



## wwPDB EM Validation Summary Report ⓘ

Oct 28, 2024 – 11:32 AM JST

PDB ID : 7FJ1  
EMDB ID : EMD-31611  
Title : Cryo-EM structure of pseudorabies virus C-capsid  
Authors : Zheng, Q.; Li, S.; Zha, Z.; Sun, H.  
Deposited on : 2021-08-02  
Resolution : 4.43 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

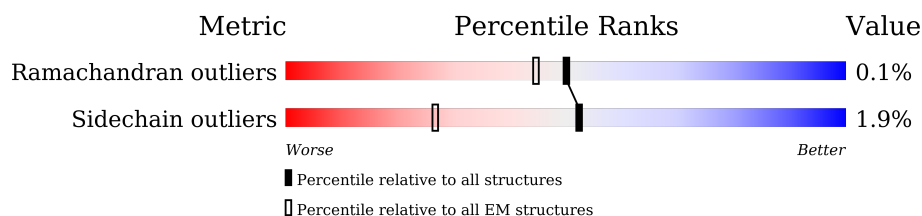
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.43 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)
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	0	1330	<div> <div>27%</div> <div>98%</div> </div>
1	A	1330	<div> <div>22%</div> <div>98%</div> </div>
1	S	1330	<div> <div>27%</div> <div>97%</div> </div>
1	U	1330	<div> <div>23%</div> <div>98%</div> </div>
1	a	1330	<div> <div>27%</div> <div>97%</div> </div>
1	e	1330	<div> <div>35%</div> <div>85%</div> <div>15%</div> </div>
1	f	1330	<div> <div>23%</div> <div>98%</div> </div>
1	g	1330	<div> <div>26%</div> <div>98%</div> </div>
1	l	1330	<div> <div>25%</div> <div>98%</div> </div>

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Mol	Chain	Length	Quality of chain
1	m	1330	25% 98% .
1	n	1330	27% 98% ..
1	p	1330	25% 98% .
1	q	1330	27% 98% .
1	u	1330	22% 98% .
1	w	1330	27% 98% .
1	y	1330	23% 98% ..
2	1	296	26% 94% 6%
2	2	296	27% 93% 6%
2	3	296	30% 94% 6%
2	j	296	53% 90% 10%
2	k	296	50% 94% 6%
2	o	296	29% 100%
2	s	296	25% 94% 6%
2	v	296	29% 97% ..
2	x	296	36% 100%
2	z	296	34% 99% .
3	B	597	72% 87% 12%
4	E	103	11% 78% 11% 12%
4	F	103	16% 78% 11% 12%
4	G	103	21% 78% 11% 12%
4	H	103	10% 78% 11% 12%
4	I	103	21% 78% 11% 12%
4	J	103	14% 76% 13% 12%
4	K	103	10% 77% 12% 12%

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Mol	Chain	Length	Quality of chain
4	L	103	
4	M	103	
4	N	103	
4	O	103	
4	P	103	
4	Q	103	
4	R	103	
4	V	103	
5	T	368	
5	h	368	
5	i	368	
5	r	368	
5	t	368	
6	X	534	
6	c	534	
7	Y	62	
7	Z	62	

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 210927 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	0	1311	Total	C	N	O	S	0	0
			10129	6403	1824	1841	61		
1	A	1308	Total	C	N	O	S	0	0
			10112	6393	1820	1837	62		
1	S	1289	Total	C	N	O	S	0	0
			9975	6307	1797	1812	59		
1	U	1311	Total	C	N	O	S	0	0
			10129	6403	1824	1841	61		
1	a	1289	Total	C	N	O	S	0	0
			9974	6311	1797	1805	61		
1	e	1126	Total	C	N	O	S	0	0
			8722	5528	1561	1579	54		
1	f	1311	Total	C	N	O	S	0	0
			10129	6403	1824	1841	61		
1	g	1310	Total	C	N	O	S	0	0
			10125	6401	1823	1840	61		
1	l	1311	Total	C	N	O	S	0	0
			10129	6403	1824	1841	61		
1	m	1311	Total	C	N	O	S	0	0
			10129	6403	1824	1841	61		
1	n	1311	Total	C	N	O	S	0	0
			10129	6403	1824	1841	61		
1	p	1311	Total	C	N	O	S	0	0
			10129	6403	1824	1841	61		
1	q	1311	Total	C	N	O	S	0	0
			10129	6403	1824	1841	61		
1	u	1311	Total	C	N	O	S	0	0
			10129	6403	1824	1841	61		
1	w	1311	Total	C	N	O	S	0	0
			10129	6403	1824	1841	61		
1	y	1311	Total	C	N	O	S	0	0
			10129	6403	1824	1841	61		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	277	Total	C	N	O	S	0	0
			2088	1318	382	377	11		
2	2	277	Total	C	N	O	S	0	0
			2088	1318	382	377	11		
2	3	277	Total	C	N	O	S	0	0
			2088	1318	382	377	11		
2	j	267	Total	C	N	O	S	0	0
			2009	1269	365	364	11		
2	k	277	Total	C	N	O	S	0	0
			2088	1318	382	377	11		
2	o	296	Total	C	N	O	S	0	0
			2229	1403	414	401	11		
2	s	277	Total	C	N	O	S	0	0
			2088	1318	382	377	11		
2	v	289	Total	C	N	O	S	0	0
			2189	1380	404	394	11		
2	x	296	Total	C	N	O	S	0	0
			2229	1403	414	401	11		
2	z	294	Total	C	N	O	S	0	0
			2210	1391	412	396	11		

- Molecule 3 is a protein called Capsid vertex component 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	524	Total	C	N	O	S	0	0
			4023	2540	764	706	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	91	Total	C	N	O	S	0	0
			722	453	139	128	2		
4	F	91	Total	C	N	O	S	0	0
			722	453	139	128	2		
4	G	91	Total	C	N	O	S	0	0
			722	453	139	128	2		
4	H	91	Total	C	N	O	S	0	0
			722	453	139	128	2		
4	I	91	Total	C	N	O	S	0	0
			722	453	139	128	2		
4	J	91	Total	C	N	O	S	0	0
			722	453	139	128	2		
4	K	91	Total	C	N	O	S	0	0
			722	453	139	128	2		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	L	91	Total	C	N	O	S	0	0
			722	453	139	128	2		
4	M	91	Total	C	N	O	S	0	0
			722	453	139	128	2		
4	N	91	Total	C	N	O	S	0	0
			722	453	139	128	2		
4	O	91	Total	C	N	O	S	0	0
			722	453	139	128	2		
4	P	91	Total	C	N	O	S	0	0
			722	453	139	128	2		
4	Q	91	Total	C	N	O	S	0	0
			722	453	139	128	2		
4	R	91	Total	C	N	O	S	0	0
			722	453	139	128	2		
4	V	91	Total	C	N	O	S	0	0
			722	453	139	128	2		

- Molecule 5 is a protein called Triplex capsid protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	T	327	Total	C	N	O	S	0	0
			2538	1582	494	450	12		
5	h	327	Total	C	N	O	S	0	0
			2538	1582	494	450	12		
5	i	327	Total	C	N	O	S	0	0
			2538	1582	494	450	12		
5	r	327	Total	C	N	O	S	0	0
			2538	1582	494	450	12		
5	t	327	Total	C	N	O	S	0	0
			2538	1582	494	450	12		

- Molecule 6 is a protein called DNA packaging tegument protein UL25.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	X	73	Total	C	N	O	S	0	0
			552	346	109	96	1		
6	c	75	Total	C	N	O	S	0	0
			558	350	111	96	1		

- Molecule 7 is a protein called VP1/2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	Y	45	Total	C	N	O	S	0	0
			353	224	72	56	1		
7	Z	35	Total	C	N	O	S	0	0
			288	180	62	45	1		

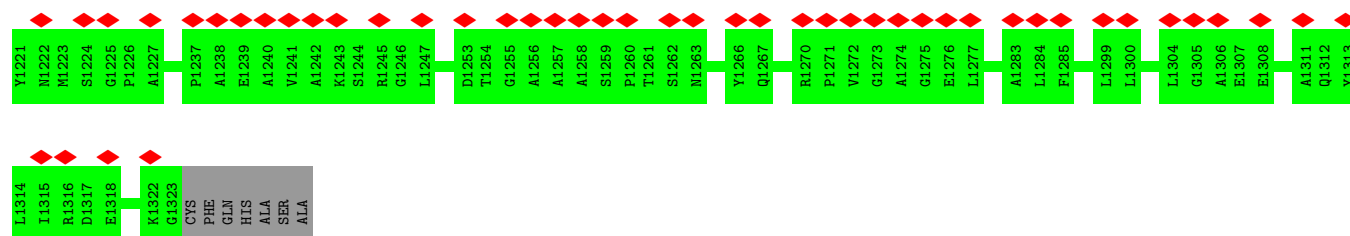


### 3 Residue-property plots

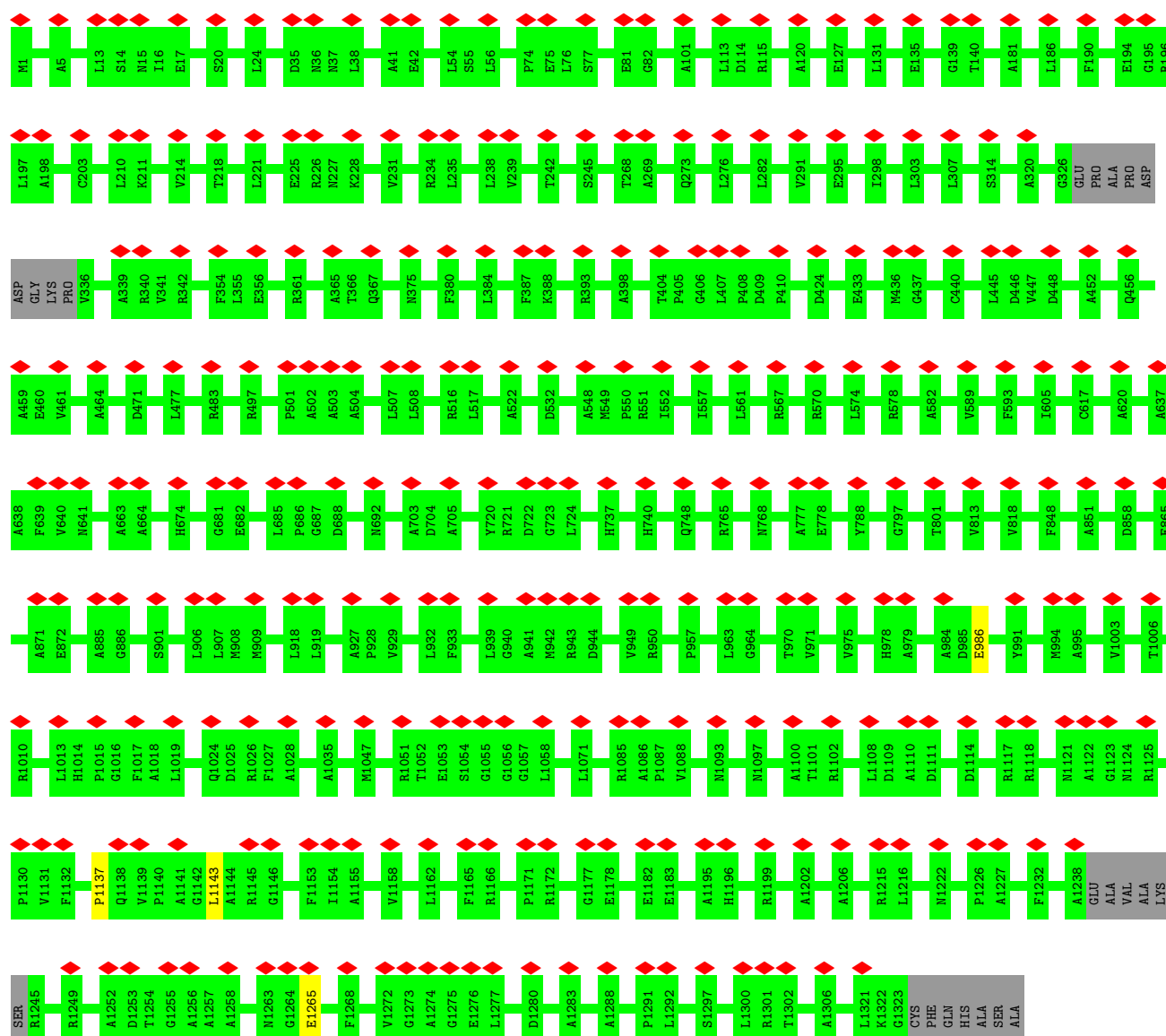
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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

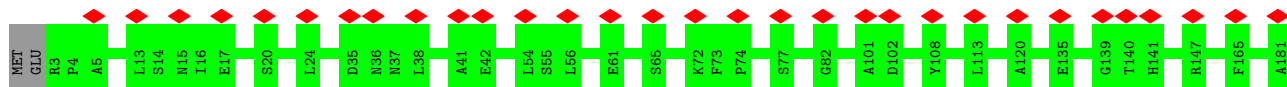


• Molecule 1: Major capsid protein



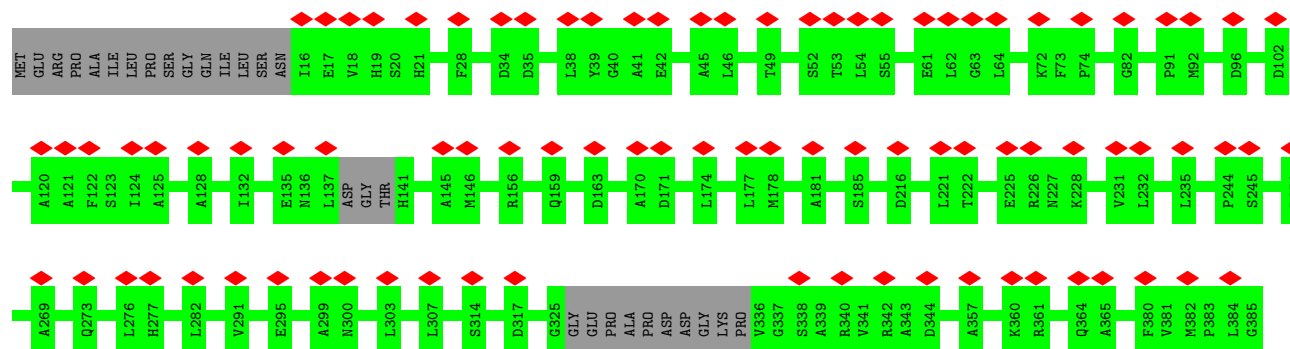


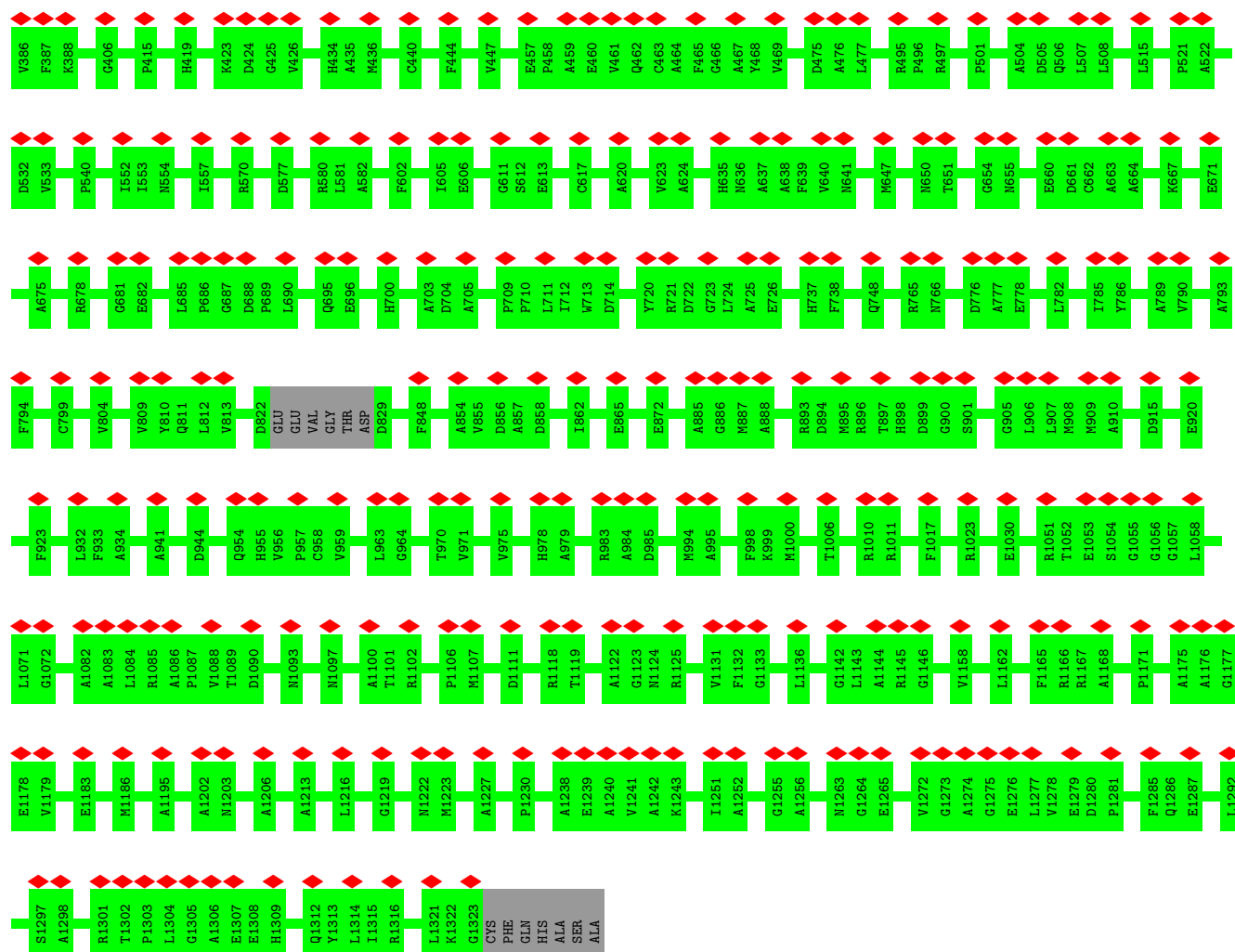
- Molecule 1: Major capsid protein



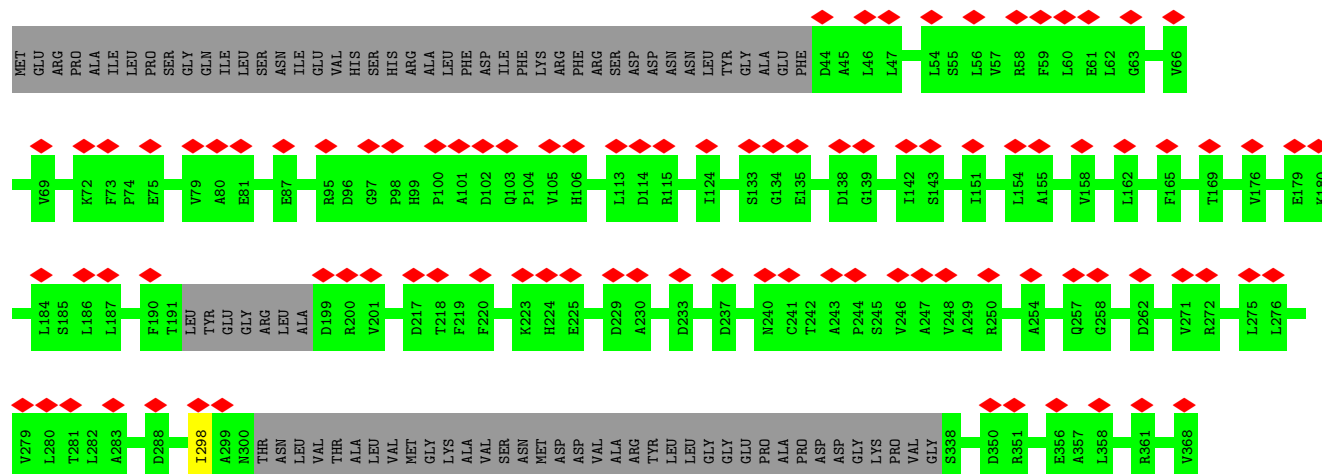
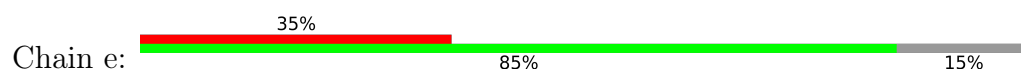


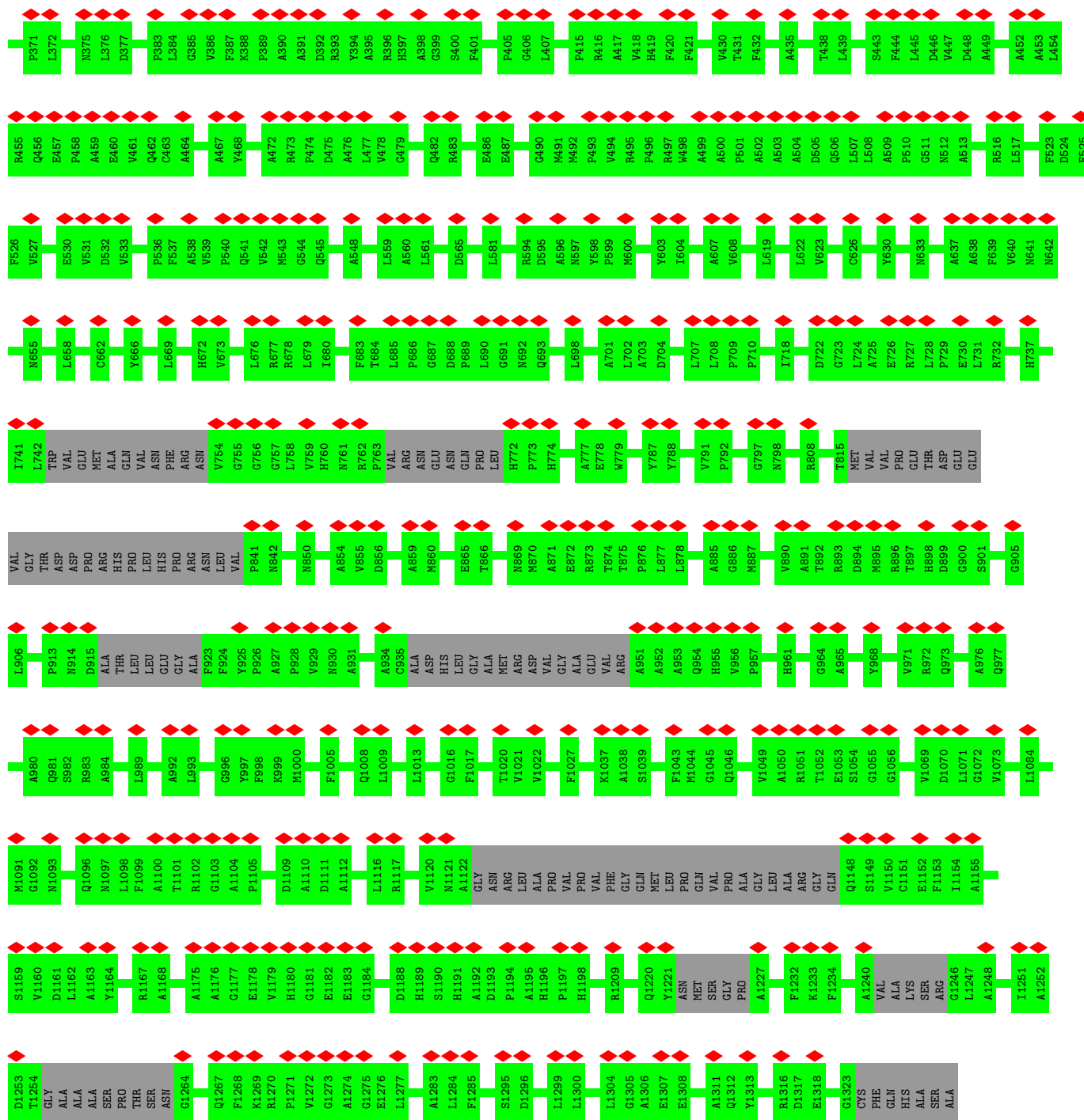
• Molecule 1: Major capsid protein



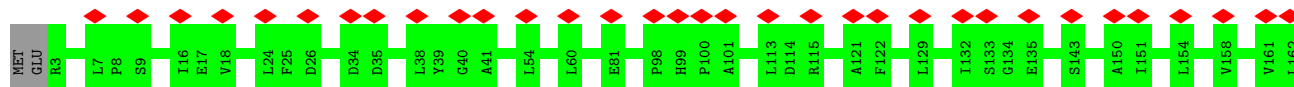


### • Molecule 1: Major capsid protein





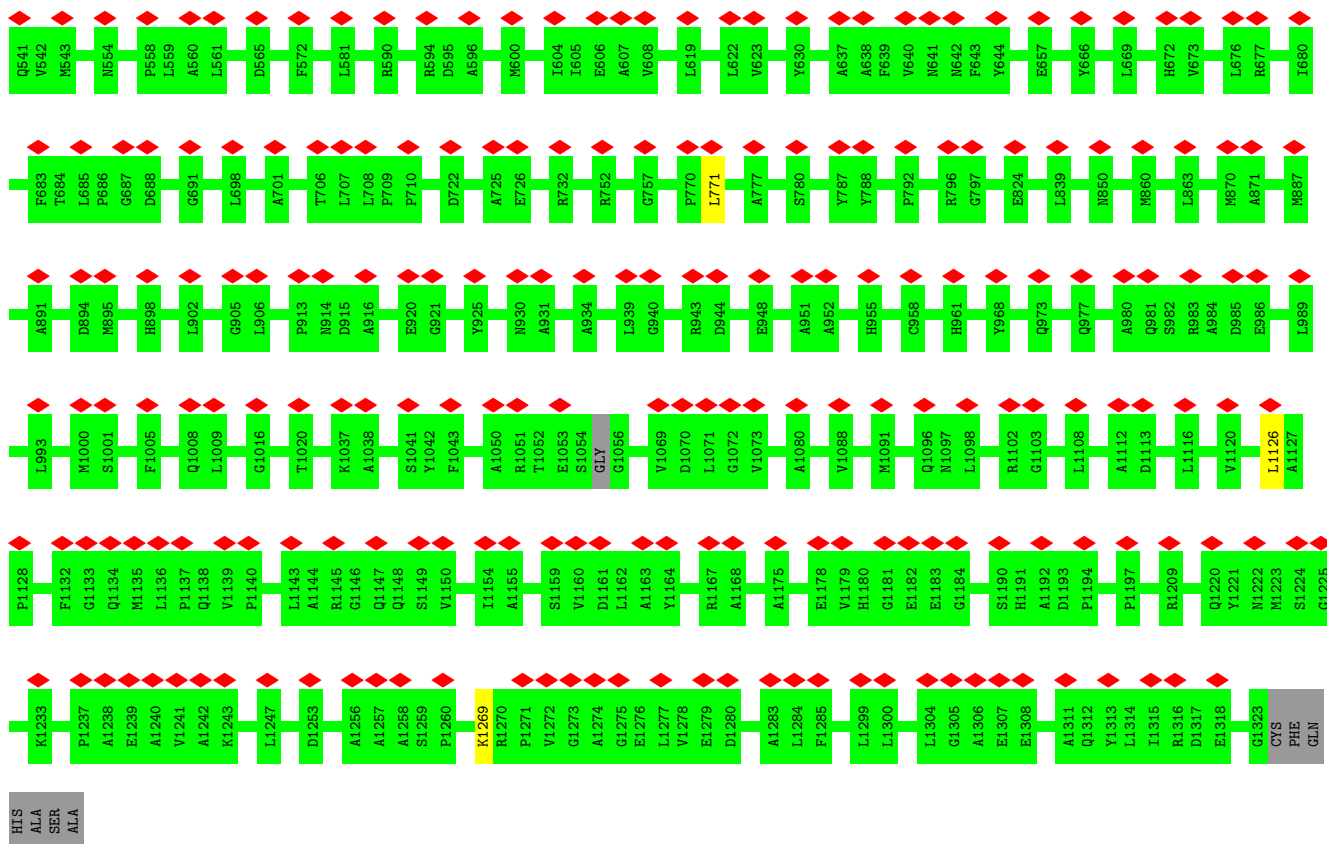
• Molecule 1: Major capsid protein



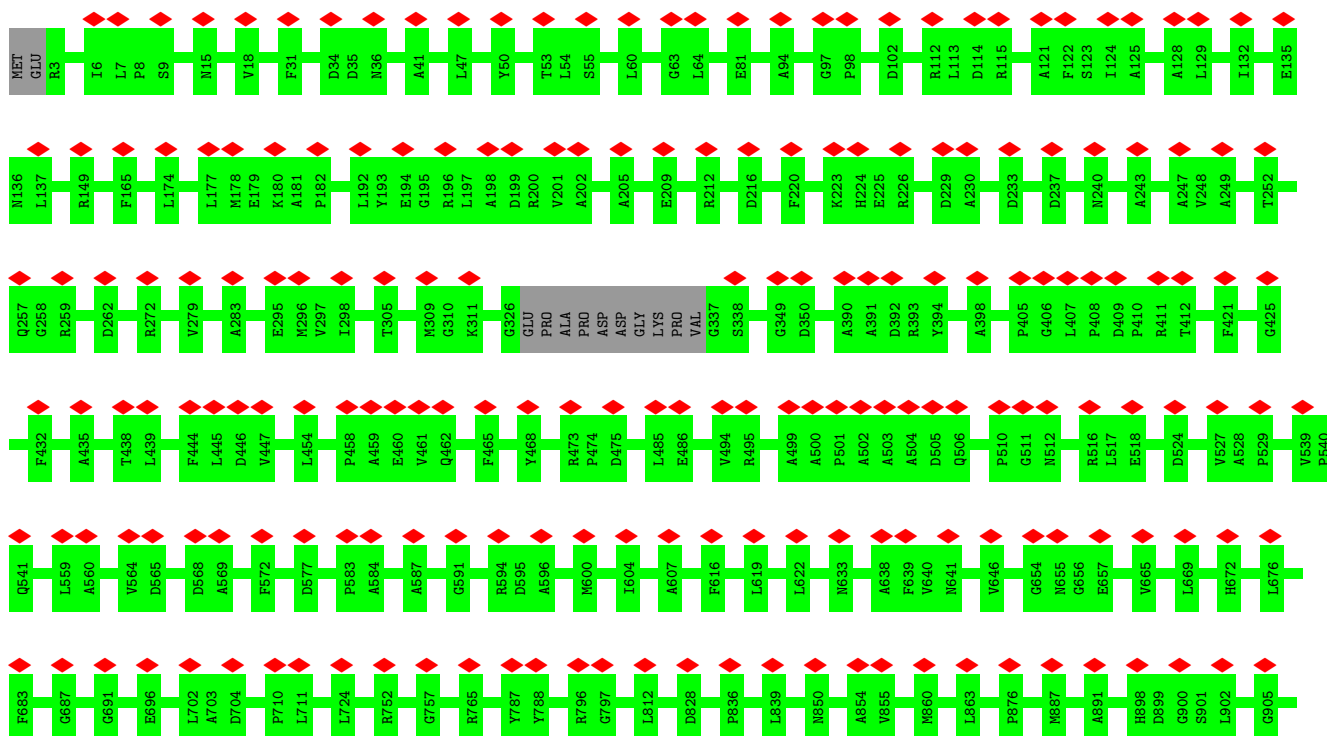


• Molecule 1: Major capsid protein

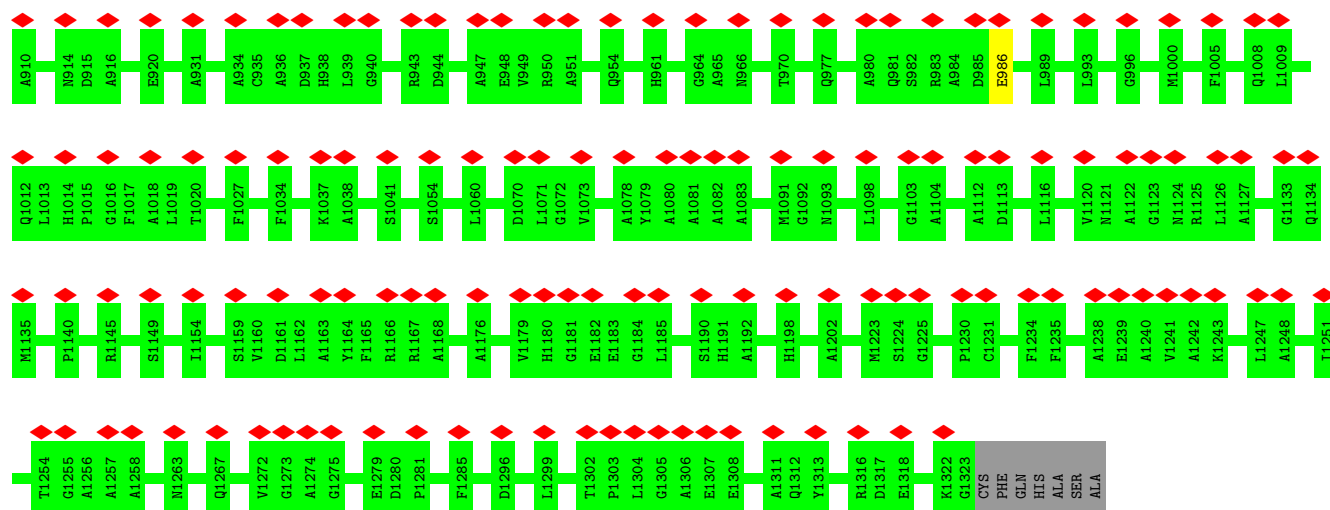




• Molecule 1: Major capsid protein

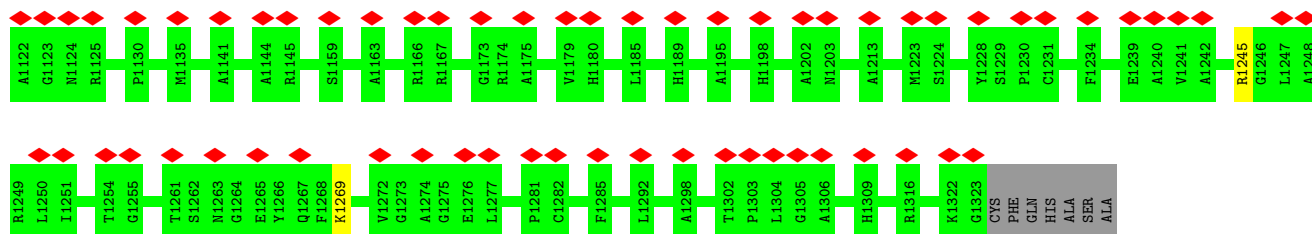




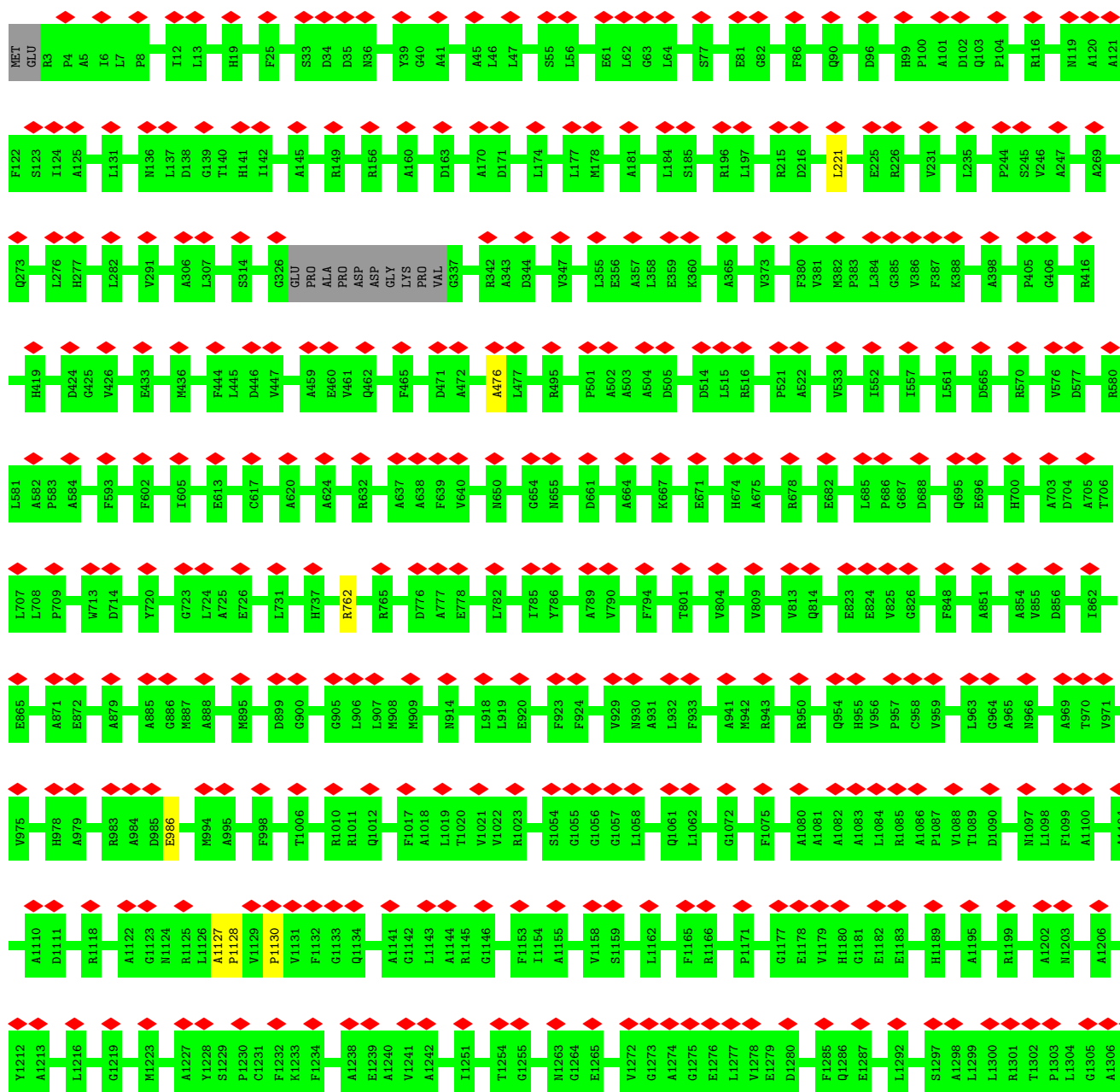


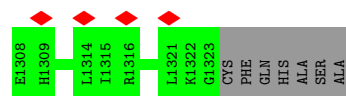
• Molecule 1: Major capsid protein



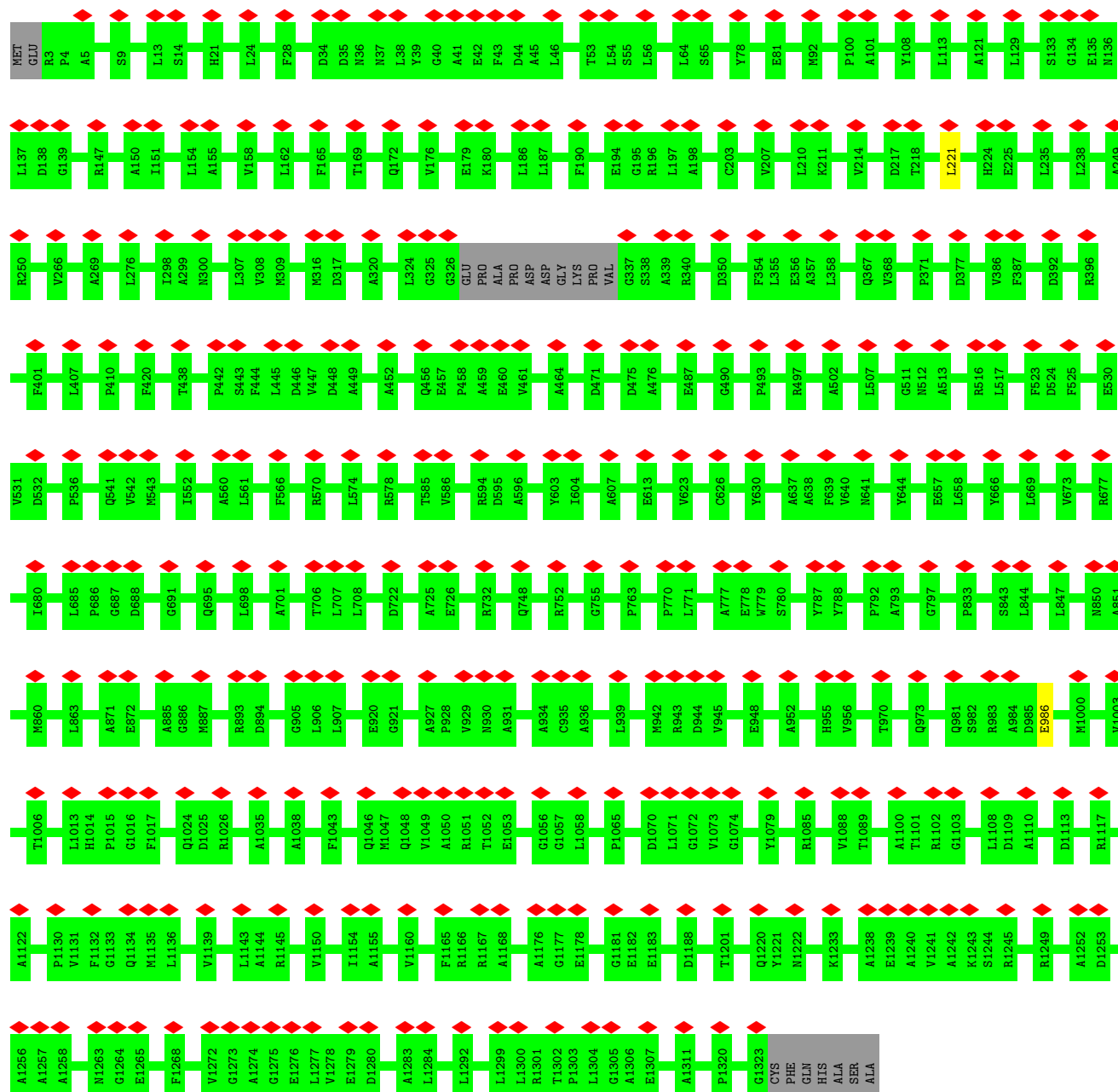


• Molecule 1: Major capsid protein



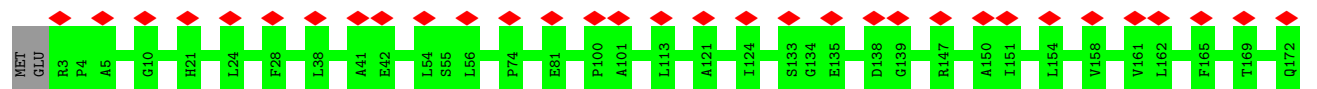


• Molecule 1: Major capsid protein



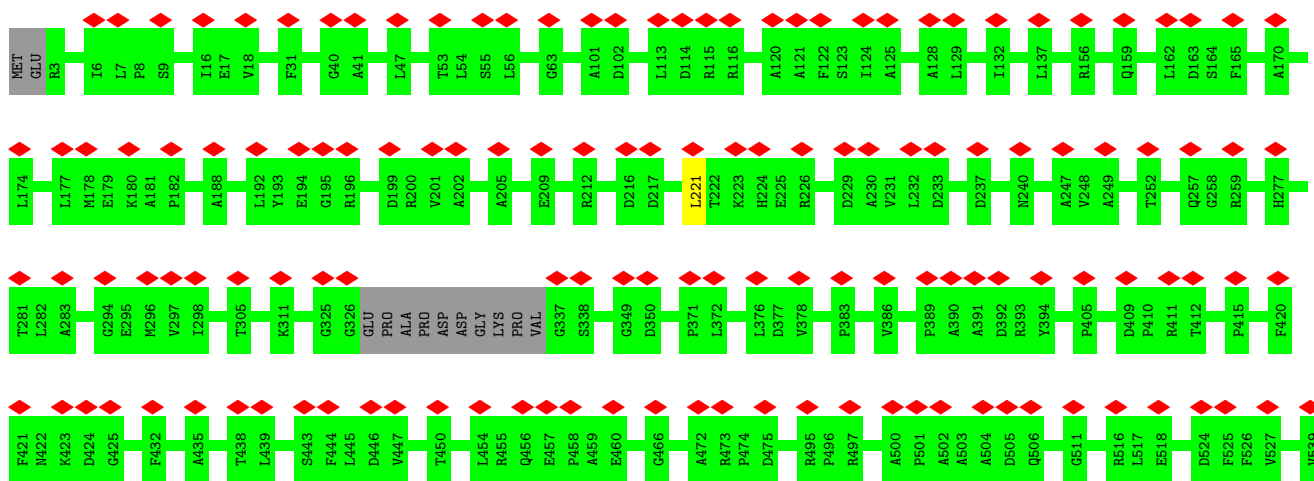
• Molecule 1: Major capsid protein

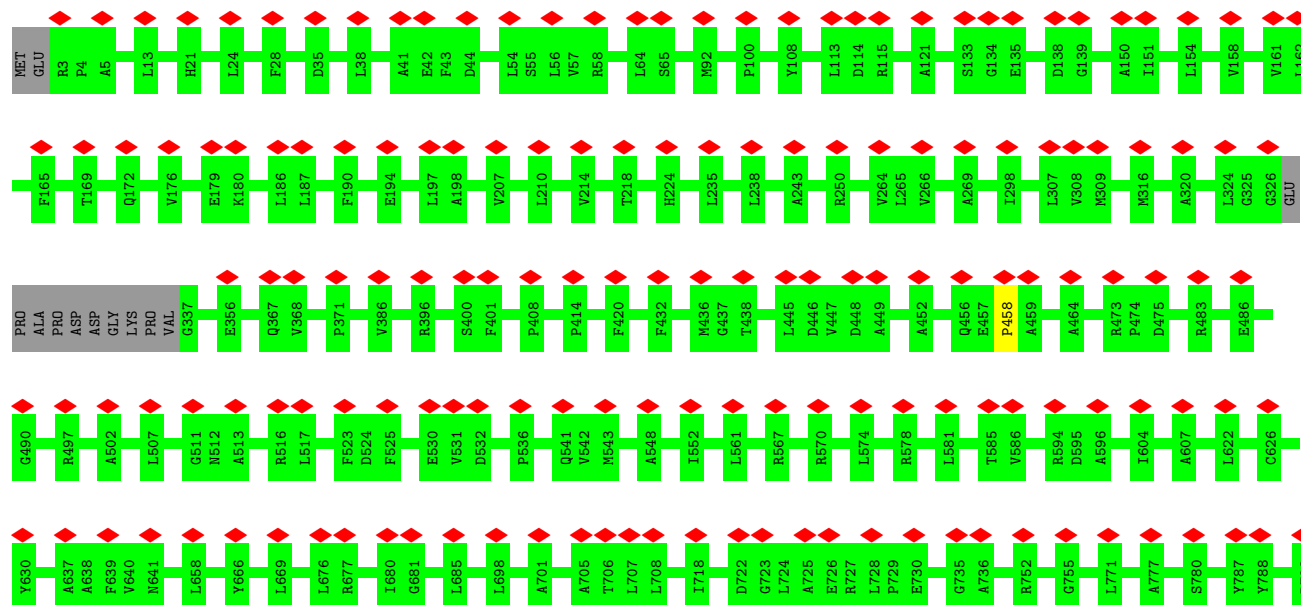


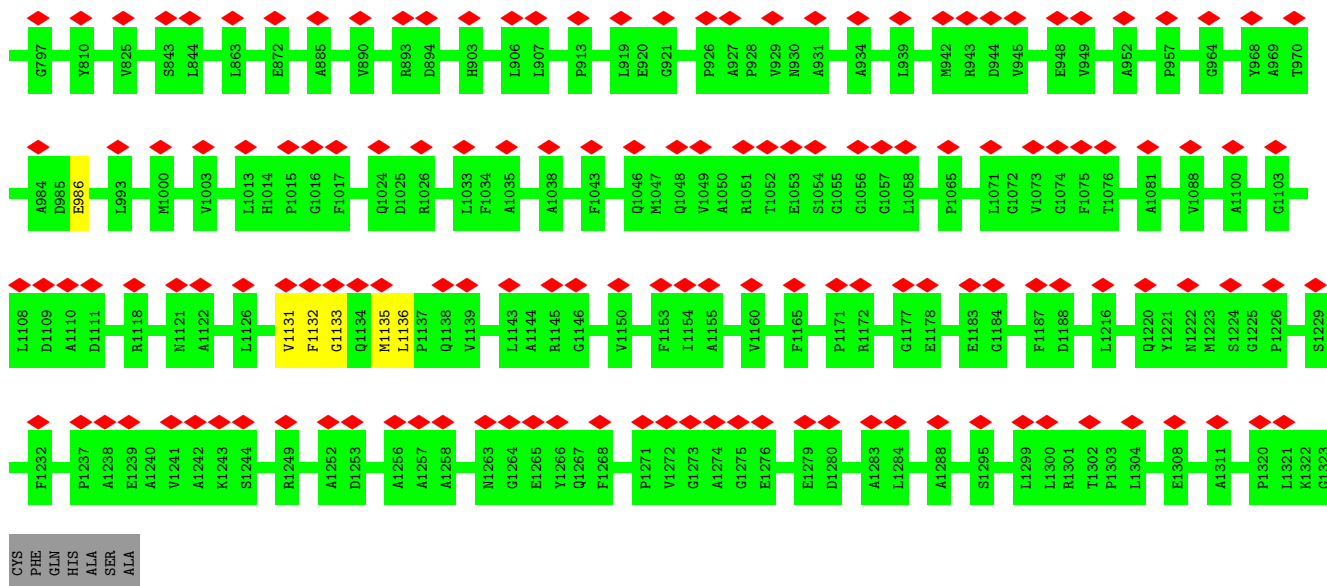




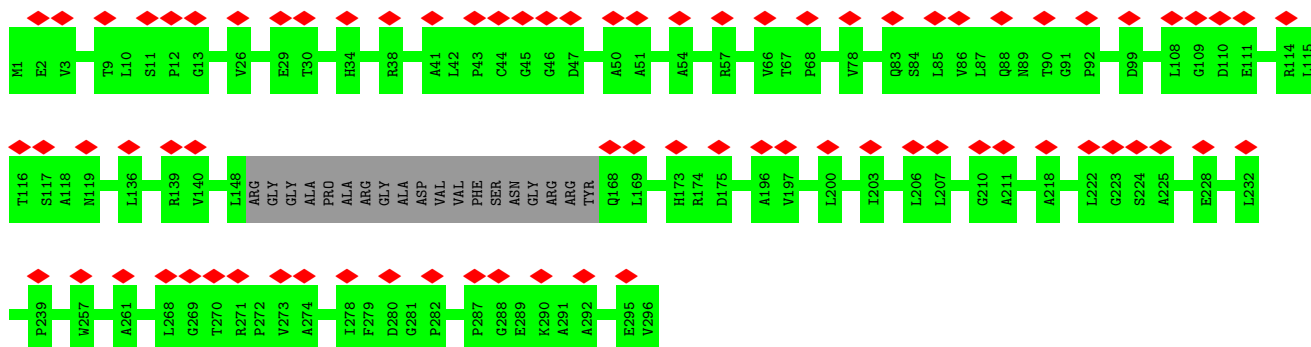
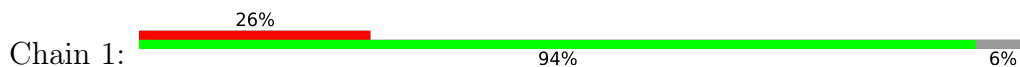
• Molecule 1: Major capsid protein



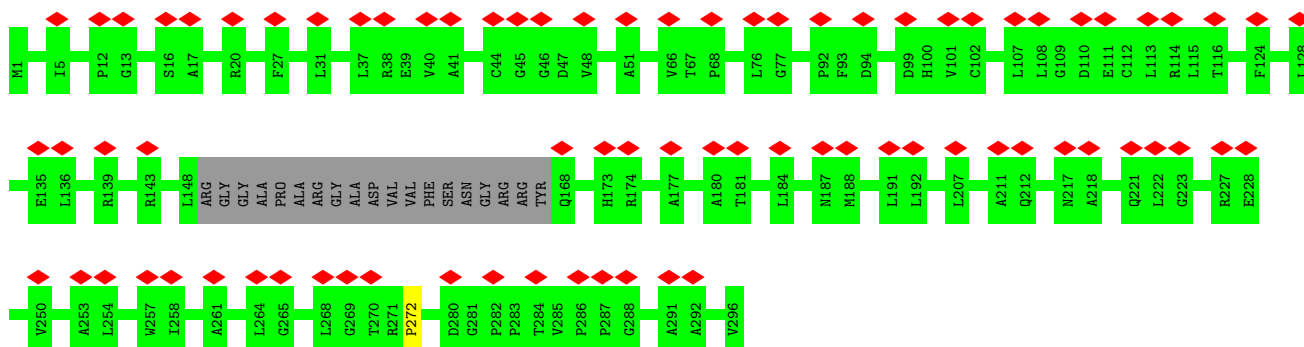
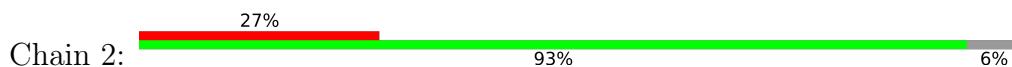




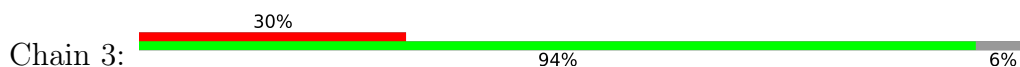
- Molecule 2: Triplex capsid protein 2

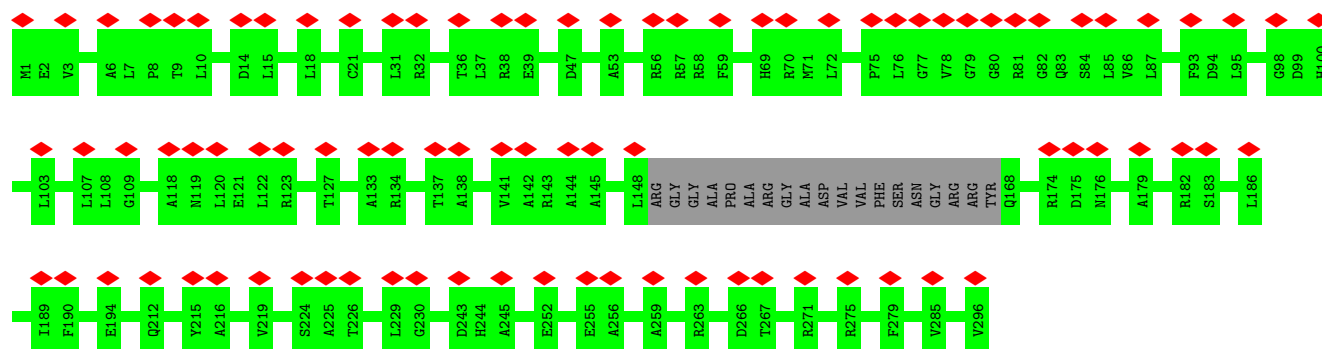


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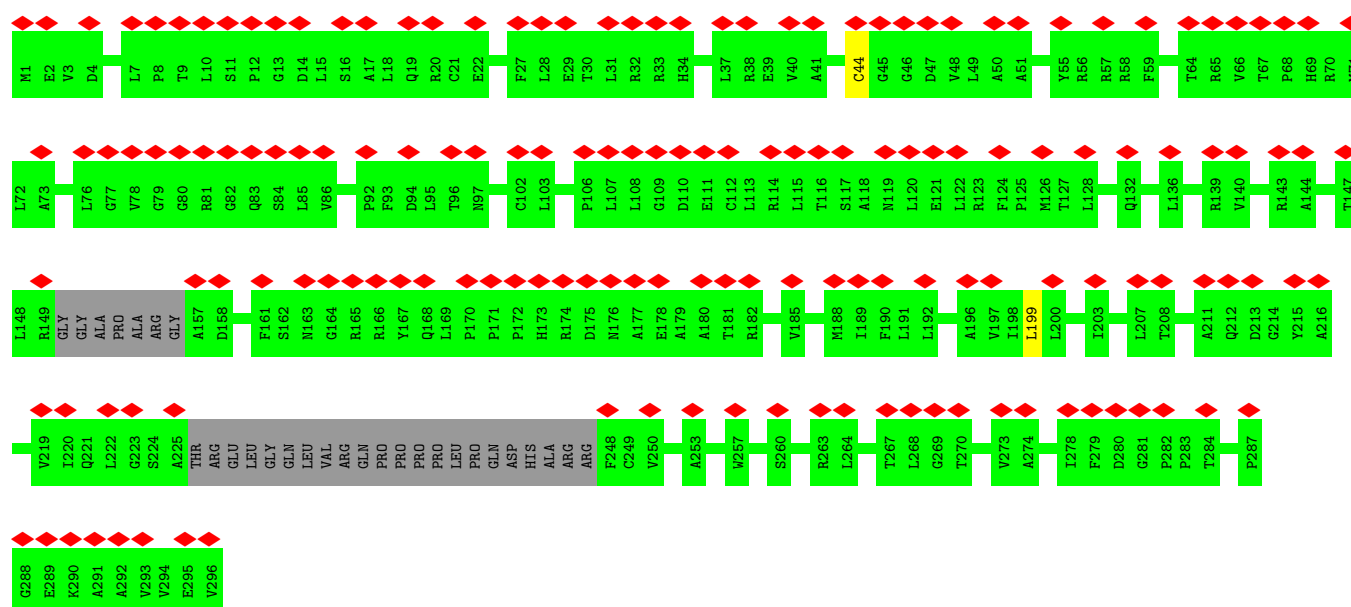
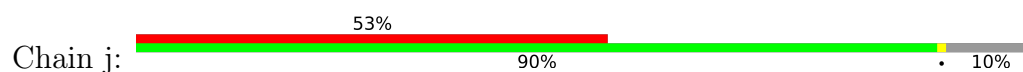


- Molecule 2: Triplex capsid protein 2

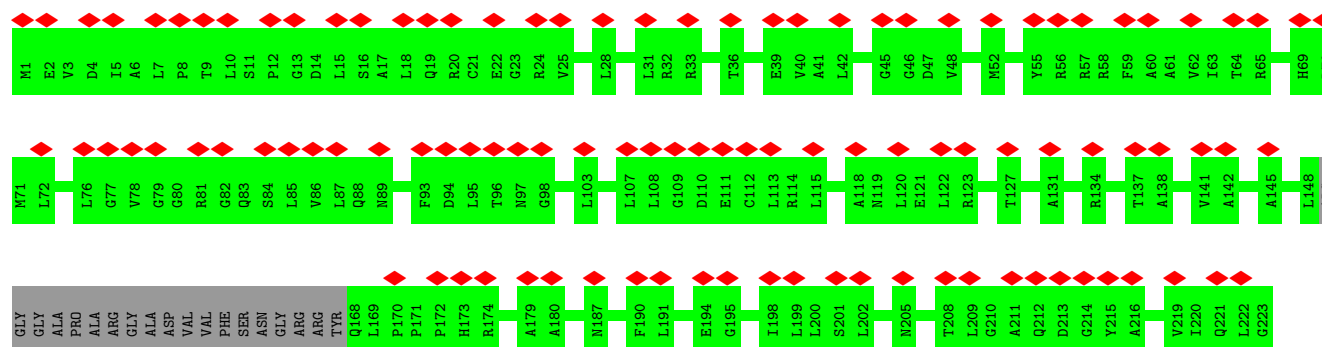




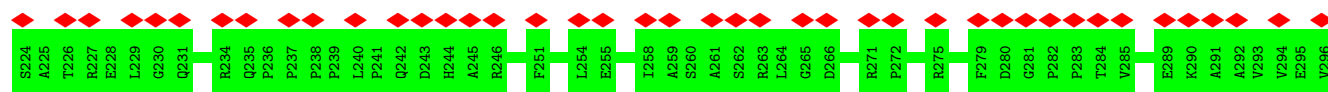
• Molecule 2: Triplex capsid protein 2



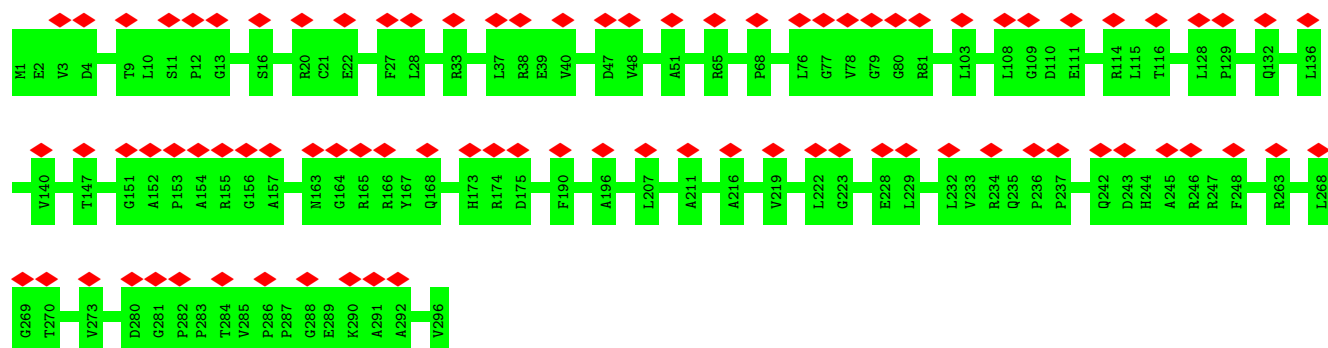
• Molecule 2: Triplex capsid protein 2



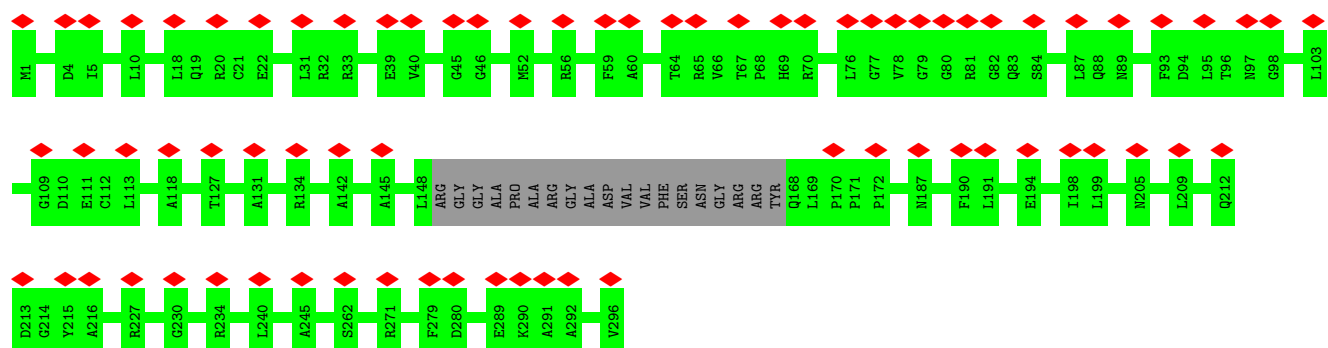
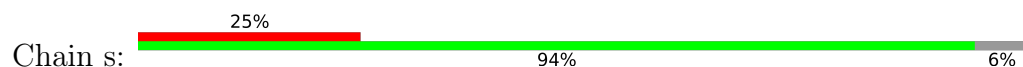




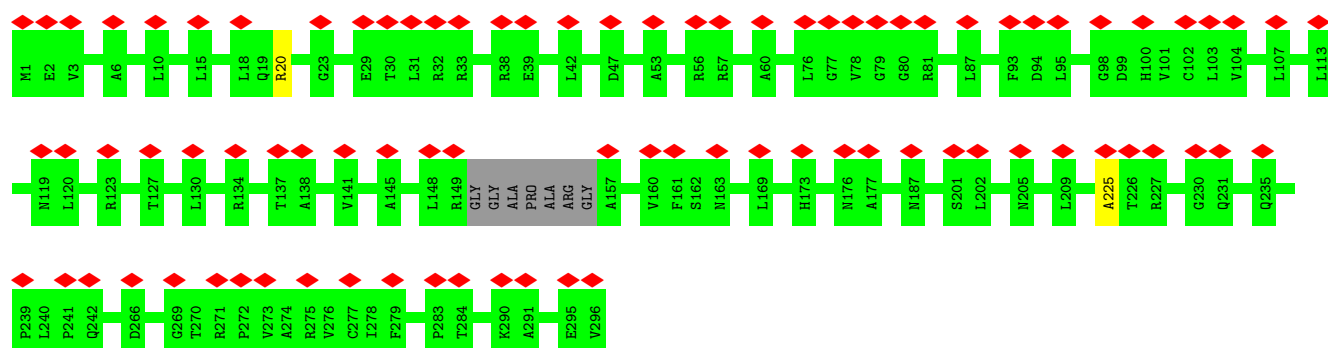
• Molecule 2: Triplex capsid protein 2



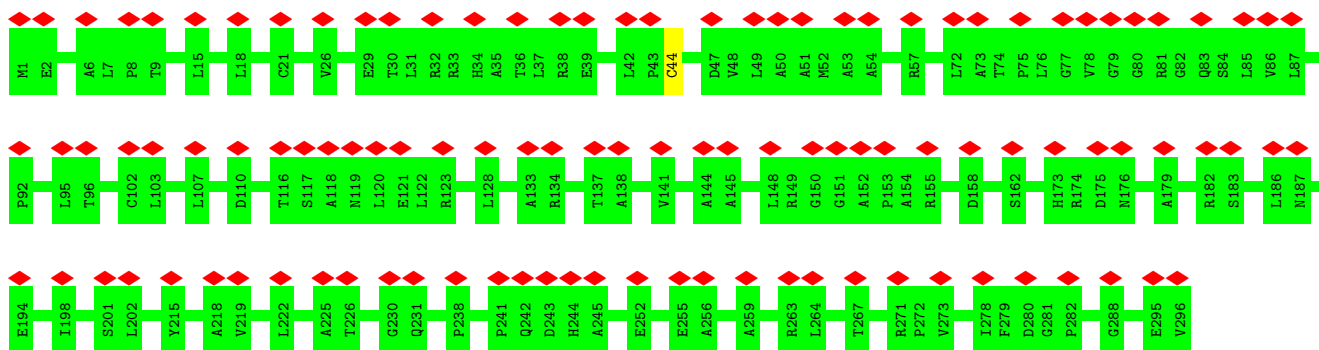
• Molecule 2: Triplex capsid protein 2



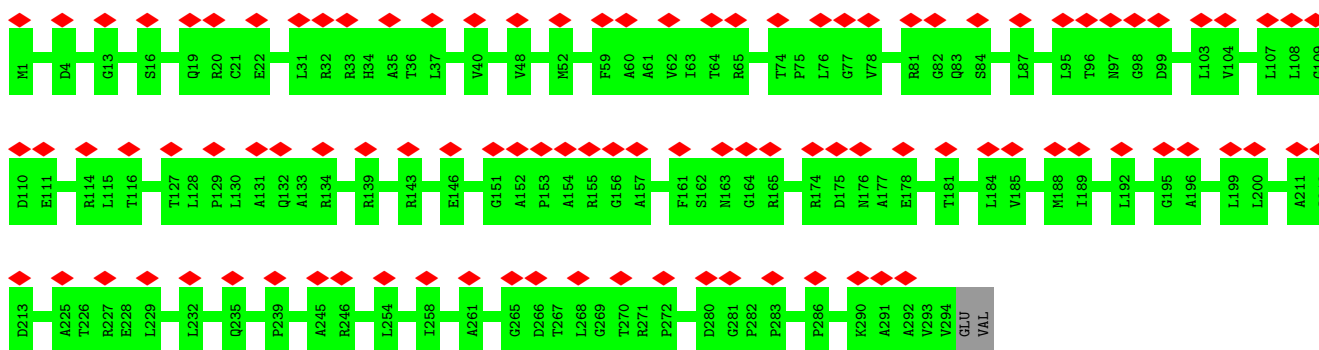
• Molecule 2: Triplex capsid protein 2



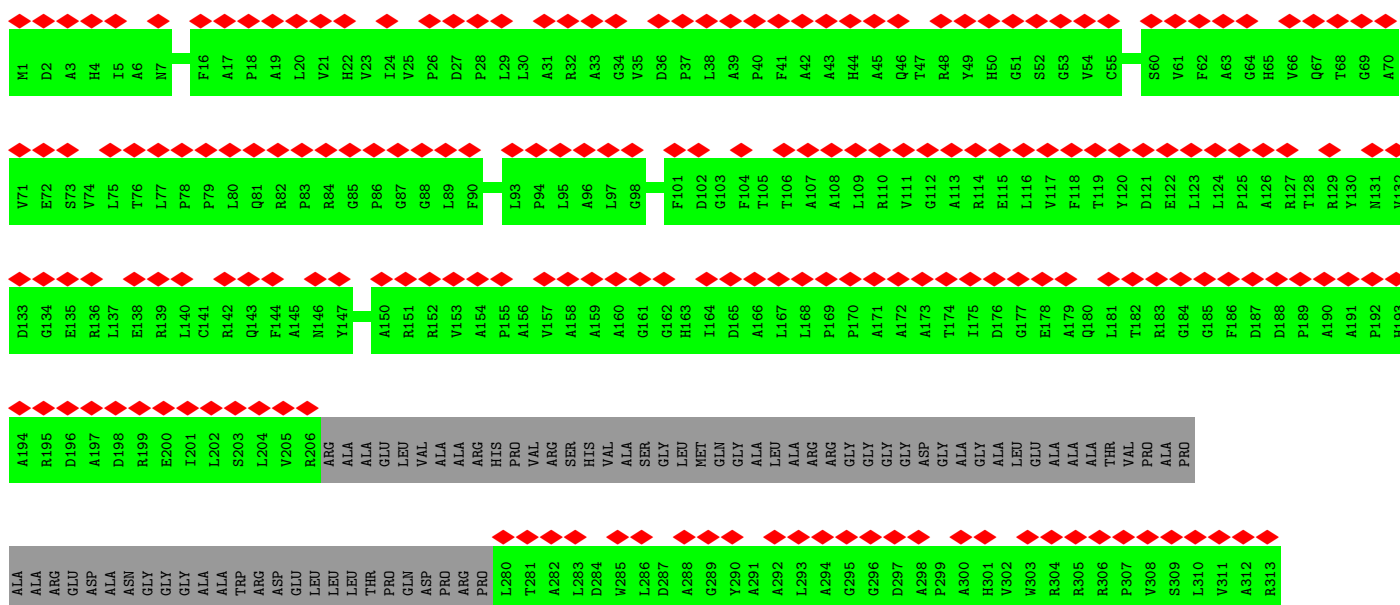
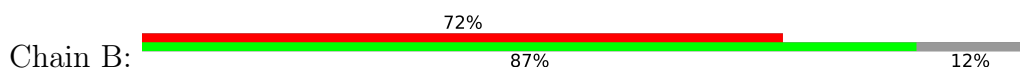
• Molecule 2: Triplex capsid protein 2



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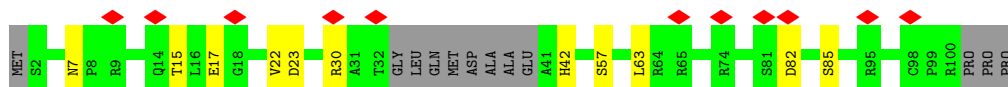
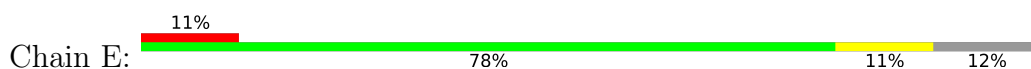


• Molecule 3: Capsid vertex component 1

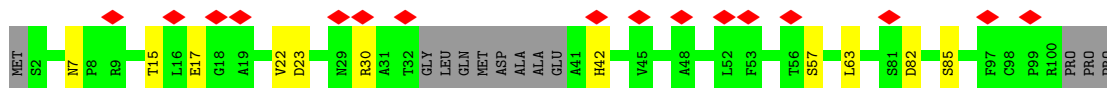
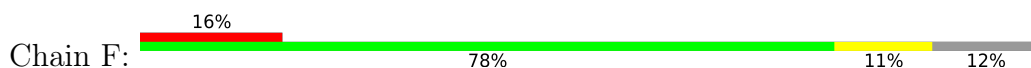




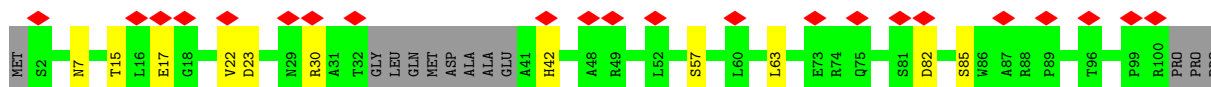
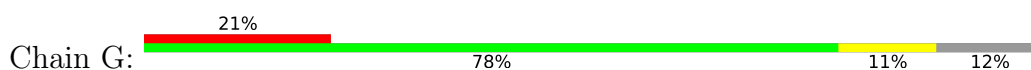
- Molecule 4: Small capsomere-interacting protein



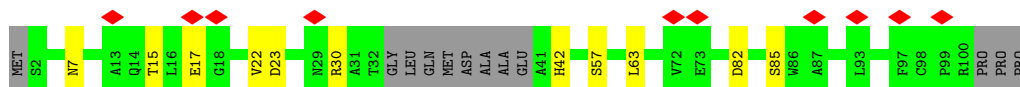
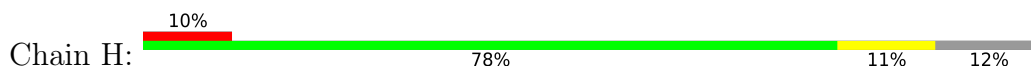
- Molecule 4: Small capsomere-interacting protein



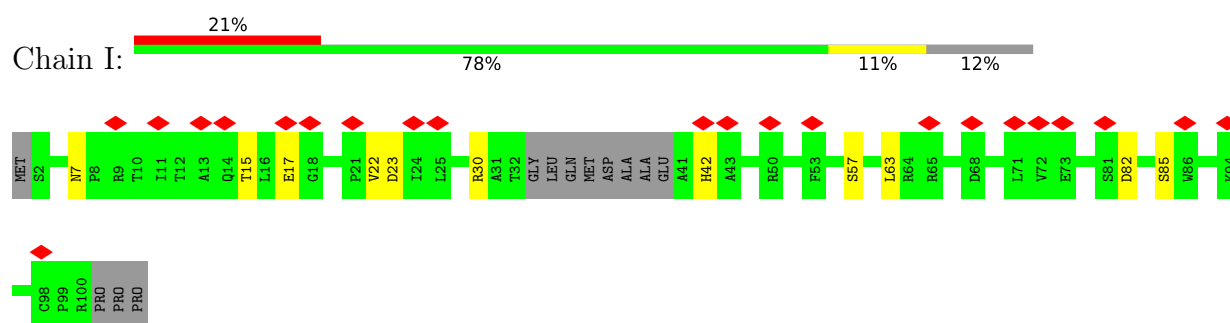
- Molecule 4: Small capsomere-interacting protein



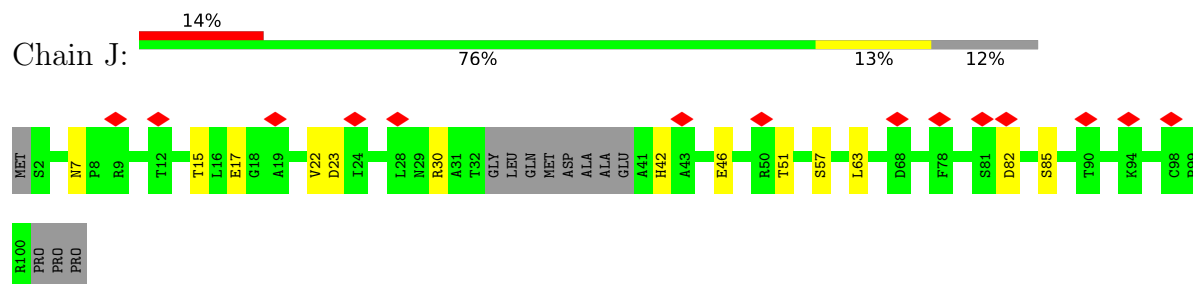
- Molecule 4: Small capsomere-interacting protein



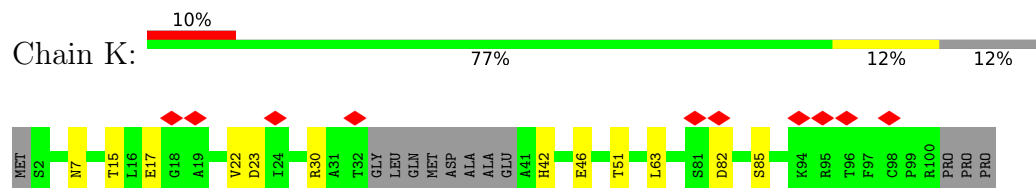
- Molecule 4: Small capsomere-interacting protein



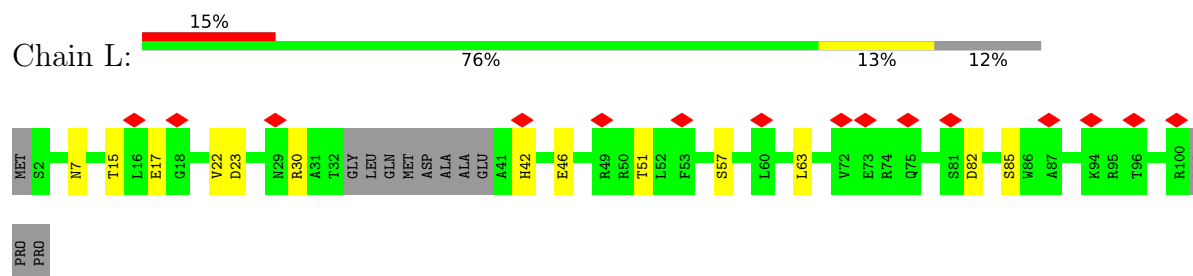
- Molecule 4: Small capsomere-interacting protein



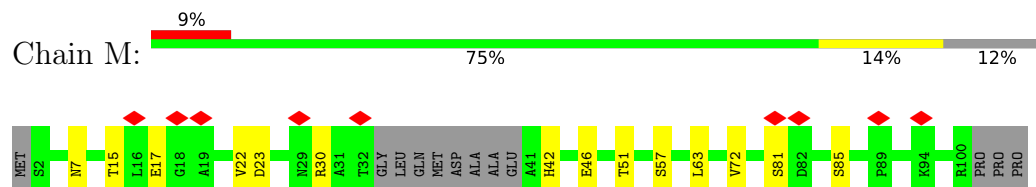
- Molecule 4: Small capsomere-interacting protein



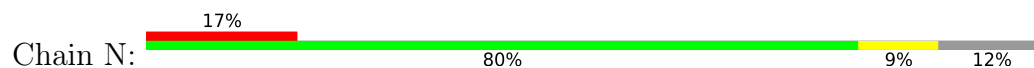
- Molecule 4: Small capsomere-interacting protein

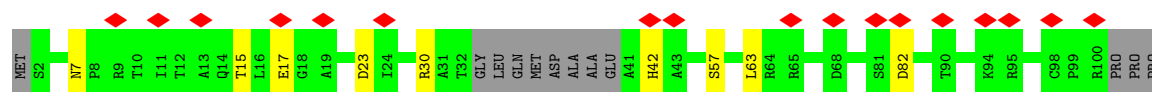


- Molecule 4: Small capsomere-interacting protein

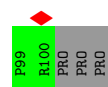
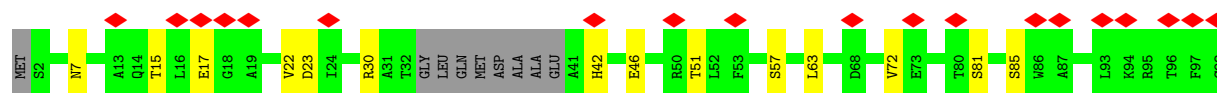
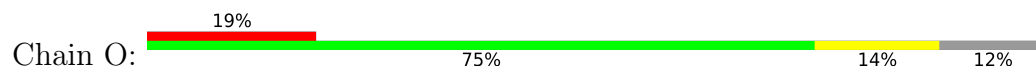


- Molecule 4: Small capsomere-interacting protein

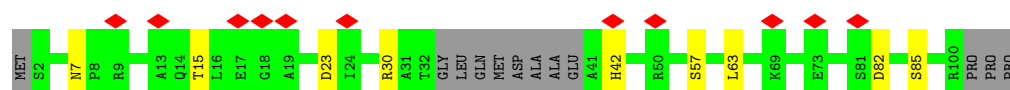
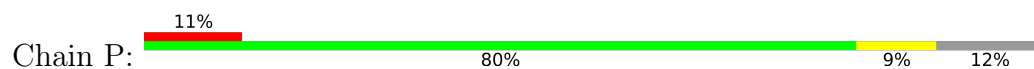




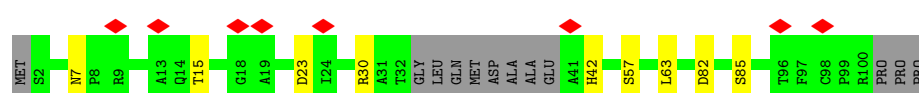
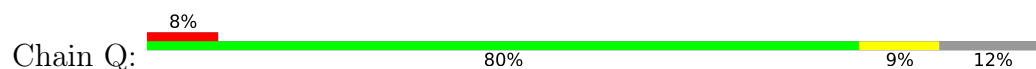
- Molecule 4: Small capsomere-interacting protein



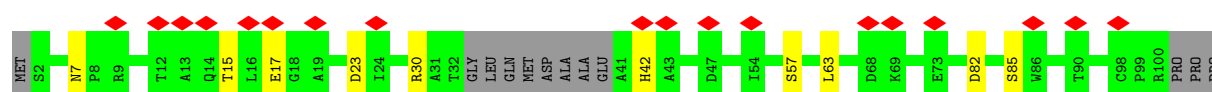
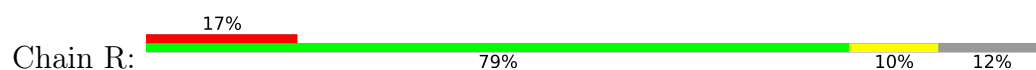
- Molecule 4: Small capsomere-interacting protein



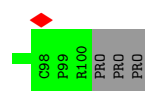
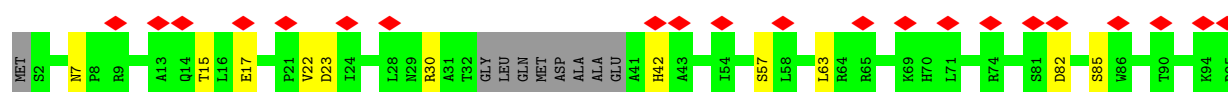
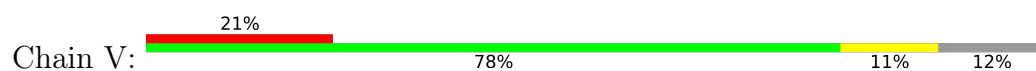
- Molecule 4: Small capsomere-interacting protein




- Molecule 4: Small capsomere-interacting protein

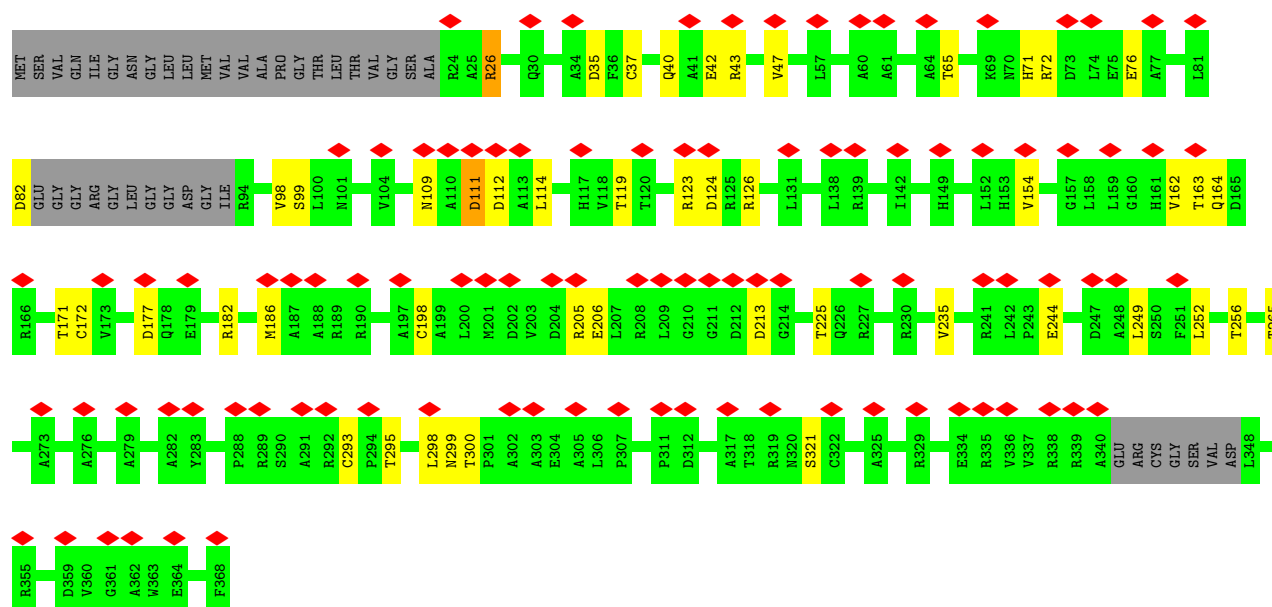


- Molecule 4: Small capsomere-interacting protein




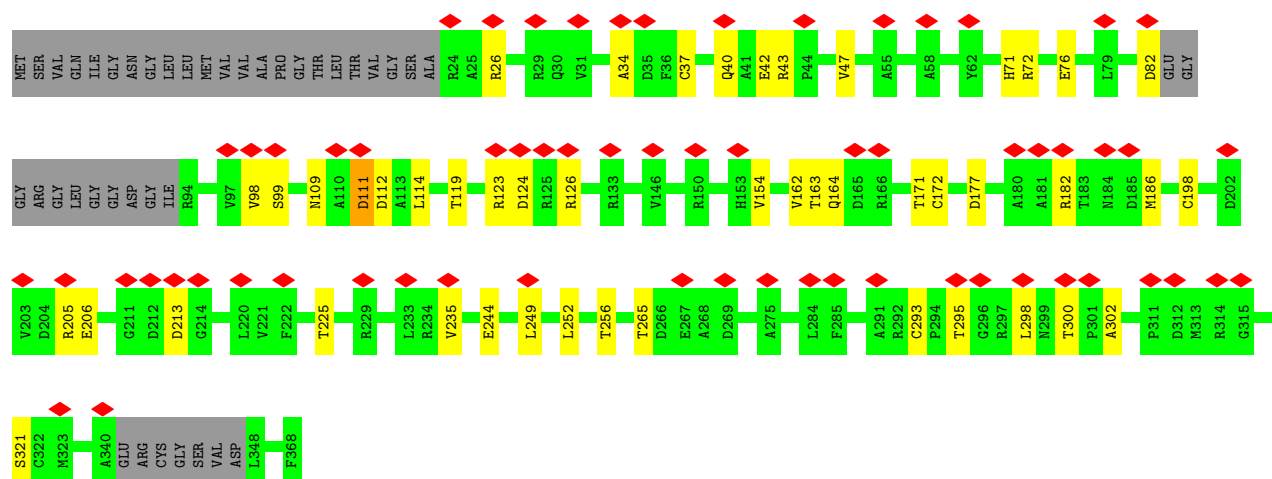
- Molecule 5: Triplex capsid protein 1

Chain T: 




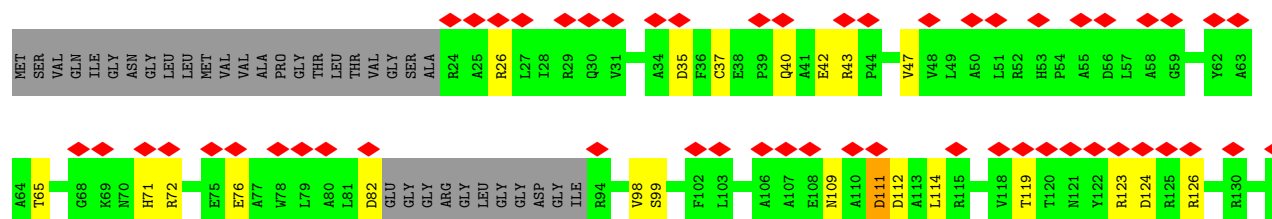
• Molecule 5: Triplex capsid protein 1

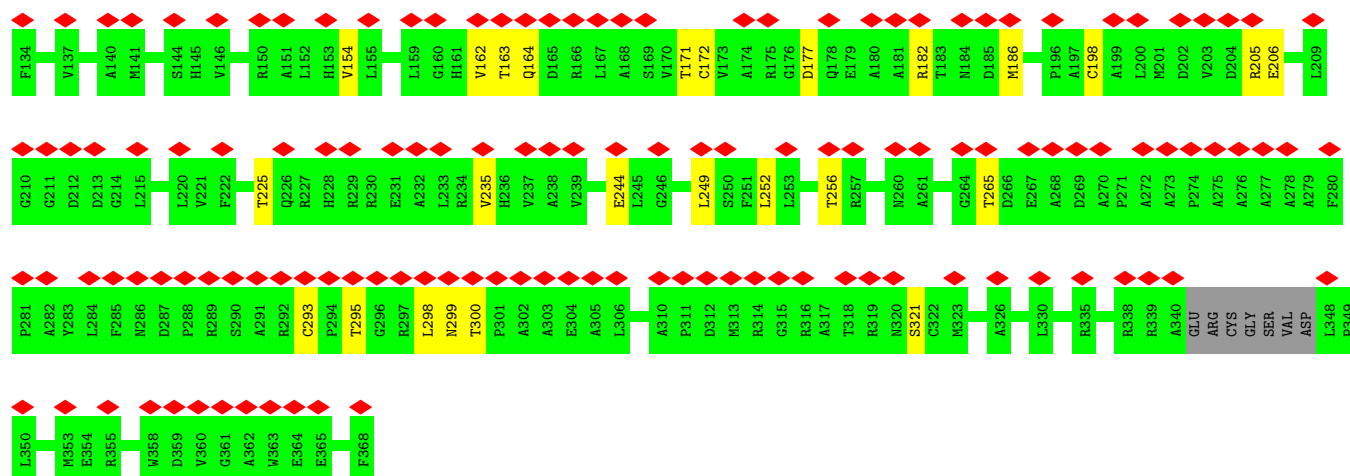
Chain h: 



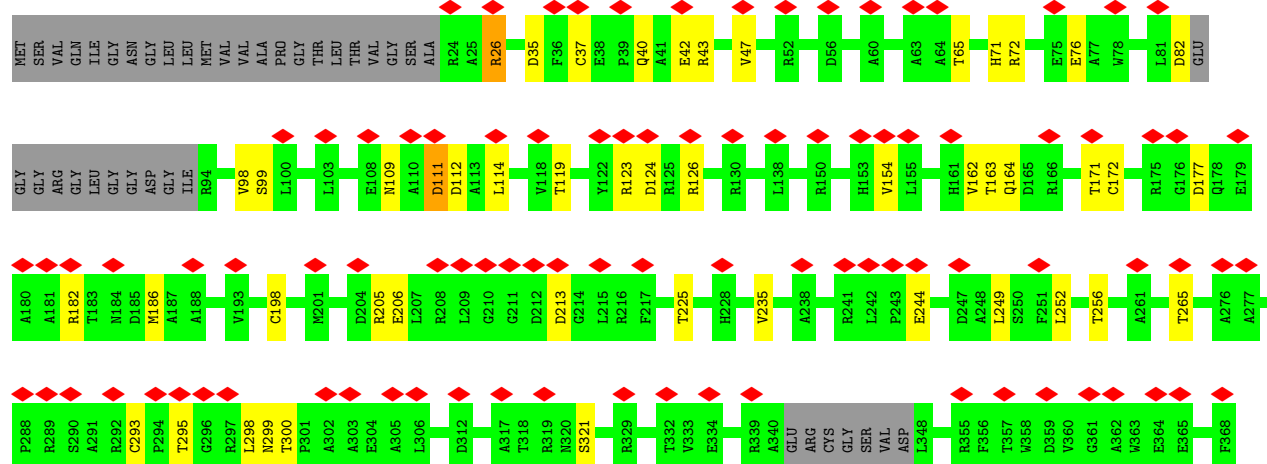
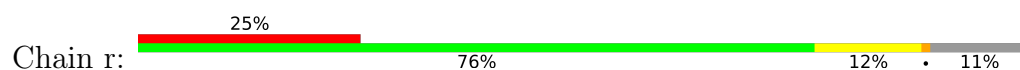
• Molecule 5: Triplex capsid protein 1

Chain i: 

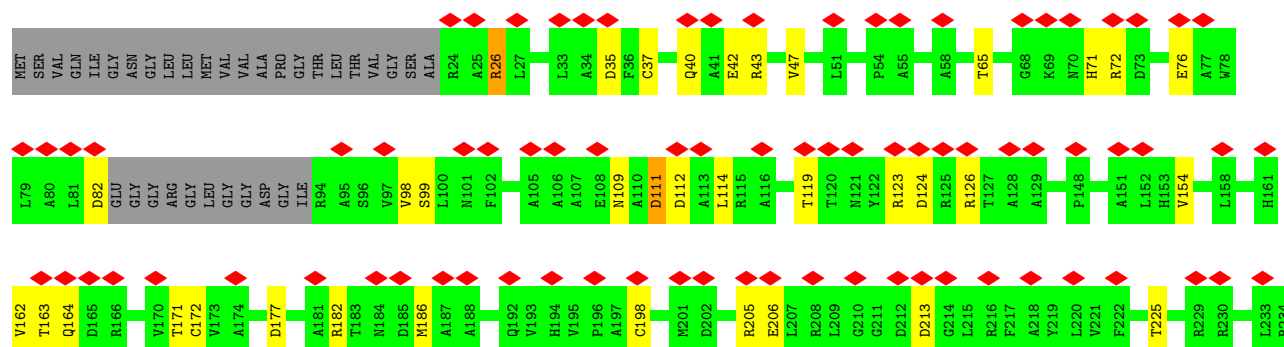
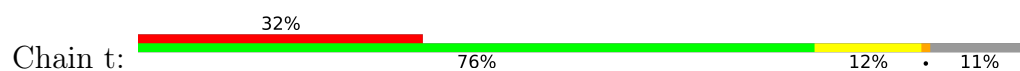


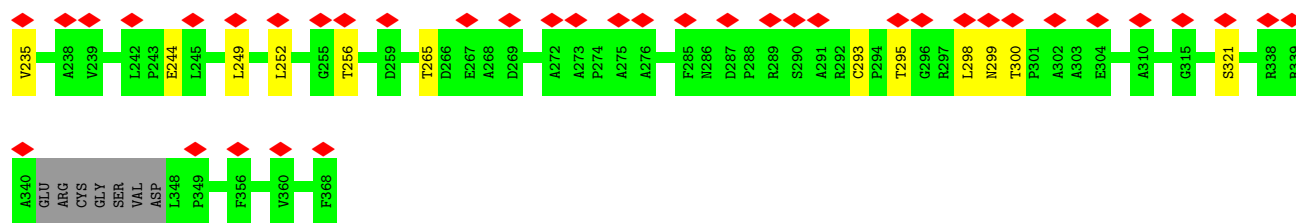


• Molecule 5: Triplex capsid protein 1

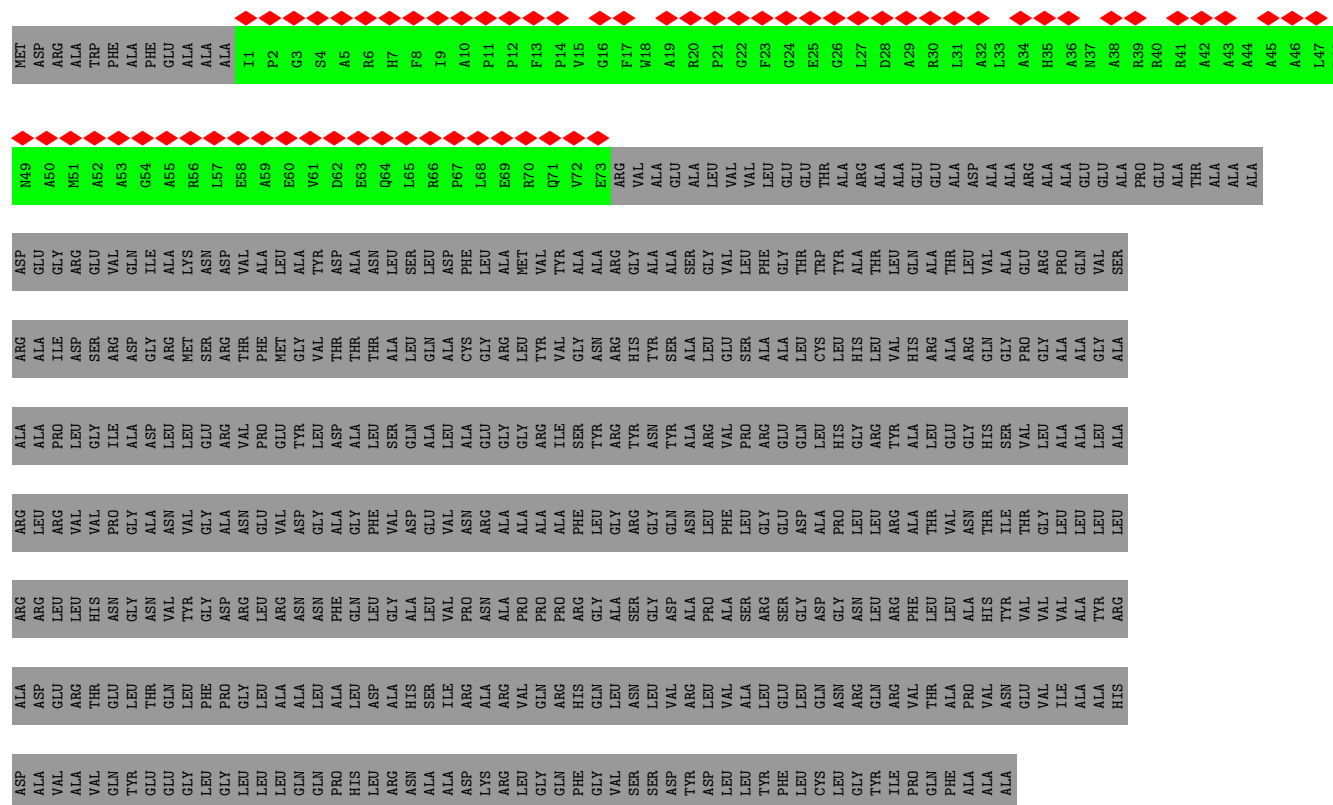


• Molecule 5: Triplex capsid protein 1

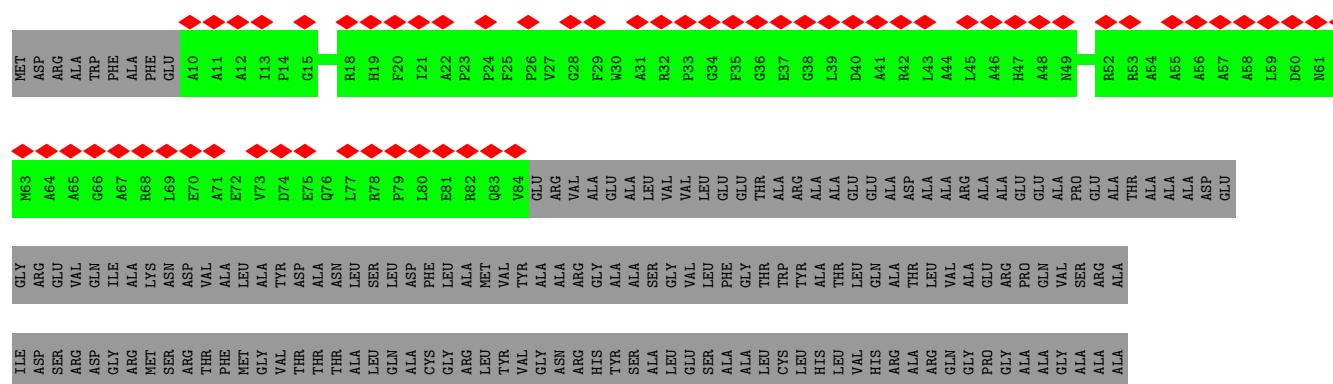




• Molecule 6: DNA packaging tegument protein UL25

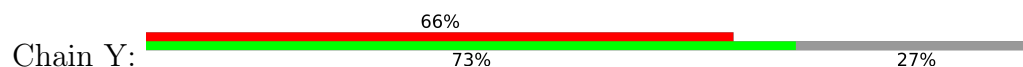


• Molecule 6: DNA packaging tegument protein UL25





- Molecule 7: VP1/2



L3137 GLY	◆	ARG	◆
		VAL	◆
		VAL	◆
		GLU	◆
		SER	◆
		ASP	◆
		THR	◆
		LEU	◆
		ILE	◆
		ASN	◆
		ARG	◆
		ARG	◆
		TYR	◆
		MET	◆
		ARG	◆
		ALA	◆
		T3093	◆
		G3094	◆
		L3095	◆
		G3096	◆
		A3097	◆
		L3098	◆
		A3099	◆
		L3100	◆
		L3101	◆
		T3102	◆
		A3103	◆
		A3104	◆
		C3105	◆
		R3106	◆
		L3107	◆
		T3108	◆
		A3109	◆
		R3110	◆
		R3111	◆
		L3112	◆
		R3113	◆
		E3114	◆
		T3115	◆
		R3116	◆
		T3117	◆
		T3118	◆
		L3119	◆
		K3120	◆
		G3121	◆
		S3122	◆
		A3123	◆
		R3124	◆
		R3125	◆
		F3126	◆
		N3127	◆
		V3128	◆
		D3129	◆
		L3130	◆
		F3131	◆
		Q3132	◆
		V3133	◆
		R3134	◆
		L3135	◆
		T3136	◆

- Molecule 7: VP1/2



L3137	GLY	ARG	VAL	VAL	GLU	SER	ASP	THR	LEU	ILE	ASN	ARG	ARG	TYR	MET	ARG	ALA	THR	THR	GLY	LEU	GLY	ALA	LEU	ALA	LEU	LEU	ILE	A3103	A3104	C3105	R3106	L3107	T3108	A3109	R3110	R3111	L3112	R3113	F3114	T3115	R3116	T3117	T3118	L3119	K3120	G3121	S3122	A3123	R3124	R3125	F3126	K3127	V3128	D3129	L3130	F3131	Q3132	V3133	R3134	L3135	T3136
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## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	14252	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TECNAI F30	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	25	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	9.391	Depositor
Minimum map value	-6.027	Depositor
Average map value	0.006	Depositor
Map value standard deviation	0.915	Depositor
Recommended contour level	2	Depositor
Map size ( $\text{\AA}$ )	1429.76, 1429.76, 1429.76	wwPDB
Map dimensions	1280, 1280, 1280	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.117, 1.117, 1.117	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	0	0.26	0/10384	0.48	2/14158 (0.0%)
1	A	0.26	0/10366	0.48	1/14132 (0.0%)
1	S	0.26	0/10229	0.48	0/13950
1	U	0.27	0/10384	0.47	1/14158 (0.0%)
1	a	0.26	0/10225	0.46	0/13938
1	e	0.28	0/8938	0.46	0/12175
1	f	0.26	0/10384	0.47	1/14158 (0.0%)
1	g	0.26	0/10379	0.46	2/14150 (0.0%)
1	l	0.26	0/10384	0.47	0/14158
1	m	0.27	0/10384	0.47	1/14158 (0.0%)
1	n	0.28	1/10384 (0.0%)	0.48	3/14158 (0.0%)
1	p	0.26	0/10384	0.47	1/14158 (0.0%)
1	q	0.26	0/10384	0.47	1/14158 (0.0%)
1	u	0.26	0/10384	0.46	1/14158 (0.0%)
1	w	0.26	0/10384	0.47	1/14158 (0.0%)
1	y	0.26	0/10384	0.47	0/14158
2	1	0.31	0/2127	0.50	0/2903
2	2	0.37	1/2127 (0.0%)	0.54	2/2903 (0.1%)
2	3	0.30	0/2127	0.50	0/2903
2	j	0.31	0/2043	0.54	1/2783 (0.0%)
2	k	0.28	0/2127	0.49	0/2903
2	o	0.32	0/2272	0.50	0/3099
2	s	0.33	0/2127	0.49	0/2903
2	v	0.31	0/2230	0.48	0/3041
2	x	0.30	0/2272	0.52	0/3099
2	z	0.29	0/2253	0.50	0/3074
3	B	0.35	0/4120	0.49	0/5609
4	E	0.28	0/736	0.55	0/999
4	F	0.28	0/736	0.58	0/999
4	G	0.29	0/736	0.58	0/999
4	H	0.29	0/736	0.62	0/999
4	I	0.29	0/736	0.63	0/999
4	J	0.29	0/736	0.55	0/999
4	K	0.28	0/736	0.56	0/999

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
4	L	0.28	0/736	0.59	0/999
4	M	0.28	0/736	0.50	0/999
4	N	0.31	0/736	0.64	1/999 (0.1%)
4	O	0.28	0/736	0.51	0/999
4	P	0.29	0/736	0.64	0/999
4	Q	0.29	0/736	0.64	0/999
4	R	0.29	0/736	0.63	0/999
4	V	0.28	0/736	0.58	0/999
5	T	0.33	0/2591	0.63	2/3521 (0.1%)
5	h	0.33	0/2591	0.65	3/3521 (0.1%)
5	i	0.33	0/2591	0.62	2/3521 (0.1%)
5	r	0.33	0/2591	0.62	2/3521 (0.1%)
5	t	0.33	0/2591	0.62	2/3521 (0.1%)
6	X	0.31	0/565	0.43	0/766
6	c	0.29	0/571	0.41	0/775
7	Y	0.28	0/354	0.48	0/474
7	Z	0.26	0/289	0.47	0/385
All	All	0.28	2/215960 (0.0%)	0.49	30/294293 (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	0	0	1
1	U	0	1
1	e	0	1
1	n	0	2
1	w	0	1
2	v	0	1
3	B	0	1
All	All	0	8

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	n	1130	PRO	N-CD	-11.74	1.31	1.47
2	2	272	PRO	N-CD	10.50	1.62	1.47

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	n	1130	PRO	CA-N-CD	7.38	122.04	111.70
5	T	111	ASP	CB-CG-OD1	-7.36	111.68	118.30
5	i	111	ASP	CB-CG-OD1	-7.31	111.72	118.30
5	h	111	ASP	CB-CG-OD1	-7.27	111.76	118.30
5	t	111	ASP	CB-CG-OD1	-7.26	111.77	118.30

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	762	ARG	Peptide
3	B	545	LEU	Peptide
1	U	762	ARG	Peptide
1	e	298	ILE	Peptide
1	n	476	ALA	Peptide

## 5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all 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	0	1307/1330 (98%)	1200 (92%)	107 (8%)	0	100	100
1	A	1302/1330 (98%)	1193 (92%)	106 (8%)	3 (0%)	44	78
1	S	1285/1330 (97%)	1174 (91%)	108 (8%)	3 (0%)	44	78
1	U	1307/1330 (98%)	1184 (91%)	122 (9%)	1 (0%)	48	83
1	a	1281/1330 (96%)	1143 (89%)	138 (11%)	0	100	100
1	e	1102/1330 (83%)	993 (90%)	109 (10%)	0	100	100
1	f	1307/1330 (98%)	1182 (90%)	123 (9%)	2 (0%)	44	78

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	g	1304/1330 (98%)	1174 (90%)	130 (10%)	0	100	100
1	l	1307/1330 (98%)	1200 (92%)	106 (8%)	1 (0%)	48	83
1	m	1307/1330 (98%)	1197 (92%)	110 (8%)	0	100	100
1	n	1307/1330 (98%)	1201 (92%)	103 (8%)	3 (0%)	44	78
1	p	1307/1330 (98%)	1199 (92%)	107 (8%)	1 (0%)	48	83
1	q	1307/1330 (98%)	1214 (93%)	92 (7%)	1 (0%)	48	83
1	u	1307/1330 (98%)	1186 (91%)	120 (9%)	1 (0%)	48	83
1	w	1307/1330 (98%)	1189 (91%)	118 (9%)	0	100	100
1	y	1307/1330 (98%)	1190 (91%)	112 (9%)	5 (0%)	30	68
2	1	273/296 (92%)	252 (92%)	21 (8%)	0	100	100
2	2	273/296 (92%)	251 (92%)	22 (8%)	0	100	100
2	3	273/296 (92%)	250 (92%)	23 (8%)	0	100	100
2	j	261/296 (88%)	236 (90%)	25 (10%)	0	100	100
2	k	273/296 (92%)	252 (92%)	21 (8%)	0	100	100
2	o	294/296 (99%)	264 (90%)	30 (10%)	0	100	100
2	s	273/296 (92%)	248 (91%)	25 (9%)	0	100	100
2	v	285/296 (96%)	256 (90%)	29 (10%)	0	100	100
2	x	294/296 (99%)	257 (87%)	37 (13%)	0	100	100
2	z	292/296 (99%)	260 (89%)	32 (11%)	0	100	100
3	B	520/597 (87%)	459 (88%)	60 (12%)	1 (0%)	44	78
4	E	87/103 (84%)	81 (93%)	6 (7%)	0	100	100
4	F	87/103 (84%)	81 (93%)	6 (7%)	0	100	100
4	G	87/103 (84%)	81 (93%)	6 (7%)	0	100	100
4	H	87/103 (84%)	81 (93%)	6 (7%)	0	100	100
4	I	87/103 (84%)	81 (93%)	6 (7%)	0	100	100
4	J	87/103 (84%)	81 (93%)	6 (7%)	0	100	100
4	K	87/103 (84%)	81 (93%)	6 (7%)	0	100	100
4	L	87/103 (84%)	80 (92%)	7 (8%)	0	100	100
4	M	87/103 (84%)	81 (93%)	6 (7%)	0	100	100
4	N	87/103 (84%)	80 (92%)	7 (8%)	0	100	100
4	O	87/103 (84%)	80 (92%)	7 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	P	87/103 (84%)	80 (92%)	7 (8%)	0	100	100
4	Q	87/103 (84%)	80 (92%)	7 (8%)	0	100	100
4	R	87/103 (84%)	81 (93%)	6 (7%)	0	100	100
4	V	87/103 (84%)	81 (93%)	6 (7%)	0	100	100
5	T	321/368 (87%)	292 (91%)	29 (9%)	0	100	100
5	h	321/368 (87%)	294 (92%)	26 (8%)	1 (0%)	37	72
5	i	321/368 (87%)	292 (91%)	29 (9%)	0	100	100
5	r	321/368 (87%)	292 (91%)	29 (9%)	0	100	100
5	t	321/368 (87%)	292 (91%)	29 (9%)	0	100	100
6	X	71/534 (13%)	67 (94%)	4 (6%)	0	100	100
6	c	73/534 (14%)	67 (92%)	6 (8%)	0	100	100
7	Y	43/62 (69%)	42 (98%)	1 (2%)	0	100	100
7	Z	33/62 (53%)	32 (97%)	1 (3%)	0	100	100
All	All	27092/29414 (92%)	24684 (91%)	2385 (9%)	23 (0%)	50	83

5 of 23 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	h	302	ALA
1	U	986	GLU
1	n	1127	ALA
1	p	986	GLU
1	y	986	GLU

### 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	0	1057/1072 (99%)	1056 (100%)	1 (0%)	92	95
1	A	1056/1072 (98%)	1056 (100%)	0	100	100
1	S	1042/1072 (97%)	1042 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	U	1057/1072 (99%)	1057 (100%)	0	100	100
1	a	1040/1072 (97%)	1040 (100%)	0	100	100
1	e	909/1072 (85%)	909 (100%)	0	100	100
1	f	1057/1072 (99%)	1056 (100%)	1 (0%)	92	95
1	g	1057/1072 (99%)	1056 (100%)	1 (0%)	92	95
1	l	1057/1072 (99%)	1057 (100%)	0	100	100
1	m	1057/1072 (99%)	1056 (100%)	1 (0%)	92	95
1	n	1057/1072 (99%)	1057 (100%)	0	100	100
1	p	1057/1072 (99%)	1057 (100%)	0	100	100
1	q	1057/1072 (99%)	1056 (100%)	1 (0%)	92	95
1	u	1057/1072 (99%)	1057 (100%)	0	100	100
1	w	1057/1072 (99%)	1057 (100%)	0	100	100
1	y	1057/1072 (99%)	1055 (100%)	2 (0%)	92	93
2	1	223/235 (95%)	223 (100%)	0	100	100
2	2	223/235 (95%)	223 (100%)	0	100	100
2	3	223/235 (95%)	223 (100%)	0	100	100
2	j	213/235 (91%)	212 (100%)	1 (0%)	86	89
2	k	223/235 (95%)	223 (100%)	0	100	100
2	o	235/235 (100%)	235 (100%)	0	100	100
2	s	223/235 (95%)	223 (100%)	0	100	100
2	v	233/235 (99%)	232 (100%)	1 (0%)	89	90
2	x	235/235 (100%)	234 (100%)	1 (0%)	89	90
2	z	232/235 (99%)	232 (100%)	0	100	100
3	B	396/440 (90%)	393 (99%)	3 (1%)	79	84
4	E	78/87 (90%)	67 (86%)	11 (14%)	3	14
4	F	78/87 (90%)	67 (86%)	11 (14%)	3	14
4	G	78/87 (90%)	67 (86%)	11 (14%)	3	14
4	H	78/87 (90%)	67 (86%)	11 (14%)	3	14
4	I	78/87 (90%)	67 (86%)	11 (14%)	3	14
4	J	78/87 (90%)	65 (83%)	13 (17%)	2	10
4	K	78/87 (90%)	66 (85%)	12 (15%)	2	12

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	L	78/87 (90%)	65 (83%)	13 (17%)	2	10
4	M	78/87 (90%)	64 (82%)	14 (18%)	1	9
4	N	78/87 (90%)	70 (90%)	8 (10%)	6	21
4	O	78/87 (90%)	64 (82%)	14 (18%)	1	9
4	P	78/87 (90%)	69 (88%)	9 (12%)	4	18
4	Q	78/87 (90%)	69 (88%)	9 (12%)	4	18
4	R	78/87 (90%)	68 (87%)	10 (13%)	3	15
4	V	78/87 (90%)	67 (86%)	11 (14%)	3	14
5	T	251/279 (90%)	203 (81%)	48 (19%)	1	7
5	h	251/279 (90%)	207 (82%)	44 (18%)	1	9
5	i	251/279 (90%)	205 (82%)	46 (18%)	1	8
5	r	251/279 (90%)	203 (81%)	48 (19%)	1	7
5	t	251/279 (90%)	203 (81%)	48 (19%)	1	7
6	X	49/387 (13%)	49 (100%)	0	100	100
6	c	48/387 (12%)	48 (100%)	0	100	100
7	Y	36/51 (71%)	36 (100%)	0	100	100
7	Z	30/51 (59%)	30 (100%)	0	100	100
All	All	21978/23518 (94%)	21563 (98%)	415 (2%)	52	69

5 of 415 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	h	98	VAL
5	i	126	ARG
5	t	235	VAL
5	h	123	ARG
5	h	265	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 451 such sidechains are listed below:

Mol	Chain	Res	Type
2	j	97	ASN
1	y	1121	ASN
1	n	106	HIS
1	y	869	ASN

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Mol	Chain	Res	Type
1	w	397	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

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

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.

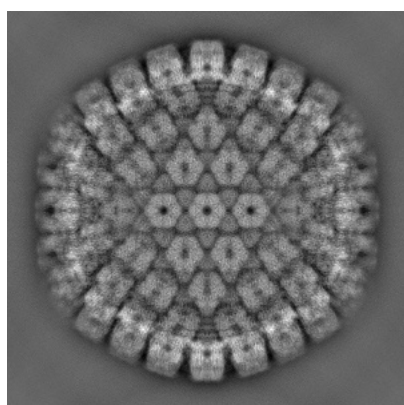
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31611. These allow visual inspection of the internal detail of the map and identification of artifacts.

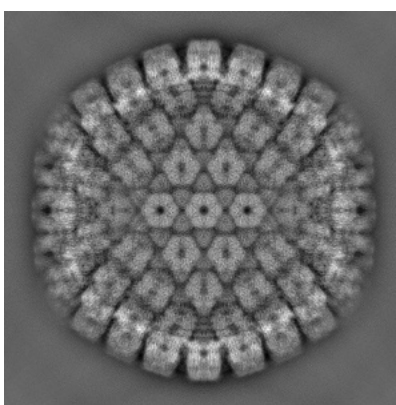
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

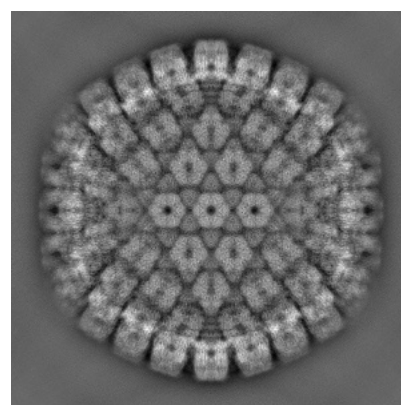
#### 6.1.1 Primary map



X



Y

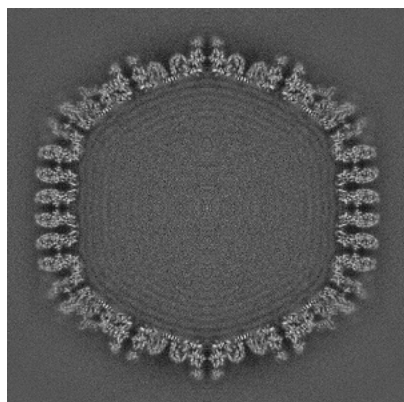


Z

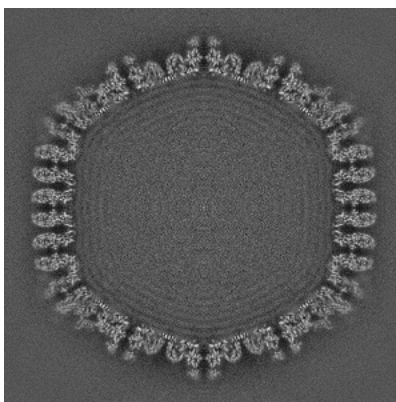
The images above show the map projected in three orthogonal directions.

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

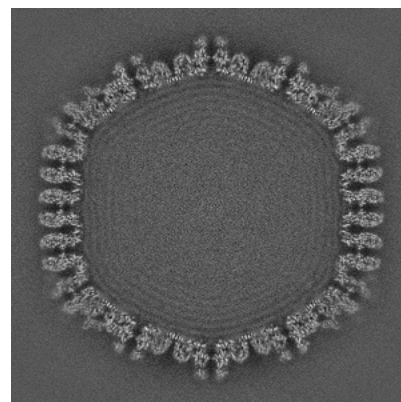
#### 6.2.1 Primary map



X Index: 640



Y Index: 640

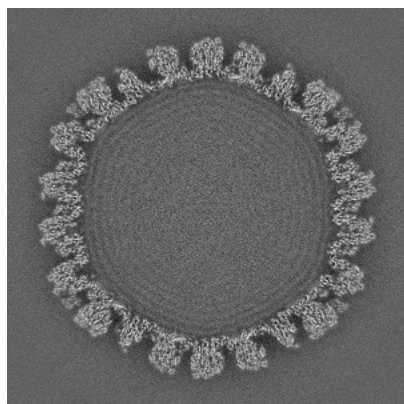


Z Index: 640

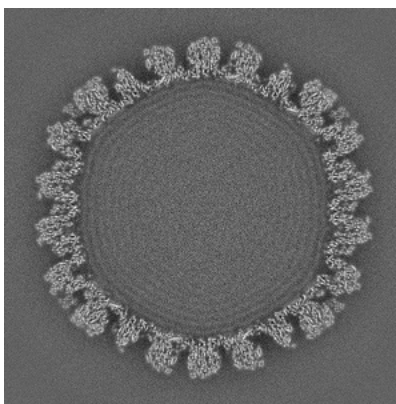
The images above show central slices of the map in three orthogonal directions.

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

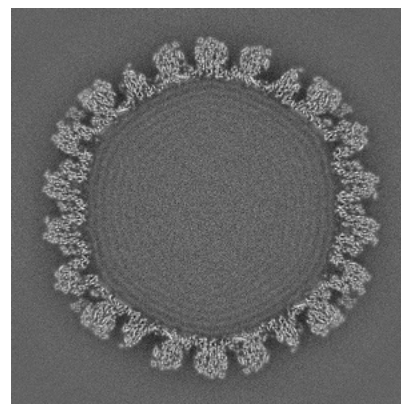
### 6.3.1 Primary map



X Index: 750



Y Index: 750

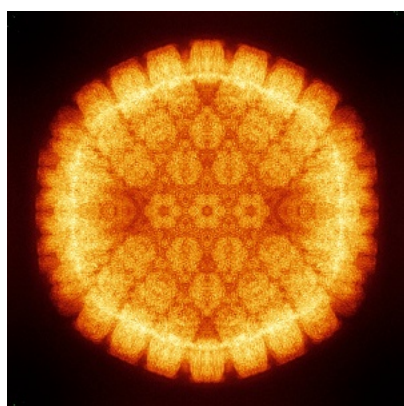


Z Index: 529

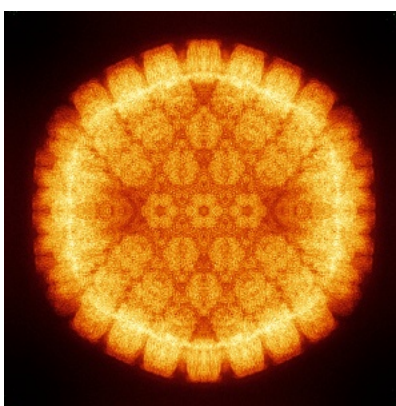
The images above show the largest variance slices of the map in three orthogonal directions.

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

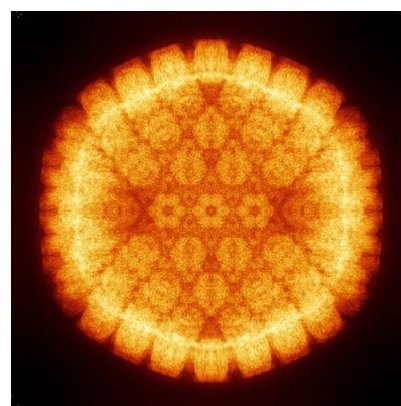
### 6.4.1 Primary map



X



Y

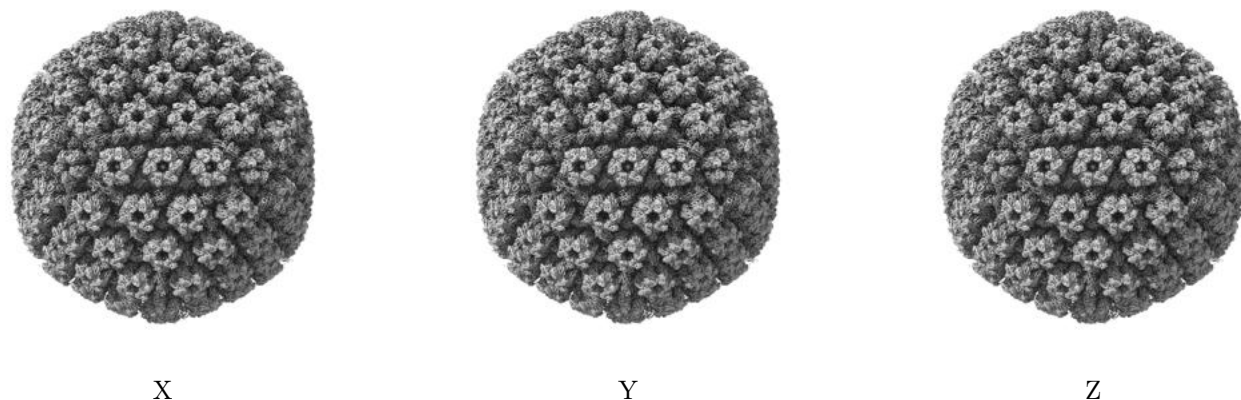


Z

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 2.0. 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](#)

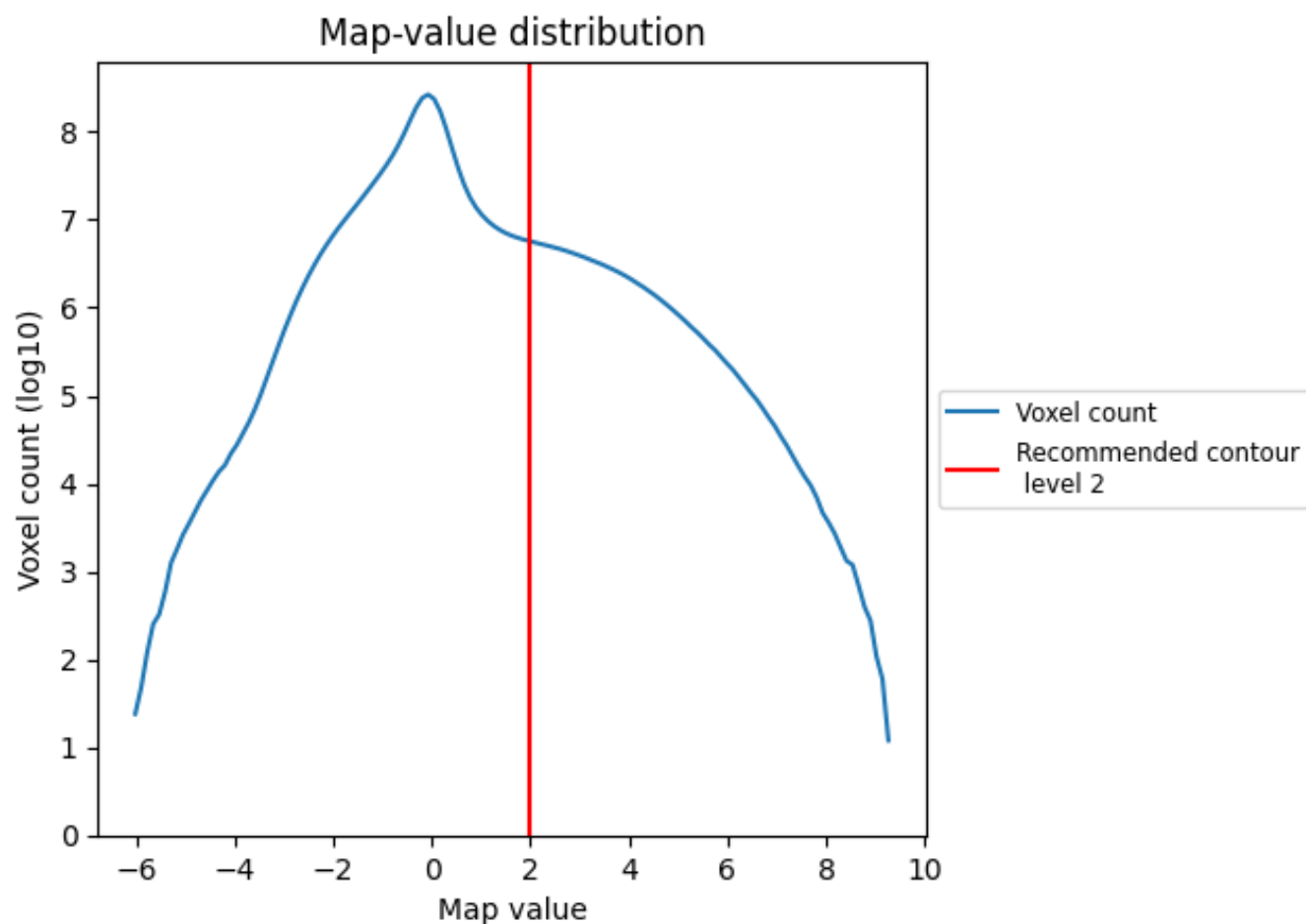
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis [i](#)

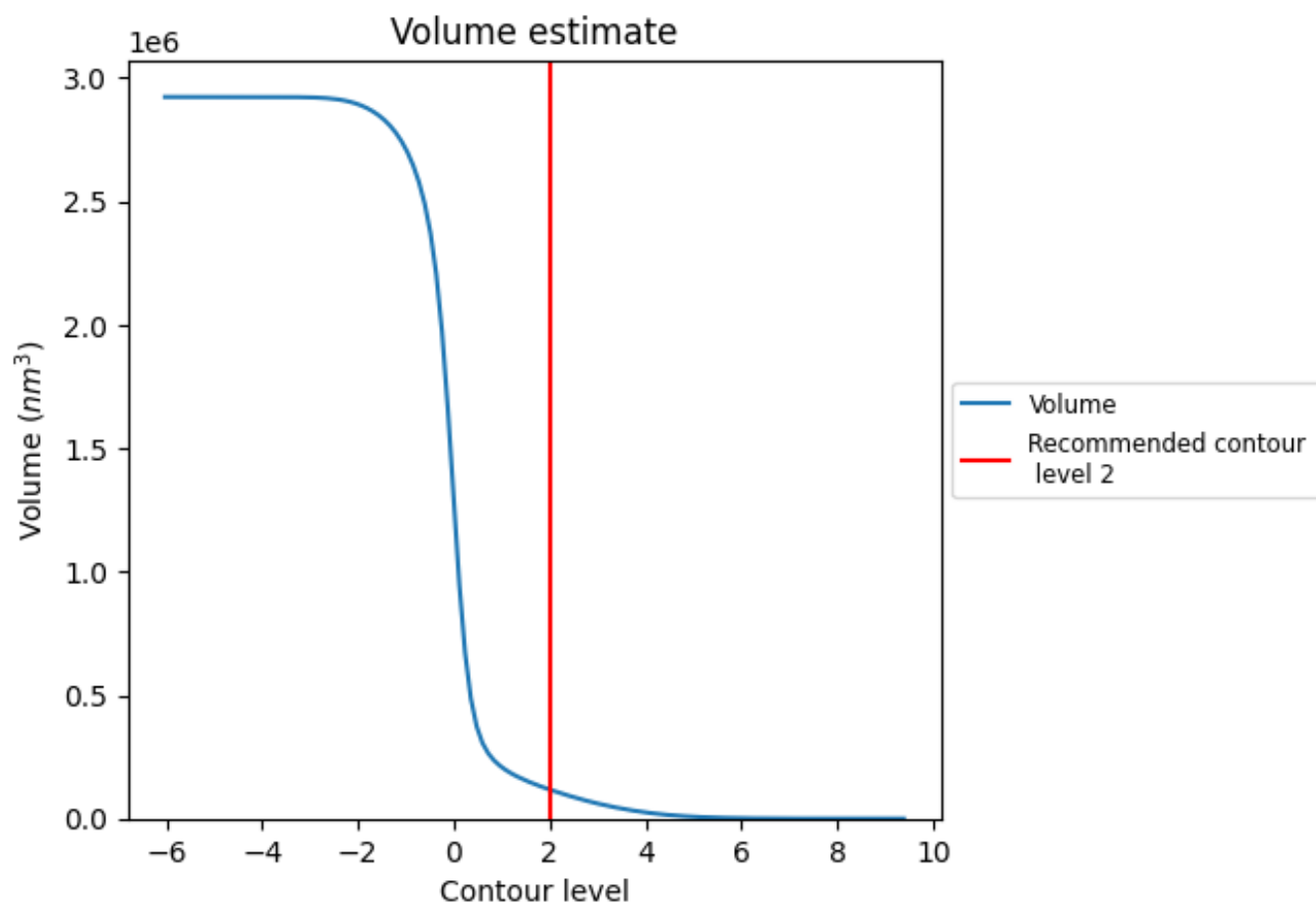
This section contains the results of statistical analysis of the map.

### 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.

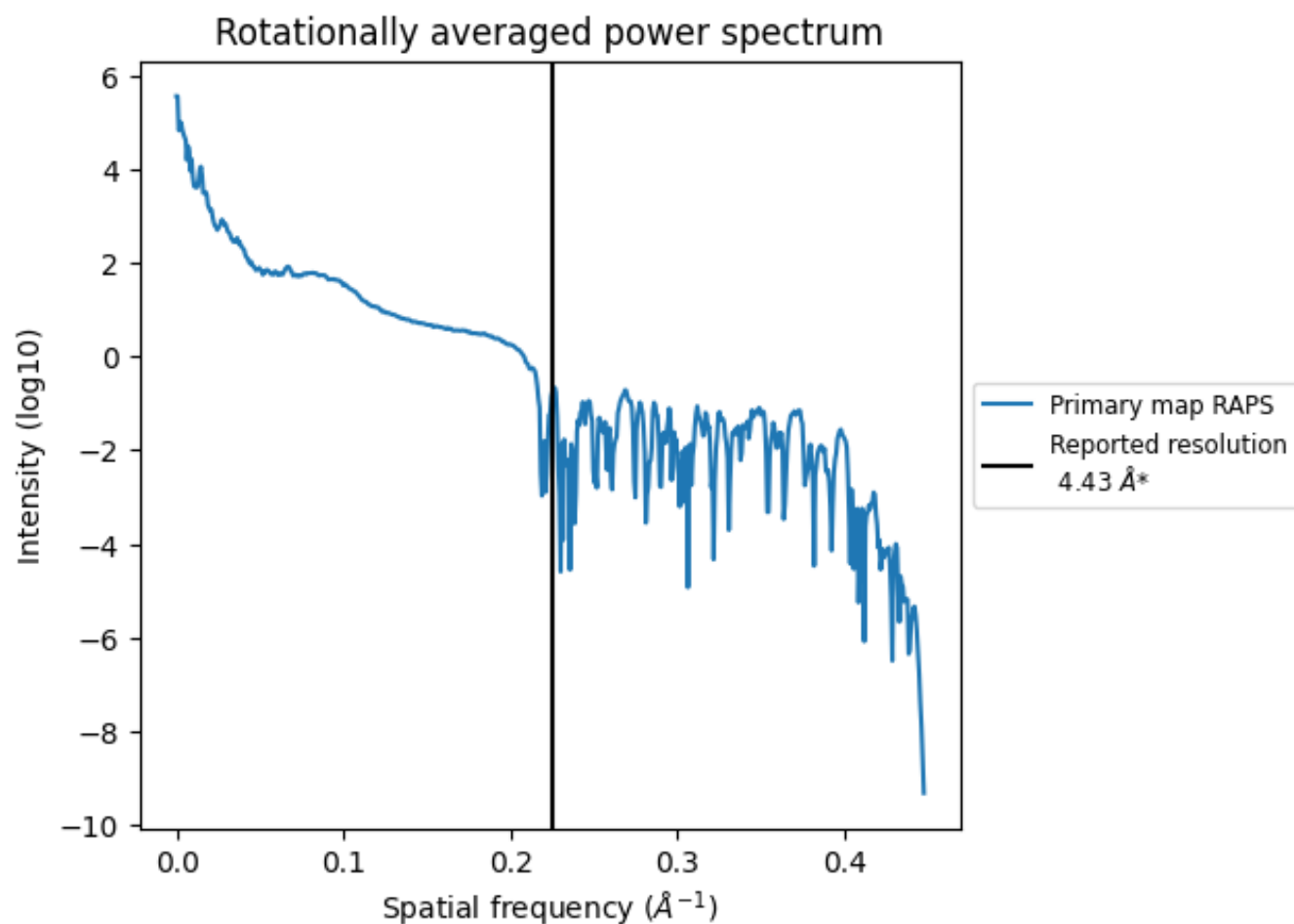
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 117685 nm<sup>3</sup>; this corresponds to an approximate mass of 106308 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 0.226 Å<sup>-1</sup>



## 8 Fourier-Shell correlation

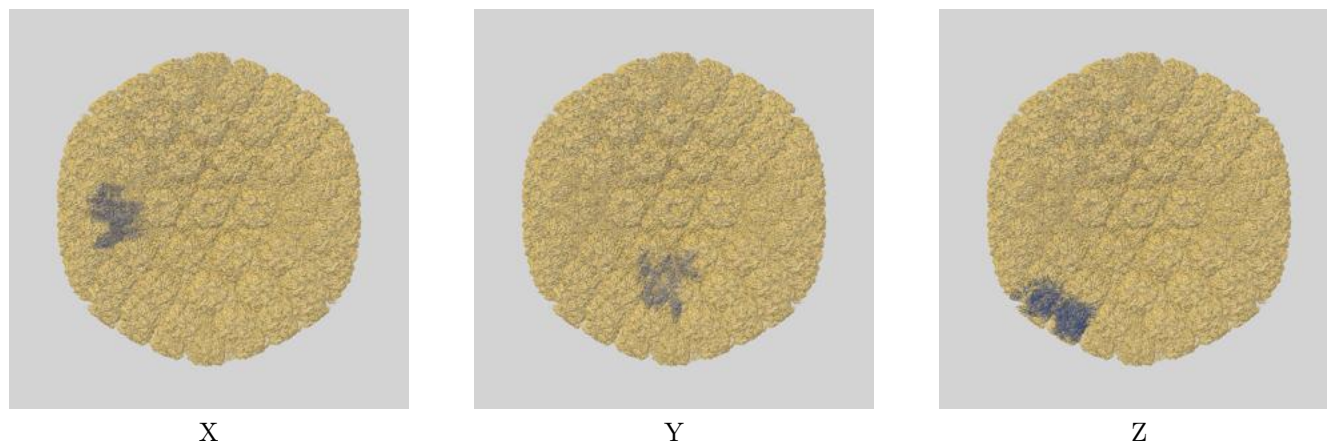
This section was not generated. No FSC curve or half-maps provided.

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

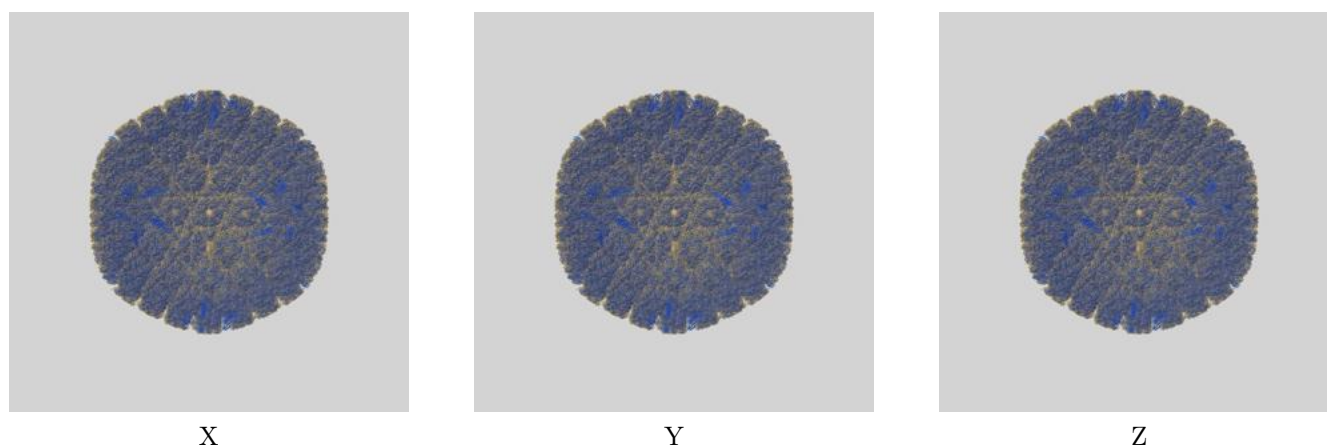
This section contains information regarding the fit between EMDB map EMD-31611 and PDB model 7FJ1. Per-residue inclusion information can be found in section 3 on page 9.

### 9.1 Map-model overlays

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

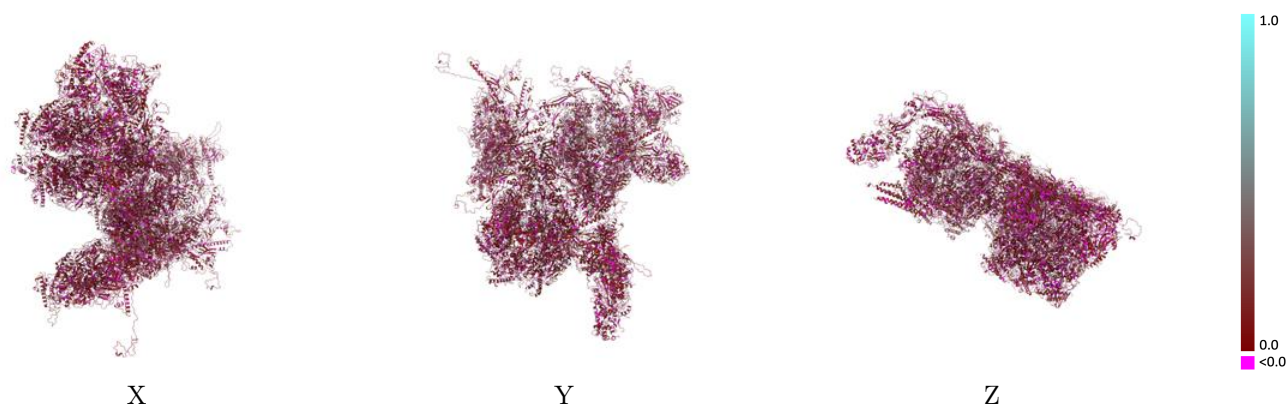


#### 9.1.2 Map-model assembly overlay [i](#)



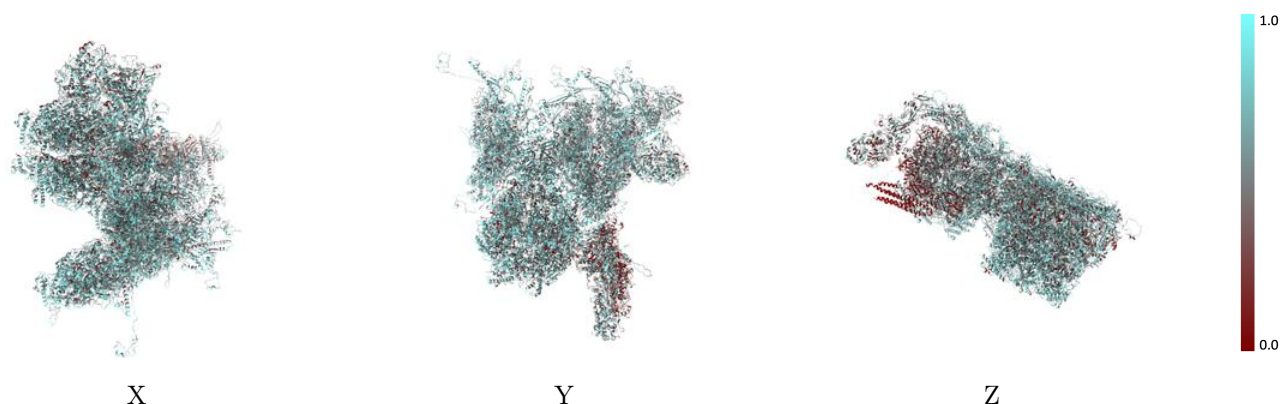
The images above show the 3D surface view of the map at the recommended contour level 2.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



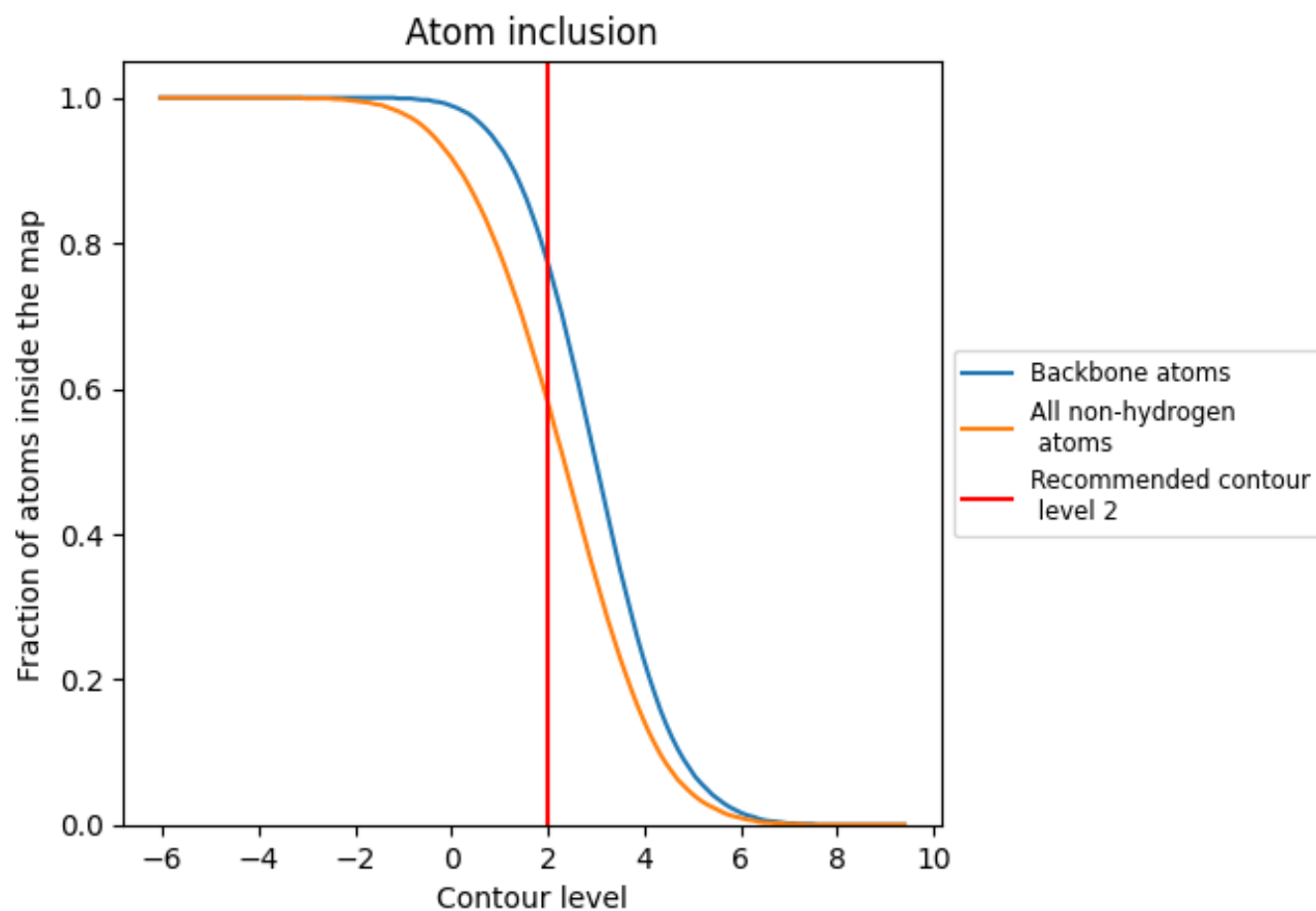
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (2).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 77% of all backbone atoms, 58% 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 (2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5810	 0.1420
0	 0.6010	 0.1380
1	 0.5760	 0.1580
2	 0.5600	 0.1460
3	 0.5650	 0.1330
A	 0.6230	 0.1420
B	 0.1850	 0.1400
E	 0.6680	 0.1500
F	 0.6750	 0.1480
G	 0.6800	 0.1350
H	 0.6800	 0.1420
I	 0.6060	 0.1580
J	 0.6690	 0.1530
K	 0.6950	 0.1700
L	 0.6630	 0.1610
M	 0.7030	 0.1710
N	 0.6760	 0.1590
O	 0.6150	 0.1490
P	 0.6760	 0.1820
Q	 0.7220	 0.1670
R	 0.6620	 0.1600
S	 0.5820	 0.1450
T	 0.5940	 0.1400
U	 0.6080	 0.1450
V	 0.6400	 0.1450
X	 0.1330	 0.1370
Y	 0.1220	 0.1220
Z	 0.0550	 0.0980
a	 0.5870	 0.1370
c	 0.2060	 0.1530
e	 0.4760	 0.1350
f	 0.6240	 0.1460
g	 0.6070	 0.1440
h	 0.6340	 0.1690
i	 0.3910	 0.1260



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Chain	Atom inclusion	Q-score
j	 0.3620	 0.1500
k	 0.3820	 0.1550
l	 0.6030	 0.1430
m	 0.6150	 0.1380
n	 0.6030	 0.1360
o	 0.5490	 0.1580
p	 0.6080	 0.1440
q	 0.6000	 0.1400
r	 0.5780	 0.1310
s	 0.5790	 0.1550
t	 0.5590	 0.1180
u	 0.6260	 0.1480
v	 0.5680	 0.1420
w	 0.5980	 0.1420
x	 0.5280	 0.1360
y	 0.6200	 0.1400
z	 0.5370	 0.1330