



wwPDB EM Validation Summary Report

Nov 20, 2022 – 09:22 am GMT

PDB ID : 6HHT
EMDB ID : EMD-0217
Title : Echovirus 18 Open particle without two pentamers
Authors : Buchta, D.; Fuzik, T.; Hrebik, D.; Levdansky, Y.; Moravcova, J.; Plevka, P.
Deposited on : 2018-08-29
Resolution : 4.05 Å (reported)
Based on initial model : 6HBH

This is a wwPDB EM Validation Summary 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.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

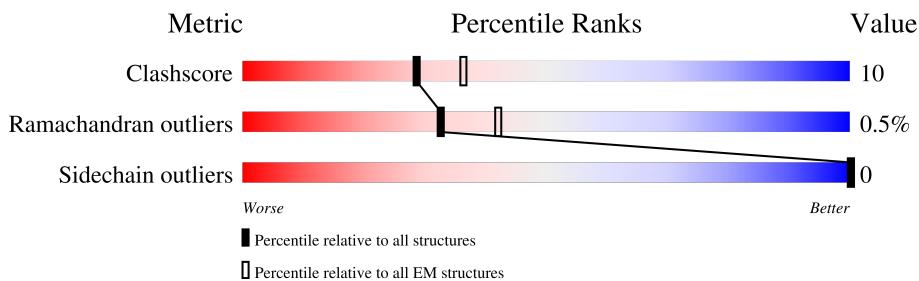
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.05 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	287	21% (red) 63% (green) 15% (yellow) 22% (grey)
1	A2	287	60% (green) 60% (green) 18% (yellow) 22% (grey)
1	D1	287	60% (green) 60% (green) 18% (yellow) 22% (grey)
1	D2	287	66% (green) 61% (green) 17% (yellow) 22% (grey)
1	G1	287	59% (green) 59% (green) 19% (yellow) 22% (grey)
1	G2	287	62% (green) 62% (green) 16% (yellow) 22% (grey)
1	J1	287	40% (red) 61% (green) 17% (yellow) 22% (grey)
1	J2	287	41% (red) 61% (green) 17% (yellow) 22% (grey)

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Mol	Chain	Length	Quality of chain
1	M1	287	60% 18% 22%
1	M2	287	62% 16% 22%
1	P1	287	5% 61% 17% 22%
1	P2	287	13% 61% 17% 22%
1	S1	287	13% 63% 15% 22%
1	S2	287	12% 62% 16% 22%
1	V1	287	5% 60% 18% 22%
1	V2	287	62% 18% 22%
1	Y2	287	8% 65% 13% 22%
1	b2	287	20% 78% 22%
1	e2	287	5% 78% 22%
1	h2	287	21% 78% 22%
1	k2	287	9% 78% 22%
1	n2	287	78% 22%
1	q2	287	26% 78% 22%
1	t2	287	12% 78% 22%
1	w2	287	78% 22%
2	B1	260	37% 71% 21% 8%
2	B2	260	63% 68% 23% 8%
2	E1	260	69% 22% 8%
2	E2	260	83% 68% 23% 8%
2	H1	260	67% 25% 8%
2	H2	260	11% 69% 22% 8%
2	K1	260	30% 68% 23% 8%
2	K2	260	29% 69% 22% 8%









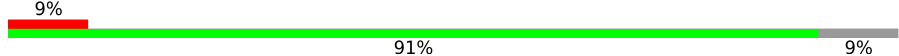
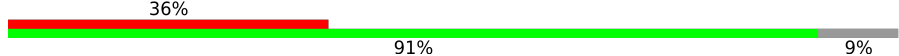
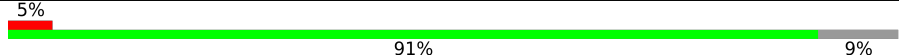
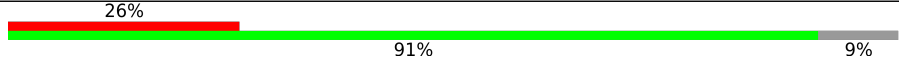
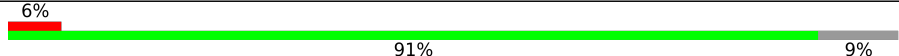
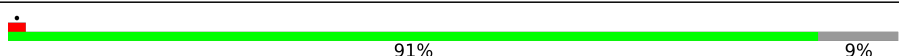
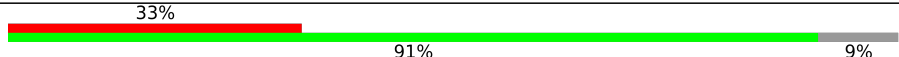
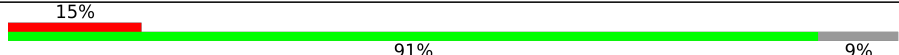
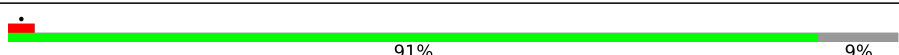
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Mol	Chain	Length	Quality of chain
2	N1	260	68% 23% 8%
2	N2	260	68% 23% 8%
2	Q1	260	67% 25% 8% 6%
2	Q2	260	68% 24% 8% 19%
2	T1	260	67% 24% 8% 23%
2	T2	260	65% 26% 8% 13%
2	W1	260	66% 25% 8% 5%
2	W2	260	68% 23% 8% 80%
2	Z2	260	68% 24% 8% 7%
2	c2	260	90% 8% 8% 34%
2	f2	260	90% 8% 8% 8%
2	i2	260	90% 8% 8% 39%
2	l2	260	90% 8% 8% 5%
2	o2	260	90% 8% 8%
2	r2	260	90% 8% 8% 51%
2	u2	260	90% 8% 8% 10%
2	x2	260	90% 8% 8%
3	C1	239	74% 18% 9% 41%
3	C2	239	72% 19% 9% 76%
3	F1	239	72% 19% 9%
3	F2	239	72% 19% 9% 89%
3	I1	239	70% 21% 9%
3	I2	239	73% 18% 9% 5%
3	L1	239	72% 19% 9% 31%
3	L2	239	70% 21% 9% 32%

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Mol	Chain	Length	Quality of chain
3	O1	239	 72% 19% 9%
3	O2	239	 71% 21% 9%
3	R1	239	 6% 70% 21% 9%
3	R2	239	 10% 72% 19% 9%
3	U1	239	 11% 73% 18% 9%
3	U2	239	 17% 72% 19% 9%
3	X1	239	 72% 19% 9%
3	X2	239	 69% 72% 19% 9%
3	a2	239	 9% 91% 9%
3	d2	239	 36% 91% 9%
3	g2	239	 5% 91% 9%
3	j2	239	 26% 91% 9%
3	m2	239	 6% 91% 9%
3	p2	239	 91% 9%
3	s2	239	 33% 91% 9%
3	v2	239	 15% 91% 9%
3	y2	239	 91% 9%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 129900 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 Echovirus 18 capsid protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A1	224	1741	1117	305	305	14	0	0
1	V1	224	1741	1117	305	305	14	0	0
1	S1	224	1741	1117	305	305	14	0	0
1	P1	224	1741	1117	305	305	14	0	0
1	M1	224	1741	1117	305	305	14	0	0
1	J1	224	1741	1117	305	305	14	0	0
1	G1	224	1741	1117	305	305	14	0	0
1	D1	224	1741	1117	305	305	14	0	0
1	A2	224	1741	1117	305	305	14	0	0
1	w2	224	1741	1117	305	305	14	0	0
1	t2	224	1741	1117	305	305	14	0	0
1	q2	224	1741	1117	305	305	14	0	0
1	n2	224	1741	1117	305	305	14	0	0
1	k2	224	1741	1117	305	305	14	0	0
1	h2	224	1741	1117	305	305	14	0	0
1	e2	224	1741	1117	305	305	14	0	0
1	b2	224	1741	1117	305	305	14	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	Y2	224	Total	C	N	O	S	0	0
			1741	1117	305	305	14		
1	V2	224	Total	C	N	O	S	0	0
			1741	1117	305	305	14		
1	S2	224	Total	C	N	O	S	0	0
			1741	1117	305	305	14		
1	P2	224	Total	C	N	O	S	0	0
			1741	1117	305	305	14		
1	M2	224	Total	C	N	O	S	0	0
			1741	1117	305	305	14		
1	J2	224	Total	C	N	O	S	0	0
			1741	1117	305	305	14		
1	G2	224	Total	C	N	O	S	0	0
			1741	1117	305	305	14		
1	D2	224	Total	C	N	O	S	0	0
			1741	1117	305	305	14		

- Molecule 2 is a protein called Echovirus 18 capsid protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	W1	238	Total	C	N	O	S	0	0
			1821	1172	302	332	15		
2	T1	238	Total	C	N	O	S	0	0
			1821	1172	302	332	15		
2	Q1	238	Total	C	N	O	S	0	0
			1821	1172	302	332	15		
2	N1	238	Total	C	N	O	S	0	0
			1821	1172	302	332	15		
2	K1	238	Total	C	N	O	S	0	0
			1821	1172	302	332	15		
2	H1	238	Total	C	N	O	S	0	0
			1821	1172	302	332	15		
2	E1	238	Total	C	N	O	S	0	0
			1821	1172	302	332	15		
2	B1	238	Total	C	N	O	S	0	0
			1821	1172	302	332	15		
2	x2	238	Total	C	N	O	S	0	0
			1821	1172	302	332	15		
2	u2	238	Total	C	N	O	S	0	0
			1821	1172	302	332	15		
2	r2	238	Total	C	N	O	S	0	0
			1821	1172	302	332	15		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	o2	238	Total	C	N	O	S	0	0
			1821	1172	302	332	15		
2	l2	238	Total	C	N	O	S	0	0
			1821	1172	302	332	15		
2	i2	238	Total	C	N	O	S	0	0
			1821	1172	302	332	15		
2	f2	238	Total	C	N	O	S	0	0
			1821	1172	302	332	15		
2	c2	238	Total	C	N	O	S	0	0
			1821	1172	302	332	15		
2	Z2	238	Total	C	N	O	S	0	0
			1821	1172	302	332	15		
2	W2	238	Total	C	N	O	S	0	0
			1821	1172	302	332	15		
2	T2	238	Total	C	N	O	S	0	0
			1821	1172	302	332	15		
2	Q2	238	Total	C	N	O	S	0	0
			1821	1172	302	332	15		
2	N2	238	Total	C	N	O	S	0	0
			1821	1172	302	332	15		
2	K2	238	Total	C	N	O	S	0	0
			1821	1172	302	332	15		
2	H2	238	Total	C	N	O	S	0	0
			1821	1172	302	332	15		
2	E2	238	Total	C	N	O	S	0	0
			1821	1172	302	332	15		
2	B2	238	Total	C	N	O	S	0	0
			1821	1172	302	332	15		

- Molecule 3 is a protein called Echovirus 18 capsid protein 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	X1	218	Total	C	N	O	S	0	0
			1634	1045	265	308	16		
3	U1	218	Total	C	N	O	S	0	0
			1634	1045	265	308	16		
3	R1	218	Total	C	N	O	S	0	0
			1634	1045	265	308	16		
3	O1	218	Total	C	N	O	S	0	0
			1634	1045	265	308	16		
3	L1	218	Total	C	N	O	S	0	0
			1634	1045	265	308	16		

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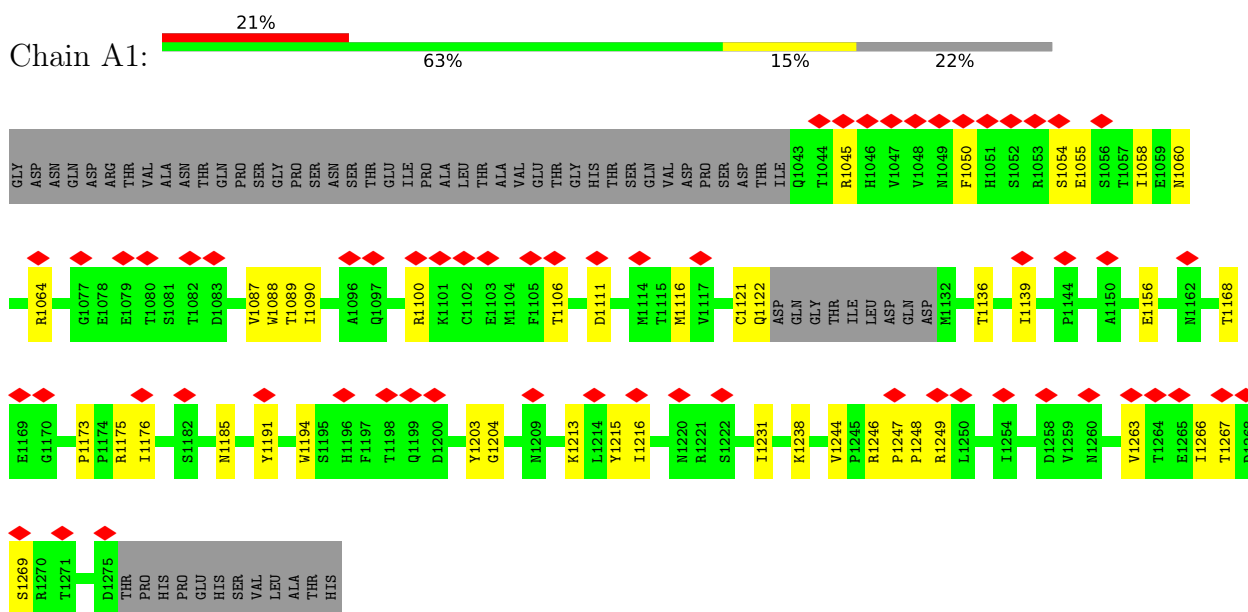
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Mol	Chain	Residues	Atoms					AltConf	Trace
3	I1	218	Total	C	N	O	S	0	0
			1634	1045	265	308	16		
3	F1	218	Total	C	N	O	S	0	0
			1634	1045	265	308	16		
3	C1	218	Total	C	N	O	S	0	0
			1634	1045	265	308	16		
3	y2	218	Total	C	N	O	S	0	0
			1634	1045	265	308	16		
3	v2	218	Total	C	N	O	S	0	0
			1634	1045	265	308	16		
3	s2	218	Total	C	N	O	S	0	0
			1634	1045	265	308	16		
3	p2	218	Total	C	N	O	S	0	0
			1634	1045	265	308	16		
3	m2	218	Total	C	N	O	S	0	0
			1634	1045	265	308	16		
3	j2	218	Total	C	N	O	S	0	0
			1634	1045	265	308	16		
3	g2	218	Total	C	N	O	S	0	0
			1634	1045	265	308	16		
3	d2	218	Total	C	N	O	S	0	0
			1634	1045	265	308	16		
3	a2	218	Total	C	N	O	S	0	0
			1634	1045	265	308	16		
3	X2	218	Total	C	N	O	S	0	0
			1634	1045	265	308	16		
3	U2	218	Total	C	N	O	S	0	0
			1634	1045	265	308	16		
3	R2	218	Total	C	N	O	S	0	0
			1634	1045	265	308	16		
3	O2	218	Total	C	N	O	S	0	0
			1634	1045	265	308	16		
3	L2	218	Total	C	N	O	S	0	0
			1634	1045	265	308	16		
3	I2	218	Total	C	N	O	S	0	0
			1634	1045	265	308	16		
3	F2	218	Total	C	N	O	S	0	0
			1634	1045	265	308	16		
3	C2	218	Total	C	N	O	S	0	0
			1634	1045	265	308	16		

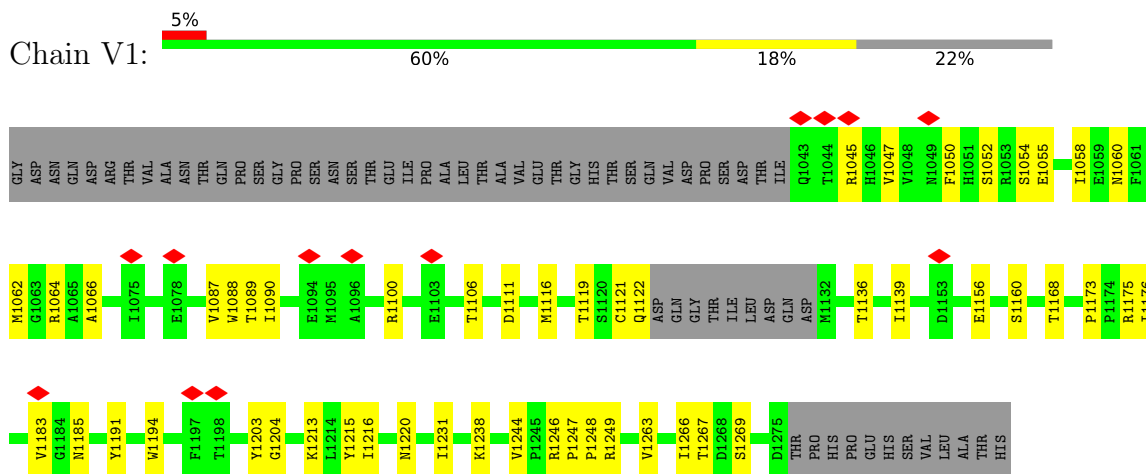
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

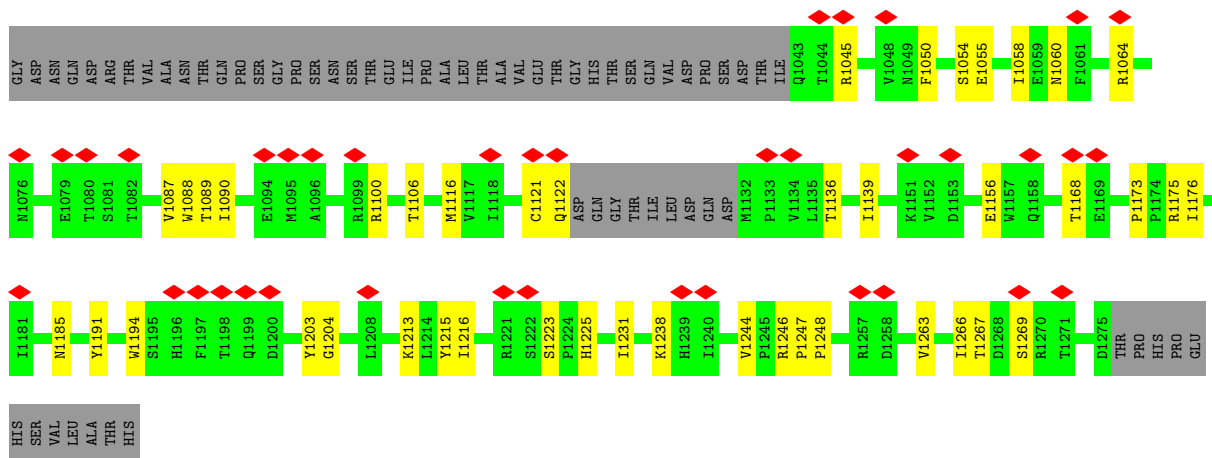
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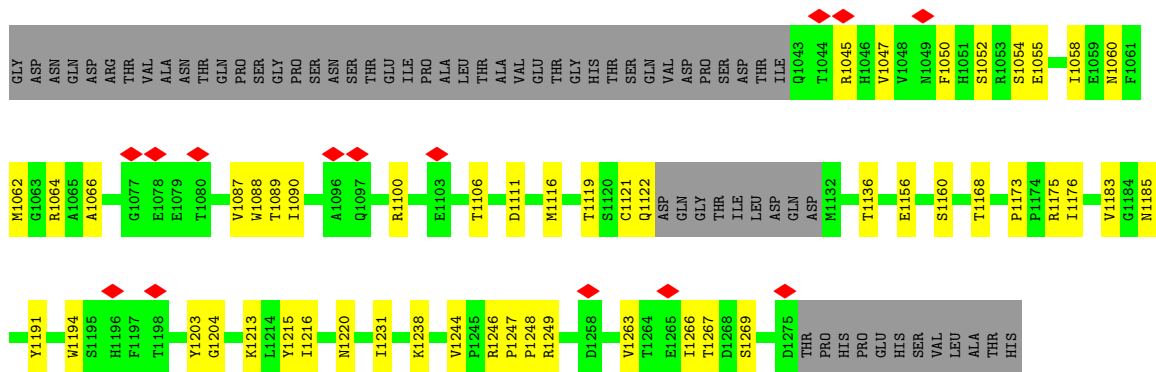
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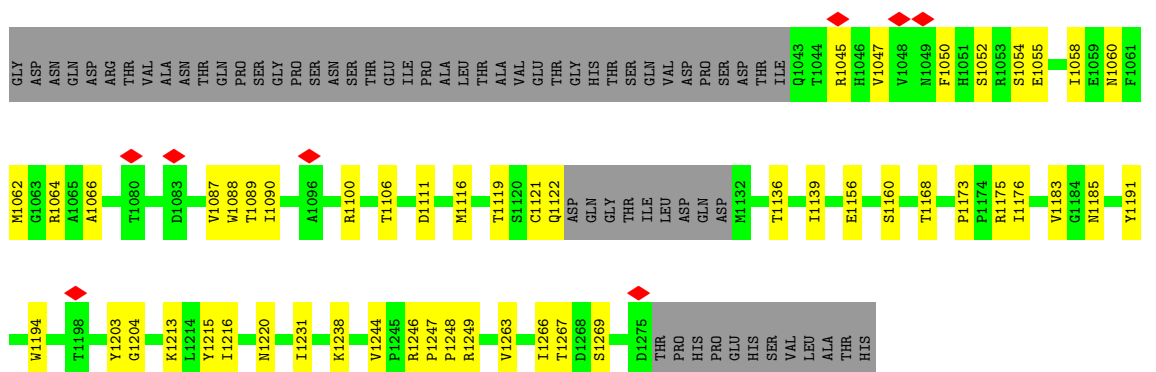
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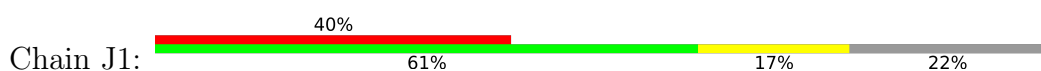
• Molecule 1: Echovirus 18 capsid protein 1



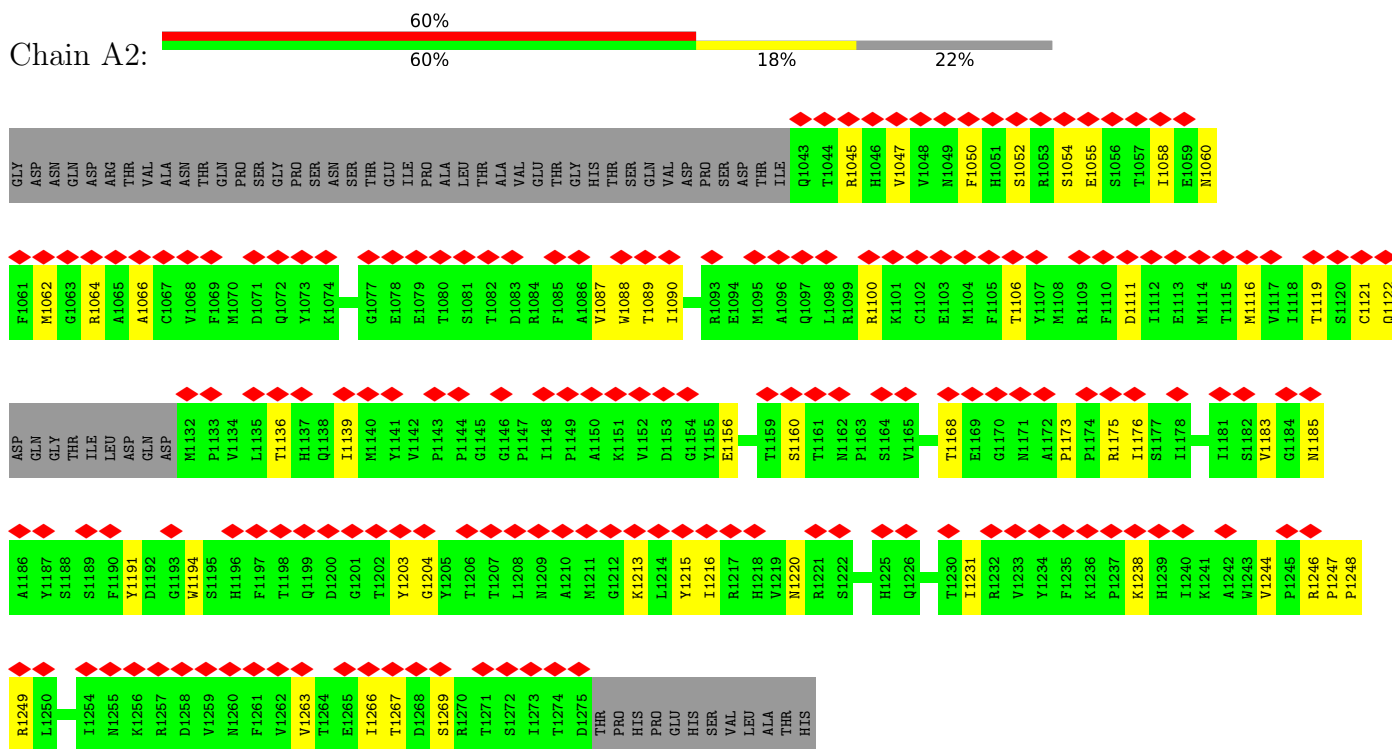
• Molecule 1: Echovirus 18 capsid protein 1



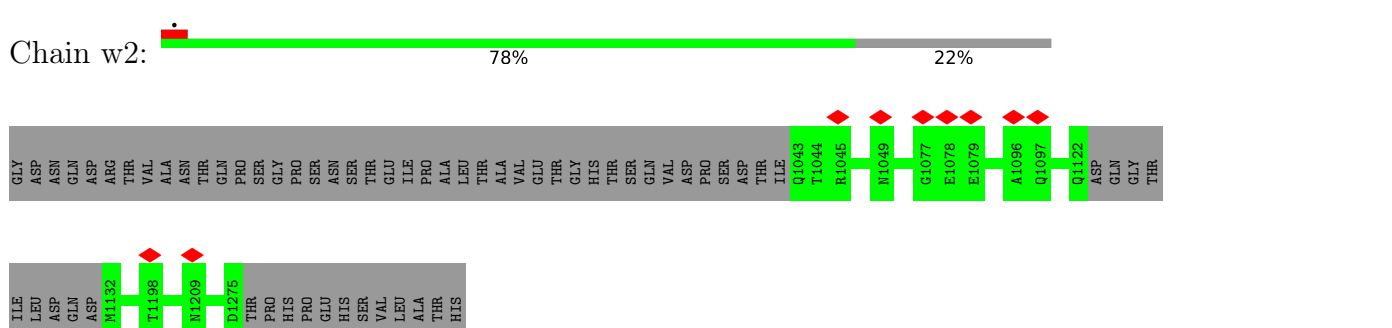
• Molecule 1: Echovirus 18 capsid protein 1



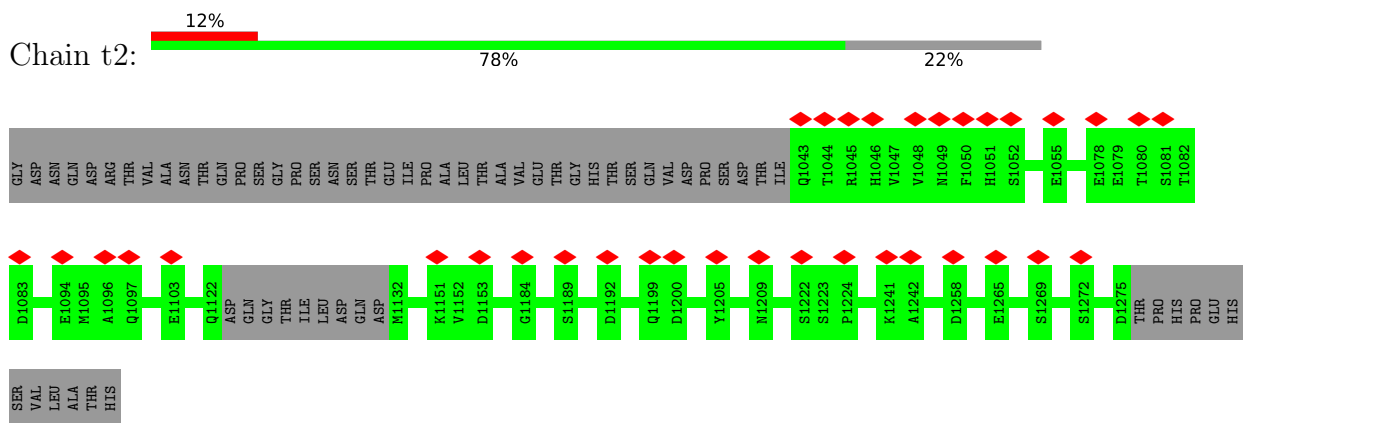
• Molecule 1: Echovirus 18 capsid protein 1



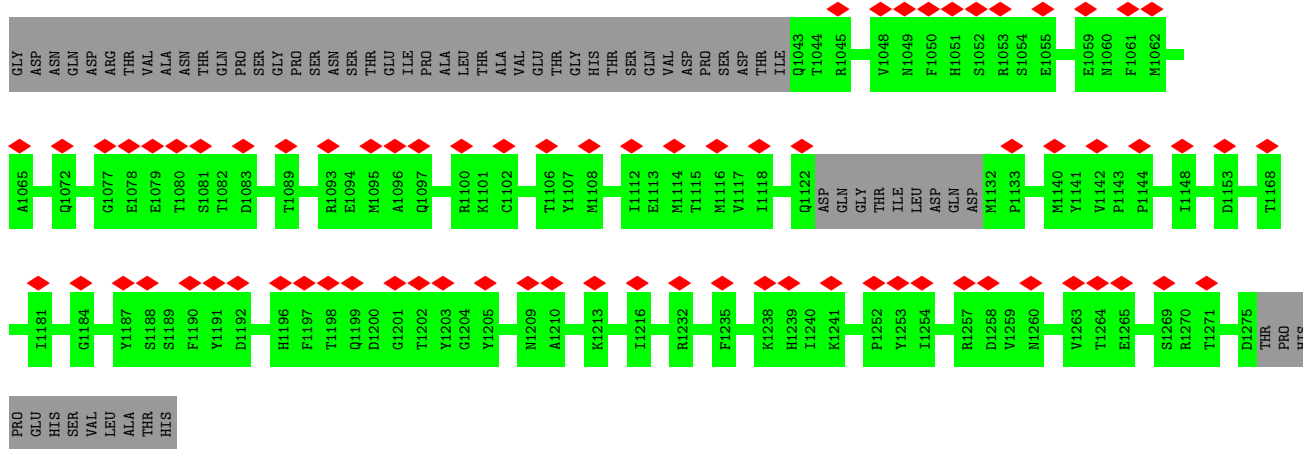
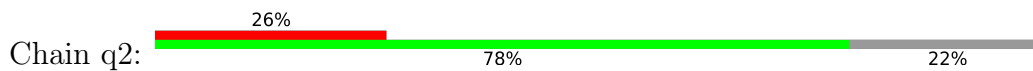
• Molecule 1: Echovirus 18 capsid protein 1



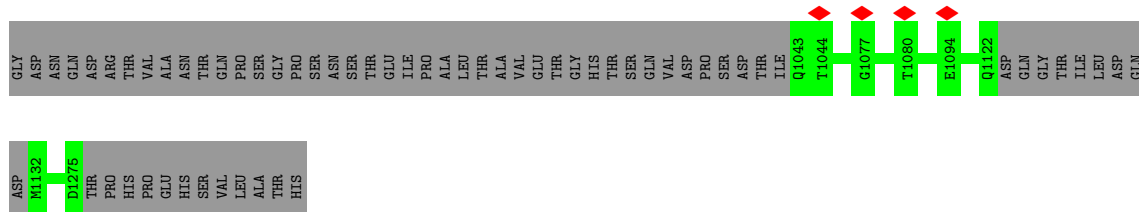
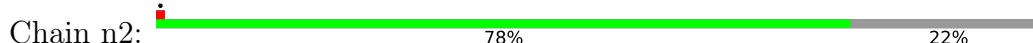
• Molecule 1: Echovirus 18 capsid protein 1



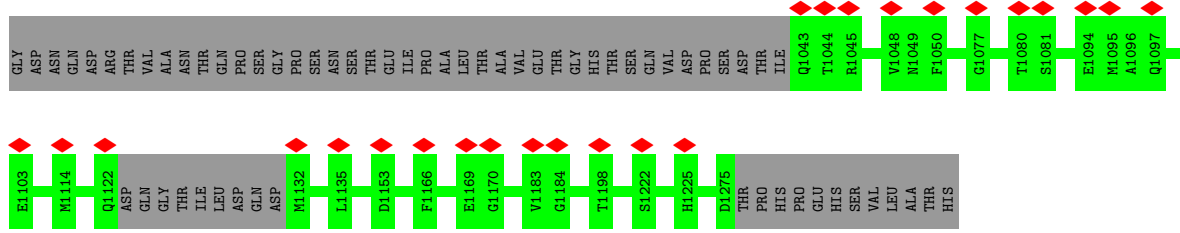
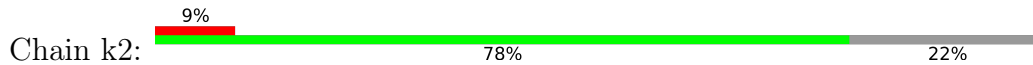
• Molecule 1: Echovirus 18 capsid protein 1



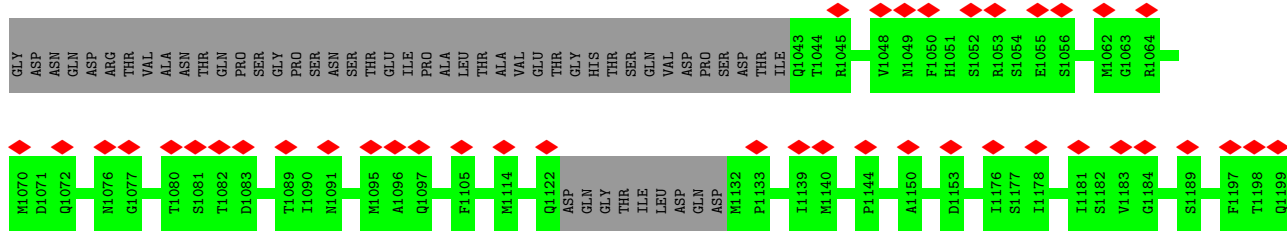
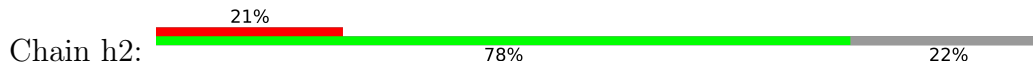
- Molecule 1: Echovirus 18 capsid protein 1

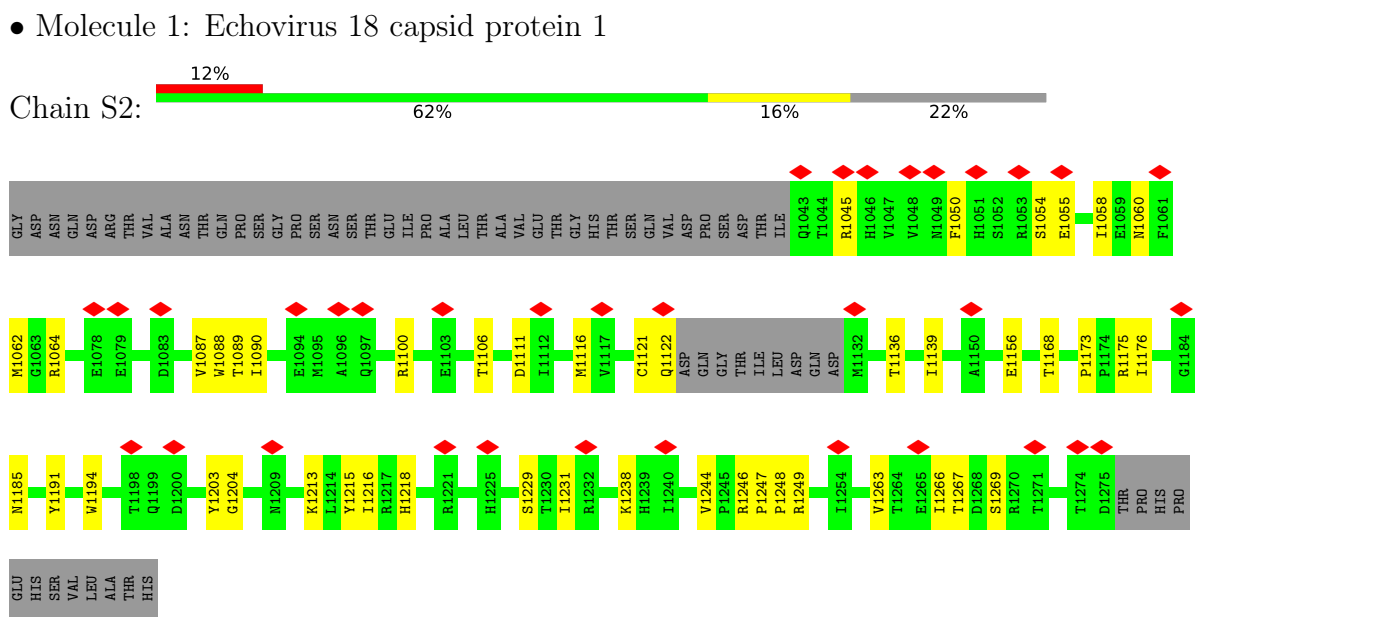
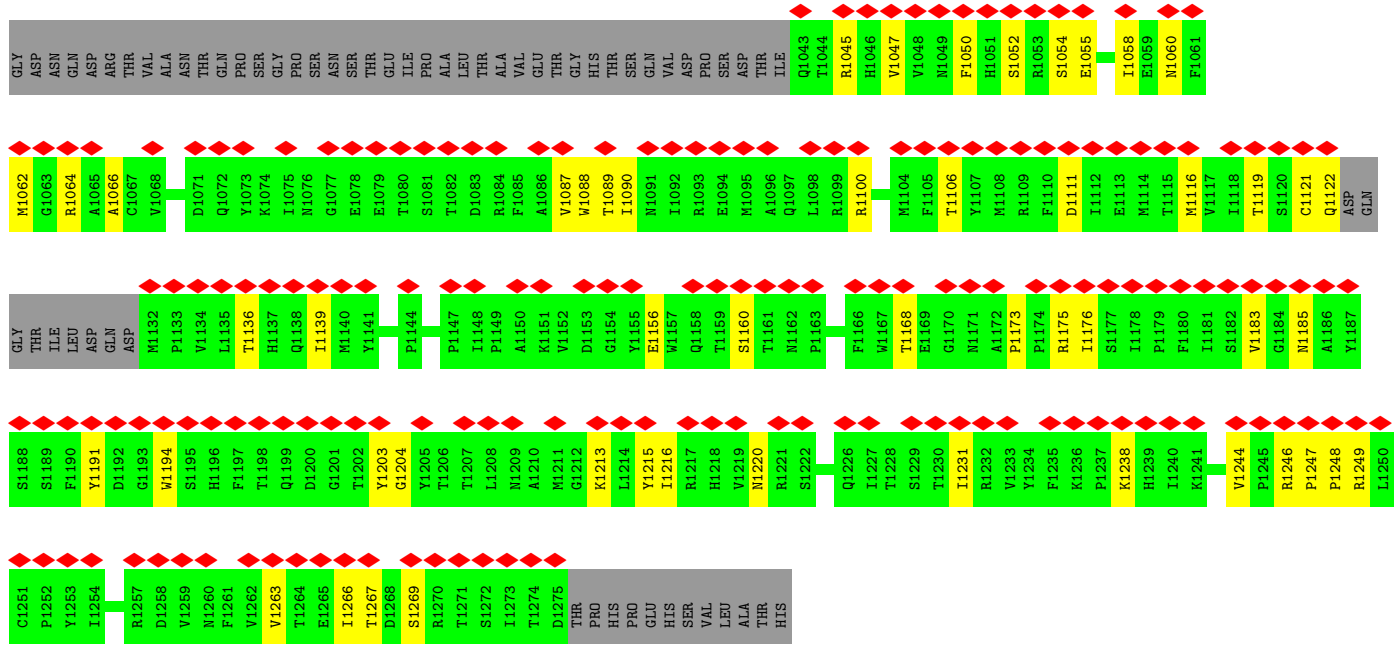


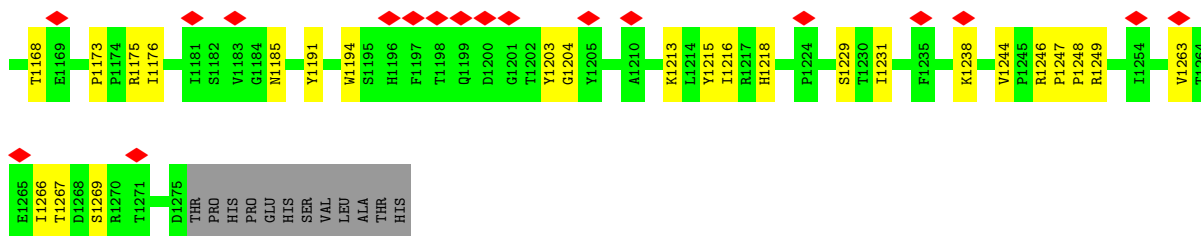
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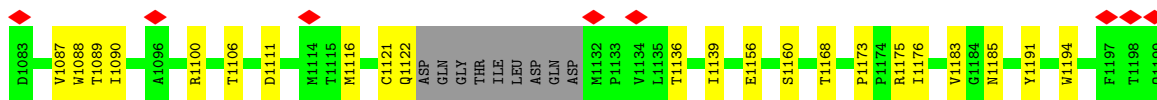
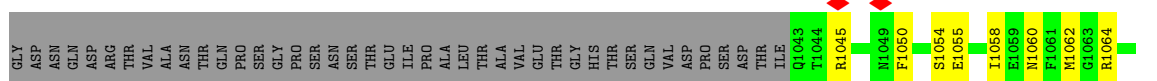
- Molecule 1: Echovirus 18 capsid protein 1



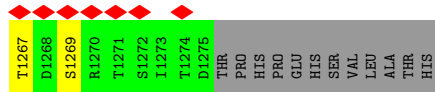
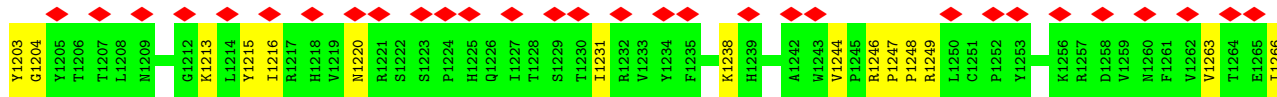
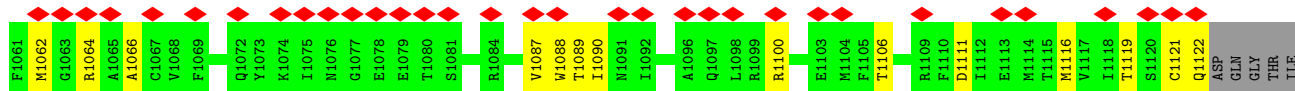
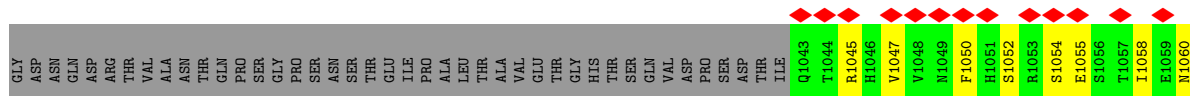
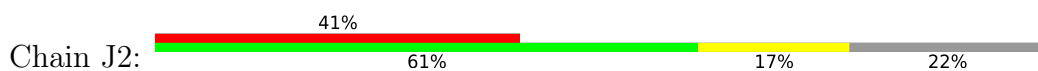




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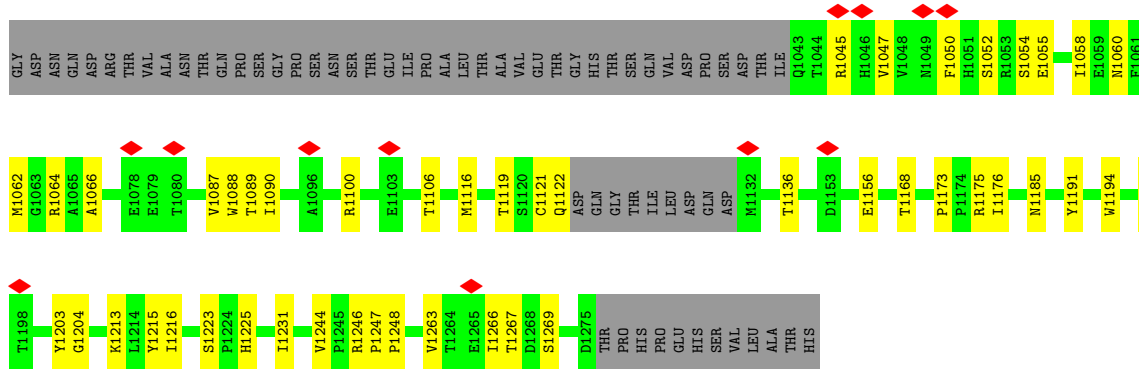


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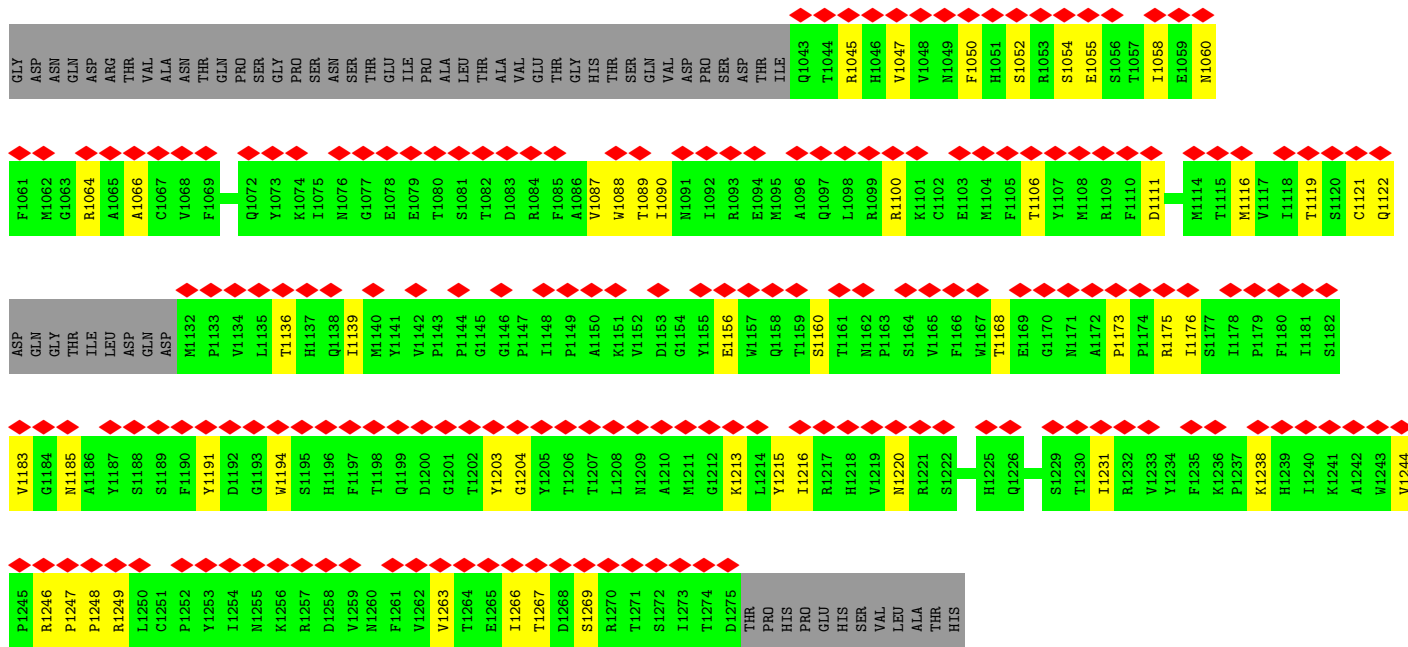


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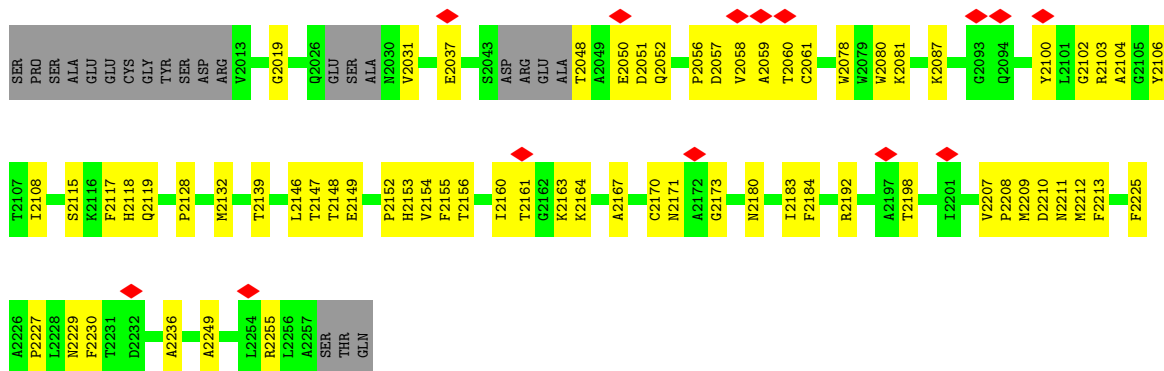


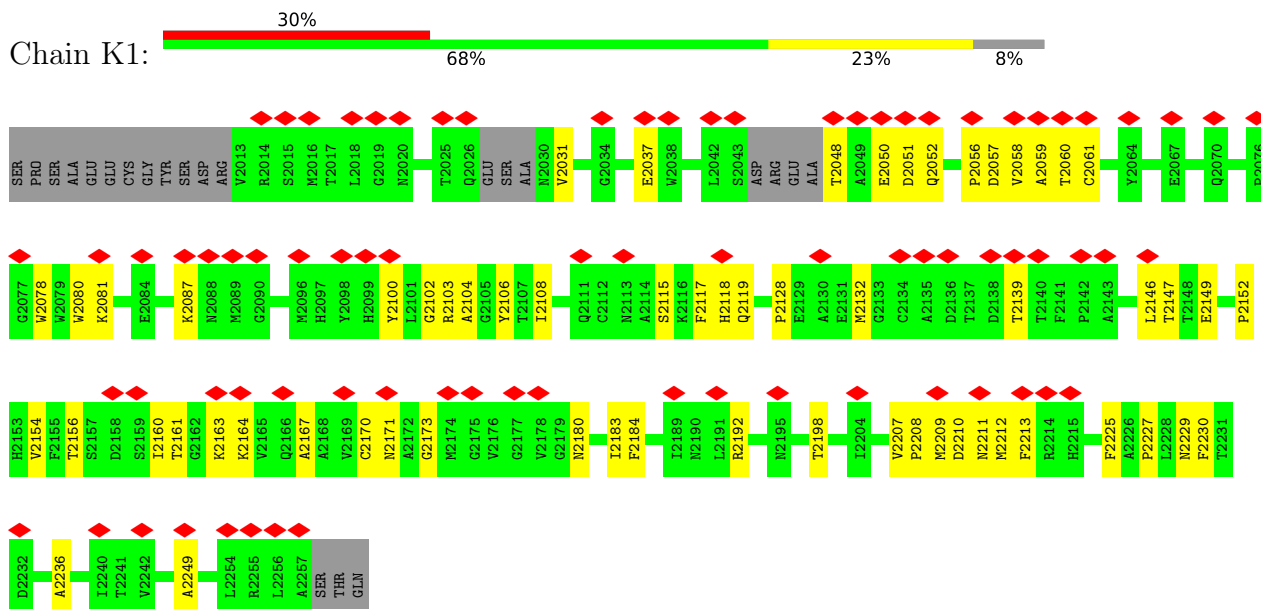


• Molecule 1: Echovirus 18 capsid protein 1

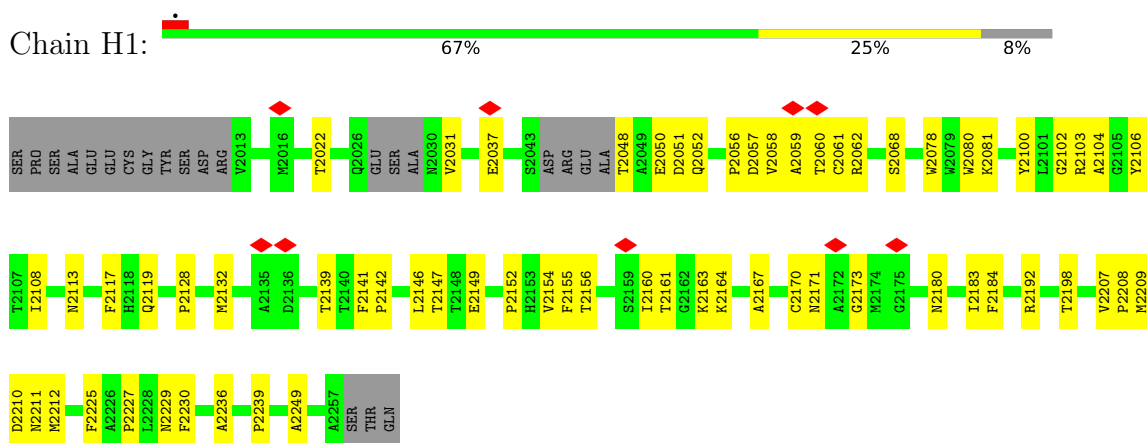


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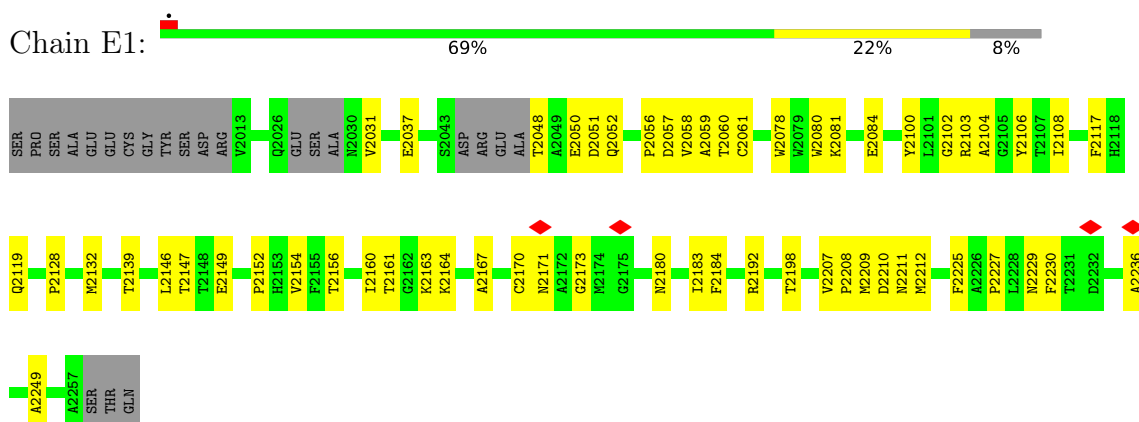




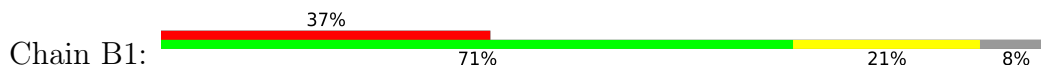
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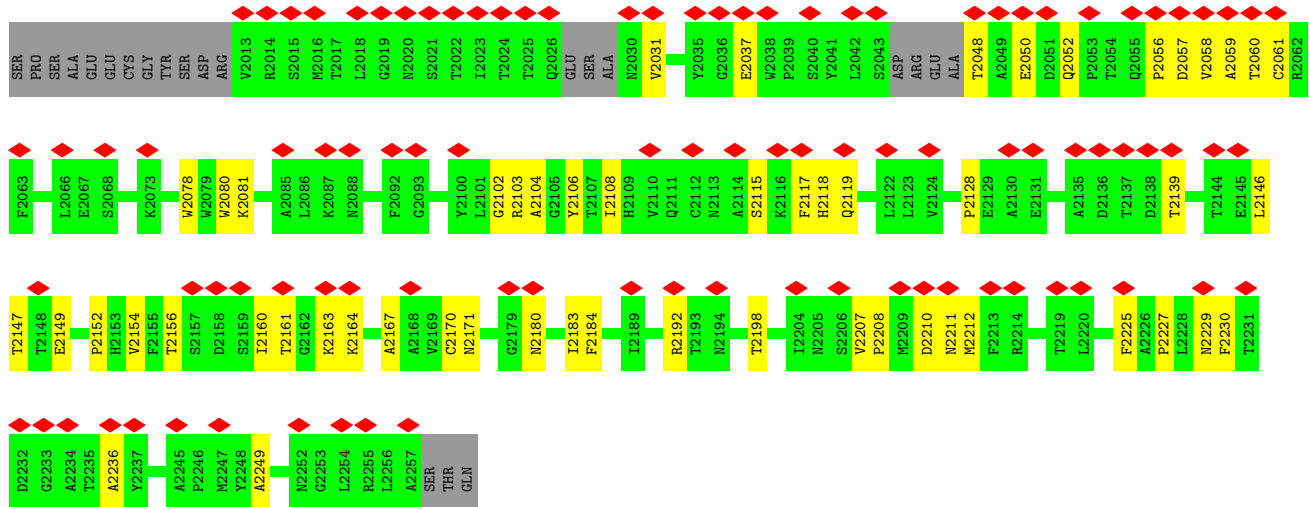


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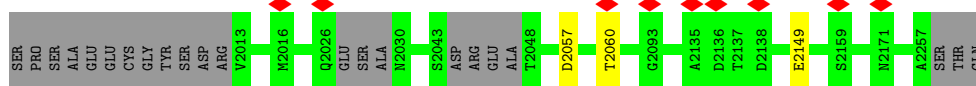
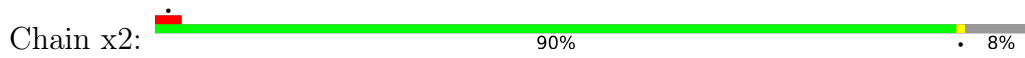


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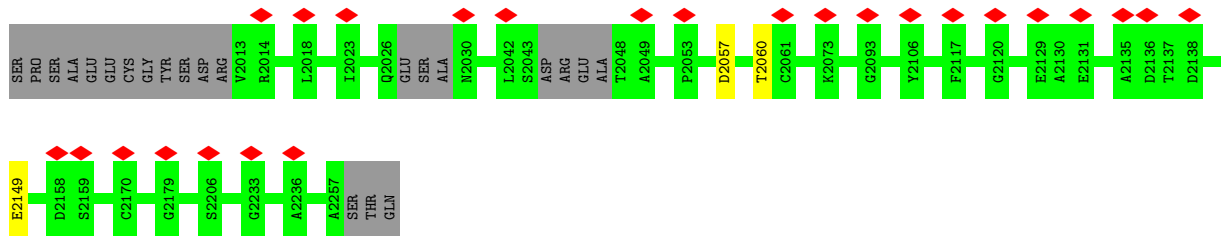
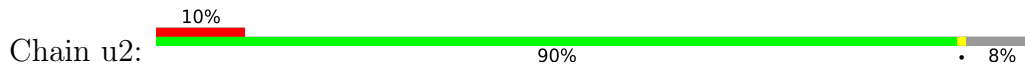




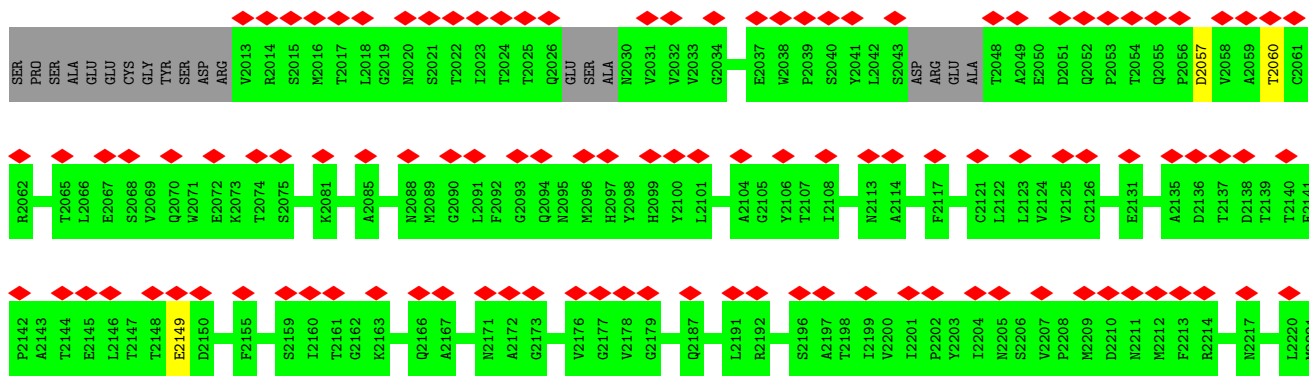
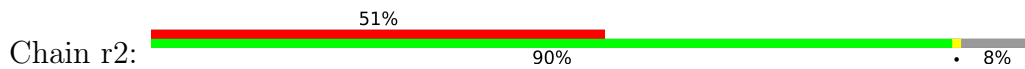
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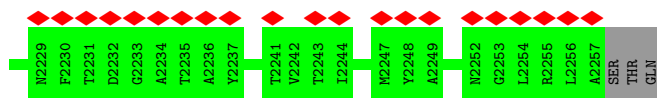


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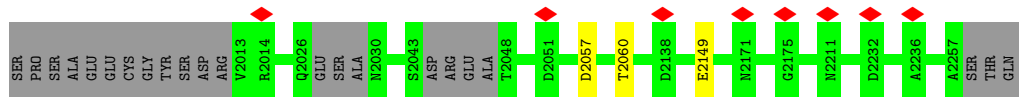


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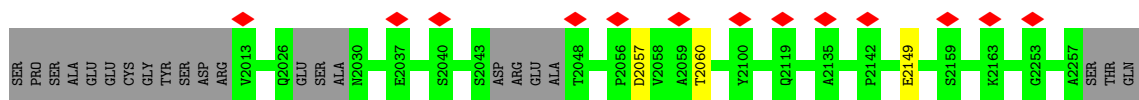
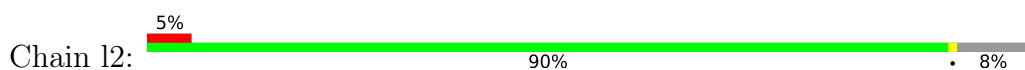




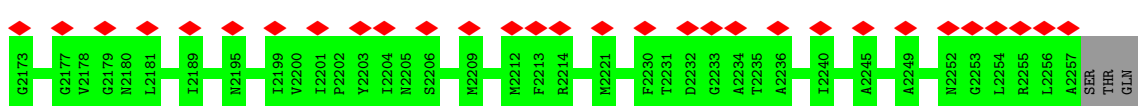
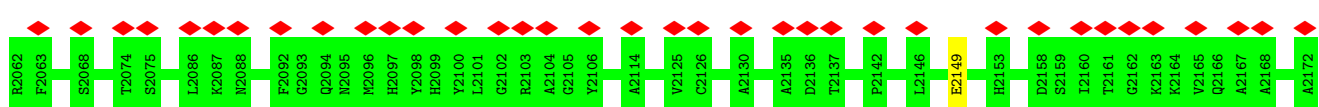
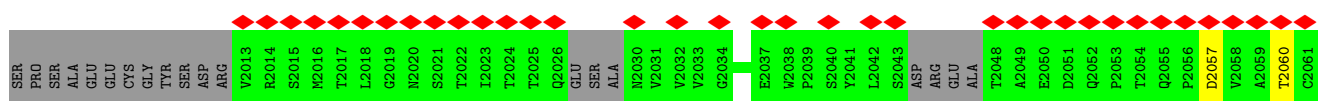
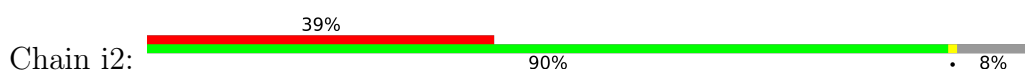
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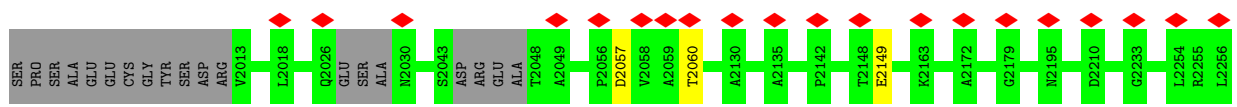
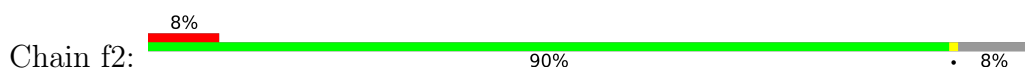
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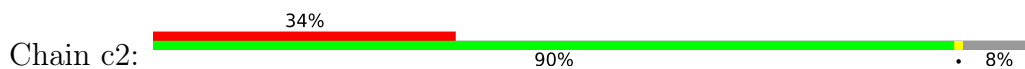
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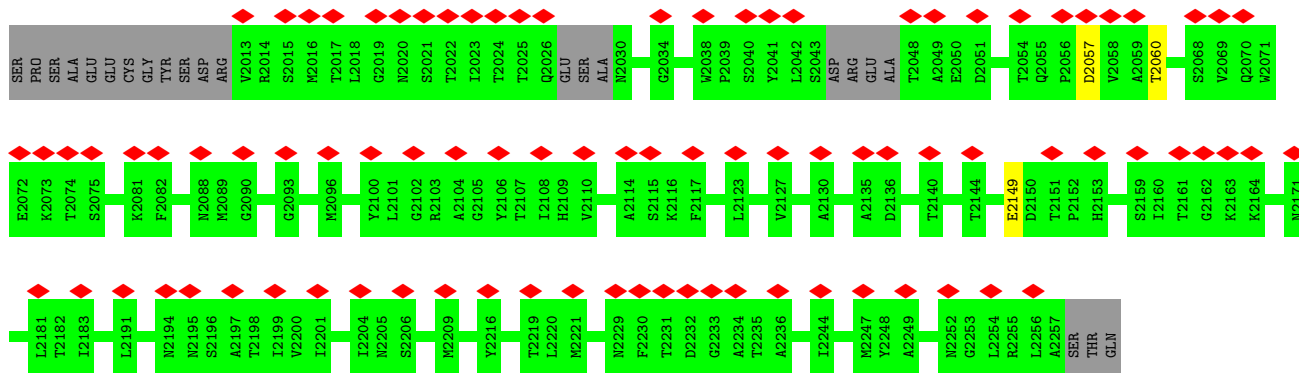


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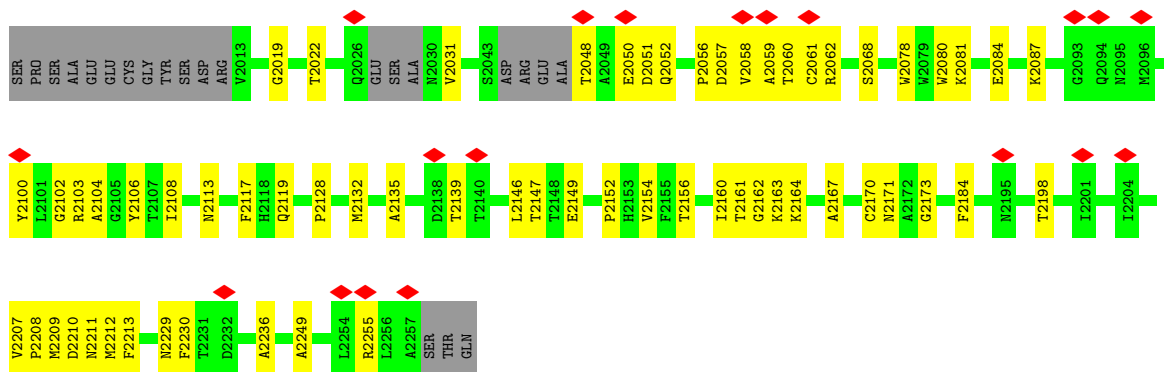


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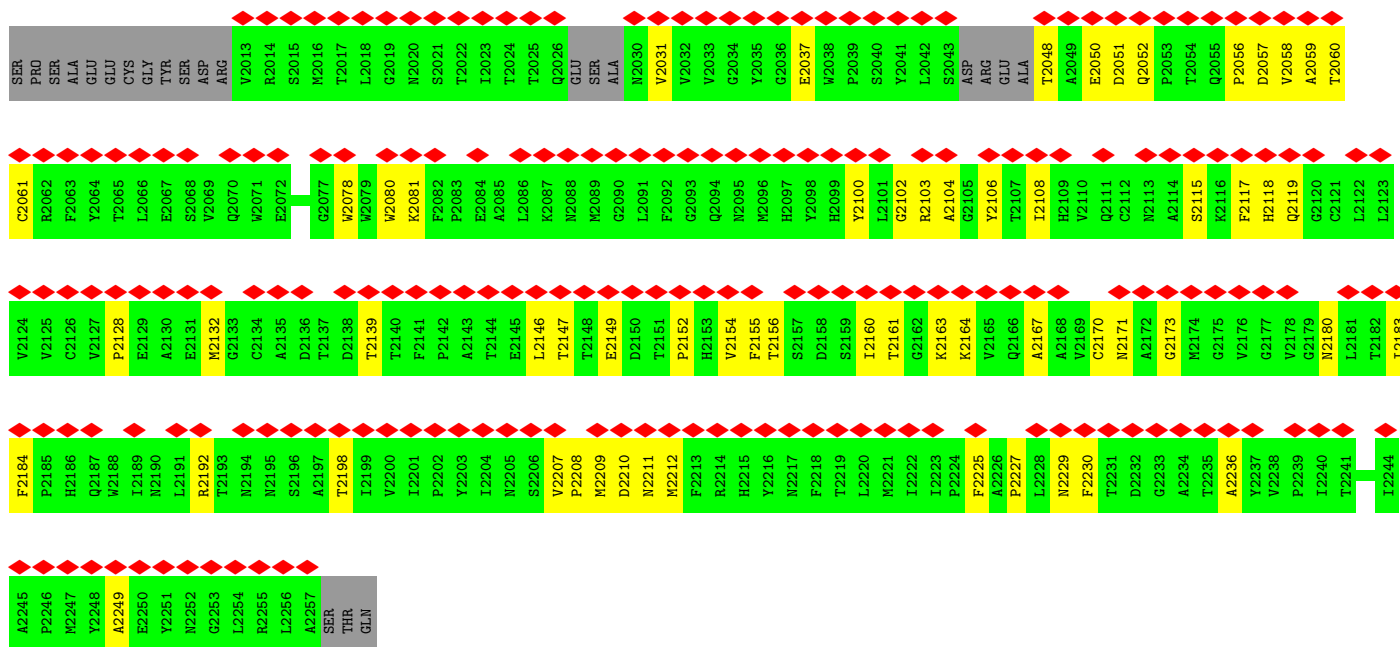
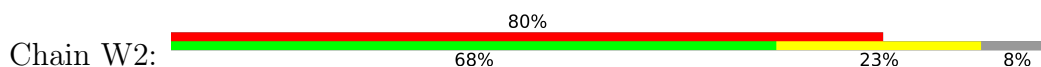




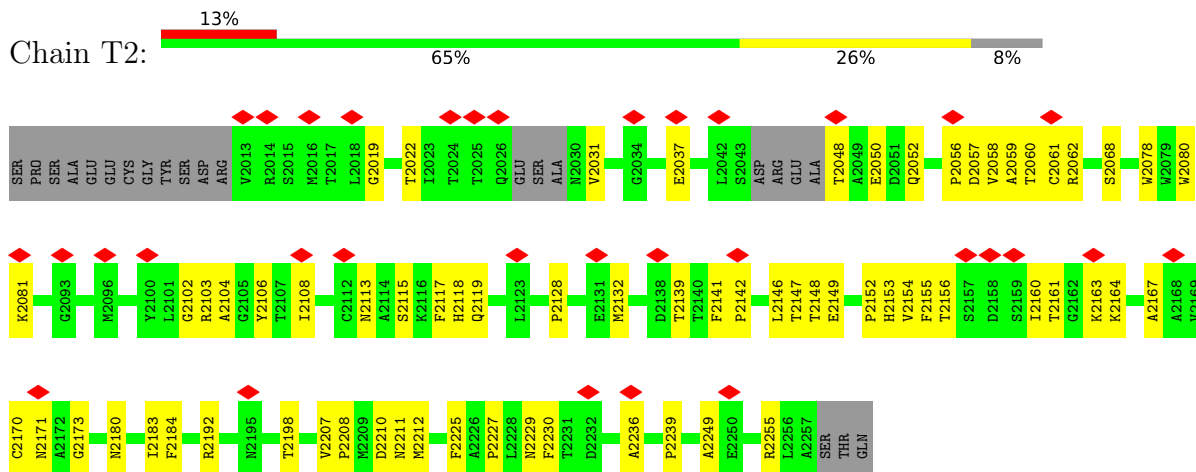
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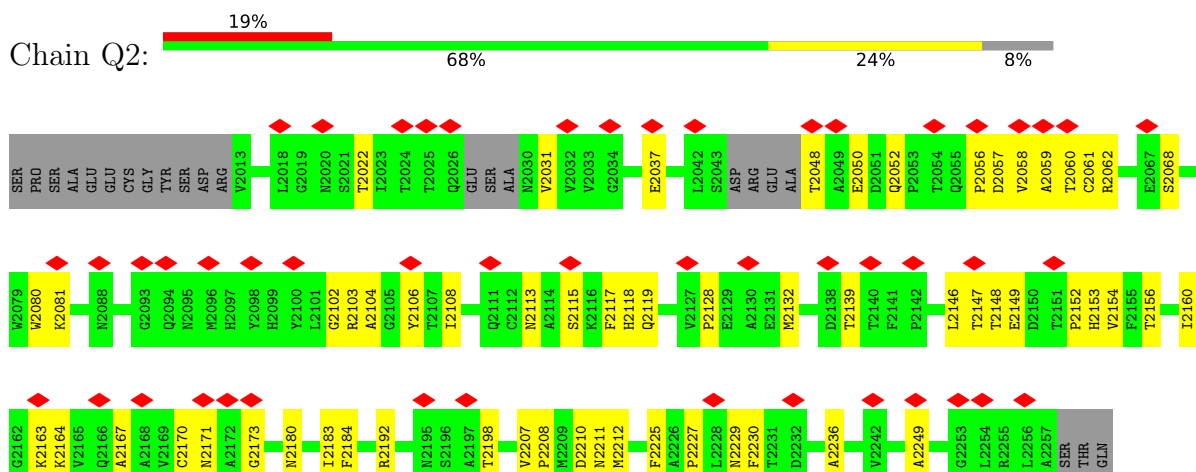
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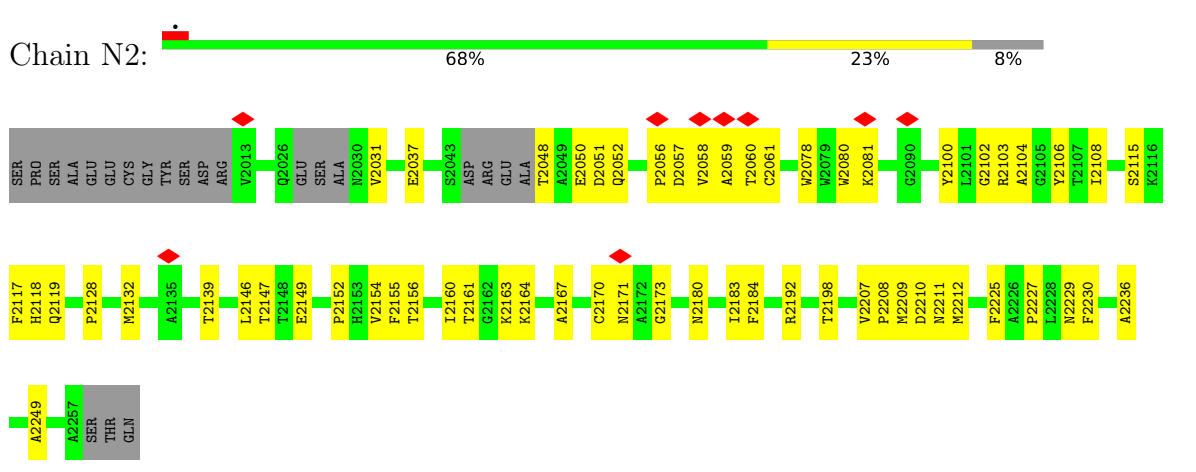
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• Molecule 2: Echovirus 18 capsid protein 2

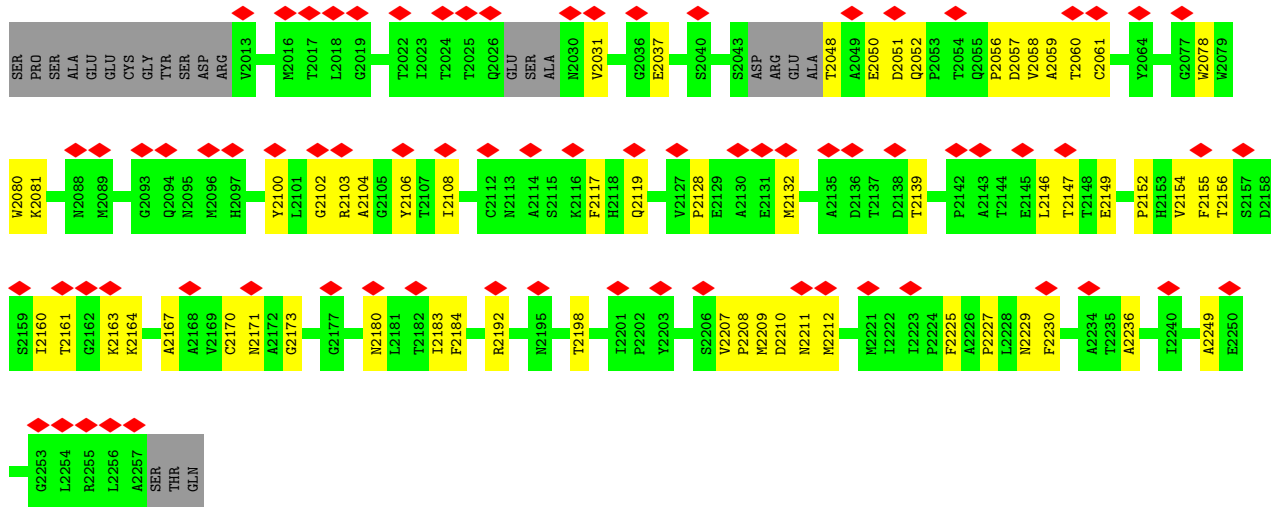


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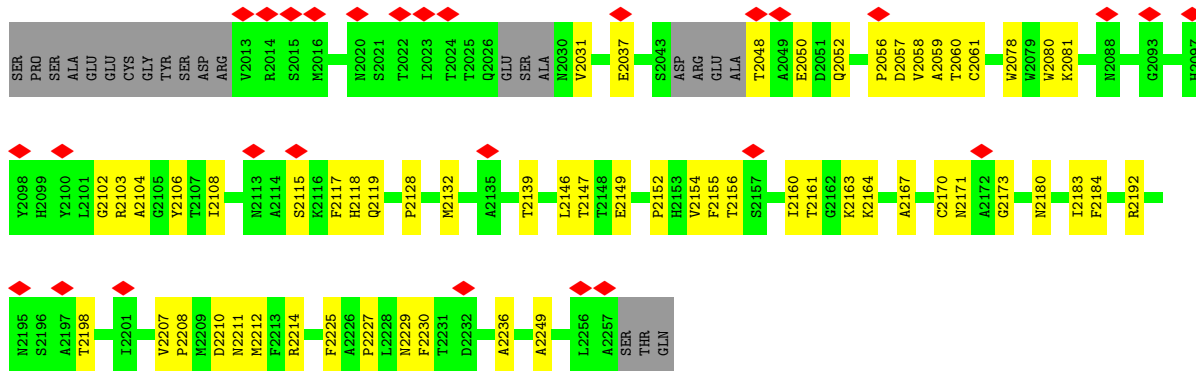
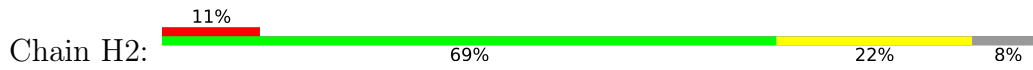


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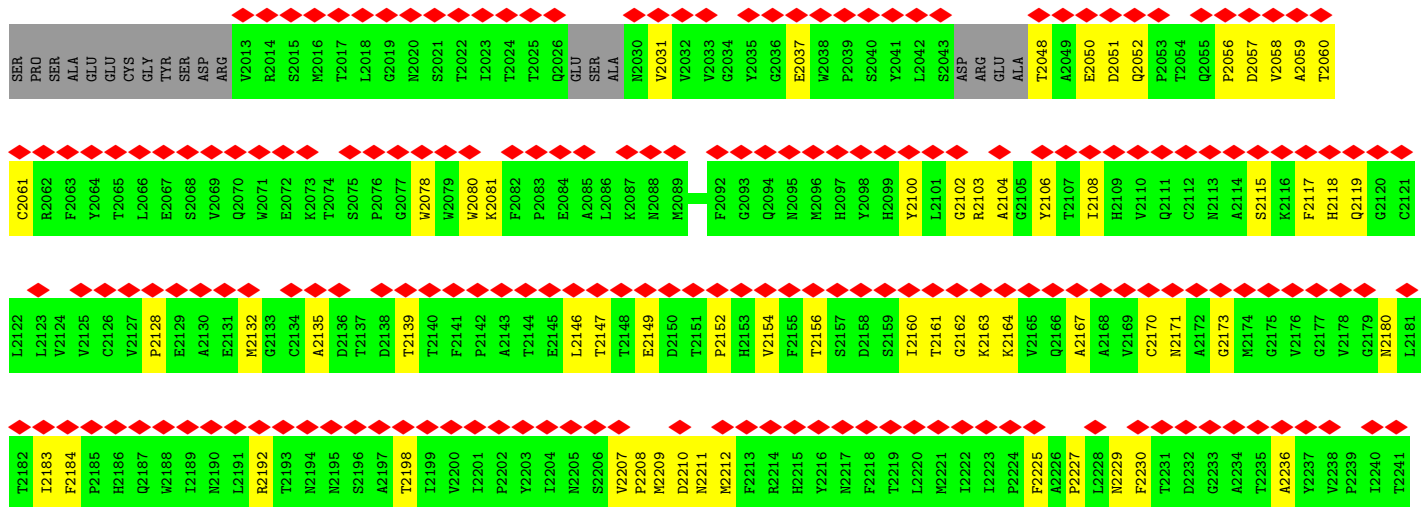
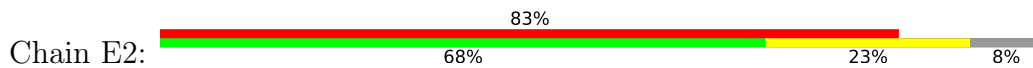


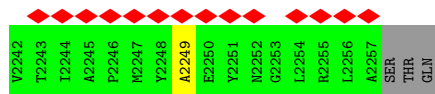


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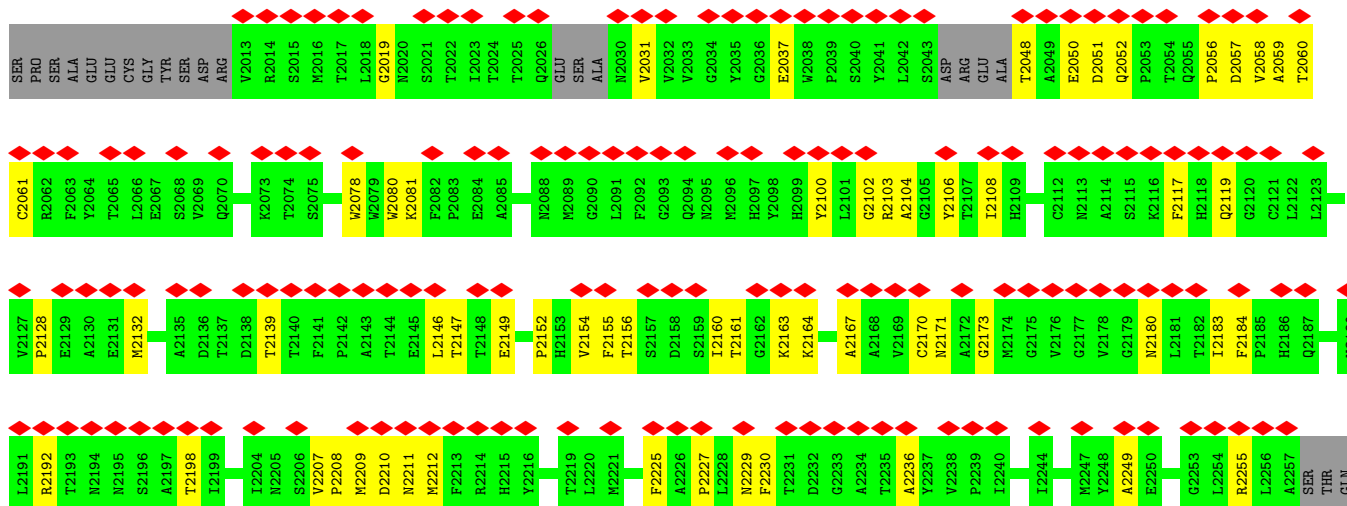


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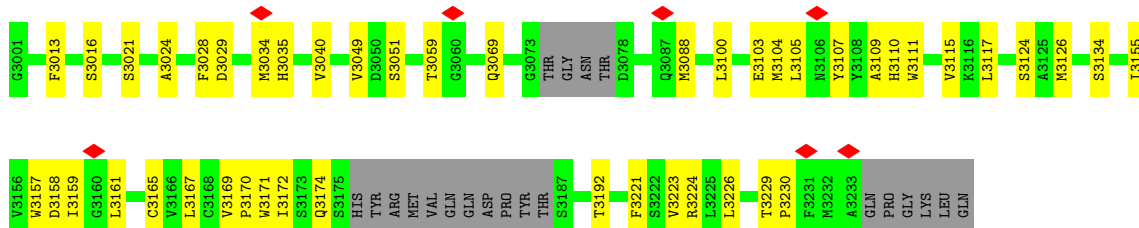




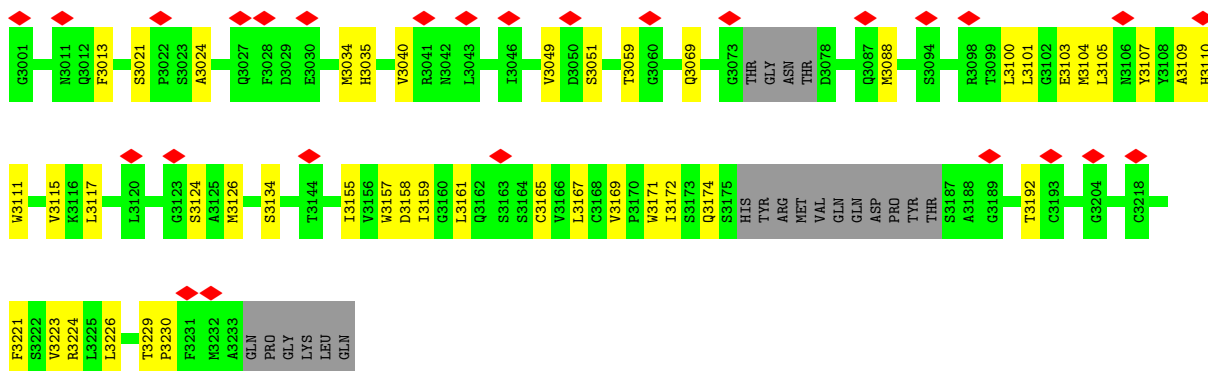
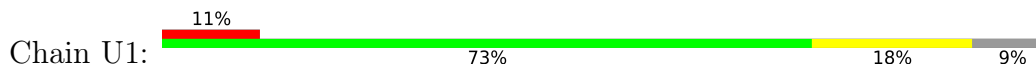
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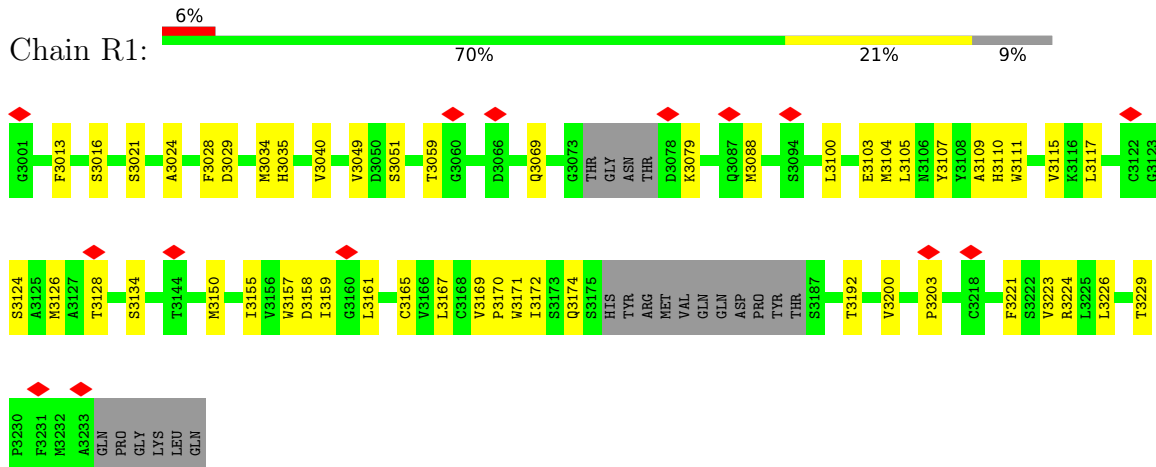
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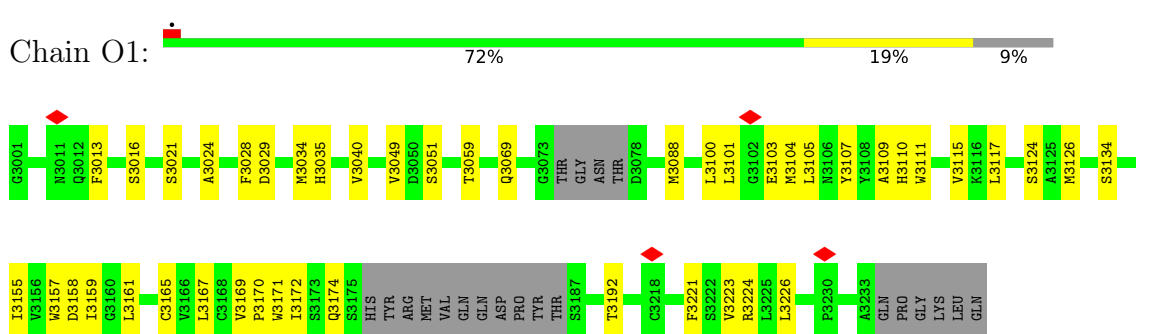
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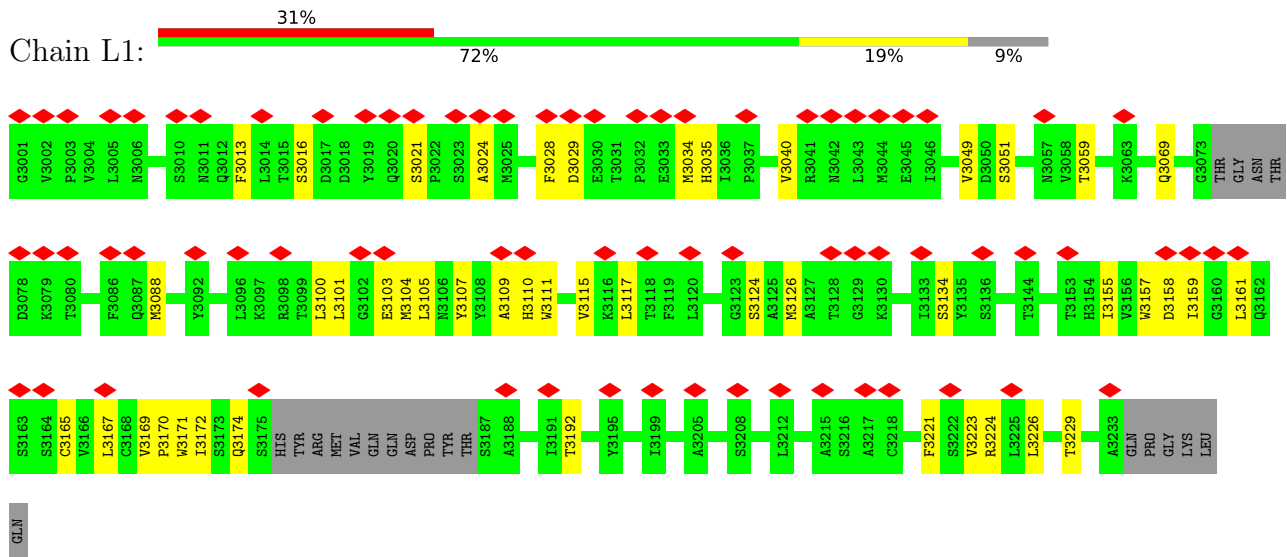
● Molecule 3: Echovirus 18 capsid protein 3



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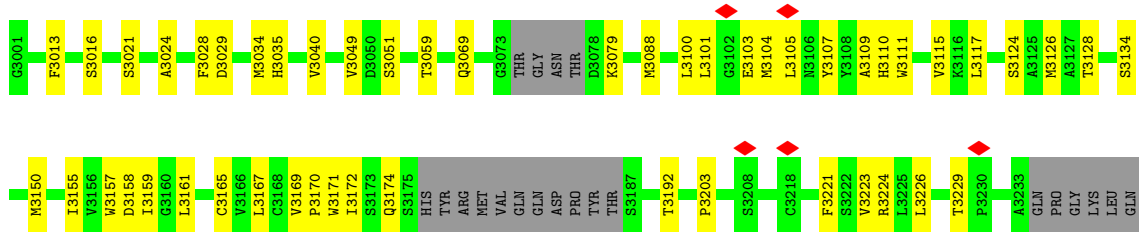


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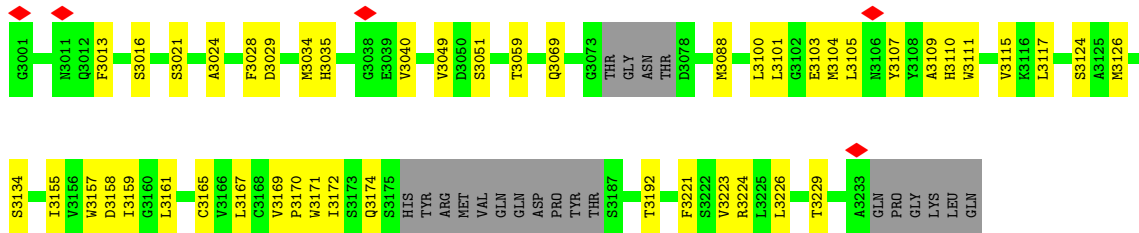


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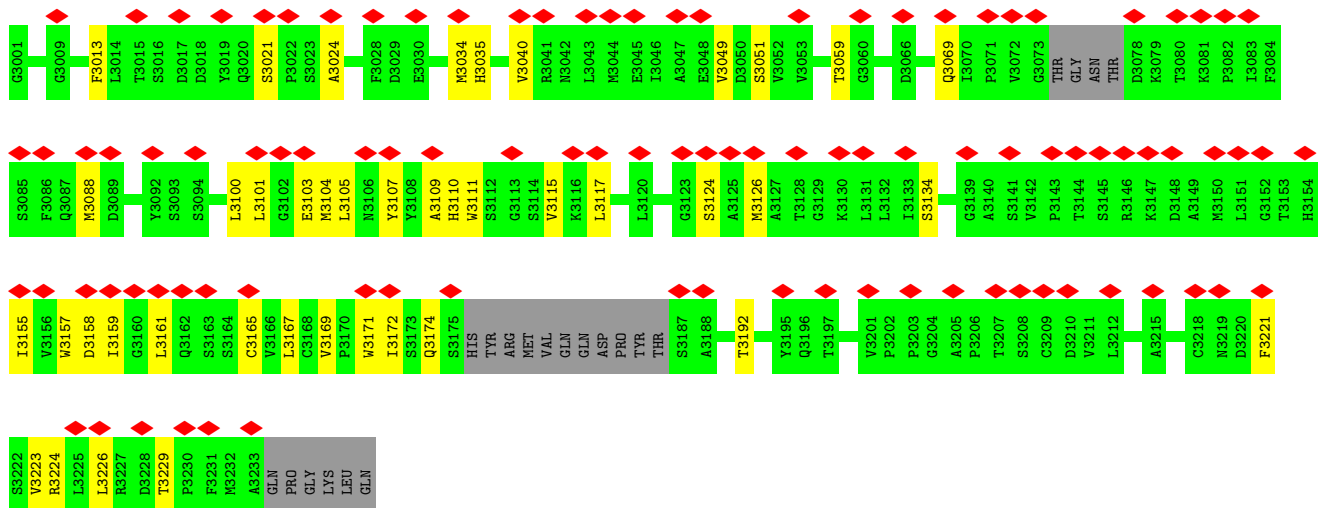
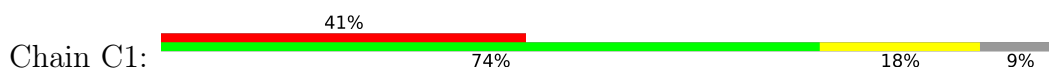




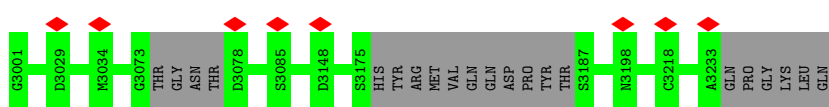
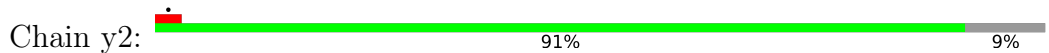
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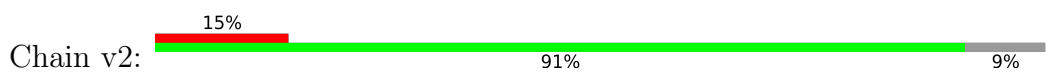
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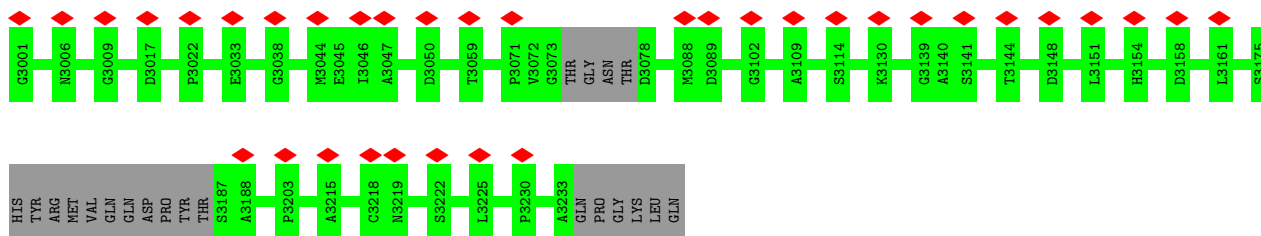


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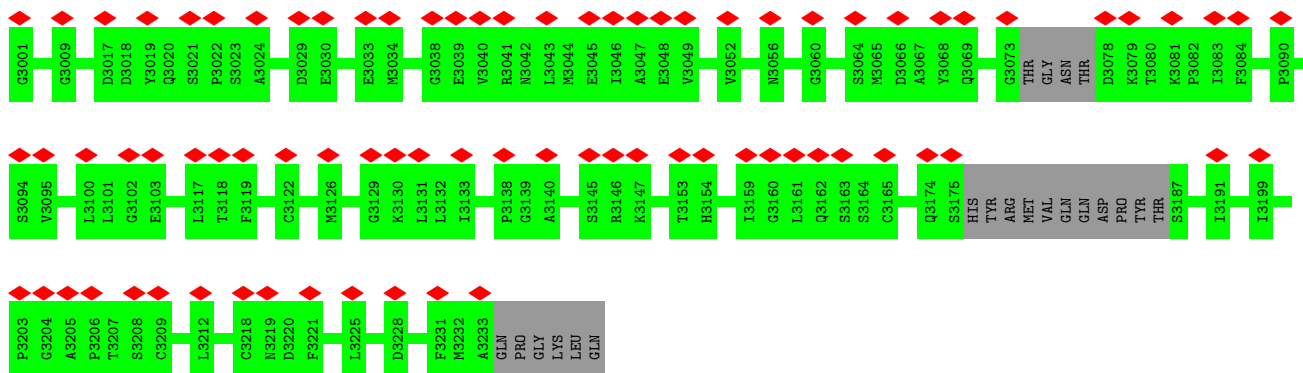
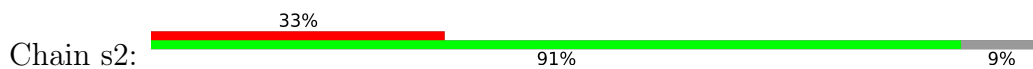


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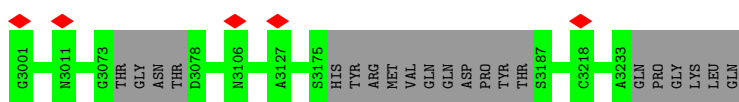




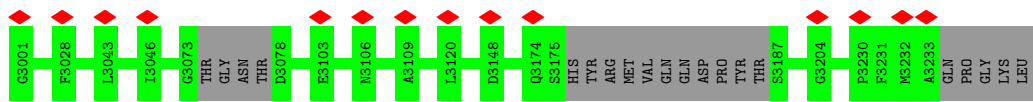
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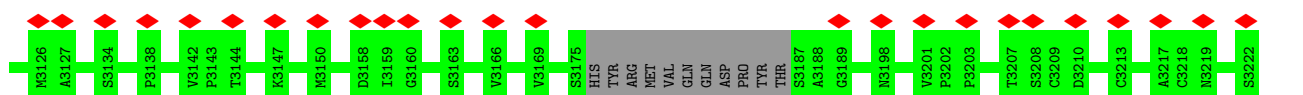
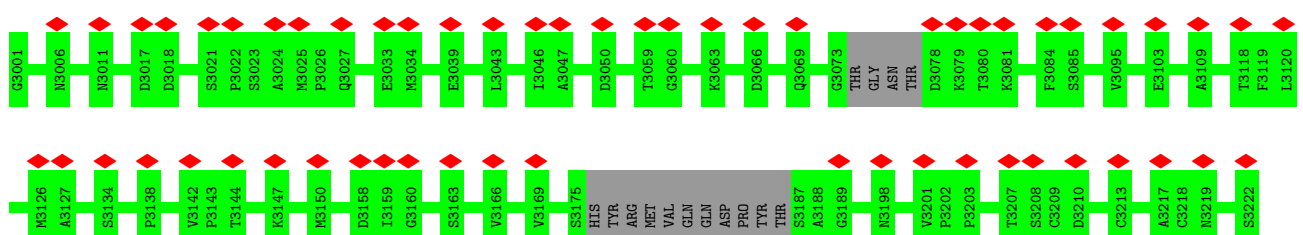
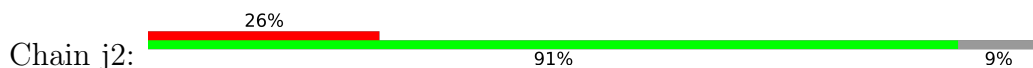
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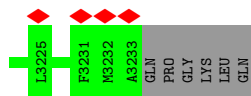


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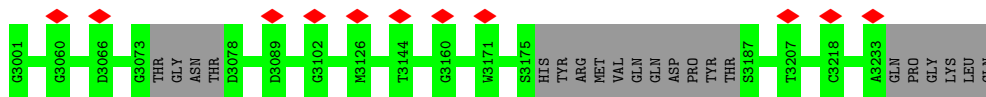
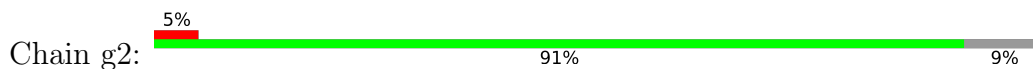


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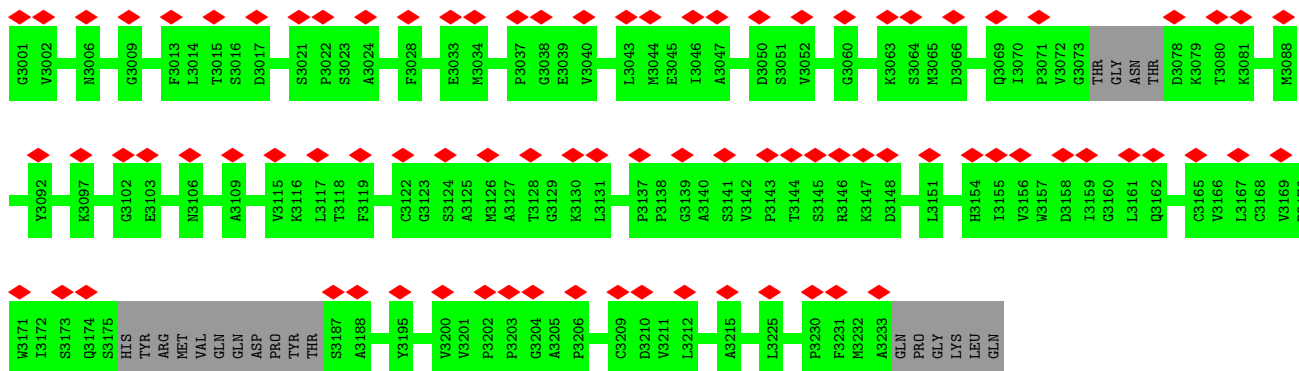
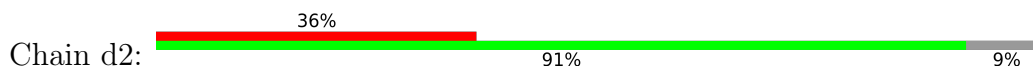




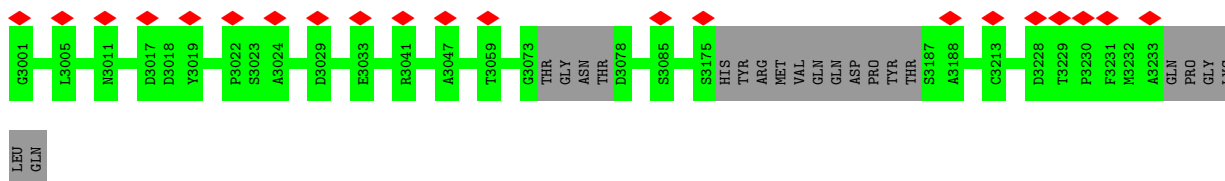
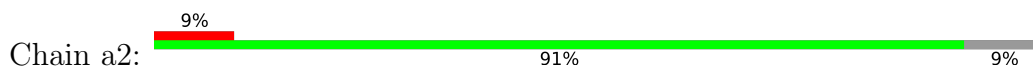
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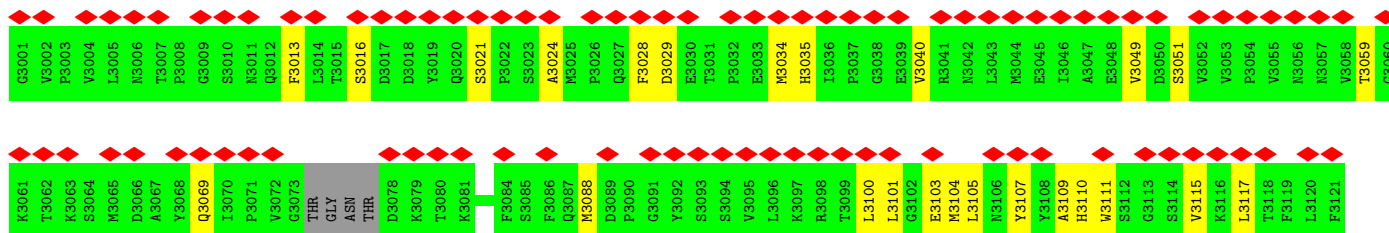
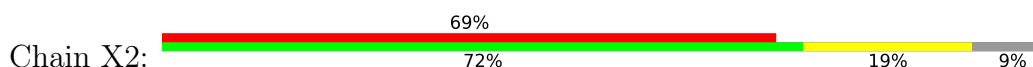
• Molecule 3: Echovirus 18 capsid protein 3



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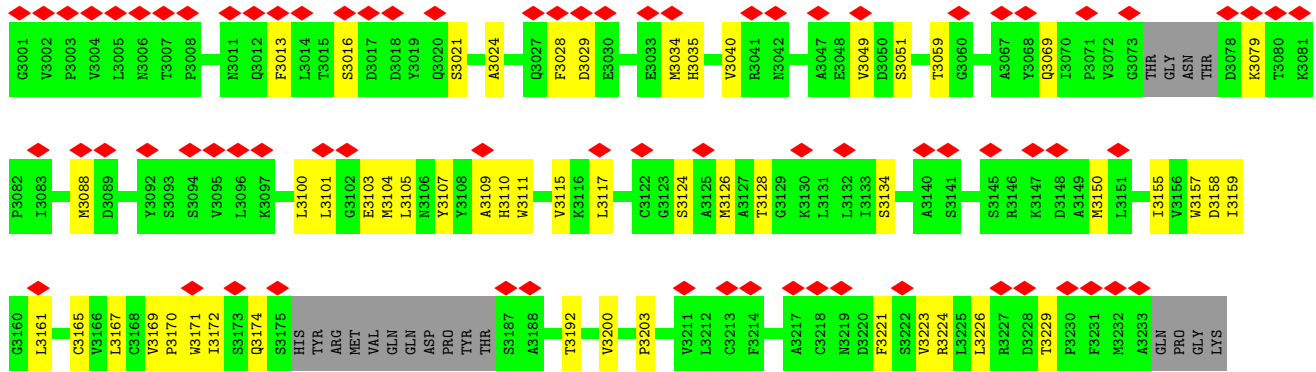


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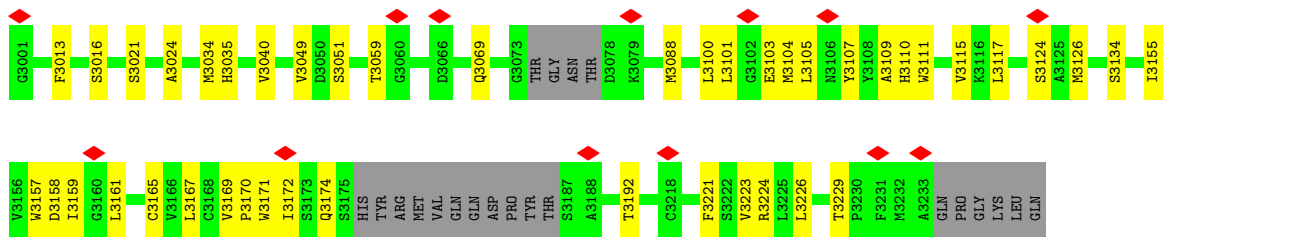
LYS
LEU
GLN

• Molecule 3: Echovirus 18 capsid protein 3

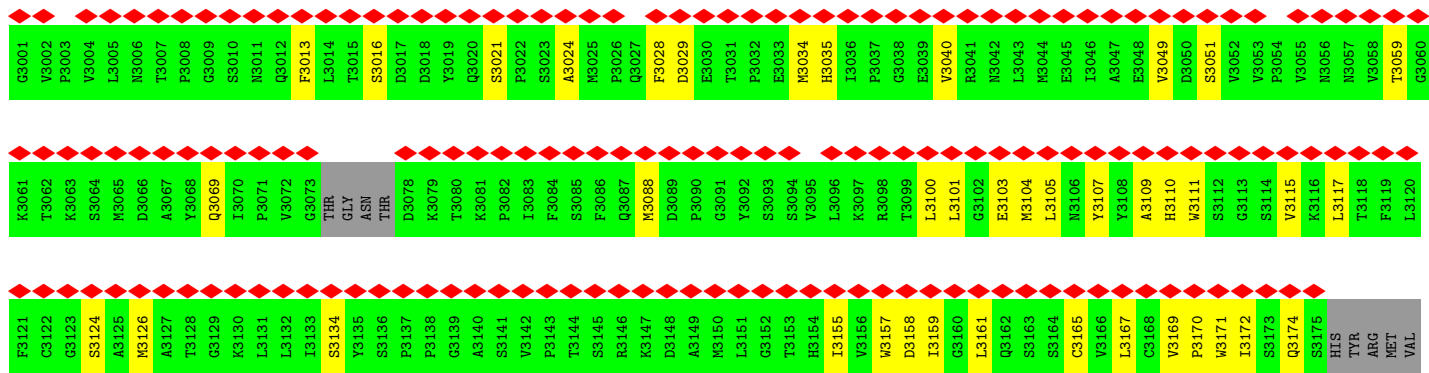
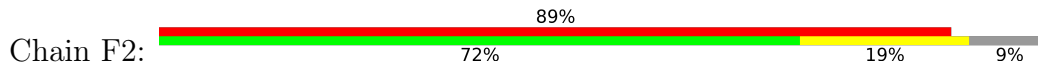


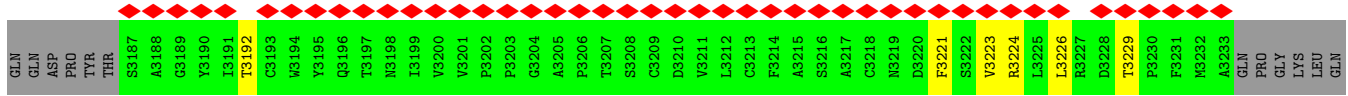
LEU
GLN

• Molecule 3: Echovirus 18 capsid protein 3

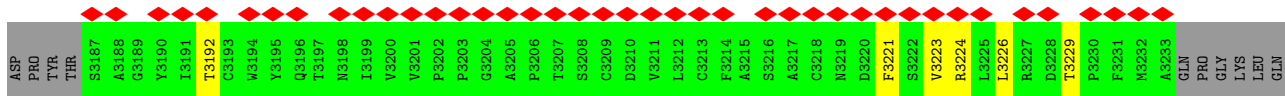
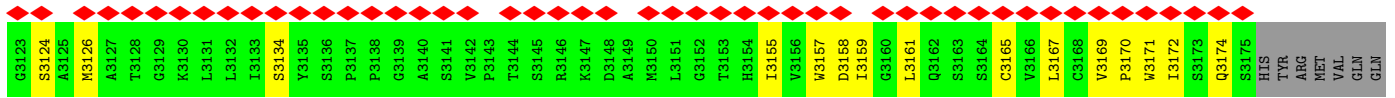
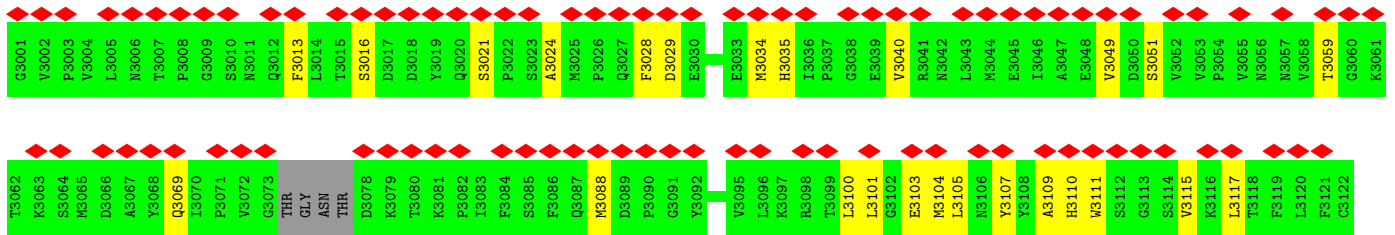
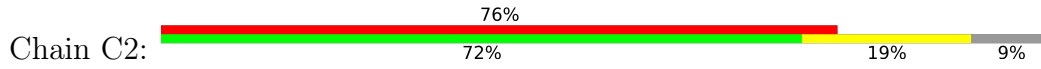


• Molecule 3: Echovirus 18 capsid protein 3





● Molecule 3: Echovirus 18 capsid protein 3



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	7635	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	45.2	Depositor
Minimum defocus (nm)	651	Depositor
Maximum defocus (nm)	3282	Depositor
Magnification	79575	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.439	Depositor
Minimum map value	-0.251	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.028	Depositor
Recommended contour level	0.07	Depositor
Map size (\AA)	371.35, 371.35, 371.35	wwPDB
Map dimensions	350, 350, 350	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.061, 1.061, 1.061	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	0.27	0/1791	0.47	0/2442
1	A2	0.27	0/1791	0.47	0/2442
1	D1	0.27	0/1791	0.47	0/2442
1	D2	0.27	0/1791	0.47	0/2442
1	G1	0.27	0/1791	0.47	0/2442
1	G2	0.27	0/1791	0.47	0/2442
1	J1	0.27	0/1791	0.47	0/2442
1	J2	0.27	0/1791	0.47	0/2442
1	M1	0.27	0/1791	0.47	0/2442
1	M2	0.27	0/1791	0.47	0/2442
1	P1	0.27	0/1791	0.47	0/2442
1	P2	0.27	0/1791	0.47	0/2442
1	S1	0.27	0/1791	0.47	0/2442
1	S2	0.27	0/1791	0.47	0/2442
1	V1	0.27	0/1791	0.47	0/2442
1	V2	0.27	0/1791	0.47	0/2442
1	Y2	0.27	0/1791	0.47	0/2442
1	b2	0.27	0/1791	0.47	0/2442
1	e2	0.27	0/1791	0.47	0/2442
1	h2	0.27	0/1791	0.47	0/2442
1	k2	0.27	0/1791	0.47	0/2442
1	n2	0.27	0/1791	0.47	0/2442
1	q2	0.27	0/1791	0.47	0/2442
1	t2	0.27	0/1791	0.47	0/2442
1	w2	0.27	0/1791	0.47	0/2442
2	B1	0.27	0/1874	0.53	0/2567
2	B2	0.27	0/1874	0.53	0/2567
2	E1	0.27	0/1874	0.53	0/2567
2	E2	0.27	0/1874	0.53	0/2567
2	H1	0.27	0/1874	0.53	0/2567
2	H2	0.27	0/1874	0.53	0/2567
2	K1	0.27	0/1874	0.53	0/2567
2	K2	0.27	0/1874	0.53	0/2567
2	N1	0.27	0/1874	0.53	0/2567

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	N2	0.27	0/1874	0.53	0/2567
2	Q1	0.27	0/1874	0.53	0/2567
2	Q2	0.27	0/1874	0.53	0/2567
2	T1	0.27	0/1874	0.53	0/2567
2	T2	0.27	0/1874	0.53	0/2567
2	W1	0.26	0/1874	0.53	0/2567
2	W2	0.26	0/1874	0.53	0/2567
2	Z2	0.26	0/1874	0.53	0/2567
2	c2	0.26	0/1874	0.53	0/2567
2	f2	0.27	0/1874	0.53	0/2567
2	i2	0.27	0/1874	0.53	0/2567
2	l2	0.27	0/1874	0.53	0/2567
2	o2	0.27	0/1874	0.53	0/2567
2	r2	0.27	0/1874	0.53	0/2567
2	u2	0.27	0/1874	0.53	0/2567
2	x2	0.27	0/1874	0.53	0/2567
3	C1	0.26	0/1676	0.48	0/2287
3	C2	0.26	0/1676	0.48	0/2287
3	F1	0.26	0/1676	0.48	0/2287
3	F2	0.26	0/1676	0.48	0/2287
3	I1	0.26	0/1676	0.48	0/2287
3	I2	0.26	0/1676	0.48	0/2287
3	L1	0.26	0/1676	0.48	0/2287
3	L2	0.26	0/1676	0.48	0/2287
3	O1	0.26	0/1676	0.48	0/2287
3	O2	0.26	0/1676	0.48	0/2287
3	R1	0.26	0/1676	0.48	0/2287
3	R2	0.26	0/1676	0.48	0/2287
3	U1	0.26	0/1676	0.48	0/2287
3	U2	0.26	0/1676	0.48	0/2287
3	X1	0.26	0/1676	0.48	0/2287
3	X2	0.26	0/1676	0.48	0/2287
3	a2	0.26	0/1676	0.48	0/2287
3	d2	0.26	0/1676	0.48	0/2287
3	g2	0.26	0/1676	0.48	0/2287
3	j2	0.26	0/1676	0.48	0/2287
3	m2	0.26	0/1676	0.48	0/2287
3	p2	0.26	0/1676	0.48	0/2287
3	s2	0.26	0/1676	0.48	0/2287
3	v2	0.26	0/1676	0.48	0/2287
3	y2	0.26	0/1676	0.48	0/2287
All	All	0.27	0/133525	0.49	0/182400

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A1	1741	0	1659	36	0
1	A2	1741	0	1659	46	0
1	D1	1741	0	1659	45	0
1	D2	1741	0	1659	45	0
1	G1	1741	0	1659	46	0
1	G2	1741	0	1659	41	0
1	J1	1741	0	1659	43	0
1	J2	1741	0	1659	44	0
1	M1	1741	0	1659	45	0
1	M2	1741	0	1659	40	0
1	P1	1741	0	1659	44	0
1	P2	1741	0	1659	42	0
1	S1	1741	0	1659	36	0
1	S2	1741	0	1659	38	0
1	V1	1741	0	1659	45	0
1	V2	1741	0	1659	45	0
1	Y2	1741	0	1659	28	0
1	b2	1741	0	1659	0	0
1	e2	1741	0	1659	0	0
1	h2	1741	0	1659	0	0
1	k2	1741	0	1659	0	0
1	n2	1741	0	1659	0	0
1	q2	1741	0	1659	0	0
1	t2	1741	0	1659	0	0
1	w2	1741	0	1659	0	0
2	B1	1821	0	1739	38	0
2	B2	1821	0	1739	45	0
2	E1	1821	0	1739	43	0
2	E2	1821	0	1739	44	0
2	H1	1821	0	1739	51	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H2	1821	0	1739	42	0
2	K1	1821	0	1739	44	0
2	K2	1821	0	1739	43	0
2	N1	1821	0	1739	46	0
2	N2	1821	0	1739	44	0
2	Q1	1821	0	1739	50	0
2	Q2	1821	0	1739	45	0
2	T1	1821	0	1739	47	0
2	T2	1821	0	1739	50	0
2	W1	1821	0	1739	49	0
2	W2	1821	0	1739	44	0
2	Z2	1821	0	1739	42	0
2	c2	1821	0	1739	0	0
2	f2	1821	0	1739	0	0
2	i2	1821	0	1739	0	0
2	l2	1821	0	1739	0	0
2	o2	1821	0	1739	0	0
2	r2	1821	0	1739	0	0
2	u2	1821	0	1739	0	0
2	x2	1821	0	1739	0	0
3	C1	1634	0	1596	40	0
3	C2	1634	0	1596	48	0
3	F1	1634	0	1596	49	0
3	F2	1634	0	1596	49	0
3	I1	1634	0	1596	54	0
3	I2	1634	0	1596	45	0
3	L1	1634	0	1596	49	0
3	L2	1634	0	1596	55	0
3	O1	1634	0	1596	47	0
3	O2	1634	0	1596	49	0
3	R1	1634	0	1596	54	0
3	R2	1634	0	1596	48	0
3	U1	1634	0	1596	41	0
3	U2	1634	0	1596	46	0
3	X1	1634	0	1596	50	0
3	X2	1634	0	1596	48	0
3	a2	1634	0	1596	0	0
3	d2	1634	0	1596	0	0
3	g2	1634	0	1596	0	0
3	j2	1634	0	1596	0	0
3	m2	1634	0	1596	0	0
3	p2	1634	0	1596	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	s2	1634	0	1596	0	0
3	v2	1634	0	1596	0	0
3	y2	1634	0	1596	0	0
All	All	129900	0	124850	1686	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 10.

The worst 5 of 1686 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:J1:1216:ILE:HD13	1:J1:1231:ILE:HD13	1.56	0.88
1:S1:1216:ILE:HD13	1:S1:1231:ILE:HD13	1.56	0.87
1:M1:1216:ILE:HD13	1:M1:1231:ILE:HD13	1.56	0.87
1:V1:1216:ILE:HD13	1:V1:1231:ILE:HD13	1.56	0.87
1:P2:1216:ILE:HD13	1:P2:1231:ILE:HD13	1.56	0.86

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	220/287 (77%)	200 (91%)	20 (9%)	0	100	100
1	A2	220/287 (77%)	200 (91%)	20 (9%)	0	100	100
1	D1	220/287 (77%)	200 (91%)	20 (9%)	0	100	100
1	D2	220/287 (77%)	200 (91%)	20 (9%)	0	100	100
1	G1	220/287 (77%)	200 (91%)	20 (9%)	0	100	100
1	G2	220/287 (77%)	199 (90%)	21 (10%)	0	100	100
1	J1	220/287 (77%)	200 (91%)	20 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	J2	220/287 (77%)	199 (90%)	21 (10%)	0	100	100
1	M1	220/287 (77%)	200 (91%)	20 (9%)	0	100	100
1	M2	220/287 (77%)	200 (91%)	20 (9%)	0	100	100
1	P1	220/287 (77%)	199 (90%)	21 (10%)	0	100	100
1	P2	220/287 (77%)	199 (90%)	21 (10%)	0	100	100
1	S1	220/287 (77%)	199 (90%)	21 (10%)	0	100	100
1	S2	220/287 (77%)	199 (90%)	21 (10%)	0	100	100
1	V1	220/287 (77%)	199 (90%)	21 (10%)	0	100	100
1	V2	220/287 (77%)	200 (91%)	20 (9%)	0	100	100
1	Y2	220/287 (77%)	200 (91%)	20 (9%)	0	100	100
1	b2	220/287 (77%)	199 (90%)	21 (10%)	0	100	100
1	e2	220/287 (77%)	199 (90%)	21 (10%)	0	100	100
1	h2	220/287 (77%)	199 (90%)	21 (10%)	0	100	100
1	k2	220/287 (77%)	200 (91%)	20 (9%)	0	100	100
1	n2	220/287 (77%)	200 (91%)	20 (9%)	0	100	100
1	q2	220/287 (77%)	200 (91%)	20 (9%)	0	100	100
1	t2	220/287 (77%)	200 (91%)	20 (9%)	0	100	100
1	w2	220/287 (77%)	200 (91%)	20 (9%)	0	100	100
2	B1	232/260 (89%)	204 (88%)	25 (11%)	3 (1%)	12	48
2	B2	232/260 (89%)	204 (88%)	25 (11%)	3 (1%)	12	48
2	E1	232/260 (89%)	204 (88%)	25 (11%)	3 (1%)	12	48
2	E2	232/260 (89%)	204 (88%)	25 (11%)	3 (1%)	12	48
2	H1	232/260 (89%)	204 (88%)	25 (11%)	3 (1%)	12	48
2	H2	232/260 (89%)	204 (88%)	25 (11%)	3 (1%)	12	48
2	K1	232/260 (89%)	204 (88%)	25 (11%)	3 (1%)	12	48
2	K2	232/260 (89%)	204 (88%)	25 (11%)	3 (1%)	12	48
2	N1	232/260 (89%)	204 (88%)	25 (11%)	3 (1%)	12	48
2	N2	232/260 (89%)	204 (88%)	25 (11%)	3 (1%)	12	48
2	Q1	232/260 (89%)	204 (88%)	25 (11%)	3 (1%)	12	48
2	Q2	232/260 (89%)	204 (88%)	25 (11%)	3 (1%)	12	48
2	T1	232/260 (89%)	204 (88%)	25 (11%)	3 (1%)	12	48

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	T2	232/260 (89%)	204 (88%)	25 (11%)	3 (1%)	12	48
2	W1	232/260 (89%)	204 (88%)	25 (11%)	3 (1%)	12	48
2	W2	232/260 (89%)	204 (88%)	25 (11%)	3 (1%)	12	48
2	Z2	232/260 (89%)	204 (88%)	25 (11%)	3 (1%)	12	48
2	c2	232/260 (89%)	204 (88%)	25 (11%)	3 (1%)	12	48
2	f2	232/260 (89%)	204 (88%)	25 (11%)	3 (1%)	12	48
2	i2	232/260 (89%)	204 (88%)	25 (11%)	3 (1%)	12	48
2	l2	232/260 (89%)	204 (88%)	25 (11%)	3 (1%)	12	48
2	o2	232/260 (89%)	204 (88%)	25 (11%)	3 (1%)	12	48
2	r2	232/260 (89%)	204 (88%)	25 (11%)	3 (1%)	12	48
2	u2	232/260 (89%)	204 (88%)	25 (11%)	3 (1%)	12	48
2	x2	232/260 (89%)	204 (88%)	25 (11%)	3 (1%)	12	48
3	C1	212/239 (89%)	197 (93%)	15 (7%)	0	100	100
3	C2	212/239 (89%)	197 (93%)	15 (7%)	0	100	100
3	F1	212/239 (89%)	197 (93%)	15 (7%)	0	100	100
3	F2	212/239 (89%)	197 (93%)	15 (7%)	0	100	100
3	I1	212/239 (89%)	197 (93%)	15 (7%)	0	100	100
3	I2	212/239 (89%)	197 (93%)	15 (7%)	0	100	100
3	L1	212/239 (89%)	197 (93%)	15 (7%)	0	100	100
3	L2	212/239 (89%)	197 (93%)	15 (7%)	0	100	100
3	O1	212/239 (89%)	197 (93%)	15 (7%)	0	100	100
3	O2	212/239 (89%)	197 (93%)	15 (7%)	0	100	100
3	R1	212/239 (89%)	197 (93%)	15 (7%)	0	100	100
3	R2	212/239 (89%)	197 (93%)	15 (7%)	0	100	100
3	U1	212/239 (89%)	197 (93%)	15 (7%)	0	100	100
3	U2	212/239 (89%)	197 (93%)	15 (7%)	0	100	100
3	X1	212/239 (89%)	197 (93%)	15 (7%)	0	100	100
3	X2	212/239 (89%)	197 (93%)	15 (7%)	0	100	100
3	a2	212/239 (89%)	197 (93%)	15 (7%)	0	100	100
3	d2	212/239 (89%)	197 (93%)	15 (7%)	0	100	100
3	g2	212/239 (89%)	197 (93%)	15 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	j2	212/239 (89%)	197 (93%)	15 (7%)	0	100	100
3	m2	212/239 (89%)	197 (93%)	15 (7%)	0	100	100
3	p2	212/239 (89%)	197 (93%)	15 (7%)	0	100	100
3	s2	212/239 (89%)	197 (93%)	15 (7%)	0	100	100
3	v2	212/239 (89%)	197 (93%)	15 (7%)	0	100	100
3	y2	212/239 (89%)	197 (93%)	15 (7%)	0	100	100
All	All	16600/19650 (84%)	15015 (90%)	1510 (9%)	75 (0%)	32	67

5 of 75 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	W1	2060	THR
2	W1	2149	GLU
2	T1	2060	THR
2	T1	2149	GLU
2	Q1	2060	THR

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all 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	A1	182/259 (70%)	182 (100%)	0	100	100
1	A2	182/259 (70%)	182 (100%)	0	100	100
1	D1	182/259 (70%)	182 (100%)	0	100	100
1	D2	182/259 (70%)	182 (100%)	0	100	100
1	G1	182/259 (70%)	182 (100%)	0	100	100
1	G2	182/259 (70%)	182 (100%)	0	100	100
1	J1	182/259 (70%)	182 (100%)	0	100	100
1	J2	182/259 (70%)	182 (100%)	0	100	100
1	M1	182/259 (70%)	182 (100%)	0	100	100
1	M2	182/259 (70%)	182 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	P1	182/259 (70%)	182 (100%)	0	100	100
1	P2	182/259 (70%)	182 (100%)	0	100	100
1	S1	182/259 (70%)	182 (100%)	0	100	100
1	S2	182/259 (70%)	182 (100%)	0	100	100
1	V1	182/259 (70%)	182 (100%)	0	100	100
1	V2	182/259 (70%)	182 (100%)	0	100	100
1	Y2	182/259 (70%)	182 (100%)	0	100	100
1	b2	182/259 (70%)	182 (100%)	0	100	100
1	e2	182/259 (70%)	182 (100%)	0	100	100
1	h2	182/259 (70%)	182 (100%)	0	100	100
1	k2	182/259 (70%)	182 (100%)	0	100	100
1	n2	182/259 (70%)	182 (100%)	0	100	100
1	q2	182/259 (70%)	182 (100%)	0	100	100
1	t2	182/259 (70%)	182 (100%)	0	100	100
1	w2	182/259 (70%)	182 (100%)	0	100	100
2	B1	193/221 (87%)	193 (100%)	0	100	100
2	B2	193/221 (87%)	193 (100%)	0	100	100
2	E1	193/221 (87%)	193 (100%)	0	100	100
2	E2	193/221 (87%)	193 (100%)	0	100	100
2	H1	193/221 (87%)	193 (100%)	0	100	100
2	H2	193/221 (87%)	193 (100%)	0	100	100
2	K1	193/221 (87%)	193 (100%)	0	100	100
2	K2	193/221 (87%)	193 (100%)	0	100	100
2	N1	193/221 (87%)	193 (100%)	0	100	100
2	N2	193/221 (87%)	193 (100%)	0	100	100
2	Q1	193/221 (87%)	193 (100%)	0	100	100
2	Q2	193/221 (87%)	193 (100%)	0	100	100
2	T1	193/221 (87%)	193 (100%)	0	100	100
2	T2	193/221 (87%)	193 (100%)	0	100	100
2	W1	193/221 (87%)	193 (100%)	0	100	100
2	W2	193/221 (87%)	193 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	Z2	193/221 (87%)	193 (100%)	0	100	100
2	c2	193/221 (87%)	193 (100%)	0	100	100
2	f2	193/221 (87%)	193 (100%)	0	100	100
2	i2	193/221 (87%)	193 (100%)	0	100	100
2	l2	193/221 (87%)	193 (100%)	0	100	100
2	o2	193/221 (87%)	193 (100%)	0	100	100
2	r2	193/221 (87%)	193 (100%)	0	100	100
2	u2	193/221 (87%)	193 (100%)	0	100	100
2	x2	193/221 (87%)	193 (100%)	0	100	100
3	C1	184/209 (88%)	184 (100%)	0	100	100
3	C2	184/209 (88%)	184 (100%)	0	100	100
3	F1	184/209 (88%)	184 (100%)	0	100	100
3	F2	184/209 (88%)	184 (100%)	0	100	100
3	I1	184/209 (88%)	184 (100%)	0	100	100
3	I2	184/209 (88%)	184 (100%)	0	100	100
3	L1	184/209 (88%)	184 (100%)	0	100	100
3	L2	184/209 (88%)	184 (100%)	0	100	100
3	O1	184/209 (88%)	184 (100%)	0	100	100
3	O2	184/209 (88%)	184 (100%)	0	100	100
3	R1	184/209 (88%)	184 (100%)	0	100	100
3	R2	184/209 (88%)	184 (100%)	0	100	100
3	U1	184/209 (88%)	184 (100%)	0	100	100
3	U2	184/209 (88%)	184 (100%)	0	100	100
3	X1	184/209 (88%)	184 (100%)	0	100	100
3	X2	184/209 (88%)	184 (100%)	0	100	100
3	a2	184/209 (88%)	184 (100%)	0	100	100
3	d2	184/209 (88%)	184 (100%)	0	100	100
3	g2	184/209 (88%)	184 (100%)	0	100	100
3	j2	184/209 (88%)	184 (100%)	0	100	100
3	m2	184/209 (88%)	184 (100%)	0	100	100
3	p2	184/209 (88%)	184 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	s2	184/209 (88%)	184 (100%)	0	100	100
3	v2	184/209 (88%)	184 (100%)	0	100	100
3	y2	184/209 (88%)	184 (100%)	0	100	100
All	All	13975/17225 (81%)	13975 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 91 such sidechains are listed below:

Mol	Chain	Res	Type
3	a2	3110	HIS
3	R2	3198	ASN
3	a2	3198	ASN
3	U2	3154	HIS
3	O2	3154	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 monosaccharides 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

There are no chain breaks in this entry.

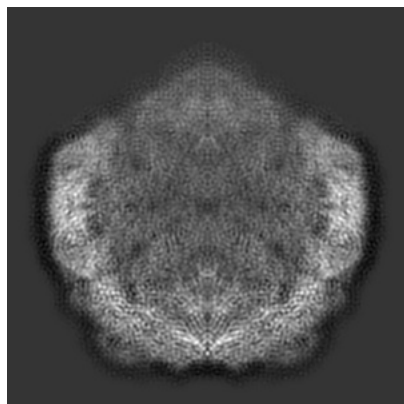
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0217. These allow visual inspection of the internal detail of the map and identification of artifacts.

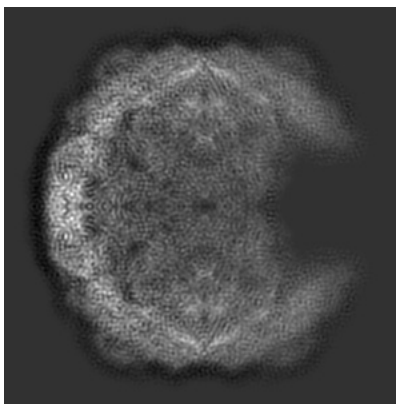
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

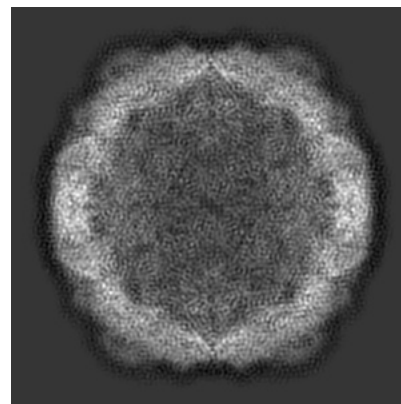
6.1.1 Primary map



X

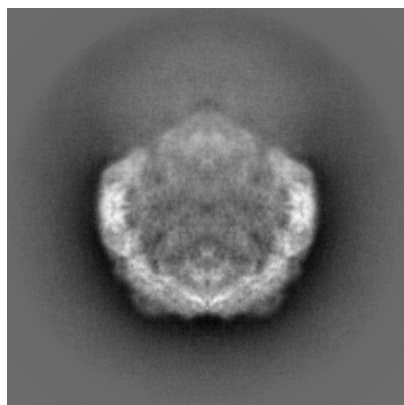


Y

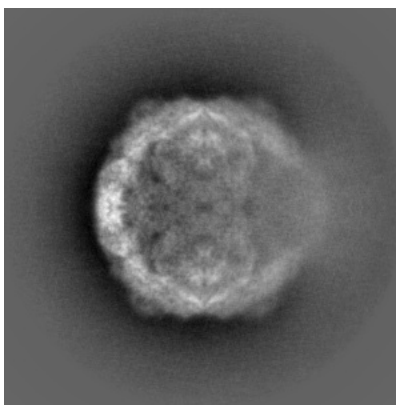


Z

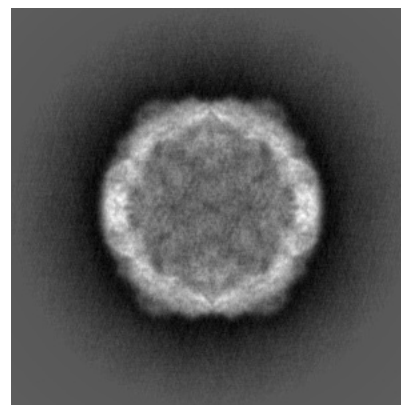
6.1.2 Raw map



X



Y



Z

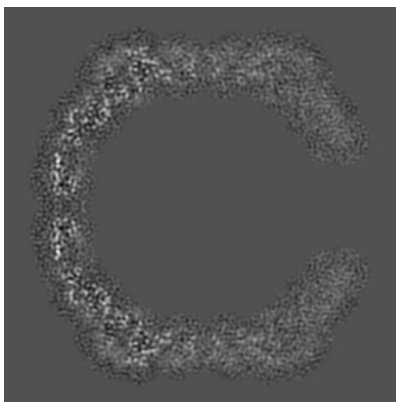
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

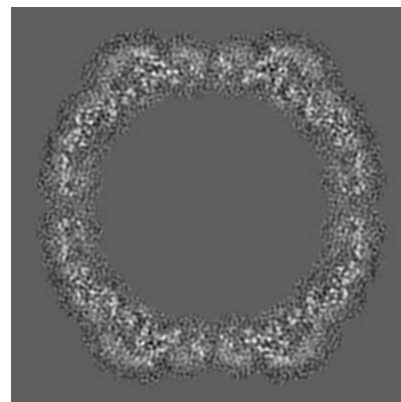
6.2.1 Primary map



X Index: 175

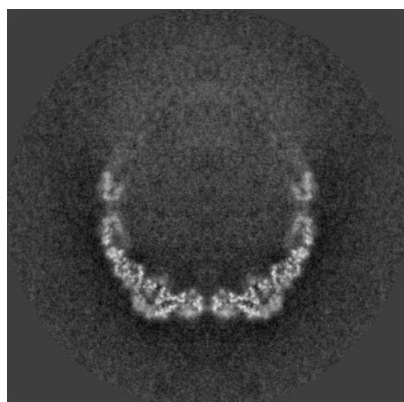


Y Index: 175

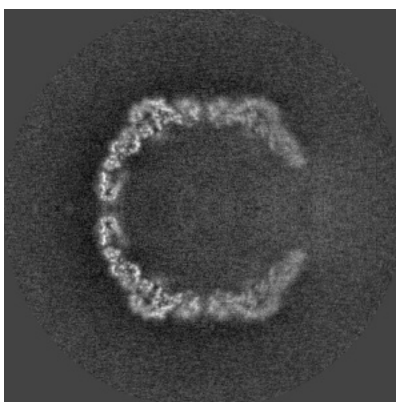


Z Index: 175

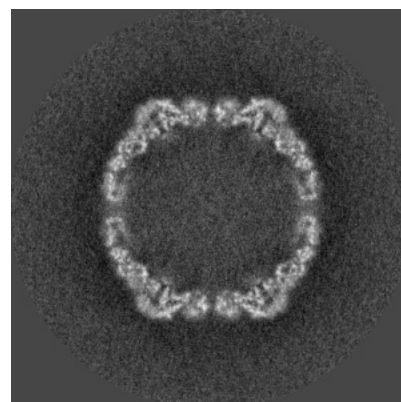
6.2.2 Raw map



X Index: 256



Y Index: 256

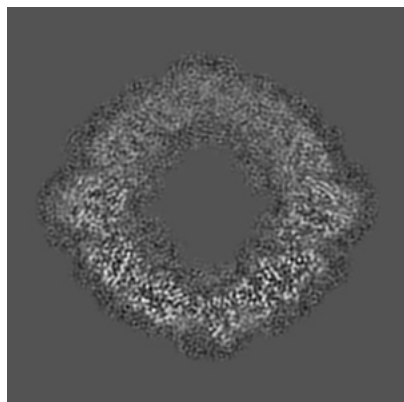


Z Index: 256

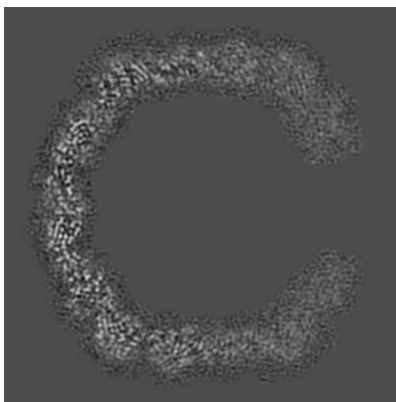
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

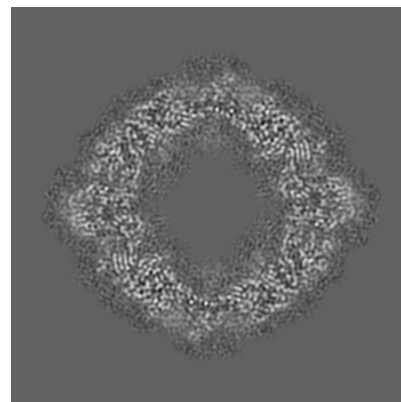
6.3.1 Primary map



X Index: 263

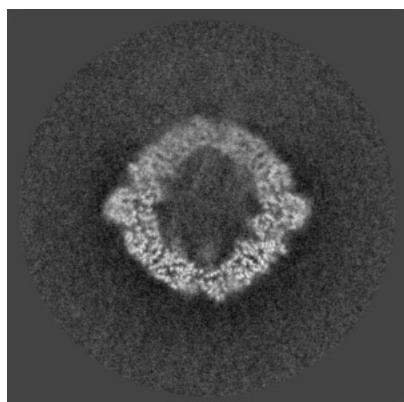


Y Index: 159

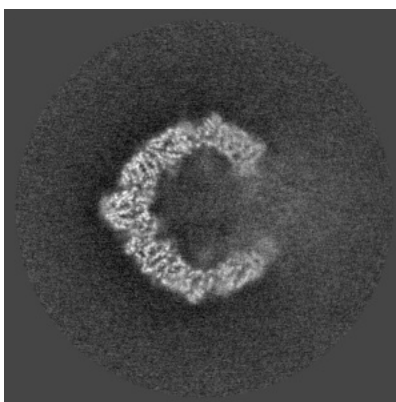


Z Index: 85

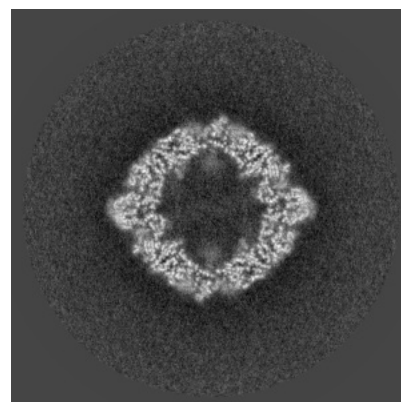
6.3.2 Raw map



X Index: 346



Y Index: 168

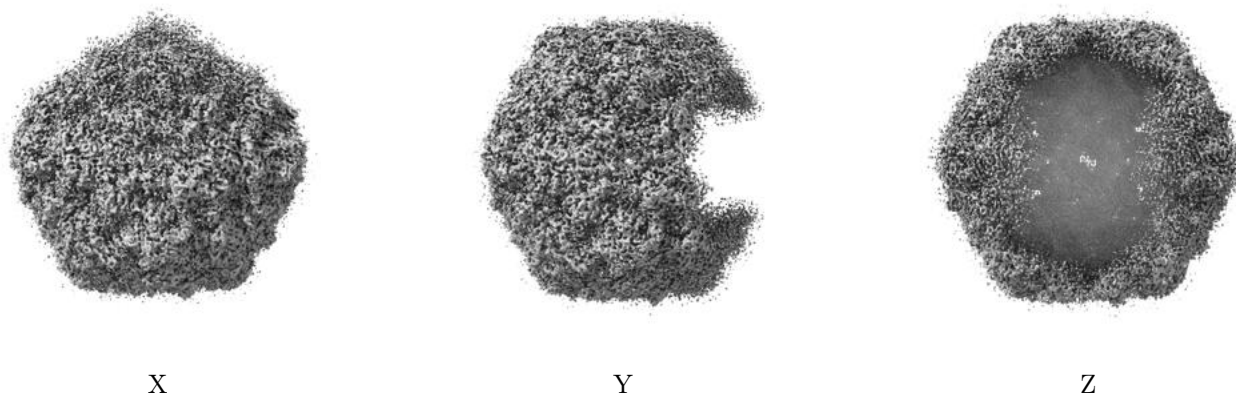


Z Index: 166

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

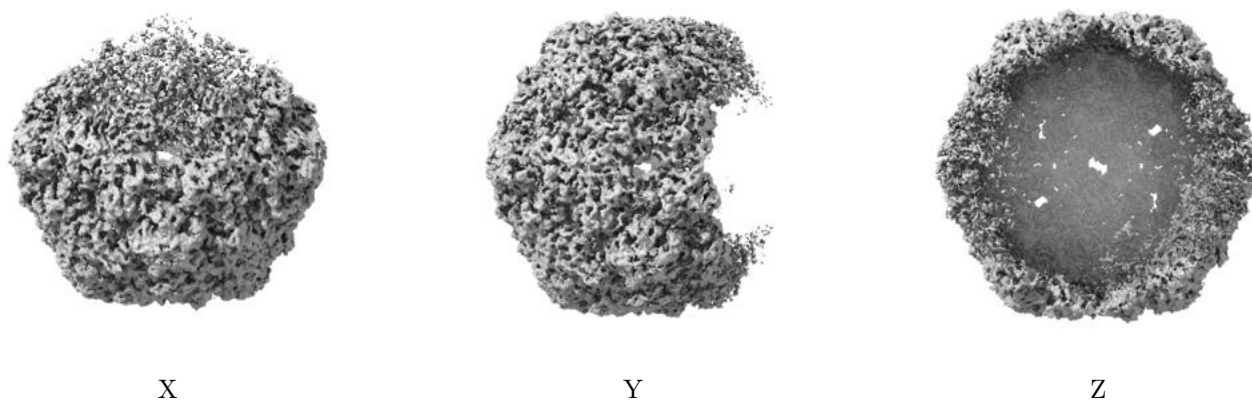
6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.07. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

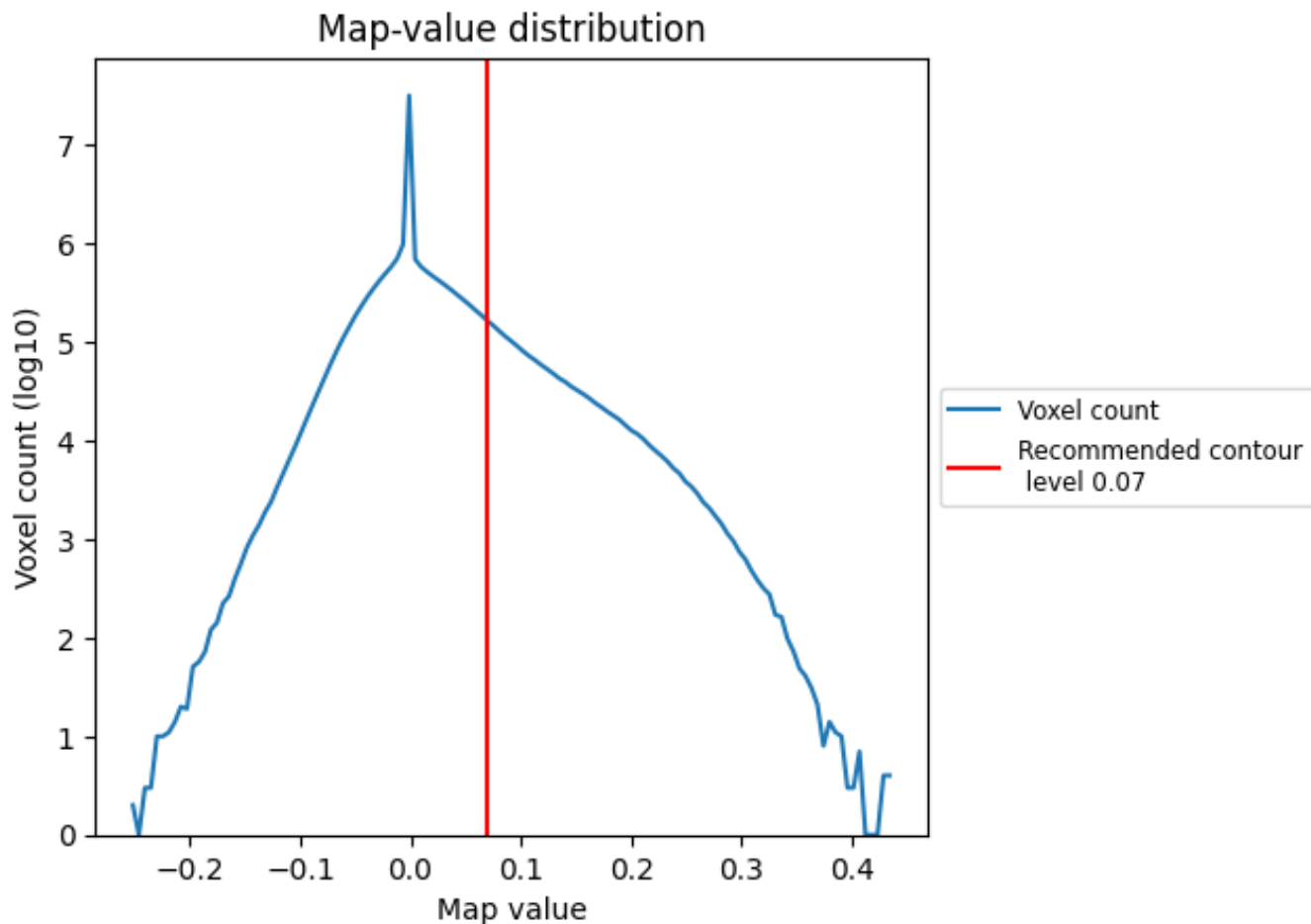
6.5 Mask visualisation [i](#)

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

7 Map analysis [i](#)

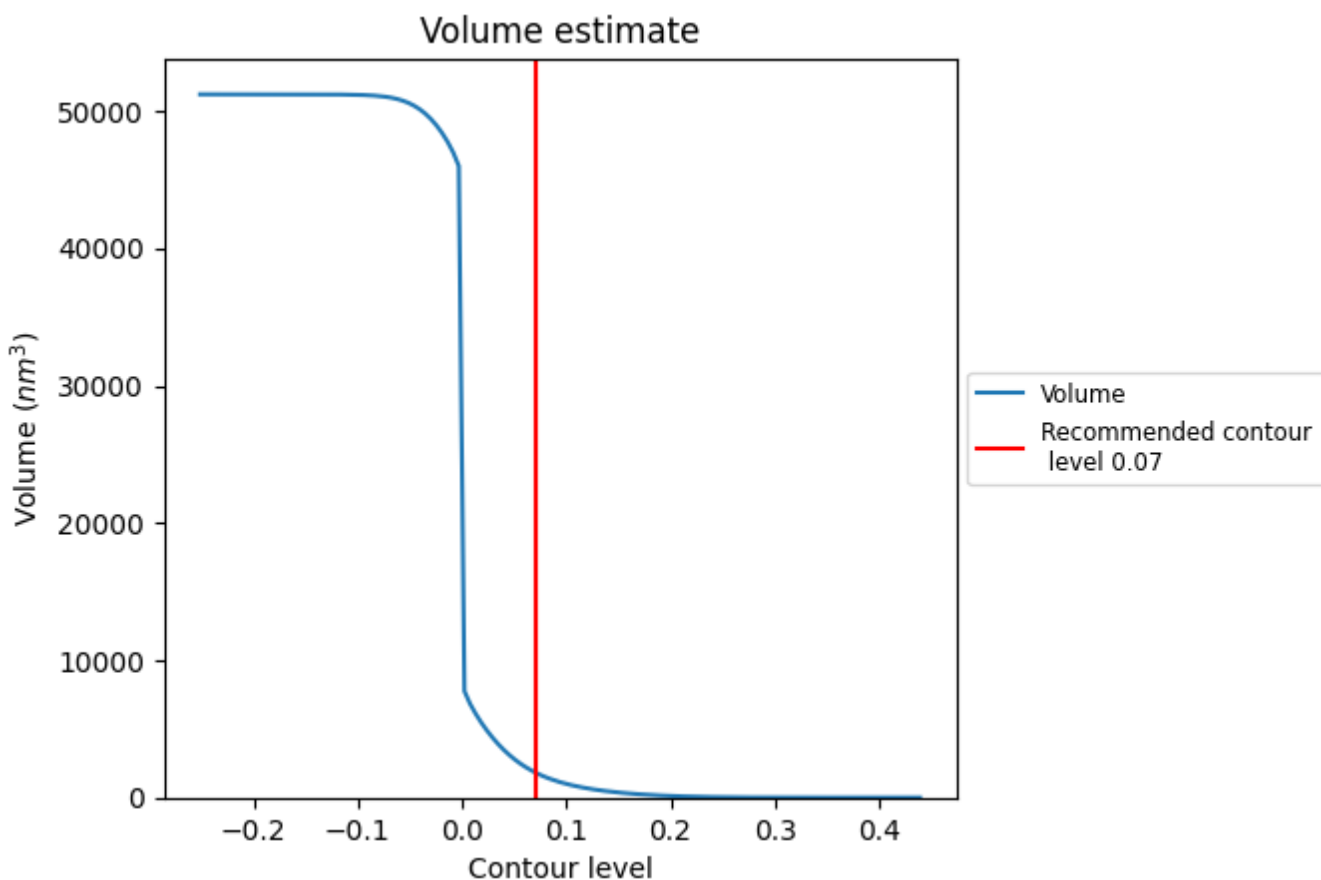
This section contains the results of statistical analysis of the map.

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.

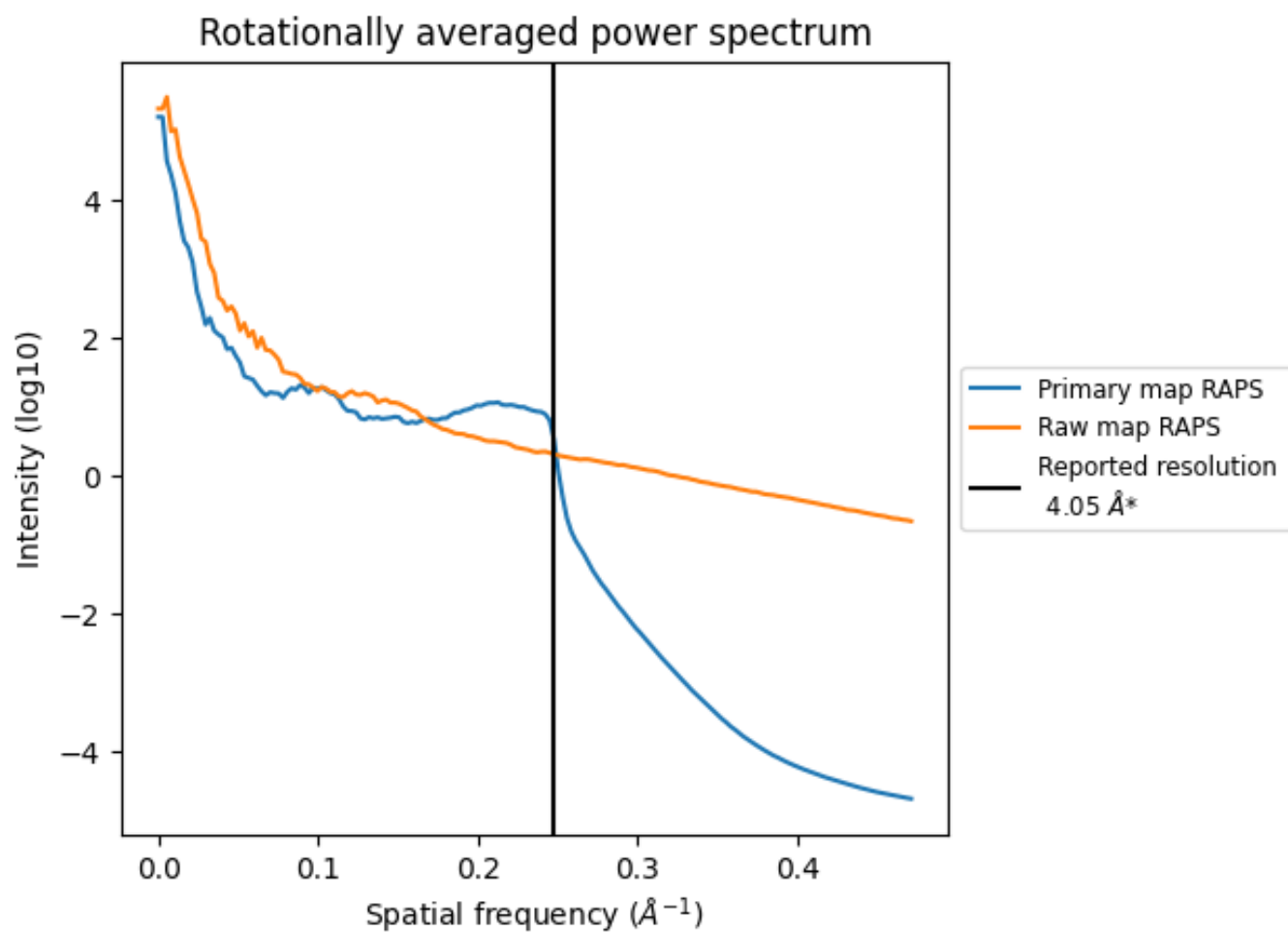
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1838 nm³; this corresponds to an approximate mass of 1661 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 i

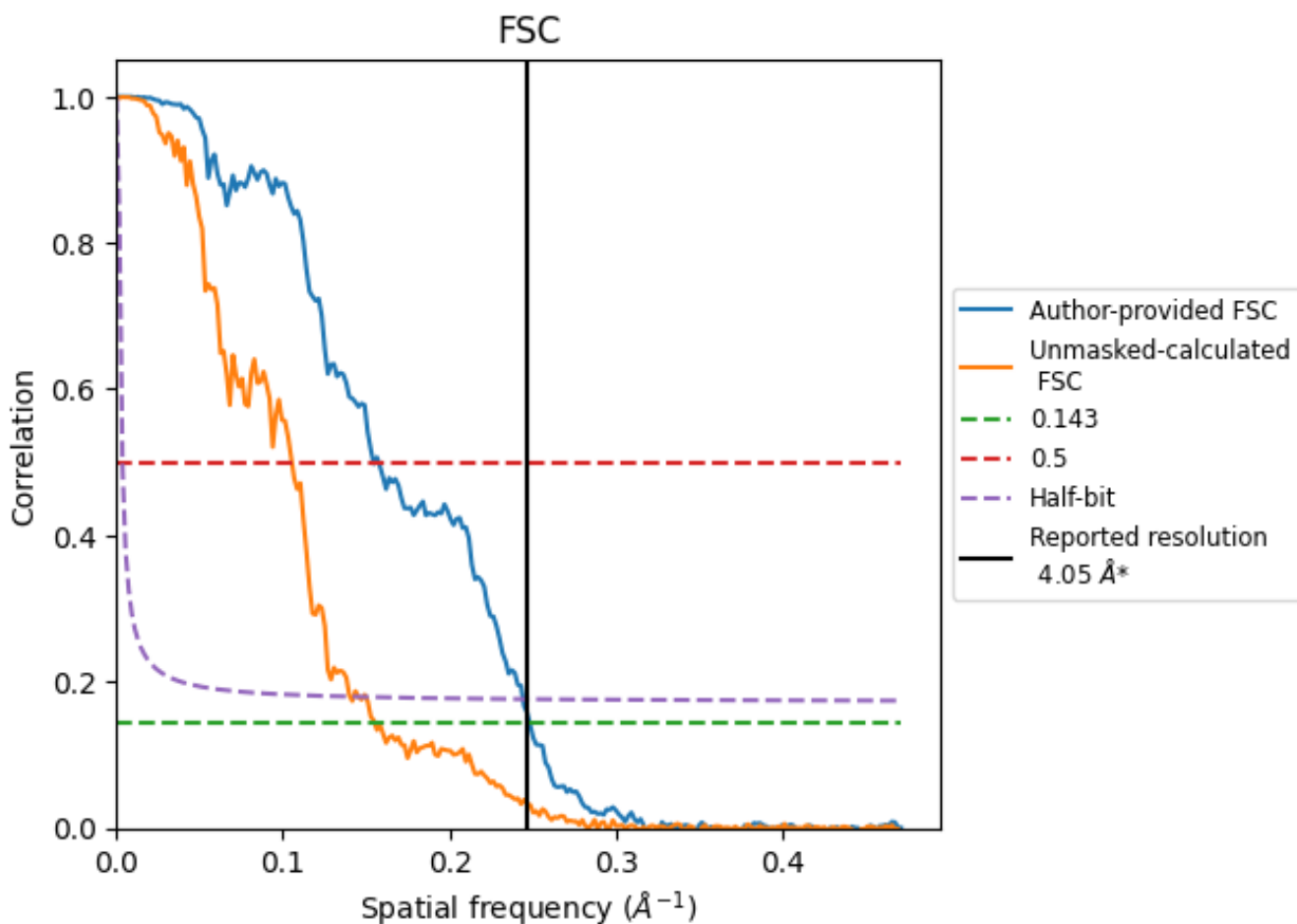


*Reported resolution corresponds to spatial frequency of 0.247 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.247 Å⁻¹

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.05	-	-
Author-provided FSC curve	4.03	6.48	4.10
Unmasked-calculated*	6.44	9.49	7.13

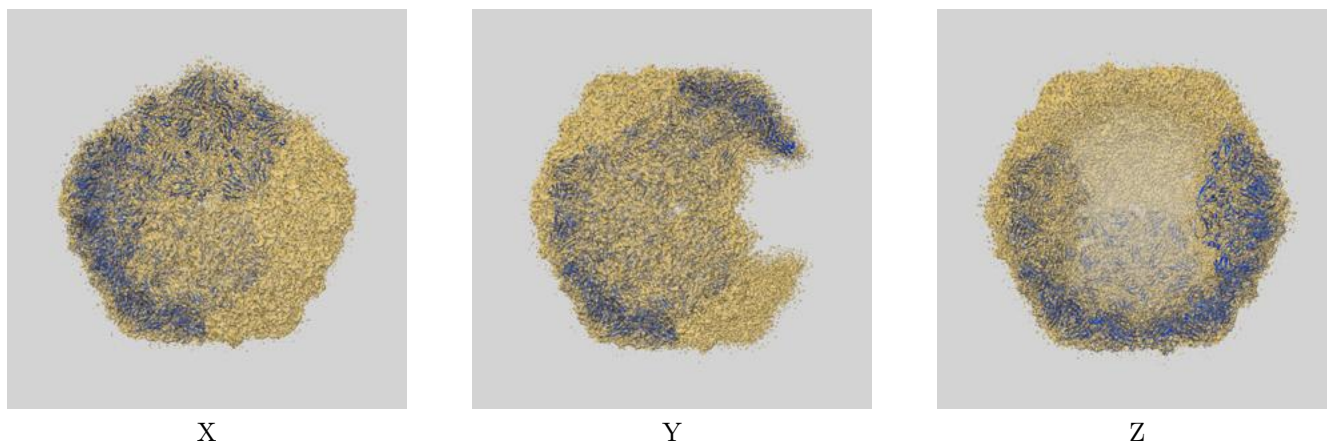
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.44 differs from the reported value 4.05 by more than 10 %

9 Map-model fit [i](#)

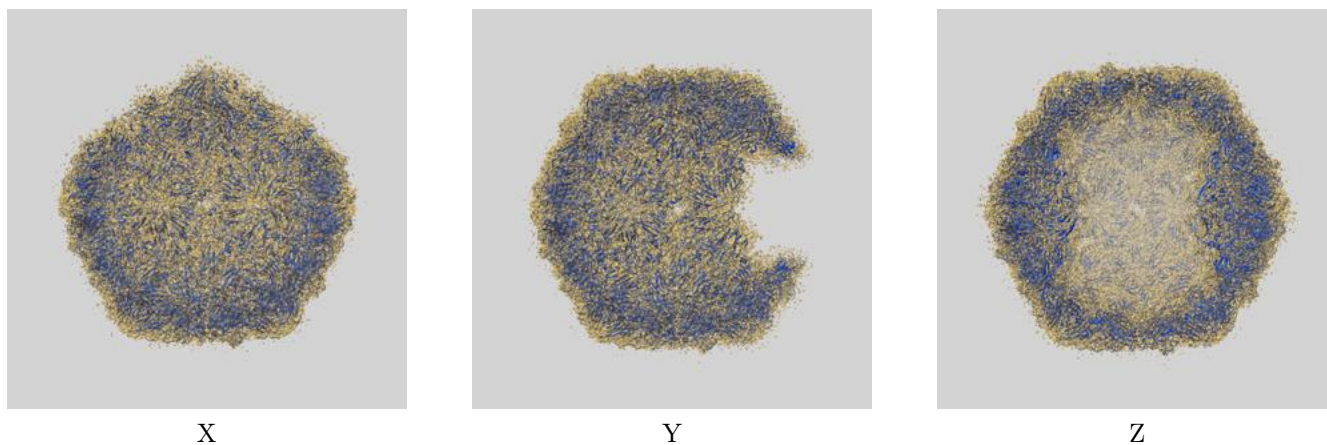
This section contains information regarding the fit between EMDB map EMD-0217 and PDB model 6HHT. Per-residue inclusion information can be found in section 3 on page 10.

9.1 Map-model overlays

9.1.1 Map-model overlay [i](#)

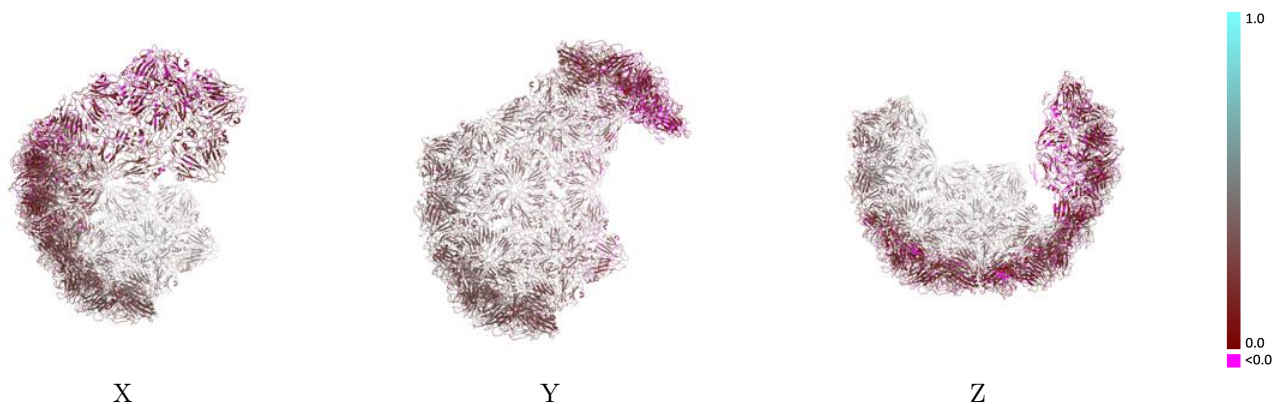


9.1.2 Map-model assembly overlay [i](#)



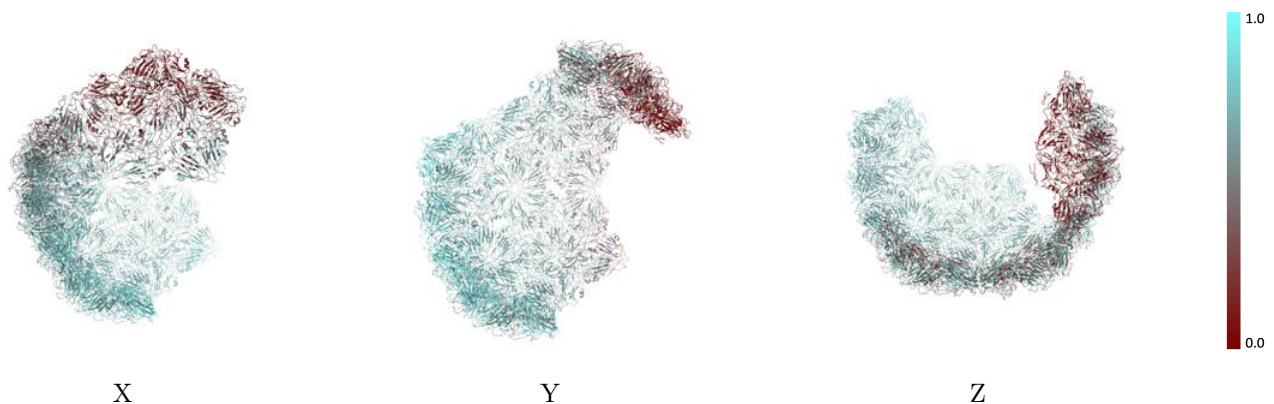
The images above show the 3D surface view of the map at the recommended contour level 0.07 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



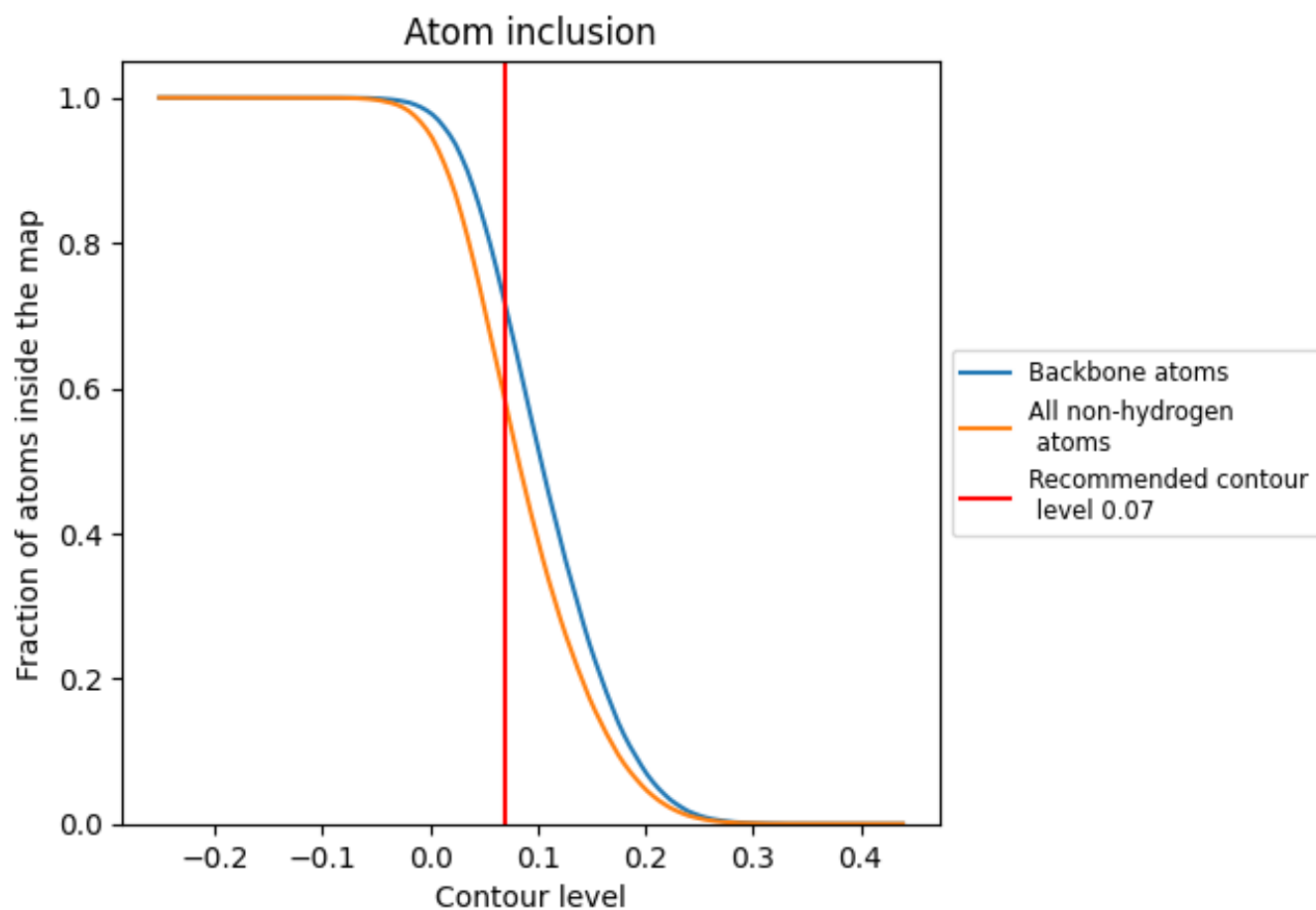
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.07).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 71% 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 (0.07) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5807	 0.2530
A1	 0.5445	 0.2090
A2	 0.2675	 0.1100
B1	 0.4543	 0.1680
B2	 0.3066	 0.1490
C1	 0.4327	 0.1480
C2	 0.2250	 0.1140
D1	 0.7301	 0.3280
D2	 0.2157	 0.0950
E1	 0.7425	 0.3340
E2	 0.1215	 0.0750
F1	 0.7402	 0.3420
F2	 0.1110	 0.0810
G1	 0.7336	 0.3220
G2	 0.7006	 0.3370
H1	 0.7246	 0.3350
H2	 0.6628	 0.3120
I1	 0.7278	 0.3200
I2	 0.6931	 0.3360
J1	 0.3972	 0.1770
J2	 0.4007	 0.1810
K1	 0.4983	 0.2370
K2	 0.5067	 0.2400
L1	 0.4786	 0.2390
L2	 0.4780	 0.2150
M1	 0.7407	 0.3260
M2	 0.7283	 0.3520
N1	 0.7336	 0.3380
N2	 0.7202	 0.3360
O1	 0.7539	 0.3440
O2	 0.7198	 0.3390
P1	 0.7171	 0.3070
P2	 0.5981	 0.2290
Q1	 0.6795	 0.2690
Q2	 0.5948	 0.2260



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Chain	Atom inclusion	Q-score
R1	 0.6894	 0.2900
R2	 0.6348	 0.2440
S1	 0.6193	 0.2430
S2	 0.6229	 0.2380
T1	 0.5825	 0.2580
T2	 0.6237	 0.2460
U1	 0.6404	 0.2730
U2	 0.5797	 0.2150
V1	 0.7101	 0.3080
V2	 0.2581	 0.1220
W1	 0.6990	 0.3020
W2	 0.1784	 0.0930
X1	 0.7099	 0.3290
X2	 0.2722	 0.1550
Y2	 0.6612	 0.2670
Z2	 0.6817	 0.2930
a2	 0.6615	 0.2980
b2	 0.5463	 0.1820
c2	 0.4922	 0.1700
d2	 0.4768	 0.1500
e2	 0.7036	 0.3350
f2	 0.6845	 0.3200
g2	 0.6844	 0.3170
h2	 0.5327	 0.1960
i2	 0.4565	 0.1890
j2	 0.5307	 0.2020
k2	 0.6517	 0.2670
l2	 0.6851	 0.2950
m2	 0.6720	 0.2870
n2	 0.7596	 0.3590
o2	 0.7553	 0.3540
p2	 0.7415	 0.3560
q2	 0.5115	 0.2000
r2	 0.3902	 0.1630
s2	 0.4916	 0.1970
t2	 0.6358	 0.2640
u2	 0.6466	 0.2650
v2	 0.6113	 0.2450
w2	 0.7278	 0.3520
x2	 0.7358	 0.3410
y2	 0.7291	 0.3440