



# Full wwPDB NMR Structure Validation Report ⓘ

Feb 13, 2017 – 12:54 am GMT

PDB ID : 2M8N  
Title : HIV-1 capsid monomer structure  
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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

Cyrange : Kirchner and Güntert (2011)  
NmrClust : Kelley et al. (1996)  
MolProbity : 4.02b-467  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
RCI : v\_1n\_11\_5\_13\_A (Berjanski et al., 2005)  
PANAV : Wang et al. (2010)  
ShiftChecker : trunk28760  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

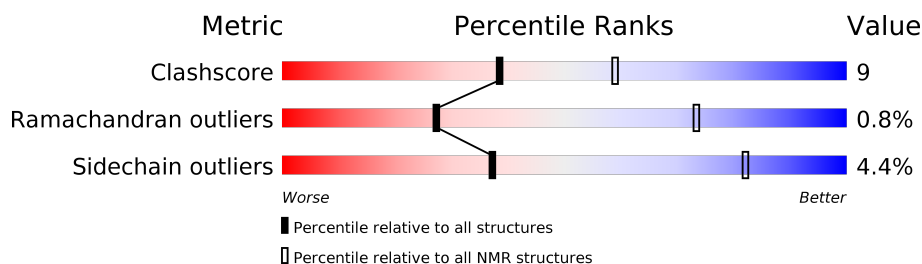
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 33%.

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	125131	11601
Ramachandran outliers	121729	10391
Sidechain outliers	121581	10367

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and a grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A	231	 79% 14% ...

## 2 Ensemble composition and analysis

This entry contains 100 models. Model 46 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)	0.03	46
2	A:150-A:221 (72)	0.03	13

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 7 clusters and 2 single-model clusters were found.

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

### 3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 3457 atoms, of which 1732 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Capsid protein p24.

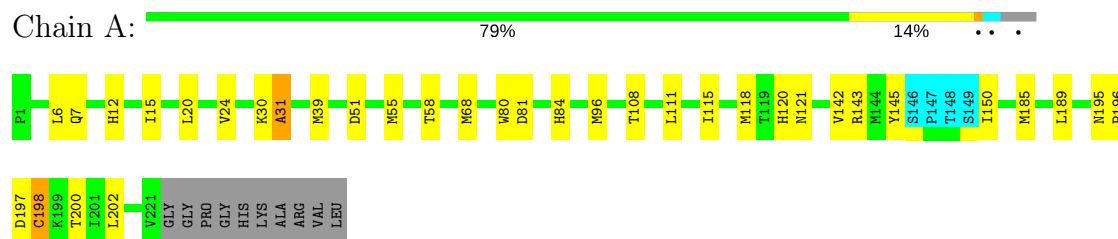
Mol	Chain	Residues	Atoms						Trace
1	A	221	Total	C	H	N	O	S	0
			3457	1088	1732	301	323	13	

## 4 Residue-property plots

### 4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA and DNA 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

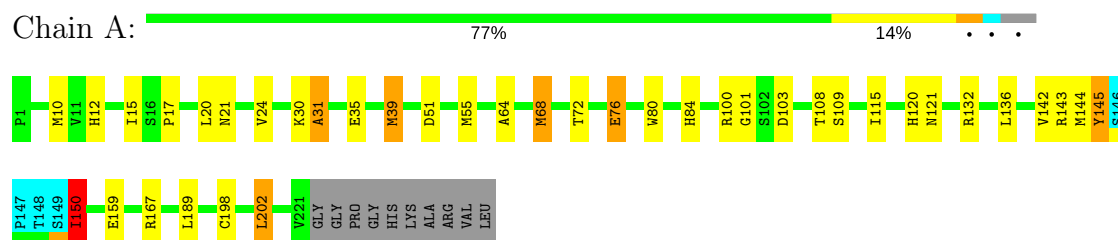


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

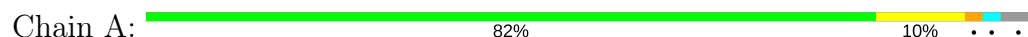
#### 4.2.1 Score per residue for model 1

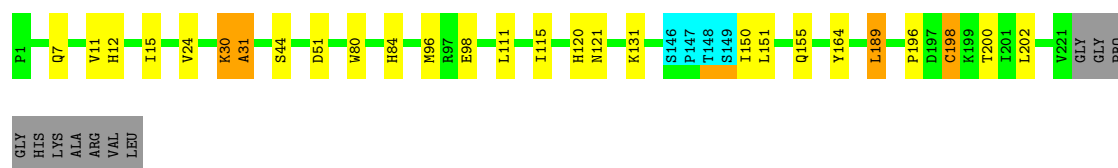
- Molecule 1: Capsid protein p24



#### 4.2.2 Score per residue for model 2

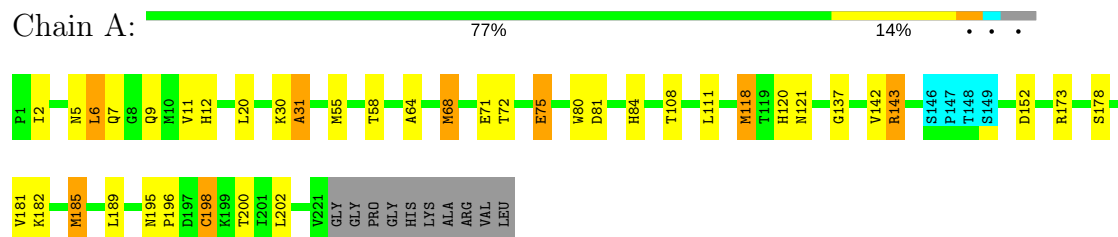
- Molecule 1: Capsid protein p24





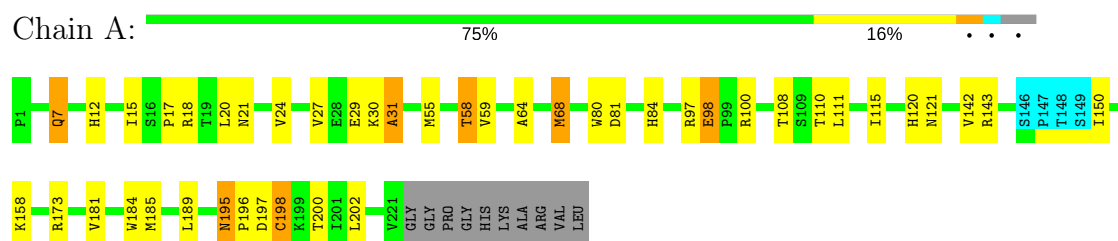
#### 4.2.3 Score per residue for model 3

- Molecule 1: Capsid protein p24



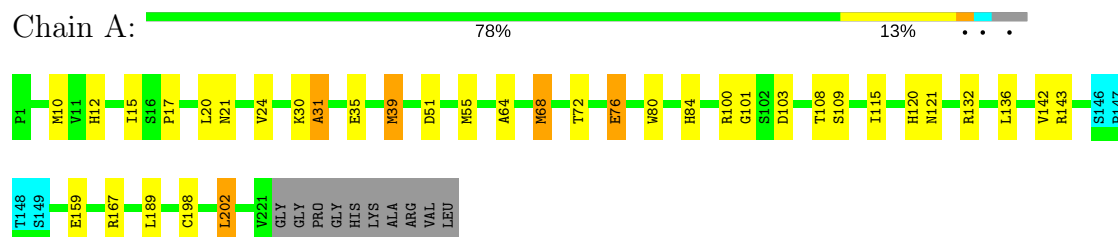
#### 4.2.4 Score per residue for model 4

- Molecule 1: Capsid protein p24



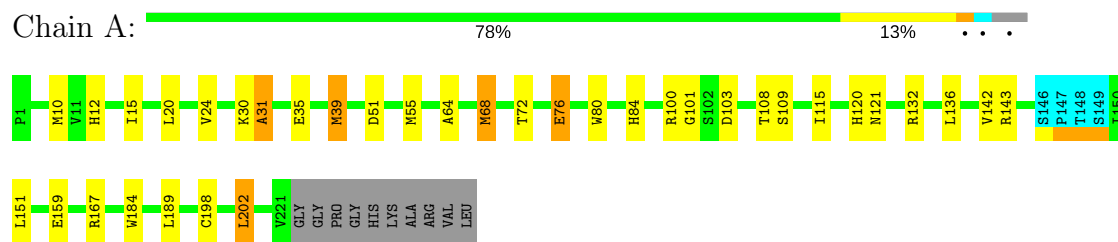
#### 4.2.5 Score per residue for model 5

- Molecule 1: Capsid protein p24



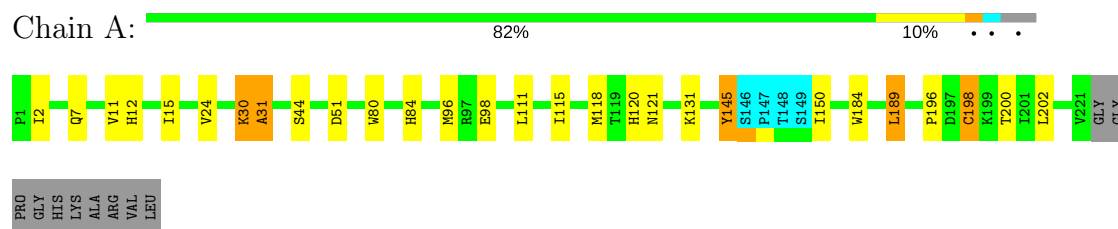
#### 4.2.6 Score per residue for model 6

- Molecule 1: Capsid protein p24



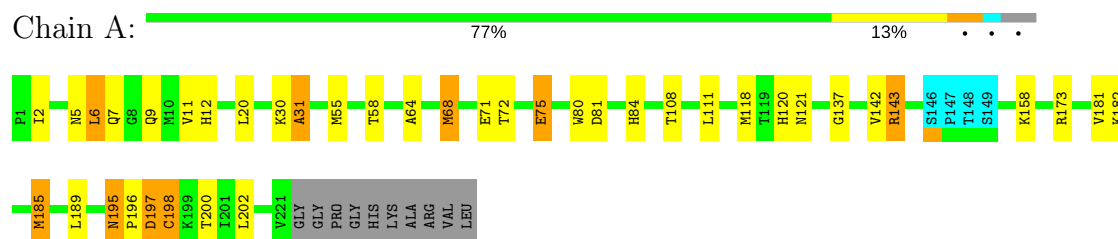
#### 4.2.7 Score per residue for model 7

- Molecule 1: Capsid protein p24



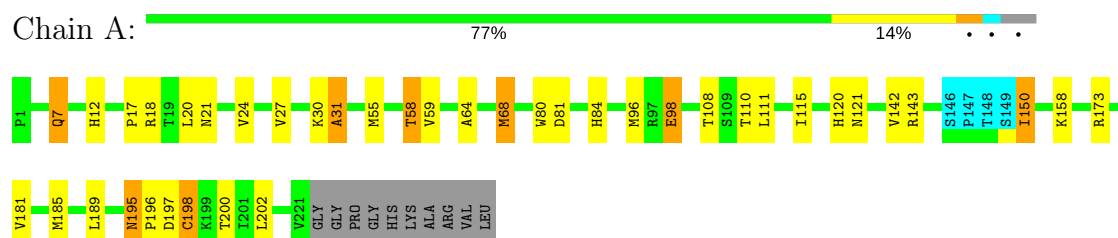
#### 4.2.8 Score per residue for model 8

- Molecule 1: Capsid protein p24



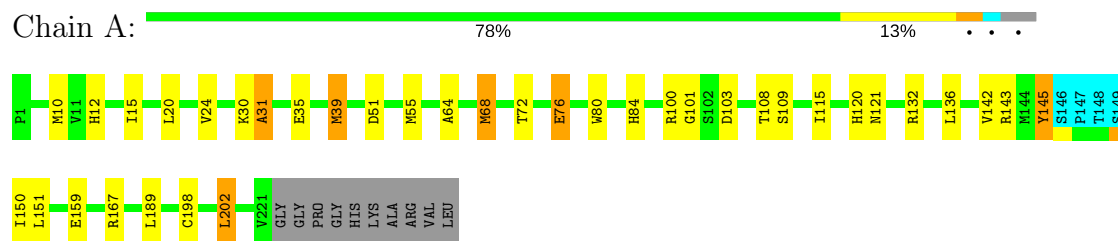
#### 4.2.9 Score per residue for model 9

- Molecule 1: Capsid protein p24



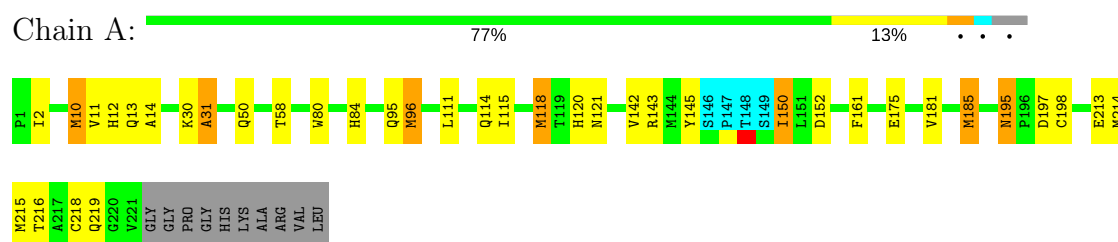
### 4.2.10 Score per residue for model 10

- Molecule 1: Capsid protein p24



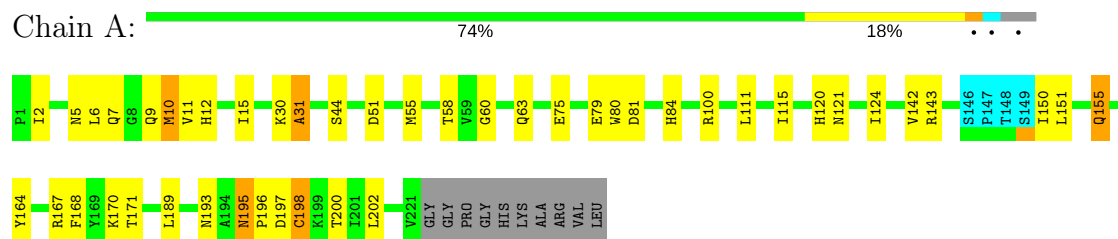
### 4.2.11 Score per residue for model 11

- Molecule 1: Capsid protein p24



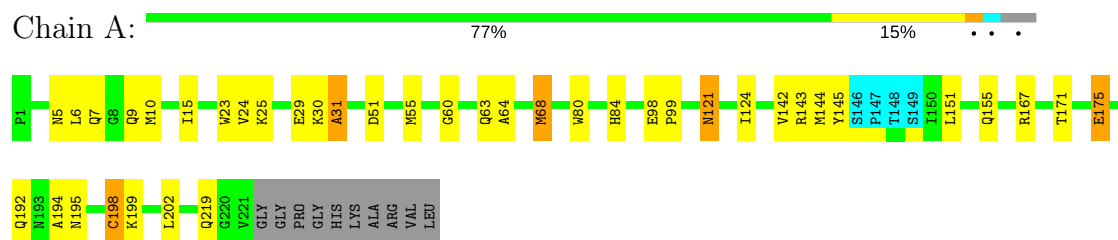
### 4.2.12 Score per residue for model 12

- Molecule 1: Capsid protein p24



### 4.2.13 Score per residue for model 13

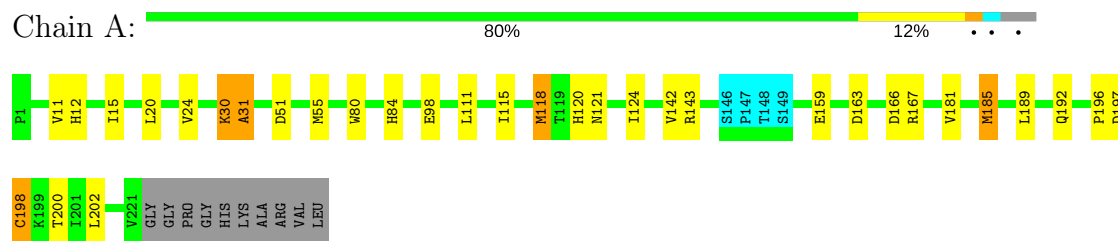
- Molecule 1: Capsid protein p24





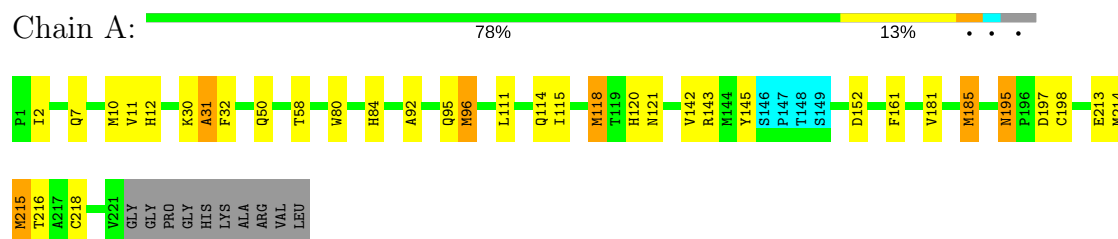
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- Molecule 1: Capsid protein p24



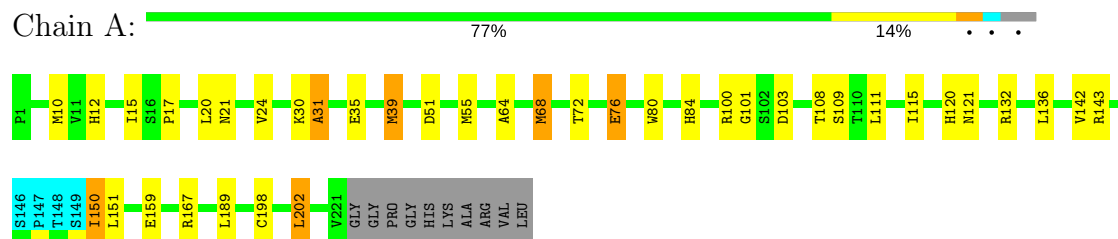
#### 4.2.15 Score per residue for model 15

- Molecule 1: Capsid protein p24



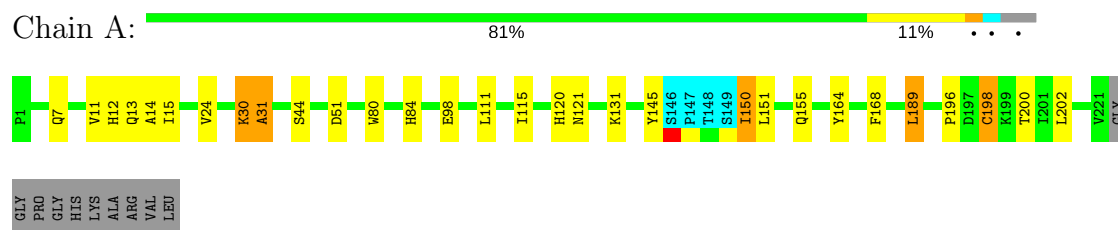
#### 4.2.16 Score per residue for model 16

- Molecule 1: Capsid protein p24



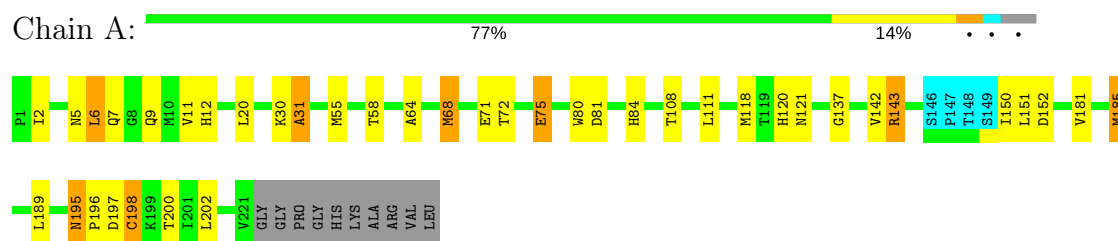
#### 4.2.17 Score per residue for model 17

- Molecule 1: Capsid protein p24



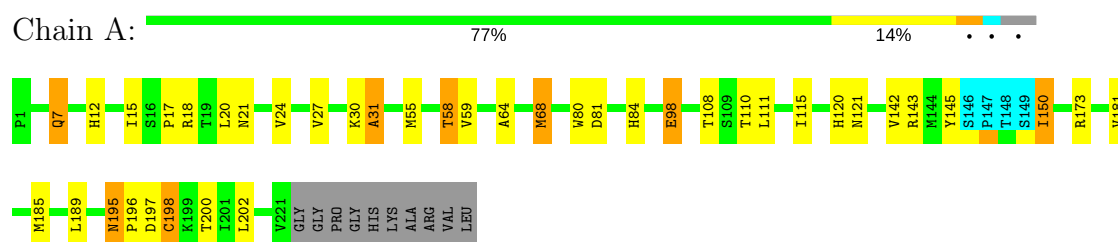
## 4.2.18 Score per residue for model 18

- Molecule 1: Capsid protein p24



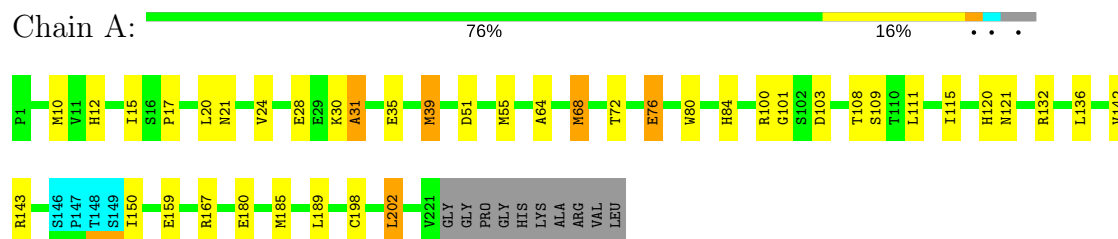
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- Molecule 1: Capsid protein p24



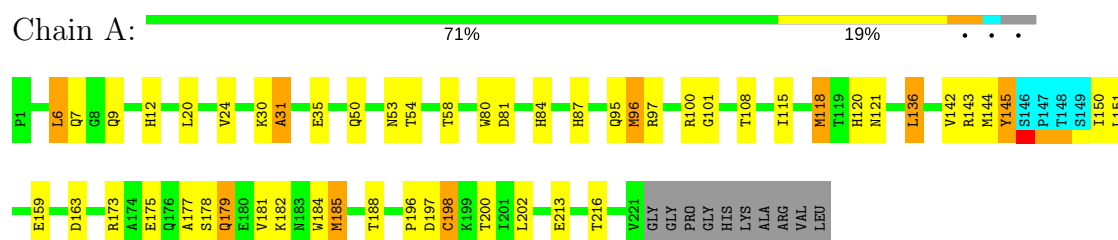
## 4.2.20 Score per residue for model 20

- Molecule 1: Capsid protein p24



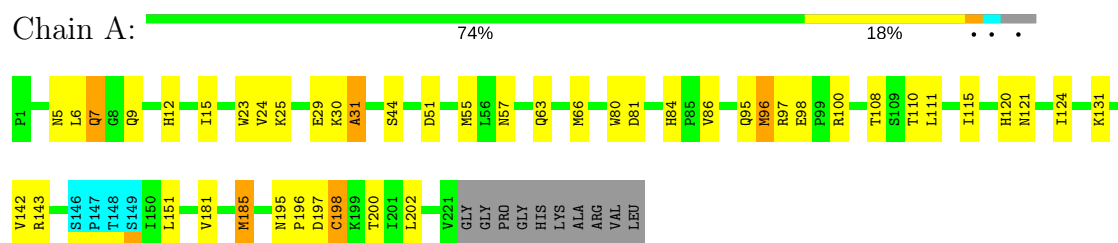
## 4.2.21 Score per residue for model 21

- Molecule 1: Capsid protein p24



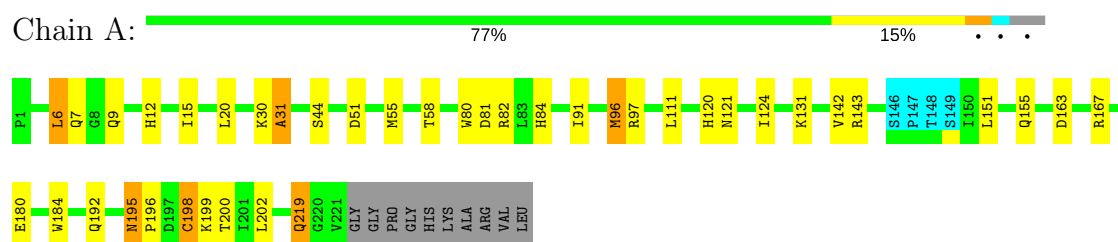
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- Molecule 1: Capsid protein p24



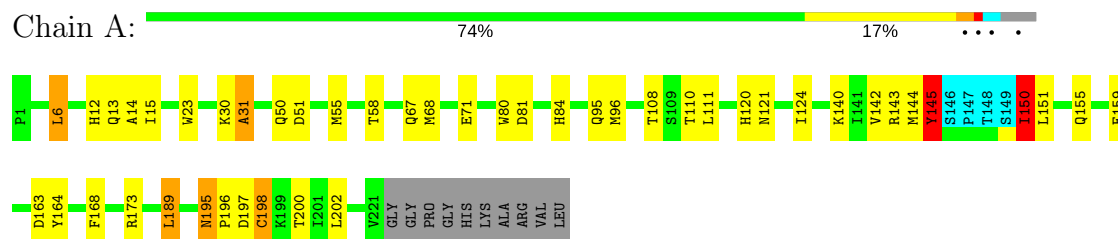
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- Molecule 1: Capsid protein p24



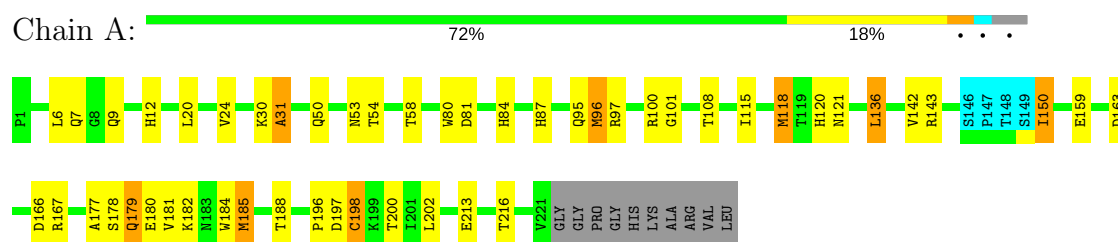
### 4.2.24 Score per residue for model 24

- Molecule 1: Capsid protein p24



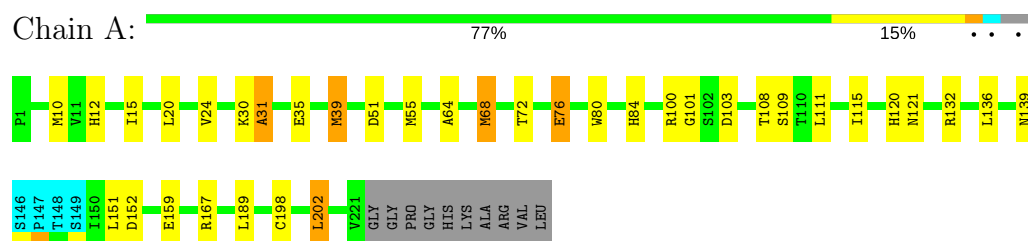
### 4.2.25 Score per residue for model 25

- Molecule 1: Capsid protein p24



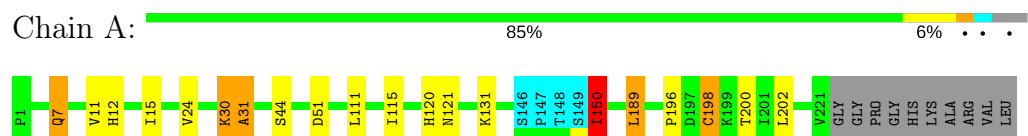
### 4.2.26 Score per residue for model 26

- Molecule 1: Capsid protein p24



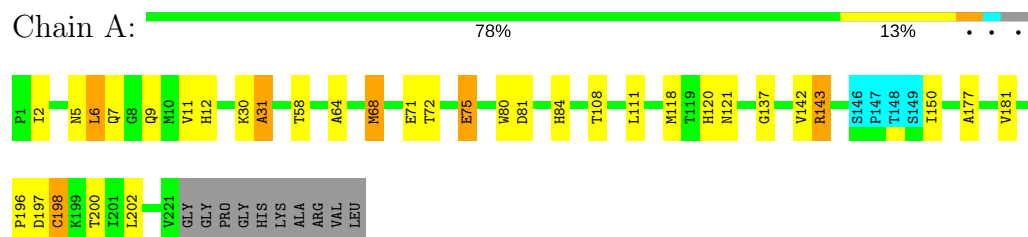
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- Molecule 1: Capsid protein p24



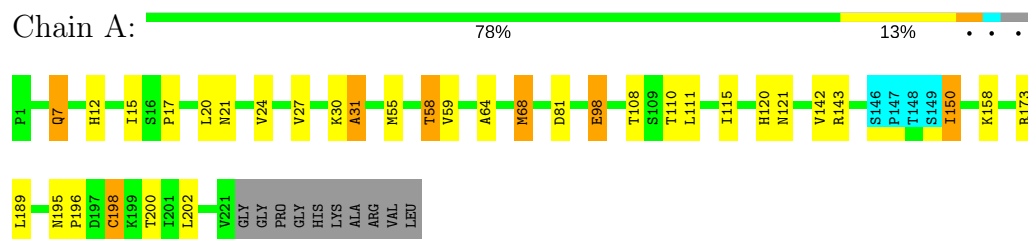
### 4.2.28 Score per residue for model 28

- Molecule 1: Capsid protein p24



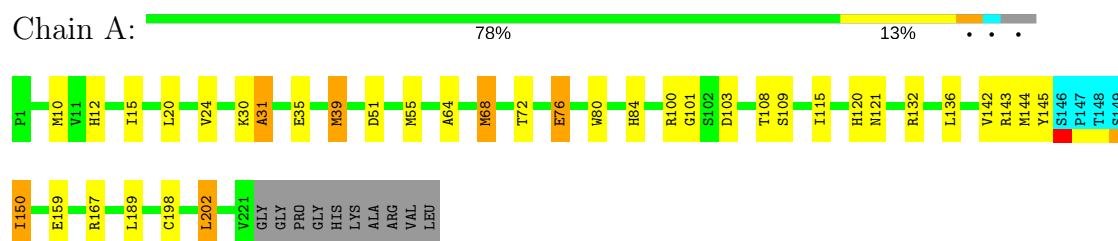
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- Molecule 1: Capsid protein p24



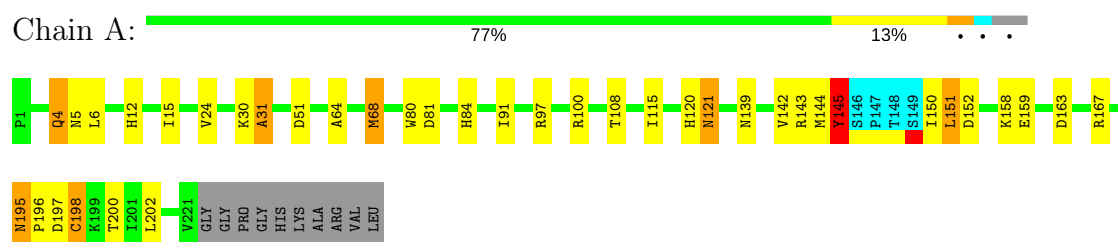
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- Molecule 1: Capsid protein p24



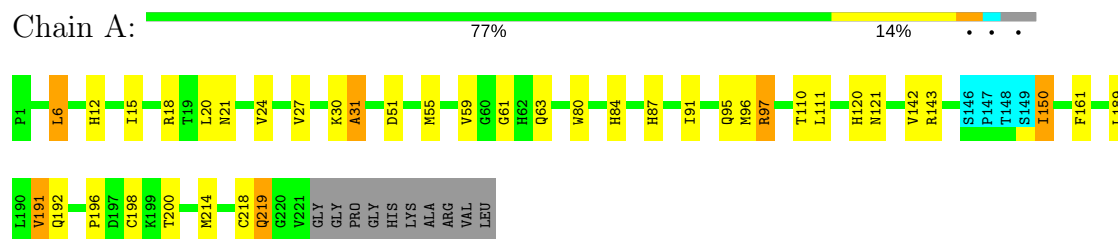
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- Molecule 1: Capsid protein p24



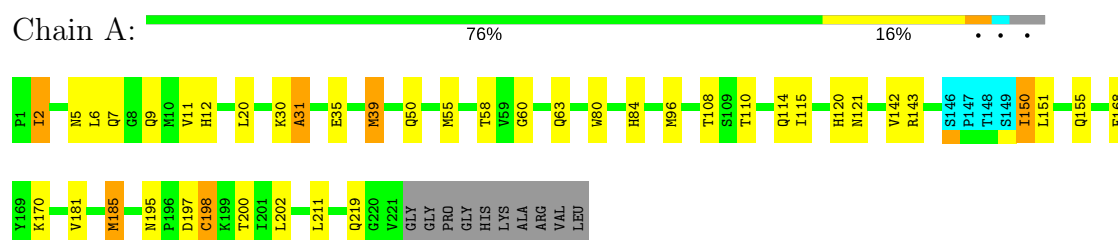
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- Molecule 1: Capsid protein p24



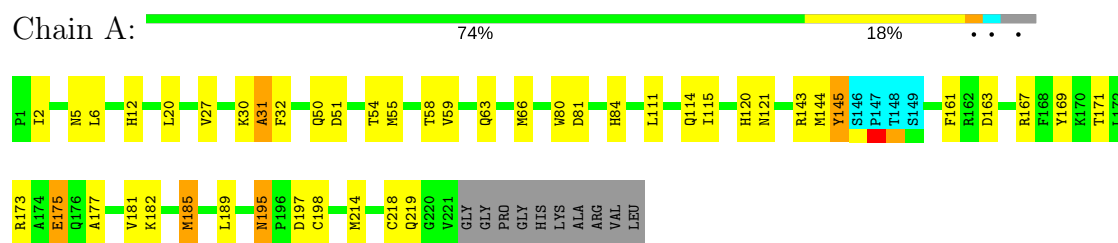
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- Molecule 1: Capsid protein p24



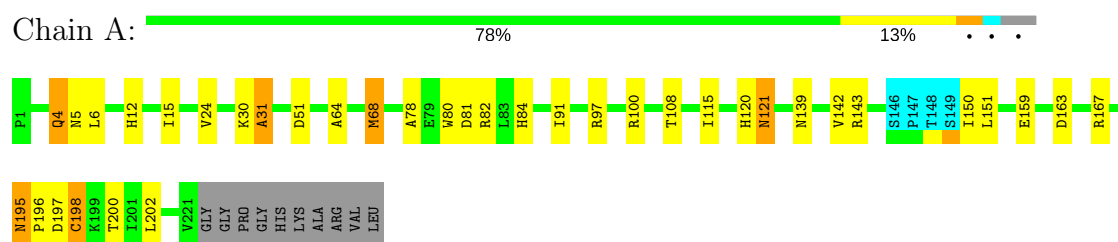
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- Molecule 1: Capsid protein p24



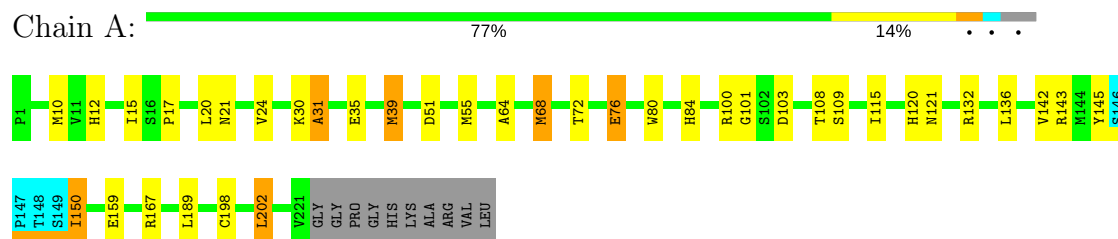
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- Molecule 1: Capsid protein p24



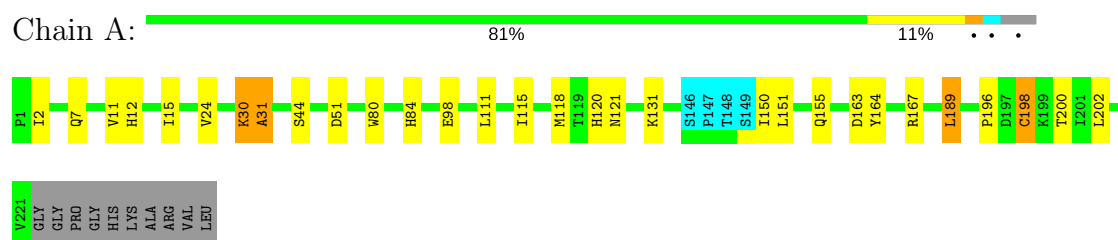
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- Molecule 1: Capsid protein p24



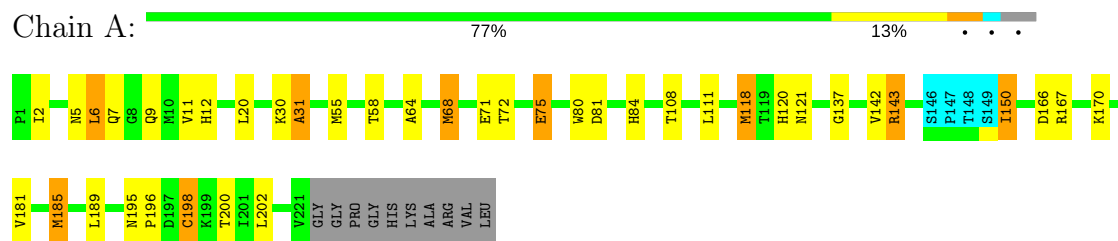
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- Molecule 1: Capsid protein p24



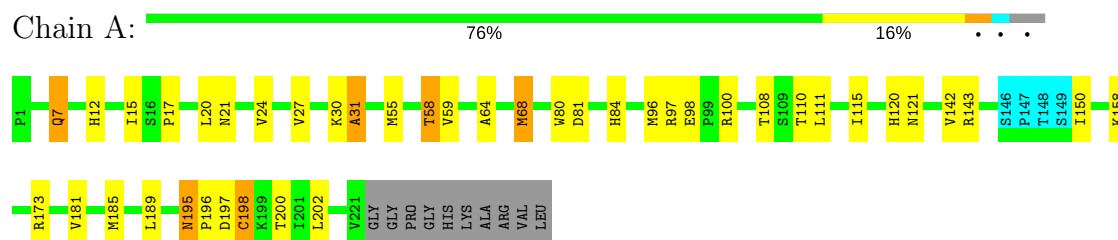
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- Molecule 1: Capsid protein p24



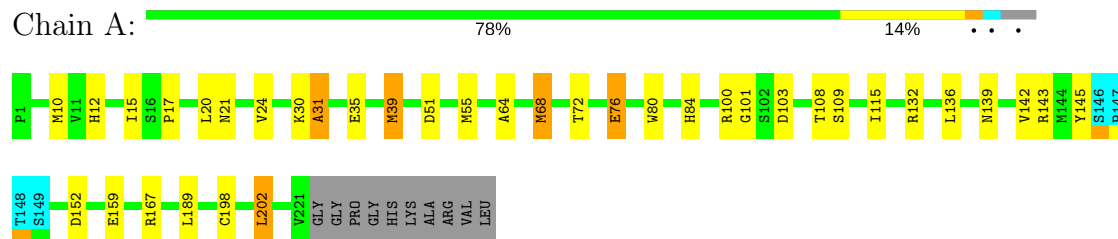
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- Molecule 1: Capsid protein p24



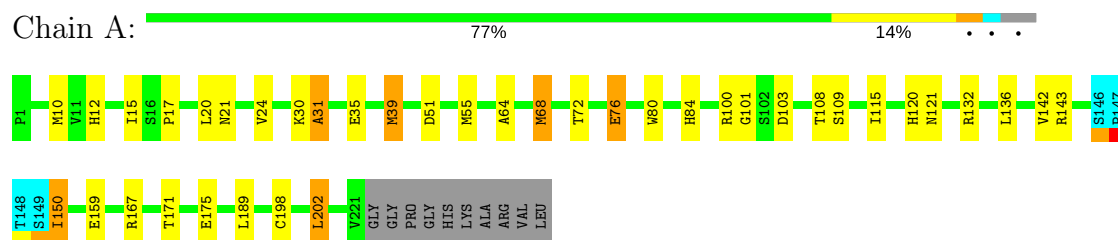
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- Molecule 1: Capsid protein p24



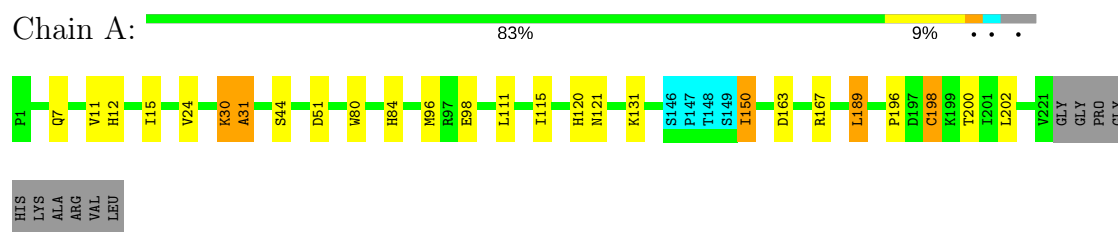
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- Molecule 1: Capsid protein p24



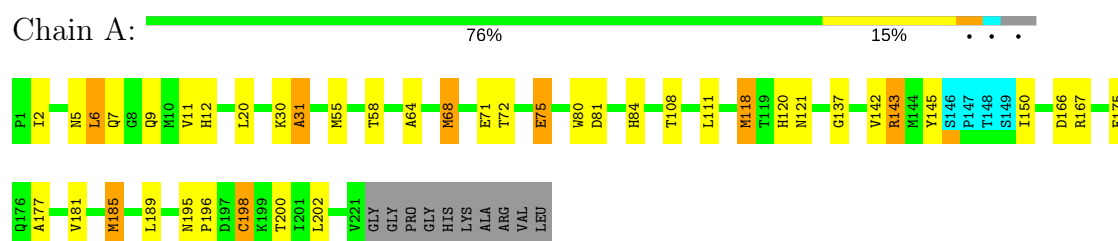
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- Molecule 1: Capsid protein p24



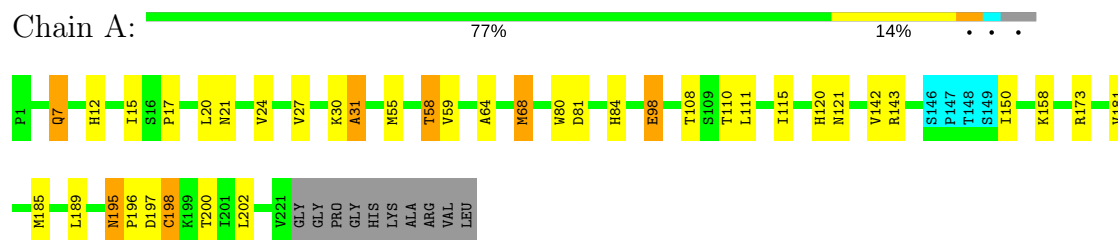
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- Molecule 1: Capsid protein p24



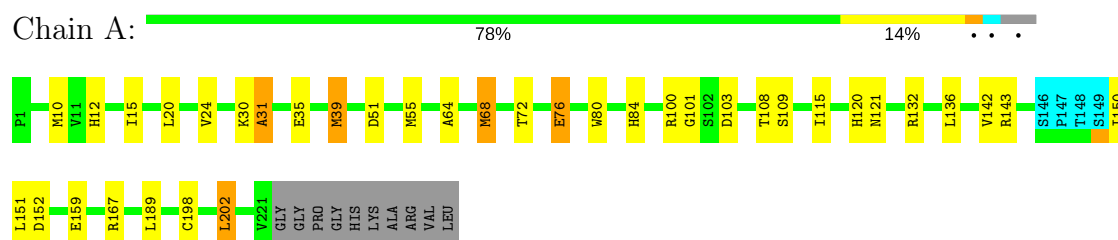
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- Molecule 1: Capsid protein p24



## 4.2.45 Score per residue for model 45

- Molecule 1: Capsid protein p24

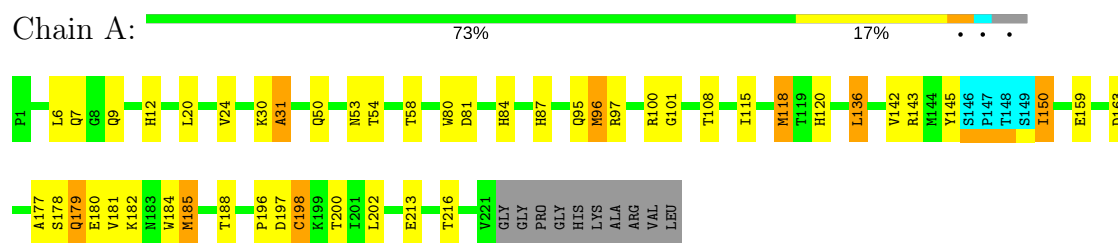






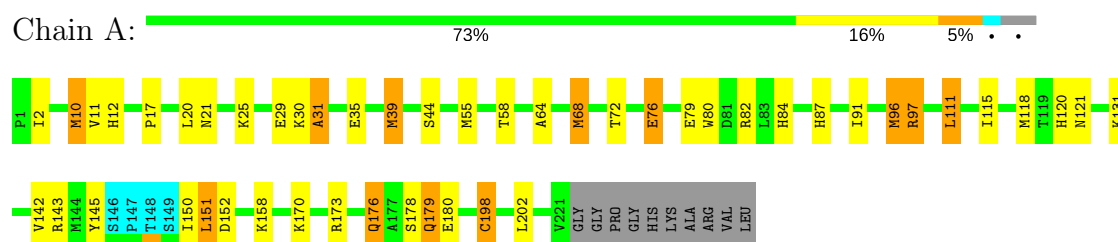
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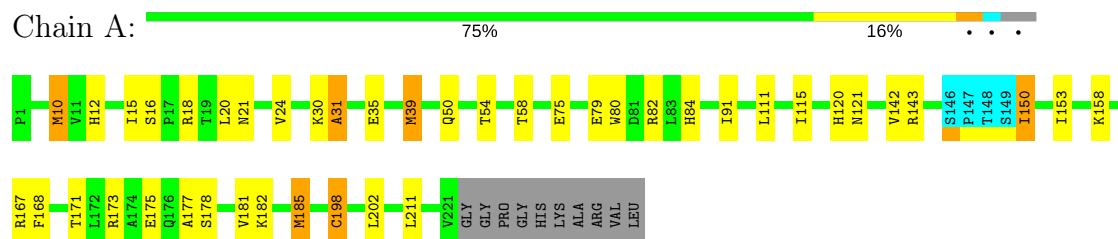
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- Molecule 1: Capsid protein p24



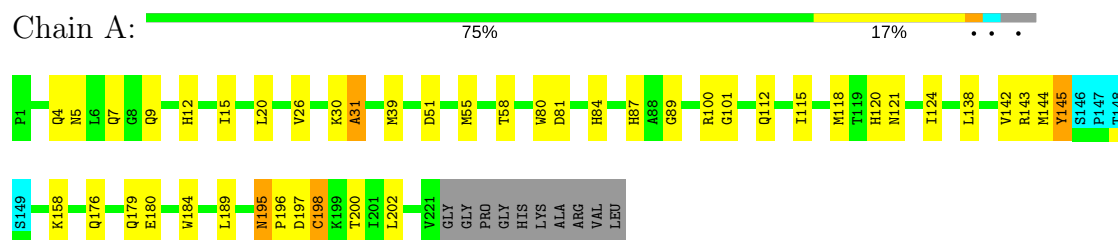
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- Molecule 1: Capsid protein p24



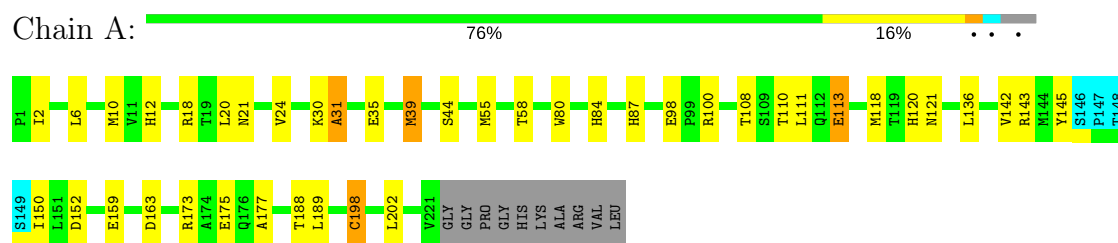
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- Molecule 1: Capsid protein p24



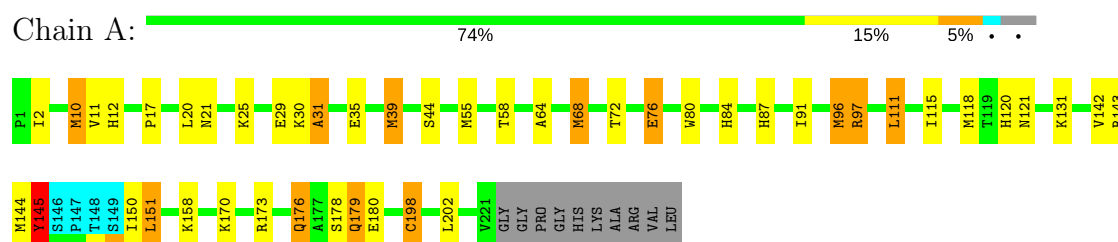
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- Molecule 1: Capsid protein p24



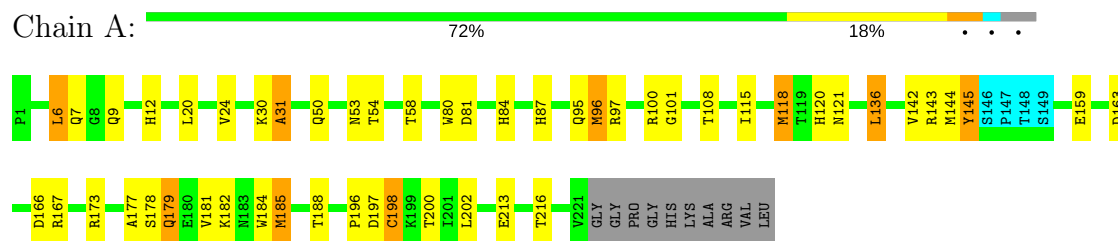
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- Molecule 1: Capsid protein p24



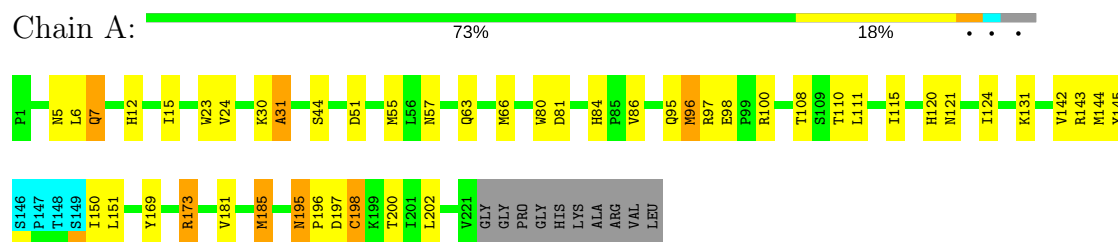
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- Molecule 1: Capsid protein p24



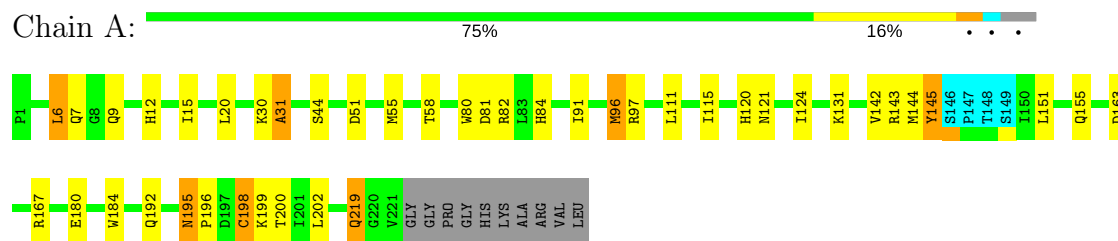
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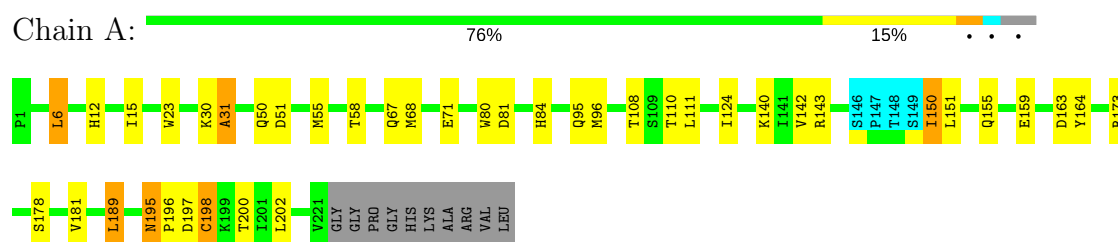
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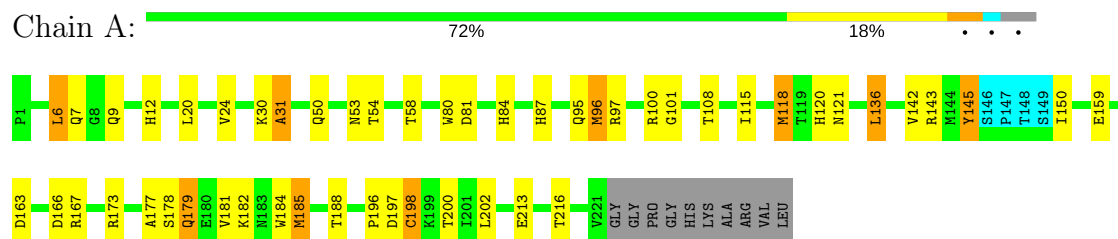
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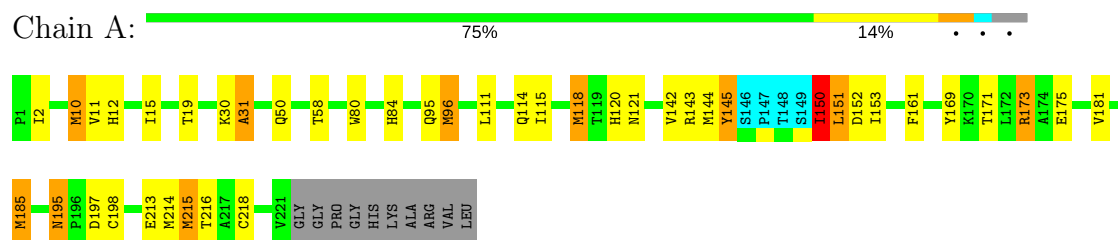
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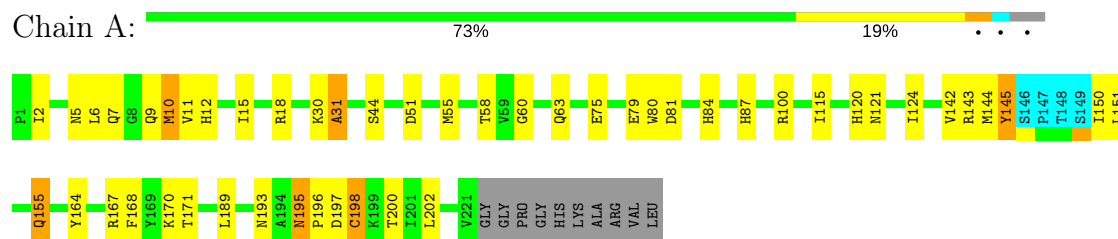
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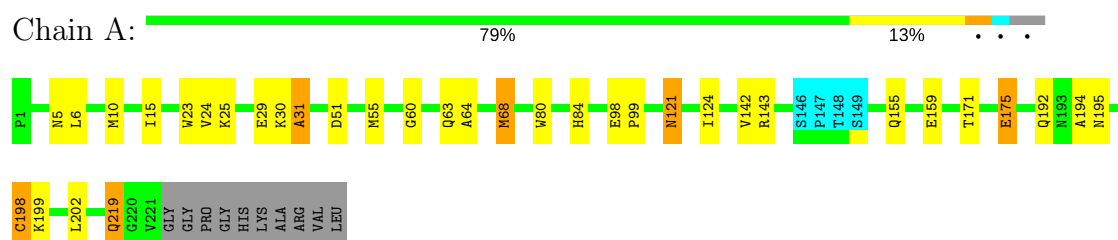
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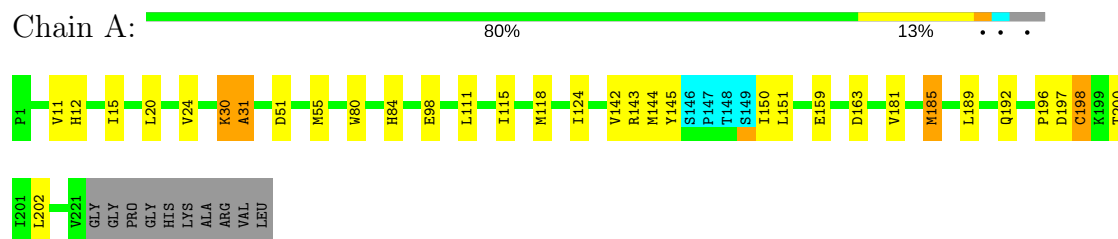
### 4.2.63 Score per residue for model 63

- Molecule 1: Capsid protein p24



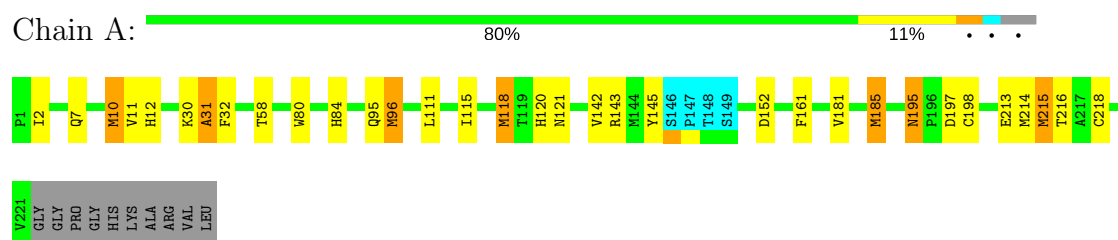
### 4.2.64 Score per residue for model 64

- Molecule 1: Capsid protein p24



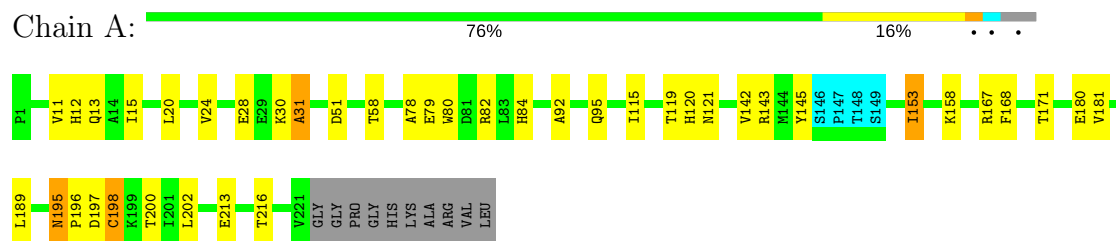
### 4.2.65 Score per residue for model 65

- Molecule 1: Capsid protein p24



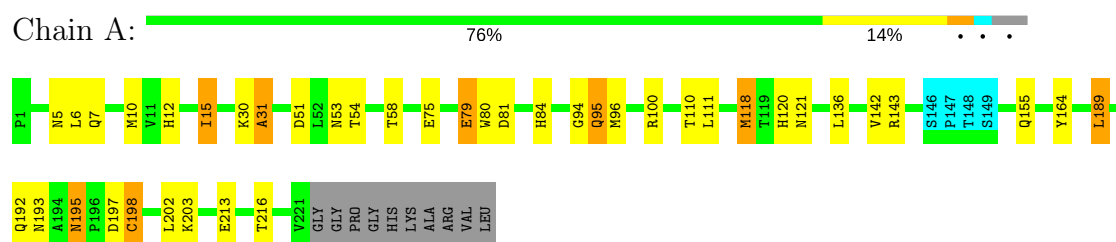
#### 4.2.66 Score per residue for model 66

- Molecule 1: Capsid protein p24



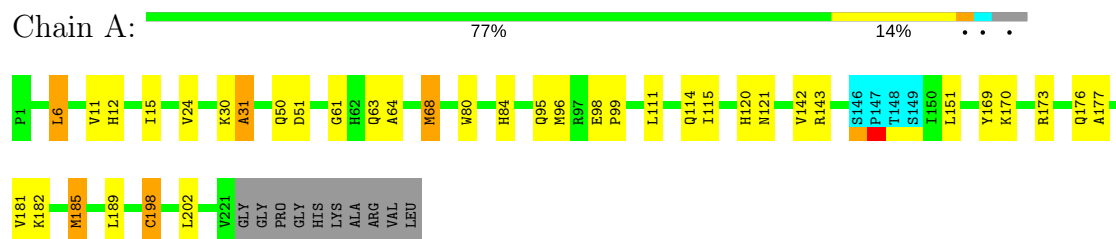
#### 4.2.67 Score per residue for model 67

- Molecule 1: Capsid protein p24



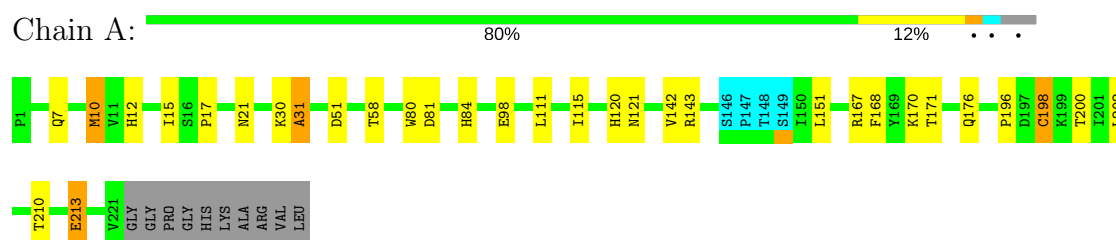
#### 4.2.68 Score per residue for model 68

- Molecule 1: Capsid protein p24



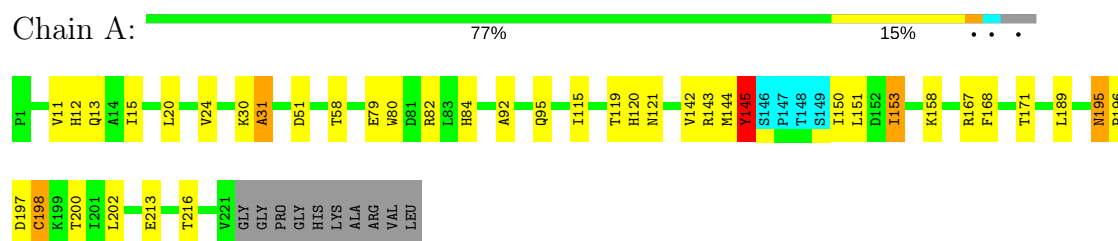
#### 4.2.69 Score per residue for model 69

- Molecule 1: Capsid protein p24



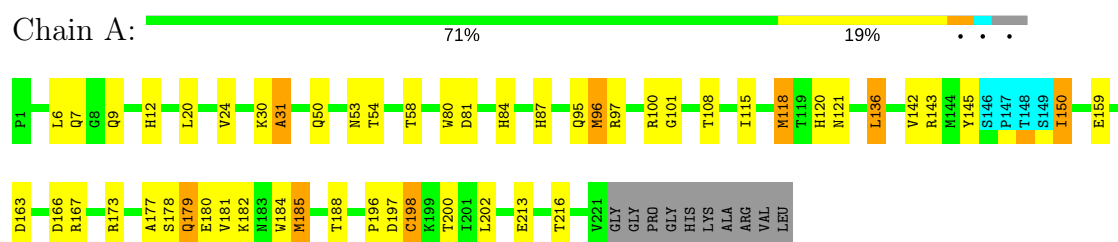
## 4.2.70 Score per residue for model 70

- Molecule 1: Capsid protein p24



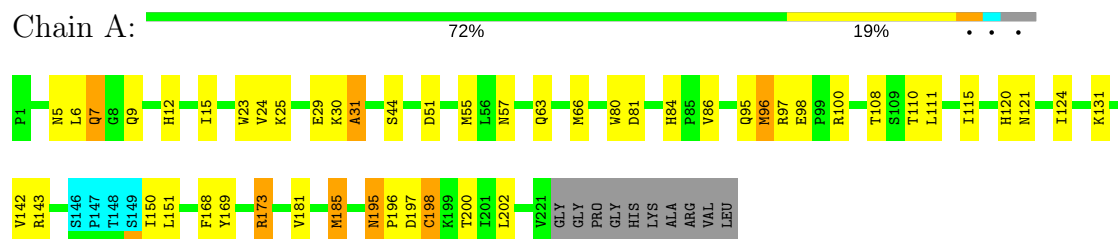
## 4.2.71 Score per residue for model 71

- Molecule 1: Capsid protein p24



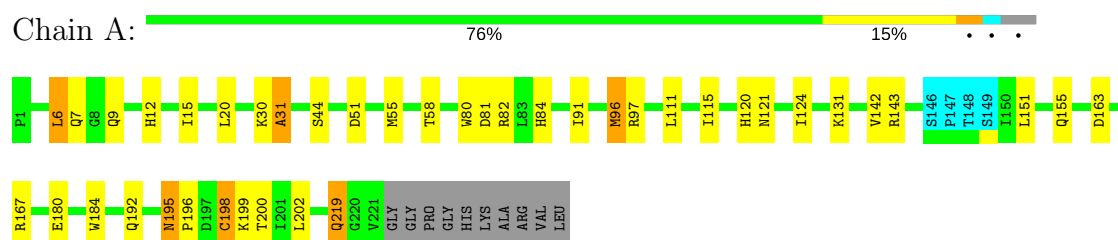
## 4.2.72 Score per residue for model 72

- Molecule 1: Capsid protein p24



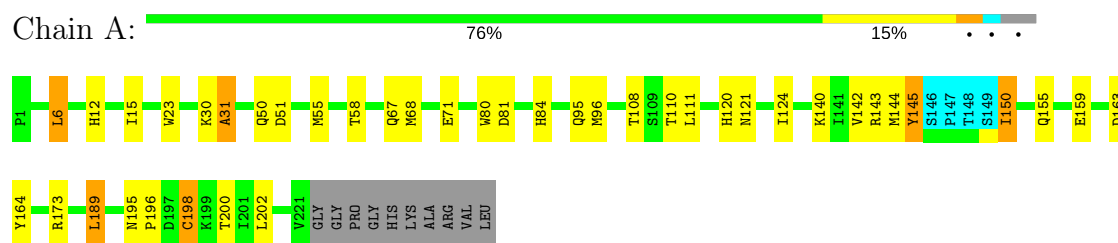
## 4.2.73 Score per residue for model 73

- Molecule 1: Capsid protein p24



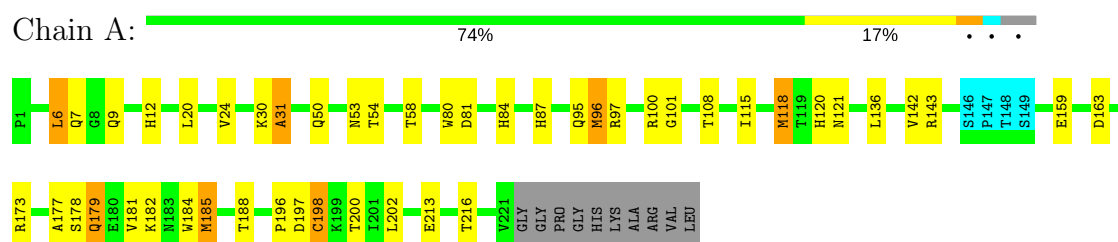
## 4.2.74 Score per residue for model 74

- Molecule 1: Capsid protein p24



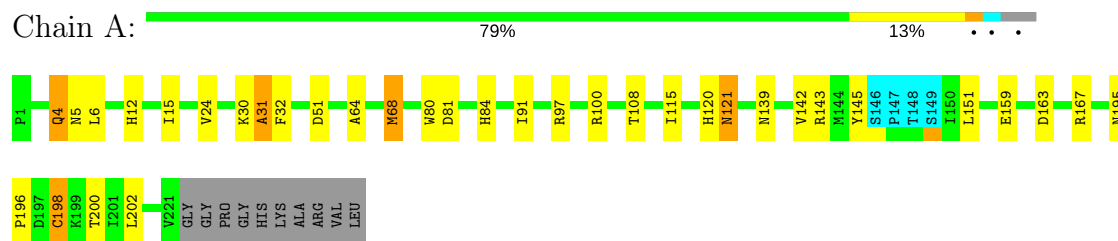
## 4.2.75 Score per residue for model 75

- Molecule 1: Capsid protein p24



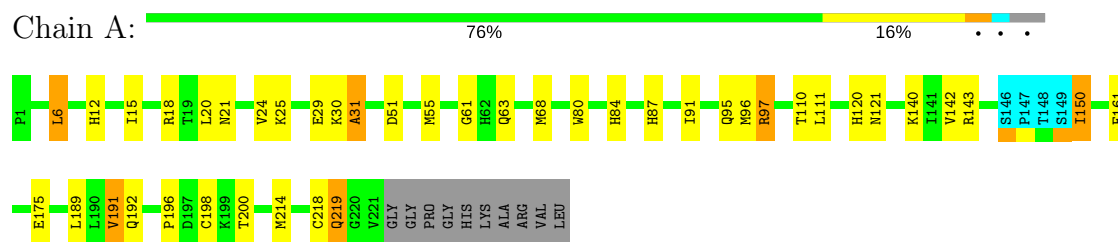
## 4.2.76 Score per residue for model 76

- Molecule 1: Capsid protein p24



## 4.2.77 Score per residue for model 77

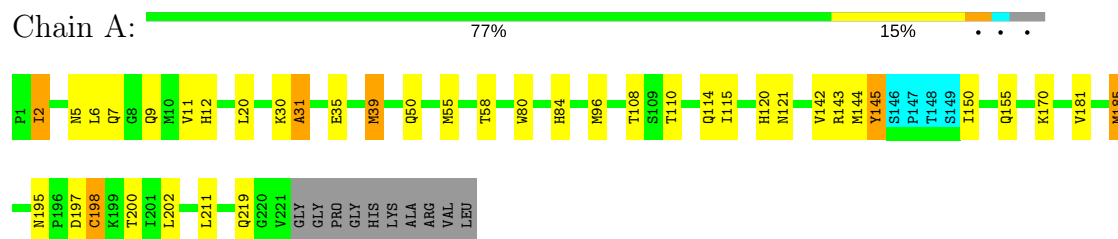
- Molecule 1: Capsid protein p24





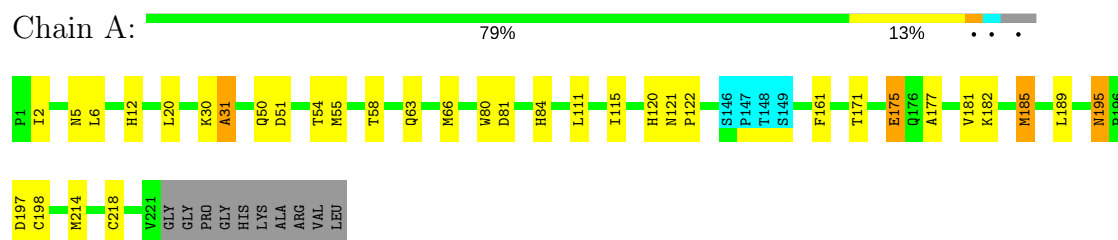
## 4.2.78 Score per residue for model 78

- Molecule 1: Capsid protein p24



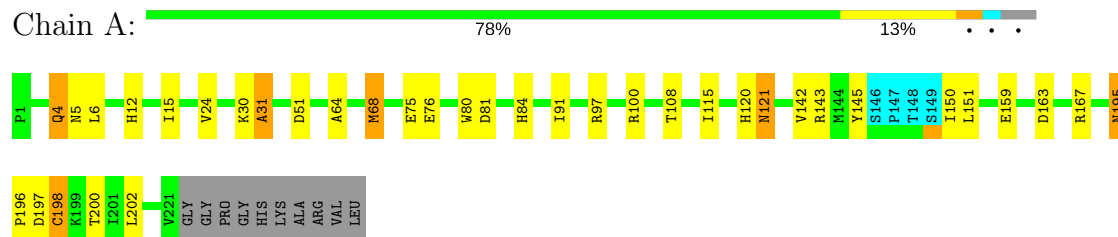
## 4.2.79 Score per residue for model 79

- Molecule 1: Capsid protein p24



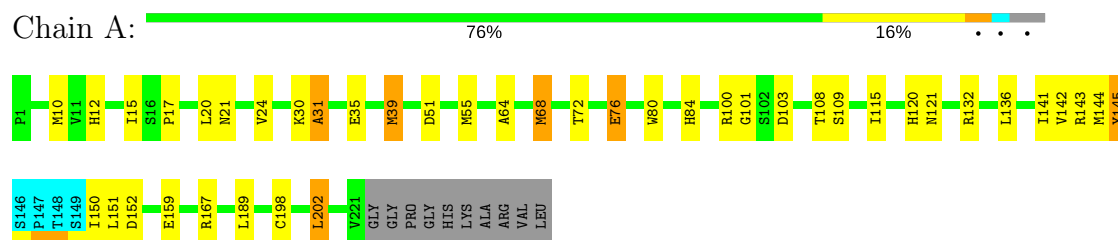
## 4.2.80 Score per residue for model 80

- Molecule 1: Capsid protein p24



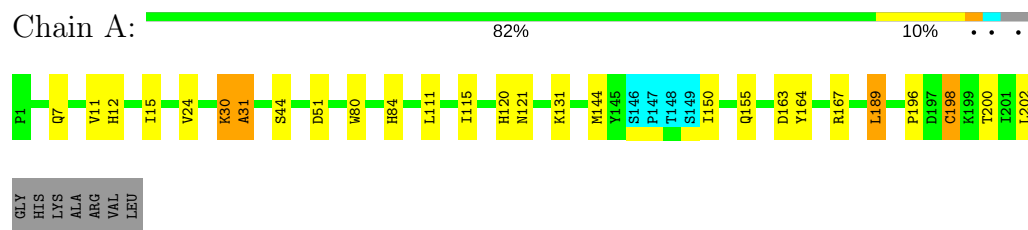
## 4.2.81 Score per residue for model 81

- Molecule 1: Capsid protein p24



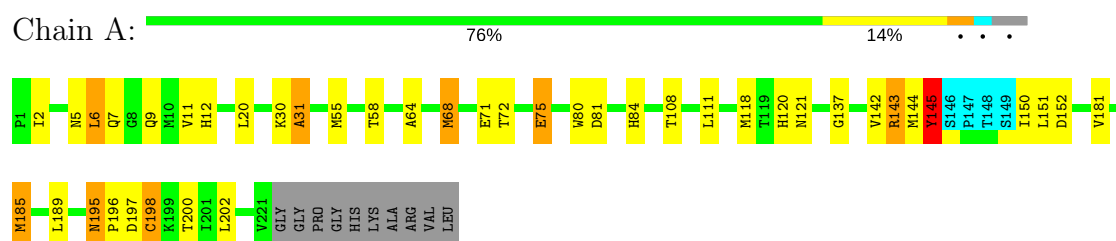
### 4.2.82 Score per residue for model 82

- Molecule 1: Capsid protein p24



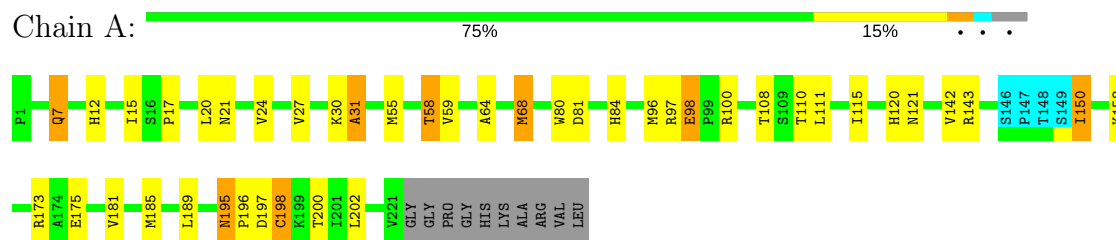
### 4.2.83 Score per residue for model 83

- Molecule 1: Capsid protein p24



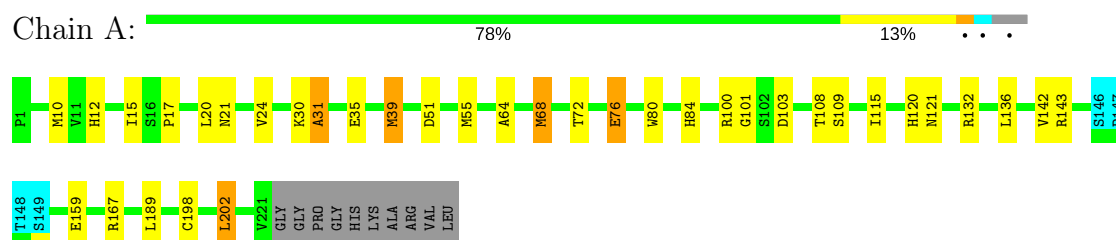
### 4.2.84 Score per residue for model 84

- Molecule 1: Capsid protein p24



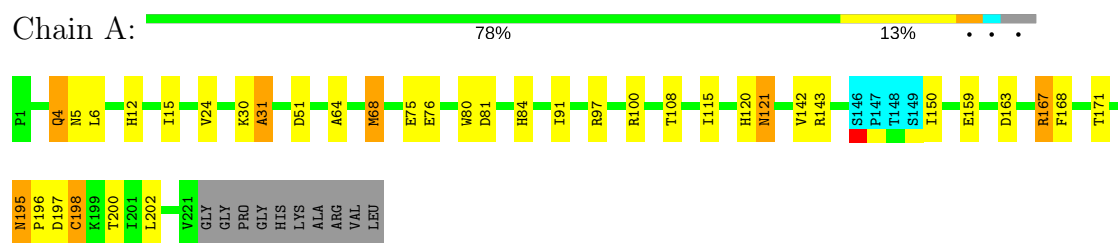
### 4.2.85 Score per residue for model 85

- Molecule 1: Capsid protein p24



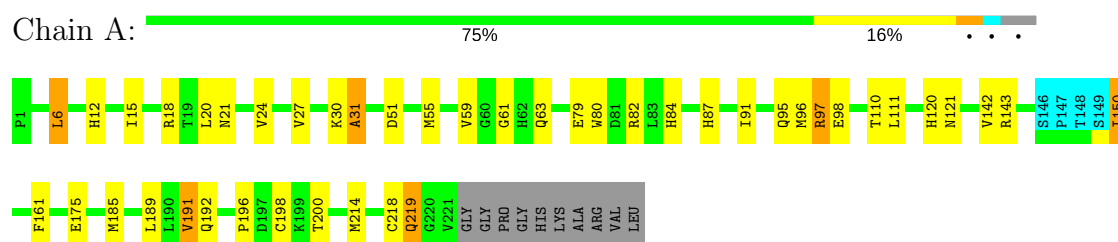
## 4.2.86 Score per residue for model 86

- Molecule 1: Capsid protein p24



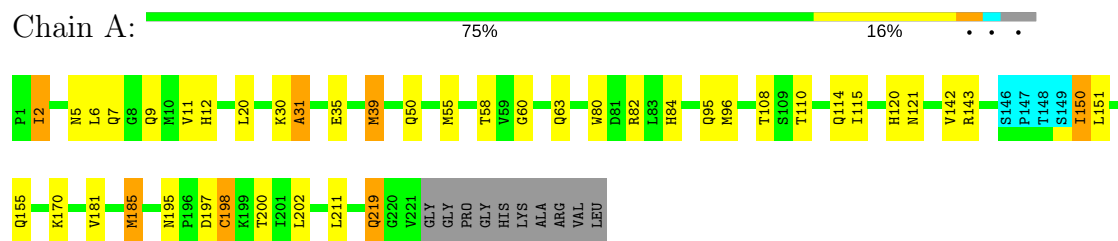
## 4.2.87 Score per residue for model 87

- Molecule 1: Capsid protein p24



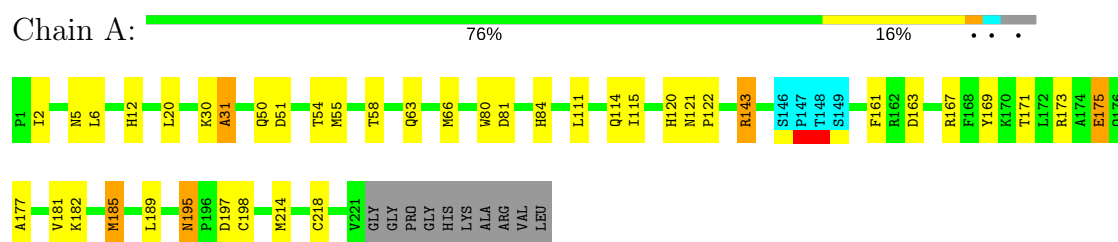
## 4.2.88 Score per residue for model 88

- Molecule 1: Capsid protein p24



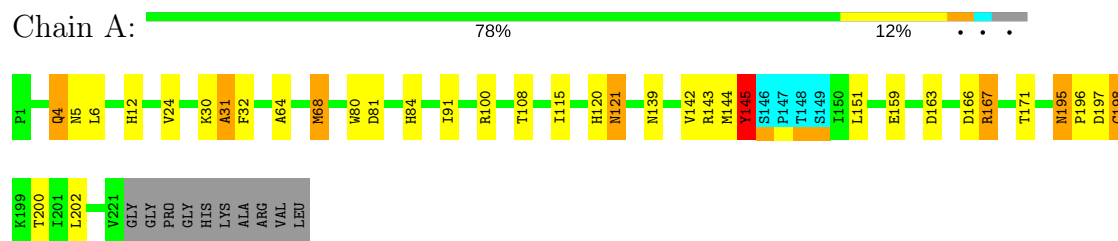
## 4.2.89 Score per residue for model 89

- Molecule 1: Capsid protein p24



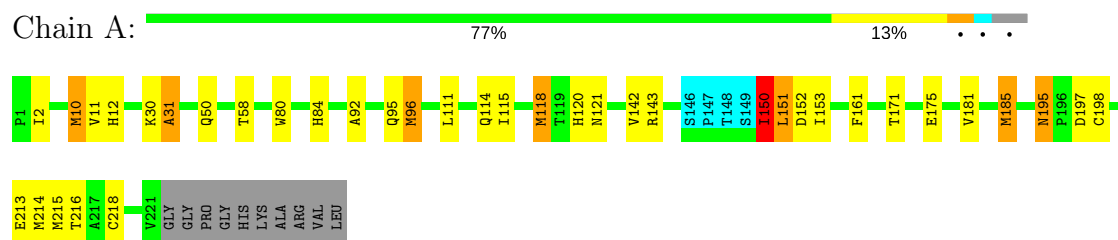
### 4.2.90 Score per residue for model 90

- Molecule 1: Capsid protein p24



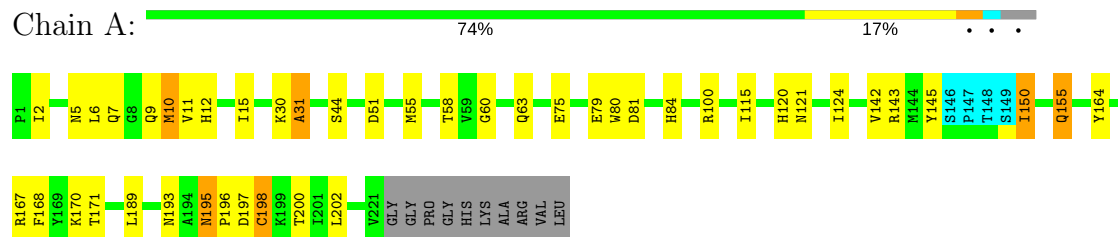
### 4.2.91 Score per residue for model 91

- Molecule 1: Capsid protein p24



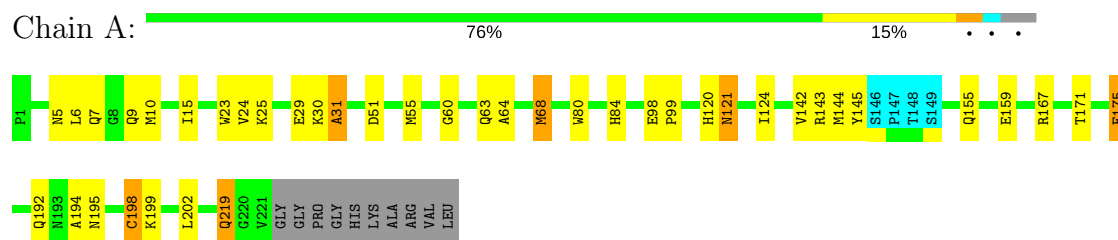
### 4.2.92 Score per residue for model 92

- Molecule 1: Capsid protein p24



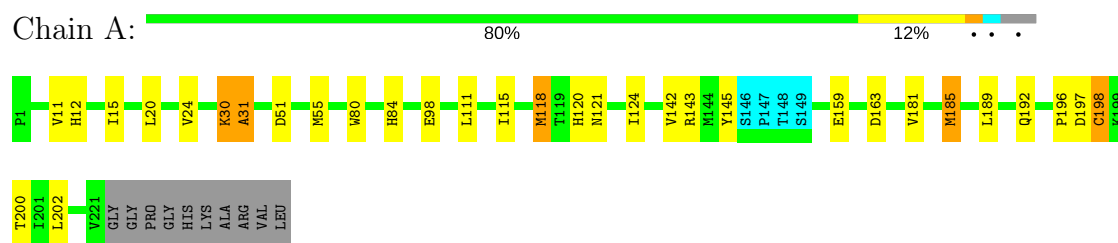
### 4.2.93 Score per residue for model 93

- Molecule 1: Capsid protein p24



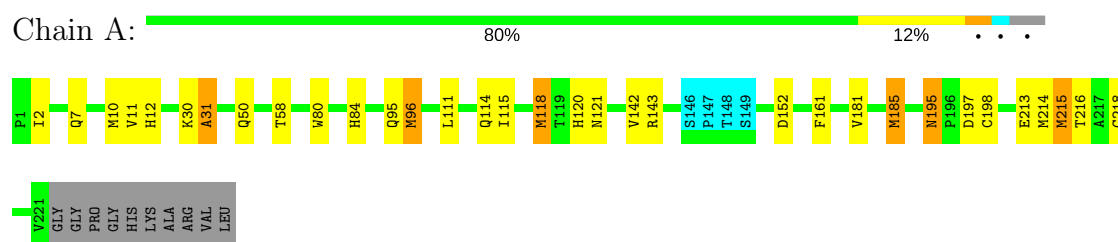
## 4.2.94 Score per residue for model 94

- Molecule 1: Capsid protein p24



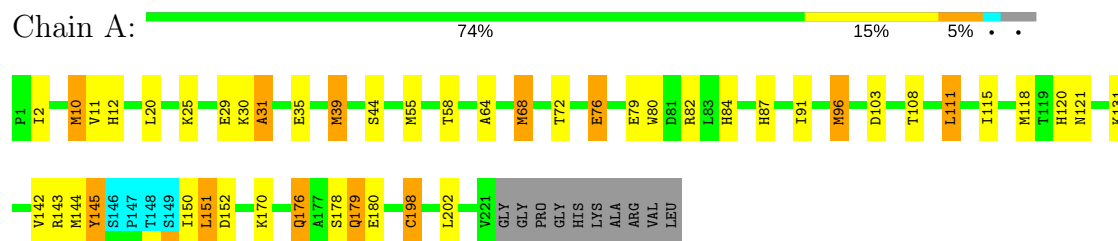
## 4.2.95 Score per residue for model 95

- Molecule 1: Capsid protein p24



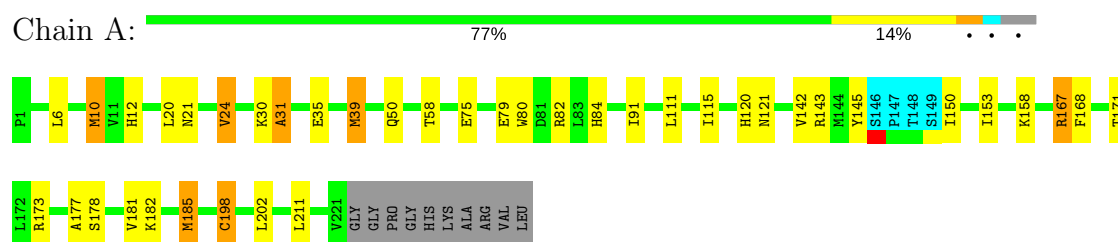
## 4.2.96 Score per residue for model 96

- Molecule 1: Capsid protein p24



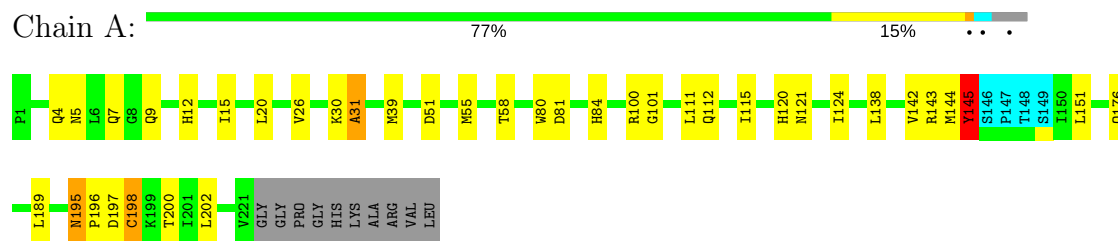
## 4.2.97 Score per residue for model 97

- Molecule 1: Capsid protein p24



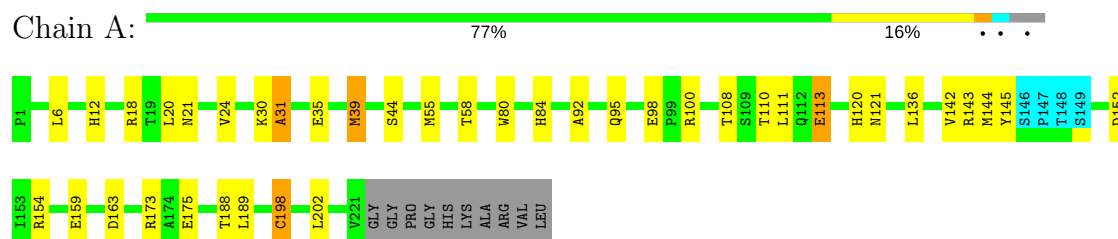
### 4.2.98 Score per residue for model 98

- Molecule 1: Capsid protein p24



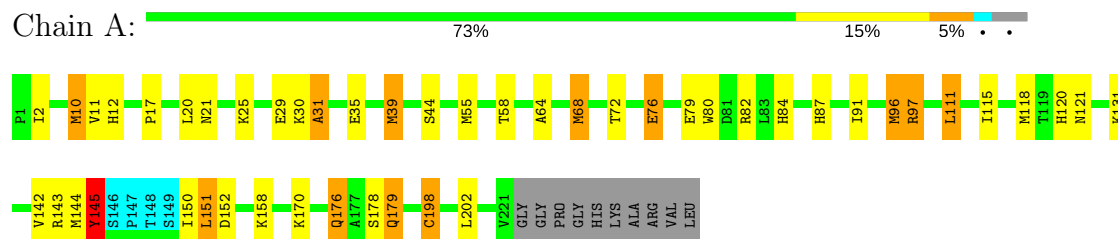
### 4.2.99 Score per residue for model 99

- Molecule 1: Capsid protein p24



### 4.2.100 Score per residue for model 100

- Molecule 1: Capsid protein p24



## 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)	2m8n_cs.str
Number of chemical shift lists	1
Total number of shifts	919
Number of shifts mapped to atoms	919
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	33%

No validations of the models with respect to experimental NMR restraints is performed at this time.

## 6 Model quality i

### 6.1 Standard geometry i

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the (average) root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.40±0.01	0±0/1737 (0.0±0.0%)	0.56±0.01	0±0/2360 (0.0±0.0%)
All	All	0.40	0/173700 (0.0%)	0.56	11/236000 (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	0.0±0.0	0.1±0.2
All	All	0	5

There are no bond-length outliers.

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	150	ILE	CB-CA-C	-6.48	98.65	111.60	41	1
1	A	150	ILE	CA-C-N	-6.08	103.83	117.20	36	3
1	A	144	MET	C-N-CA	-5.65	107.58	121.70	30	1
1	A	145	TYR	CA-CB-CG	-5.63	102.71	113.40	81	1
1	A	145	TYR	CB-CG-CD1	-5.40	117.76	121.00	26	2
1	A	145	TYR	N-CA-C	5.18	124.98	111.00	10	1
1	A	145	TYR	CB-CG-CD2	-5.13	117.92	121.00	98	1
1	A	150	ILE	N-CA-CB	-5.04	99.22	110.80	61	1

There are no chirality outliers.

All unique planar outliers are listed below.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	150	ILE	Mainchain	5



## 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	1699	1708	1703	31±6
All	All	169900	170800	170300	3111

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:6:LEU:H	1:A:6:LEU:HD22	1.04	1.13	75	4
1:A:6:LEU:HD22	1:A:6:LEU:H	0.98	1.14	46	6
1:A:144:MET:O	1:A:145:TYR:O	0.97	1.82	56	8
1:A:150:ILE:HD13	1:A:150:ILE:H	0.89	1.27	38	1
1:A:6:LEU:HD22	1:A:6:LEU:N	0.83	1.88	62	11
1:A:6:LEU:N	1:A:6:LEU:HD22	0.81	1.89	60	3
1:A:12:HIS:CD2	1:A:111:LEU:HD11	0.79	2.13	67	30
1:A:143:ARG:NH2	1:A:184:TRP:CZ2	0.78	2.52	6	1
1:A:20:LEU:O	1:A:24:VAL:HG23	0.78	1.79	44	7
1:A:51:ASP:O	1:A:54:THR:OG1	0.76	2.04	79	3
1:A:6:LEU:H	1:A:6:LEU:CD2	0.76	1.94	21	14
1:A:150:ILE:H	1:A:150:ILE:HD12	0.75	1.38	7	2
1:A:6:LEU:CD2	1:A:6:LEU:H	0.73	1.94	56	10
1:A:161:PHE:CG	1:A:218:CYS:SG	0.73	2.81	77	12
1:A:53:ASN:OD1	1:A:54:THR:N	0.73	2.22	75	8
1:A:150:ILE:HD12	1:A:150:ILE:H	0.73	1.43	21	1
1:A:185:MET:SD	1:A:189:LEU:HD22	0.72	2.25	29	7
1:A:150:ILE:HD12	1:A:150:ILE:N	0.71	2.01	42	2
1:A:158:LYS:O	1:A:158:LYS:CG	0.69	2.40	44	6
1:A:176:GLN:NE2	1:A:176:GLN:H	0.69	1.86	51	2
1:A:150:ILE:HG21	1:A:175:GLU:OE2	0.69	1.86	61	1
1:A:108:THR:O	1:A:108:THR:HG22	0.69	1.88	3	24
1:A:176:GLN:H	1:A:176:GLN:NE2	0.69	1.86	55	2
1:A:32:PHE:CE2	1:A:145:TYR:CE2	0.69	2.81	76	2
1:A:108:THR:HG22	1:A:108:THR:O	0.68	1.88	28	14
1:A:158:LYS:CG	1:A:158:LYS:O	0.68	2.41	52	4
1:A:91:ILE:HD12	1:A:91:ILE:N	0.68	2.04	73	10

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:91:ILE:N	1:A:91:ILE:HD12	0.68	2.04	48	9
1:A:167:ARG:O	1:A:171:THR:HG23	0.68	1.87	12	8
1:A:91:ILE:HD11	1:A:97:ARG:HH21	0.66	1.50	76	5
1:A:161:PHE:CD2	1:A:218:CYS:SG	0.66	2.87	91	6
1:A:142:VAL:O	1:A:145:TYR:CD2	0.66	2.49	74	1
1:A:80:TRP:CZ3	1:A:84:HIS:CE1	0.65	2.84	31	75
1:A:161:PHE:CD1	1:A:218:CYS:SG	0.65	2.90	32	6
1:A:92:ALA:HB3	1:A:95:GLN:OE1	0.65	1.91	70	2
1:A:144:MET:O	1:A:145:TYR:C	0.65	2.33	83	10
1:A:145:TYR:O	1:A:145:TYR:CG	0.65	2.49	83	4
1:A:2:ILE:HD13	1:A:2:ILE:H	0.64	1.52	88	3
1:A:144:MET:O	1:A:145:TYR:CD2	0.63	2.51	53	2
1:A:144:MET:O	1:A:145:TYR:CG	0.63	2.51	98	3
1:A:97:ARG:NE	1:A:100:ARG:NH1	0.63	2.47	4	2
1:A:150:ILE:O	1:A:153:ILE:N	0.63	2.24	91	2
1:A:6:LEU:CD2	1:A:6:LEU:N	0.63	2.62	50	6
1:A:50:GLN:OE1	1:A:111:LEU:HD13	0.63	1.94	24	6
1:A:80:TRP:CZ3	1:A:84:HIS:NE2	0.62	2.67	2	18
1:A:32:PHE:CZ	1:A:145:TYR:CZ	0.62	2.88	76	2
1:A:87:HIS:CE1	1:A:97:ARG:NH2	0.62	2.68	55	3
1:A:150:ILE:HG22	1:A:171:THR:CG2	0.62	2.25	61	1
1:A:150:ILE:HG12	1:A:175:GLU:OE2	0.62	1.95	61	1
1:A:143:ARG:NH1	1:A:143:ARG:O	0.61	2.33	43	3
1:A:68:MET:SD	1:A:68:MET:N	0.61	2.73	40	24
1:A:150:ILE:HG13	1:A:151:LEU:H	0.61	1.55	61	1
1:A:150:ILE:HD13	1:A:151:LEU:N	0.61	2.10	59	1
1:A:161:PHE:CD1	1:A:198:CYS:SG	0.61	2.93	95	6
1:A:150:ILE:C	1:A:150:ILE:HD12	0.61	2.15	91	1
1:A:10:MET:N	1:A:10:MET:SD	0.61	2.74	67	9
1:A:96:MET:SD	1:A:120:HIS:CE1	0.61	2.94	60	18
1:A:32:PHE:CE2	1:A:145:TYR:CZ	0.61	2.88	76	3
1:A:68:MET:N	1:A:68:MET:SD	0.61	2.74	43	18
1:A:144:MET:O	1:A:145:TYR:HB2	0.61	1.94	100	1
1:A:13:GLN:N	1:A:13:GLN:NE2	0.61	2.49	66	2
1:A:142:VAL:O	1:A:145:TYR:CD1	0.61	2.54	24	2
1:A:95:GLN:NE2	1:A:95:GLN:N	0.60	2.49	67	1
1:A:11:VAL:HG22	1:A:12:HIS:N	0.60	2.12	91	16
1:A:96:MET:SD	1:A:97:ARG:N	0.60	2.75	48	4
1:A:171:THR:HG22	1:A:175:GLU:OE2	0.60	1.97	79	3
1:A:6:LEU:H	1:A:6:LEU:HD23	0.60	1.56	28	10
1:A:18:ARG:NH1	1:A:21:ASN:HD22	0.60	1.94	87	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:155:GLN:HE21	1:A:195:ASN:H	0.59	1.38	63	11
1:A:30:LYS:O	1:A:31:ALA:C	0.59	2.41	2	100
1:A:80:TRP:CH2	1:A:84:HIS:NE2	0.59	2.70	34	28
1:A:20:LEU:HD23	1:A:55:MET:SD	0.59	2.38	6	42
1:A:150:ILE:CD1	1:A:150:ILE:N	0.59	2.65	71	2
1:A:176:GLN:CD	1:A:176:GLN:H	0.59	2.01	100	2
1:A:158:LYS:O	1:A:158:LYS:HG2	0.59	1.98	70	10
1:A:181:VAL:O	1:A:185:MET:SD	0.59	2.61	33	37
1:A:10:MET:SD	1:A:10:MET:N	0.59	2.75	69	6
1:A:11:VAL:HG12	1:A:12:HIS:N	0.58	2.13	2	13
1:A:144:MET:O	1:A:145:TYR:CD1	0.58	2.56	99	2
1:A:155:GLN:HE22	1:A:195:ASN:ND2	0.58	1.96	92	3
1:A:87:HIS:CE1	1:A:97:ARG:HH21	0.58	2.15	55	3
1:A:176:GLN:H	1:A:176:GLN:CD	0.58	2.01	96	2
1:A:5:ASN:OD1	1:A:6:LEU:N	0.58	2.36	12	23
1:A:28:GLU:O	1:A:180:GLU:OE2	0.58	2.22	66	1
1:A:214:MET:O	1:A:218:CYS:SG	0.58	2.62	87	12
1:A:97:ARG:HE	1:A:100:ARG:NH1	0.58	1.97	4	3
1:A:50:GLN:O	1:A:54:THR:HG23	0.58	1.98	79	3
1:A:144:MET:O	1:A:145:TYR:CB	0.58	2.50	55	3
1:A:145:TYR:OH	1:A:181:VAL:CG2	0.58	2.52	66	1
1:A:161:PHE:CD2	1:A:198:CYS:SG	0.57	2.97	79	6
1:A:60:GLY:O	1:A:63:GLN:NE2	0.57	2.37	13	6
1:A:153:ILE:N	1:A:153:ILE:CD1	0.57	2.66	97	3
1:A:87:HIS:CD2	1:A:97:ARG:HH12	0.57	2.17	77	3
1:A:142:VAL:O	1:A:145:TYR:O	0.57	2.22	71	2
1:A:96:MET:SD	1:A:120:HIS:NE2	0.57	2.78	100	4
1:A:97:ARG:NE	1:A:100:ARG:HH12	0.57	1.97	4	1
1:A:63:GLN:NE2	1:A:66:MET:CE	0.57	2.68	34	6
1:A:72:THR:HG21	1:A:137:GLY:HA2	0.57	1.77	83	7
1:A:177:ALA:O	1:A:182:LYS:NZ	0.57	2.34	71	14
1:A:120:HIS:CD2	1:A:121:ASN:H	0.57	2.18	52	4
1:A:153:ILE:N	1:A:153:ILE:HD12	0.57	2.14	97	1
1:A:153:ILE:CD1	1:A:153:ILE:N	0.57	2.67	70	1
1:A:158:LYS:HG2	1:A:158:LYS:O	0.57	2.00	53	6
1:A:169:TYR:OH	1:A:173:ARG:NH2	0.57	2.38	34	2
1:A:150:ILE:O	1:A:152:ASP:N	0.56	2.38	91	2
1:A:143:ARG:O	1:A:145:TYR:CE2	0.56	2.58	96	3
1:A:111:LEU:H	1:A:111:LEU:HD23	0.56	1.60	55	3
1:A:96:MET:N	1:A:96:MET:SD	0.56	2.79	55	11
1:A:150:ILE:CG2	1:A:175:GLU:OE2	0.56	2.53	61	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:12:HIS:HB2	1:A:115:ILE:HD11	0.56	1.78	96	33
1:A:150:ILE:HD12	1:A:151:LEU:N	0.56	2.16	91	1
1:A:95:GLN:OE1	1:A:95:GLN:N	0.56	2.39	66	1
1:A:6:LEU:HD23	1:A:6:LEU:H	0.56	1.61	49	5
1:A:97:ARG:NH2	1:A:98:GLU:OE1	0.56	2.39	72	4
1:A:20:LEU:HD11	1:A:58:THR:OG1	0.56	2.01	56	14
1:A:163:ASP:OD1	1:A:167:ARG:NH1	0.56	2.39	34	12
1:A:79:GLU:OE2	1:A:82:ARG:NH2	0.56	2.39	66	2
1:A:153:ILE:HD12	1:A:153:ILE:N	0.56	2.16	52	3
1:A:7:GLN:O	1:A:9:GLN:NE2	0.55	2.39	50	32
1:A:111:LEU:HD23	1:A:111:LEU:H	0.55	1.61	100	1
1:A:64:ALA:O	1:A:68:MET:SD	0.55	2.65	45	42
1:A:96:MET:SD	1:A:96:MET:N	0.55	2.79	51	11
1:A:150:ILE:N	1:A:150:ILE:HD12	0.55	2.16	71	2
1:A:81:ASP:OD1	1:A:100:ARG:NH1	0.55	2.39	56	17
1:A:168:PHE:O	1:A:171:THR:OG1	0.55	2.23	52	8
1:A:87:HIS:O	1:A:97:ARG:NH1	0.55	2.40	50	8
1:A:159:GLU:OE1	1:A:159:GLU:N	0.54	2.40	93	2
1:A:95:GLN:N	1:A:95:GLN:OE1	0.54	2.40	70	1
1:A:185:MET:N	1:A:185:MET:SD	0.54	2.80	89	21
1:A:121:ASN:H	1:A:121:ASN:ND2	0.54	2.00	13	3
1:A:111:LEU:CD2	1:A:111:LEU:H	0.54	2.16	55	2
1:A:184:TRP:CE2	1:A:188:THR:OG1	0.54	2.59	75	8
1:A:177:ALA:H	1:A:182:LYS:NZ	0.54	2.00	89	6
1:A:189:LEU:HD21	1:A:193:ASN:ND2	0.54	2.18	62	3
1:A:219:GLN:O	1:A:219:GLN:OE1	0.54	2.26	77	5
1:A:18:ARG:NH2	1:A:21:ASN:OD1	0.54	2.40	54	2
1:A:121:ASN:HD22	1:A:121:ASN:H	0.54	1.46	63	6
1:A:111:LEU:N	1:A:111:LEU:HD23	0.54	2.18	51	2
1:A:139:ASN:HD21	1:A:143:ARG:HH21	0.54	1.45	26	1
1:A:35:GLU:O	1:A:39:MET:SD	0.54	2.66	40	25
1:A:167:ARG:NH1	1:A:171:THR:OG1	0.54	2.41	90	2
1:A:185:MET:SD	1:A:185:MET:N	0.54	2.81	33	16
1:A:196:PRO:O	1:A:200:THR:HG23	0.54	2.03	50	61
1:A:192:GLN:O	1:A:199:LYS:NZ	0.54	2.40	23	4
1:A:68:MET:SD	1:A:140:LYS:NZ	0.54	2.81	24	4
1:A:80:TRP:CE3	1:A:84:HIS:CE1	0.53	2.96	90	28
1:A:166:ASP:OD2	1:A:167:ARG:NH2	0.53	2.41	14	7
1:A:161:PHE:CE1	1:A:198:CYS:SG	0.53	3.01	95	6
1:A:111:LEU:HD23	1:A:111:LEU:N	0.53	2.18	55	2
1:A:111:LEU:H	1:A:111:LEU:CD2	0.53	2.16	96	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:151:LEU:HD23	1:A:152:ASP:N	0.53	2.19	100	3
1:A:86:VAL:CG2	1:A:100:ARG:CZ	0.53	2.87	72	4
1:A:96:MET:SD	1:A:120:HIS:ND1	0.53	2.82	88	9
1:A:10:MET:SD	1:A:10:MET:O	0.53	2.67	12	2
1:A:120:HIS:CG	1:A:121:ASN:N	0.53	2.77	89	83
1:A:91:ILE:CD1	1:A:97:ARG:HH21	0.53	2.16	76	5
1:A:113:GLU:OE1	1:A:113:GLU:N	0.53	2.42	54	1
1:A:12:HIS:NE2	1:A:111:LEU:HD11	0.52	2.19	54	3
1:A:120:HIS:ND1	1:A:121:ASN:N	0.52	2.58	23	23
1:A:25:LYS:NZ	1:A:29:GLU:OE2	0.52	2.41	13	4
1:A:44:SER:O	1:A:131:LYS:NZ	0.52	2.41	22	19
1:A:145:TYR:O	1:A:145:TYR:CD1	0.52	2.62	31	1
1:A:98:GLU:H	1:A:98:GLU:CD	0.52	2.08	94	5
1:A:18:ARG:HE	1:A:18:ARG:N	0.52	2.03	99	2
1:A:12:HIS:CG	1:A:111:LEU:HD21	0.52	2.40	68	30
1:A:18:ARG:HH12	1:A:21:ASN:HD22	0.52	1.46	87	3
1:A:10:MET:O	1:A:10:MET:SD	0.52	2.68	62	1
1:A:35:GLU:OE1	1:A:184:TRP:NE1	0.52	2.42	21	1
1:A:180:GLU:OE2	1:A:184:TRP:NE1	0.52	2.42	23	3
1:A:118:MET:O	1:A:118:MET:SD	0.52	2.67	50	7
1:A:24:VAL:HG22	1:A:58:THR:CG2	0.52	2.35	19	7
1:A:139:ASN:OD1	1:A:143:ARG:NE	0.52	2.43	90	4
1:A:6:LEU:HD12	1:A:6:LEU:N	0.52	2.20	88	1
1:A:181:VAL:O	1:A:185:MET:HG2	0.52	2.05	19	7
1:A:150:ILE:CD1	1:A:150:ILE:H	0.52	2.06	38	4
1:A:87:HIS:O	1:A:97:ARG:NH2	0.52	2.42	100	1
1:A:4:GLN:NE2	1:A:5:ASN:O	0.51	2.43	35	6
1:A:150:ILE:HG13	1:A:175:GLU:OE2	0.51	2.04	11	1
1:A:139:ASN:HD21	1:A:143:ARG:NH2	0.51	2.03	40	2
1:A:159:GLU:OE1	1:A:167:ARG:NH2	0.51	2.42	10	14
1:A:12:HIS:CD2	1:A:111:LEU:CD1	0.51	2.93	54	2
1:A:150:ILE:N	1:A:150:ILE:HD13	0.51	2.08	38	2
1:A:87:HIS:O	1:A:87:HIS:CG	0.51	2.63	51	3
1:A:113:GLU:N	1:A:113:GLU:OE1	0.51	2.44	99	1
1:A:79:GLU:N	1:A:79:GLU:OE1	0.51	2.44	67	1
1:A:12:HIS:HB3	1:A:115:ILE:HD11	0.51	1.83	26	45
1:A:50:GLN:O	1:A:53:ASN:OD1	0.51	2.29	56	8
1:A:108:THR:CG2	1:A:108:THR:O	0.51	2.59	47	18
1:A:18:ARG:NH1	1:A:21:ASN:OD1	0.51	2.44	4	3
1:A:179:GLN:HE21	1:A:179:GLN:C	0.51	2.09	25	6
1:A:121:ASN:N	1:A:121:ASN:ND2	0.51	2.59	13	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:150:ILE:N	1:A:150:ILE:CD1	0.51	2.70	42	1
1:A:219:GLN:OE1	1:A:219:GLN:O	0.51	2.29	23	8
1:A:118:MET:SD	1:A:118:MET:O	0.50	2.69	60	12
1:A:145:TYR:CD1	1:A:145:TYR:O	0.50	2.64	83	1
1:A:121:ASN:ND2	1:A:121:ASN:H	0.50	2.05	76	6
1:A:87:HIS:CG	1:A:87:HIS:O	0.50	2.64	55	2
1:A:95:GLN:C	1:A:96:MET:SD	0.50	2.90	50	18
1:A:124:ILE:N	1:A:124:ILE:HD12	0.50	2.21	92	11
1:A:179:GLN:NE2	1:A:179:GLN:C	0.50	2.65	60	6
1:A:95:GLN:O	1:A:96:MET:SD	0.50	2.70	68	9
1:A:108:THR:O	1:A:108:THR:CG2	0.50	2.59	59	20
1:A:177:ALA:HB3	1:A:182:LYS:HZ1	0.50	1.66	89	6
1:A:150:ILE:CG2	1:A:171:THR:CG2	0.50	2.90	91	1
1:A:91:ILE:N	1:A:91:ILE:CD1	0.50	2.74	48	11
1:A:79:GLU:OE1	1:A:82:ARG:NH2	0.50	2.45	100	1
1:A:28:GLU:OE2	1:A:180:GLU:OE1	0.50	2.30	20	1
1:A:178:SER:OG	1:A:181:VAL:HG23	0.50	2.06	49	2
1:A:39:MET:SD	1:A:39:MET:N	0.50	2.85	40	10
1:A:53:ASN:OD1	1:A:53:ASN:C	0.50	2.50	50	7
1:A:194:ALA:O	1:A:199:LYS:NZ	0.50	2.41	13	3
1:A:6:LEU:N	1:A:6:LEU:HD12	0.50	2.21	33	1
1:A:12:HIS:CG	1:A:111:LEU:HD11	0.50	2.42	87	21
1:A:98:GLU:OE1	1:A:98:GLU:N	0.50	2.45	47	7
1:A:44:SER:HB2	1:A:131:LYS:HZ2	0.50	1.67	72	4
1:A:179:GLN:H	1:A:179:GLN:NE2	0.50	2.05	53	1
1:A:124:ILE:HD12	1:A:124:ILE:N	0.50	2.22	12	12
1:A:169:TYR:OH	1:A:173:ARG:NE	0.50	2.45	72	2
1:A:197:ASP:O	1:A:200:THR:CG2	0.49	2.60	33	3
1:A:150:ILE:HG21	1:A:168:PHE:CE1	0.49	2.41	17	1
1:A:11:VAL:CG1	1:A:12:HIS:N	0.49	2.75	37	13
1:A:96:MET:SD	1:A:97:ARG:O	0.49	2.70	48	4
1:A:53:ASN:C	1:A:53:ASN:OD1	0.49	2.50	25	1
1:A:29:GLU:O	1:A:184:TRP:CH2	0.49	2.65	4	1
1:A:155:GLN:NE2	1:A:195:ASN:H	0.49	2.05	93	6
1:A:198:CYS:SG	1:A:202:LEU:HD11	0.49	2.47	99	74
1:A:91:ILE:CD1	1:A:91:ILE:N	0.49	2.74	73	8
1:A:6:LEU:O	1:A:6:LEU:HD13	0.49	2.07	32	2
1:A:84:HIS:O	1:A:100:ARG:NH2	0.49	2.45	67	1
1:A:30:LYS:CD	1:A:30:LYS:N	0.49	2.76	17	4
1:A:87:HIS:CD2	1:A:97:ARG:NH1	0.49	2.81	77	3
1:A:150:ILE:HD11	1:A:168:PHE:CZ	0.49	2.43	72	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:84:HIS:O	1:A:100:ARG:NH1	0.49	2.45	67	1
1:A:94:GLY:C	1:A:95:GLN:NE2	0.49	2.66	67	1
1:A:50:GLN:H	1:A:114:GLN:HE22	0.49	1.51	68	11
1:A:98:GLU:O	1:A:100:ARG:NH1	0.49	2.44	99	2
1:A:150:ILE:HG21	1:A:175:GLU:CD	0.48	2.28	61	1
1:A:150:ILE:HD11	1:A:175:GLU:OE1	0.48	2.08	41	2
1:A:184:TRP:CD2	1:A:188:THR:OG1	0.48	2.66	50	6
1:A:179:GLN:C	1:A:179:GLN:NE2	0.48	2.67	71	2
1:A:143:ARG:NH2	1:A:184:TRP:CE2	0.48	2.80	6	1
1:A:11:VAL:CG2	1:A:12:HIS:N	0.48	2.77	14	16
1:A:2:ILE:HD12	1:A:118:MET:SD	0.48	2.48	100	5
1:A:179:GLN:C	1:A:179:GLN:HE21	0.48	2.12	50	2
1:A:171:THR:O	1:A:175:GLU:CD	0.48	2.52	79	3
1:A:98:GLU:CD	1:A:98:GLU:H	0.48	2.11	84	5
1:A:6:LEU:CD1	1:A:6:LEU:N	0.48	2.75	88	1
1:A:103:ASP:CB	1:A:109:SER:OG	0.48	2.62	41	14
1:A:12:HIS:CE1	1:A:112:GLN:HE22	0.48	2.27	53	2
1:A:121:ASN:HD22	1:A:121:ASN:N	0.48	2.06	13	3
1:A:173:ARG:NH2	1:A:182:LYS:NZ	0.48	2.62	8	2
1:A:32:PHE:CE2	1:A:145:TYR:CE1	0.48	3.02	65	1
1:A:100:ARG:HG2	1:A:101:GLY:N	0.48	2.23	20	13
1:A:177:ALA:HB3	1:A:182:LYS:NZ	0.48	2.24	89	6
1:A:145:TYR:C	1:A:145:TYR:CD1	0.48	2.87	50	1
1:A:100:ARG:CG	1:A:101:GLY:N	0.48	2.77	98	19
1:A:6:LEU:N	1:A:6:LEU:CD2	0.48	2.76	79	2
1:A:25:LYS:O	1:A:29:GLU:OE1	0.48	2.32	72	7
1:A:72:THR:O	1:A:76:GLU:OE1	0.47	2.32	6	18
1:A:121:ASN:H	1:A:121:ASN:HD22	0.47	1.52	80	3
1:A:80:TRP:CH2	1:A:84:HIS:CE1	0.47	3.02	11	24
1:A:171:THR:O	1:A:175:GLU:OE1	0.47	2.33	13	3
1:A:7:GLN:CG	1:A:7:GLN:O	0.47	2.62	65	1
1:A:30:LYS:N	1:A:30:LYS:CD	0.47	2.77	7	3
1:A:44:SER:CB	1:A:131:LYS:HZ2	0.47	2.23	96	16
1:A:98:GLU:OE1	1:A:99:PRO:O	0.47	2.32	68	4
1:A:32:PHE:CD2	1:A:145:TYR:CE2	0.47	3.02	76	1
1:A:141:ILE:O	1:A:145:TYR:HD1	0.47	1.92	81	1
1:A:175:GLU:OE1	1:A:175:GLU:N	0.47	2.46	89	2
1:A:32:PHE:CZ	1:A:145:TYR:OH	0.47	2.64	34	2
1:A:173:ARG:HH22	1:A:182:LYS:NZ	0.47	2.07	8	2
1:A:15:ILE:HD12	1:A:15:ILE:N	0.47	2.24	67	1
1:A:81:ASP:O	1:A:81:ASP:OD1	0.47	2.33	19	18

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:121:ASN:O	1:A:121:ASN:OD1	0.47	2.33	20	16
1:A:2:ILE:HD13	1:A:2:ILE:N	0.47	2.23	33	1
1:A:150:ILE:HG21	1:A:168:PHE:CD1	0.47	2.44	17	1
1:A:210:THR:OG1	1:A:213:GLU:OE1	0.47	2.32	69	1
1:A:17:PRO:O	1:A:21:ASN:ND2	0.47	2.48	55	3
1:A:167:ARG:CZ	1:A:171:THR:OG1	0.47	2.62	90	1
1:A:155:GLN:NE2	1:A:195:ASN:ND2	0.46	2.63	92	3
1:A:78:ALA:O	1:A:82:ARG:HG2	0.46	2.10	35	1
1:A:39:MET:N	1:A:39:MET:SD	0.46	2.88	52	11
1:A:159:GLU:OE2	1:A:163:ASP:OD2	0.46	2.33	35	23
1:A:4:GLN:OE1	1:A:5:ASN:O	0.46	2.33	53	2
1:A:115:ILE:O	1:A:119:THR:HG22	0.46	2.10	70	2
1:A:79:GLU:OE1	1:A:82:ARG:CZ	0.46	2.63	96	2
1:A:12:HIS:CG	1:A:111:LEU:CD2	0.46	2.99	2	27
1:A:21:ASN:O	1:A:24:VAL:HG12	0.46	2.11	77	7
1:A:6:LEU:HD13	1:A:6:LEU:O	0.46	2.09	77	1
1:A:166:ASP:OD1	1:A:170:LYS:NZ	0.46	2.42	38	1
1:A:159:GLU:CD	1:A:167:ARG:HH21	0.46	2.13	6	12
1:A:155:GLN:N	1:A:164:TYR:CE1	0.46	2.84	92	12
1:A:6:LEU:N	1:A:6:LEU:CD1	0.46	2.78	33	1
1:A:121:ASN:OD1	1:A:121:ASN:O	0.46	2.33	79	10
1:A:7:GLN:N	1:A:7:GLN:CD	0.46	2.68	22	2
1:A:198:CYS:SG	1:A:202:LEU:CD1	0.46	3.04	24	74
1:A:75:GLU:O	1:A:79:GLU:OE1	0.46	2.34	52	3
1:A:61:GLY:O	1:A:63:GLN:OE1	0.46	2.33	77	4
1:A:191:VAL:CG2	1:A:192:GLN:N	0.46	2.78	32	3
1:A:98:GLU:N	1:A:98:GLU:OE1	0.46	2.49	17	4
1:A:169:TYR:CE2	1:A:173:ARG:NE	0.46	2.83	68	1
1:A:143:ARG:HH22	1:A:177:ALA:HB1	0.46	1.71	28	1
1:A:7:GLN:O	1:A:7:GLN:CG	0.46	2.63	15	2
1:A:96:MET:SD	1:A:120:HIS:CD2	0.46	3.09	100	4
1:A:78:ALA:CB	1:A:82:ARG:HH22	0.46	2.24	66	1
1:A:2:ILE:CD1	1:A:118:MET:SD	0.46	3.04	61	6
1:A:71:GLU:O	1:A:75:GLU:OE2	0.46	2.34	8	7
1:A:152:ASP:OD1	1:A:154:ARG:NH1	0.46	2.49	99	1
1:A:110:THR:HG22	1:A:111:LEU:N	0.46	2.26	19	11
1:A:163:ASP:CG	1:A:167:ARG:NH1	0.46	2.70	73	4
1:A:32:PHE:CE1	1:A:145:TYR:CE2	0.46	3.03	34	1
1:A:176:GLN:CD	1:A:176:GLN:N	0.46	2.68	100	2
1:A:192:GLN:OE1	1:A:193:ASN:OD1	0.46	2.34	67	1
1:A:215:MET:C	1:A:215:MET:SD	0.45	2.95	15	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:81:ASP:OD1	1:A:81:ASP:O	0.45	2.34	43	15
1:A:75:GLU:OE2	1:A:79:GLU:OE2	0.45	2.34	62	3
1:A:121:ASN:N	1:A:121:ASN:HD22	0.45	2.09	63	1
1:A:7:GLN:OE1	1:A:7:GLN:O	0.45	2.34	44	5
1:A:79:GLU:CD	1:A:82:ARG:HE	0.45	2.14	70	2
1:A:15:ILE:HD11	1:A:51:ASP:HB3	0.45	1.89	94	56
1:A:44:SER:OG	1:A:55:MET:SD	0.45	2.70	92	5
1:A:176:GLN:N	1:A:176:GLN:CD	0.45	2.68	96	2
1:A:202:LEU:HD13	1:A:202:LEU:O	0.45	2.12	40	4
1:A:161:PHE:CE2	1:A:198:CYS:SG	0.45	3.10	79	3
1:A:167:ARG:NH2	1:A:171:THR:OG1	0.45	2.49	13	1
1:A:32:PHE:CZ	1:A:145:TYR:CE2	0.45	3.05	90	2
1:A:7:GLN:O	1:A:7:GLN:HG3	0.45	2.12	65	1
1:A:150:ILE:HD13	1:A:171:THR:HG22	0.45	1.89	41	1
1:A:7:GLN:O	1:A:7:GLN:OE1	0.45	2.35	84	9
1:A:219:GLN:O	1:A:219:GLN:CG	0.45	2.65	77	1
1:A:152:ASP:OD1	1:A:152:ASP:O	0.45	2.35	54	3
1:A:203:LYS:CB	1:A:203:LYS:NZ	0.45	2.80	67	1
1:A:179:GLN:OE1	1:A:180:GLU:OE2	0.45	2.35	71	3
1:A:150:ILE:HG23	1:A:189:LEU:CD2	0.45	2.42	84	1
1:A:80:TRP:CD2	1:A:84:HIS:CD2	0.45	3.05	82	14
1:A:23:TRP:CD1	1:A:55:MET:SD	0.45	3.10	63	11
1:A:152:ASP:O	1:A:152:ASP:OD1	0.45	2.35	15	5
1:A:2:ILE:N	1:A:2:ILE:CD1	0.45	2.80	78	2
1:A:150:ILE:HD13	1:A:150:ILE:C	0.45	2.32	59	1
1:A:195:ASN:OD1	1:A:197:ASP:N	0.45	2.49	79	37
1:A:189:LEU:O	1:A:189:LEU:HD13	0.45	2.11	67	8
1:A:60:GLY:O	1:A:63:GLN:OE1	0.45	2.35	88	2
1:A:2:ILE:N	1:A:2:ILE:HD13	0.45	2.23	78	1
1:A:57:ASN:ND2	1:A:57:ASN:O	0.44	2.51	22	4
1:A:132:ARG:O	1:A:136:LEU:HD13	0.44	2.12	40	14
1:A:189:LEU:HD13	1:A:189:LEU:O	0.44	2.11	74	4
1:A:27:VAL:HG21	1:A:59:VAL:HG11	0.44	1.90	4	10
1:A:5:ASN:HD21	1:A:11:VAL:CG1	0.44	2.24	43	7
1:A:145:TYR:CG	1:A:145:TYR:O	0.44	2.70	80	1
1:A:17:PRO:O	1:A:21:ASN:OD1	0.44	2.35	39	17
1:A:184:TRP:N	1:A:184:TRP:CD1	0.44	2.85	7	1
1:A:176:GLN:O	1:A:176:GLN:CD	0.44	2.56	98	2
1:A:81:ASP:CG	1:A:100:ARG:HH12	0.44	2.16	60	5
1:A:4:GLN:OE1	1:A:4:GLN:O	0.44	2.35	80	4
1:A:150:ILE:HG12	1:A:150:ILE:O	0.44	2.12	33	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:121:ASN:ND2	1:A:121:ASN:N	0.44	2.65	76	3
1:A:202:LEU:O	1:A:202:LEU:HD13	0.44	2.13	20	10
1:A:118:MET:C	1:A:118:MET:SD	0.44	2.96	14	6
1:A:13:GLN:OE1	1:A:14:ALA:N	0.44	2.51	17	3
1:A:7:GLN:CG	1:A:9:GLN:HE22	0.44	2.25	50	2
1:A:80:TRP:CE2	1:A:84:HIS:CD2	0.44	3.06	96	4
1:A:44:SER:CB	1:A:131:LYS:NZ	0.44	2.81	47	19
1:A:150:ILE:HG23	1:A:151:LEU:N	0.44	2.28	83	3
1:A:2:ILE:CD1	1:A:2:ILE:N	0.44	2.80	88	1
1:A:213:GLU:O	1:A:216:THR:OG1	0.44	2.31	46	17
1:A:197:ASP:OD1	1:A:197:ASP:O	0.44	2.35	56	9
1:A:176:GLN:O	1:A:176:GLN:CG	0.44	2.66	51	3
1:A:150:ILE:HD11	1:A:168:PHE:CD1	0.44	2.47	33	1
1:A:150:ILE:CD1	1:A:168:PHE:CE1	0.44	3.01	24	1
1:A:197:ASP:O	1:A:197:ASP:OD1	0.44	2.35	14	9
1:A:180:GLU:O	1:A:184:TRP:CE2	0.44	2.71	53	1
1:A:67:GLN:HE22	1:A:71:GLU:CD	0.44	2.16	24	4
1:A:55:MET:O	1:A:58:THR:HG22	0.44	2.13	84	7
1:A:176:GLN:CG	1:A:176:GLN:O	0.43	2.66	96	3
1:A:32:PHE:CD1	1:A:145:TYR:CE2	0.43	3.06	34	1
1:A:145:TYR:CD2	1:A:145:TYR:O	0.43	2.71	13	1
1:A:176:GLN:O	1:A:176:GLN:OE1	0.43	2.35	100	3
1:A:80:TRP:CE3	1:A:84:HIS:CD2	0.43	3.07	68	8
1:A:164:TYR:OH	1:A:193:ASN:CB	0.43	2.66	92	3
1:A:150:ILE:H	1:A:150:ILE:CD1	0.43	2.14	7	1
1:A:169:TYR:OH	1:A:173:ARG:CZ	0.43	2.67	61	1
1:A:178:SER:OG	1:A:179:GLN:OE1	0.43	2.36	96	4
1:A:176:GLN:OE1	1:A:176:GLN:O	0.43	2.36	96	1
1:A:175:GLU:N	1:A:175:GLU:OE1	0.43	2.51	79	1
1:A:2:ILE:N	1:A:2:ILE:HD12	0.43	2.29	34	2
1:A:87:HIS:O	1:A:87:HIS:ND1	0.43	2.51	77	1
1:A:6:LEU:HD23	1:A:6:LEU:O	0.43	2.14	68	1
1:A:5:ASN:CG	1:A:7:GLN:H	0.43	2.17	67	1
1:A:142:VAL:HG23	1:A:143:ARG:N	0.43	2.29	25	90
1:A:16:SER:OG	1:A:18:ARG:NH1	0.43	2.51	52	1
1:A:150:ILE:HD13	1:A:185:MET:SD	0.43	2.53	20	1
1:A:15:ILE:HD11	1:A:54:THR:HG21	0.43	1.89	67	1
1:A:79:GLU:CD	1:A:82:ARG:HH21	0.43	2.17	66	2
1:A:6:LEU:N	1:A:6:LEU:HD23	0.43	2.25	28	1
1:A:7:GLN:CD	1:A:7:GLN:N	0.43	2.72	72	1
1:A:2:ILE:HD12	1:A:2:ILE:N	0.42	2.29	79	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:95:GLN:CG	1:A:96:MET:N	0.42	2.82	88	1
1:A:111:LEU:CD2	1:A:111:LEU:N	0.42	2.81	55	3
1:A:215:MET:SD	1:A:215:MET:C	0.42	2.98	61	1
1:A:151:LEU:HD23	1:A:152:ASP:H	0.42	1.73	51	2
1:A:202:LEU:CD1	1:A:202:LEU:O	0.42	2.67	40	5
1:A:143:ARG:NH2	1:A:178:SER:H	0.42	2.13	3	1
1:A:75:GLU:O	1:A:79:GLU:CD	0.42	2.57	97	2
1:A:120:HIS:ND1	1:A:122:PRO:O	0.42	2.49	79	2
1:A:202:LEU:O	1:A:202:LEU:CD1	0.42	2.67	81	9
1:A:26:VAL:HG13	1:A:39:MET:SD	0.42	2.54	98	2
1:A:175:GLU:OE2	1:A:177:ALA:HB2	0.42	2.15	54	1
1:A:4:GLN:O	1:A:4:GLN:OE1	0.42	2.37	86	2
1:A:75:GLU:OE1	1:A:75:GLU:N	0.42	2.53	8	1
1:A:216:THR:O	1:A:219:GLN:OE1	0.42	2.37	11	1
1:A:51:ASP:O	1:A:51:ASP:OD1	0.42	2.38	67	1
1:A:110:THR:OG1	1:A:113:GLU:CD	0.42	2.58	99	2
1:A:118:MET:SD	1:A:118:MET:C	0.42	2.98	61	8
1:A:81:ASP:CG	1:A:100:ARG:NH1	0.42	2.73	46	1
1:A:171:THR:O	1:A:175:GLU:OE2	0.42	2.38	79	1
1:A:103:ASP:OD1	1:A:108:THR:OG1	0.42	2.34	96	1
1:A:87:HIS:CD2	1:A:89:GLY:H	0.42	2.33	53	1
1:A:71:GLU:O	1:A:75:GLU:CD	0.42	2.58	8	2
1:A:167:ARG:HH21	1:A:171:THR:N	0.41	2.13	13	2
1:A:171:THR:HG22	1:A:175:GLU:OE1	0.41	2.15	13	2
1:A:150:ILE:HG21	1:A:185:MET:SD	0.41	2.55	87	1
1:A:103:ASP:CG	1:A:109:SER:OG	0.41	2.58	16	13
1:A:44:SER:OG	1:A:131:LYS:NZ	0.41	2.41	7	2
1:A:2:ILE:HD13	1:A:118:MET:SD	0.41	2.56	61	5
1:A:24:VAL:HG22	1:A:58:THR:HG21	0.41	1.93	19	3
1:A:15:ILE:CD1	1:A:55:MET:SD	0.41	3.09	19	6
1:A:136:LEU:HD13	1:A:136:LEU:O	0.41	2.16	71	4
1:A:179:GLN:OE1	1:A:180:GLU:N	0.41	2.47	55	3
1:A:152:ASP:O	1:A:152:ASP:CG	0.41	2.58	96	2
1:A:150:ILE:CD1	1:A:175:GLU:OE1	0.41	2.69	43	1
1:A:166:ASP:OD1	1:A:166:ASP:C	0.41	2.59	90	1
1:A:78:ALA:C	1:A:82:ARG:NH2	0.41	2.73	66	1
1:A:150:ILE:C	1:A:150:ILE:CD1	0.41	2.88	91	1
1:A:145:TYR:O	1:A:145:TYR:CD2	0.41	2.73	60	1
1:A:177:ALA:N	1:A:182:LYS:NZ	0.41	2.67	89	4
1:A:136:LEU:O	1:A:136:LEU:HD13	0.41	2.16	50	3
1:A:92:ALA:HB3	1:A:95:GLN:HG2	0.41	1.92	91	3

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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	0.41	2.45	51	1
1:A:111:LEU:N	1:A:111:LEU:CD2	0.41	2.81	51	1
1:A:159:GLU:OE2	1:A:163:ASP:CG	0.41	2.59	14	3
1:A:96:MET:SD	1:A:96:MET:C	0.41	2.99	73	4
1:A:12:HIS:C	1:A:13:GLN:NE2	0.41	2.74	70	2
1:A:95:GLN:HG2	1:A:96:MET:N	0.41	2.30	88	1
1:A:150:ILE:O	1:A:150:ILE:CG1	0.41	2.68	33	1
1:A:96:MET:CE	1:A:120:HIS:ND1	0.41	2.84	39	1
1:A:7:GLN:HG3	1:A:9:GLN:HE22	0.41	1.75	60	1
1:A:53:ASN:O	1:A:53:ASN:OD1	0.41	2.39	67	1
1:A:61:GLY:O	1:A:63:GLN:CD	0.41	2.59	32	1
1:A:75:GLU:OE1	1:A:76:GLU:OE2	0.41	2.38	80	2
1:A:79:GLU:CG	1:A:82:ARG:NH2	0.41	2.84	87	1
1:A:166:ASP:CG	1:A:167:ARG:NH2	0.41	2.75	71	1
1:A:155:GLN:NE2	1:A:195:ASN:HD22	0.41	2.14	12	2
1:A:143:ARG:HH22	1:A:177:ALA:CB	0.40	2.29	28	1
1:A:143:ARG:HH21	1:A:177:ALA:HB1	0.40	1.76	43	1
1:A:75:GLU:CA	1:A:75:GLU:OE1	0.40	2.70	83	2
1:A:4:GLN:CD	1:A:5:ASN:O	0.40	2.59	31	1
1:A:15:ILE:HD11	1:A:54:THR:CG2	0.40	2.46	52	1
1:A:13:GLN:OE1	1:A:14:ALA:O	0.40	2.40	17	1
1:A:87:HIS:NE2	1:A:97:ARG:NH1	0.40	2.68	87	1
1:A:121:ASN:CG	1:A:121:ASN:O	0.40	2.60	35	1
1:A:195:ASN:OD1	1:A:195:ASN:C	0.40	2.60	80	1
1:A:63:GLN:HE22	1:A:66:MET:CE	0.40	2.30	57	1
1:A:75:GLU:OE1	1:A:75:GLU:CA	0.40	2.70	38	1
1:A:169:TYR:CE2	1:A:173:ARG:CD	0.40	3.04	68	1
1:A:87:HIS:ND1	1:A:87:HIS:O	0.40	2.55	32	1
1:A:110:THR:OG1	1:A:113:GLU:OE2	0.40	2.37	54	1
1:A:15:ILE:CG1	1:A:19:THR:OG1	0.40	2.70	61	1
1:A:15:ILE:CD1	1:A:15:ILE:N	0.40	2.84	67	1

## 6.3 Torsion angles ⓘ

### 6.3.1 Protein backbone ⓘ

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	215/231 (93%)	211±1 (98±0%)	2±1 (1±0%)	2±1 (1±0%)	27 73
All	All	21500/23100 (93%)	21092 (98%)	244 (1%)	164 (1%)	27 73

All 4 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	31	ALA	100
1	A	150	ILE	38
1	A	145	TYR	23
1	A	151	LEU	3

### 6.3.2 Protein sidechains ⓘ

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	184/194 (95%)	176±2 (96±1%)	8±2 (4±1%)	37 82
All	All	18400/19400 (95%)	17588 (96%)	812 (4%)	37 82

All 55 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	88
1	A	195	ASN	49
1	A	24	VAL	49
1	A	189	LEU	49
1	A	58	THR	45
1	A	68	MET	42
1	A	185	MET	37
1	A	10	MET	31
1	A	173	ARG	27
1	A	6	LEU	27
1	A	96	MET	26
1	A	39	MET	25
1	A	118	MET	24
1	A	76	GLU	18

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Mol	Chain	Res	Type	Models (Total)
1	A	108	THR	17
1	A	145	TYR	16
1	A	202	LEU	14
1	A	2	ILE	13
1	A	7	GLN	12
1	A	179	GLN	12
1	A	150	ILE	12
1	A	170	LYS	12
1	A	219	GLN	11
1	A	136	LEU	11
1	A	110	THR	10
1	A	30	LYS	10
1	A	178	SER	10
1	A	121	ASN	9
1	A	143	ARG	8
1	A	167	ARG	7
1	A	75	GLU	7
1	A	82	ARG	7
1	A	175	GLU	6
1	A	215	MET	6
1	A	97	ARG	6
1	A	176	GLN	6
1	A	192	GLN	6
1	A	98	GLU	6
1	A	4	GLN	6
1	A	211	LEU	5
1	A	151	LEU	4
1	A	111	LEU	4
1	A	155	GLN	3
1	A	191	VAL	3
1	A	153	ILE	2
1	A	138	LEU	2
1	A	188	THR	2
1	A	113	GLU	2
1	A	87	HIS	2
1	A	213	GLU	1
1	A	18	ARG	1
1	A	79	GLU	1
1	A	95	GLN	1
1	A	197	ASP	1
1	A	15	ILE	1

### 6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 6.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

### 6.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.6 Ligand geometry [i](#)

There are no ligands in this entry.

### 6.7 Other polymers [i](#)

There are no such molecules in this entry.

### 6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 33% for the well-defined parts and 32% for the entire structure.

### 7.1 Chemical shift list 1

File name: 2m8n\_cs.str

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	919
Number of shifts mapped to atoms	919
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

#### 7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	200	$0.09 \pm 0.14$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}_\beta$	173	$1.36 \pm 0.05$	Should be applied
$^{13}\text{C}'$	190	$-0.38 \pm 0.11$	None needed ( $< 0.5$ ppm)
$^{15}\text{N}$	178	$0.07 \pm 0.30$	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 33%, i.e. 875 atoms were assigned a chemical shift out of a possible 2679. 0 out of 31 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	709/1053 (67%)	169/418 (40%)	371/434 (85%)	169/201 (84%)
Sidechain	166/1458 (11%)	0/857 (0%)	166/536 (31%)	0/65 (0%)

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	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Aromatic	0/168 (0%)	0/86 (0%)	0/67 (0%)	0/15 (0%)
Overall	875/2679 (33%)	169/1361 (12%)	537/1037 (52%)	169/281 (60%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 32%, i.e. 875 atoms were assigned a chemical shift out of a possible 2716. 0 out of 31 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Backbone	709/1071 (66%)	169/425 (40%)	371/442 (84%)	169/204 (83%)
Sidechain	166/1477 (11%)	0/869 (0%)	166/543 (31%)	0/65 (0%)
Aromatic	0/168 (0%)	0/86 (0%)	0/67 (0%)	0/15 (0%)
Overall	875/2716 (32%)	169/1380 (12%)	537/1052 (51%)	169/284 (60%)

#### 7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

#### 7.1.5 Random Coil Index (RCI) plots [i](#)

The 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.

Random coil index (RCI) for chain A:

