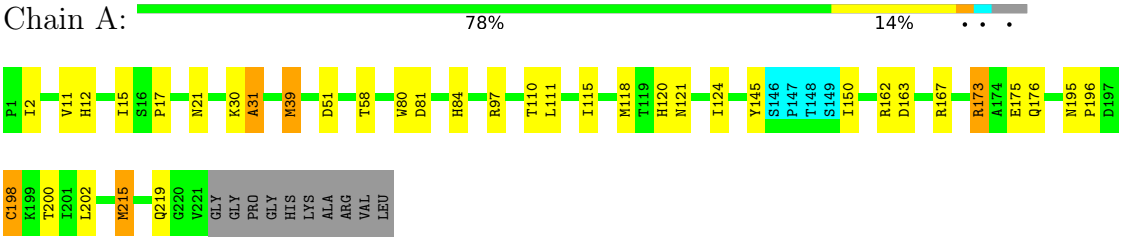
Chain A:



4.2.96 Score per residue for model 96

• Molecule 1: Capsid protein p24

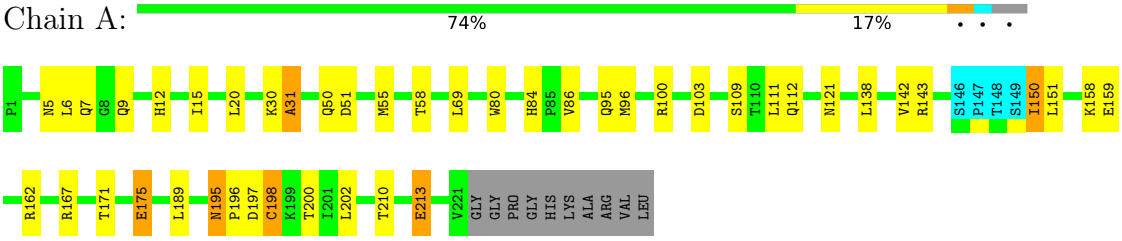
Chain A:



4.2.97 Score per residue for model 97

• Molecule 1: Capsid protein p24

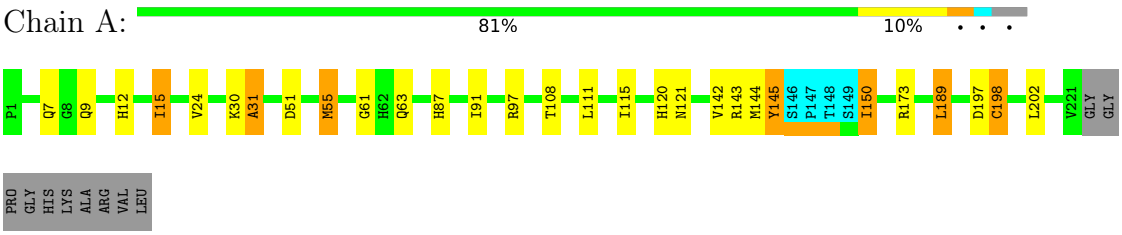
Chain A:



4.2.98 Score per residue for model 98

• Molecule 1: Capsid protein p24

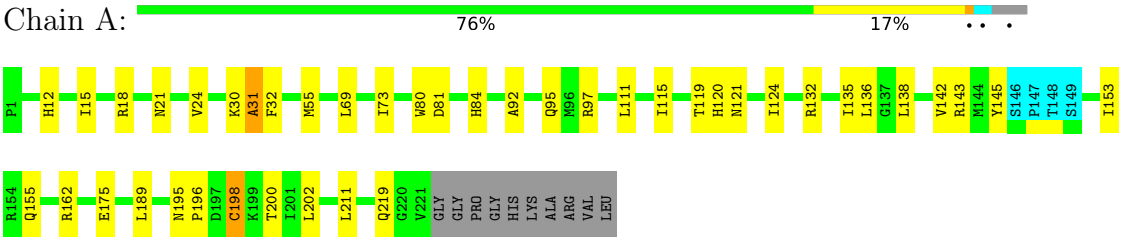
Chain A:



4.2.99 Score per residue for model 99

• Molecule 1: Capsid protein p24

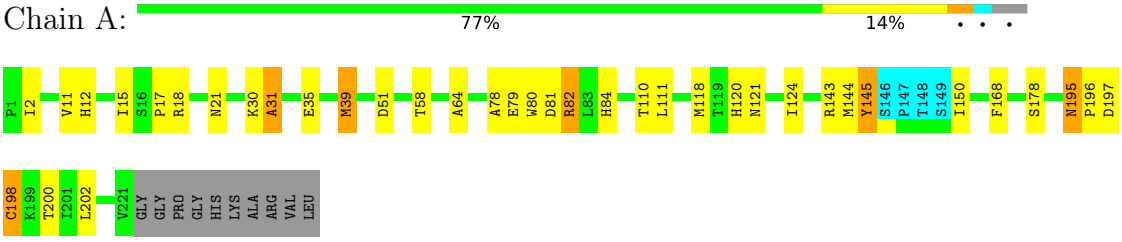
Chain A:



4.2.100 Score per residue for model 100

• Molecule 1: Capsid protein p24

Chain A:



5 Refinement protocol and experimental data overview

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

Of the 480 calculated structures, 100 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	refinement	2.32

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	1060
Number of shifts mapped to atoms	1016
Number of unparsed shifts	0
Number of shifts with mapping errors	44
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	34%

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	0.39±0.01	0±0/1723 (0.0± 0.0%)	0.56±0.01	0±0/2341 (0.0± 0.0%)
All	All	0.39	0/172300 (0.0%)	0.56	3/234100 (0.0%)

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(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	150	ILE	CA-C-N	-5.23	105.69	117.20	37	2
1	A	145	TYR	CA-CB-CG	-5.16	103.60	113.40	11	1

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	1687	1699	1694	30±5
All	All	168700	169900	169399	2954

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:150:ILE:HG22	1:A:171:THR:HG22	0.88	1.45	27	8
1:A:12:HIS:CD2	1:A:111:LEU:HD11	0.82	2.10	21	41
1:A:145:TYR:CG	1:A:145:TYR:O	0.81	2.33	7	2
1:A:150:ILE:HD12	1:A:150:ILE:O	0.74	1.83	47	2
1:A:150:ILE:N	1:A:150:ILE:HD13	0.73	1.98	37	2
1:A:144:MET:O	1:A:145:TYR:C	0.72	2.27	31	12
1:A:150:ILE:HD11	1:A:168:PHE:CZ	0.72	2.20	100	2
1:A:2:ILE:HD13	1:A:118:MET:SD	0.69	2.27	95	46
1:A:32:PHE:CE2	1:A:145:TYR:CE1	0.68	2.82	48	3
1:A:108:THR:O	1:A:108:THR:HG22	0.68	1.89	28	20
1:A:150:ILE:HG23	1:A:151:LEU:H	0.67	1.49	95	1
1:A:150:ILE:HG22	1:A:171:THR:CG2	0.66	2.20	47	6
1:A:32:PHE:CE1	1:A:145:TYR:CD2	0.66	2.84	25	2
1:A:80:TRP:CZ3	1:A:84:HIS:NE2	0.66	2.64	75	50
1:A:32:PHE:CE1	1:A:145:TYR:CD1	0.66	2.84	86	1
1:A:162:ARG:NH2	1:A:219:GLN:NE2	0.65	2.45	94	2
1:A:80:TRP:CE3	1:A:84:HIS:CE1	0.64	2.85	52	35
1:A:150:ILE:C	1:A:150:ILE:HD13	0.64	2.13	87	2
1:A:80:TRP:CZ3	1:A:84:HIS:CE1	0.64	2.86	57	39
1:A:5:ASN:HD22	1:A:9:GLN:HE22	0.63	1.37	27	14
1:A:97:ARG:HE	1:A:98:GLU:H	0.63	1.36	51	1
1:A:96:MET:SD	1:A:97:ARG:N	0.63	2.72	36	4
1:A:5:ASN:HD22	1:A:9:GLN:NE2	0.62	1.93	77	14
1:A:12:HIS:CG	1:A:111:LEU:HD11	0.62	2.29	42	39
1:A:32:PHE:CZ	1:A:145:TYR:CD2	0.62	2.87	41	5
1:A:80:TRP:CE3	1:A:84:HIS:CD2	0.62	2.88	66	46
1:A:173:ARG:NH2	1:A:182:LYS:NZ	0.62	2.48	8	2
1:A:173:ARG:O	1:A:173:ARG:NE	0.61	2.33	66	39
1:A:144:MET:O	1:A:145:TYR:CG	0.61	2.53	44	3
1:A:68:MET:N	1:A:68:MET:SD	0.61	2.74	91	2
1:A:91:ILE:HD11	1:A:97:ARG:NH2	0.61	2.11	53	20
1:A:32:PHE:CZ	1:A:145:TYR:CD1	0.61	2.87	80	4
1:A:5:ASN:ND2	1:A:9:GLN:HE22	0.61	1.93	52	9
1:A:144:MET:O	1:A:145:TYR:CD2	0.60	2.53	68	1
1:A:155:GLN:HE21	1:A:195:ASN:H	0.60	1.37	69	20
1:A:11:VAL:HG22	1:A:12:HIS:N	0.60	2.12	10	40
1:A:32:PHE:CE1	1:A:145:TYR:CG	0.60	2.89	31	2
1:A:35:GLU:O	1:A:39:MET:SD	0.60	2.60	91	30
1:A:162:ARG:NH1	1:A:219:GLN:HE21	0.59	1.94	13	16
1:A:171:THR:O	1:A:175:GLU:OE2	0.59	2.21	37	2
1:A:30:LYS:O	1:A:31:ALA:C	0.59	2.41	85	100
1:A:173:ARG:HH22	1:A:182:LYS:NZ	0.59	1.95	8	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:5:ASN:OD1	1:A:6:LEU:N	0.59	2.35	52	32
1:A:78:ALA:O	1:A:82:ARG:NE	0.59	2.35	31	28
1:A:20:LEU:HD23	1:A:55:MET:SD	0.59	2.38	27	20
1:A:18:ARG:NH2	1:A:21:ASN:HD22	0.59	1.96	84	10
1:A:18:ARG:NH1	1:A:21:ASN:HD22	0.59	1.95	14	4
1:A:162:ARG:HH12	1:A:219:GLN:HE22	0.59	1.39	56	1
1:A:162:ARG:NE	1:A:219:GLN:HE22	0.59	1.95	64	2
1:A:153:ILE:HD12	1:A:153:ILE:N	0.58	2.13	89	8
1:A:50:GLN:OE1	1:A:111:LEU:HD13	0.58	1.97	42	20
1:A:162:ARG:NE	1:A:219:GLN:NE2	0.58	2.50	64	2
1:A:120:HIS:ND1	1:A:121:ASN:N	0.58	2.51	1	89
1:A:162:ARG:HH12	1:A:219:GLN:HE21	0.58	1.39	14	9
1:A:162:ARG:CZ	1:A:219:GLN:NE2	0.58	2.66	74	2
1:A:67:GLN:HE22	1:A:151:LEU:CD1	0.57	2.12	59	2
1:A:173:ARG:O	1:A:173:ARG:CZ	0.57	2.53	11	17
1:A:142:VAL:O	1:A:145:TYR:CE1	0.57	2.58	5	4
1:A:18:ARG:HH12	1:A:21:ASN:ND2	0.57	1.98	69	3
1:A:144:MET:O	1:A:145:TYR:CB	0.56	2.52	59	5
1:A:162:ARG:NH2	1:A:219:GLN:HE21	0.56	1.99	38	2
1:A:69:LEU:O	1:A:73:ILE:HD13	0.56	2.01	39	20
1:A:153:ILE:N	1:A:153:ILE:CD1	0.56	2.68	29	19
1:A:87:HIS:CG	1:A:87:HIS:O	0.56	2.59	7	5
1:A:150:ILE:HG23	1:A:151:LEU:N	0.56	2.16	94	5
1:A:145:TYR:CD2	1:A:145:TYR:O	0.56	2.58	53	8
1:A:80:TRP:CZ3	1:A:84:HIS:CD2	0.56	2.94	75	13
1:A:175:GLU:N	1:A:175:GLU:OE1	0.56	2.39	42	7
1:A:18:ARG:HH22	1:A:21:ASN:HD22	0.56	1.43	69	4
1:A:150:ILE:HD13	1:A:168:PHE:CE1	0.56	2.36	47	2
1:A:162:ARG:NH1	1:A:219:GLN:HE22	0.55	1.98	56	1
1:A:162:ARG:NE	1:A:219:GLN:OE1	0.55	2.39	94	1
1:A:86:VAL:HG12	1:A:100:ARG:NE	0.55	2.16	97	17
1:A:144:MET:O	1:A:145:TYR:HB2	0.55	2.02	8	1
1:A:215:MET:SD	1:A:215:MET:O	0.55	2.64	95	12
1:A:162:ARG:NH1	1:A:219:GLN:NE2	0.55	2.54	48	3
1:A:153:ILE:N	1:A:153:ILE:HD12	0.55	2.16	94	11
1:A:162:ARG:HH12	1:A:219:GLN:NE2	0.55	1.98	84	8
1:A:97:ARG:HE	1:A:98:GLU:N	0.55	2.00	51	1
1:A:7:GLN:O	1:A:9:GLN:NE2	0.55	2.40	13	18
1:A:144:MET:O	1:A:145:TYR:CD1	0.55	2.60	53	1
1:A:51:ASP:O	1:A:55:MET:SD	0.55	2.65	68	20
1:A:67:GLN:HE22	1:A:151:LEU:CB	0.55	2.15	59	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:91:ILE:HD11	1:A:97:ARG:CZ	0.54	2.32	98	7
1:A:113:GLU:OE1	1:A:117:TRP:CE3	0.54	2.60	36	3
1:A:145:TYR:CD1	1:A:145:TYR:O	0.54	2.60	2	1
1:A:81:ASP:OD2	1:A:100:ARG:NH2	0.54	2.40	26	10
1:A:113:GLU:OE1	1:A:117:TRP:CZ3	0.54	2.59	6	2
1:A:32:PHE:CE1	1:A:145:TYR:O	0.54	2.61	16	3
1:A:18:ARG:HH12	1:A:21:ASN:HD22	0.54	1.43	69	4
1:A:15:ILE:HD12	1:A:15:ILE:H	0.54	1.63	98	20
1:A:163:ASP:OD1	1:A:167:ARG:NH1	0.54	2.40	90	26
1:A:80:TRP:CH2	1:A:84:HIS:NE2	0.54	2.76	86	39
1:A:145:TYR:O	1:A:145:TYR:CG	0.54	2.60	2	3
1:A:167:ARG:HH21	1:A:171:THR:N	0.54	2.00	9	3
1:A:142:VAL:O	1:A:145:TYR:CD1	0.54	2.60	79	6
1:A:150:ILE:HG22	1:A:150:ILE:O	0.54	2.02	2	1
1:A:92:ALA:HB3	1:A:95:GLN:HG2	0.54	1.80	12	25
1:A:87:HIS:O	1:A:97:ARG:NH2	0.53	2.42	46	20
1:A:158:LYS:CD	1:A:158:LYS:O	0.53	2.56	76	3
1:A:32:PHE:CD2	1:A:145:TYR:CE1	0.53	2.97	48	3
1:A:79:GLU:OE2	1:A:82:ARG:NH2	0.53	2.42	35	27
1:A:167:ARG:NH2	1:A:171:THR:OG1	0.53	2.42	34	1
1:A:32:PHE:CE1	1:A:145:TYR:CE2	0.53	2.97	57	2
1:A:12:HIS:CG	1:A:111:LEU:HD21	0.53	2.39	33	59
1:A:213:GLU:OE1	1:A:213:GLU:N	0.53	2.42	37	3
1:A:81:ASP:CG	1:A:100:ARG:NH2	0.52	2.63	6	6
1:A:32:PHE:CE2	1:A:145:TYR:CZ	0.52	2.97	48	2
1:A:12:HIS:HB2	1:A:115:ILE:HD11	0.52	1.81	80	30
1:A:15:ILE:CD1	1:A:55:MET:SD	0.52	2.98	49	20
1:A:68:MET:SD	1:A:140:LYS:NZ	0.52	2.74	52	9
1:A:189:LEU:HD13	1:A:189:LEU:O	0.52	2.03	28	17
1:A:145:TYR:O	1:A:145:TYR:CD2	0.52	2.62	7	2
1:A:150:ILE:HD11	1:A:168:PHE:CD1	0.52	2.40	20	5
1:A:12:HIS:HB3	1:A:115:ILE:HD11	0.52	1.82	88	40
1:A:124:ILE:HD12	1:A:124:ILE:N	0.51	2.21	64	60
1:A:144:MET:SD	1:A:181:VAL:CG2	0.51	2.99	71	3
1:A:7:GLN:O	1:A:9:GLN:OE1	0.51	2.28	2	17
1:A:145:TYR:O	1:A:145:TYR:CD1	0.51	2.63	7	1
1:A:163:ASP:OD1	1:A:167:ARG:CZ	0.51	2.59	76	8
1:A:32:PHE:CD1	1:A:145:TYR:O	0.51	2.63	75	1
1:A:158:LYS:O	1:A:158:LYS:CG	0.51	2.59	76	4
1:A:95:GLN:O	1:A:96:MET:SD	0.51	2.69	67	15
1:A:112:GLN:NE2	1:A:112:GLN:H	0.51	2.04	32	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:155:GLN:N	1:A:164:TYR:CE1	0.51	2.79	37	7
1:A:17:PRO:O	1:A:21:ASN:OD1	0.51	2.28	65	40
1:A:87:HIS:O	1:A:97:ARG:NH1	0.51	2.44	83	4
1:A:69:LEU:HD21	1:A:138:LEU:HD12	0.50	1.84	62	20
1:A:162:ARG:CZ	1:A:219:GLN:HE21	0.50	2.19	48	2
1:A:143:ARG:O	1:A:145:TYR:CE2	0.50	2.64	85	1
1:A:39:MET:SD	1:A:39:MET:N	0.50	2.85	91	28
1:A:145:TYR:CE1	1:A:178:SER:OG	0.50	2.60	90	1
1:A:18:ARG:CZ	1:A:21:ASN:HD22	0.50	2.20	14	4
1:A:150:ILE:HD11	1:A:168:PHE:O	0.50	2.06	25	3
1:A:32:PHE:CE2	1:A:145:TYR:CE2	0.50	2.99	63	2
1:A:198:CYS:SG	1:A:202:LEU:HD11	0.50	2.47	22	100
1:A:150:ILE:HD13	1:A:150:ILE:O	0.50	2.06	12	1
1:A:96:MET:SD	1:A:97:ARG:O	0.50	2.70	36	1
1:A:132:ARG:NH2	1:A:135:ILE:HG21	0.49	2.22	9	6
1:A:108:THR:O	1:A:108:THR:CG2	0.49	2.60	33	20
1:A:144:MET:O	1:A:145:TYR:O	0.49	2.31	83	3
1:A:120:HIS:CG	1:A:121:ASN:N	0.49	2.80	36	22
1:A:139:ASN:ND2	1:A:143:ARG:HH11	0.49	2.05	11	2
1:A:145:TYR:C	1:A:145:TYR:CD1	0.49	2.86	54	2
1:A:69:LEU:HD21	1:A:138:LEU:CD1	0.49	2.38	12	20
1:A:215:MET:SD	1:A:215:MET:C	0.49	2.91	76	1
1:A:162:ARG:NH2	1:A:219:GLN:HE22	0.49	2.05	94	1
1:A:196:PRO:O	1:A:200:THR:HG23	0.49	2.08	4	80
1:A:159:GLU:CD	1:A:167:ARG:NH1	0.49	2.66	47	11
1:A:79:GLU:CD	1:A:82:ARG:NH2	0.49	2.67	76	6
1:A:175:GLU:CD	1:A:176:GLN:N	0.48	2.67	66	10
1:A:150:ILE:CG2	1:A:151:LEU:N	0.48	2.75	94	4
1:A:103:ASP:CB	1:A:109:SER:OG	0.48	2.62	47	20
1:A:11:VAL:CG2	1:A:12:HIS:N	0.48	2.77	5	40
1:A:81:ASP:O	1:A:81:ASP:OD1	0.48	2.32	65	60
1:A:86:VAL:CG1	1:A:100:ARG:CZ	0.48	2.91	36	7
1:A:210:THR:OG1	1:A:213:GLU:OE1	0.48	2.32	92	11
1:A:25:LYS:NZ	1:A:29:GLU:OE2	0.47	2.42	32	12
1:A:150:ILE:HD12	1:A:150:ILE:C	0.47	2.30	47	2
1:A:145:TYR:CD2	1:A:145:TYR:C	0.47	2.87	25	1
1:A:171:THR:O	1:A:175:GLU:OE1	0.47	2.32	42	8
1:A:155:GLN:NE2	1:A:195:ASN:H	0.47	2.05	14	20
1:A:150:ILE:O	1:A:150:ILE:CG1	0.47	2.62	12	1
1:A:7:GLN:CG	1:A:9:GLN:HE22	0.47	2.23	48	3
1:A:215:MET:C	1:A:215:MET:SD	0.47	2.93	51	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:16:SER:OG	1:A:18:ARG:CZ	0.47	2.63	56	2
1:A:121:ASN:OD1	1:A:121:ASN:O	0.47	2.33	52	4
1:A:21:ASN:O	1:A:24:VAL:HG12	0.47	2.10	79	20
1:A:67:GLN:NE2	1:A:151:LEU:HD13	0.47	2.25	59	1
1:A:12:HIS:CD2	1:A:111:LEU:HD21	0.46	2.46	53	23
1:A:145:TYR:CD1	1:A:145:TYR:C	0.46	2.88	86	1
1:A:61:GLY:O	1:A:63:GLN:OE1	0.46	2.34	88	20
1:A:152:ASP:CG	1:A:152:ASP:O	0.46	2.54	89	5
1:A:15:ILE:HD13	1:A:55:MET:SD	0.46	2.50	54	1
1:A:64:ALA:HB2	1:A:178:SER:OG	0.46	2.10	73	1
1:A:110:THR:HG22	1:A:111:LEU:N	0.46	2.25	65	40
1:A:80:TRP:CD2	1:A:84:HIS:CD2	0.46	3.04	48	53
1:A:15:ILE:H	1:A:15:ILE:CD1	0.46	2.24	43	14
1:A:7:GLN:HG3	1:A:9:GLN:HE22	0.46	1.69	13	3
1:A:7:GLN:CB	1:A:9:GLN:HE22	0.46	2.23	72	2
1:A:198:CYS:SG	1:A:202:LEU:CD1	0.45	3.04	94	100
1:A:12:HIS:CG	1:A:111:LEU:CD2	0.45	3.00	13	40
1:A:197:ASP:O	1:A:197:ASP:OD1	0.45	2.34	48	20
1:A:5:ASN:OD1	1:A:9:GLN:O	0.45	2.34	6	3
1:A:39:MET:N	1:A:39:MET:SD	0.45	2.89	1	8
1:A:115:ILE:O	1:A:119:THR:HG22	0.45	2.12	9	20
1:A:81:ASP:CG	1:A:100:ARG:HH21	0.45	2.14	95	2
1:A:173:ARG:NH2	1:A:174:ALA:HB2	0.45	2.26	76	1
1:A:32:PHE:CE2	1:A:145:TYR:CD1	0.45	3.05	81	2
1:A:195:ASN:OD1	1:A:197:ASP:N	0.45	2.49	2	30
1:A:142:VAL:O	1:A:145:TYR:O	0.45	2.34	80	1
1:A:132:ARG:O	1:A:136:LEU:HD13	0.45	2.12	59	20
1:A:162:ARG:H	1:A:162:ARG:CD	0.45	2.23	76	2
1:A:150:ILE:O	1:A:150:ILE:CD1	0.45	2.65	12	3
1:A:5:ASN:CG	1:A:7:GLN:H	0.45	2.14	68	10
1:A:103:ASP:OD1	1:A:108:THR:OG1	0.45	2.33	95	6
1:A:15:ILE:HD11	1:A:51:ASP:HB3	0.45	1.89	2	60
1:A:28:GLU:OE1	1:A:29:GLU:OE1	0.45	2.35	43	1
1:A:75:GLU:OE1	1:A:76:GLU:OE2	0.44	2.36	6	4
1:A:150:ILE:HG23	1:A:171:THR:CG2	0.44	2.42	68	2
1:A:132:ARG:HH21	1:A:135:ILE:HD13	0.44	1.72	99	6
1:A:12:HIS:CE1	1:A:50:GLN:OE1	0.44	2.71	76	3
1:A:150:ILE:CD1	1:A:175:GLU:OE1	0.44	2.66	37	1
1:A:145:TYR:CD1	1:A:145:TYR:N	0.44	2.86	45	1
1:A:32:PHE:CZ	1:A:145:TYR:CZ	0.44	3.05	57	1
1:A:173:ARG:O	1:A:173:ARG:CD	0.44	2.66	73	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:175:GLU:OE1	1:A:175:GLU:N	0.44	2.51	77	1
1:A:86:VAL:HG13	1:A:100:ARG:NH2	0.44	2.28	6	1
1:A:144:MET:C	1:A:145:TYR:CD2	0.44	2.92	44	1
1:A:175:GLU:OE2	1:A:176:GLN:O	0.44	2.36	66	2
1:A:121:ASN:O	1:A:121:ASN:CG	0.43	2.56	7	8
1:A:64:ALA:CB	1:A:178:SER:OG	0.43	2.66	100	1
1:A:5:ASN:OD1	1:A:7:GLN:OE1	0.43	2.36	23	3
1:A:150:ILE:HD11	1:A:168:PHE:CG	0.43	2.47	60	2
1:A:145:TYR:OH	1:A:178:SER:OG	0.43	2.36	35	1
1:A:113:GLU:OE1	1:A:113:GLU:O	0.43	2.36	36	1
1:A:23:TRP:CG	1:A:55:MET:CE	0.43	3.01	75	2
1:A:32:PHE:CZ	1:A:145:TYR:CE2	0.43	3.07	17	1
1:A:162:ARG:HH11	1:A:219:GLN:HE21	0.43	1.54	41	1
1:A:150:ILE:N	1:A:150:ILE:CD1	0.43	2.80	85	1
1:A:142:VAL:HG23	1:A:143:ARG:N	0.43	2.29	29	60
1:A:159:GLU:OE2	1:A:167:ARG:CZ	0.43	2.67	7	2
1:A:32:PHE:CZ	1:A:145:TYR:CE1	0.43	3.07	80	1
1:A:81:ASP:OD1	1:A:100:ARG:NH2	0.43	2.52	6	1
1:A:150:ILE:HG13	1:A:150:ILE:O	0.43	2.14	91	3
1:A:86:VAL:HG21	1:A:100:ARG:NH2	0.43	2.29	44	11
1:A:132:ARG:HH21	1:A:135:ILE:HG21	0.43	1.74	29	1
1:A:96:MET:SD	1:A:96:MET:C	0.43	2.97	36	1
1:A:53:ASN:OD1	1:A:53:ASN:O	0.43	2.37	1	3
1:A:18:ARG:NH1	1:A:21:ASN:ND2	0.43	2.63	14	2
1:A:32:PHE:CE2	1:A:145:TYR:CD2	0.43	3.07	65	1
1:A:78:ALA:O	1:A:82:ARG:HG2	0.42	2.14	22	3
1:A:159:GLU:OE2	1:A:167:ARG:NH1	0.42	2.52	77	2
1:A:144:MET:C	1:A:145:TYR:CG	0.42	2.92	44	1
1:A:86:VAL:HG12	1:A:100:ARG:HE	0.42	1.74	82	2
1:A:150:ILE:N	1:A:150:ILE:HD12	0.42	2.30	90	1
1:A:32:PHE:CD2	1:A:145:TYR:CZ	0.42	3.07	73	1
1:A:143:ARG:O	1:A:145:TYR:CE1	0.42	2.73	100	1
1:A:132:ARG:HH21	1:A:135:ILE:CD1	0.42	2.28	99	3
1:A:5:ASN:ND2	1:A:7:GLN:OE1	0.42	2.53	23	2
1:A:5:ASN:ND2	1:A:7:GLN:CB	0.42	2.83	33	2
1:A:103:ASP:CG	1:A:109:SER:OG	0.42	2.58	2	10
1:A:144:MET:O	1:A:145:TYR:HB3	0.42	2.15	40	1
1:A:162:ARG:HE	1:A:219:GLN:HE22	0.42	1.53	64	1
1:A:164:TYR:OH	1:A:193:ASN:CB	0.42	2.68	37	1
1:A:150:ILE:C	1:A:150:ILE:CD1	0.41	2.83	87	1
1:A:167:ARG:HH21	1:A:171:THR:CA	0.41	2.28	34	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:67:GLN:NE2	1:A:151:LEU:CD1	0.41	2.82	59	1
1:A:179:GLN:O	1:A:183:ASN:OD1	0.41	2.37	67	6
1:A:173:ARG:NH2	1:A:182:LYS:HZ3	0.41	2.13	8	1
1:A:112:GLN:NE2	1:A:112:GLN:N	0.41	2.69	32	1
1:A:154:ARG:NH1	1:A:155:GLN:O	0.41	2.53	36	1
1:A:5:ASN:CB	1:A:9:GLN:NE2	0.41	2.84	52	1
1:A:121:ASN:O	1:A:121:ASN:OD1	0.41	2.39	7	1
1:A:18:ARG:HH22	1:A:21:ASN:ND2	0.41	2.12	69	1
1:A:152:ASP:OD1	1:A:154:ARG:NH1	0.41	2.53	64	1
1:A:87:HIS:O	1:A:87:HIS:CG	0.41	2.74	62	2
1:A:80:TRP:CE2	1:A:84:HIS:CD2	0.41	3.09	83	3
1:A:80:TRP:CH2	1:A:84:HIS:CE1	0.41	3.09	92	2
1:A:195:ASN:OD1	1:A:195:ASN:C	0.40	2.60	2	1
1:A:32:PHE:CD2	1:A:32:PHE:O	0.40	2.75	21	2
1:A:143:ARG:O	1:A:145:TYR:CD1	0.40	2.74	100	1
1:A:216:THR:O	1:A:219:GLN:OE1	0.40	2.39	7	2
1:A:174:ALA:O	1:A:176:GLN:OE1	0.40	2.38	76	1
1:A:150:ILE:HG23	1:A:189:LEU:CD2	0.40	2.46	80	1
1:A:121:ASN:CG	1:A:121:ASN:O	0.40	2.60	32	1
1:A:211:LEU:O	1:A:211:LEU:HD23	0.40	2.15	34	3
1:A:152:ASP:O	1:A:152:ASP:CG	0.40	2.59	74	1
1:A:63:GLN:CD	1:A:180:GLU:CG	0.40	2.90	93	1
1:A:162:ARG:CZ	1:A:219:GLN:OE1	0.40	2.69	94	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	215/231 (93%)	211±1 (98±0%)	2±1 (1±0%)	2±1 (1±0%)	20	68
All	All	21500/23100 (93%)	21055 (98%)	235 (1%)	210 (1%)	20	68

All 3 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	31	ALA	100
1	A	150	ILE	73
1	A	145	TYR	37

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	182/192 (95%)	176±1 (97±1%)	6±1 (3±1%)	39 86
All	All	18200/19200 (95%)	17568 (97%)	632 (3%)	39 86

All 29 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	198	CYS	100
1	A	58	THR	60
1	A	189	LEU	60
1	A	195	ASN	57
1	A	39	MET	37
1	A	173	ARG	33
1	A	162	ARG	30
1	A	82	ARG	28
1	A	145	TYR	21
1	A	15	ILE	20
1	A	24	VAL	20
1	A	55	MET	20
1	A	138	LEU	20
1	A	211	LEU	20
1	A	18	ARG	18
1	A	150	ILE	15
1	A	215	MET	12
1	A	213	GLU	12
1	A	158	LYS	9
1	A	175	GLU	8
1	A	97	ARG	7
1	A	9	GLN	6
1	A	153	ILE	6

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Mol	Chain	Res	Type	Models (Total)
1	A	132	ARG	5
1	A	113	GLU	2
1	A	68	MET	2
1	A	112	GLN	2
1	A	32	PHE	1
1	A	7	GLN	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

The completeness of assignment taking into account all chemical shift lists is 34% for the well-defined parts and 34% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping

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

Total number of shifts	1060
Number of shifts mapped to atoms	1016
Number of unparsed shifts	0
Number of shifts with mapping errors	44
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	1

The following assigned chemical shifts were not mapped to the molecules present in the coordinate file.

- No matching atom found in the structure. All 44 occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	222	GLY	H	8.566	0.02	.
1	A	222	GLY	C	174.119	0.2	.
1	A	222	GLY	CA	44.634	0.2	.
1	A	222	GLY	N	115.64	0.2	.
1	A	223	GLY	H	7.917	0.02	.
1	A	223	GLY	C	172.071	0.2	.
1	A	223	GLY	CA	44.124	0.2	.
1	A	223	GLY	N	108.671	0.2	.
1	A	224	PRO	C	177.881	0.2	.
1	A	224	PRO	CA	63.264	0.2	.
1	A	224	PRO	CB	31.122	0.2	.
1	A	225	GLY	H	8.414	0.02	.
1	A	225	GLY	C	174.067	0.2	.
1	A	225	GLY	CA	44.876	0.2	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	225	GLY	N	109.295	0.2	.
1	A	226	HIS	H	8.048	0.02	.
1	A	226	HIS	CA	55.859	0.2	.
1	A	226	HIS	CB	28.879	0.2	.
1	A	226	HIS	N	119.97	0.2	.
1	A	227	LYS	H	8.106	0.02	.
1	A	227	LYS	C	175.898	0.2	.
1	A	227	LYS	CA	55.692	0.2	.
1	A	227	LYS	CB	31.835	0.2	.
1	A	227	LYS	N	123.511	0.2	.
1	A	228	ALA	H	8.139	0.02	.
1	A	228	ALA	C	177.383	0.2	.
1	A	228	ALA	CA	51.91	0.2	.
1	A	228	ALA	CB	18.4	0.2	.
1	A	228	ALA	N	125.583	0.2	.
1	A	229	ARG	H	8.16	0.02	.
1	A	229	ARG	C	175.894	0.2	.
1	A	229	ARG	CA	55.678	0.2	.
1	A	229	ARG	CB	29.898	0.2	.
1	A	229	ARG	N	121.105	0.2	.
1	A	230	VAL	H	8.088	0.02	.
1	A	230	VAL	C	175.019	0.2	.
1	A	230	VAL	CA	61.949	0.2	.
1	A	230	VAL	CB	31.655	0.2	.
1	A	230	VAL	N	123.049	0.2	.
1	A	231	LEU	H	7.757	0.02	.
1	A	231	LEU	C	182.069	0.2	.
1	A	231	LEU	CA	56.348	0.2	.
1	A	231	LEU	CB	42.393	0.2	.
1	A	231	LEU	N	131.889	0.2	.

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	226	0.14 ± 0.17	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	205	1.33 ± 0.12	Should be checked
$^{13}C'$	217	-0.35 ± 0.10	None needed (< 0.5 ppm)
^{15}N	206	0.08 ± 0.20	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 34%, i.e. 999 atoms were assigned a chemical shift out of a possible 2957. 0 out of 31 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	805/1068 (75%)	194/433 (45%)	417/434 (96%)	194/201 (97%)
Sidechain	194/1725 (11%)	0/1126 (0%)	194/534 (36%)	0/65 (0%)
Aromatic	0/164 (0%)	0/80 (0%)	0/70 (0%)	0/14 (0%)
Overall	999/2957 (34%)	194/1639 (12%)	611/1038 (59%)	194/280 (69%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 34%, i.e. 1016 atoms were assigned a chemical shift out of a possible 2996. 0 out of 31 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	818/1086 (75%)	197/440 (45%)	424/442 (96%)	197/204 (97%)
Sidechain	198/1746 (11%)	0/1140 (0%)	198/541 (37%)	0/65 (0%)
Aromatic	0/164 (0%)	0/80 (0%)	0/70 (0%)	0/14 (0%)
Overall	1016/2996 (34%)	197/1660 (12%)	622/1053 (59%)	197/283 (70%)

7.1.4 Statistically unusual chemical shifts

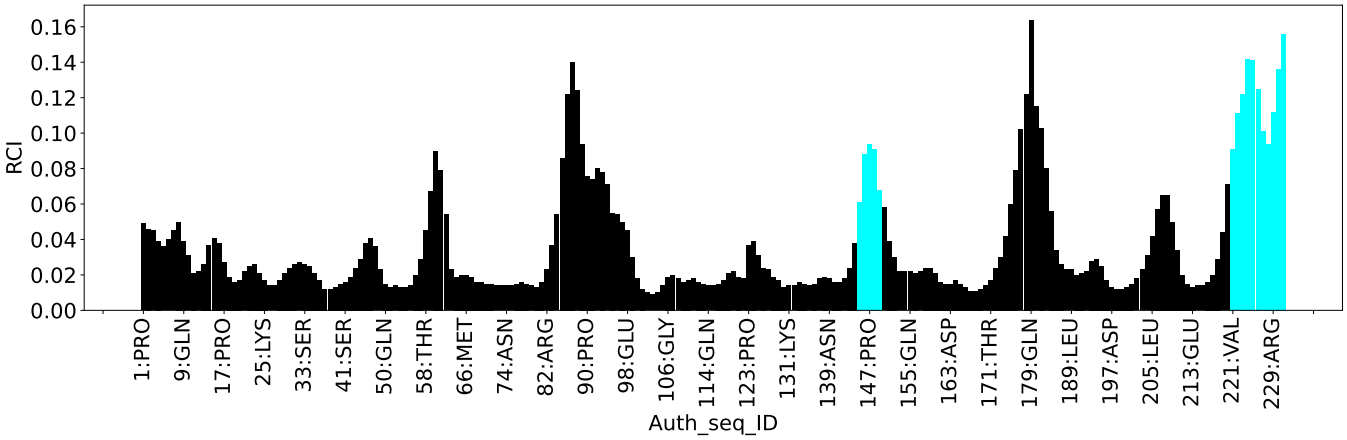
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	101	GLY	H	11.57	5.23 – 11.42	5.2

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:


RCI
0.16
0.14
0.12
0.10
0.08
0.06
0.04
0.02
0.00
1:PRO
9:GLN
17:PRO
25:LYS
33:SER
41:SER
50:GLN
58:THR
66:MET
74:ASN
82:ARG
90:PRO
98:GLU
106:GLY
114:GLN
123:PRO
131:LYS
139:ASN
147:PRO
155:GLN
163:ASP
171:THR
179:GLN
189:LEU
197:ASP
205:LEU
213:GLU
221:VAL
229:ARG
Auth_seq_ID

8 NMR restraints analysis (i)

No restraints data found

9 Distance violation analysis (i)

No distance restraints data found

10 Dihedral-angle violation analysis (i)

No dihedral-angle restraints found