



## wwPDB EM Validation Summary Report ⓘ

Oct 21, 2024 – 12:24 PM JST

PDB ID : 6M6H  
EMDB ID : EMD-30124  
Title : Structure of HSV2 C-capsid portal vertex  
Authors : Wang, X.X.; Wang, N.  
Deposited on : 2020-03-14  
Resolution : 4.50 Å(reported)

This is a wwPDB EM Validation Summary 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

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.dev113  
MolProbity : 4.02b-467  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

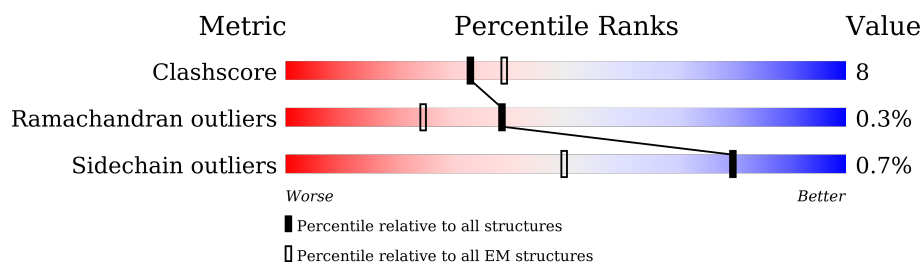
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.50 Å.

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)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. 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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1374	
1	B	1374	
1	C	1374	
1	D	1374	
1	E	1374	
1	F	1374	
2	G	702	
3	H	585	

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Mol	Chain	Length	Quality of chain
3	I	585	
4	J	112	
4	K	112	
4	L	112	
4	M	112	
4	N	112	
4	O	112	
5	P	3122	
5	Q	3122	
6	R	318	
6	S	318	
7	T	466	

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 77884 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Major capsid protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1319	Total	C	N	O	S	0	0
			9828	6232	1783	1759	54		
1	B	1362	Total	C	N	O	S	0	0
			10173	6459	1839	1821	54		
1	C	1362	Total	C	N	O	S	0	0
			10209	6479	1843	1833	54		
1	D	1362	Total	C	N	O	S	0	0
			10221	6485	1847	1835	54		
1	E	1351	Total	C	N	O	S	0	0
			10162	6452	1836	1820	54		
1	F	1351	Total	C	N	O	S	0	0
			9978	6343	1803	1781	51		

- Molecule 2 is a protein called Capsid vertex component 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	G	554	Total	C	N	O	S	0	0
			4241	2699	774	749	19		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	44	MET	VAL	conflict	UNP P89440
G	89	LEU	ILE	conflict	UNP P89440
G	90	ILE	LEU	conflict	UNP P89440
G	94	VAL	ILE	conflict	UNP P89440
G	198	MET	LEU	conflict	UNP P89440
G	200	LEU	MET	conflict	UNP P89440

- Molecule 3 is a protein called Capsid vertex component 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	94	Total	C	N	O	S	0	0
			759	482	138	137	2		
3	I	80	Total	C	N	O		0	0
			644	406	122	116			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	36	TYR	TRP	conflict	UNP P89448
H	38	SER	LEU	conflict	UNP P89448
H	106	THR	ALA	conflict	UNP P89448
H	540	LEU	PRO	conflict	UNP P89448
H	555	ALA	THR	conflict	UNP P89448
I	36	TYR	TRP	conflict	UNP P89448
I	38	SER	LEU	conflict	UNP P89448
I	106	THR	ALA	conflict	UNP P89448
I	540	LEU	PRO	conflict	UNP P89448
I	555	ALA	THR	conflict	UNP P89448

- Molecule 4 is a protein called Small capsomere-interacting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	J	101	Total	C	N	O	S	0	0
			773	489	143	138	3		
4	K	101	Total	C	N	O	S	0	0
			773	489	143	138	3		
4	L	101	Total	C	N	O	S	0	0
			773	489	143	138	3		
4	M	101	Total	C	N	O	S	0	0
			773	489	143	138	3		
4	N	101	Total	C	N	O	S	0	0
			773	489	143	138	3		
4	O	101	Total	C	N	O	S	0	0
			773	489	143	138	3		

- Molecule 5 is a protein called Large tegument protein deneddylase.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	P	47	Total	C	N	O	S	0	0
			388	237	90	59	2		
5	Q	47	Total	C	N	O	S	0	0
			382	234	87	59	2		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	3076	ARG	SER	conflict	UNP P89459
Q	3076	ARG	SER	conflict	UNP P89459

- Molecule 6 is a protein called Triplex capsid protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	R	299	Total	C	N	O	S	0	0
			2078	1341	373	357	7		
6	S	307	Total	C	N	O	S	0	0
			2175	1405	392	370	8		

- Molecule 7 is a protein called Triplex capsid protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	T	285	Total	C	N	O	S	0	0
			2008	1283	360	348	17		

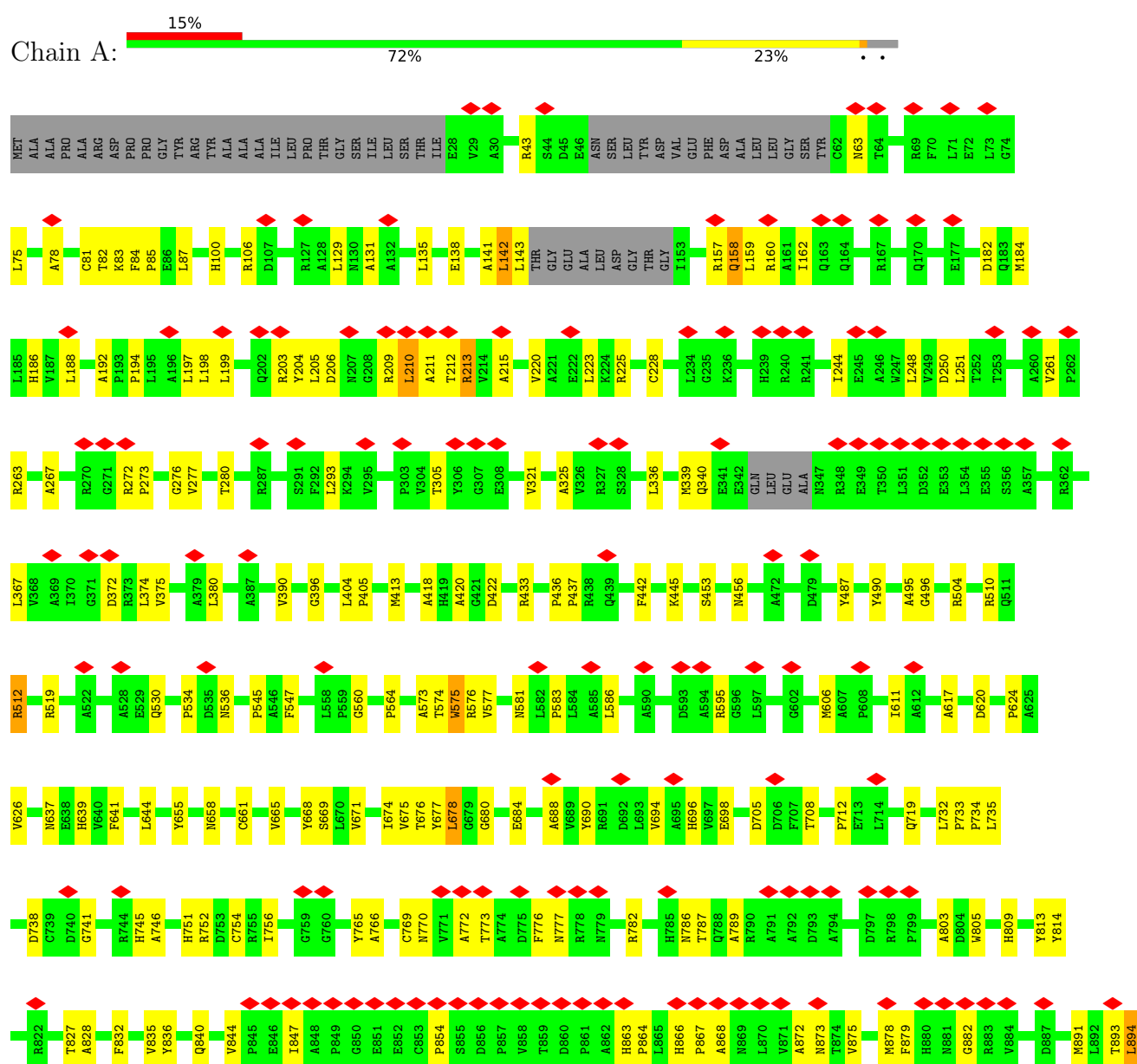
There is a discrepancy between the modelled and reference sequences:

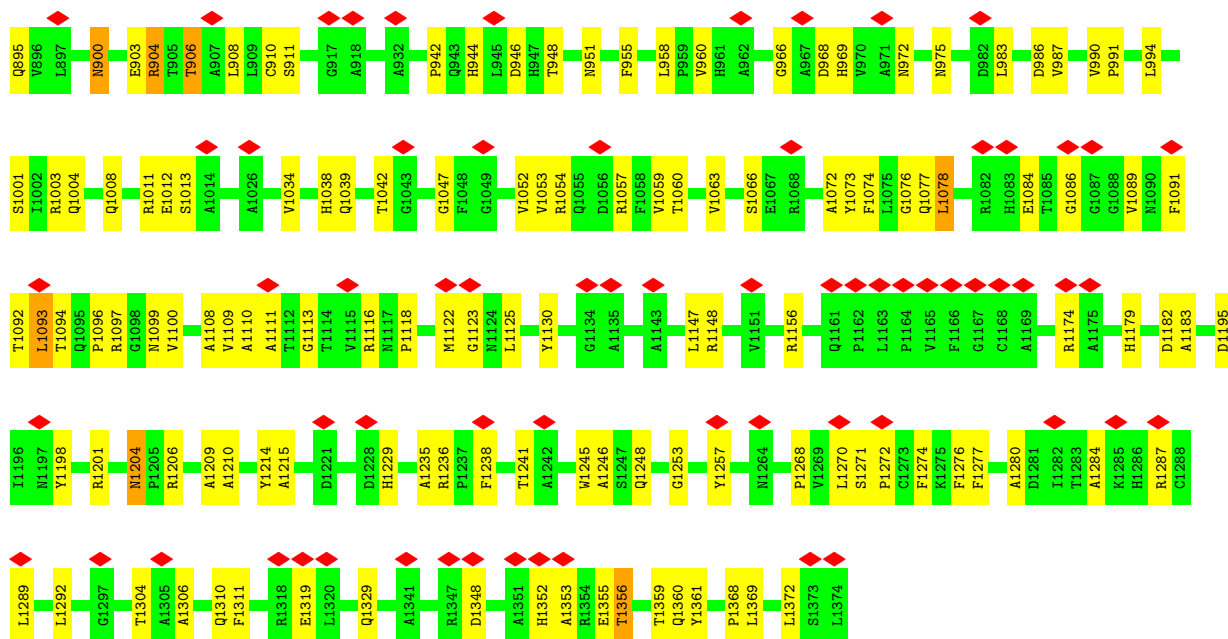
Chain	Residue	Modelled	Actual	Comment	Reference
T	283	CYS	ARG	conflict	UNP G9I260

### 3 Residue-property plots [i](#)

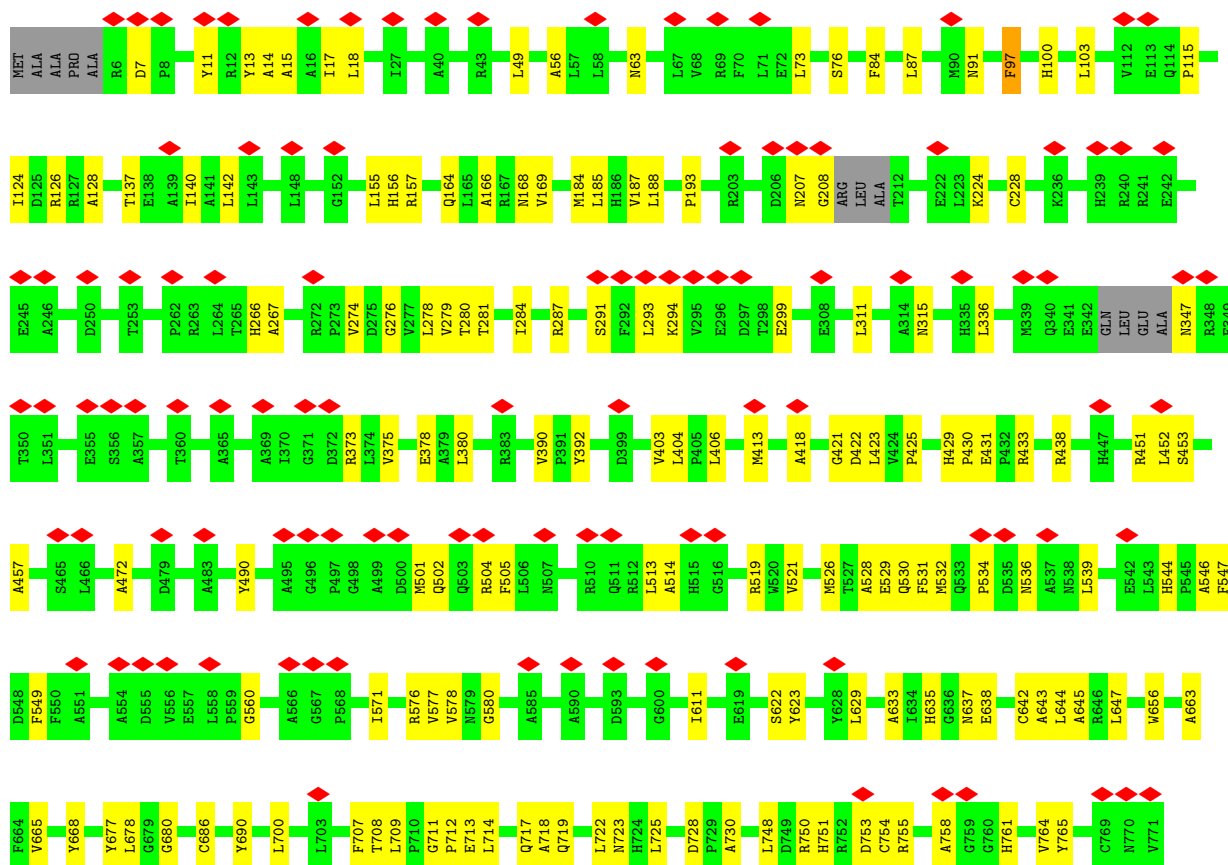
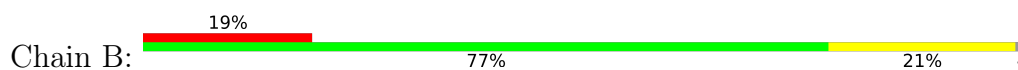
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-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. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

#### • Molecule 1: Major capsid protein

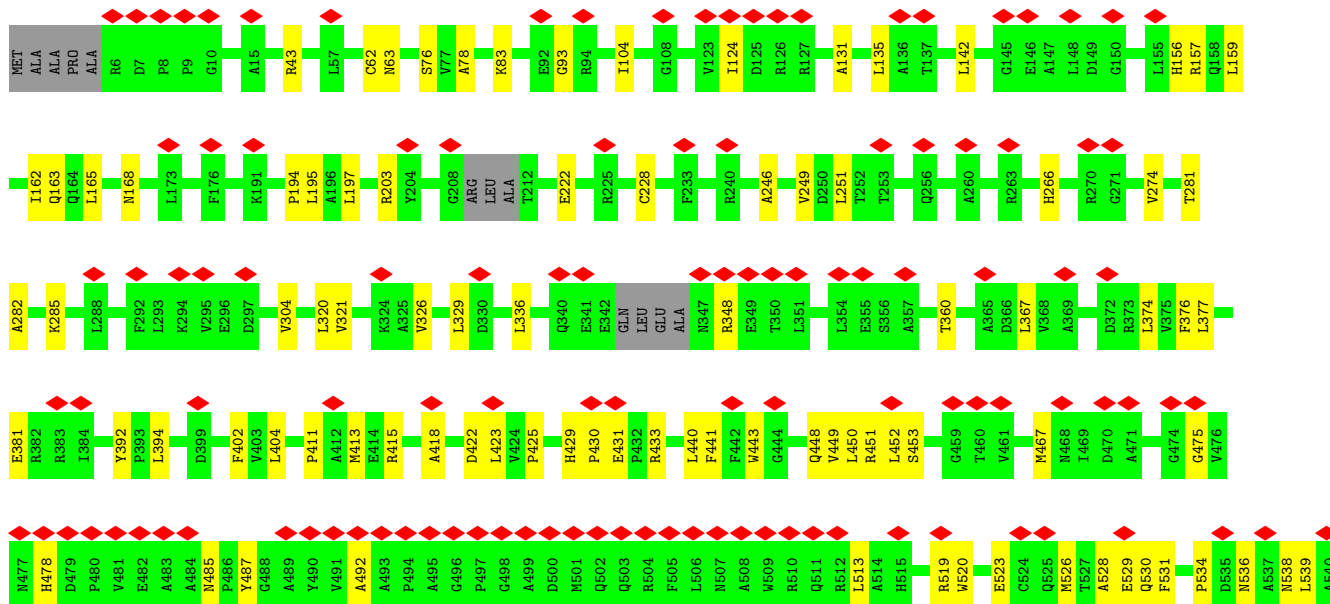


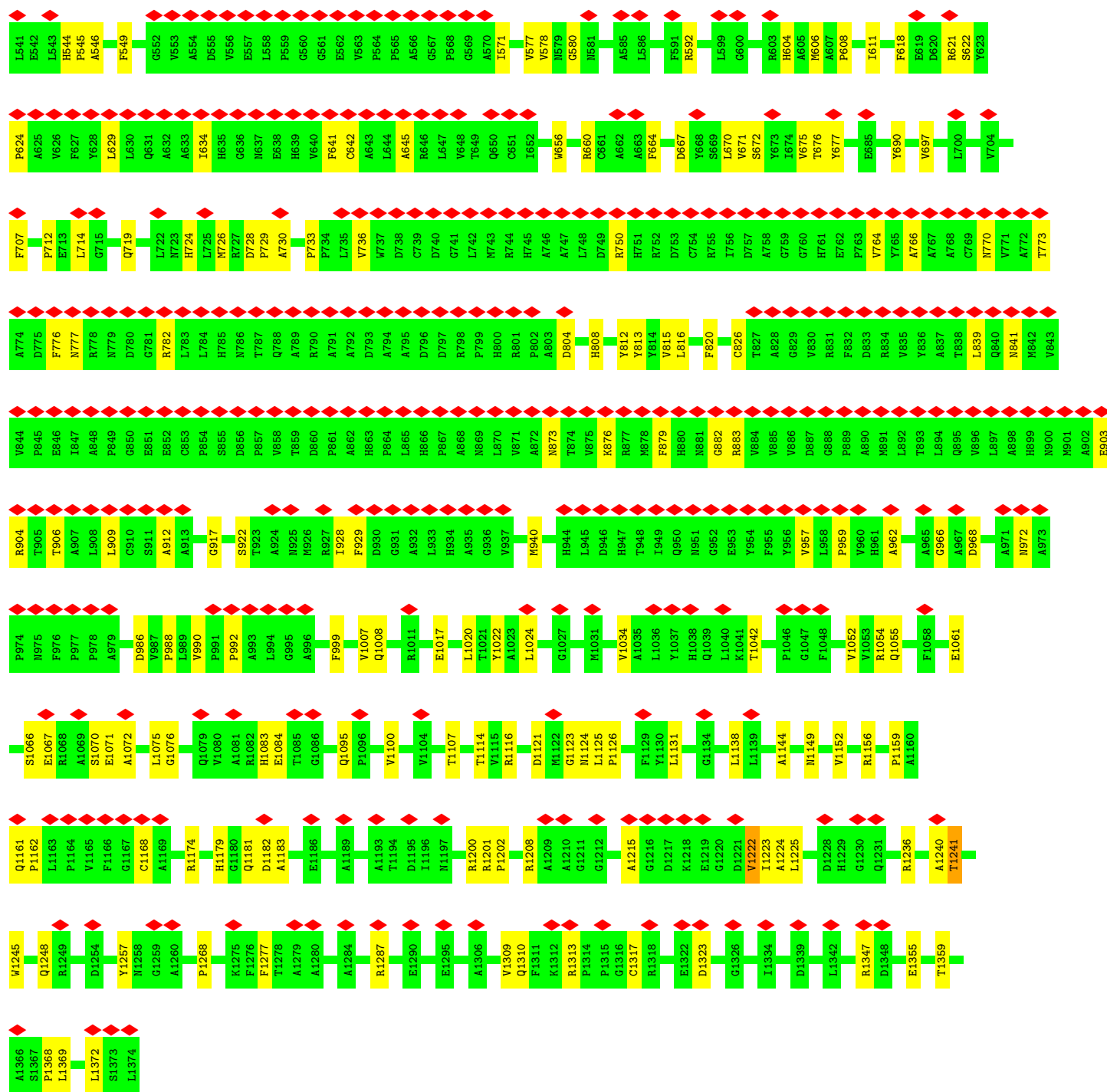


• Molecule 1: Major capsid protein

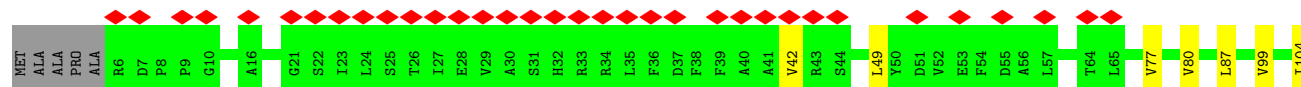
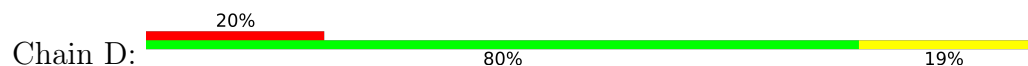


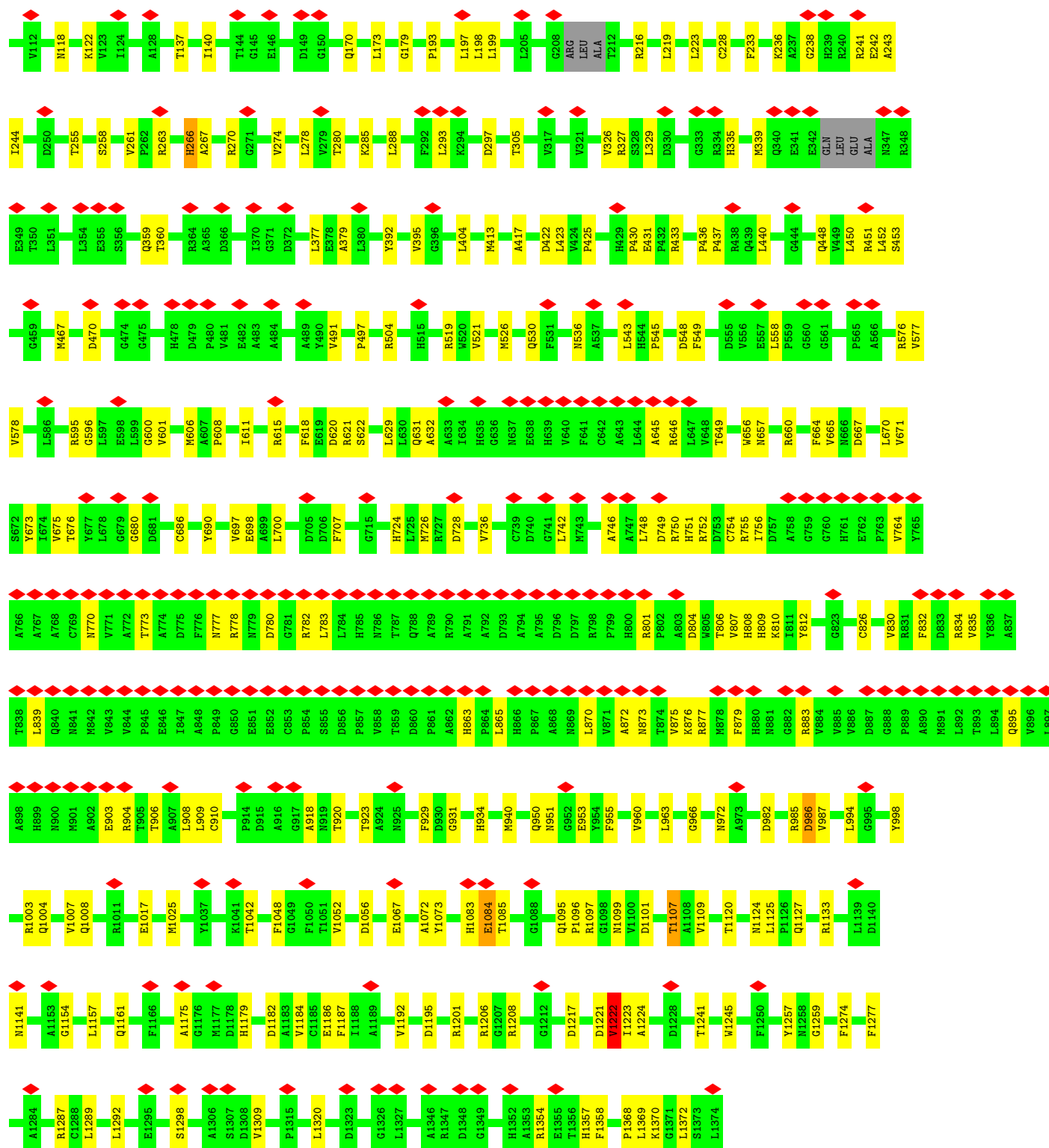






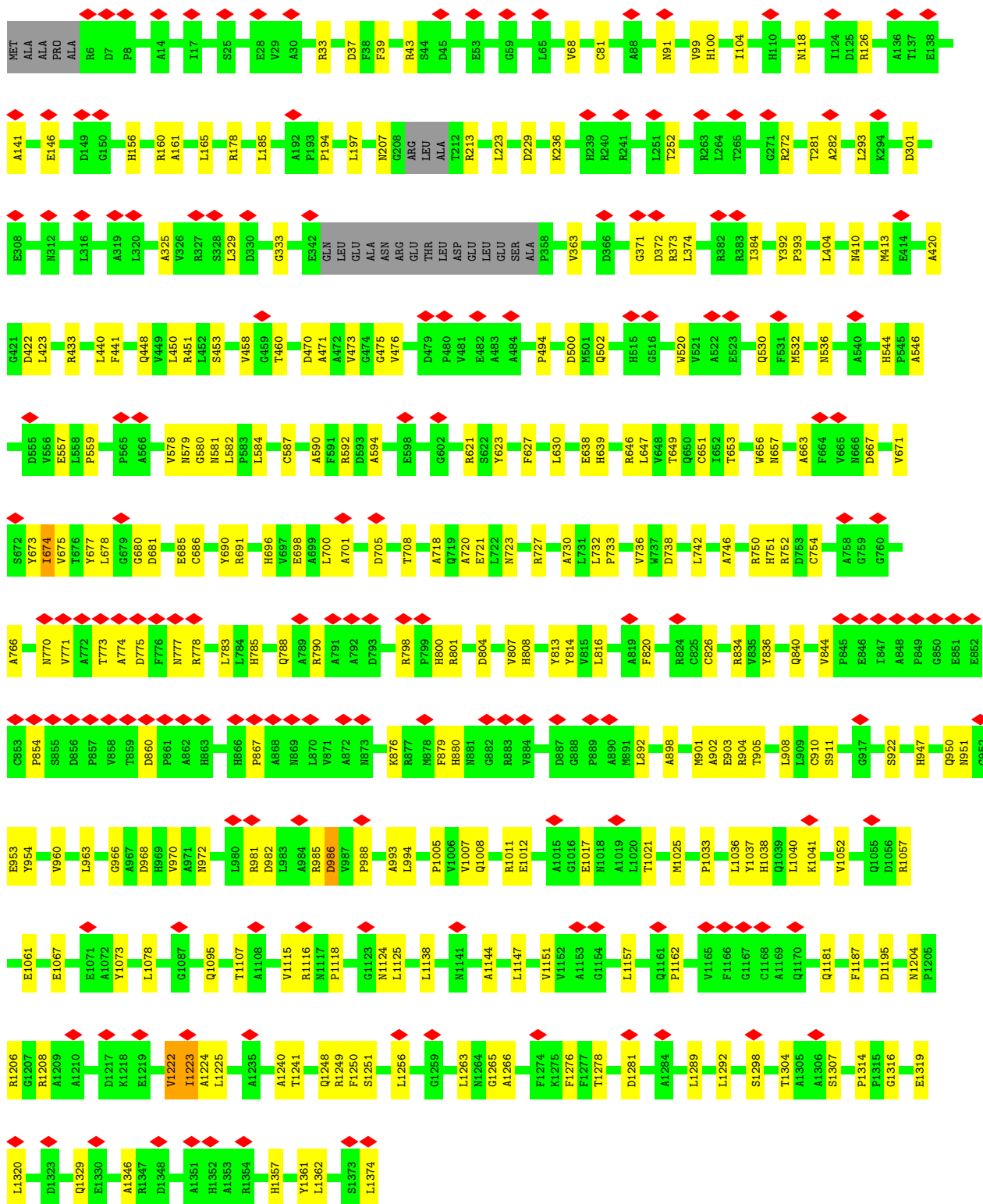
• Molecule 1: Major capsid protein



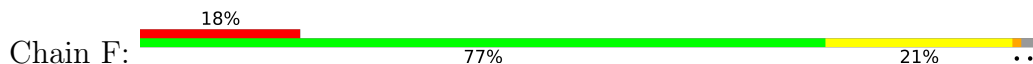


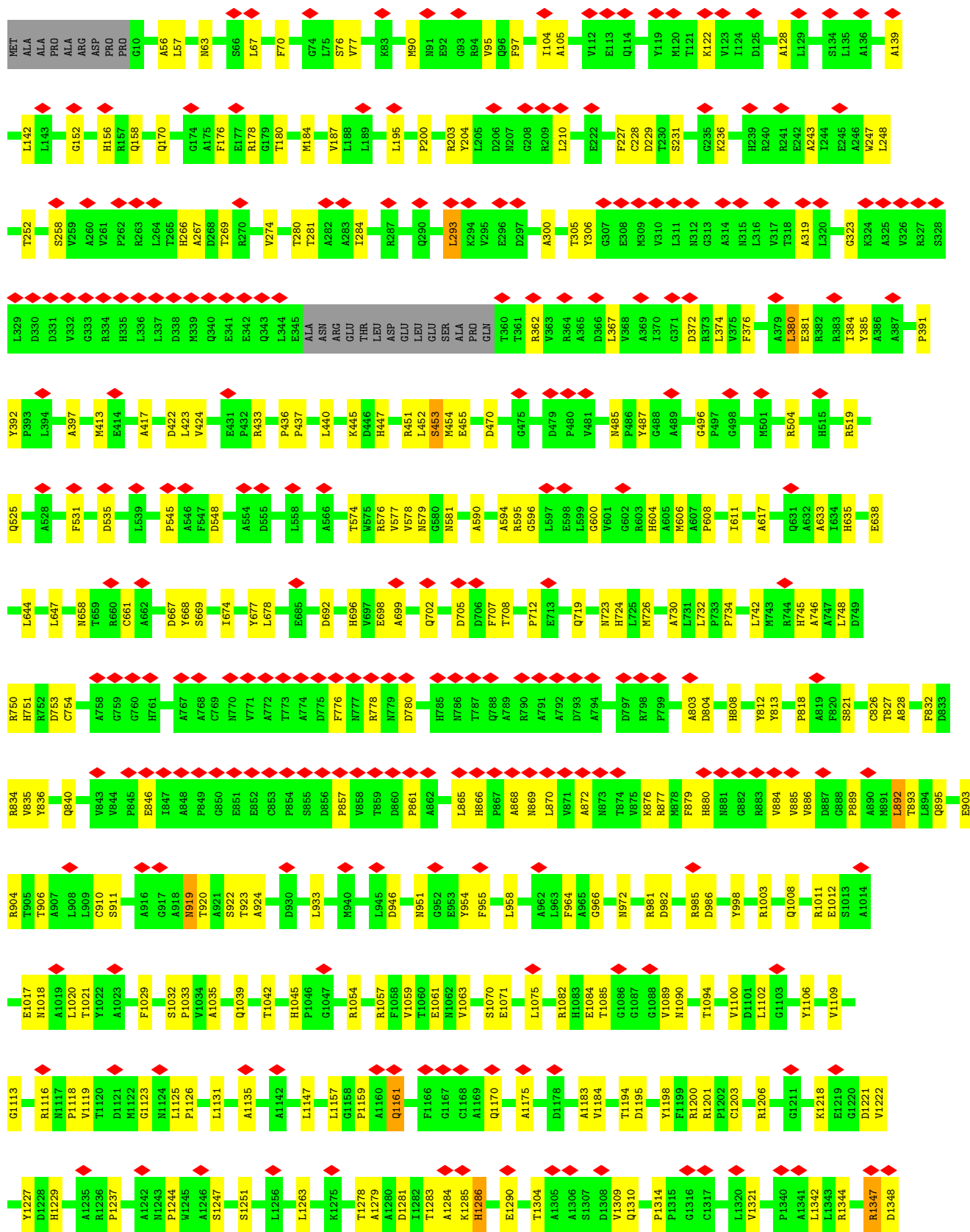
• Molecule 1: Major capsid protein

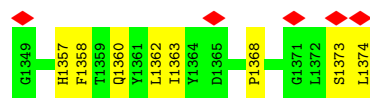




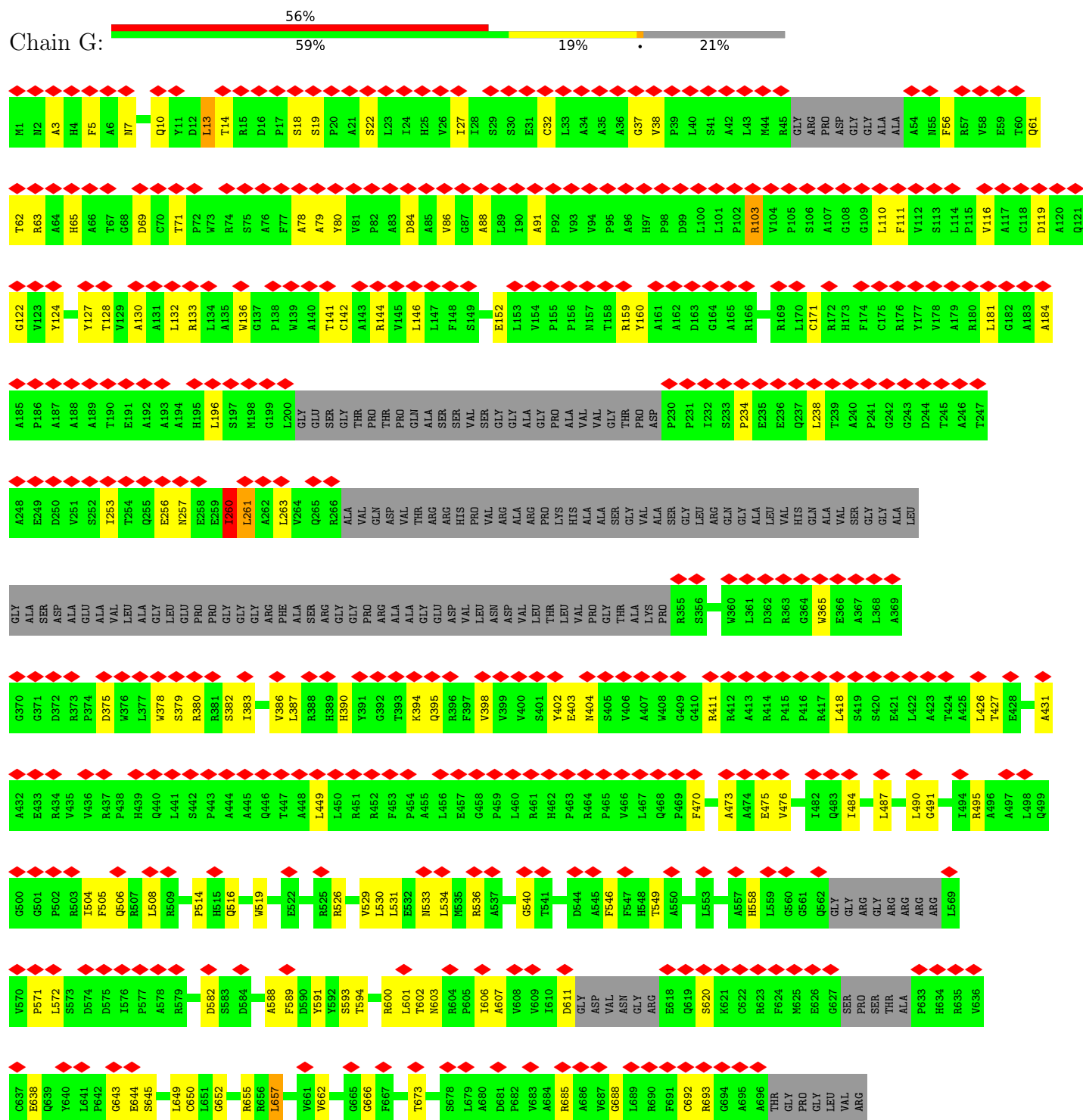
• Molecule 1: Major capsid protein



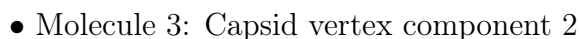


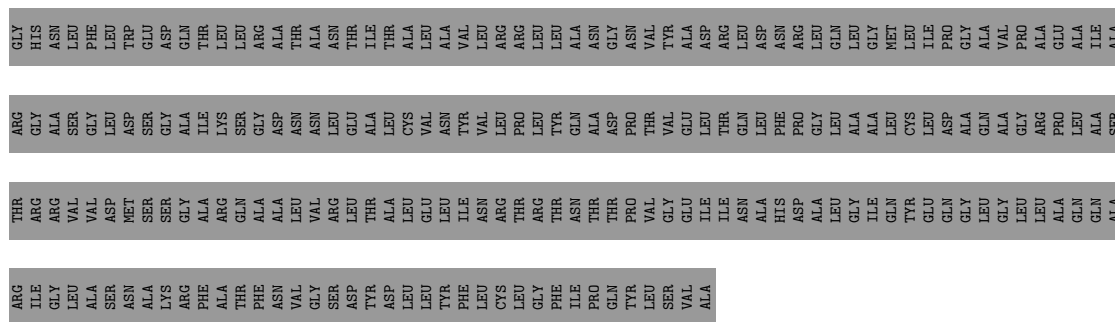


• Molecule 2: Capsid vertex component 1

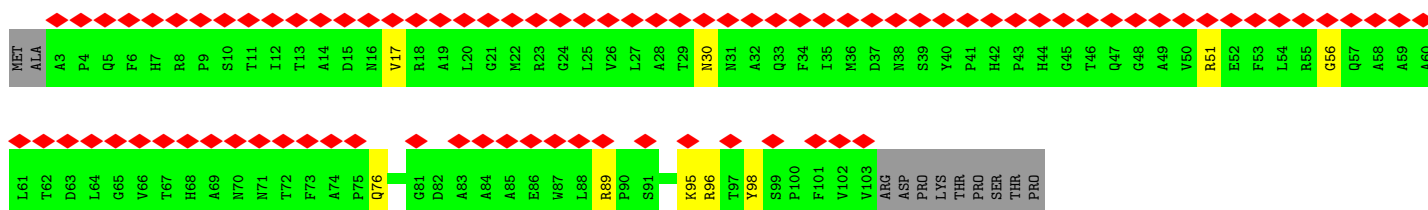
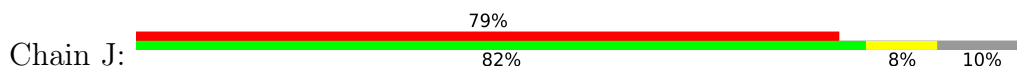


• Molecule 3: Capsid vertex component 2

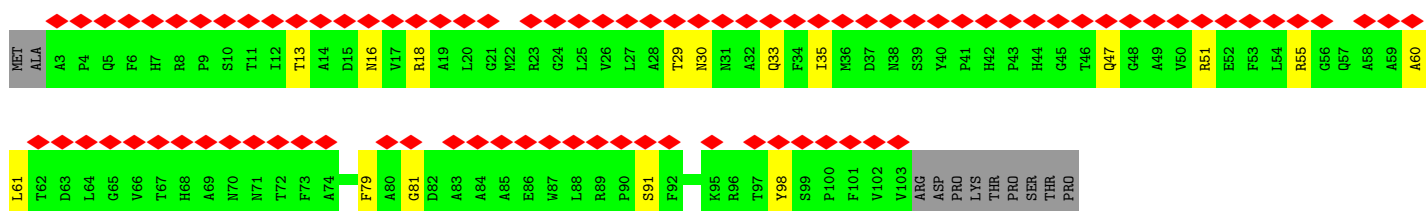
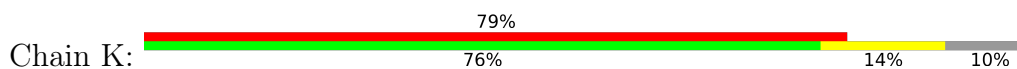




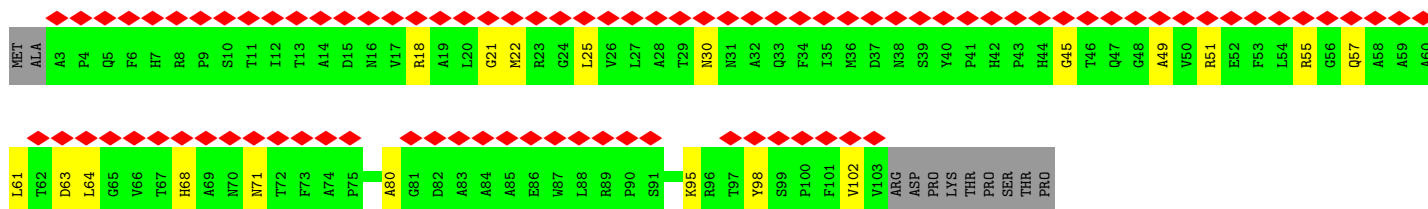
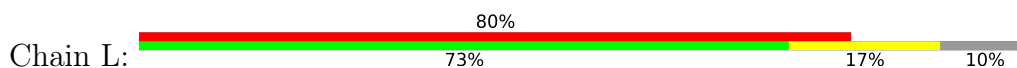
- Molecule 4: Small capsomere-interacting protein



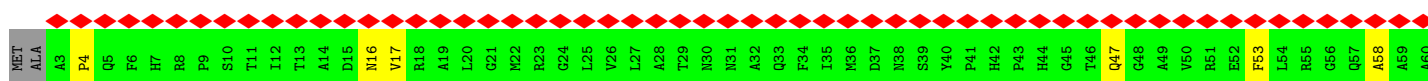
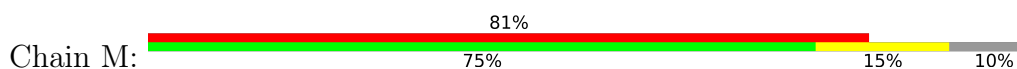
- Molecule 4: Small capsomere-interacting protein



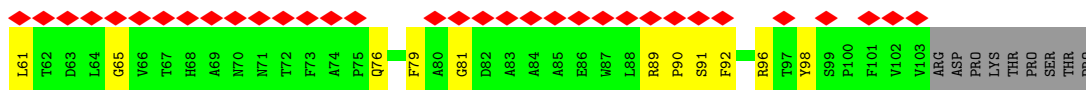
- Molecule 4: Small capsomere-interacting protein



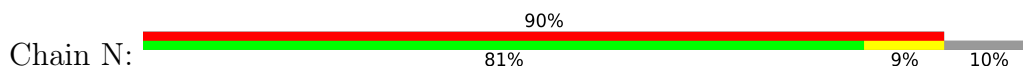
- Molecule 4: Small capsomere-interacting protein



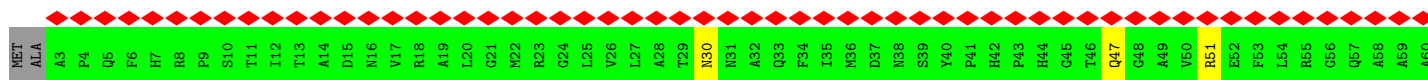
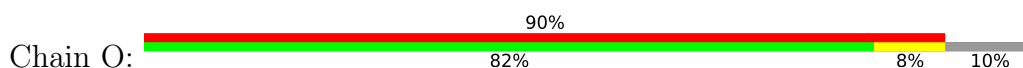




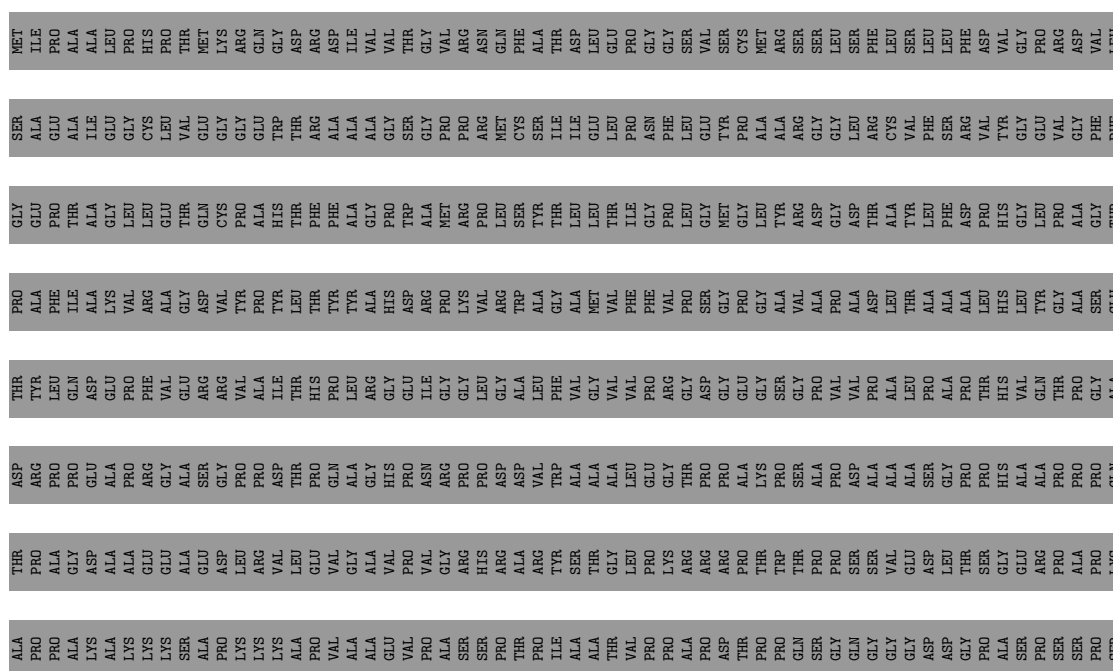
• Molecule 4: Small capsomere-interacting protein



• Molecule 4: Small capsomere-interacting protein



• Molecule 5: Large tegument protein deneddylase



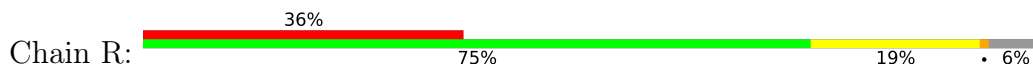


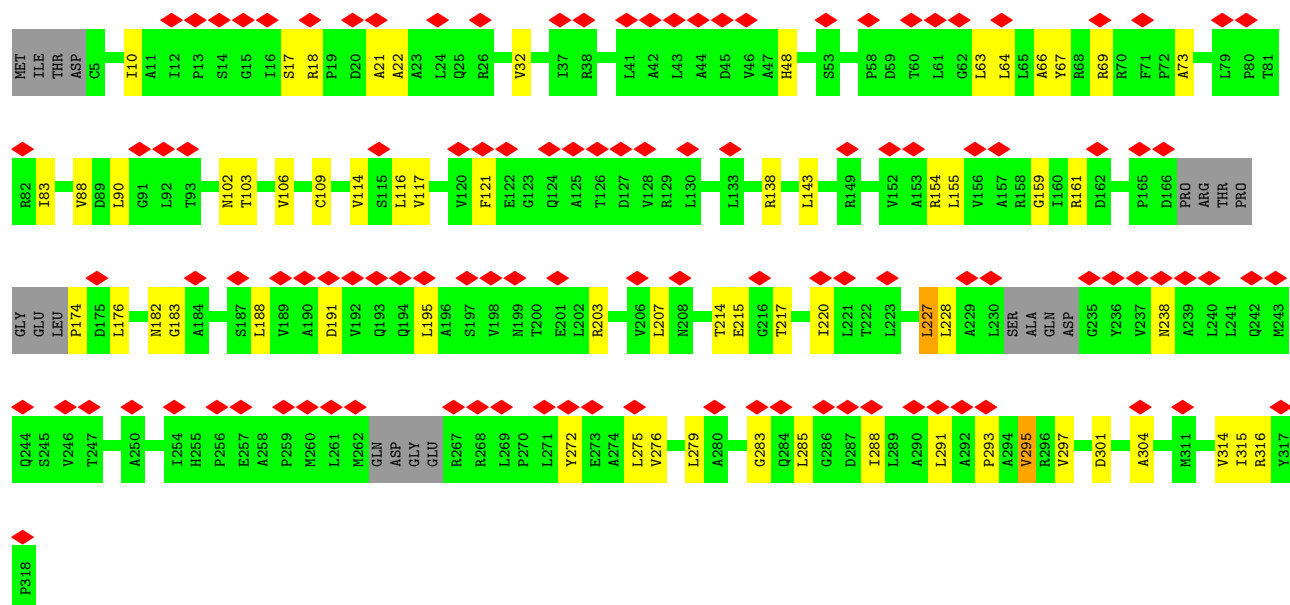




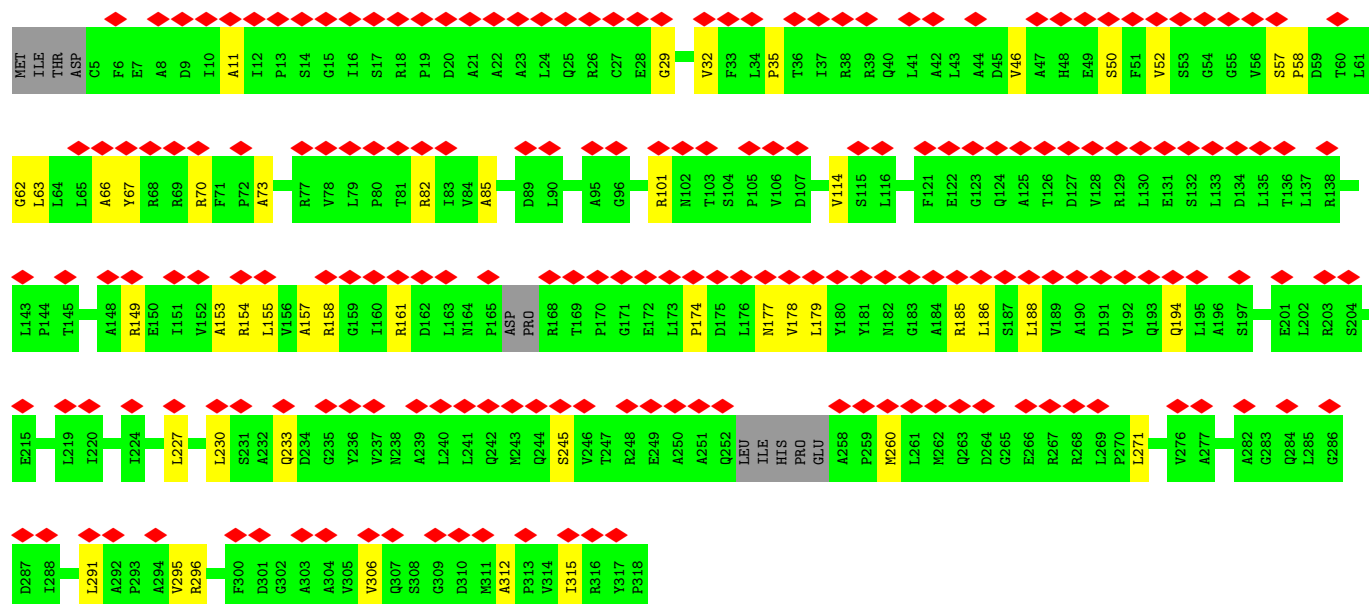
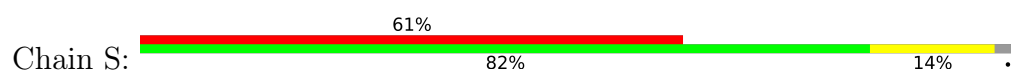


- Molecule 6: Triplex capsid protein 2

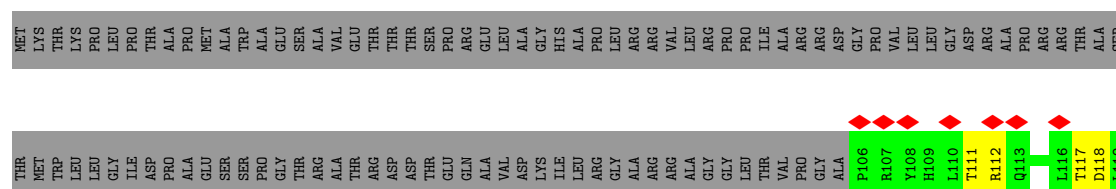


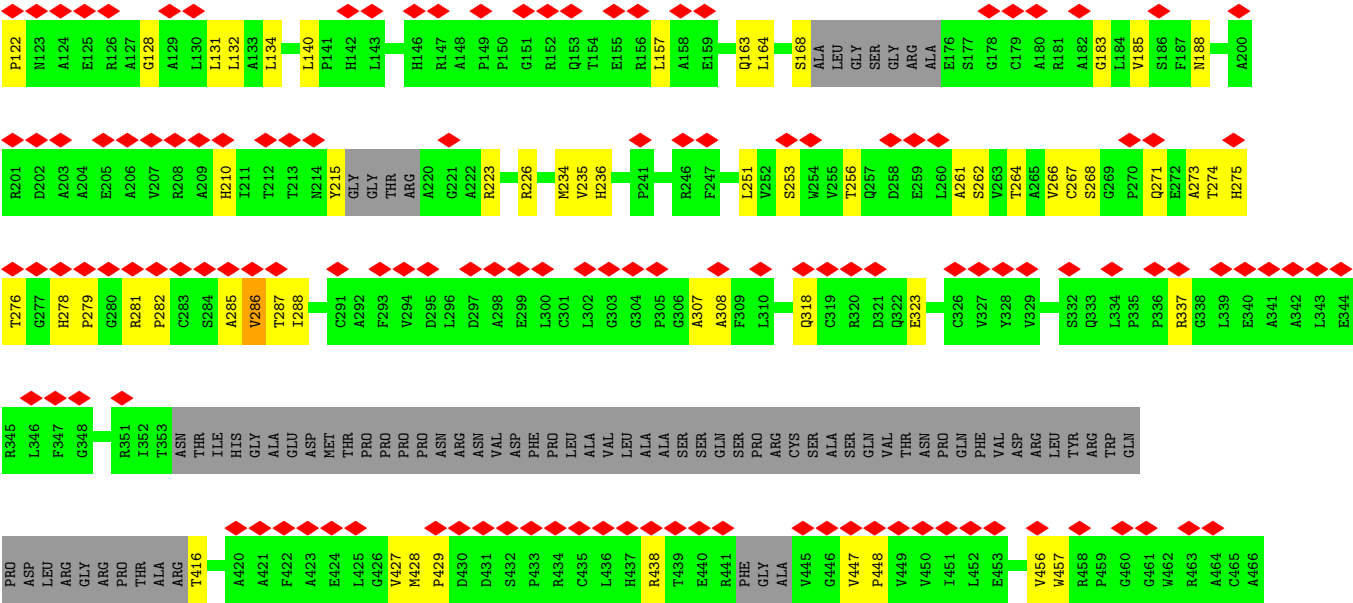


- Molecule 6: Triplex capsid protein 2



- Molecule 7: Triplex capsid protein 1







## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	35698	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	30.0, 30	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k), FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.109	Depositor
Minimum map value	-0.078	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.012	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	414.0, 414.0, 414.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.38, 1.38, 1.38	Depositor

## 5 Model quality

### 5.1 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 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	0.41	0/10068	0.66	4/13767 (0.0%)
1	B	0.39	0/10427	0.63	2/14259 (0.0%)
1	C	0.36	0/10464	0.59	1/14307 (0.0%)
1	D	0.37	0/10475	0.62	4/14319 (0.0%)
1	E	0.39	0/10416	0.62	3/14235 (0.0%)
1	F	0.40	0/10227	0.66	9/13997 (0.1%)
2	G	0.34	1/4350 (0.0%)	0.55	1/5933 (0.0%)
3	H	0.30	0/779	0.54	0/1062
3	I	0.31	0/659	0.55	0/897
4	J	0.30	0/795	0.53	0/1084
4	K	0.32	0/795	0.56	0/1084
4	L	0.30	0/795	0.55	0/1084
4	M	0.29	0/795	0.51	0/1084
4	N	0.26	0/795	0.46	0/1084
4	O	0.26	0/795	0.48	0/1084
5	P	0.23	0/390	0.50	0/520
5	Q	0.29	0/384	0.49	0/513
6	R	0.32	0/2114	0.64	0/2909
6	S	0.30	0/2215	0.62	0/3047
7	T	0.33	0/2055	0.67	0/2818
All	All	0.37	1/79793 (0.0%)	0.62	24/109087 (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 outliers	#Planarity outliers
1	A	0	7
1	B	0	5
1	C	0	8
1	D	0	6
1	E	0	6

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	F	0	7
2	G	0	2
6	R	0	2
6	S	0	1
7	T	0	1
All	All	0	45

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	19	SER	C-N	8.43	1.50	1.34

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	293	LEU	CA-CB-CG	8.59	135.06	115.30
1	F	892	LEU	CA-CB-CG	6.92	131.23	115.30
1	A	678	LEU	CA-CB-CG	6.63	130.56	115.30
1	F	1348	ASP	CB-CG-OD1	6.49	124.14	118.30
2	G	657	LEU	CA-CB-CG	6.47	130.19	115.30

There are no chirality outliers.

5 of 45 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	305	THR	Peptide
1	A	573	ALA	Peptide
1	A	665	VAL	Peptide
1	A	81	CYS	Peptide
1	A	975	ASN	Peptide

## 5.2 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 the 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 within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	9828	0	9537	215	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	10173	0	9890	200	0
1	C	10209	0	9935	152	0
1	D	10221	0	9958	164	0
1	E	10162	0	9934	165	0
1	F	9978	0	9625	188	0
2	G	4241	0	4187	96	0
3	H	759	0	737	15	0
3	I	644	0	629	22	0
4	J	773	0	748	9	0
4	K	773	0	748	16	0
4	L	773	0	748	15	0
4	M	773	0	748	15	0
4	N	773	0	748	7	0
4	O	773	0	748	8	0
5	P	388	0	426	7	0
5	Q	382	0	415	13	0
6	R	2078	0	2053	41	0
6	S	2175	0	2213	31	0
7	T	2008	0	1886	35	0
All	All	77884	0	75913	1256	0

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 8.

The worst 5 of 1256 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:321:VAL:HG22	1:B:18:LEU:CD1	1.80	1.11
1:A:43:ARG:CB	1:A:1091:PHE:CZ	2.36	1.08
1:A:43:ARG:CB	1:A:1091:PHE:CE2	2.49	0.95
2:G:257:ASN:HA	2:G:260:ILE:HD11	1.45	0.94
1:A:321:VAL:HG22	1:B:18:LEU:HD11	1.50	0.90

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 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 EM 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	1311/1374 (95%)	1118 (85%)	188 (14%)	5 (0%)	30	68
1	B	1356/1374 (99%)	1206 (89%)	143 (10%)	7 (0%)	25	64
1	C	1356/1374 (99%)	1223 (90%)	130 (10%)	3 (0%)	44	78
1	D	1356/1374 (99%)	1205 (89%)	146 (11%)	5 (0%)	30	68
1	E	1345/1374 (98%)	1193 (89%)	151 (11%)	1 (0%)	48	83
1	F	1347/1374 (98%)	1162 (86%)	183 (14%)	2 (0%)	48	83
2	G	540/702 (77%)	507 (94%)	32 (6%)	1 (0%)	44	78
3	H	92/585 (16%)	84 (91%)	8 (9%)	0	100	100
3	I	78/585 (13%)	72 (92%)	6 (8%)	0	100	100
4	J	99/112 (88%)	93 (94%)	6 (6%)	0	100	100
4	K	99/112 (88%)	89 (90%)	10 (10%)	0	100	100
4	L	99/112 (88%)	90 (91%)	9 (9%)	0	100	100
4	M	99/112 (88%)	91 (92%)	8 (8%)	0	100	100
4	N	99/112 (88%)	93 (94%)	6 (6%)	0	100	100
4	O	99/112 (88%)	96 (97%)	3 (3%)	0	100	100
5	P	45/3122 (1%)	44 (98%)	1 (2%)	0	100	100
5	Q	45/3122 (1%)	45 (100%)	0	0	100	100
6	R	291/318 (92%)	253 (87%)	38 (13%)	0	100	100
6	S	301/318 (95%)	274 (91%)	27 (9%)	0	100	100
7	T	275/466 (59%)	222 (81%)	50 (18%)	3 (1%)	12	46
All	All	10332/18134 (57%)	9160 (89%)	1145 (11%)	27 (0%)	38	72

5 of 27 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	294	LYS

*Continued on next page...*

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Mol	Chain	Res	Type
1	B	299	GLU
1	B	1223	ILE
1	C	1223	ILE
1	D	1085	THR

### 5.3.2 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 EM 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	969/1080 (90%)	952 (98%)	17 (2%)	54	71
1	B	1009/1080 (93%)	1000 (99%)	9 (1%)	75	83
1	C	1018/1080 (94%)	1014 (100%)	4 (0%)	89	90
1	D	1020/1080 (94%)	1014 (99%)	6 (1%)	84	88
1	E	1018/1080 (94%)	1017 (100%)	1 (0%)	92	94
1	F	968/1080 (90%)	963 (100%)	5 (0%)	86	89
2	G	427/529 (81%)	421 (99%)	6 (1%)	62	75
3	H	77/451 (17%)	77 (100%)	0	100	100
3	I	64/451 (14%)	63 (98%)	1 (2%)	58	74
4	J	78/88 (89%)	78 (100%)	0	100	100
4	K	78/88 (89%)	78 (100%)	0	100	100
4	L	78/88 (89%)	78 (100%)	0	100	100
4	M	78/88 (89%)	78 (100%)	0	100	100
4	N	78/88 (89%)	78 (100%)	0	100	100
4	O	78/88 (89%)	78 (100%)	0	100	100
5	P	41/2370 (2%)	40 (98%)	1 (2%)	44	63
5	Q	40/2370 (2%)	39 (98%)	1 (2%)	42	62
6	R	195/264 (74%)	193 (99%)	2 (1%)	73	81
6	S	214/264 (81%)	214 (100%)	0	100	100
7	T	184/365 (50%)	184 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	7712/14072 (55%)	7659 (99%)	53 (1%)	80 87

5 of 53 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	415	ARG
1	D	1141	ASN
5	P	3098	ARG
1	C	1107	THR
1	D	756	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 118 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	1004	GLN
4	O	16	ASN
1	E	777	ASN
4	O	7	HIS
4	K	16	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.



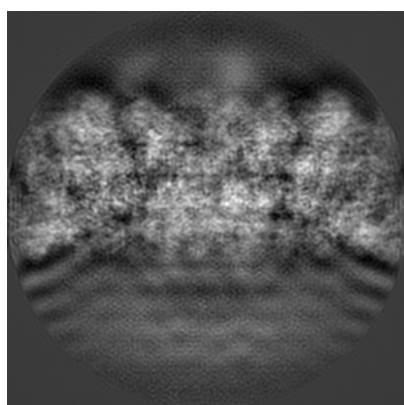
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30124. These allow visual inspection of the internal detail of the map and identification of artifacts.

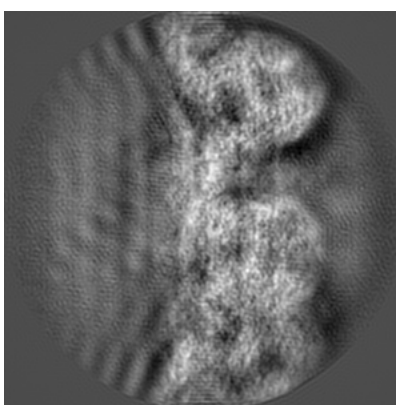
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

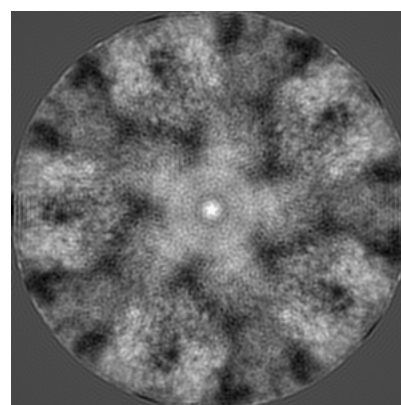
#### 6.1.1 Primary map



X



Y

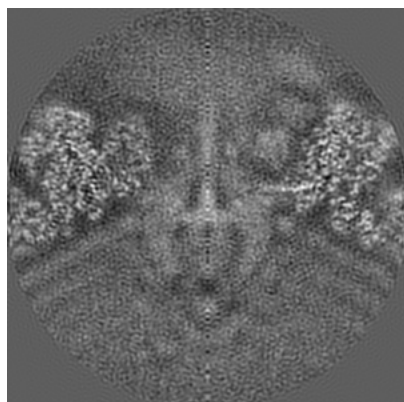


Z

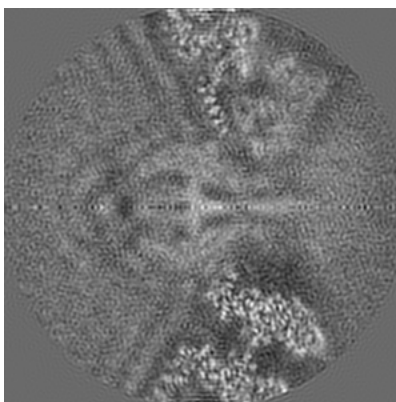
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

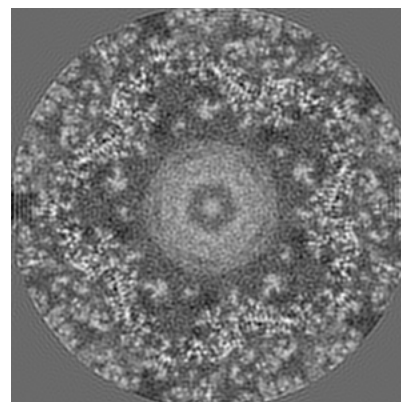
#### 6.2.1 Primary map



X Index: 150



Y Index: 150

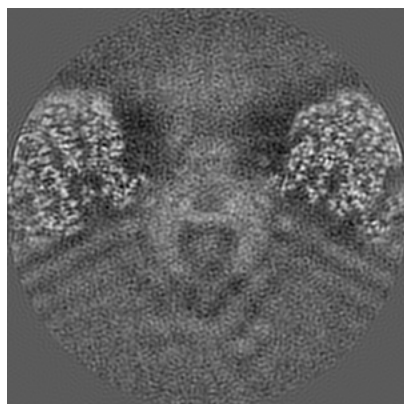


Z Index: 150

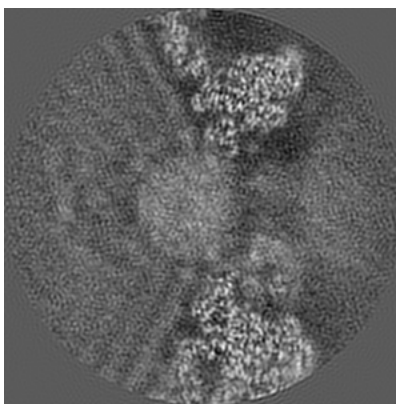
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

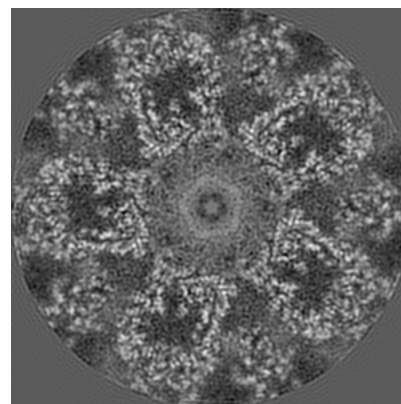
### 6.3.1 Primary map



X Index: 135



Y Index: 121

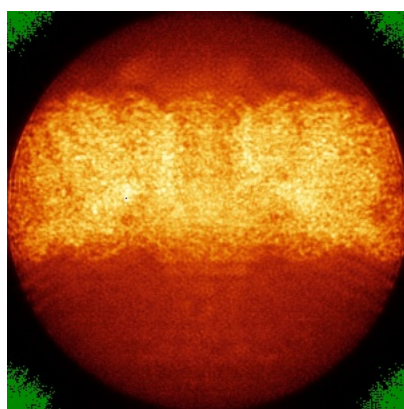


Z Index: 169

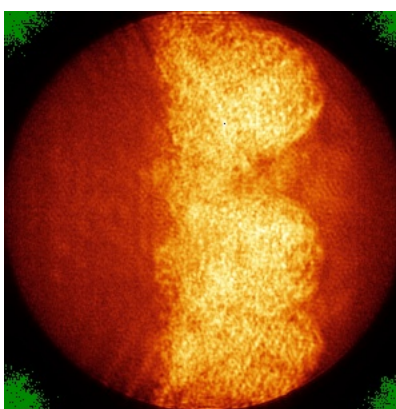
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

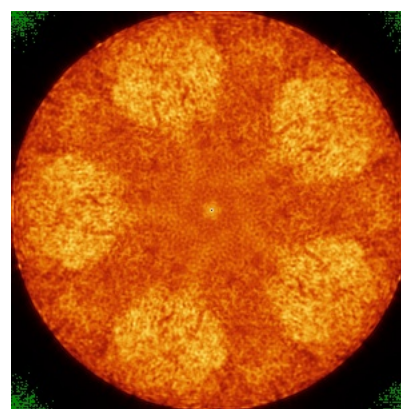
### 6.4.1 Primary map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

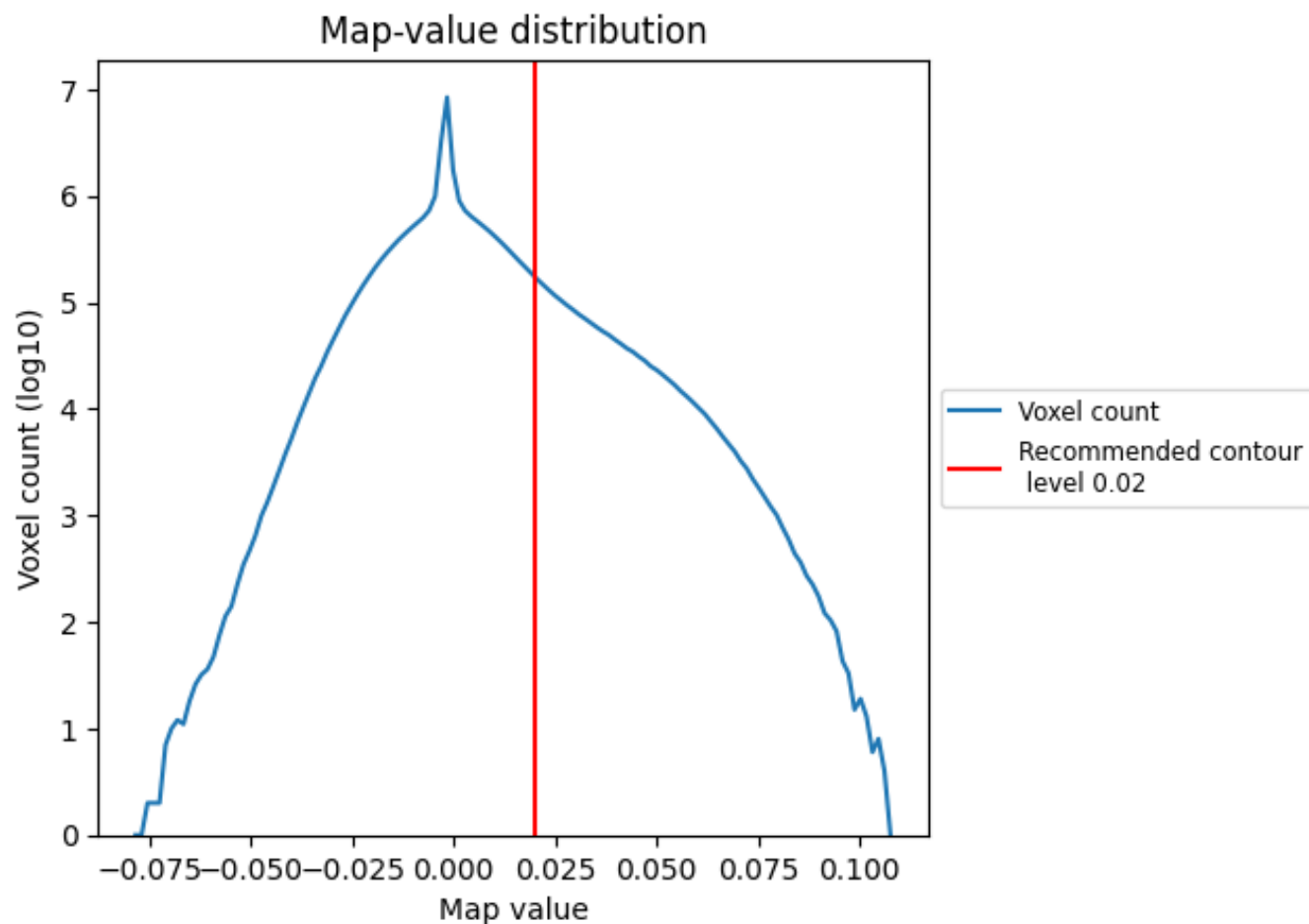
## 6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

## 7 Map analysis [i](#)

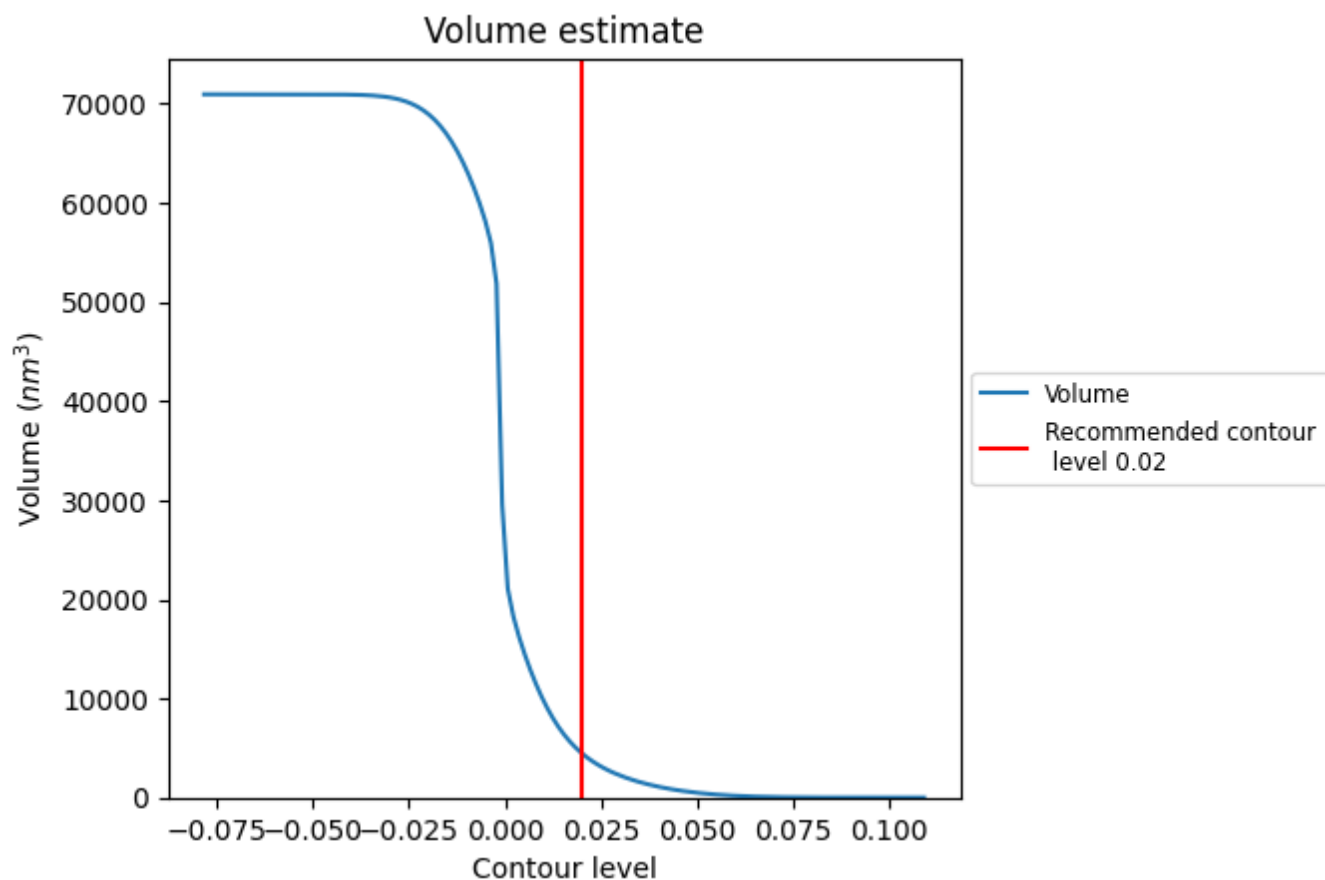
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

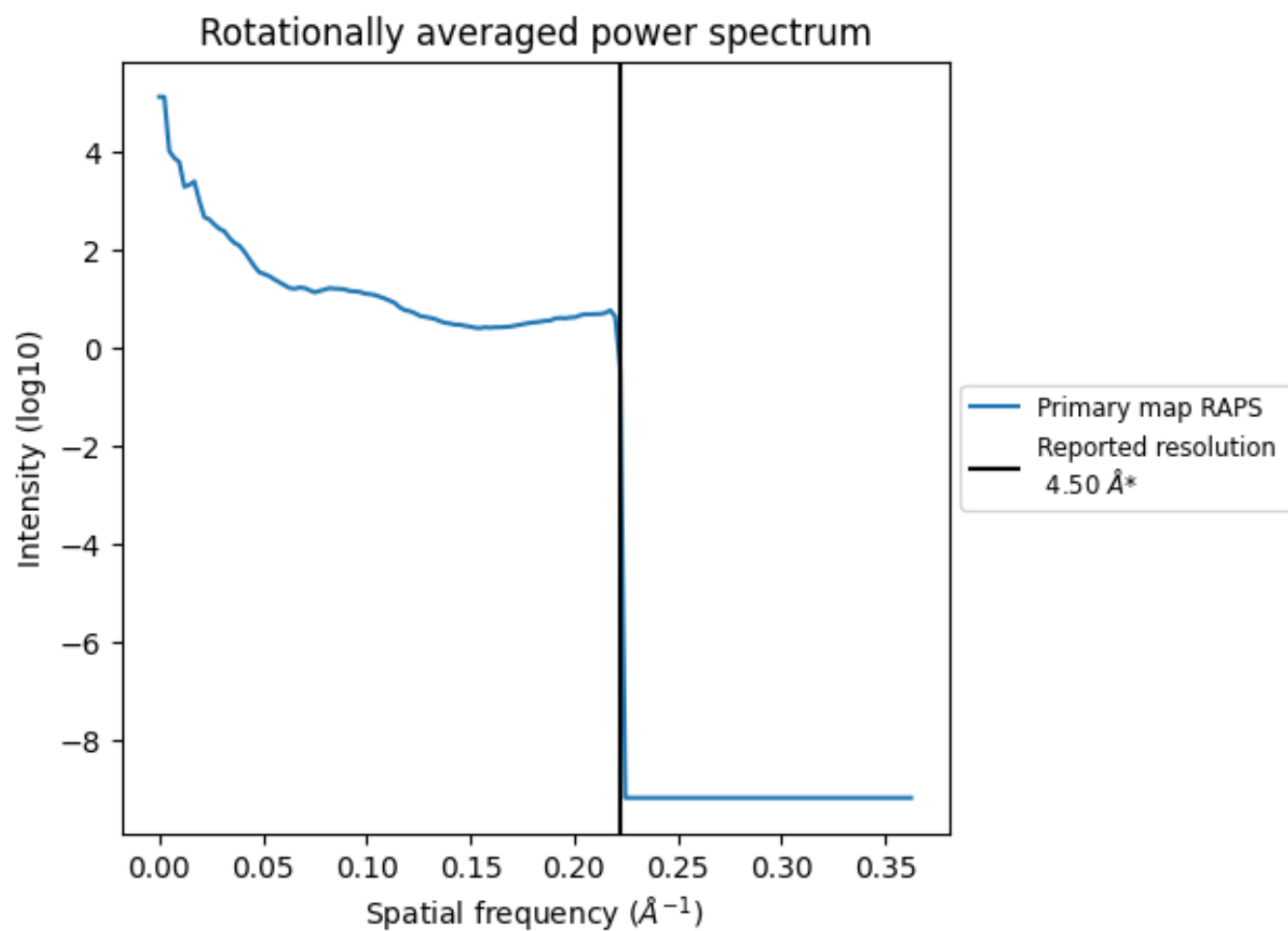
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 4481  $\text{nm}^3$ ; this corresponds to an approximate mass of 4048 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum ⓘ



\*Reported resolution corresponds to spatial frequency of 0.222  $\text{\AA}^{-1}$

## 8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

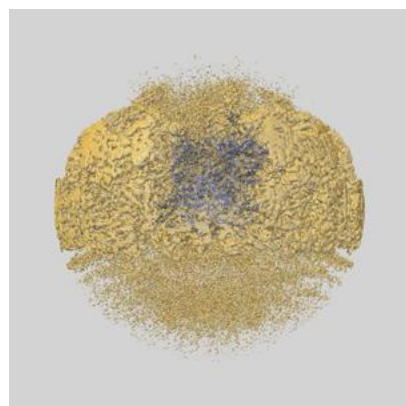


## 9 Map-model fit [i](#)

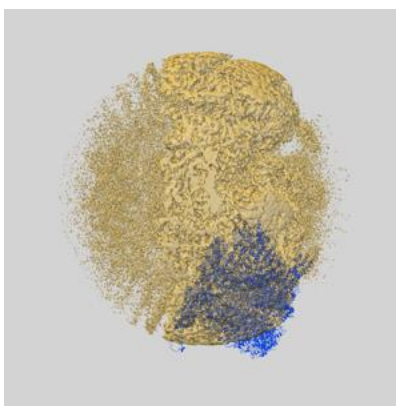
This section contains information regarding the fit between EMDB map EMD-30124 and PDB model 6M6H. Per-residue inclusion information can be found in section 3 on page 7.

### 9.1 Map-model overlays

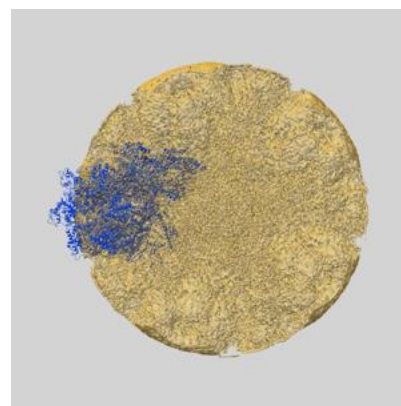
#### 9.1.1 Map-model overlay [i](#)



X

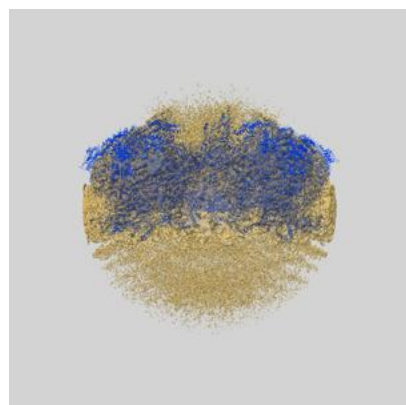


Y

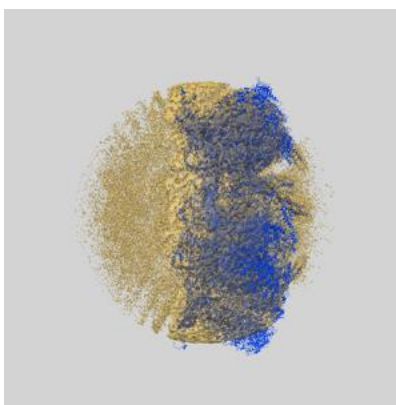


Z

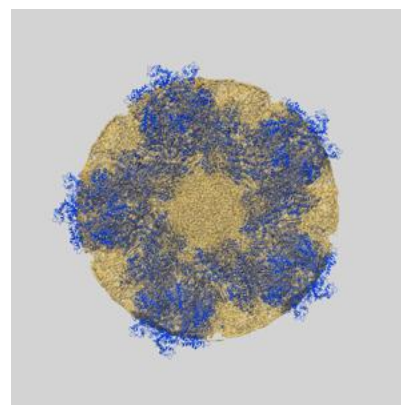
#### 9.1.2 Map-model assembly overlay [i](#)



X



Y

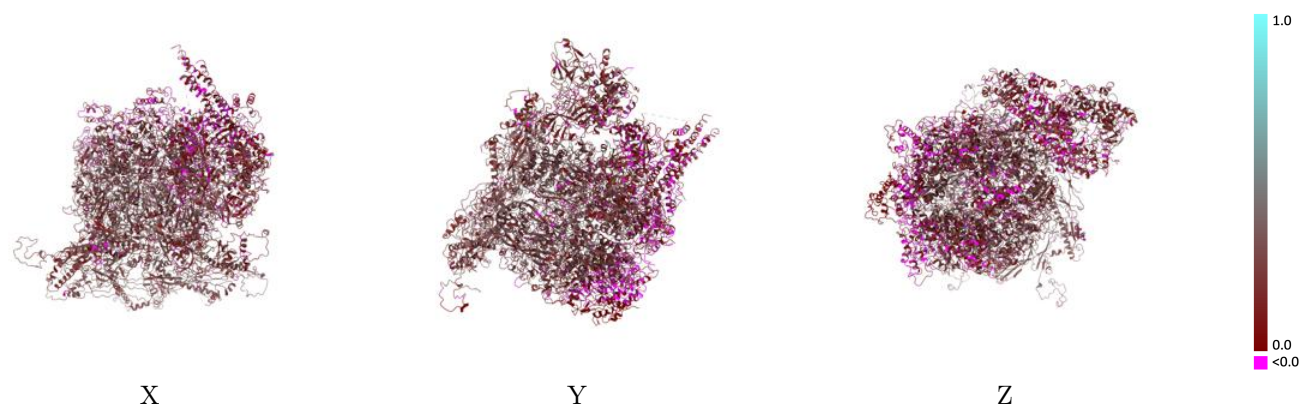


Z

The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

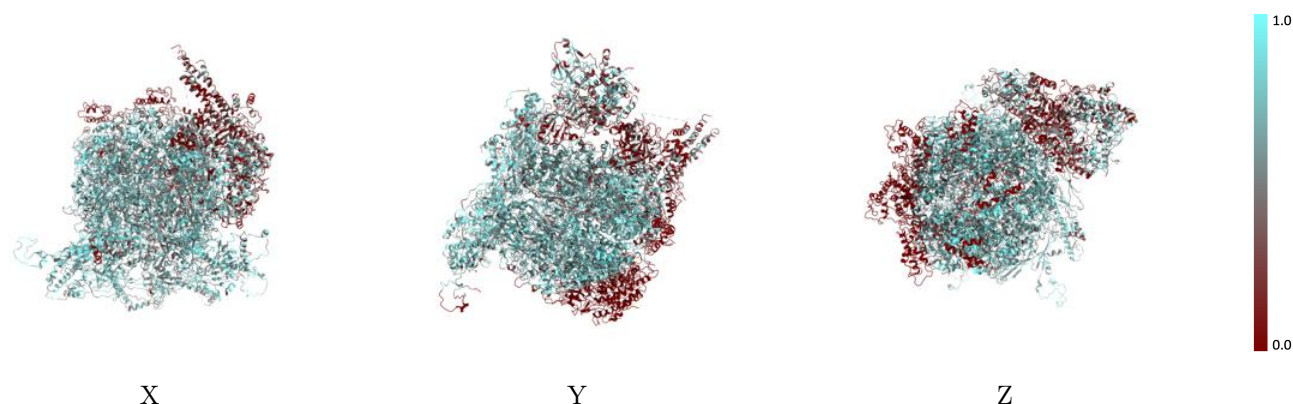


## 9.2 Q-score mapped to coordinate model [i](#)



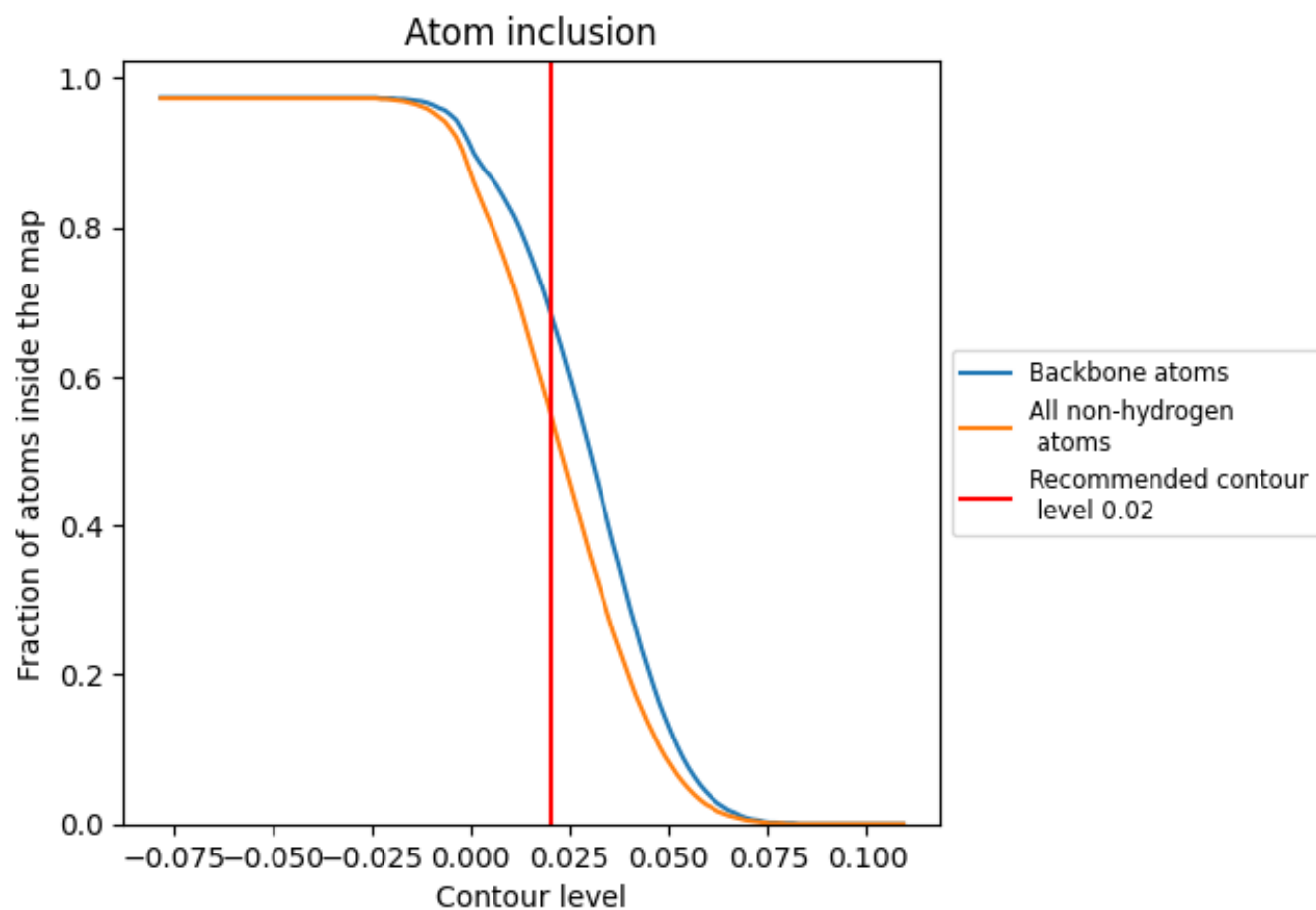
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.02).











































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 69% of all backbone atoms, 55% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5530	 0.2020
A	 0.6680	 0.2250
B	 0.6400	 0.2160
C	 0.5110	 0.1970
D	 0.6210	 0.2230
E	 0.6930	 0.2410
F	 0.6520	 0.2310
G	 0.2760	 0.1380
H	 0.2950	 0.1610
I	 0.2960	 0.1430
J	 0.1120	 0.0070
K	 0.1280	 0.0710
L	 0.1060	 0.0810
M	 0.1190	 0.0620
N	 0.0000	 0.0350
O	 0.0000	 0.0180
P	 0.2870	 0.1280
Q	 0.2620	 0.1210
R	 0.4900	 0.2060
S	 0.3410	 0.1980
T	 0.4650	 0.1500

