



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 01:47 PM UTC

PDB ID : 8RBS / pdb_00008rbs
EMDB ID : EMD-19035
Title : Emiliania huxleyi virus 201 (EhV-201) asymmetrical unit of capsid proteins predicted by AlphaFold2 fitted into the cryo-EM density of EhV-201 virion composite map.
Authors : Homola, M.; Buttner, C.R.; Fuzik, T.; Novacek, J.; Chaillet, M.; Forster, F.; Plevka, P.
Deposited on : 2023-12-04
Resolution : 18.00 Å(reported)
Based on initial model : .

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

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

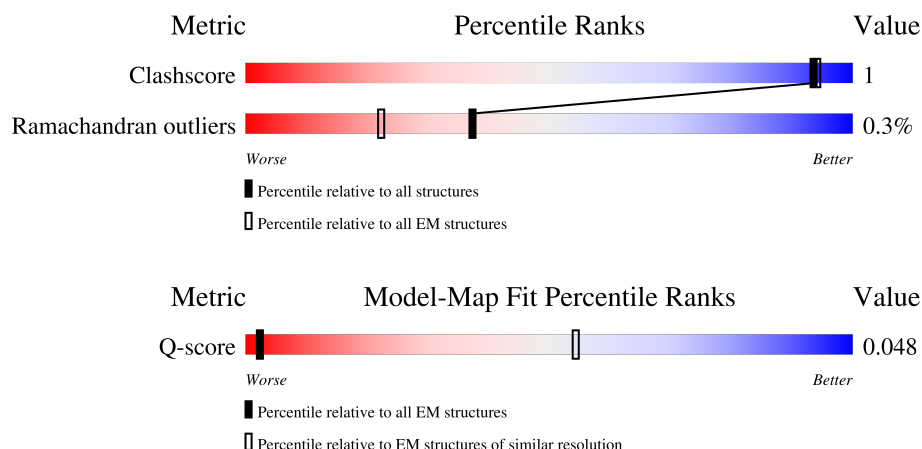
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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 18.00 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Q-score	-	25397	24 (17.50 - 18.30)

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 ≥ 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	A1	496	
1	A2	496	
1	A3	496	
1	A4	496	
1	A5	496	

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Mol	Chain	Length	Quality of chain
1	A6	496	25% 96% ..
1	A7	496	31% 96% ..
1	A8	496	23% 96% ..
1	A9	496	30% 96% ..
1	B1	496	32% 96% ..
1	B2	496	27% 96% ..
1	B3	496	31% 96% ..
1	B4	496	33% 96% ..
1	B5	496	26% 96% ..
1	B6	496	31% 96% ..
1	B7	496	34% 96% ..
1	B8	496	28% 96% ..
1	B9	496	31% 96% ..
1	C1	496	29% 96% ..
1	C2	496	35% 96% ..
1	C3	496	29% 96% ..
1	C4	496	31% 96% ..
1	C5	496	31% 96% ..
1	C6	496	31% 96% ..
1	C7	496	30% 96% ..
1	C8	496	29% 96% ..
1	C9	496	30% 96% ..
1	D1	496	33% 96% ..
1	D2	496	32% 96% ..
1	D3	496	32% 96% ..

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Mol	Chain	Length	Quality of chain
1	D4	496	30% 96% ..
1	D5	496	30% 96% ..
1	D6	496	32% 96% ..
1	D7	496	29% 96% ..
1	D8	496	30% 96% ..
1	D9	496	26% 96% ..
1	E1	496	28% 96% ..
1	E2	496	29% 96% ..
1	E3	496	30% 96% ..
1	E4	496	30% 96% ..
1	E5	496	33% 96% ..
1	E6	496	27% 96% ..
1	E7	496	31% 96% ..
1	E8	496	33% 96% ..
1	E9	496	28% 96% ..
1	F1	496	30% 96% ..
1	F2	496	30% 96% ..
1	F3	496	29% 96% ..
1	F4	496	32% 96% ..
1	F5	496	35% 96% ..
1	F6	496	29% 96% ..
1	F7	496	28% 96% ..
1	F8	496	30% 96% ..
1	F9	496	22% 96% ..
1	G1	496	29% 96% ..

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Mol	Chain	Length	Quality of chain
1	G2	496	34% 96% ..
1	G3	496	27% 96% ..
1	G4	496	24% 96% ..
1	G5	496	30% 96% ..
1	G6	496	24% 96% ..
1	G7	496	28% 96% ..
1	G8	496	30% 96% ..
1	G9	496	24% 96% ..
1	H1	496	25% 96% ..
1	H2	496	27% 96% ..
1	H3	496	22% 96% ..
1	H4	496	25% 96% ..
1	H5	496	26% 96% ..
1	H6	496	21% 96% ..
1	H7	496	23% 96% ..
1	H8	496	31% 96% ..
1	H9	496	23% 96% ..
1	I1	496	24% 96% ..
1	I2	496	28% 96% ..
1	I3	496	24% 96% ..
1	I4	496	26% 96% ..
1	I5	496	26% 96% ..
1	I6	496	25% 96% ..
1	I7	496	27% 96% ..
1	I8	496	27% 96% ..

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Mol	Chain	Length	Quality of chain
1	I9	496	26% 96% ..
1	J1	496	21% 96% ..
1	J2	496	23% 96% ..
1	J3	496	21% 96% ..
2	K	663	14% 100%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 164605 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	A1	482	Total 1928	C 964	N 482	O 482	0	0
1	A2	482	Total 1928	C 964	N 482	O 482	0	0
1	A3	482	Total 1928	C 964	N 482	O 482	0	0
1	A4	482	Total 1928	C 964	N 482	O 482	0	0
1	A5	482	Total 1928	C 964	N 482	O 482	0	0
1	A6	482	Total 1928	C 964	N 482	O 482	0	0
1	A7	482	Total 1928	C 964	N 482	O 482	0	0
1	A8	482	Total 1928	C 964	N 482	O 482	0	0
1	A9	482	Total 1928	C 964	N 482	O 482	0	0
1	B1	482	Total 1928	C 964	N 482	O 482	0	0
1	B2	482	Total 1928	C 964	N 482	O 482	0	0
1	B3	482	Total 1928	C 964	N 482	O 482	0	0
1	B4	482	Total 1928	C 964	N 482	O 482	0	0
1	B5	482	Total 1928	C 964	N 482	O 482	0	0
1	B6	482	Total 1928	C 964	N 482	O 482	0	0
1	B7	482	Total 1928	C 964	N 482	O 482	0	0
1	B8	482	Total 1928	C 964	N 482	O 482	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
1	B9	482	Total 1928	C 964	N 482	O 482	0	0
1	C1	482	Total 1928	C 964	N 482	O 482	0	0
1	C2	482	Total 1928	C 964	N 482	O 482	0	0
1	C3	482	Total 1928	C 964	N 482	O 482	0	0
1	C4	482	Total 1928	C 964	N 482	O 482	0	0
1	C5	482	Total 1928	C 964	N 482	O 482	0	0
1	C6	482	Total 1928	C 964	N 482	O 482	0	0
1	C7	482	Total 1928	C 964	N 482	O 482	0	0
1	C8	482	Total 1928	C 964	N 482	O 482	0	0
1	C9	482	Total 1928	C 964	N 482	O 482	0	0
1	D1	482	Total 1928	C 964	N 482	O 482	0	0
1	D2	482	Total 1928	C 964	N 482	O 482	0	0
1	D3	482	Total 1928	C 964	N 482	O 482	0	0
1	D4	482	Total 1928	C 964	N 482	O 482	0	0
1	D5	482	Total 1928	C 964	N 482	O 482	0	0
1	D6	482	Total 1928	C 964	N 482	O 482	0	0
1	D7	482	Total 1928	C 964	N 482	O 482	0	0
1	D8	482	Total 1928	C 964	N 482	O 482	0	0
1	D9	482	Total 1928	C 964	N 482	O 482	0	0
1	E1	482	Total 1928	C 964	N 482	O 482	0	0
1	E2	482	Total 1928	C 964	N 482	O 482	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
1	E3	482	Total 1928	C 964	N 482	O 482	0	0
1	E4	482	Total 1928	C 964	N 482	O 482	0	0
1	E5	482	Total 1928	C 964	N 482	O 482	0	0
1	E6	482	Total 1928	C 964	N 482	O 482	0	0
1	E7	482	Total 1928	C 964	N 482	O 482	0	0
1	E8	482	Total 1928	C 964	N 482	O 482	0	0
1	E9	482	Total 1928	C 964	N 482	O 482	0	0
1	F1	482	Total 1928	C 964	N 482	O 482	0	0
1	F2	482	Total 1928	C 964	N 482	O 482	0	0
1	F3	482	Total 1928	C 964	N 482	O 482	0	0
1	F4	482	Total 1928	C 964	N 482	O 482	0	0
1	F5	482	Total 1928	C 964	N 482	O 482	0	0
1	F6	482	Total 1928	C 964	N 482	O 482	0	0
1	F7	482	Total 1928	C 964	N 482	O 482	0	0
1	F8	482	Total 1928	C 964	N 482	O 482	0	0
1	F9	482	Total 1928	C 964	N 482	O 482	0	0
1	G1	482	Total 1928	C 964	N 482	O 482	0	0
1	G2	482	Total 1928	C 964	N 482	O 482	0	0
1	G3	482	Total 1928	C 964	N 482	O 482	0	0
1	G4	482	Total 1928	C 964	N 482	O 482	0	0
1	G5	482	Total 1928	C 964	N 482	O 482	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
1	G6	482	Total 1928	C 964	N 482	O 482	0	0
1	G7	482	Total 1928	C 964	N 482	O 482	0	0
1	G8	482	Total 1928	C 964	N 482	O 482	0	0
1	G9	482	Total 1928	C 964	N 482	O 482	0	0
1	H1	482	Total 1928	C 964	N 482	O 482	0	0
1	H2	482	Total 1928	C 964	N 482	O 482	0	0
1	H3	482	Total 1928	C 964	N 482	O 482	0	0
1	H4	482	Total 1928	C 964	N 482	O 482	0	0
1	H5	482	Total 1928	C 964	N 482	O 482	0	0
1	H6	482	Total 1928	C 964	N 482	O 482	0	0
1	H7	482	Total 1928	C 964	N 482	O 482	0	0
1	H8	482	Total 1928	C 964	N 482	O 482	0	0
1	H9	482	Total 1928	C 964	N 482	O 482	0	0
1	I1	482	Total 1928	C 964	N 482	O 482	0	0
1	I2	482	Total 1928	C 964	N 482	O 482	0	0
1	I3	482	Total 1928	C 964	N 482	O 482	0	0
1	I4	482	Total 1928	C 964	N 482	O 482	0	0
1	I5	482	Total 1928	C 964	N 482	O 482	0	0
1	I6	482	Total 1928	C 964	N 482	O 482	0	0
1	I7	482	Total 1928	C 964	N 482	O 482	0	0
1	I8	482	Total 1928	C 964	N 482	O 482	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
1	I9	482	Total 1928	C 964	N 482	O 482	0	0
1	J1	482	Total 1928	C 964	N 482	O 482	0	0
1	J2	482	Total 1928	C 964	N 482	O 482	0	0
1	J3	482	Total 1928	C 964	N 482	O 482	0	0

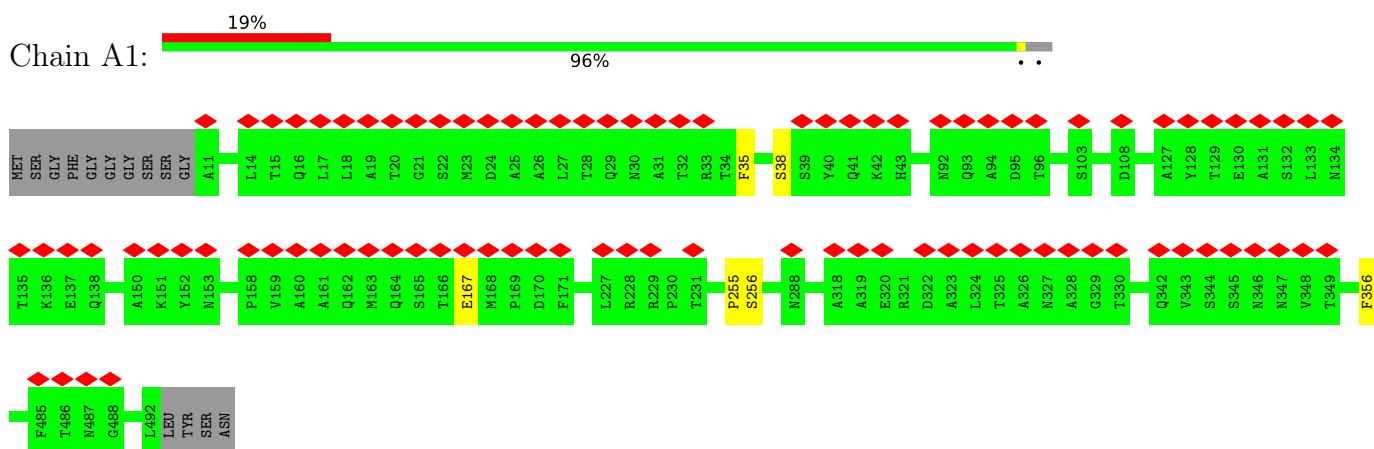
- Molecule 2 is a protein called Penton protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	K	663	Total 2653	C 1326	N 663	O 664	0	0

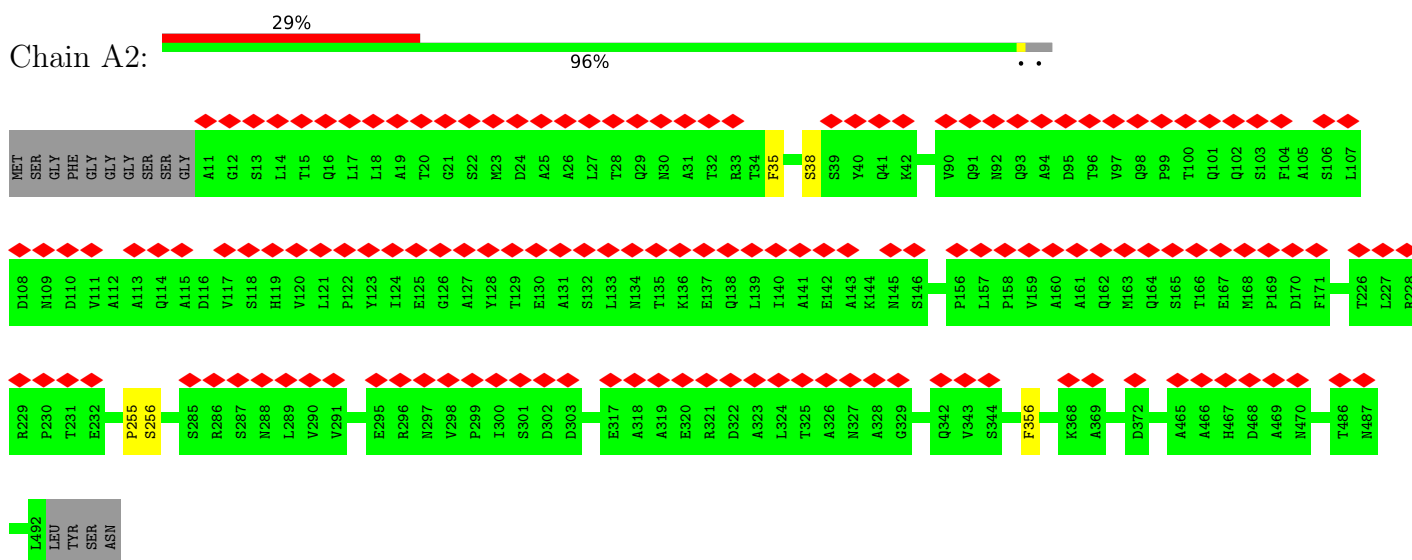
3 Residue-property plots

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

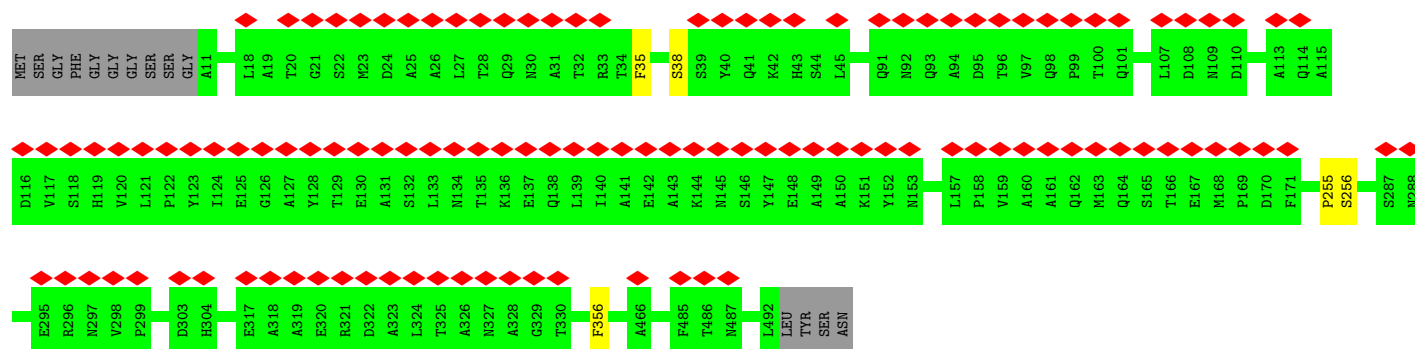


- Molecule 1: Major capsid protein



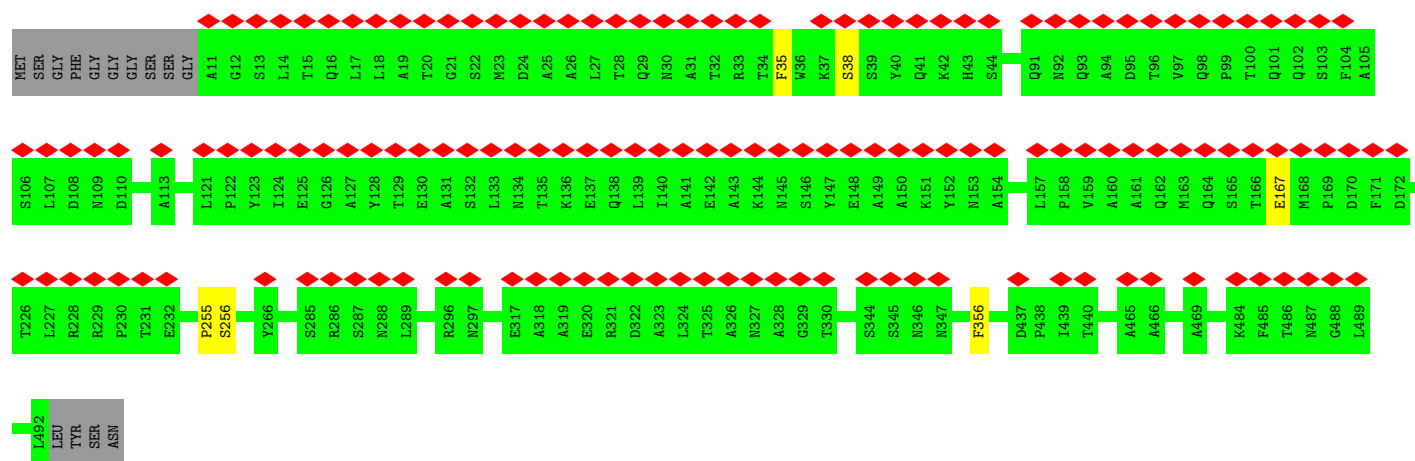
- Molecule 1: Major capsid protein





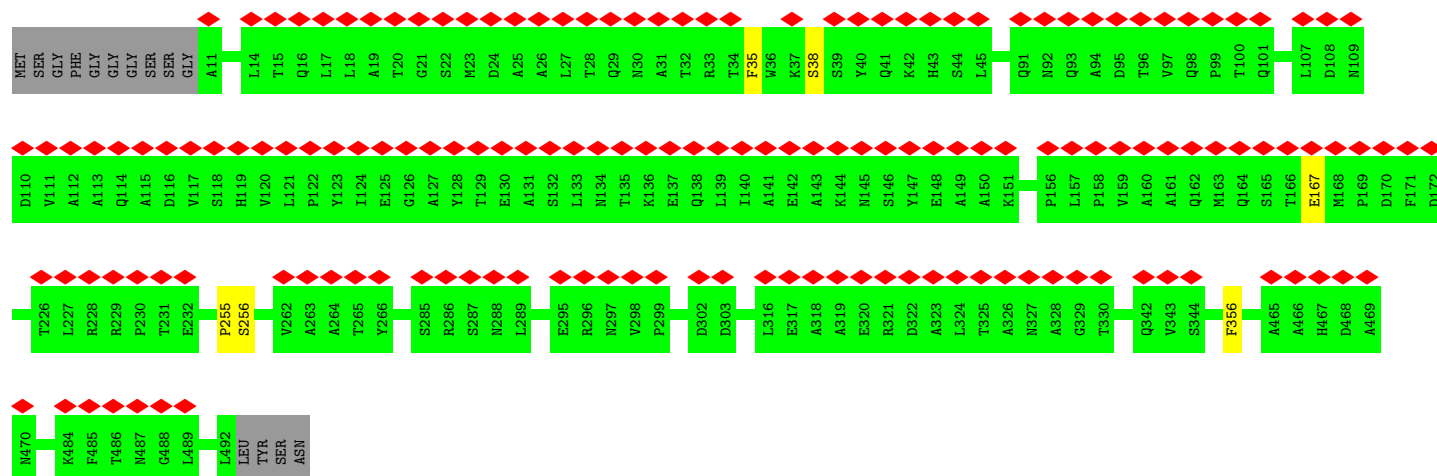
- Molecule 1: Major capsid protein

Chain A4: 30% 96%



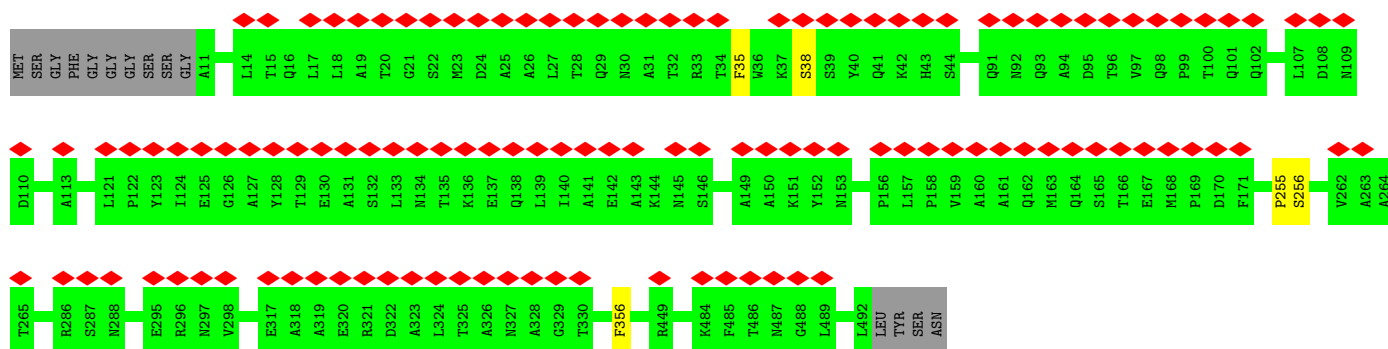
- Molecule 1: Major capsid protein

Chain A5: 32% 96%



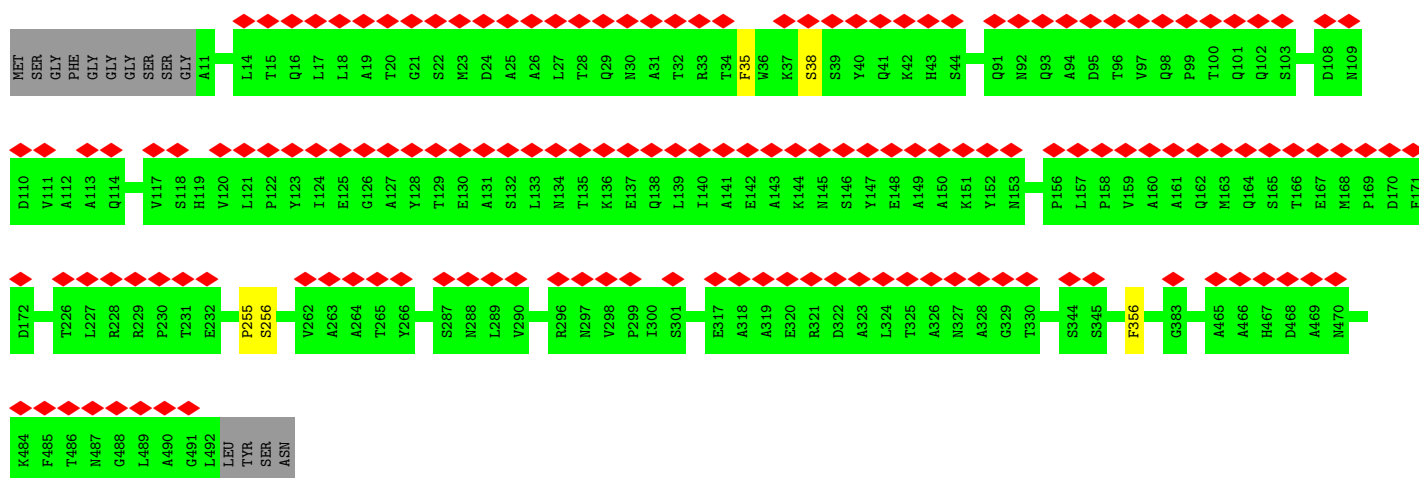
- Molecule 1: Major capsid protein

Chain A6: 25% 96%



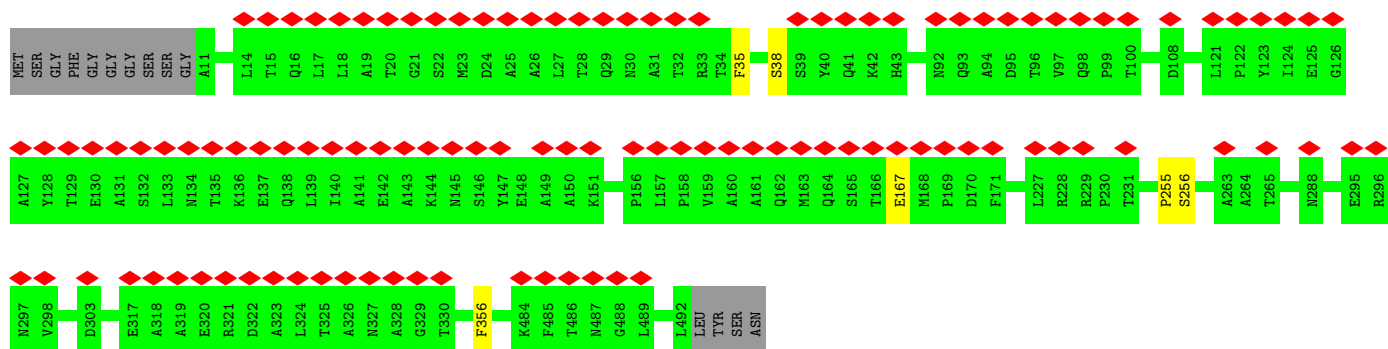
- Molecule 1: Major capsid protein

Chain A7: 31% 96%



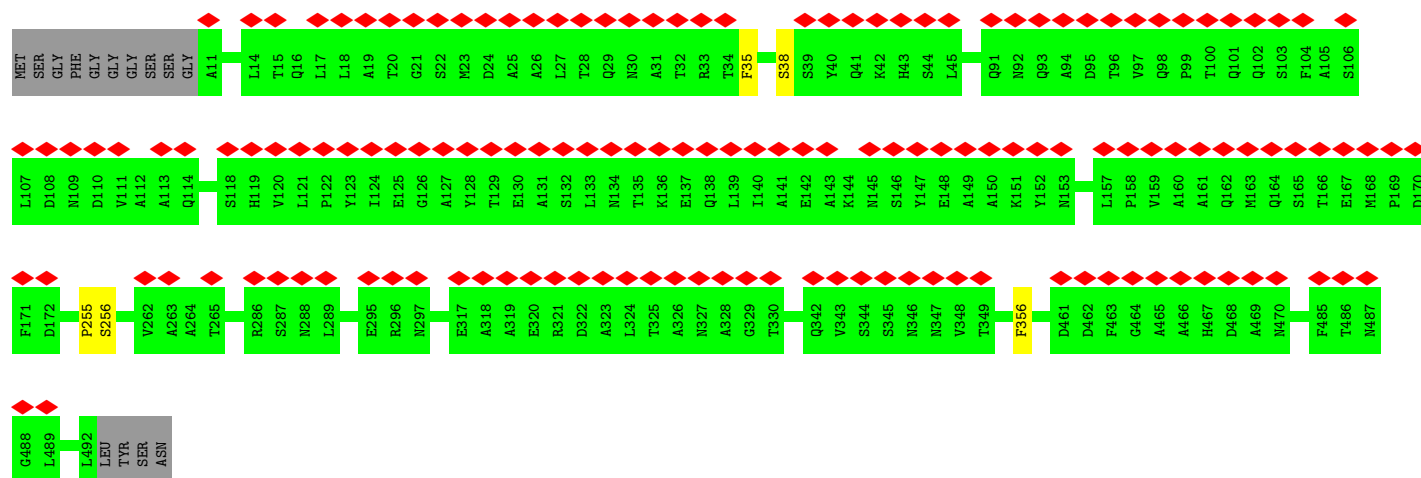
- Molecule 1: Major capsid protein

Chain A8: 23% 96%



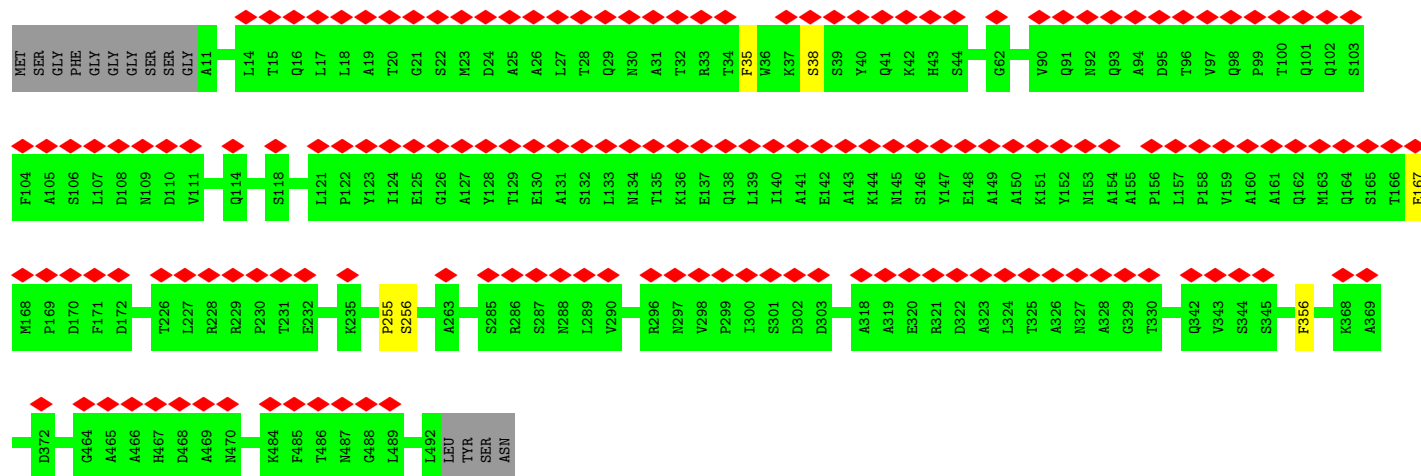
- Molecule 1: Major capsid protein

Chain A9: 30% 96%



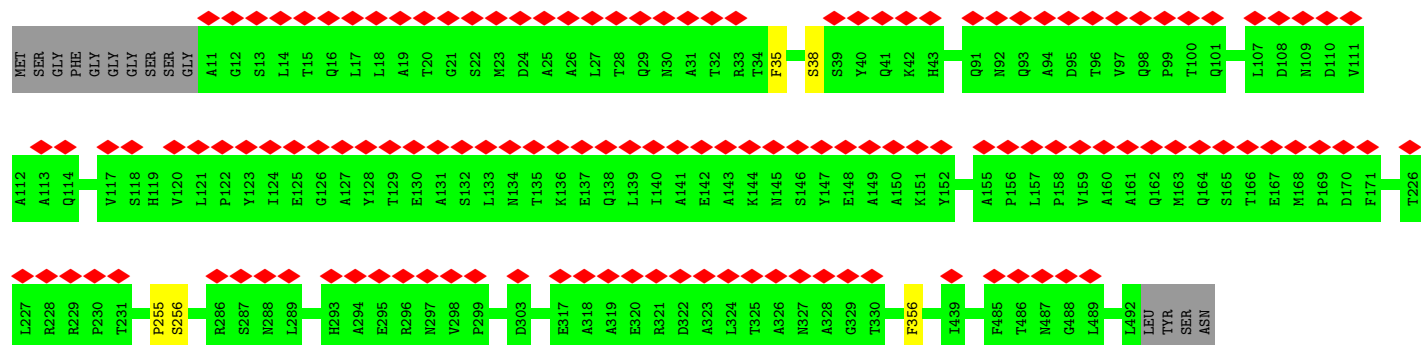
- Molecule 1: Major capsid protein

Chain B1: 32% 96%

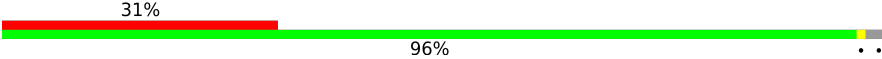


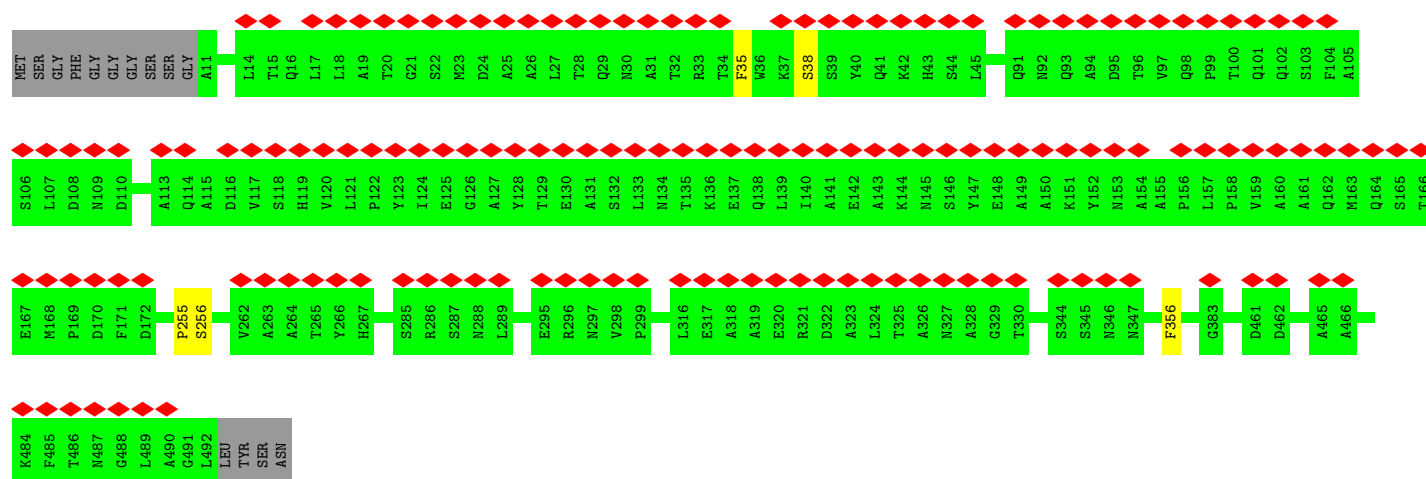
- Molecule 1: Major capsid protein

Chain B2: 27% 96%

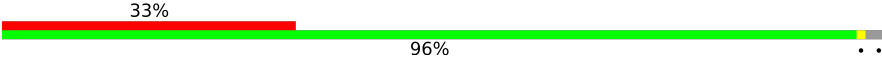


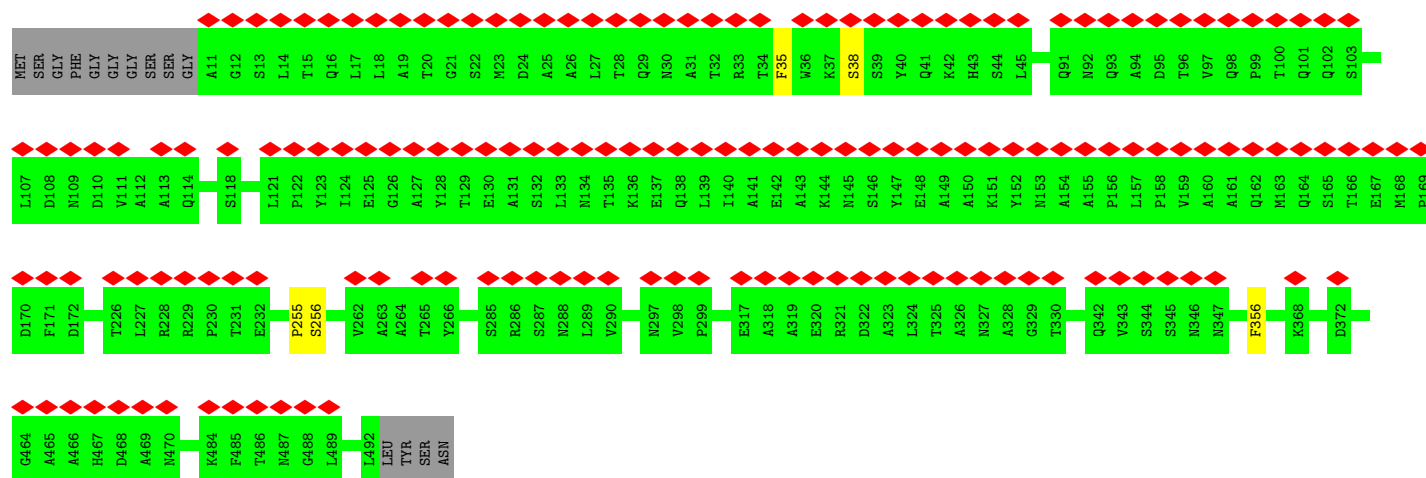
- Molecule 1: Major capsid protein

Chain B3: 

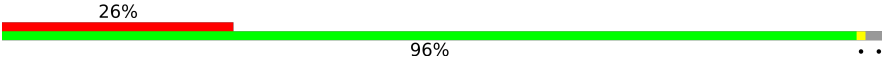


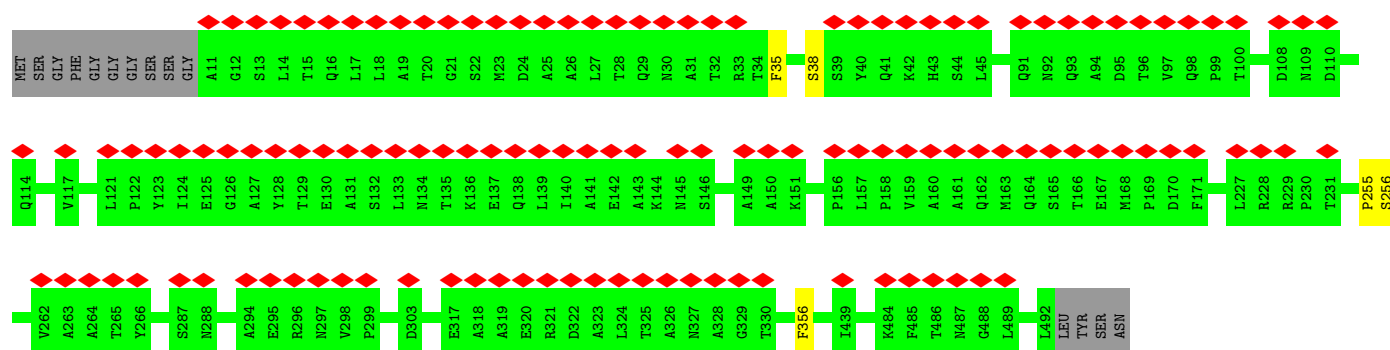
• Molecule 1: Major capsid protein

Chain B4: 



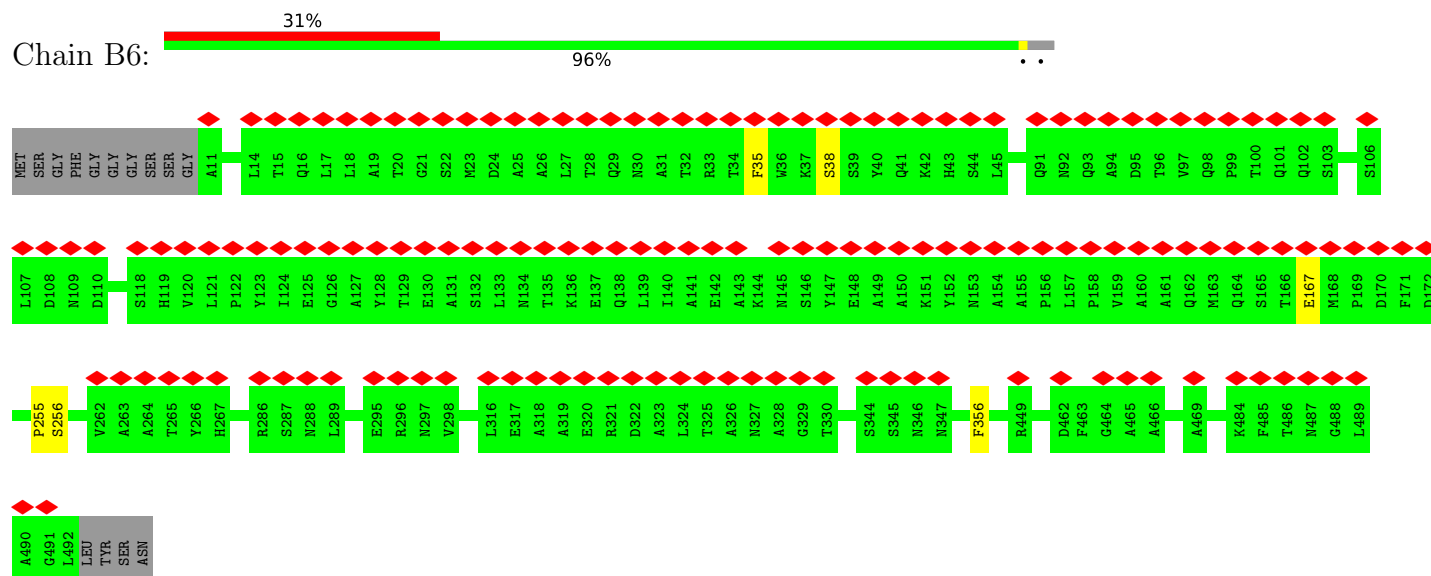
• Molecule 1: Major capsid protein

Chain B5: 



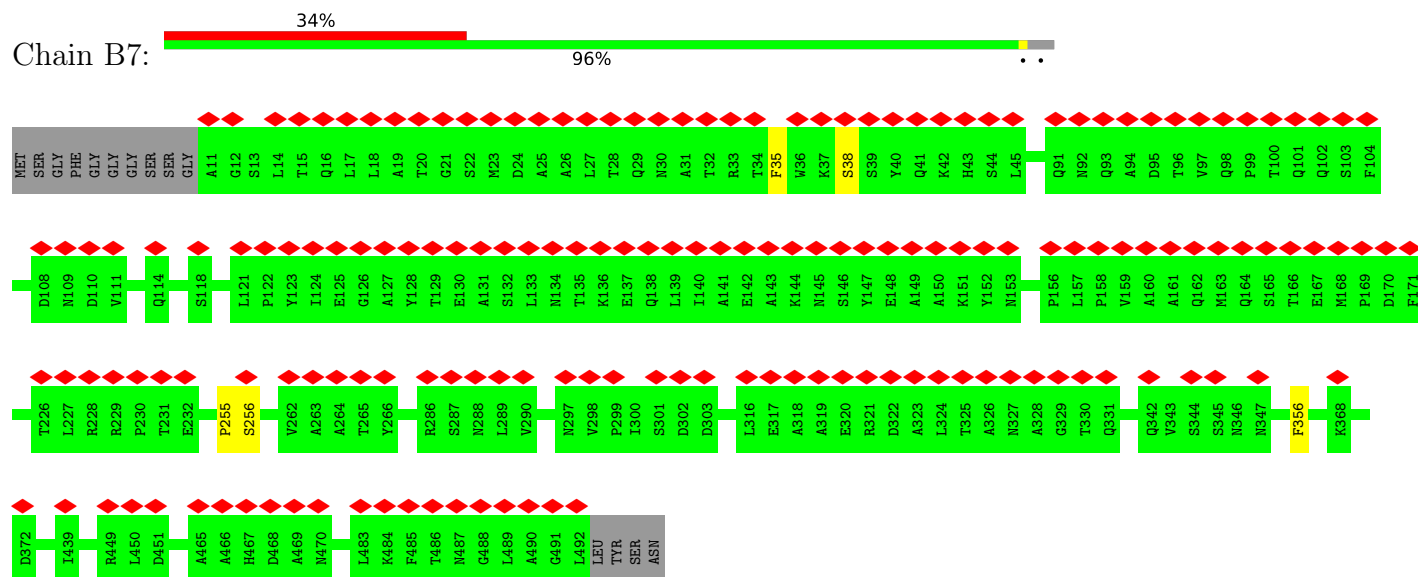
- Molecule 1: Major capsid protein

Chain B6:



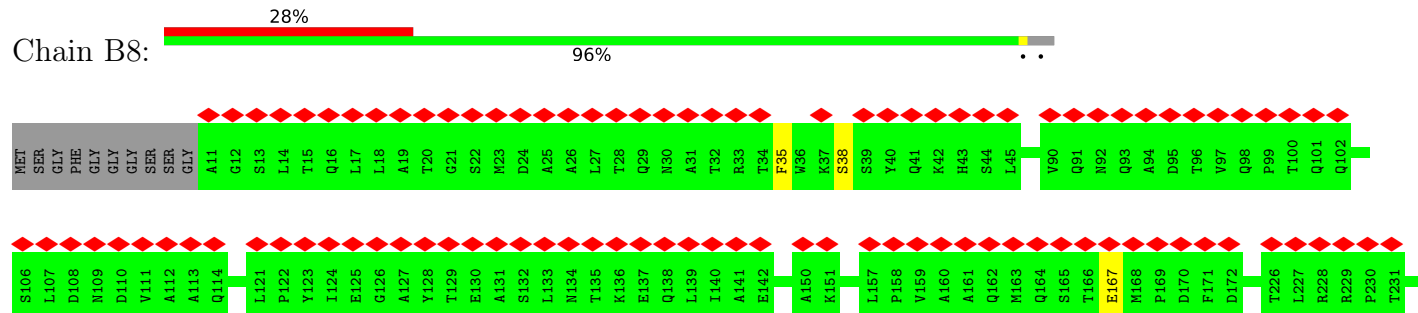
- Molecule 1: Major capsid protein

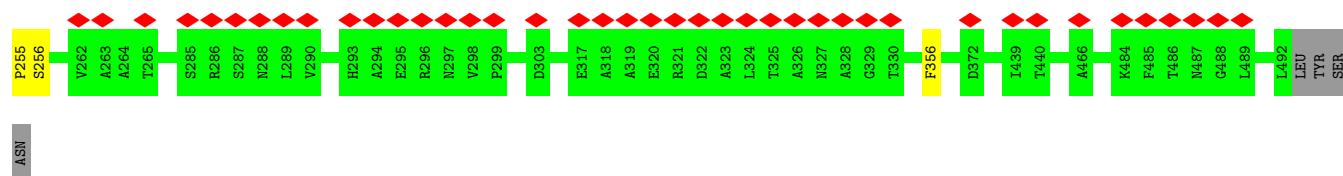
Chain B7:



- Molecule 1: Major capsid protein

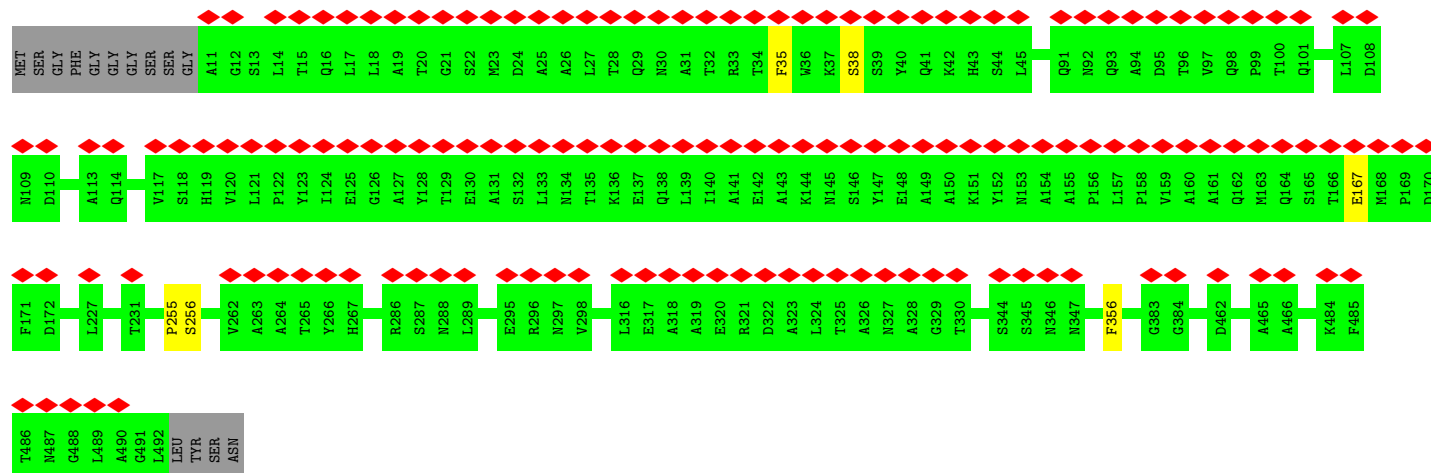
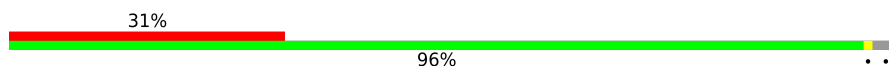
Chain B8:





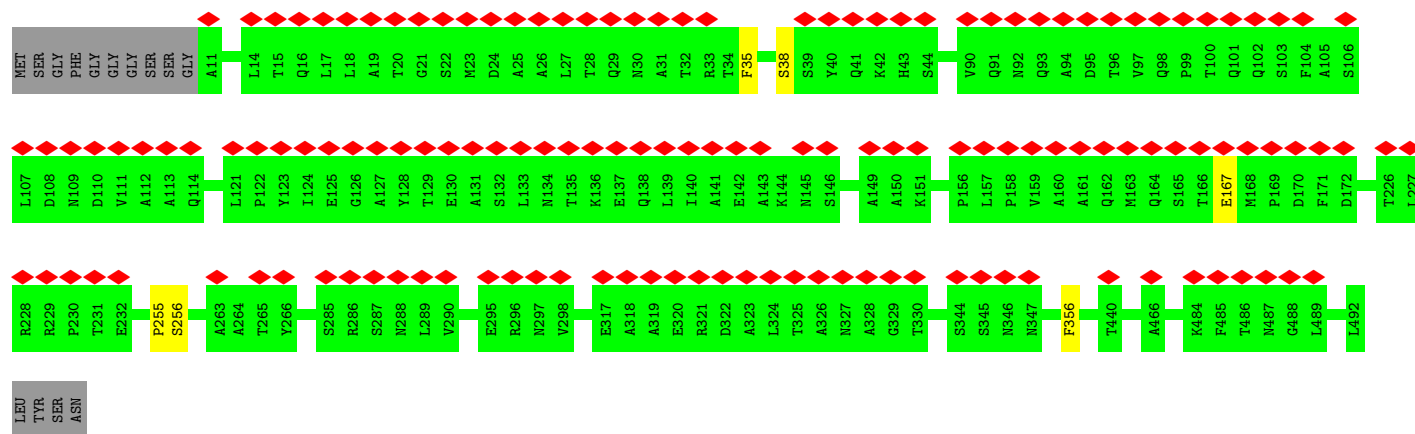
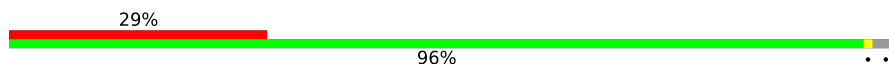
- Molecule 1: Major capsid protein

Chain B9:



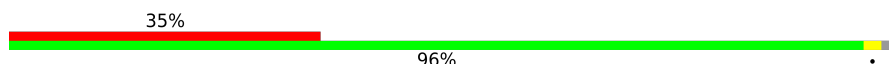
- Molecule 1: Major capsid protein

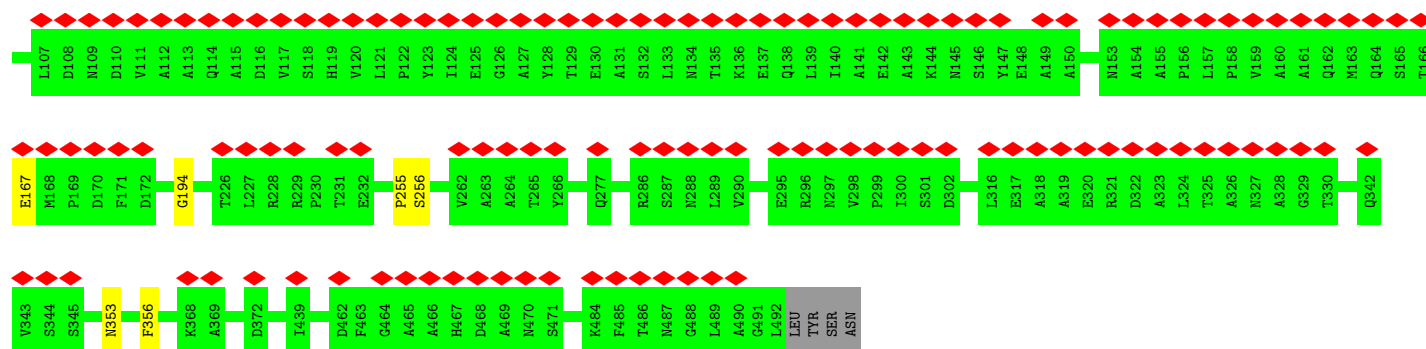
Chain C1:



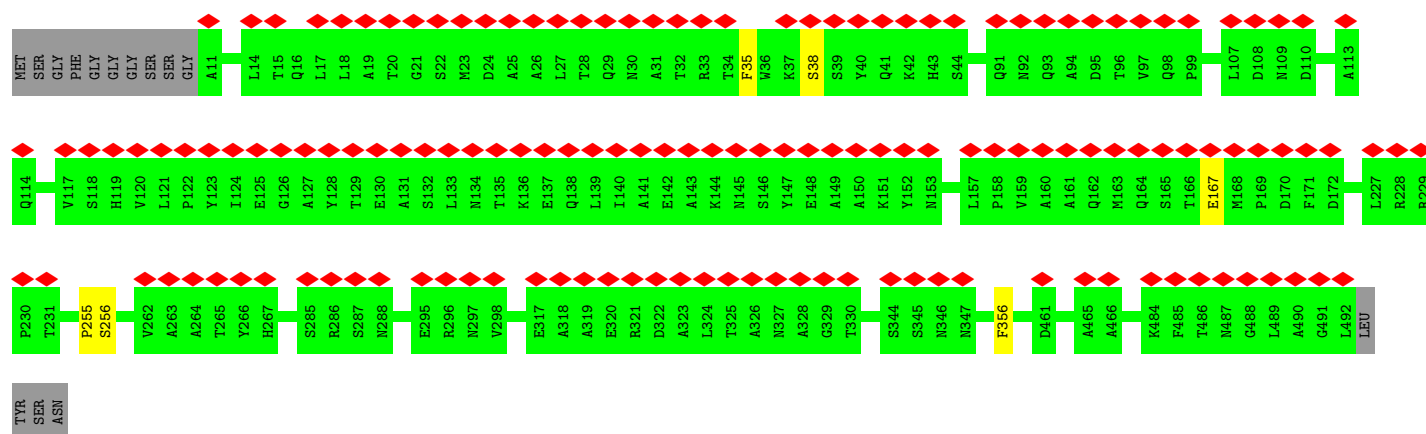
- Molecule 1: Major capsid protein

Chain C2:

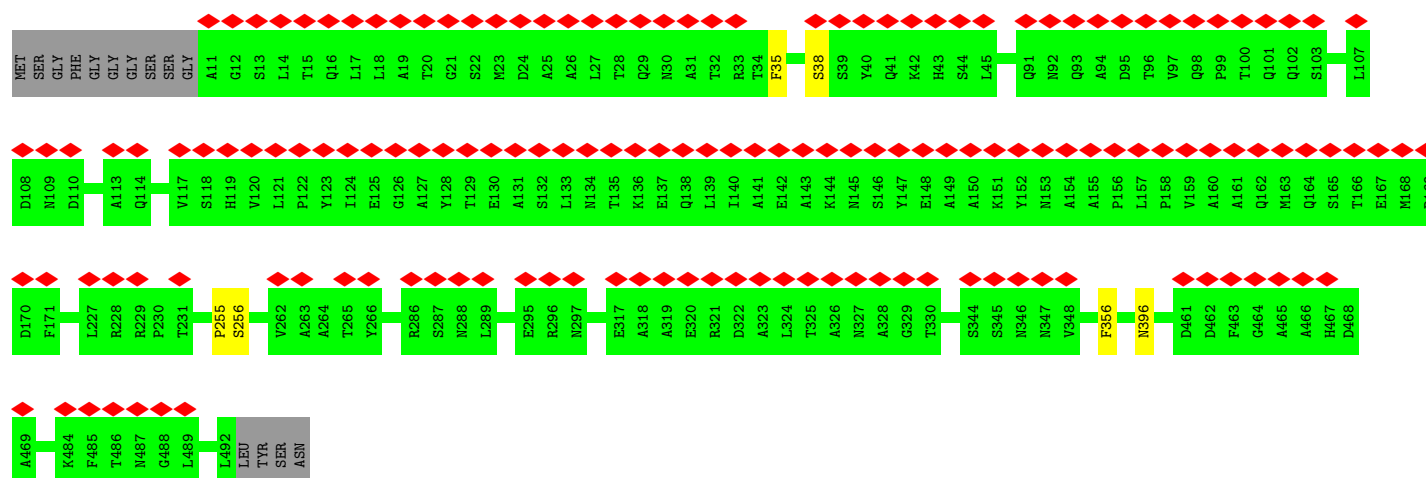




• Molecule 1: Major capsid protein

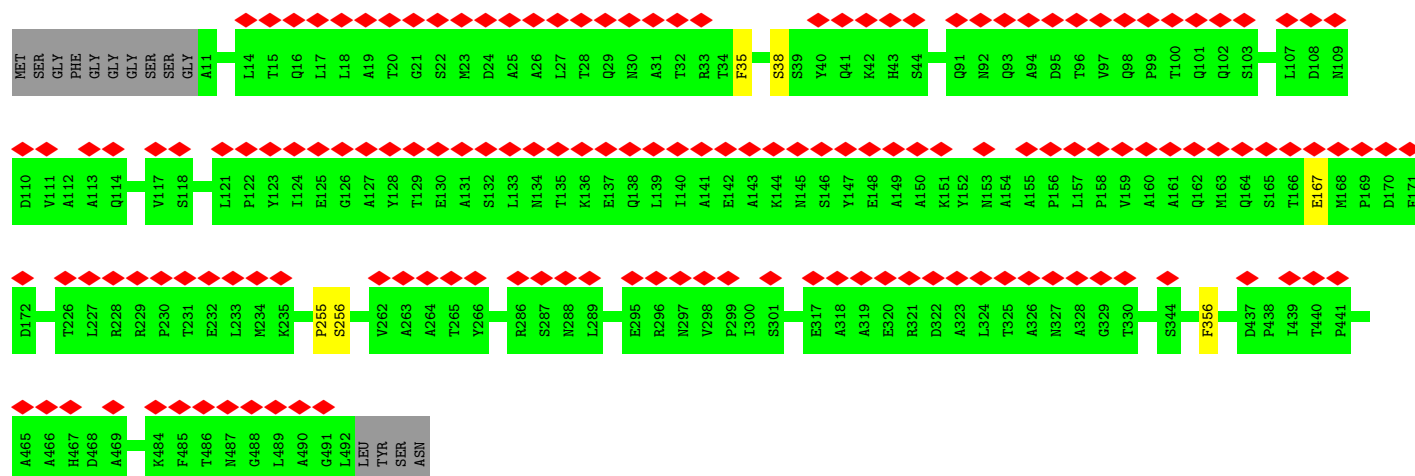


• Molecule 1: Major capsid protein



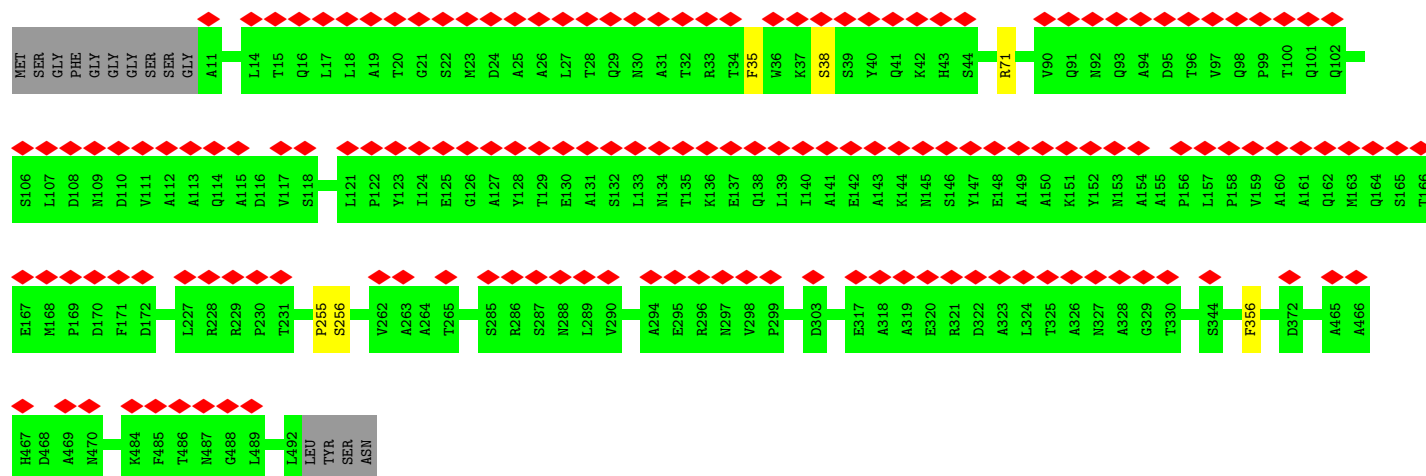
• Molecule 1: Major capsid protein





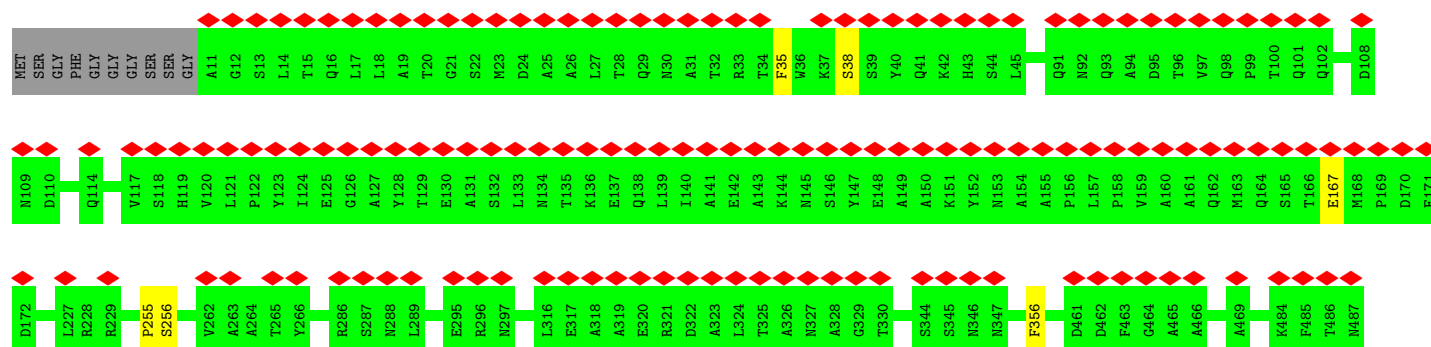
- Molecule 1: Major capsid protein

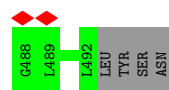
Chain C6: 31% 96%



- Molecule 1: Major capsid protein

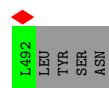
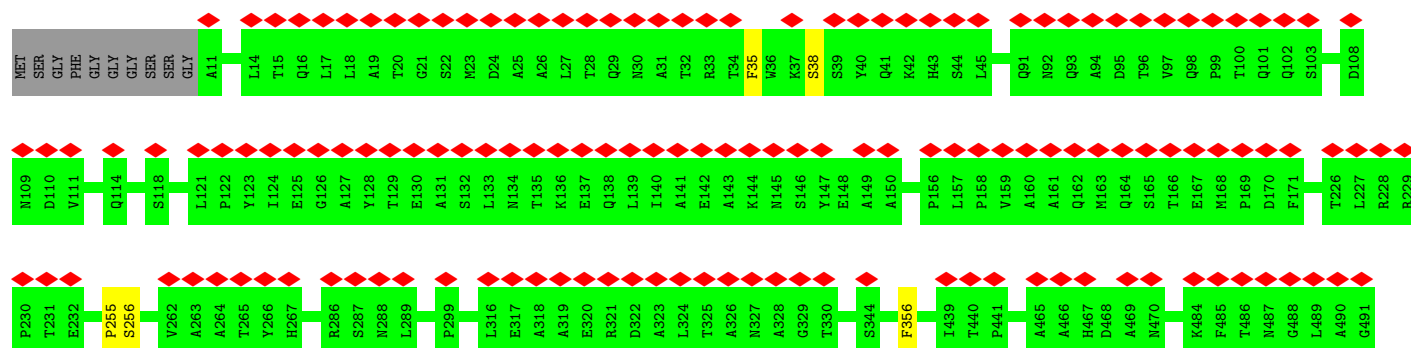
Chain C7: 30% 96%





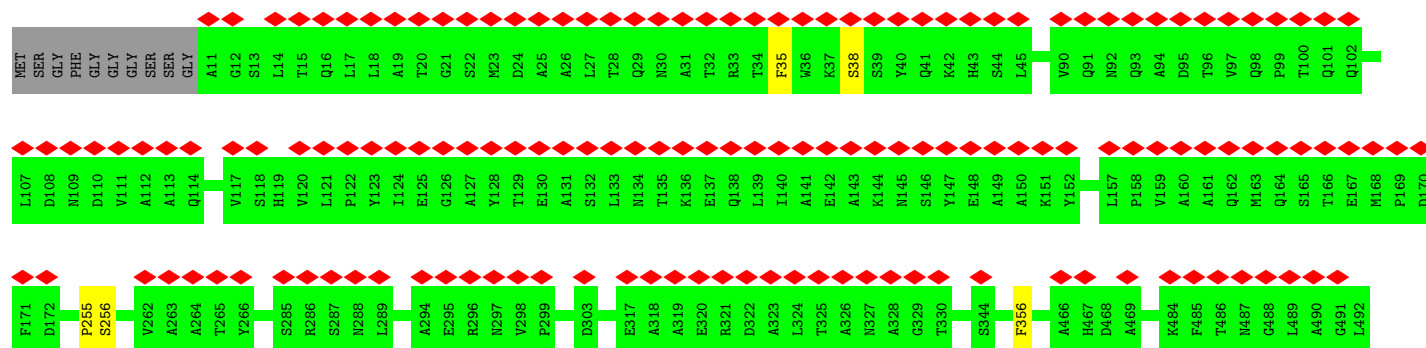
- Molecule 1: Major capsid protein

Chain C8: 29% 96%



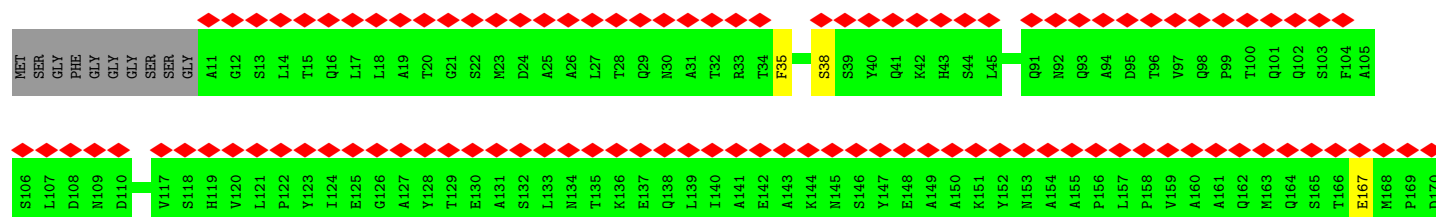
- Molecule 1: Major capsid protein

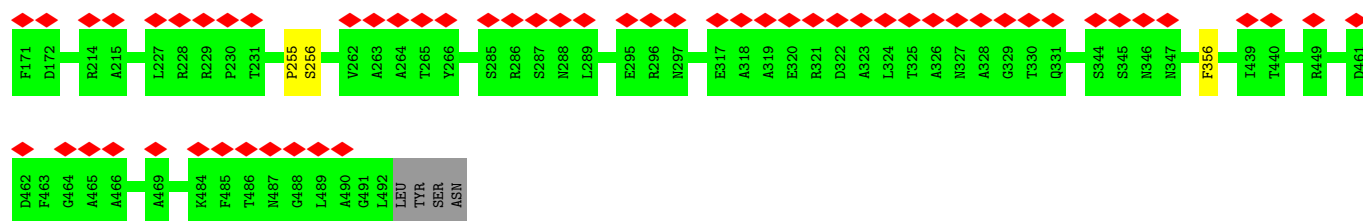
Chain C9: 30% 96%



- Molecule 1: Major capsid protein

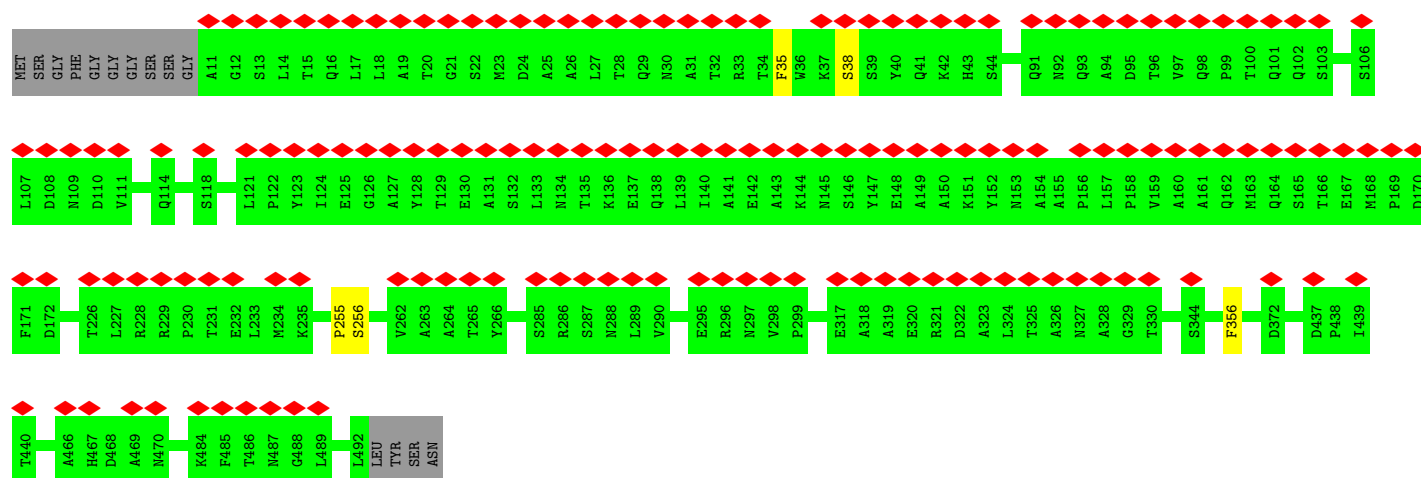
Chain D1: 33% 96%





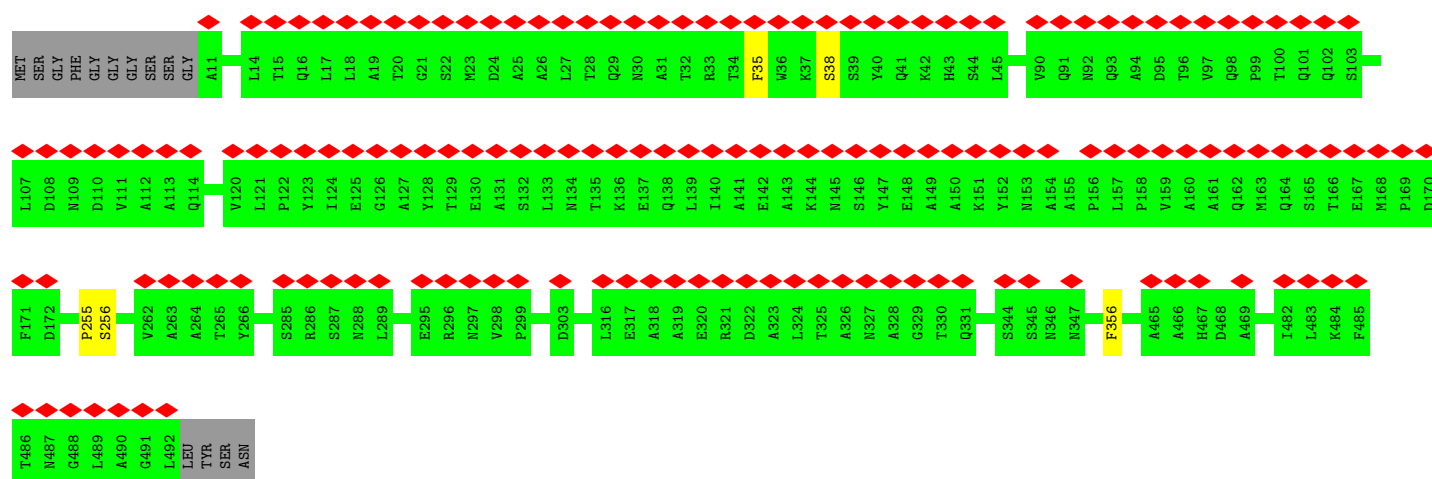
- Molecule 1: Major capsid protein

Chain D2: 32% 96%



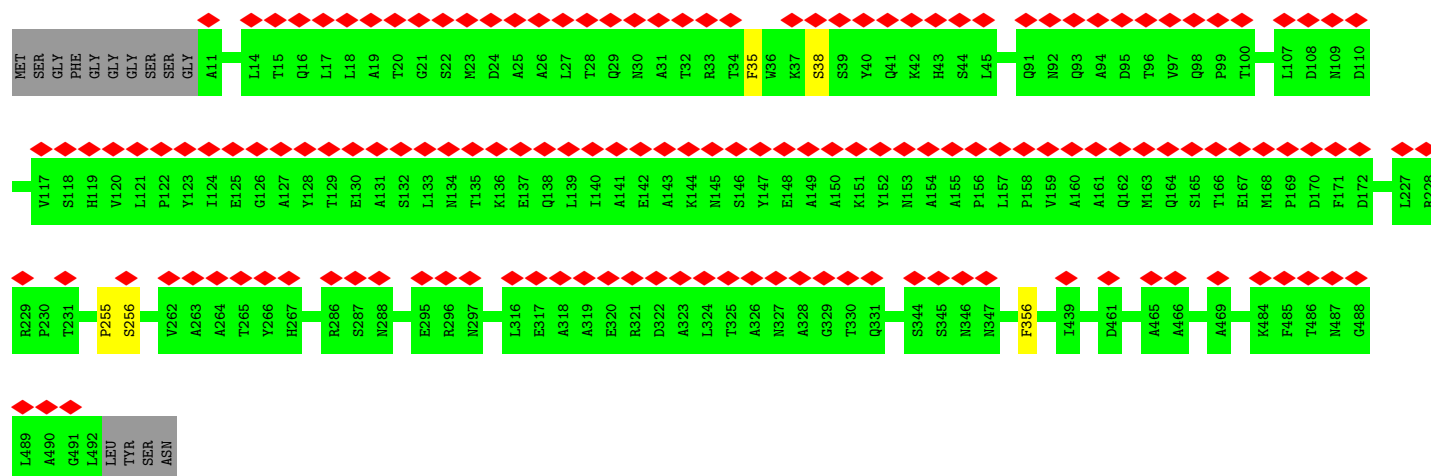
- Molecule 1: Major capsid protein

Chain D3: 32% 96%

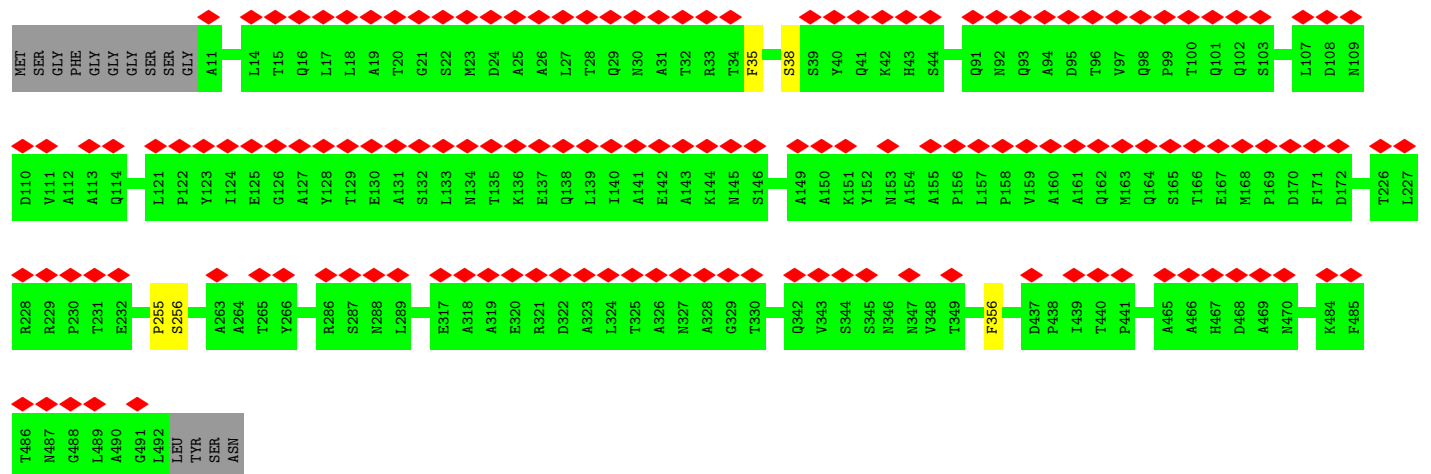


- Molecule 1: Major capsid protein

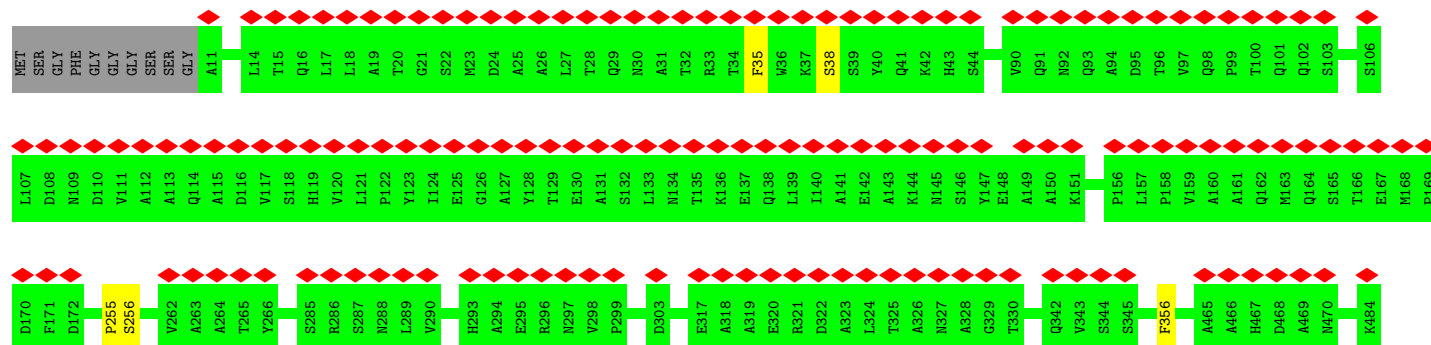
Chain D4: 30% 96%

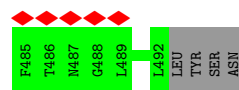


- Molecule 1: Major capsid protein

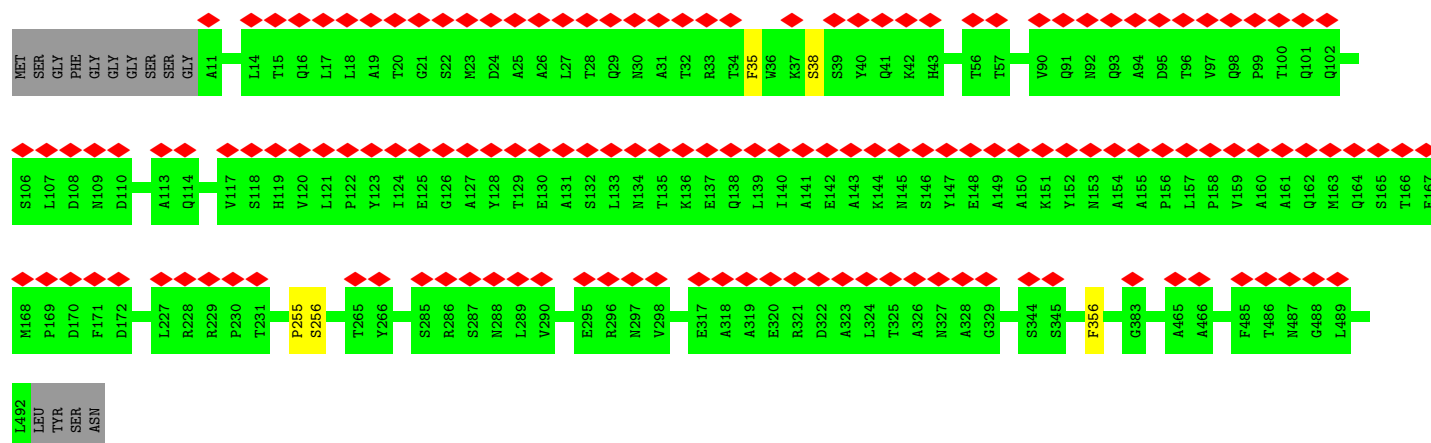


- Molecule 1: Major capsid protein

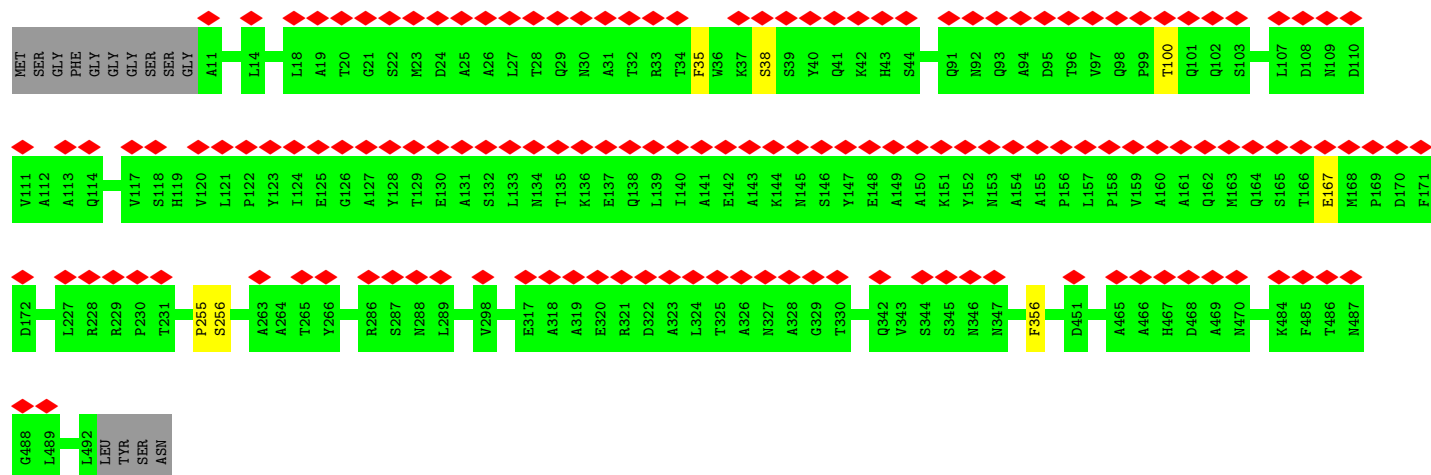




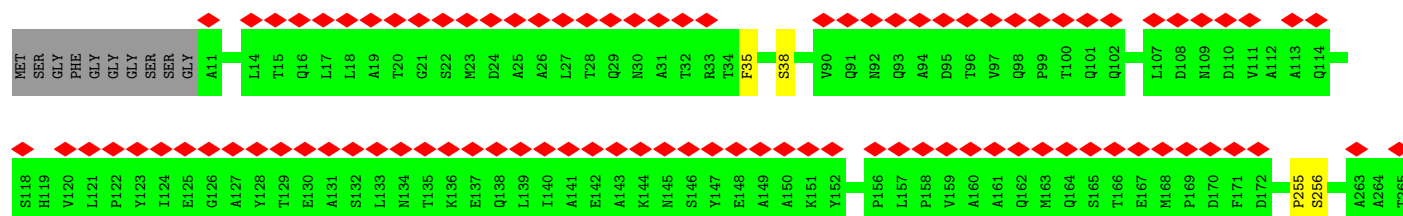
- Molecule 1: Major capsid protein

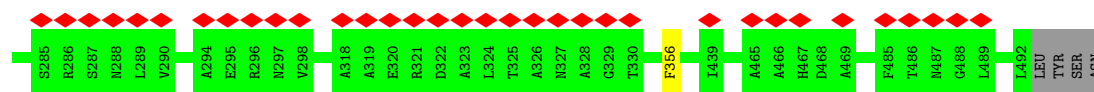


- Molecule 1: Major capsid protein



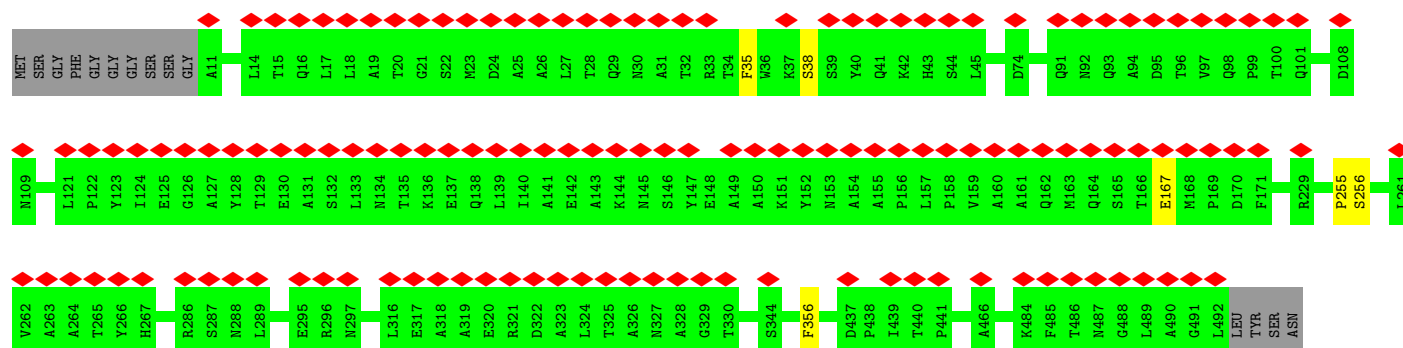
- Molecule 1: Major capsid protein





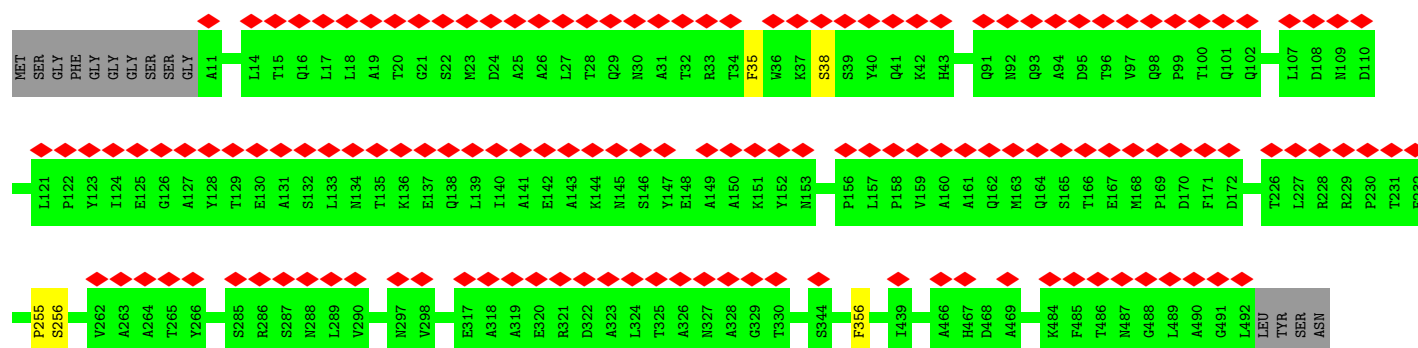
• Molecule 1: Major capsid protein

Chain E1: 28% 96%



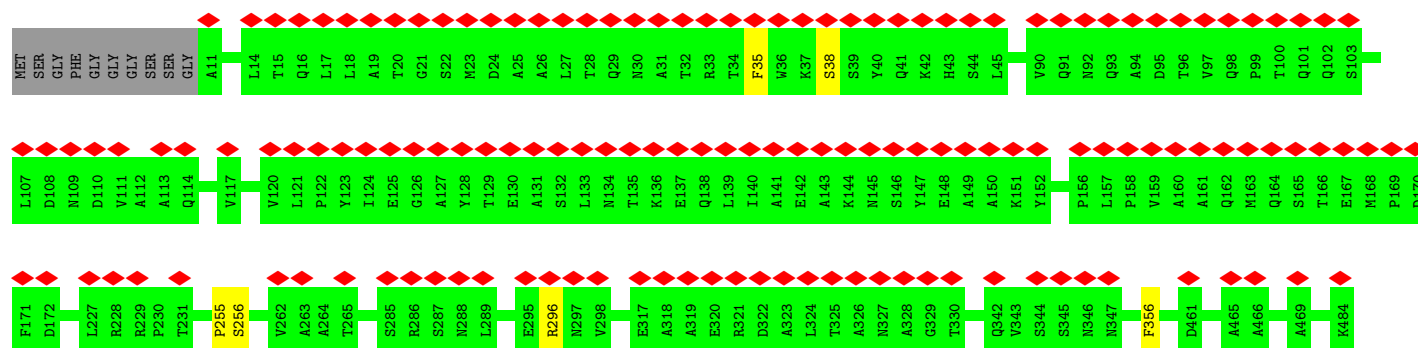
• Molecule 1: Major capsid protein

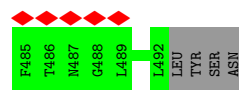
Chain E2: 29% 96%



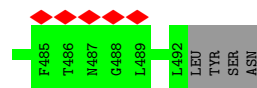
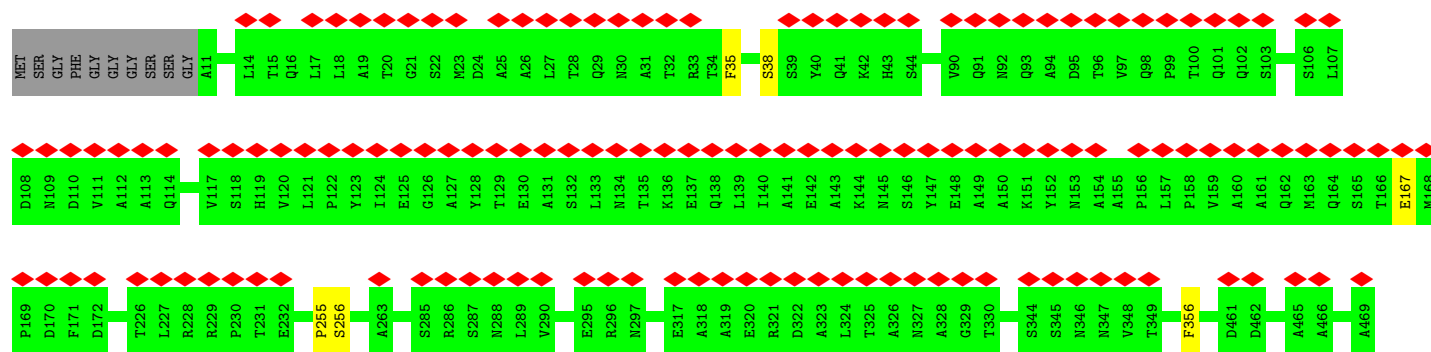
• Molecule 1: Major capsid protein

Chain E3: 30% 96%

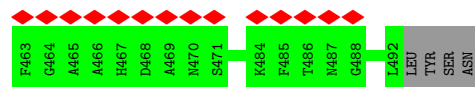
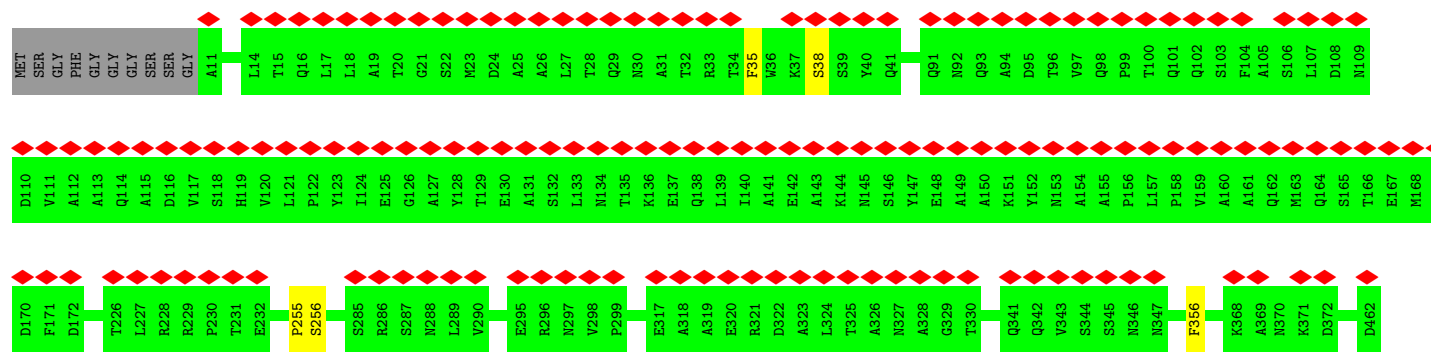




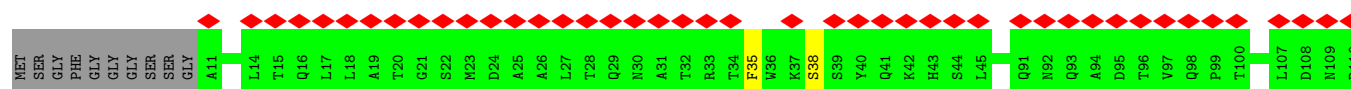
- Molecule 1: Major capsid protein



- Molecule 1: Major capsid protein



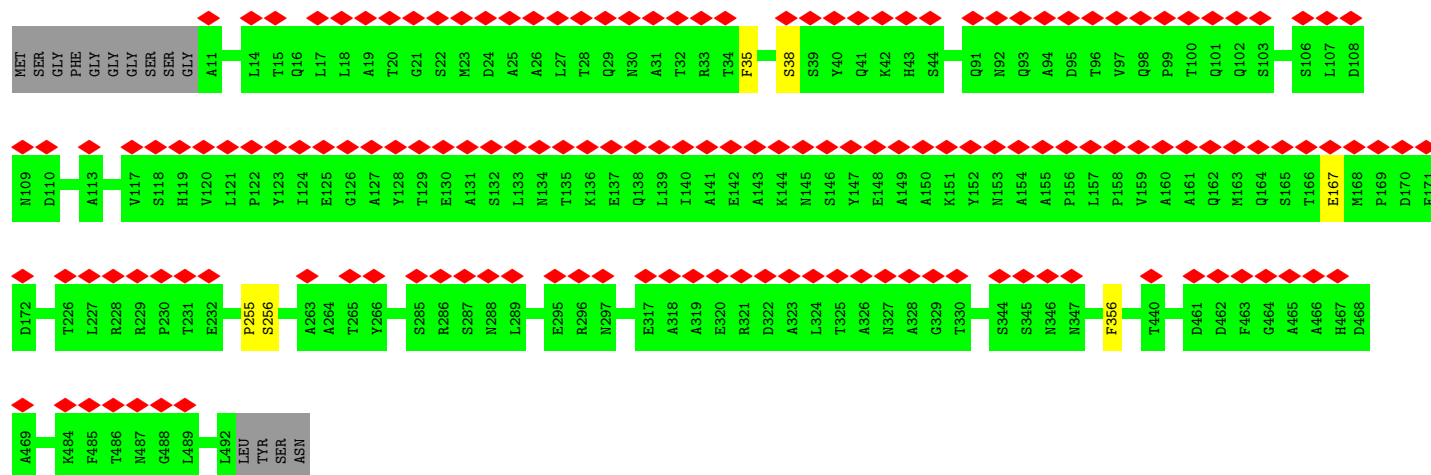
- Molecule 1: Major capsid protein





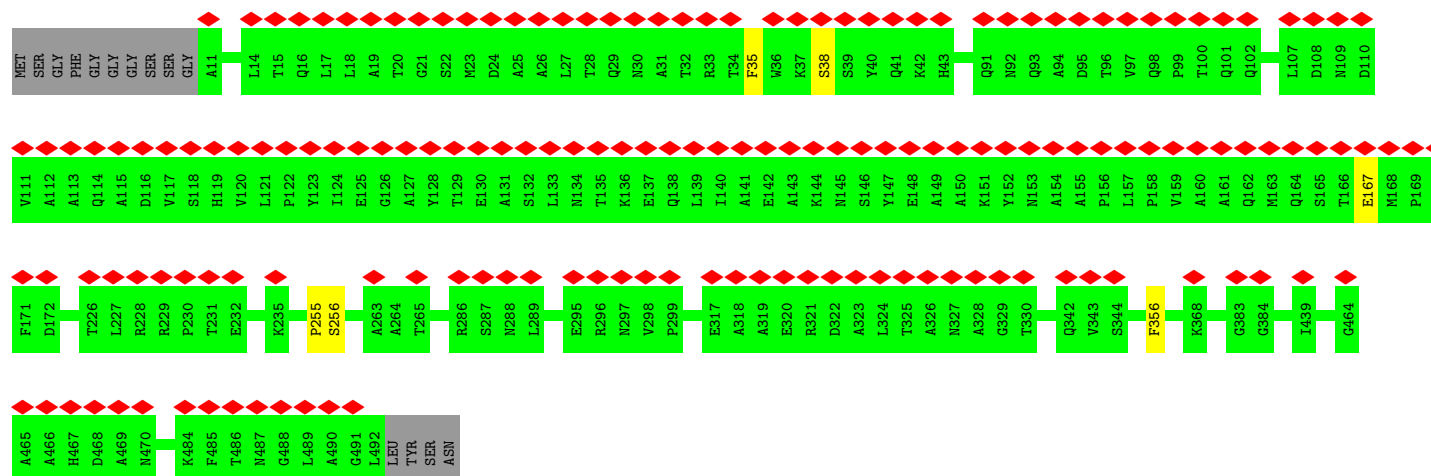
• Molecule 1: Major capsid protein

Chain E7: 31% 96%



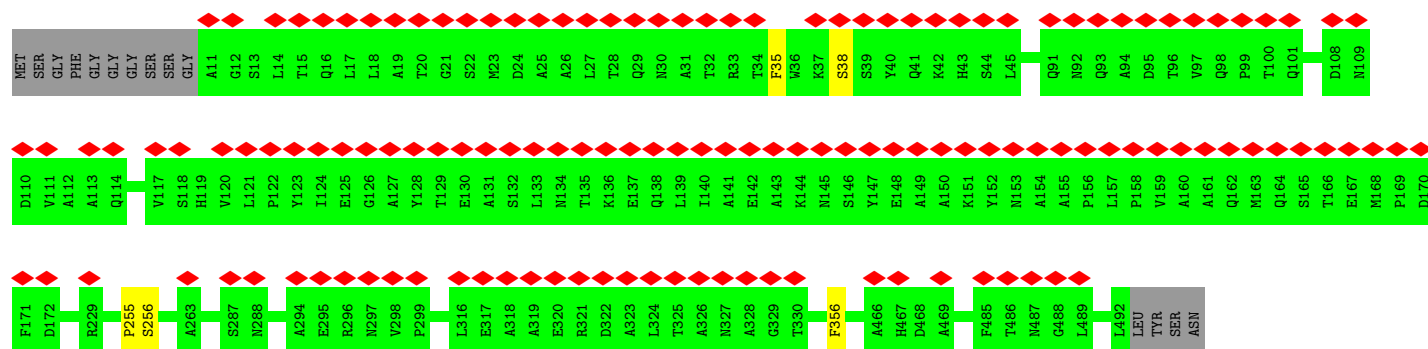
• Molecule 1: Major capsid protein

Chain E8: 33% 96%



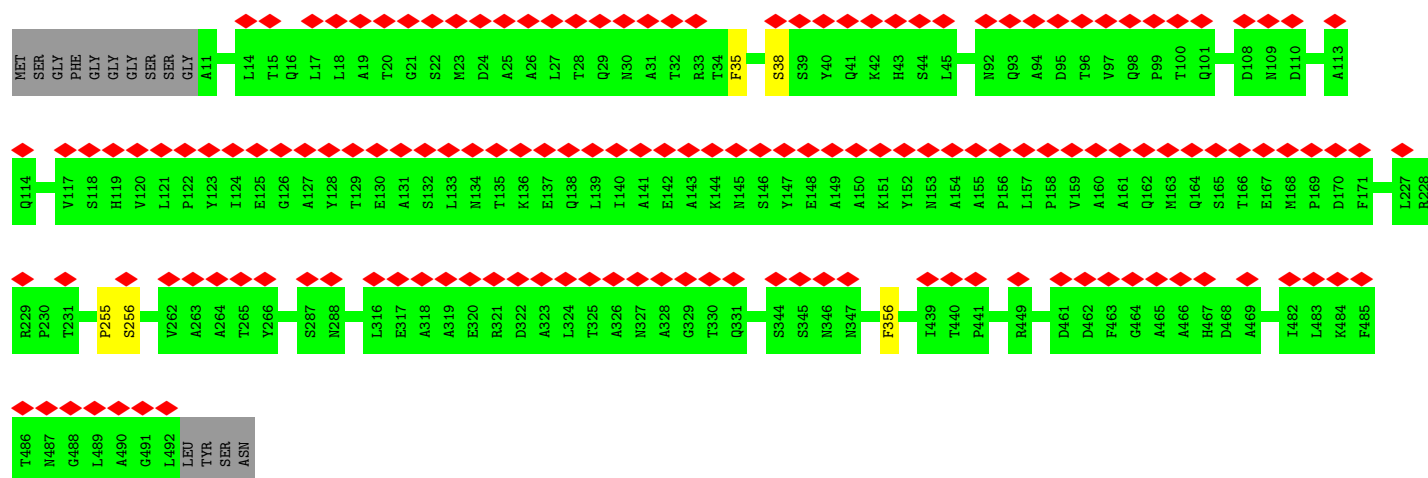
• Molecule 1: Major capsid protein

Chain E9: 28% 96%



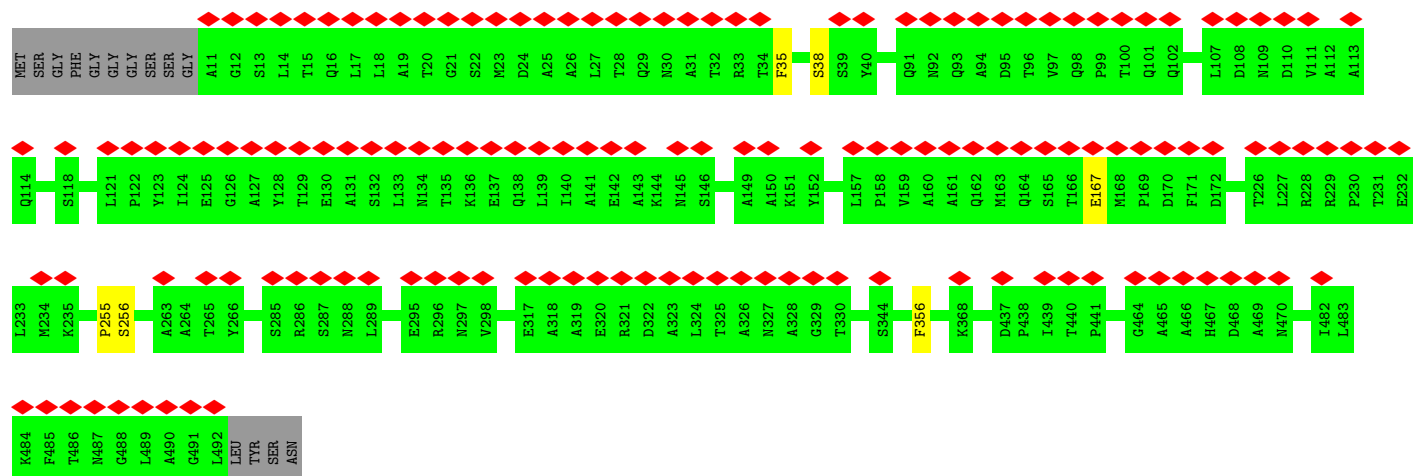
- Molecule 1: Major capsid protein

Chain F1: 30% 96%

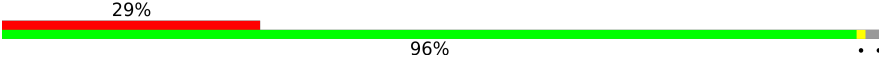


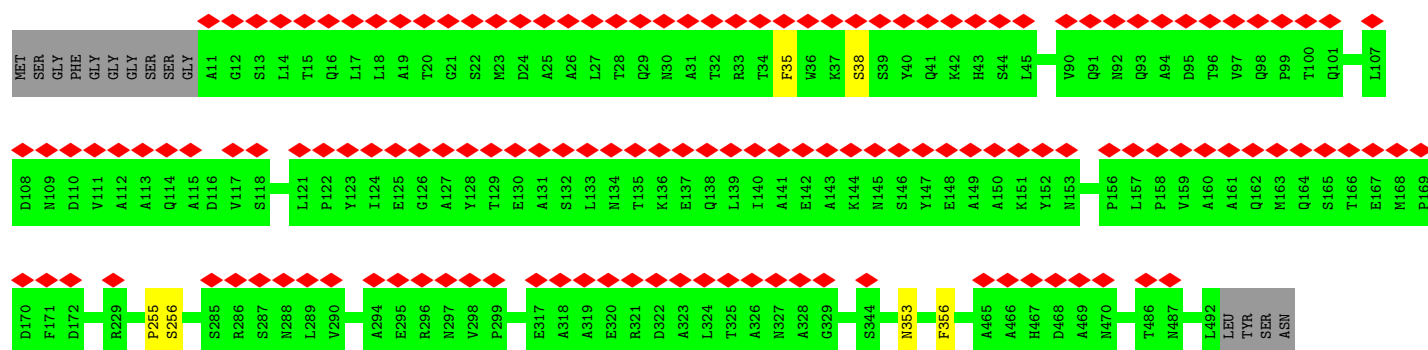
- Molecule 1: Major capsid protein

Chain F2: 30% 96%

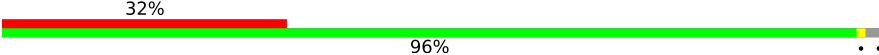


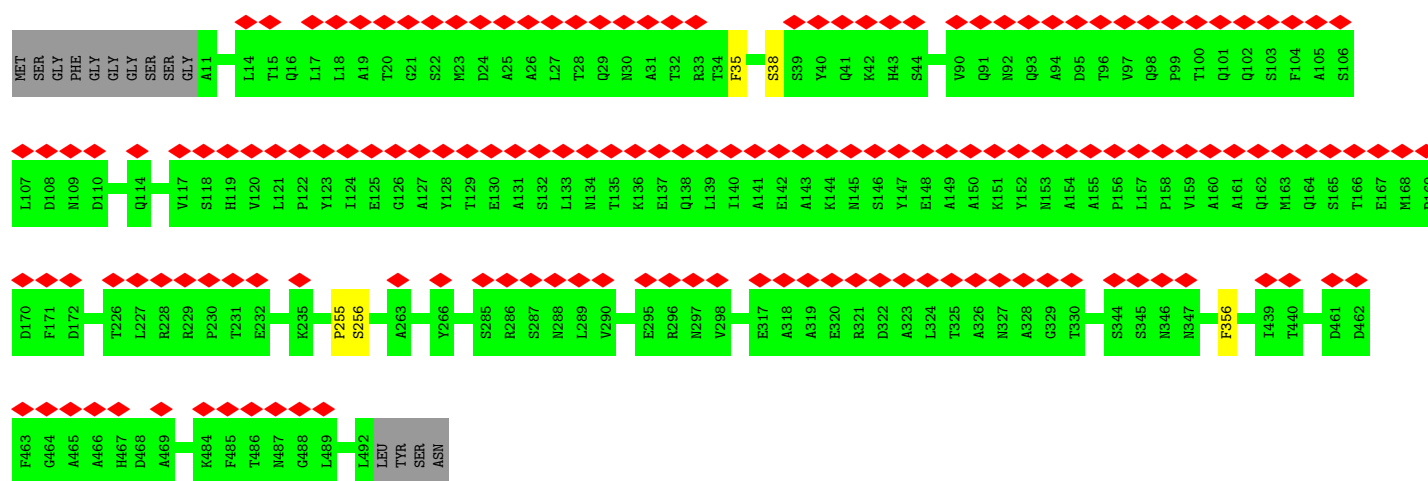
- Molecule 1: Major capsid protein

Chain F3: 

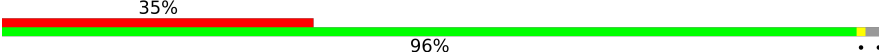


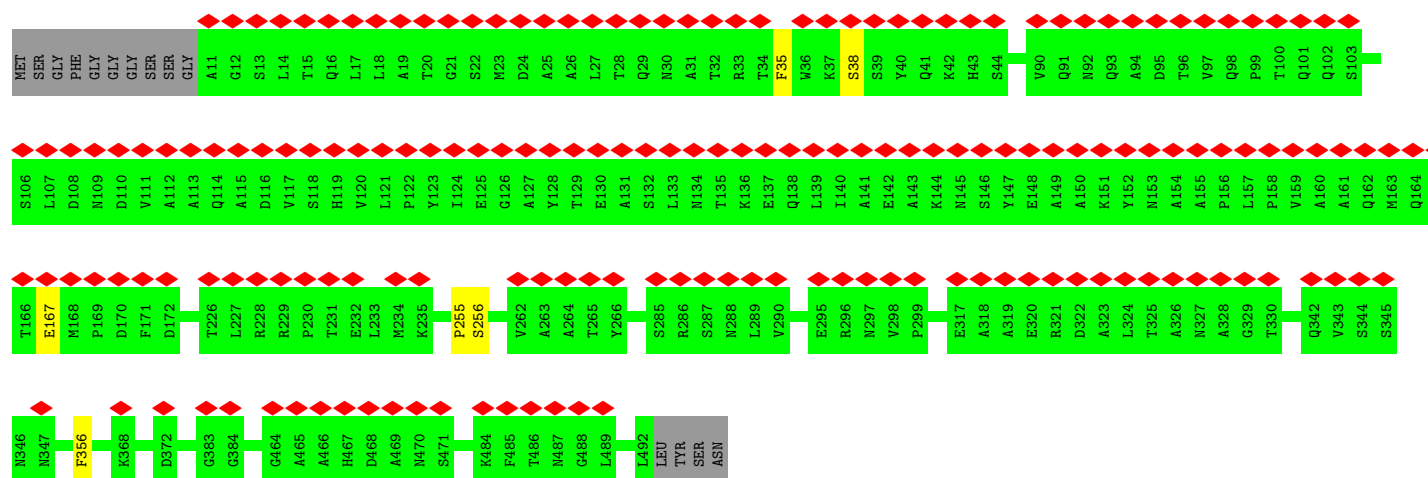
• Molecule 1: Major capsid protein

Chain F4: 



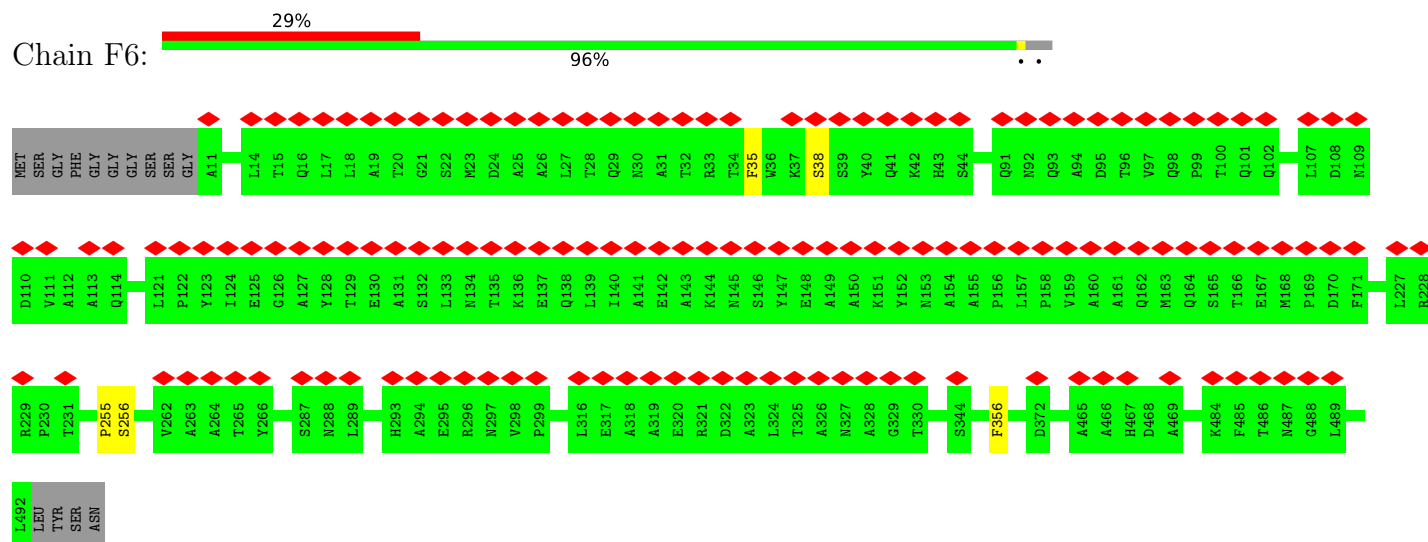
• Molecule 1: Major capsid protein

Chain F5: 



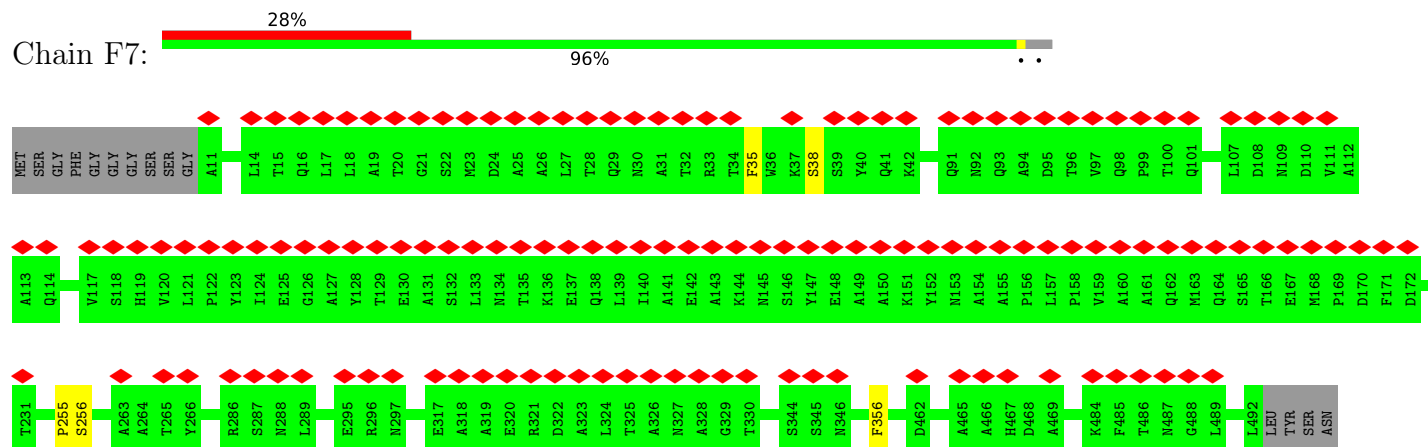
• Molecule 1: Major capsid protein

Chain F6:



• Molecule 1: Major capsid protein

Chain F7:

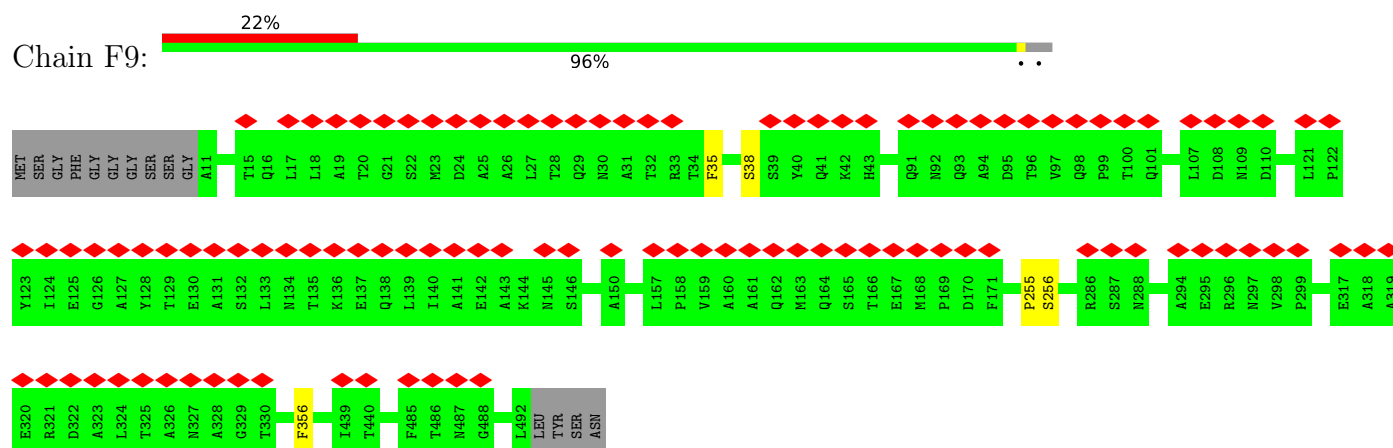


• Molecule 1: Major capsid protein

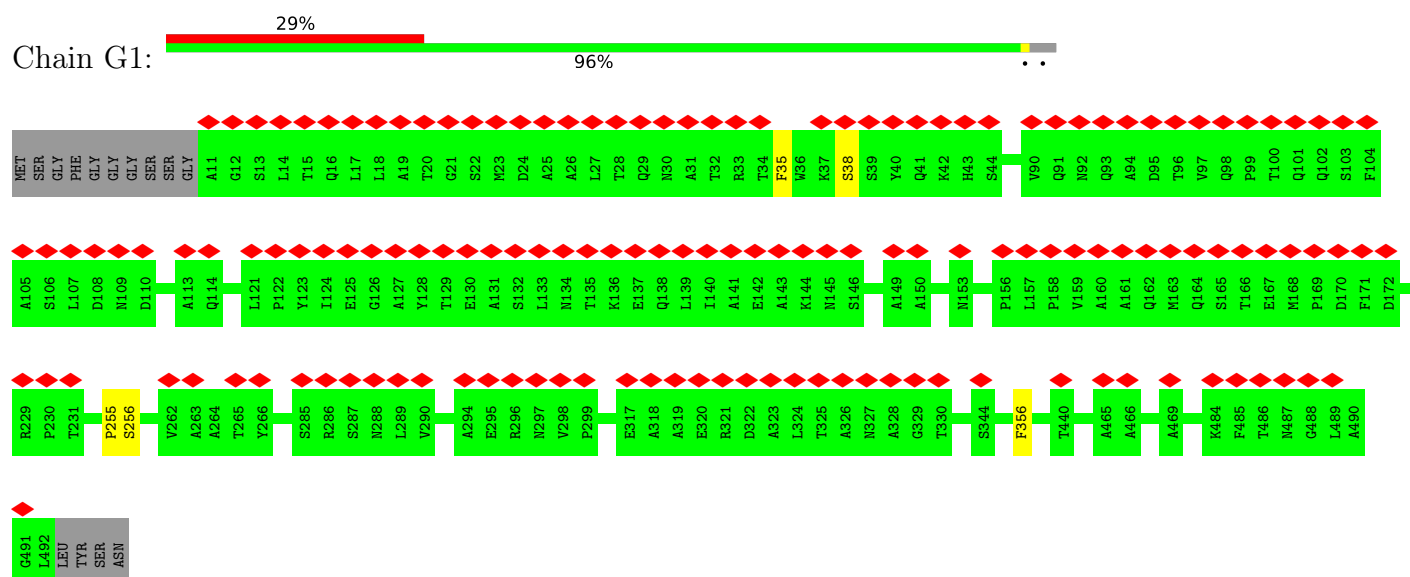
Chain F8:



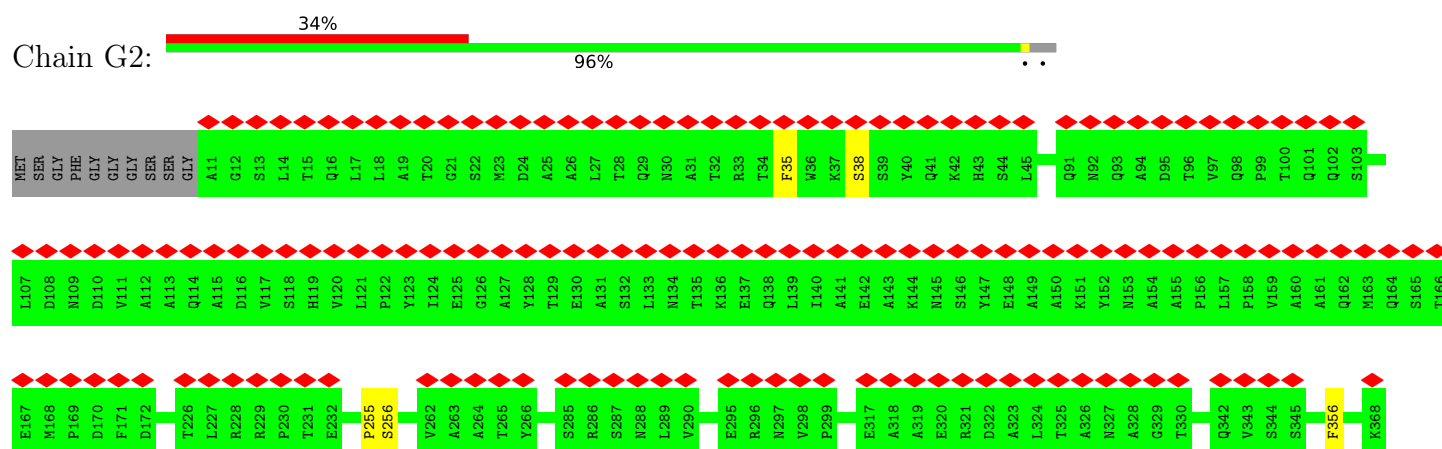
- Molecule 1: Major capsid protein

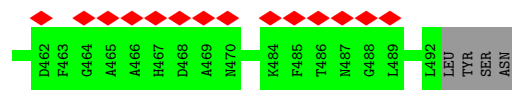


- Molecule 1: Major capsid protein

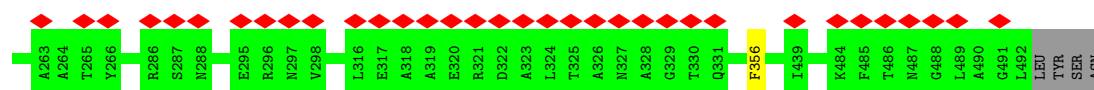
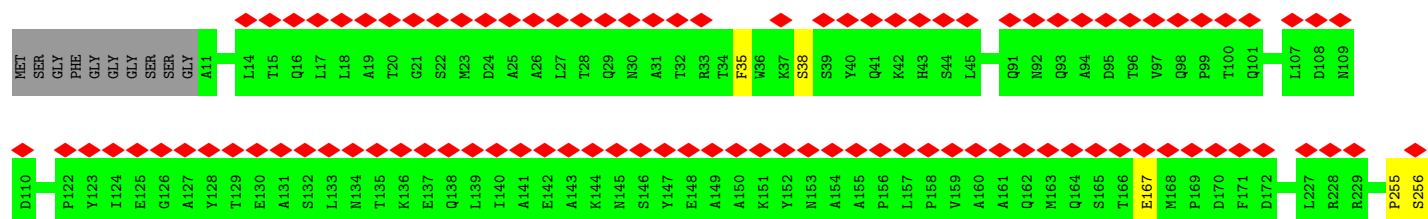


- Molecule 1: Major capsid protein

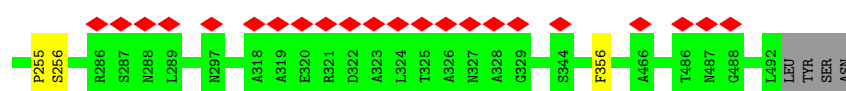
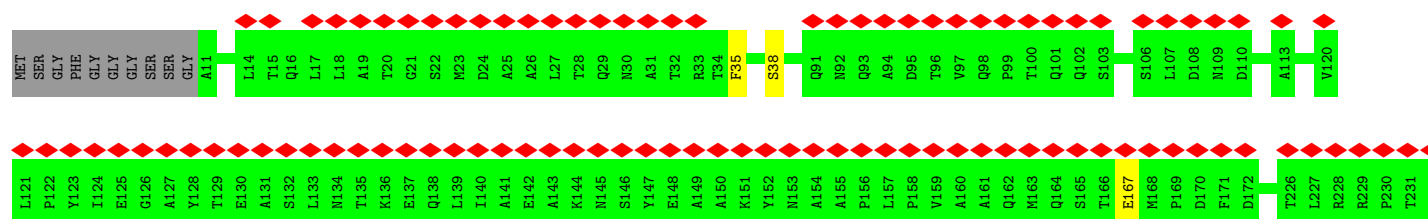




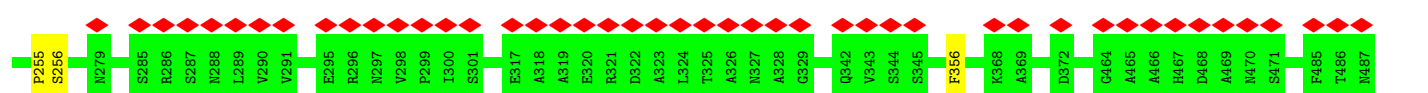
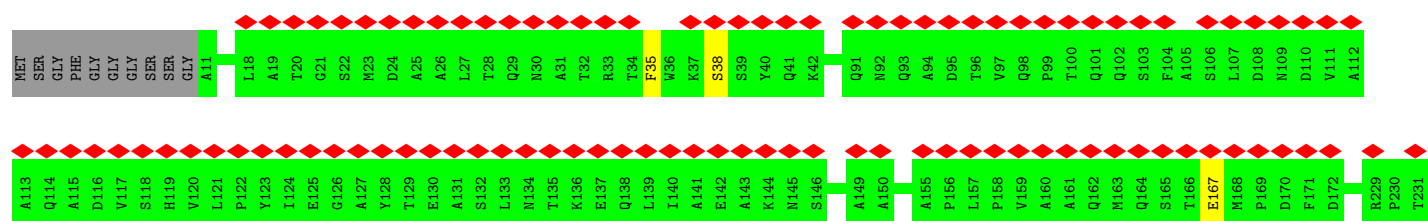
• Molecule 1: Major capsid protein

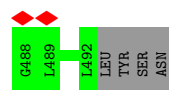


• Molecule 1: Major capsid protein

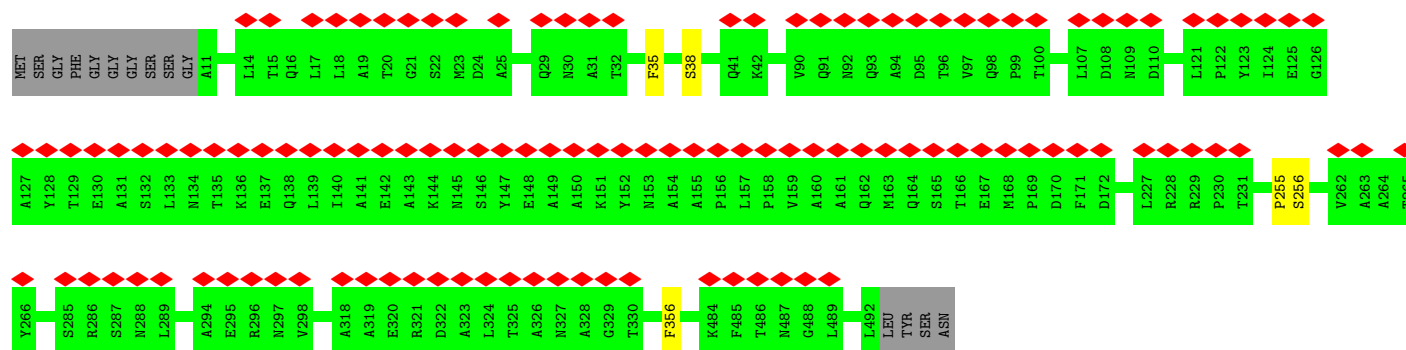


• Molecule 1: Major capsid protein

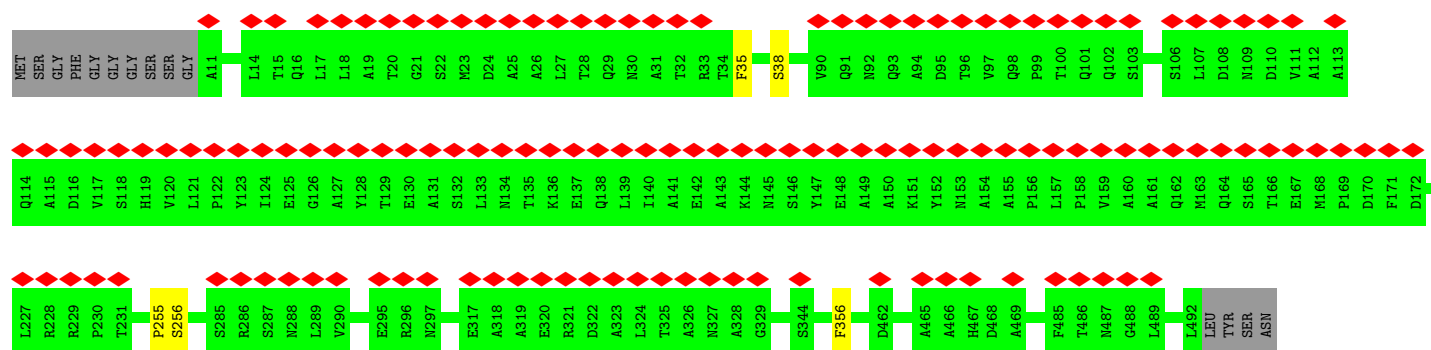




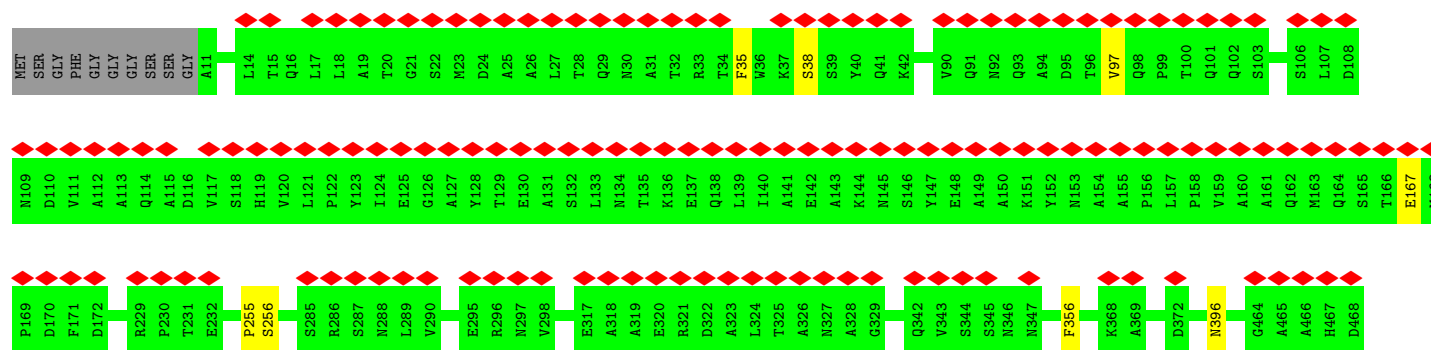
• Molecule 1: Major capsid protein

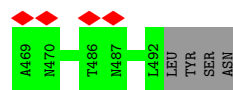


• Molecule 1: Major capsid protein

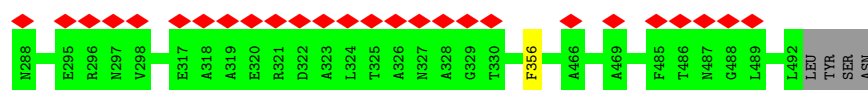
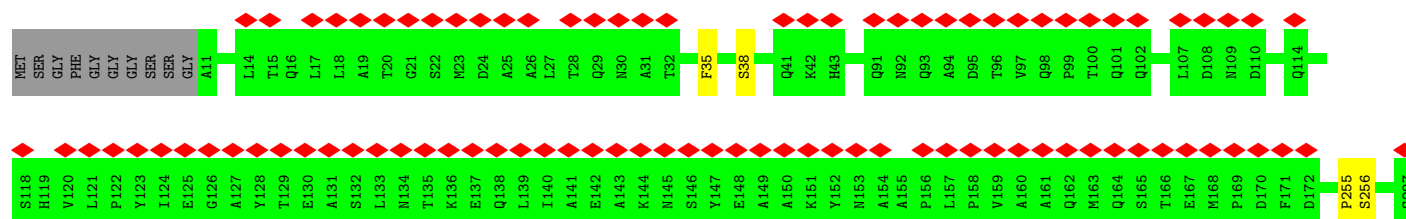


• Molecule 1: Major capsid protein

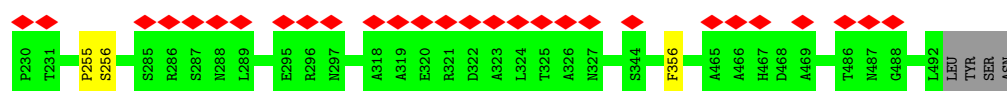
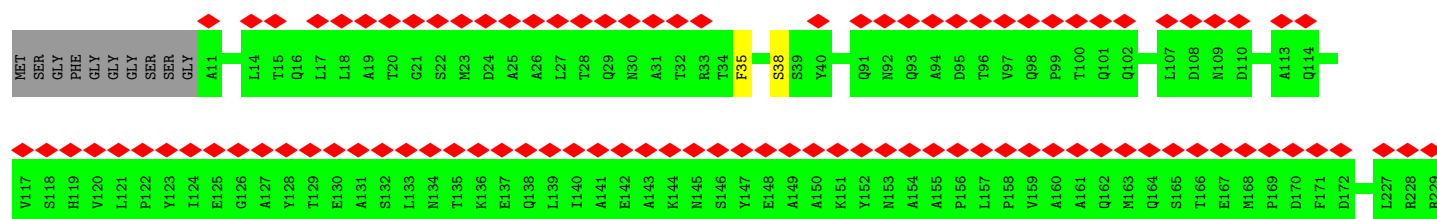




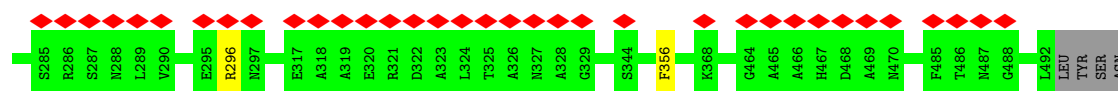
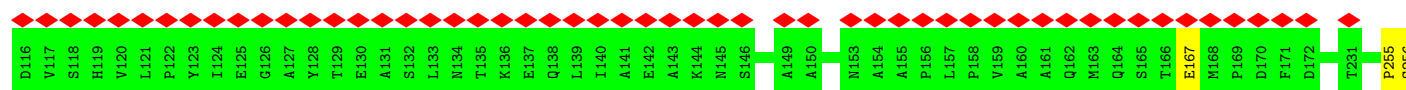
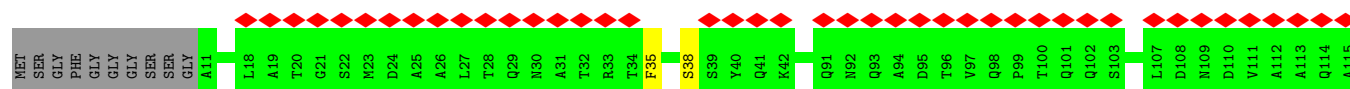
- Molecule 1: Major capsid protein



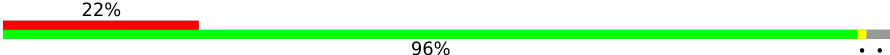
- Molecule 1: Major capsid protein

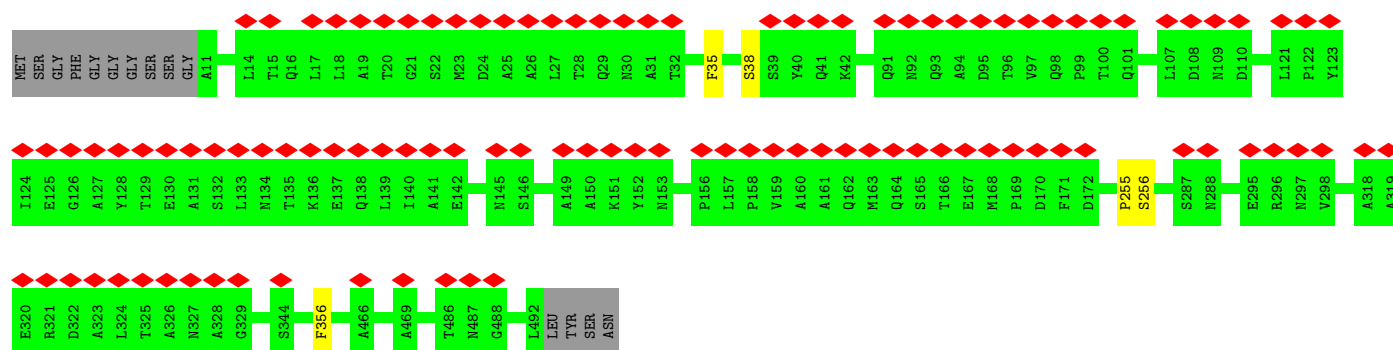


- Molecule 1: Major capsid protein

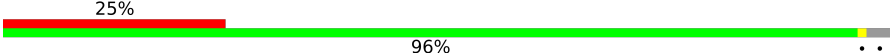


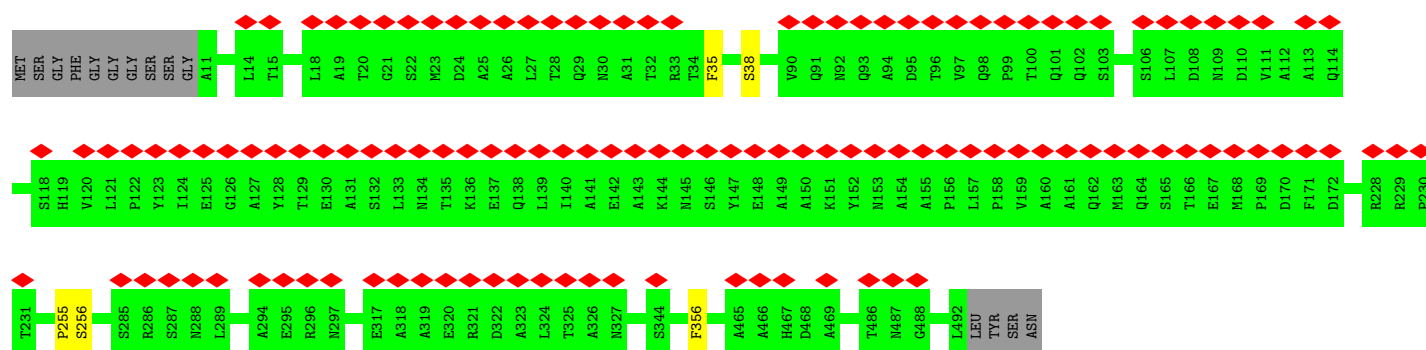
- Molecule 1: Major capsid protein

Chain H3: 

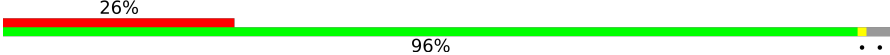


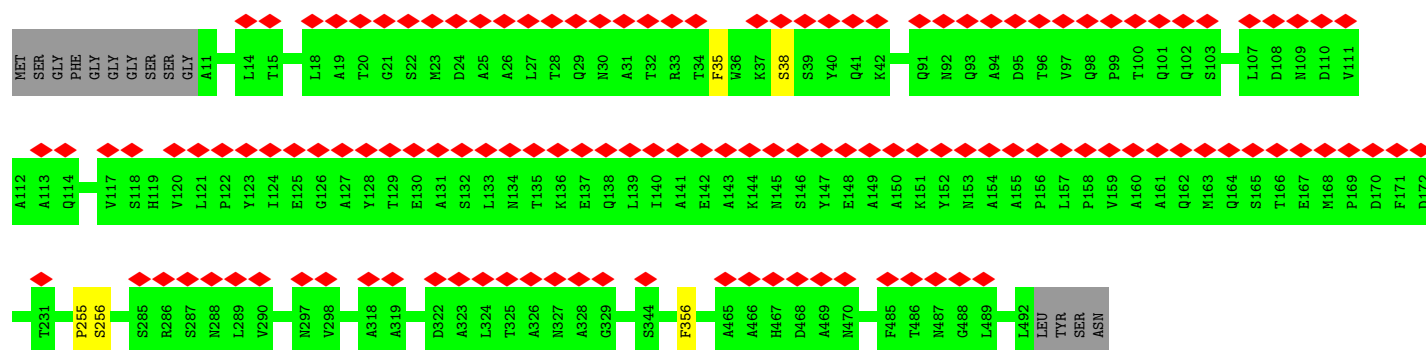
- Molecule 1: Major capsid protein

Chain H4: 

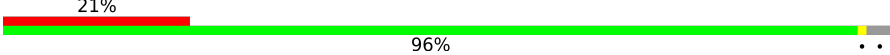


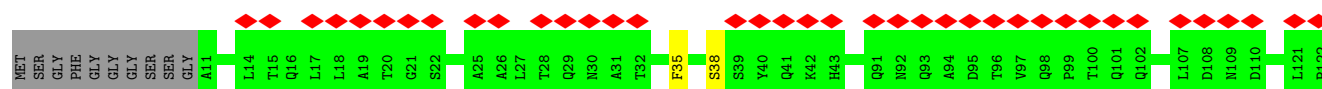
- Molecule 1: Major capsid protein

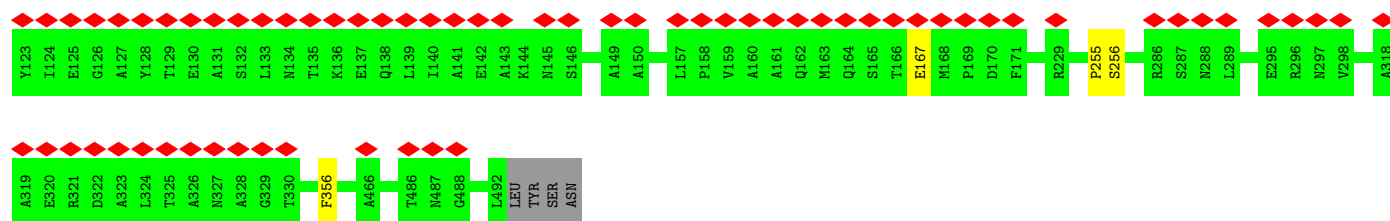
Chain H5: 



- Molecule 1: Major capsid protein

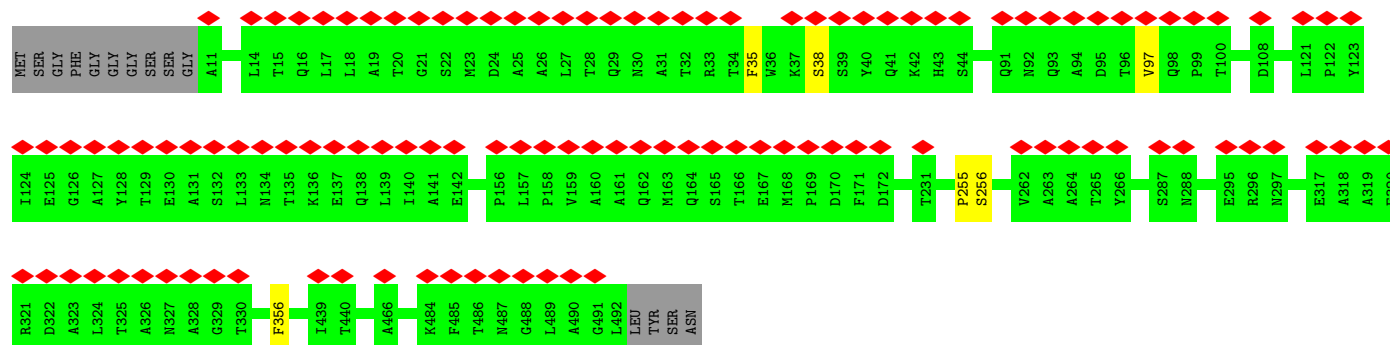
Chain H6: 





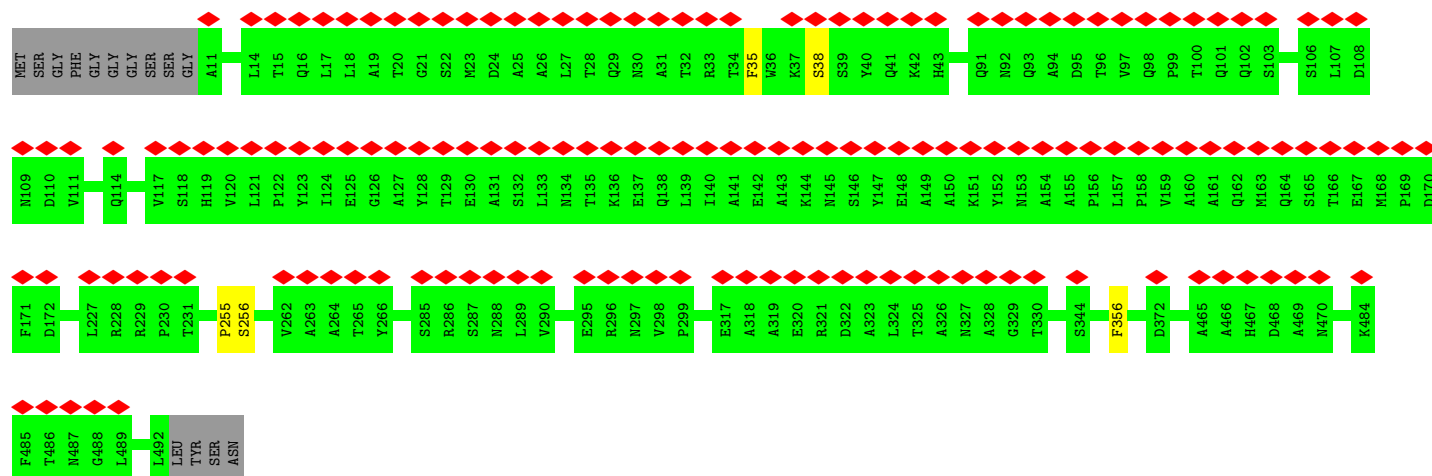
• Molecule 1: Major capsid protein

Chain H7: 23% 96%



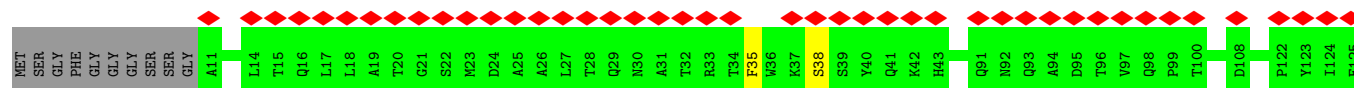
• Molecule 1: Major capsid protein

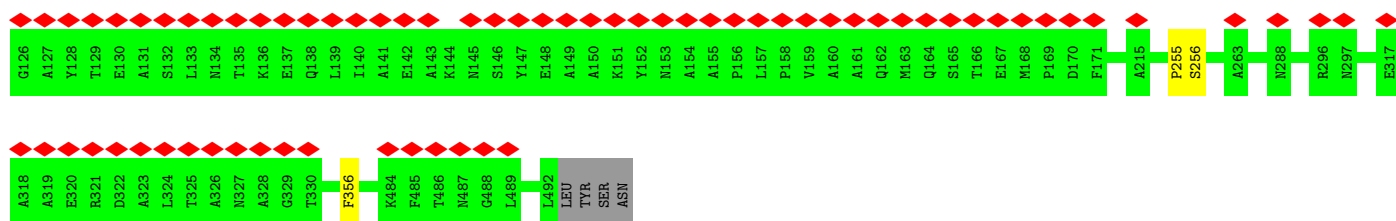
Chain H8: 31% 96%



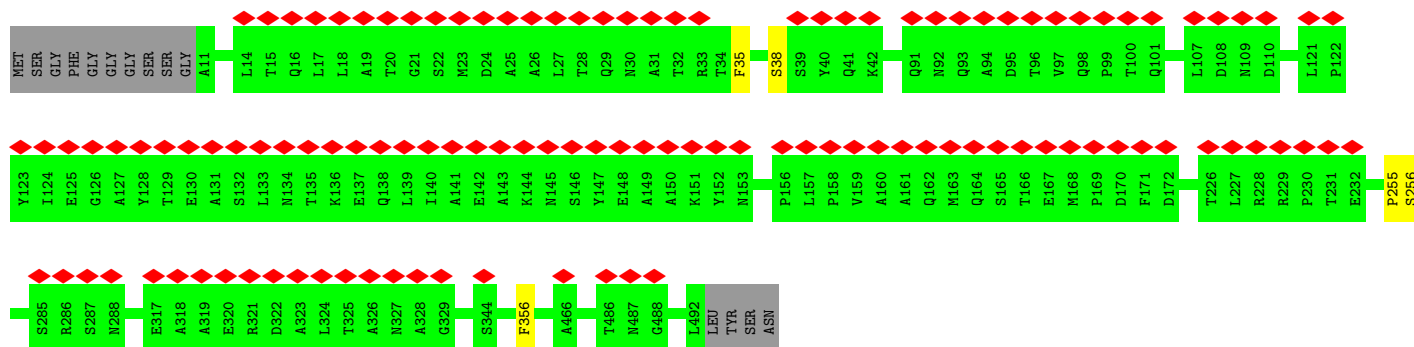
• Molecule 1: Major capsid protein

Chain H9: 23% 96%

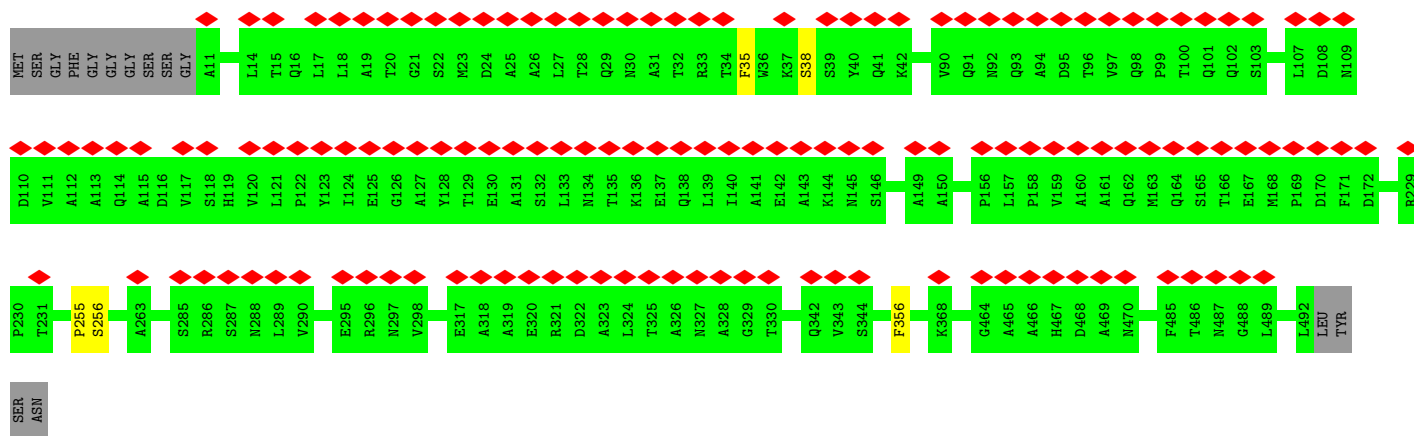




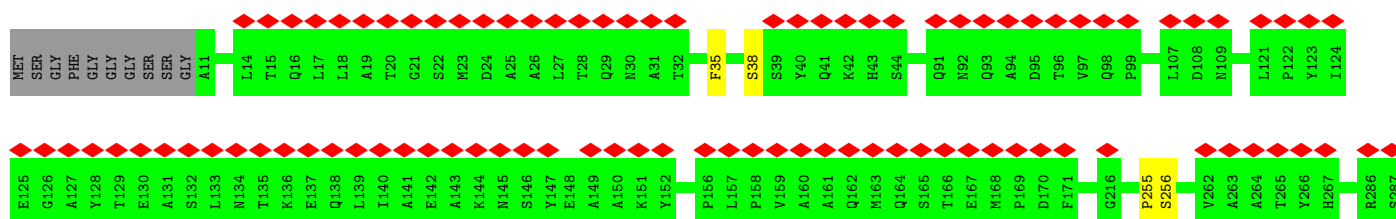
• Molecule 1: Major capsid protein

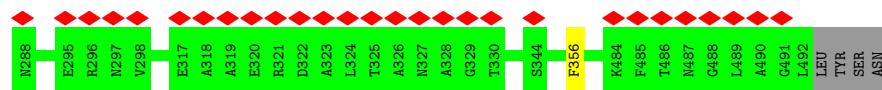


• Molecule 1: Major capsid protein



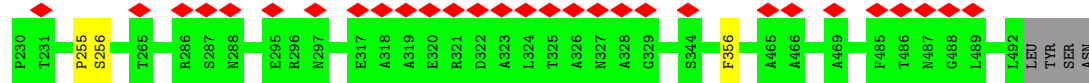
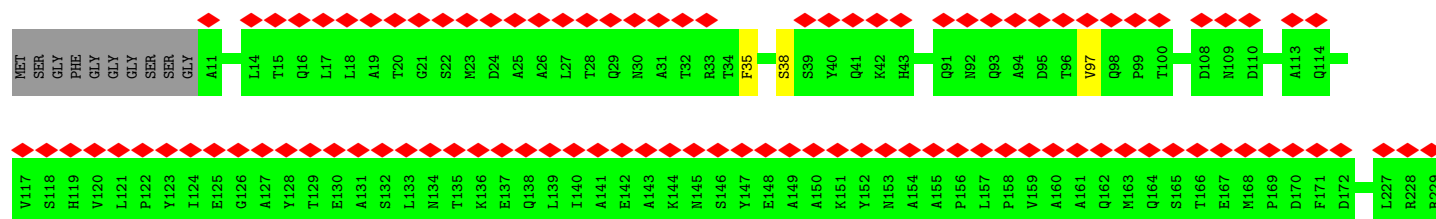
• Molecule 1: Major capsid protein





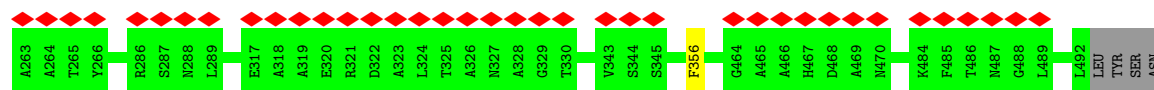
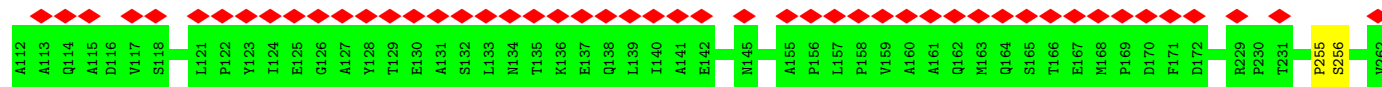
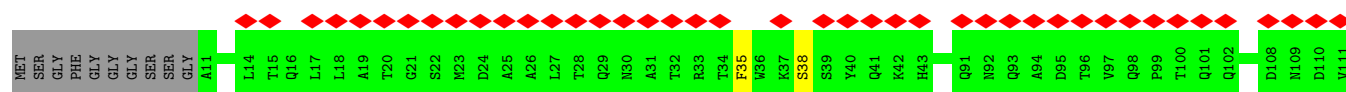
- Molecule 1: Major capsid protein

Chain I4: 26% 96%



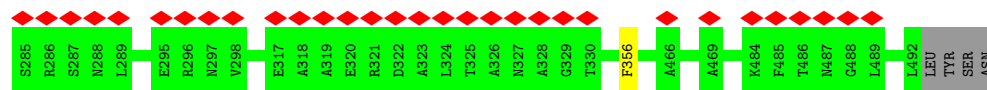
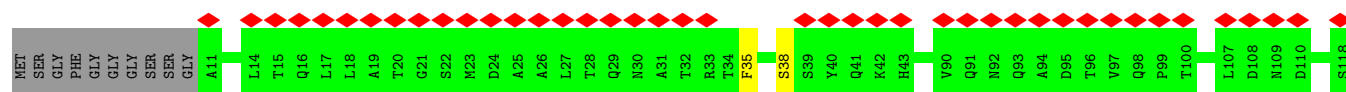
- Molecule 1: Major capsid protein

Chain I5: 26% 96%

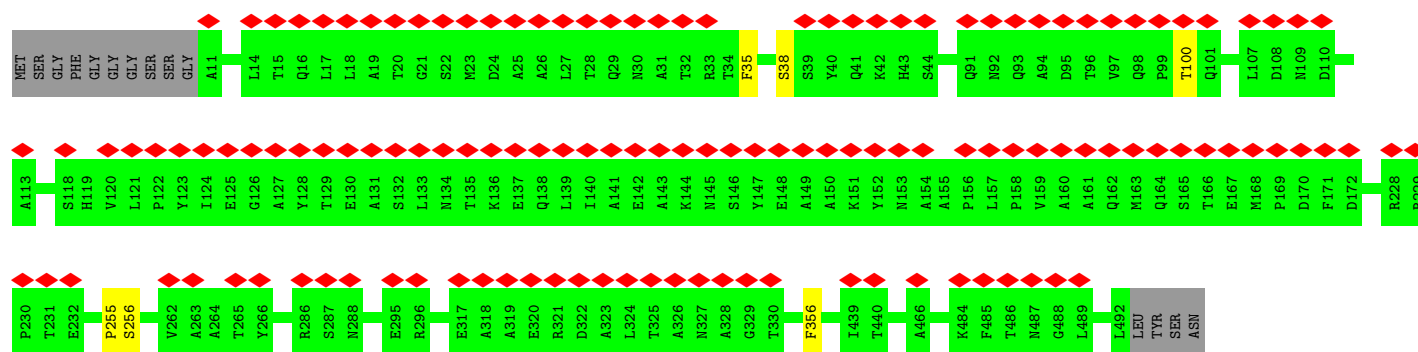


- Molecule 1: Major capsid protein

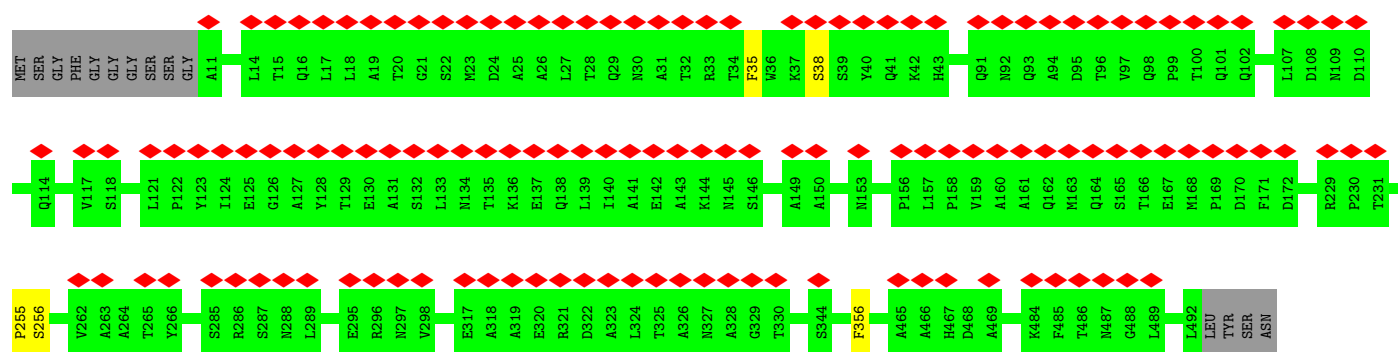
Chain I6: 25% 96%



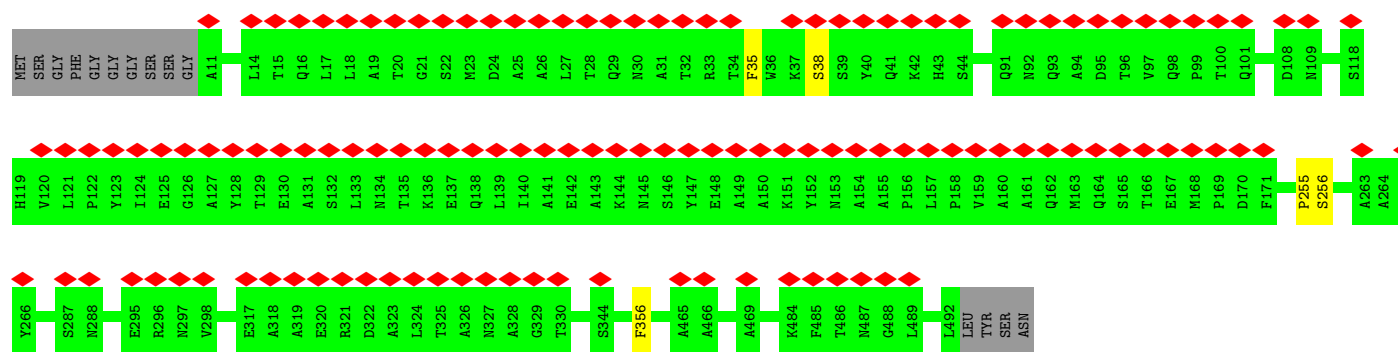
- Molecule 1: Major capsid protein



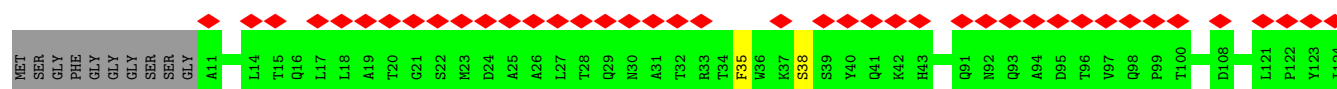
• Molecule 1: Major capsid protein

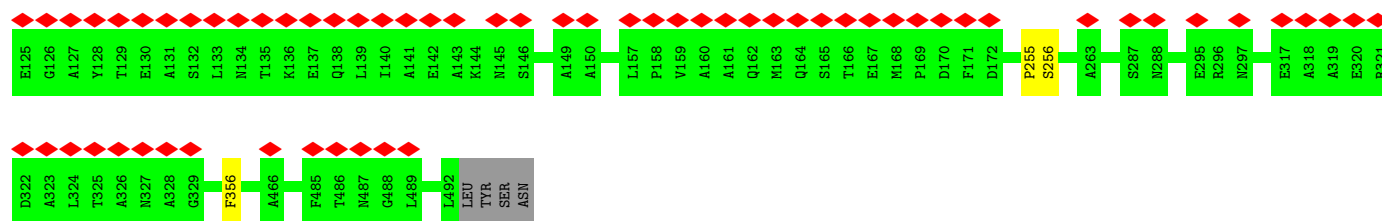


• Molecule 1: Major capsid protein

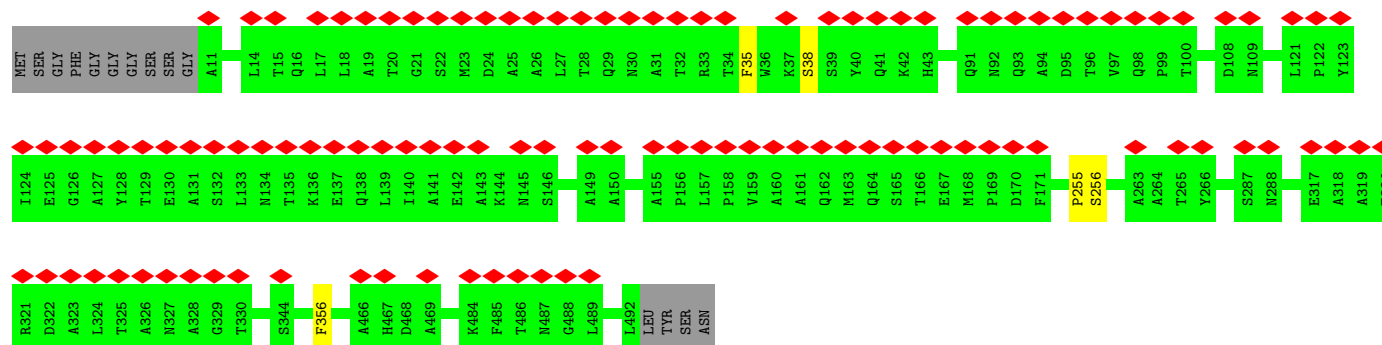


• Molecule 1: Major capsid protein

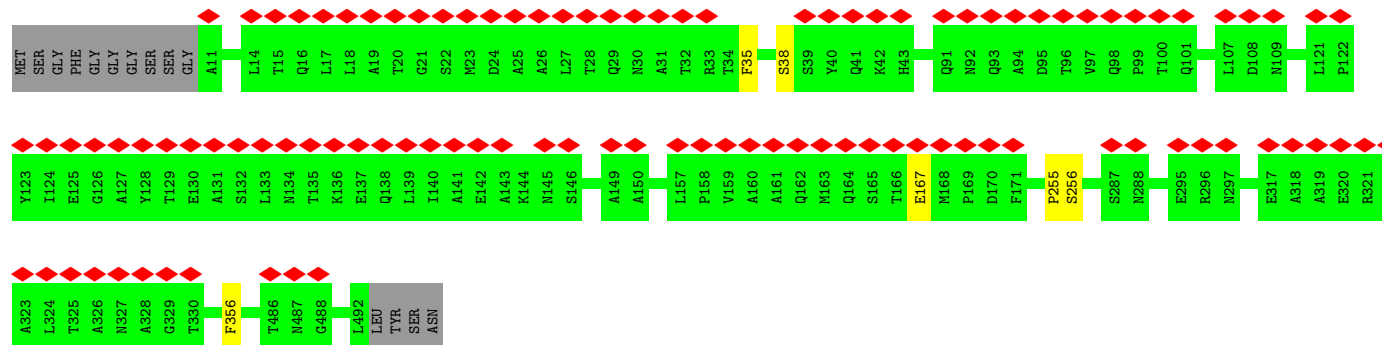




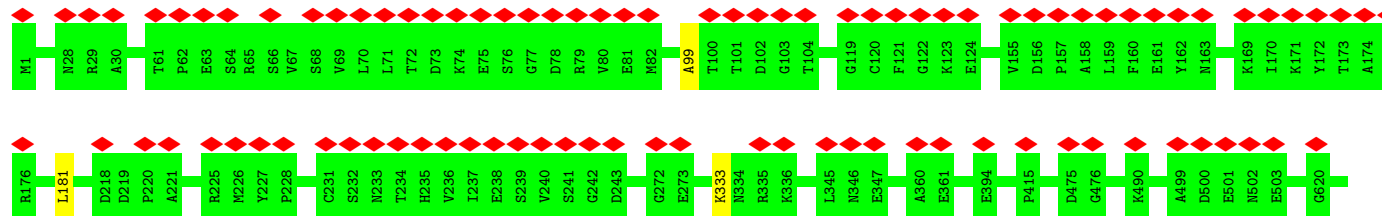
• Molecule 1: Major capsid protein

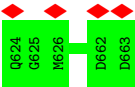


• Molecule 1: Major capsid protein



• Molecule 2: Penton protein





4 Experimental information

Property	Value	Source
EM reconstruction method	SUBTOMOGRAM AVERAGING	Depositor
Imposed symmetry	POINT, I	Depositor
Number of subtomograms used	3152	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 ($e^-/\text{\AA}^2$)	80	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	42000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.366	Depositor
Minimum map value	-0.056	Depositor
Average map value	0.102	Depositor
Map value standard deviation	0.238	Depositor
Recommended contour level	0.75	Depositor
Map size (Å)	2196.48, 2196.48, 2196.48	wwPDB
Map dimensions	352, 352, 352	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	6.24, 6.24, 6.24	Depositor

5 Model quality [i](#)

5.1 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 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	A1	0.65	0/1927	1.15	0/2407
1	A2	0.64	0/1927	1.15	0/2407
1	A3	0.64	0/1927	1.15	0/2407
1	A4	0.65	0/1927	1.15	0/2407
1	A5	0.65	0/1927	1.15	0/2407
1	A6	0.65	0/1927	1.15	0/2407
1	A7	0.65	0/1927	1.15	0/2407
1	A8	0.65	0/1927	1.16	0/2407
1	A9	0.65	0/1927	1.15	0/2407
1	B1	0.64	0/1927	1.15	0/2407
1	B2	0.65	0/1927	1.15	0/2407
1	B3	0.65	0/1927	1.15	0/2407
1	B4	0.65	0/1927	1.15	0/2407
1	B5	0.65	0/1927	1.15	0/2407
1	B6	0.65	0/1927	1.15	0/2407
1	B7	0.65	0/1927	1.15	0/2407
1	B8	0.65	0/1927	1.15	0/2407
1	B9	0.65	0/1927	1.15	0/2407
1	C1	0.64	0/1927	1.15	0/2407
1	C2	0.64	0/1927	1.15	0/2407
1	C3	0.65	0/1927	1.15	0/2407
1	C4	0.65	0/1927	1.15	0/2407
1	C5	0.65	0/1927	1.15	0/2407
1	C6	0.65	0/1927	1.15	0/2407
1	C7	0.64	0/1927	1.15	0/2407
1	C8	0.65	0/1927	1.15	0/2407
1	C9	0.65	0/1927	1.15	0/2407
1	D1	0.65	0/1927	1.15	0/2407
1	D2	0.65	0/1927	1.15	0/2407
1	D3	0.65	0/1927	1.15	0/2407
1	D4	0.65	0/1927	1.15	0/2407
1	D5	0.64	0/1927	1.15	0/2407
1	D6	0.64	0/1927	1.15	0/2407
1	D7	0.64	0/1927	1.15	0/2407

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	D8	0.65	0/1927	1.15	0/2407
1	D9	0.64	0/1927	1.15	0/2407
1	E1	0.65	0/1927	1.15	0/2407
1	E2	0.65	0/1927	1.15	0/2407
1	E3	0.65	0/1927	1.15	0/2407
1	E4	0.65	0/1927	1.15	0/2407
1	E5	0.64	0/1927	1.15	0/2407
1	E6	0.65	0/1927	1.15	0/2407
1	E7	0.65	0/1927	1.15	0/2407
1	E8	0.65	0/1927	1.15	0/2407
1	E9	0.65	0/1927	1.15	0/2407
1	F1	0.65	0/1927	1.15	0/2407
1	F2	0.64	0/1927	1.15	0/2407
1	F3	0.64	0/1927	1.15	0/2407
1	F4	0.65	0/1927	1.15	0/2407
1	F5	0.65	0/1927	1.15	0/2407
1	F6	0.65	0/1927	1.15	0/2407
1	F7	0.65	0/1927	1.15	0/2407
1	F8	0.64	0/1927	1.16	0/2407
1	F9	0.65	0/1927	1.15	0/2407
1	G1	0.65	0/1927	1.15	0/2407
1	G2	0.65	0/1927	1.15	0/2407
1	G3	0.64	0/1927	1.15	0/2407
1	G4	0.65	0/1927	1.15	0/2407
1	G5	0.64	0/1927	1.15	0/2407
1	G6	0.65	0/1927	1.15	0/2407
1	G7	0.65	0/1927	1.15	0/2407
1	G8	0.65	0/1927	1.15	0/2407
1	G9	0.64	0/1927	1.15	0/2407
1	H1	0.65	0/1927	1.15	0/2407
1	H2	0.65	0/1927	1.15	0/2407
1	H3	0.65	0/1927	1.15	0/2407
1	H4	0.65	0/1927	1.15	0/2407
1	H5	0.65	0/1927	1.15	0/2407
1	H6	0.65	0/1927	1.15	0/2407
1	H7	0.65	0/1927	1.15	0/2407
1	H8	0.65	0/1927	1.15	0/2407
1	H9	0.65	0/1927	1.15	0/2407
1	I1	0.64	0/1927	1.15	0/2407
1	I2	0.65	0/1927	1.15	0/2407
1	I3	0.65	0/1927	1.15	0/2407
1	I4	0.65	0/1927	1.15	0/2407
1	I5	0.65	0/1927	1.15	0/2407

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	I6	0.65	0/1927	1.15	0/2407
1	I7	0.64	0/1927	1.15	0/2407
1	I8	0.65	0/1927	1.15	0/2407
1	I9	0.65	0/1927	1.15	0/2407
1	J1	0.65	0/1927	1.15	0/2407
1	J2	0.65	0/1927	1.15	0/2407
1	J3	0.64	0/1927	1.15	0/2407
2	K	0.66	0/2652	1.12	0/3312
All	All	0.65	0/164520	1.15	0/205500

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
2	K	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	K	181	LEU	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in 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	A1	1928	0	503	6	0
1	A2	1928	0	503	6	0
1	A3	1928	0	503	6	0
1	A4	1928	0	503	6	0
1	A5	1928	0	503	6	0
1	A6	1928	0	503	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A7	1928	0	503	6	0
1	A8	1928	0	503	6	0
1	A9	1928	0	503	6	0
1	B1	1928	0	503	6	0
1	B2	1928	0	503	6	0
1	B3	1928	0	503	6	0
1	B4	1928	0	503	6	0
1	B5	1928	0	503	6	0
1	B6	1928	0	503	6	0
1	B7	1928	0	503	6	0
1	B8	1928	0	503	6	0
1	B9	1928	0	503	6	0
1	C1	1928	0	503	6	0
1	C2	1928	0	503	11	0
1	C3	1928	0	503	6	0
1	C4	1928	0	503	8	0
1	C5	1928	0	503	6	0
1	C6	1928	0	503	9	0
1	C7	1928	0	503	6	0
1	C8	1928	0	503	6	0
1	C9	1928	0	503	6	0
1	D1	1928	0	503	6	0
1	D2	1928	0	503	6	0
1	D3	1928	0	503	6	0
1	D4	1928	0	503	6	0
1	D5	1928	0	503	6	0
1	D6	1928	0	503	6	0
1	D7	1928	0	503	6	0
1	D8	1928	0	503	9	0
1	D9	1928	0	503	6	0
1	E1	1928	0	503	6	0
1	E2	1928	0	503	6	0
1	E3	1928	0	503	9	0
1	E4	1928	0	503	6	0
1	E5	1928	0	503	6	0
1	E6	1928	0	503	6	0
1	E7	1928	0	503	6	0
1	E8	1928	0	503	6	0
1	E9	1928	0	503	6	0
1	F1	1928	0	503	6	0
1	F2	1928	0	503	6	0
1	F3	1928	0	503	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F4	1928	0	503	6	0
1	F5	1928	0	503	6	0
1	F6	1928	0	503	6	0
1	F7	1928	0	503	6	0
1	F8	1928	0	503	7	0
1	F9	1928	0	503	6	0
1	G1	1928	0	503	6	0
1	G2	1928	0	503	6	0
1	G3	1928	0	503	6	0
1	G4	1928	0	503	6	0
1	G5	1928	0	503	6	0
1	G6	1928	0	503	6	0
1	G7	1928	0	503	6	0
1	G8	1928	0	503	8	0
1	G9	1928	0	503	6	0
1	H1	1928	0	503	6	0
1	H2	1928	0	503	8	0
1	H3	1928	0	503	6	0
1	H4	1928	0	503	6	0
1	H5	1928	0	503	6	0
1	H6	1928	0	503	6	0
1	H7	1928	0	503	7	0
1	H8	1928	0	503	6	0
1	H9	1928	0	503	6	0
1	I1	1928	0	503	6	0
1	I2	1928	0	503	6	0
1	I3	1928	0	503	6	0
1	I4	1928	0	503	7	0
1	I5	1928	0	503	6	0
1	I6	1928	0	503	6	0
1	I7	1928	0	503	8	0
1	I8	1928	0	503	6	0
1	I9	1928	0	503	6	0
1	J1	1928	0	503	6	0
1	J2	1928	0	503	6	0
1	J3	1928	0	503	6	0
2	K	2653	0	740	0	0
All	All	164605	0	42992	265	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 1.

All (265) 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:C2:194:GLY:HA3	1:C6:71:ARG:O	1.34	1.22
1:H2:296:ARG:O	1:I7:100:THR:O	1.64	1.16
1:B1:38:SER:N	1:B2:256:SER:O	1.88	1.06
1:D1:256:SER:O	1:D3:38:SER:N	1.88	1.06
1:I1:256:SER:O	1:I3:38:SER:N	1.88	1.06
1:C1:256:SER:O	1:C3:38:SER:N	1.88	1.06
1:H1:38:SER:N	1:H2:256:SER:O	1.89	1.06
1:I7:256:SER:O	1:I9:38:SER:N	1.89	1.06
1:D7:38:SER:N	1:D8:256:SER:O	1.88	1.06
1:E5:38:SER:N	1:E6:256:SER:O	1.88	1.06
1:H5:38:SER:N	1:H6:256:SER:O	1.89	1.06
1:B5:38:SER:N	1:B6:256:SER:O	1.89	1.05
1:E8:38:SER:N	1:E9:256:SER:O	1.89	1.05
1:F7:38:SER:N	1:F8:256:SER:O	1.88	1.05
1:J1:256:SER:O	1:J3:38:SER:N	1.88	1.05
1:C4:38:SER:N	1:C5:256:SER:O	1.88	1.05
1:D5:38:SER:N	1:D6:256:SER:O	1.89	1.05
1:G7:256:SER:O	1:G9:38:SER:N	1.89	1.05
1:A4:256:SER:O	1:A6:38:SER:N	1.89	1.05
1:E1:256:SER:O	1:E3:38:SER:N	1.89	1.05
1:G4:38:SER:N	1:G5:256:SER:O	1.89	1.05
1:H7:256:SER:O	1:H9:38:SER:N	1.88	1.05
1:F2:38:SER:N	1:F3:256:SER:O	1.88	1.05
1:F4:38:SER:N	1:F5:256:SER:O	1.89	1.05
1:A2:38:SER:N	1:A3:256:SER:O	1.89	1.04
1:A7:38:SER:N	1:A8:256:SER:O	1.88	1.04
1:C7:256:SER:O	1:C9:38:SER:N	1.89	1.04
1:G2:38:SER:N	1:G3:256:SER:O	1.88	1.04
1:I4:38:SER:N	1:I5:256:SER:O	1.88	1.04
1:B7:38:SER:N	1:B8:256:SER:O	1.88	1.04
1:D8:100:THR:CA	1:E3:296:ARG:O	2.10	1.00
1:F7:256:SER:O	1:F9:38:SER:N	2.13	0.81
1:I8:38:SER:N	1:I9:256:SER:O	2.14	0.81
1:A1:38:SER:N	1:A2:256:SER:O	2.13	0.81
1:B4:38:SER:N	1:B5:256:SER:O	2.13	0.81
1:C2:194:GLY:CA	1:C6:71:ARG:O	2.26	0.81
1:D2:38:SER:N	1:D3:256:SER:O	2.13	0.81
1:E4:38:SER:N	1:E5:256:SER:O	2.13	0.81
1:G1:38:SER:N	1:G2:256:SER:O	2.13	0.81
1:C2:38:SER:N	1:C3:256:SER:O	2.13	0.81
1:F1:38:SER:N	1:F2:256:SER:O	2.14	0.81
1:G8:38:SER:N	1:G9:256:SER:O	2.13	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D7:256:SER:O	1:D9:38:SER:N	2.13	0.81
1:F4:256:SER:O	1:F6:38:SER:N	2.13	0.81
1:C4:256:SER:O	1:C6:38:SER:N	2.13	0.81
1:C8:38:SER:N	1:C9:256:SER:O	2.14	0.81
1:E2:38:SER:N	1:E3:256:SER:O	2.14	0.81
1:B1:256:SER:O	1:B3:38:SER:N	2.13	0.80
1:H8:38:SER:N	1:H9:256:SER:O	2.13	0.80
1:I4:256:SER:O	1:I6:38:SER:N	2.13	0.80
1:H2:296:ARG:O	1:I7:100:THR:C	2.24	0.80
1:B7:256:SER:O	1:B9:38:SER:N	2.14	0.80
1:D4:38:SER:N	1:D5:256:SER:O	2.14	0.80
1:E7:38:SER:N	1:E8:256:SER:O	2.13	0.80
1:H1:256:SER:O	1:H3:38:SER:N	2.13	0.80
1:J2:38:SER:N	1:J3:256:SER:O	2.13	0.80
1:G4:256:SER:O	1:G6:38:SER:N	2.13	0.80
1:A7:256:SER:O	1:A9:38:SER:N	2.13	0.80
1:A5:38:SER:N	1:A6:256:SER:O	2.14	0.80
1:H4:38:SER:N	1:H5:256:SER:O	2.13	0.80
1:I2:38:SER:N	1:I3:256:SER:O	2.14	0.79
1:C2:353:ASN:O	1:C4:396:ASN:C	2.25	0.79
1:E4:256:SER:O	1:E6:38:SER:N	2.16	0.78
1:H4:256:SER:O	1:H6:38:SER:N	2.17	0.78
1:I5:38:SER:N	1:I6:256:SER:O	2.16	0.78
1:A4:38:SER:N	1:A5:256:SER:O	2.17	0.78
1:A8:38:SER:N	1:A9:256:SER:O	2.17	0.78
1:E1:38:SER:N	1:E2:256:SER:O	2.17	0.78
1:J1:38:SER:N	1:J2:256:SER:O	2.16	0.78
1:F8:38:SER:N	1:F9:256:SER:O	2.17	0.78
1:G5:38:SER:N	1:G6:256:SER:O	2.17	0.78
1:B8:38:SER:N	1:B9:256:SER:O	2.16	0.78
1:D4:256:SER:O	1:D6:38:SER:N	2.16	0.78
1:D8:38:SER:N	1:D9:256:SER:O	2.16	0.78
1:F5:38:SER:N	1:F6:256:SER:O	2.16	0.78
1:I1:38:SER:N	1:I2:256:SER:O	2.17	0.78
1:A1:256:SER:O	1:A3:38:SER:N	2.16	0.78
1:G1:256:SER:O	1:G3:38:SER:N	2.17	0.78
1:C7:38:SER:N	1:C8:256:SER:O	2.16	0.77
1:H7:38:SER:N	1:H8:256:SER:O	2.16	0.77
1:F1:256:SER:O	1:F3:38:SER:N	2.16	0.77
1:H2:38:SER:N	1:H3:256:SER:O	2.17	0.77
1:I7:38:SER:N	1:I8:256:SER:O	2.16	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E7:256:SER:O	1:E9:38:SER:N	2.17	0.77
1:B4:256:SER:O	1:B6:38:SER:N	2.17	0.77
1:C5:38:SER:N	1:C6:256:SER:O	2.17	0.77
1:C1:38:SER:N	1:C2:256:SER:O	2.16	0.77
1:B2:38:SER:N	1:B3:256:SER:O	2.17	0.77
1:D1:38:SER:N	1:D2:256:SER:O	2.17	0.77
1:G7:38:SER:N	1:G8:256:SER:O	2.16	0.76
1:D8:100:THR:C	1:E3:296:ARG:O	2.31	0.72
1:H5:38:SER:CA	1:H6:256:SER:O	2.41	0.69
1:H1:38:SER:CA	1:H2:256:SER:O	2.41	0.69
1:D1:256:SER:O	1:D3:38:SER:CA	2.41	0.69
1:E1:256:SER:O	1:E3:38:SER:CA	2.41	0.69
1:F2:38:SER:CA	1:F3:256:SER:O	2.41	0.69
1:F7:38:SER:CA	1:F8:256:SER:O	2.41	0.69
1:I4:38:SER:CA	1:I5:256:SER:O	2.41	0.69
1:G4:38:SER:CA	1:G5:256:SER:O	2.41	0.68
1:J1:256:SER:O	1:J3:38:SER:CA	2.41	0.68
1:C7:256:SER:O	1:C9:38:SER:CA	2.41	0.68
1:I1:256:SER:O	1:I3:38:SER:CA	2.41	0.68
1:A4:256:SER:O	1:A6:38:SER:CA	2.41	0.68
1:B1:38:SER:CA	1:B2:256:SER:O	2.41	0.68
1:B7:38:SER:CA	1:B8:256:SER:O	2.41	0.68
1:C4:38:SER:CA	1:C5:256:SER:O	2.41	0.68
1:G7:256:SER:O	1:G9:38:SER:CA	2.41	0.68
1:A2:38:SER:CA	1:A3:256:SER:O	2.41	0.68
1:D5:38:SER:CA	1:D6:256:SER:O	2.41	0.68
1:A7:38:SER:CA	1:A8:256:SER:O	2.41	0.68
1:D7:38:SER:CA	1:D8:256:SER:O	2.41	0.68
1:B5:38:SER:CA	1:B6:256:SER:O	2.41	0.68
1:F4:38:SER:CA	1:F5:256:SER:O	2.41	0.68
1:G2:38:SER:CA	1:G3:256:SER:O	2.41	0.68
1:E5:38:SER:CA	1:E6:256:SER:O	2.41	0.68
1:E8:38:SER:CA	1:E9:256:SER:O	2.41	0.67
1:I7:256:SER:O	1:I9:38:SER:CA	2.41	0.67
1:C1:256:SER:O	1:C3:38:SER:CA	2.41	0.67
1:H7:256:SER:O	1:H9:38:SER:CA	2.41	0.67
1:G7:255:PRO:O	1:G9:35:PHE:O	2.16	0.64
1:A2:35:PHE:O	1:A3:255:PRO:O	2.16	0.64
1:D7:35:PHE:O	1:D8:255:PRO:O	2.16	0.64
1:F2:35:PHE:O	1:F3:255:PRO:O	2.16	0.64
1:H1:35:PHE:O	1:H2:255:PRO:O	2.16	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A7:35:PHE:O	1:A8:255:PRO:O	2.16	0.64
1:F7:35:PHE:O	1:F8:255:PRO:O	2.16	0.64
1:G4:35:PHE:O	1:G5:255:PRO:O	2.16	0.64
1:I4:35:PHE:O	1:I5:255:PRO:O	2.16	0.64
1:E1:255:PRO:O	1:E3:35:PHE:O	2.16	0.64
1:E5:35:PHE:O	1:E6:255:PRO:O	2.16	0.64
1:I7:255:PRO:O	1:I9:35:PHE:O	2.16	0.64
1:C1:255:PRO:O	1:C3:35:PHE:O	2.16	0.64
1:F4:35:PHE:O	1:F5:255:PRO:O	2.16	0.64
1:D5:35:PHE:O	1:D6:255:PRO:O	2.16	0.63
1:E8:35:PHE:O	1:E9:255:PRO:O	2.16	0.63
1:B1:35:PHE:O	1:B2:255:PRO:O	2.16	0.63
1:B5:35:PHE:O	1:B6:255:PRO:O	2.16	0.63
1:G2:35:PHE:O	1:G3:255:PRO:O	2.16	0.63
1:J1:255:PRO:O	1:J3:35:PHE:O	2.16	0.63
1:B7:35:PHE:O	1:B8:255:PRO:O	2.16	0.63
1:C4:35:PHE:O	1:C5:255:PRO:O	2.16	0.63
1:H7:255:PRO:O	1:H9:35:PHE:O	2.16	0.63
1:I1:255:PRO:O	1:I3:35:PHE:O	2.16	0.63
1:D1:255:PRO:O	1:D3:35:PHE:O	2.16	0.62
1:H5:35:PHE:O	1:H6:255:PRO:O	2.16	0.62
1:A4:255:PRO:O	1:A6:35:PHE:O	2.16	0.62
1:C7:255:PRO:O	1:C9:35:PHE:O	2.16	0.62
1:D8:35:PHE:O	1:D9:255:PRO:O	2.19	0.61
1:D4:255:PRO:O	1:D6:35:PHE:O	2.19	0.61
1:H4:255:PRO:O	1:H6:35:PHE:O	2.19	0.61
1:A4:35:PHE:O	1:A5:255:PRO:O	2.19	0.61
1:C1:35:PHE:O	1:C2:255:PRO:O	2.19	0.61
1:G1:255:PRO:O	1:G3:35:PHE:O	2.19	0.61
1:E4:255:PRO:O	1:E6:35:PHE:O	2.19	0.61
1:G5:35:PHE:O	1:G6:255:PRO:O	2.19	0.61
1:D1:35:PHE:O	1:D2:255:PRO:O	2.19	0.61
1:E1:35:PHE:O	1:E2:255:PRO:O	2.19	0.60
1:E7:255:PRO:O	1:E9:35:PHE:O	2.19	0.60
1:F8:35:PHE:O	1:F9:255:PRO:O	2.19	0.60
1:H7:35:PHE:O	1:H8:255:PRO:O	2.19	0.60
1:J1:35:PHE:O	1:J2:255:PRO:O	2.19	0.60
1:A8:35:PHE:O	1:A9:255:PRO:O	2.19	0.60
1:C5:35:PHE:O	1:C6:255:PRO:O	2.19	0.60
1:H2:35:PHE:O	1:H3:255:PRO:O	2.19	0.60
1:B8:35:PHE:O	1:B9:255:PRO:O	2.19	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I1:35:PHE:O	1:I2:255:PRO:O	2.19	0.60
1:C7:35:PHE:O	1:C8:255:PRO:O	2.19	0.59
1:F5:35:PHE:O	1:F6:255:PRO:O	2.19	0.59
1:I5:35:PHE:O	1:I6:255:PRO:O	2.19	0.59
1:G7:35:PHE:O	1:G8:255:PRO:O	2.19	0.59
1:I7:35:PHE:O	1:I8:255:PRO:O	2.19	0.59
1:A1:255:PRO:O	1:A3:35:PHE:O	2.19	0.59
1:F1:255:PRO:O	1:F3:35:PHE:O	2.19	0.59
1:B4:255:PRO:O	1:B6:35:PHE:O	2.19	0.59
1:D8:100:THR:O	1:E3:296:ARG:O	2.20	0.58
1:B2:35:PHE:O	1:B3:255:PRO:O	2.19	0.58
1:G8:38:SER:CA	1:G9:256:SER:O	2.55	0.55
1:C2:38:SER:CA	1:C3:256:SER:O	2.55	0.55
1:F7:256:SER:O	1:F9:38:SER:CA	2.55	0.55
1:A1:38:SER:CA	1:A2:256:SER:O	2.55	0.55
1:E7:38:SER:CA	1:E8:256:SER:O	2.55	0.55
1:I8:38:SER:CA	1:I9:256:SER:O	2.55	0.55
1:C8:38:SER:CA	1:C9:256:SER:O	2.55	0.55
1:A7:256:SER:O	1:A9:38:SER:CA	2.55	0.55
1:E2:38:SER:CA	1:E3:256:SER:O	2.55	0.55
1:G4:256:SER:O	1:G6:38:SER:CA	2.55	0.55
1:D4:38:SER:CA	1:D5:256:SER:O	2.55	0.55
1:F1:38:SER:CA	1:F2:256:SER:O	2.55	0.55
1:H8:38:SER:CA	1:H9:256:SER:O	2.55	0.55
1:H4:38:SER:CA	1:H5:256:SER:O	2.55	0.54
1:J2:38:SER:CA	1:J3:256:SER:O	2.55	0.54
1:E4:38:SER:CA	1:E5:256:SER:O	2.55	0.54
1:H1:256:SER:O	1:H3:38:SER:CA	2.55	0.54
1:I4:256:SER:O	1:I6:38:SER:CA	2.55	0.54
1:D7:256:SER:O	1:D9:38:SER:CA	2.55	0.54
1:F4:256:SER:O	1:F6:38:SER:CA	2.55	0.54
1:B4:38:SER:CA	1:B5:256:SER:O	2.55	0.54
1:A5:38:SER:CA	1:A6:256:SER:O	2.55	0.54
1:B1:256:SER:O	1:B3:38:SER:CA	2.55	0.54
1:D2:38:SER:CA	1:D3:256:SER:O	2.55	0.54
1:I2:38:SER:CA	1:I3:256:SER:O	2.55	0.54
1:C4:256:SER:O	1:C6:38:SER:CA	2.55	0.54
1:G1:38:SER:CA	1:G2:256:SER:O	2.55	0.54
1:B7:256:SER:O	1:B9:38:SER:CA	2.55	0.53
1:C2:194:GLY:HA3	1:C6:71:ARG:C	2.27	0.51
1:D7:255:PRO:O	1:D9:35:PHE:O	2.31	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C2:35:PHE:O	1:C3:255:PRO:O	2.31	0.49
1:D4:35:PHE:O	1:D5:255:PRO:O	2.31	0.49
1:G4:255:PRO:O	1:G6:35:PHE:O	2.31	0.49
1:H4:35:PHE:O	1:H5:255:PRO:O	2.31	0.49
1:E4:35:PHE:O	1:E5:255:PRO:O	2.31	0.49
1:F7:255:PRO:O	1:F9:35:PHE:O	2.31	0.49
1:B4:35:PHE:O	1:B5:255:PRO:O	2.31	0.49
1:A1:35:PHE:O	1:A2:255:PRO:O	2.31	0.49
1:B1:255:PRO:O	1:B3:35:PHE:O	2.31	0.49
1:E2:35:PHE:O	1:E3:255:PRO:O	2.31	0.49
1:F4:255:PRO:O	1:F6:35:PHE:O	2.31	0.49
1:H8:35:PHE:O	1:H9:255:PRO:O	2.31	0.49
1:I4:255:PRO:O	1:I6:35:PHE:O	2.31	0.49
1:I8:35:PHE:O	1:I9:255:PRO:O	2.31	0.49
1:A5:35:PHE:O	1:A6:255:PRO:O	2.31	0.49
1:C2:353:ASN:O	1:C4:396:ASN:CA	2.61	0.49
1:D2:35:PHE:O	1:D3:255:PRO:O	2.31	0.49
1:F1:35:PHE:O	1:F2:255:PRO:O	2.31	0.49
1:E7:35:PHE:O	1:E8:255:PRO:O	2.31	0.49
1:G1:35:PHE:O	1:G2:255:PRO:O	2.31	0.49
1:J2:35:PHE:O	1:J3:255:PRO:O	2.31	0.49
1:C4:255:PRO:O	1:C6:35:PHE:O	2.31	0.48
1:A7:255:PRO:O	1:A9:35:PHE:O	2.31	0.48
1:B7:255:PRO:O	1:B9:35:PHE:O	2.31	0.48
1:G8:35:PHE:O	1:G9:255:PRO:O	2.31	0.48
1:H1:255:PRO:O	1:H3:35:PHE:O	2.31	0.48
1:I2:35:PHE:O	1:I3:255:PRO:O	2.31	0.48
1:C8:35:PHE:O	1:C9:255:PRO:O	2.31	0.47
1:G8:97:VAL:C	1:I4:97:VAL:O	2.59	0.45
1:B8:38:SER:CA	1:B9:256:SER:O	2.66	0.43
1:E4:256:SER:O	1:E6:38:SER:CA	2.66	0.43
1:H4:256:SER:O	1:H6:38:SER:CA	2.66	0.43
1:B2:38:SER:CA	1:B3:256:SER:O	2.67	0.43
1:C1:38:SER:CA	1:C2:256:SER:O	2.67	0.43
1:F8:38:SER:CA	1:F9:256:SER:O	2.66	0.43
1:G5:38:SER:CA	1:G6:256:SER:O	2.67	0.43
1:G7:38:SER:CA	1:G8:256:SER:O	2.66	0.43
1:J1:38:SER:CA	1:J2:256:SER:O	2.67	0.43
1:H2:38:SER:CA	1:H3:256:SER:O	2.67	0.43
1:C7:38:SER:CA	1:C8:256:SER:O	2.66	0.43
1:F5:38:SER:CA	1:F6:256:SER:O	2.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B4:256:SER:O	1:B6:38:SER:CA	2.67	0.43
1:C5:38:SER:CA	1:C6:256:SER:O	2.66	0.43
1:D1:38:SER:CA	1:D2:256:SER:O	2.67	0.43
1:I5:38:SER:CA	1:I6:256:SER:O	2.66	0.43
1:F3:353:ASN:O	1:G8:396:ASN:O	2.37	0.43
1:A4:38:SER:CA	1:A5:256:SER:O	2.66	0.43
1:F1:256:SER:O	1:F3:38:SER:CA	2.66	0.42
1:G1:256:SER:O	1:G3:38:SER:CA	2.66	0.42
1:I1:38:SER:CA	1:I2:256:SER:O	2.66	0.42
1:D4:256:SER:O	1:D6:38:SER:CA	2.66	0.42
1:A1:256:SER:O	1:A3:38:SER:CA	2.66	0.42
1:I7:38:SER:CA	1:I8:256:SER:O	2.66	0.42
1:A8:38:SER:CA	1:A9:256:SER:O	2.66	0.42
1:D8:38:SER:CA	1:D9:256:SER:O	2.66	0.42
1:E1:38:SER:CA	1:E2:256:SER:O	2.67	0.42
1:E7:256:SER:O	1:E9:38:SER:CA	2.67	0.42
1:H7:38:SER:CA	1:H8:256:SER:O	2.67	0.42
1:F8:97:VAL:CA	1:H7:97:VAL:O	2.70	0.40

There are no symmetry-related clashes.

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	A1	480/496 (97%)	463 (96%)	15 (3%)	2 (0%)	30	67
1	A2	480/496 (97%)	463 (96%)	16 (3%)	1 (0%)	43	78
1	A3	480/496 (97%)	463 (96%)	16 (3%)	1 (0%)	43	78
1	A4	480/496 (97%)	463 (96%)	15 (3%)	2 (0%)	30	67
1	A5	480/496 (97%)	463 (96%)	15 (3%)	2 (0%)	30	67
1	A6	480/496 (97%)	463 (96%)	16 (3%)	1 (0%)	43	78

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A7	480/496 (97%)	463 (96%)	16 (3%)	1 (0%)	43	78
1	A8	480/496 (97%)	463 (96%)	15 (3%)	2 (0%)	30	67
1	A9	480/496 (97%)	463 (96%)	16 (3%)	1 (0%)	43	78
1	B1	480/496 (97%)	463 (96%)	15 (3%)	2 (0%)	30	67
1	B2	480/496 (97%)	463 (96%)	16 (3%)	1 (0%)	43	78
1	B3	480/496 (97%)	463 (96%)	16 (3%)	1 (0%)	43	78
1	B4	480/496 (97%)	463 (96%)	16 (3%)	1 (0%)	43	78
1	B5	480/496 (97%)	463 (96%)	16 (3%)	1 (0%)	43	78
1	B6	480/496 (97%)	463 (96%)	15 (3%)	2 (0%)	30	67
1	B7	480/496 (97%)	463 (96%)	16 (3%)	1 (0%)	43	78
1	B8	480/496 (97%)	463 (96%)	15 (3%)	2 (0%)	30	67
1	B9	480/496 (97%)	463 (96%)	15 (3%)	2 (0%)	30	67
1	C1	480/496 (97%)	463 (96%)	15 (3%)	2 (0%)	30	67
1	C2	480/496 (97%)	463 (96%)	15 (3%)	2 (0%)	30	67
1	C3	480/496 (97%)	463 (96%)	15 (3%)	2 (0%)	30	67
1	C4	480/496 (97%)	463 (96%)	16 (3%)	1 (0%)	43	78
1	C5	480/496 (97%)	463 (96%)	15 (3%)	2 (0%)	30	67
1	C6	480/496 (97%)	463 (96%)	16 (3%)	1 (0%)	43	78
1	C7	480/496 (97%)	463 (96%)	15 (3%)	2 (0%)	30	67
1	C8	480/496 (97%)	463 (96%)	16 (3%)	1 (0%)	43	78
1	C9	480/496 (97%)	463 (96%)	16 (3%)	1 (0%)	43	78
1	D1	480/496 (97%)	463 (96%)	15 (3%)	2 (0%)	30	67
1	D2	480/496 (97%)	463 (96%)	16 (3%)	1 (0%)	43	78
1	D3	480/496 (97%)	463 (96%)	16 (3%)	1 (0%)	43	78
1	D4	480/496 (97%)	463 (96%)	16 (3%)	1 (0%)	43	78
1	D5	480/496 (97%)	463 (96%)	16 (3%)	1 (0%)	43	78
1	D6	480/496 (97%)	463 (96%)	16 (3%)	1 (0%)	43	78
1	D7	480/496 (97%)	463 (96%)	16 (3%)	1 (0%)	43	78
1	D8	480/496 (97%)	463 (96%)	15 (3%)	2 (0%)	30	67
1	D9	480/496 (97%)	463 (96%)	16 (3%)	1 (0%)	43	78
1	E1	480/496 (97%)	463 (96%)	15 (3%)	2 (0%)	30	67

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E2	480/496 (97%)	463 (96%)	16 (3%)	1 (0%)	43	78
1	E3	480/496 (97%)	463 (96%)	16 (3%)	1 (0%)	43	78
1	E4	480/496 (97%)	463 (96%)	15 (3%)	2 (0%)	30	67
1	E5	480/496 (97%)	463 (96%)	16 (3%)	1 (0%)	43	78
1	E6	480/496 (97%)	463 (96%)	16 (3%)	1 (0%)	43	78
1	E7	480/496 (97%)	463 (96%)	15 (3%)	2 (0%)	30	67
1	E8	480/496 (97%)	463 (96%)	15 (3%)	2 (0%)	30	67
1	E9	480/496 (97%)	463 (96%)	16 (3%)	1 (0%)	43	78
1	F1	480/496 (97%)	463 (96%)	16 (3%)	1 (0%)	43	78
1	F2	480/496 (97%)	463 (96%)	15 (3%)	2 (0%)	30	67
1	F3	480/496 (97%)	463 (96%)	16 (3%)	1 (0%)	43	78
1	F4	480/496 (97%)	463 (96%)	16 (3%)	1 (0%)	43	78
1	F5	480/496 (97%)	463 (96%)	15 (3%)	2 (0%)	30	67
1	F6	480/496 (97%)	463 (96%)	16 (3%)	1 (0%)	43	78
1	F7	480/496 (97%)	463 (96%)	16 (3%)	1 (0%)	43	78
1	F8	480/496 (97%)	463 (96%)	16 (3%)	1 (0%)	43	78
1	F9	480/496 (97%)	463 (96%)	16 (3%)	1 (0%)	43	78
1	G1	480/496 (97%)	463 (96%)	16 (3%)	1 (0%)	43	78
1	G2	480/496 (97%)	463 (96%)	16 (3%)	1 (0%)	43	78
1	G3	480/496 (97%)	463 (96%)	15 (3%)	2 (0%)	30	67
1	G4	480/496 (97%)	463 (96%)	15 (3%)	2 (0%)	30	67
1	G5	480/496 (97%)	463 (96%)	15 (3%)	2 (0%)	30	67
1	G6	480/496 (97%)	463 (96%)	16 (3%)	1 (0%)	43	78
1	G7	480/496 (97%)	463 (96%)	16 (3%)	1 (0%)	43	78
1	G8	480/496 (97%)	463 (96%)	15 (3%)	2 (0%)	30	67
1	G9	480/496 (97%)	463 (96%)	16 (3%)	1 (0%)	43	78
1	H1	480/496 (97%)	463 (96%)	16 (3%)	1 (0%)	43	78
1	H2	480/496 (97%)	463 (96%)	15 (3%)	2 (0%)	30	67
1	H3	480/496 (97%)	463 (96%)	16 (3%)	1 (0%)	43	78
1	H4	480/496 (97%)	463 (96%)	16 (3%)	1 (0%)	43	78
1	H5	480/496 (97%)	463 (96%)	16 (3%)	1 (0%)	43	78

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H6	480/496 (97%)	463 (96%)	15 (3%)	2 (0%)	30	67
1	H7	480/496 (97%)	463 (96%)	16 (3%)	1 (0%)	43	78
1	H8	480/496 (97%)	463 (96%)	16 (3%)	1 (0%)	43	78
1	H9	480/496 (97%)	463 (96%)	16 (3%)	1 (0%)	43	78
1	I1	480/496 (97%)	463 (96%)	16 (3%)	1 (0%)	43	78
1	I2	480/496 (97%)	463 (96%)	16 (3%)	1 (0%)	43	78
1	I3	480/496 (97%)	463 (96%)	16 (3%)	1 (0%)	43	78
1	I4	480/496 (97%)	463 (96%)	16 (3%)	1 (0%)	43	78
1	I5	480/496 (97%)	463 (96%)	16 (3%)	1 (0%)	43	78
1	I6	480/496 (97%)	463 (96%)	15 (3%)	2 (0%)	30	67
1	I7	480/496 (97%)	463 (96%)	16 (3%)	1 (0%)	43	78
1	I8	480/496 (97%)	463 (96%)	16 (3%)	1 (0%)	43	78
1	I9	480/496 (97%)	463 (96%)	16 (3%)	1 (0%)	43	78
1	J1	480/496 (97%)	463 (96%)	16 (3%)	1 (0%)	43	78
1	J2	480/496 (97%)	463 (96%)	16 (3%)	1 (0%)	43	78
1	J3	480/496 (97%)	463 (96%)	15 (3%)	2 (0%)	30	67
2	K	661/663 (100%)	635 (96%)	24 (4%)	2 (0%)	36	72
All	All	40981/42327 (97%)	39527 (96%)	1339 (3%)	115 (0%)	37	72

All (115) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	K	99	ALA
2	K	333	LYS
1	A1	167	GLU
1	A4	167	GLU
1	A5	167	GLU
1	A8	167	GLU
1	B1	167	GLU
1	B6	167	GLU
1	B8	167	GLU
1	B9	167	GLU
1	C1	167	GLU
1	C2	167	GLU
1	C3	167	GLU
1	C5	167	GLU

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Mol	Chain	Res	Type
1	C7	167	GLU
1	D1	167	GLU
1	D8	167	GLU
1	E1	167	GLU
1	E4	167	GLU
1	E7	167	GLU
1	E8	167	GLU
1	F2	167	GLU
1	F5	167	GLU
1	G3	167	GLU
1	G4	167	GLU
1	G5	167	GLU
1	G8	167	GLU
1	H2	167	GLU
1	H6	167	GLU
1	I6	167	GLU
1	J3	167	GLU
1	A1	356	PHE
1	A2	356	PHE
1	A3	356	PHE
1	A4	356	PHE
1	A5	356	PHE
1	A6	356	PHE
1	A7	356	PHE
1	A8	356	PHE
1	A9	356	PHE
1	B1	356	PHE
1	B2	356	PHE
1	B3	356	PHE
1	B4	356	PHE
1	B5	356	PHE
1	B6	356	PHE
1	B7	356	PHE
1	B8	356	PHE
1	B9	356	PHE
1	C1	356	PHE
1	C2	356	PHE
1	C3	356	PHE
1	C4	356	PHE
1	C5	356	PHE
1	C6	356	PHE
1	C7	356	PHE

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Mol	Chain	Res	Type
1	C8	356	PHE
1	C9	356	PHE
1	D1	356	PHE
1	D2	356	PHE
1	D3	356	PHE
1	D4	356	PHE
1	D5	356	PHE
1	D6	356	PHE
1	D7	356	PHE
1	D8	356	PHE
1	D9	356	PHE
1	E1	356	PHE
1	E2	356	PHE
1	E3	356	PHE
1	E4	356	PHE
1	E5	356	PHE
1	E6	356	PHE
1	E7	356	PHE
1	E8	356	PHE
1	E9	356	PHE
1	F1	356	PHE
1	F2	356	PHE
1	F3	356	PHE
1	F4	356	PHE
1	F5	356	PHE
1	F6	356	PHE
1	F7	356	PHE
1	F8	356	PHE
1	F9	356	PHE
1	G1	356	PHE
1	G2	356	PHE
1	G3	356	PHE
1	G4	356	PHE
1	G5	356	PHE
1	G6	356	PHE
1	G7	356	PHE
1	G8	356	PHE
1	G9	356	PHE
1	H1	356	PHE
1	H2	356	PHE
1	H3	356	PHE
1	H4	356	PHE

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Mol	Chain	Res	Type
1	H5	356	PHE
1	H6	356	PHE
1	H7	356	PHE
1	H8	356	PHE
1	H9	356	PHE
1	I1	356	PHE
1	I2	356	PHE
1	I3	356	PHE
1	I4	356	PHE
1	I5	356	PHE
1	I6	356	PHE
1	I7	356	PHE
1	I8	356	PHE
1	I9	356	PHE
1	J1	356	PHE
1	J2	356	PHE
1	J3	356	PHE

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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.

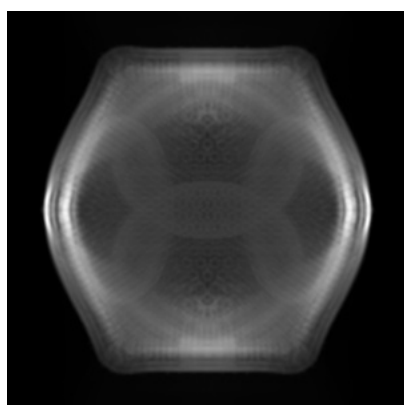
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-19035. These allow visual inspection of the internal detail of the map and identification of artifacts.

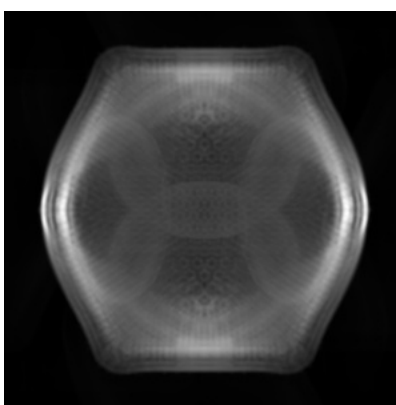
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

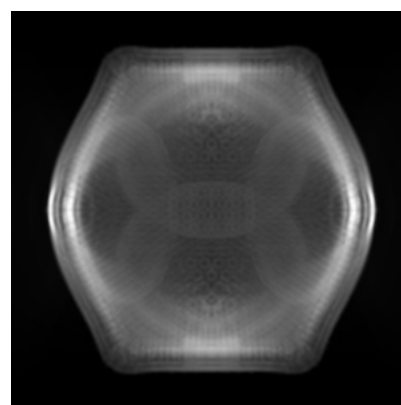
6.1.1 Primary map



X



Y

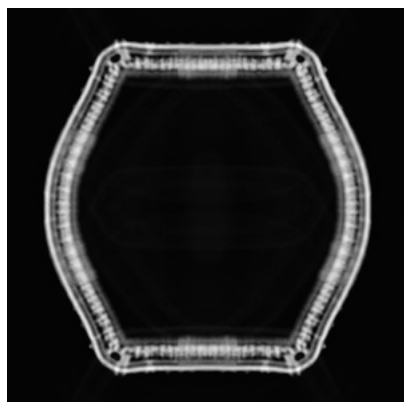


Z

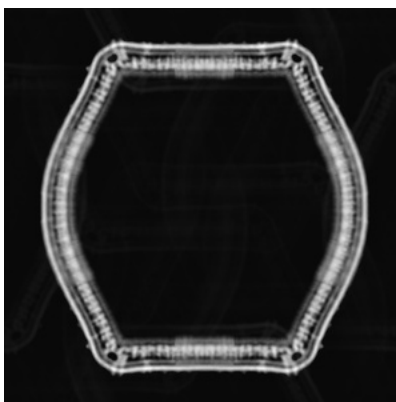
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 176



Y Index: 176

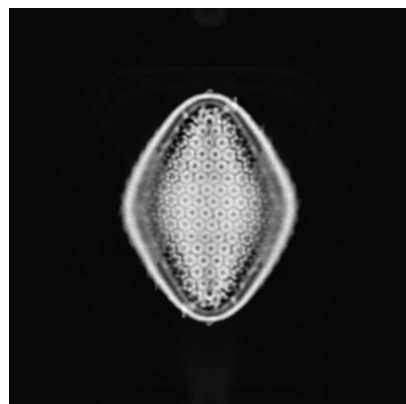


Z Index: 176

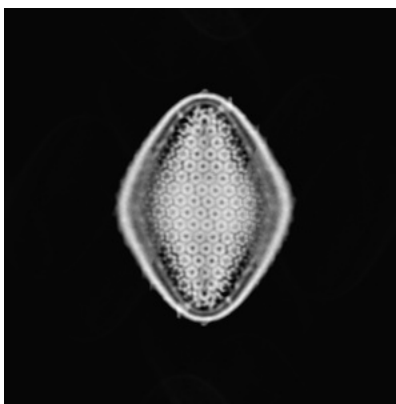
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

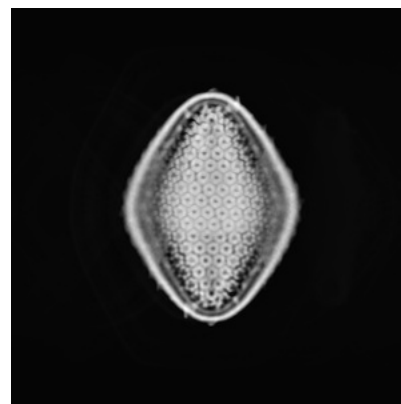
6.3.1 Primary map



X Index: 299



Y Index: 299

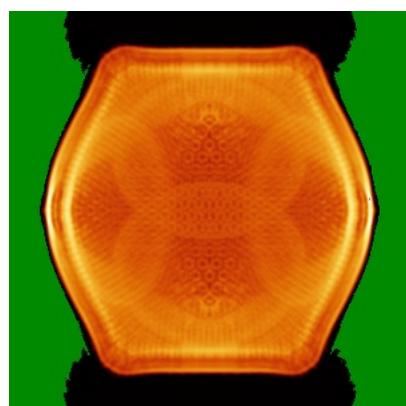


Z Index: 299

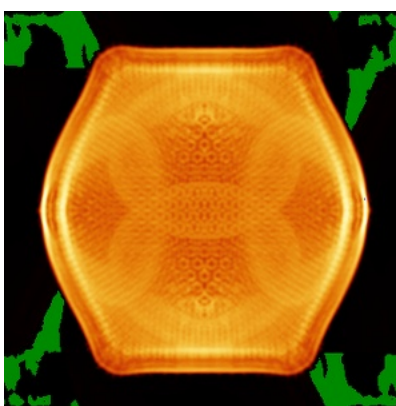
The images above show the largest variance slices of the map in three orthogonal directions.

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

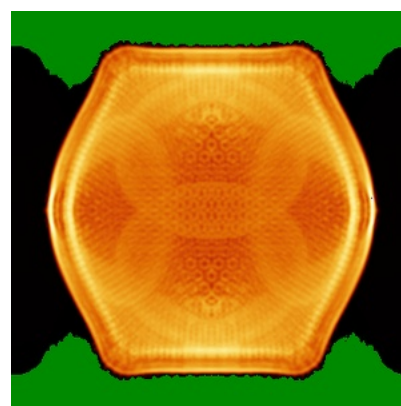
6.4.1 Primary map



X



Y

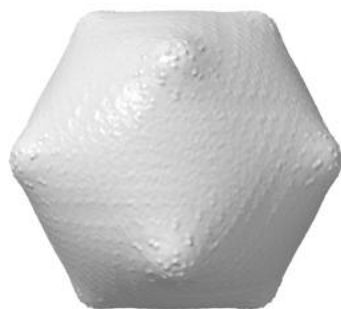


Z

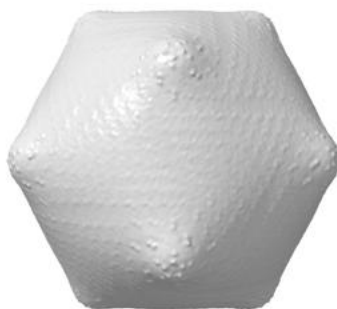
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

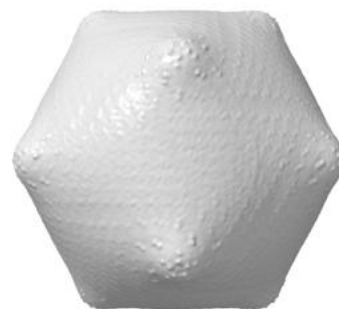
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.75. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

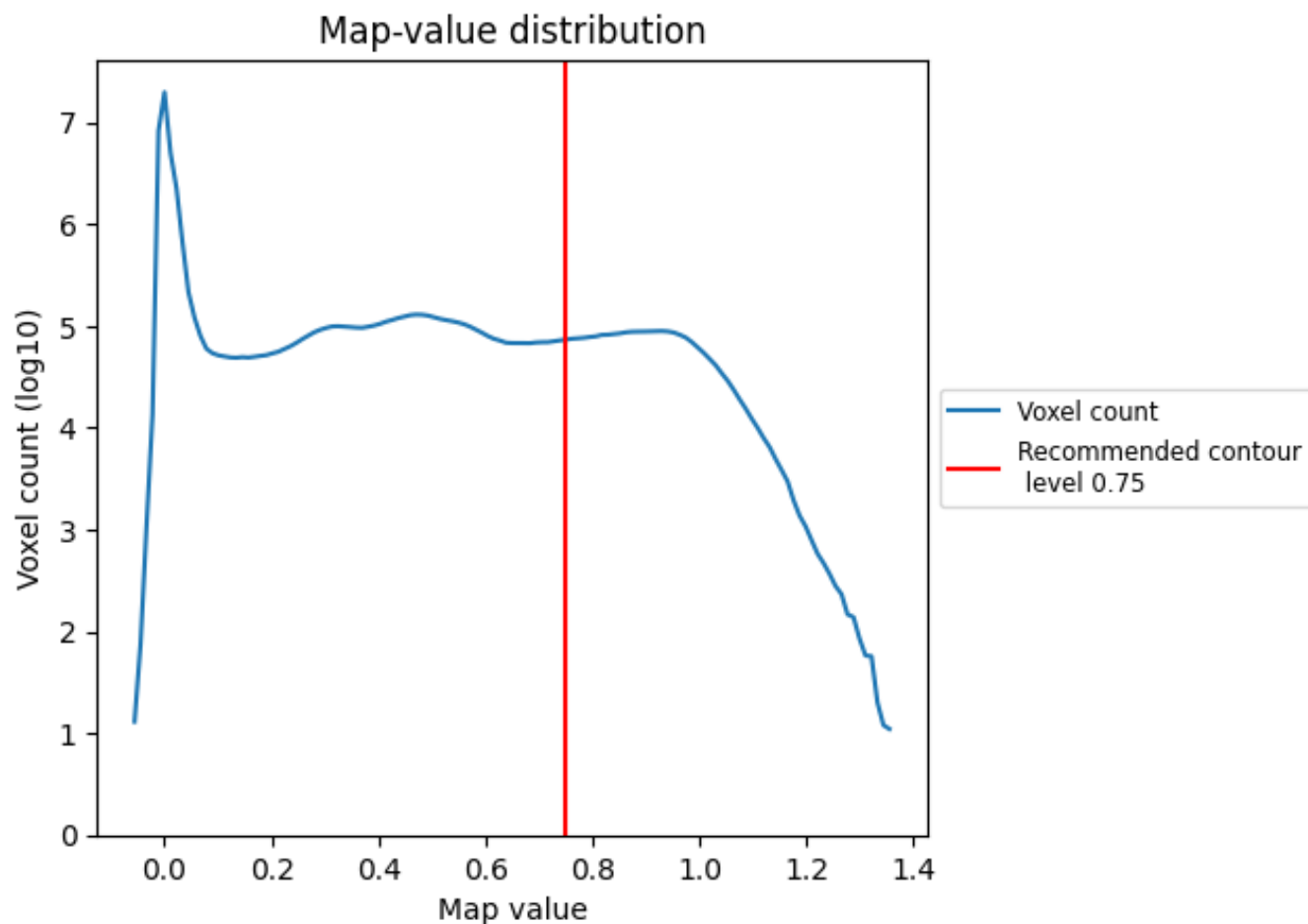
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

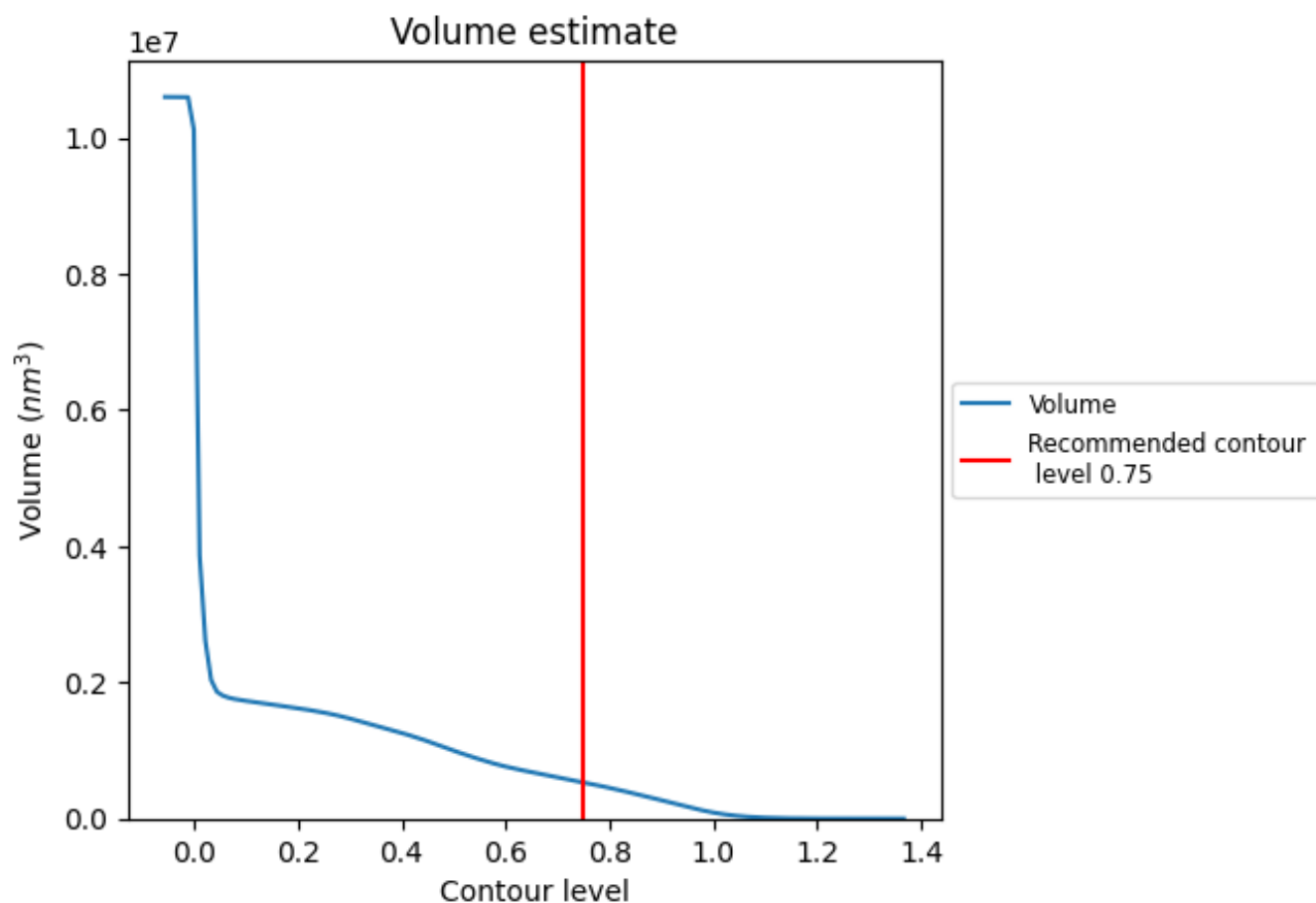
This section contains the results of statistical analysis of the map.

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.

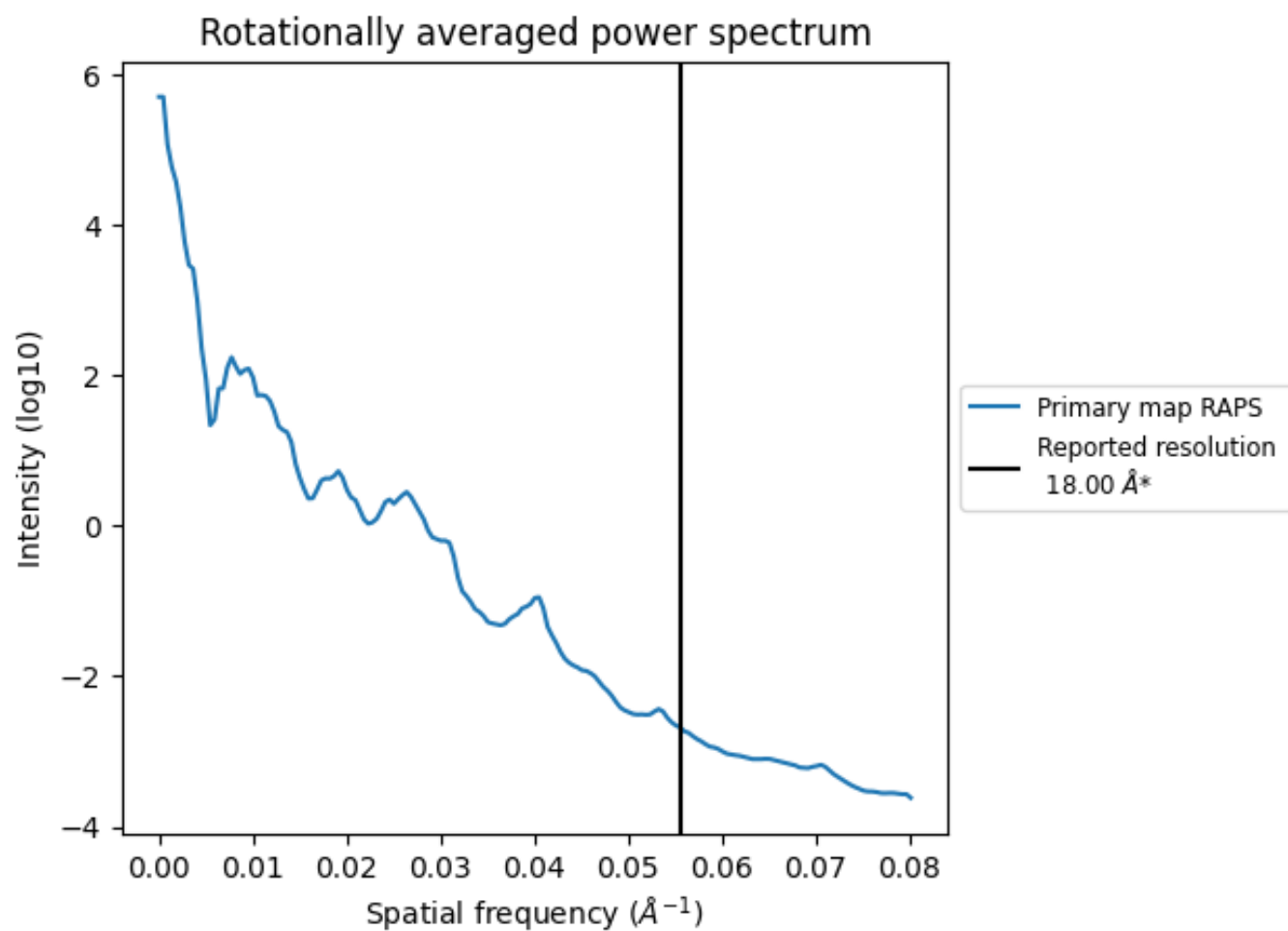
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 532934 nm³; this corresponds to an approximate mass of 481413 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 0.056 Å⁻¹

8 Fourier-Shell correlation ⓘ

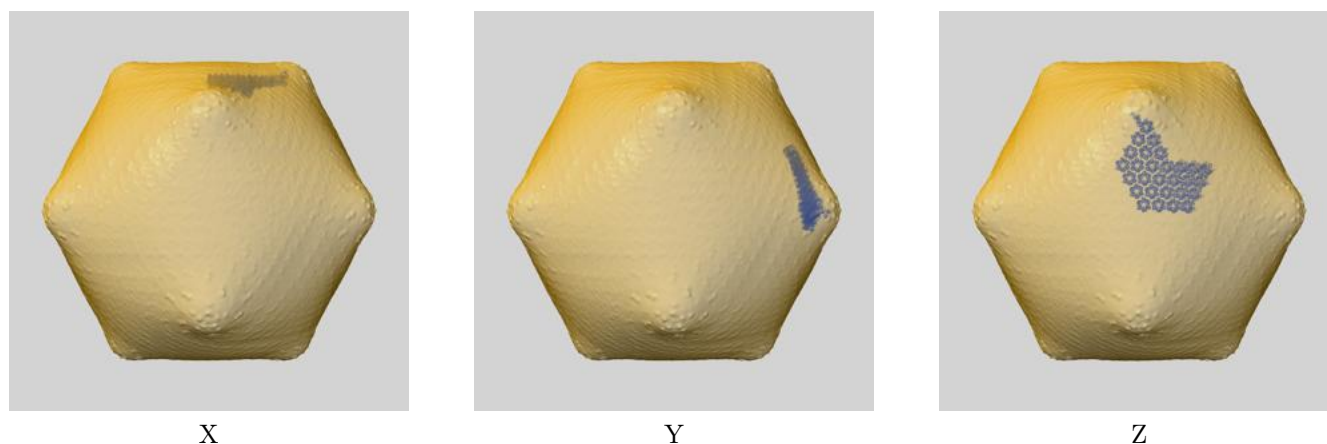
This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

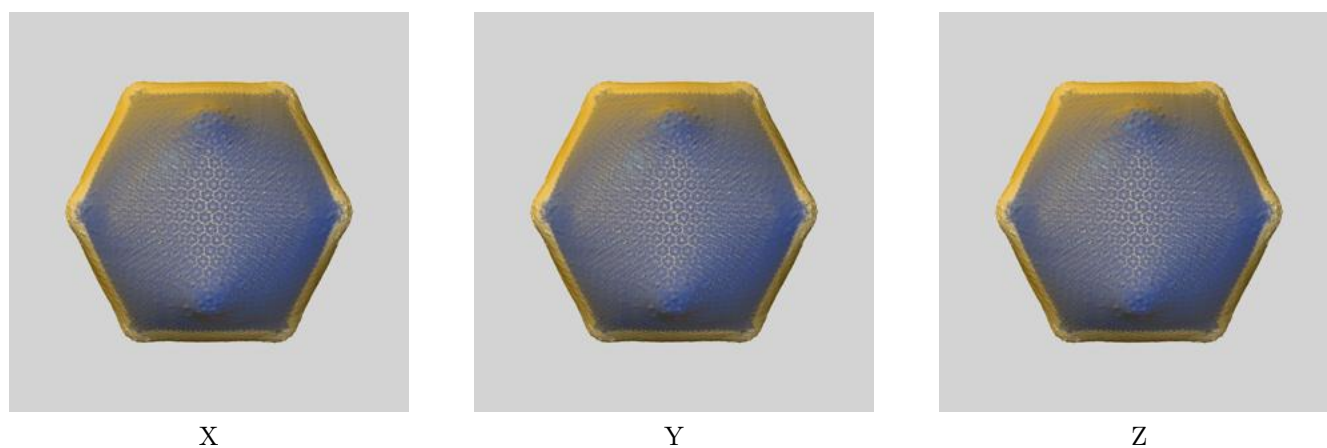
This section contains information regarding the fit between EMDB map EMD-19035 and PDB model 8RBS. Per-residue inclusion information can be found in section 3 on page 12.

9.1 Map-model overlays

9.1.1 Map-model overlay [i](#)

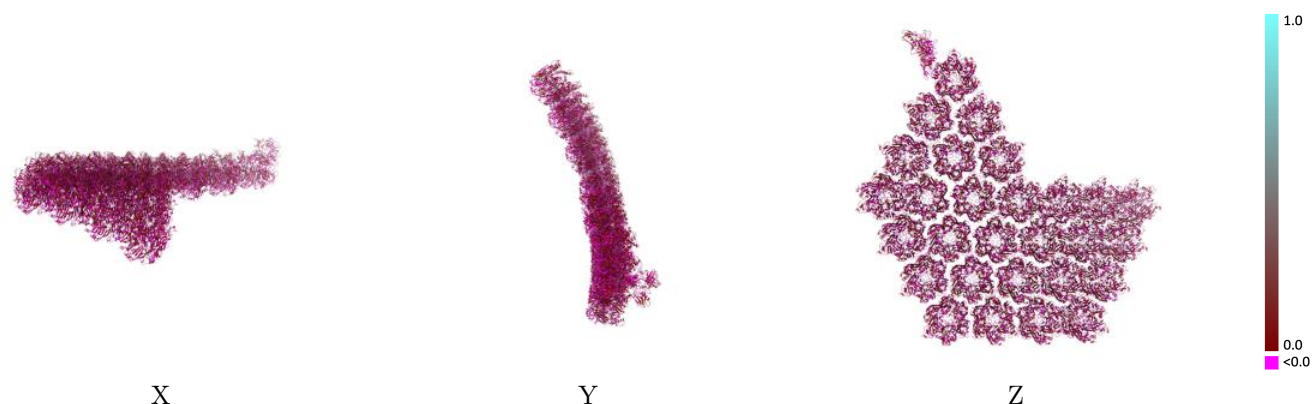


9.1.2 Map-model assembly overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.75 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](#)

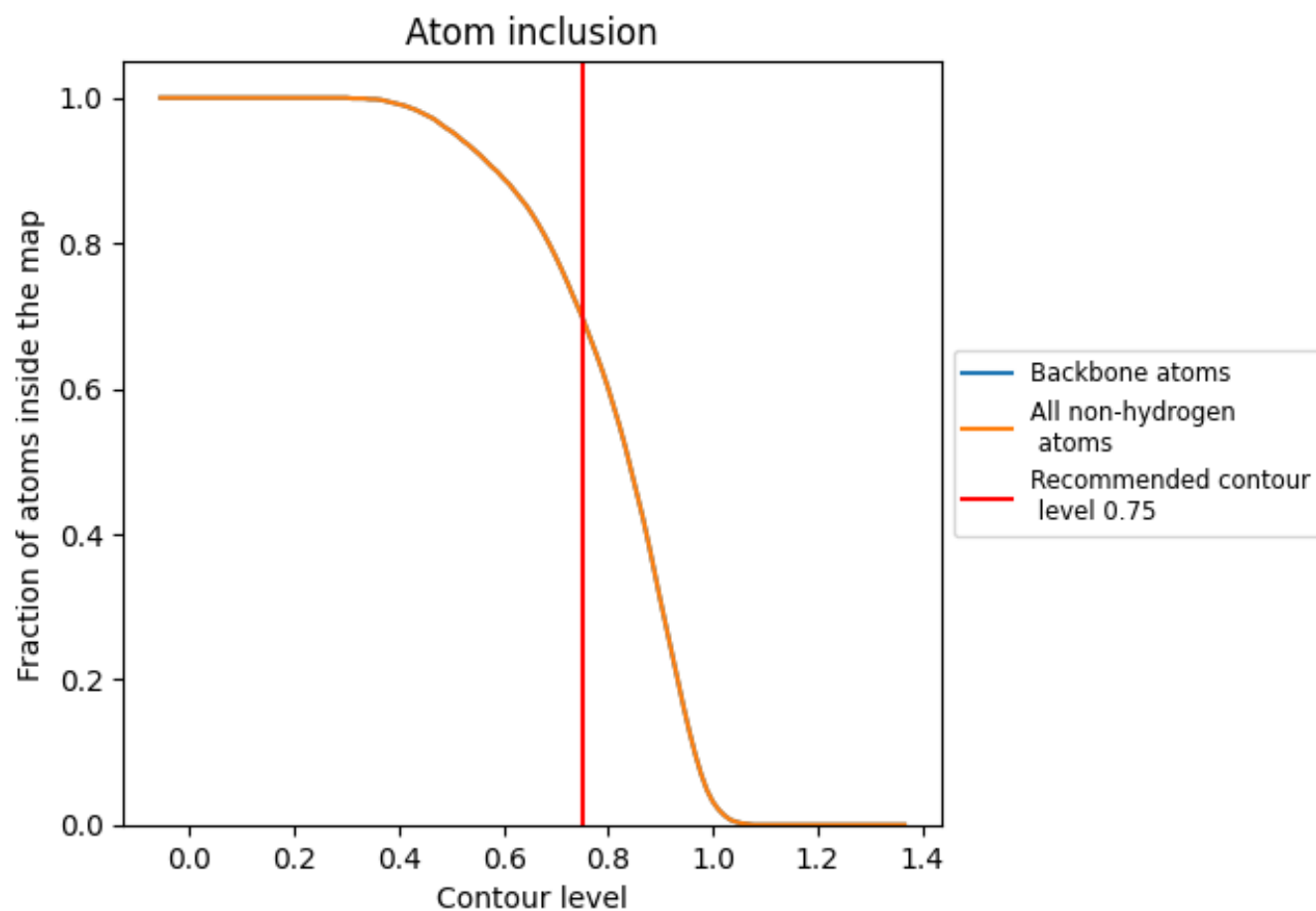


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 70% of all backbone atoms, 70% 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 (0.75) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6990	 0.0480
A1	 0.7990	 0.0420
A2	 0.6900	 0.0440
A3	 0.7360	 0.0470
A4	 0.6810	 0.0470
A5	 0.6660	 0.0550
A6	 0.7280	 0.0500
A7	 0.6740	 0.0510
A8	 0.7520	 0.0530
A9	 0.6810	 0.0490
B1	 0.6510	 0.0480
B2	 0.7020	 0.0470
B3	 0.6680	 0.0460
B4	 0.6550	 0.0570
B5	 0.7210	 0.0560
B6	 0.6680	 0.0500
B7	 0.6370	 0.0560
B8	 0.6880	 0.0520
B9	 0.6650	 0.0480
C1	 0.6940	 0.0560
C2	 0.6280	 0.0460
C3	 0.6810	 0.0520
C4	 0.6690	 0.0520
C5	 0.6630	 0.0540
C6	 0.6690	 0.0530
C7	 0.6750	 0.0470
C8	 0.6760	 0.0530
C9	 0.6780	 0.0530
D1	 0.6500	 0.0480
D2	 0.6570	 0.0540
D3	 0.6570	 0.0530
D4	 0.6750	 0.0480
D5	 0.6810	 0.0460
D6	 0.6610	 0.0500
D7	 0.6880	 0.0430



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Chain	Atom inclusion	Q-score
D8	 0.6860	 0.0470
D9	 0.7170	 0.0500
E1	 0.6970	 0.0380
E2	 0.6880	 0.0540
E3	 0.6750	 0.0530
E4	 0.6810	 0.0530
E5	 0.6480	 0.0410
E6	 0.7120	 0.0490
E7	 0.6680	 0.0490
E8	 0.6470	 0.0520
E9	 0.7050	 0.0420
F1	 0.6760	 0.0440
F2	 0.6720	 0.0490
F3	 0.6890	 0.0530
F4	 0.6600	 0.0510
F5	 0.6300	 0.0520
F6	 0.6780	 0.0490
F7	 0.6980	 0.0370
F8	 0.6780	 0.0480
F9	 0.7660	 0.0530
G1	 0.6830	 0.0430
G2	 0.6420	 0.0470
G3	 0.7080	 0.0530
G4	 0.7410	 0.0490
G5	 0.6780	 0.0430
G6	 0.7360	 0.0430
G7	 0.7020	 0.0440
G8	 0.6830	 0.0410
G9	 0.7420	 0.0530
H1	 0.7250	 0.0490
H2	 0.7130	 0.0410
H3	 0.7640	 0.0550
H4	 0.7270	 0.0440
H5	 0.7230	 0.0430
H6	 0.7680	 0.0460
H7	 0.7490	 0.0390
H8	 0.6620	 0.0370
H9	 0.7520	 0.0480
I1	 0.7390	 0.0480
I2	 0.7000	 0.0460
I3	 0.7360	 0.0410
I4	 0.7150	 0.0460

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Chain	Atom inclusion	Q-score
I5	 0.7150	 0.0430
I6	 0.7260	 0.0500
I7	 0.7120	 0.0440
I8	 0.7080	 0.0430
I9	 0.7200	 0.0450
J1	 0.7720	 0.0420
J2	 0.7500	 0.0370
J3	 0.7740	 0.0480
K	 0.8350	 0.0500