



wwPDB EM Validation Summary Report ⓘ

Nov 10, 2024 – 10:19 PM EST

PDB ID : 8TEU
EMDB ID : EMD-41202
Title : Human cytomegalovirus portal vertex, non-infectious enveloped particle (NIEP) configuration 2 - inverted (NC2-inv)
Authors : Jih, J.; Liu, Y.T.; Liu, W.; Zhou, H.
Deposited on : 2023-07-07
Resolution : 4.01 Å(reported)

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

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

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

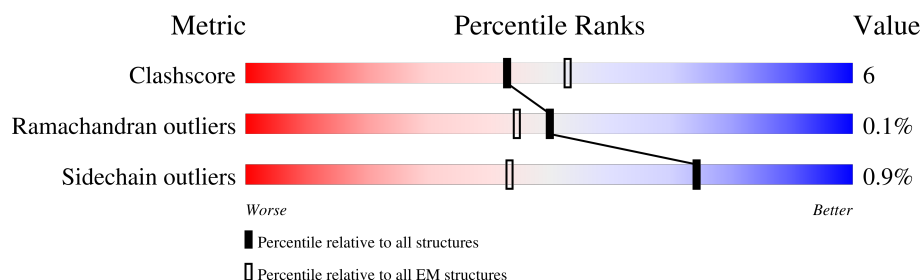
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.01 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	2241	
1	C	2241	
2	E	642	
2	F	642	
3	G	594	
4	H	1370	
4	I	1370	
4	J	1370	

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Mol	Chain	Length	Quality of chain
4	K	1370	
4	L	1370	
4	M	1370	
5	N	75	
5	O	75	
5	P	75	
5	Q	75	
5	R	75	
5	S	75	
6	T	290	
6	W	290	
7	U	306	
7	V	306	
7	X	306	
7	Y	306	
8	Z	1048	

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 96759 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 Large tegument protein deneddylase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	722	Total	C	N	O	S	0	0
			5830	3723	1027	1058	22		
1	C	40	Total	C	N	O	S	0	0
			332	213	60	58	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	495	Total	C	N	O	S	0	0
			3992	2559	706	715	12		
2	F	85	Total	C	N	O	S	0	0
			710	442	138	126	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	471	Total	C	N	O	S	0	0
			3862	2416	740	692	14		

- Molecule 4 is a protein called Major capsid protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	1309	Total	C	N	O	S	0	0
			10391	6619	1800	1911	61		
4	I	1350	Total	C	N	O	S	0	0
			10693	6809	1853	1970	61		
4	J	1317	Total	C	N	O	S	0	0
			10433	6641	1814	1919	59		
4	K	1296	Total	C	N	O	S	0	0
			10259	6529	1787	1884	59		
4	L	1350	Total	C	N	O	S	0	0
			10693	6809	1853	1970	61		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	M	1350	Total	C	N	O	S	0	0
			10693	6809	1853	1970	61		

- Molecule 5 is a protein called Small capsomere-interacting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	N	63	Total	C	N	O	S	0	0
			513	321	97	91	4		
5	O	63	Total	C	N	O	S	0	0
			513	321	97	91	4		
5	P	63	Total	C	N	O	S	0	0
			513	321	97	91	4		
5	Q	63	Total	C	N	O	S	0	0
			513	321	97	91	4		
5	R	63	Total	C	N	O	S	0	0
			513	321	97	91	4		
5	S	63	Total	C	N	O	S	0	0
			513	321	97	91	4		

- Molecule 6 is a protein called Triplex capsid protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	T	242	Total	C	N	O	S	0	0
			1939	1248	338	342	11		
6	W	290	Total	C	N	O	S	0	0
			2325	1485	411	417	12		

- Molecule 7 is a protein called Triplex capsid protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	U	292	Total	C	N	O	S	0	0
			2317	1489	399	411	18		
7	V	288	Total	C	N	O	S	0	0
			2292	1471	397	407	17		
7	X	295	Total	C	N	O	S	0	0
			2334	1501	402	412	19		
7	Y	285	Total	C	N	O	S	0	0
			2266	1456	387	405	18		

- Molecule 8 is a protein called Large structural phosphoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	Z	284	Total	C	N	O	S	0	0
			2320	1463	425	420	12		

L1741	S1742	L1743	Q1744	E1745	F1746	C1747	V1748	L1749	I1750	A1751	A1752	L1753	V1754	P1755	E1756	Y1757	I1758	Y1759	T1760	V1761	L1762	K1763	V1764	P1765	V1766	Q1767	M1768	S1769	L1770	P1771	S1772	L1773	T1774	A1775	H1776	L1777	L1778	Q1779	D1780	V1781	I1782	H1783	A1784	V1785	V1786	H1787	M1788	T1789	H1790	K1791	M1792	P1793	P1794	D1795	H1796	L1797	P1798	E1799	Q1800																																																																																																																																																																																																																																																																																																																																																																																																		
H1681	T1682	H1683	P1684	A1685	E1686	T1687	H1688	T1689	L1690	H1691	N1692	L1693	K1694	L1695	F1696	C1697	Y1698	L1699	V1700	S1701	T1702	A1703	W1704	H1705	Q1706	R1707	I1708	D1709	T1710	GLN	GLN	GLU	LEU	THR	ALA	ASP	ARG	VAL	GLY	VAL	GLY	ASP	VAL	GLY	GLN	ARG	T1736	T1737	V1738	L1739	R1740																																																																																																																																																																																																																																																																																																																																																																																																										
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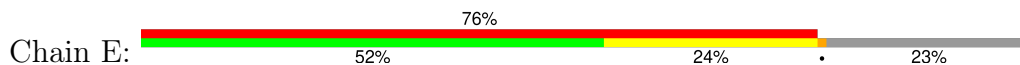


[illegible]

THR	ALA	PHE	GLY	GLY	SER	VAL	PHE	GLN	GLU	ASN	ARG	LEU	GLY	GLU	THR	PRO	LEU	CYS	ARG	ASP	GLU	LEU	VAL	ALA	VAL	ALA	PRO	GLY	ALA	SER	THR	PHE	SER	SER	ALA	SER	PRO	PRO	ILE	THR	V2202	V2203	T2204	T2205	N2206	V2207	T2208	L2209	A2210	L2211	E2212	T2213	L2214	R2215	L2216	V2217	R2218	L2219	V2220
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- Molecule 2: Capsid vertex component 2

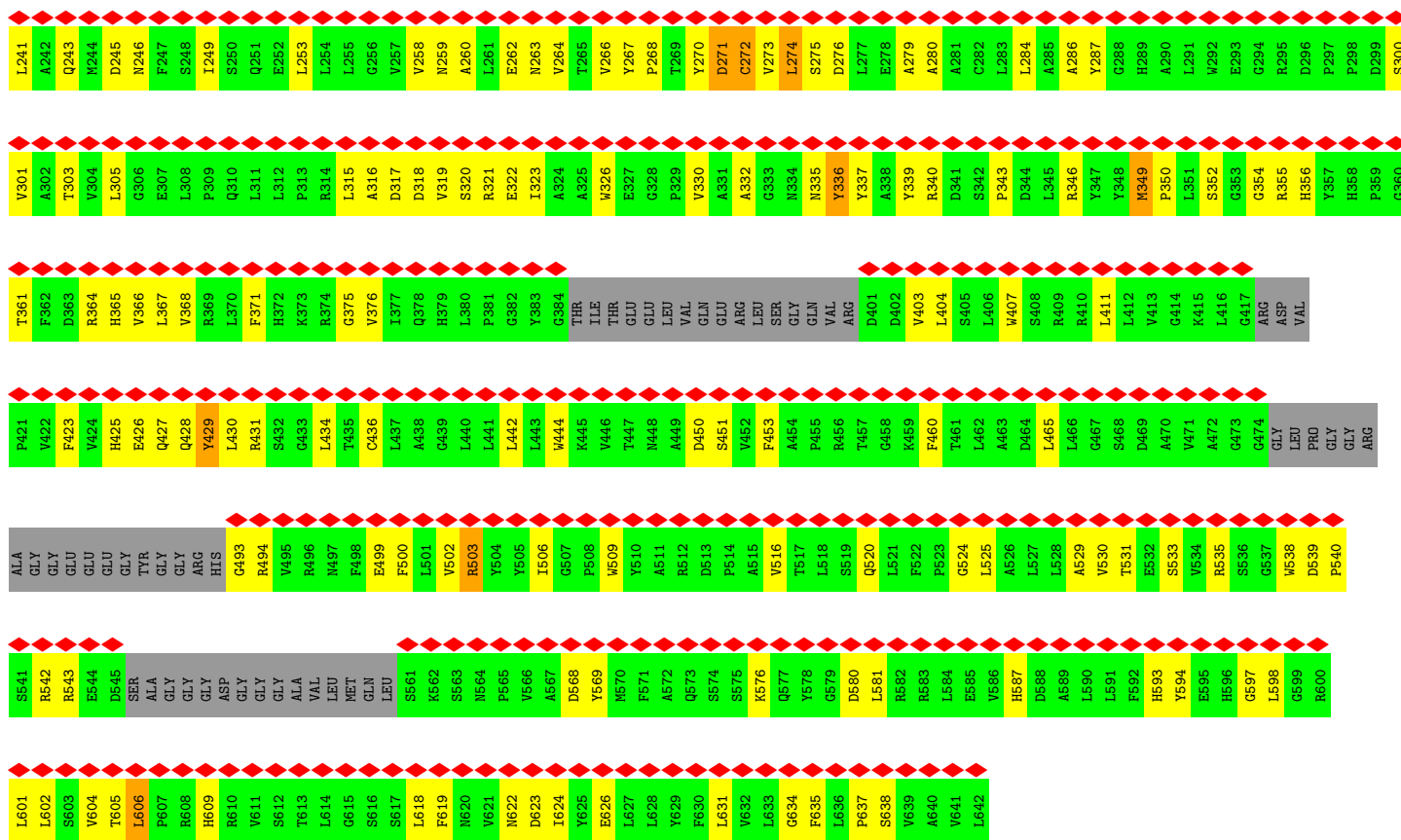


NET	SER	LEU	HIS	THR	PHE	TRP	ARG	LEU	PRO	V12	A13	V14	F15	F16	E17	F18	H19	E20	E21	V22	V23	L24	R25	C26	C27	E28	R29	V30	L31	R32	R33	L34	L35	E36	D37	A38	A39	L40	V40	T41	M42	R43	G44	G45	G46	G47	R48	E49	D50	V51	L52	M53	D54	R55	V56	R57	K58	R59	V60
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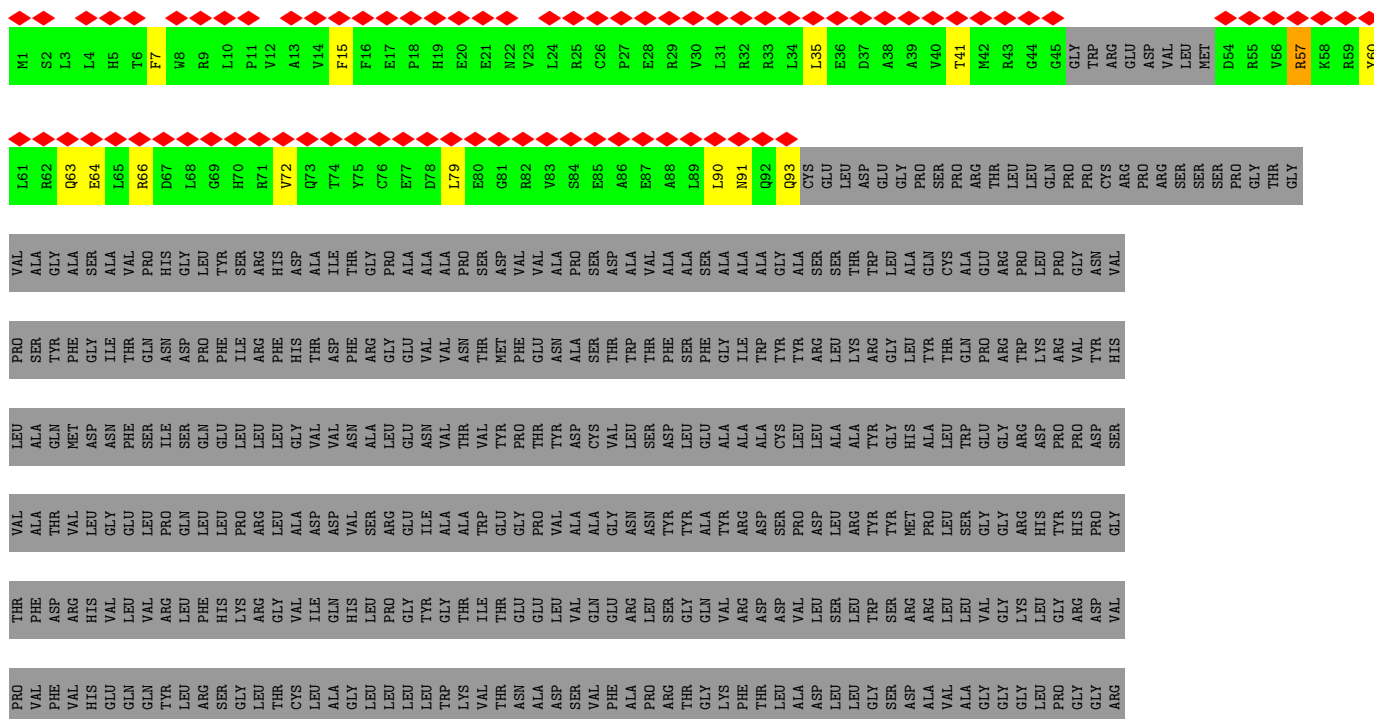
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VAL	GLY	ALA	SER	ALA	VAL	PRO	HIS	GLY	LEU	TYP	SER	ARG	HIS	ASP	ALA	ILE	THR	GLY	PRO	ALA	ALA	ALA	PRO	PRO	SER	ASP	VAL	VAL	ALA	ALA	PRO	SER	ASP	ALA	ALA	ALA	ALA	GLY	ALA	SER	SER	THR	TRP	LEU	ALA	GLN	CYS	ALA	ALA	GLU	ARG	PRO	LEU	PRO	GLY	ASN
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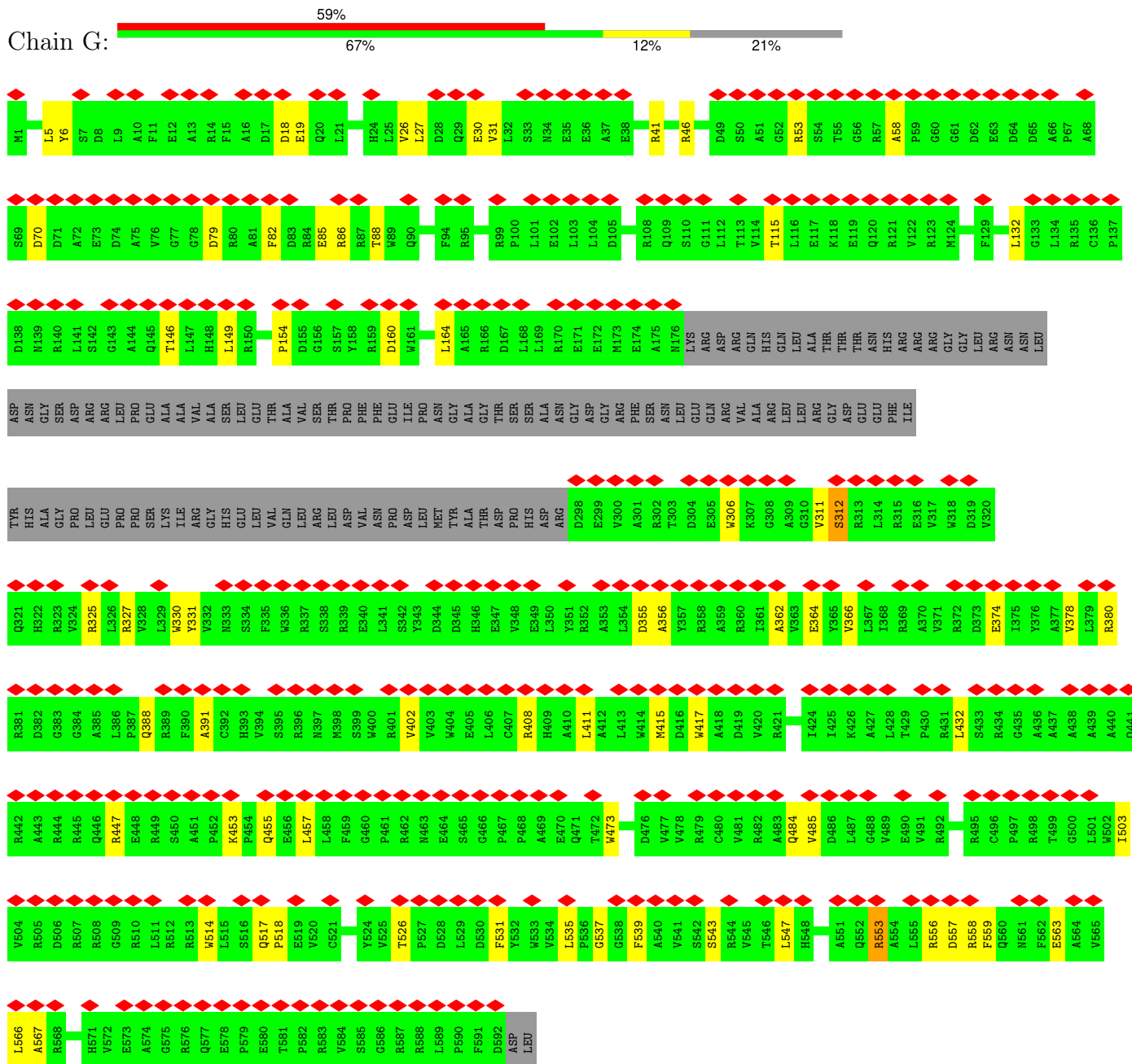
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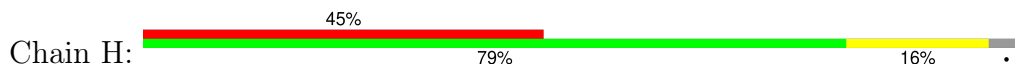
• Molecule 2: Capsid vertex component 2

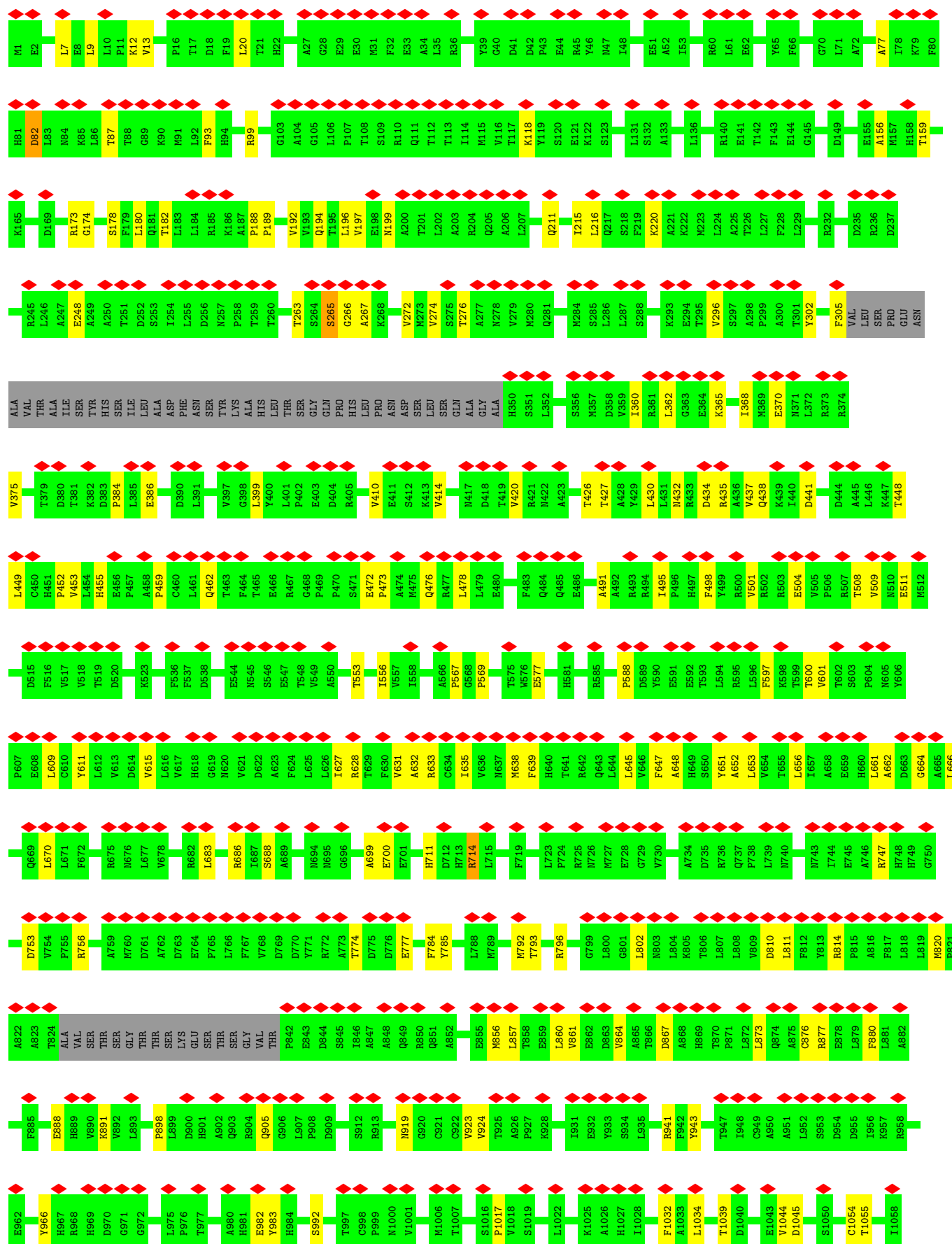


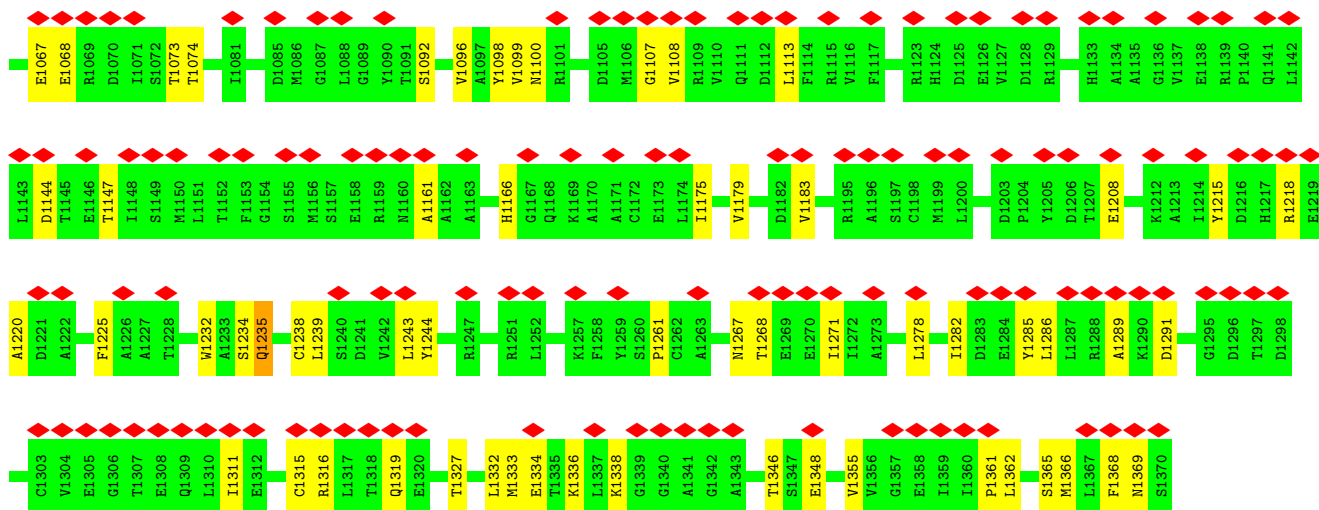
- Molecule 3: Capsid vertex component 1

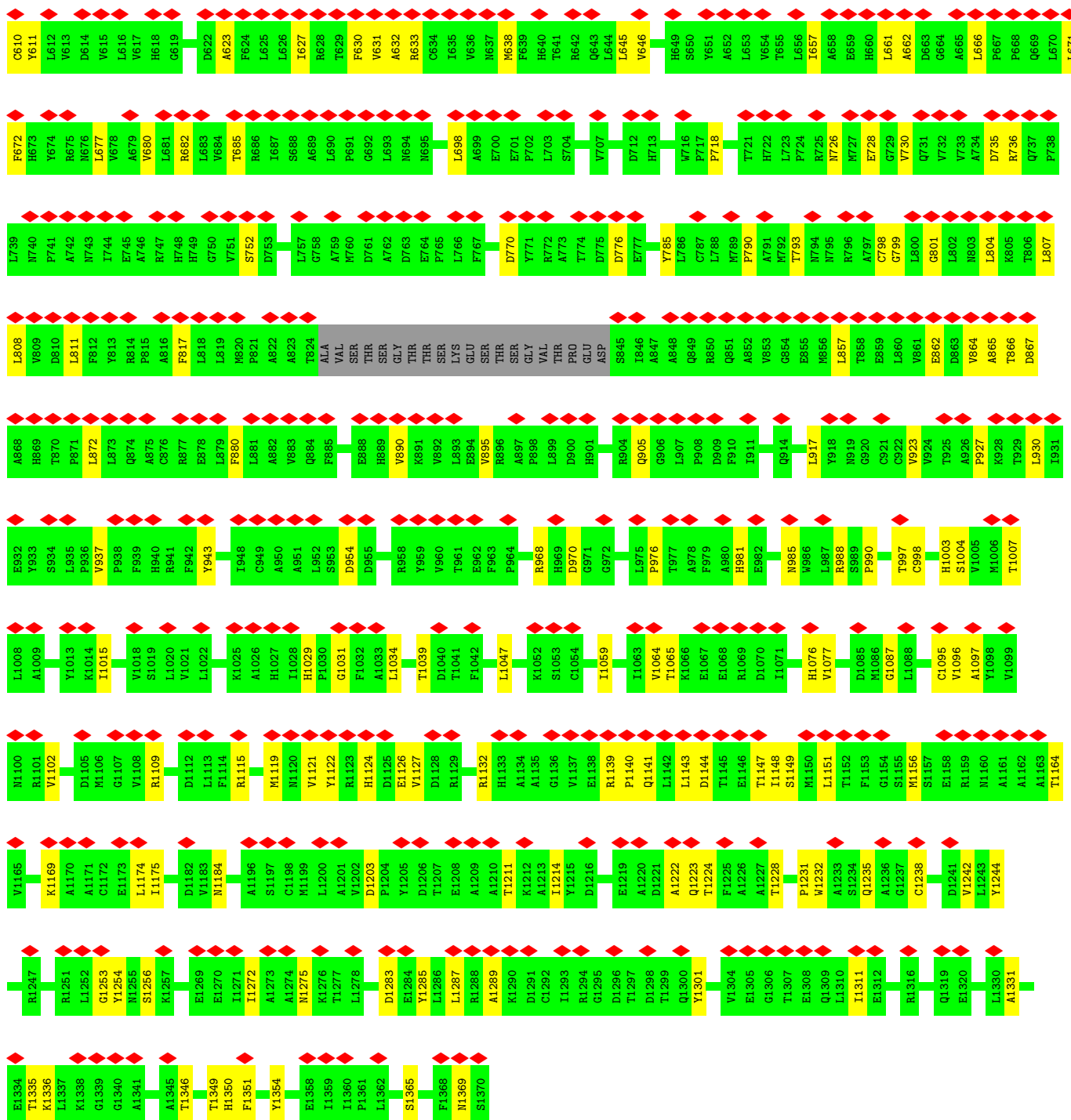


- Molecule 4: Major capsid protein

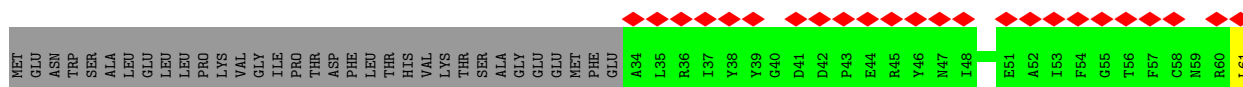
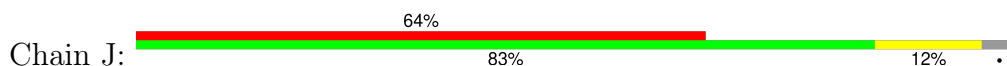




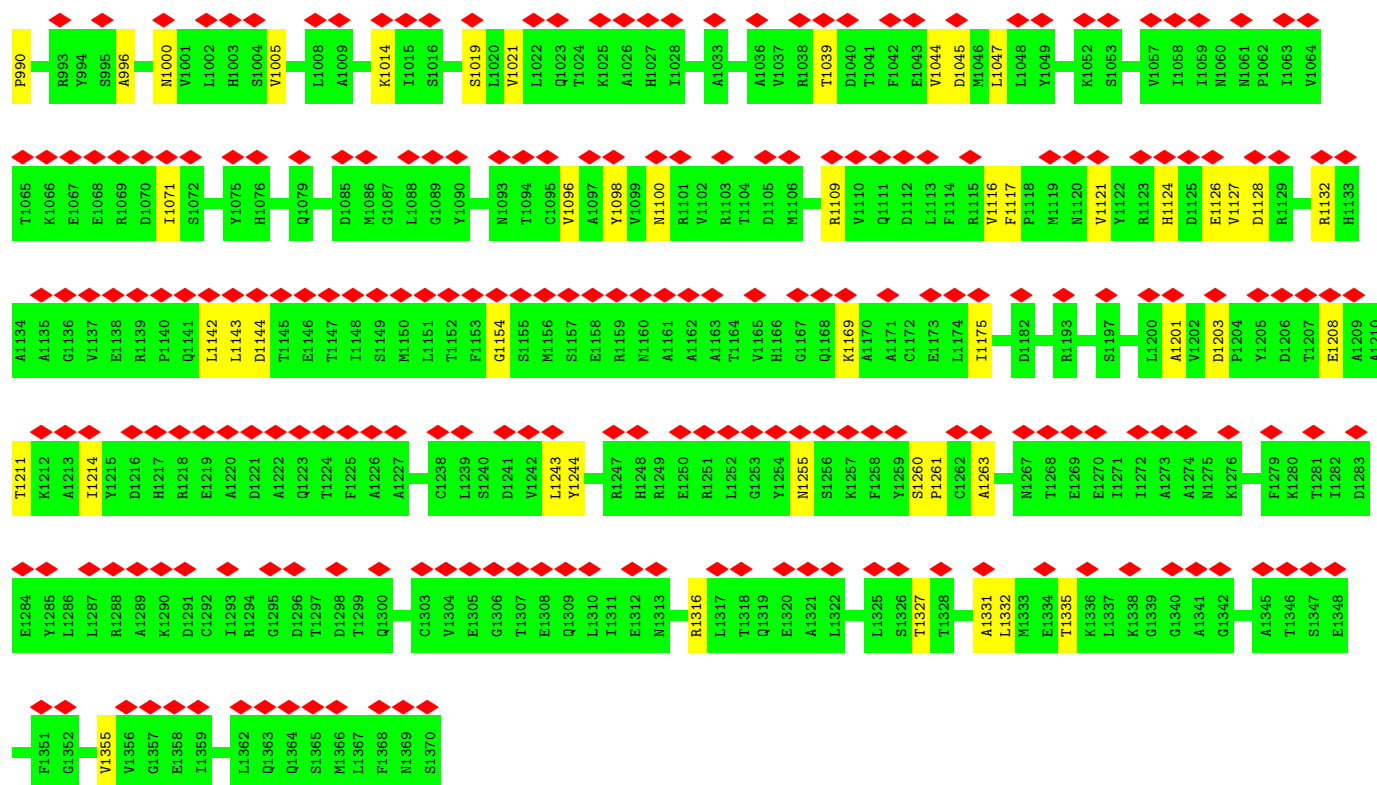




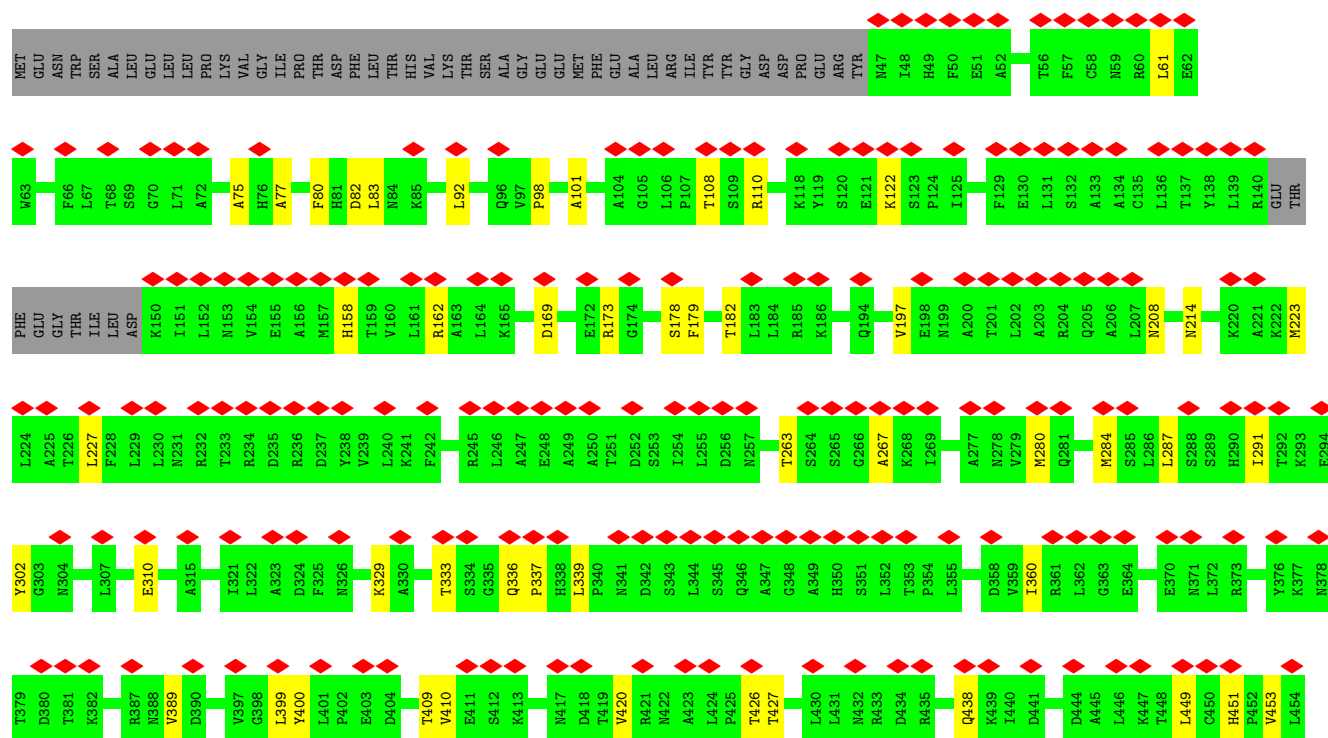
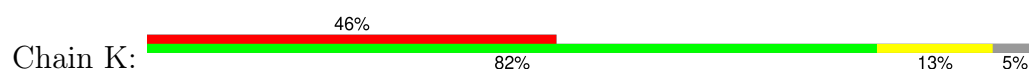
• Molecule 4: Major capsid protein

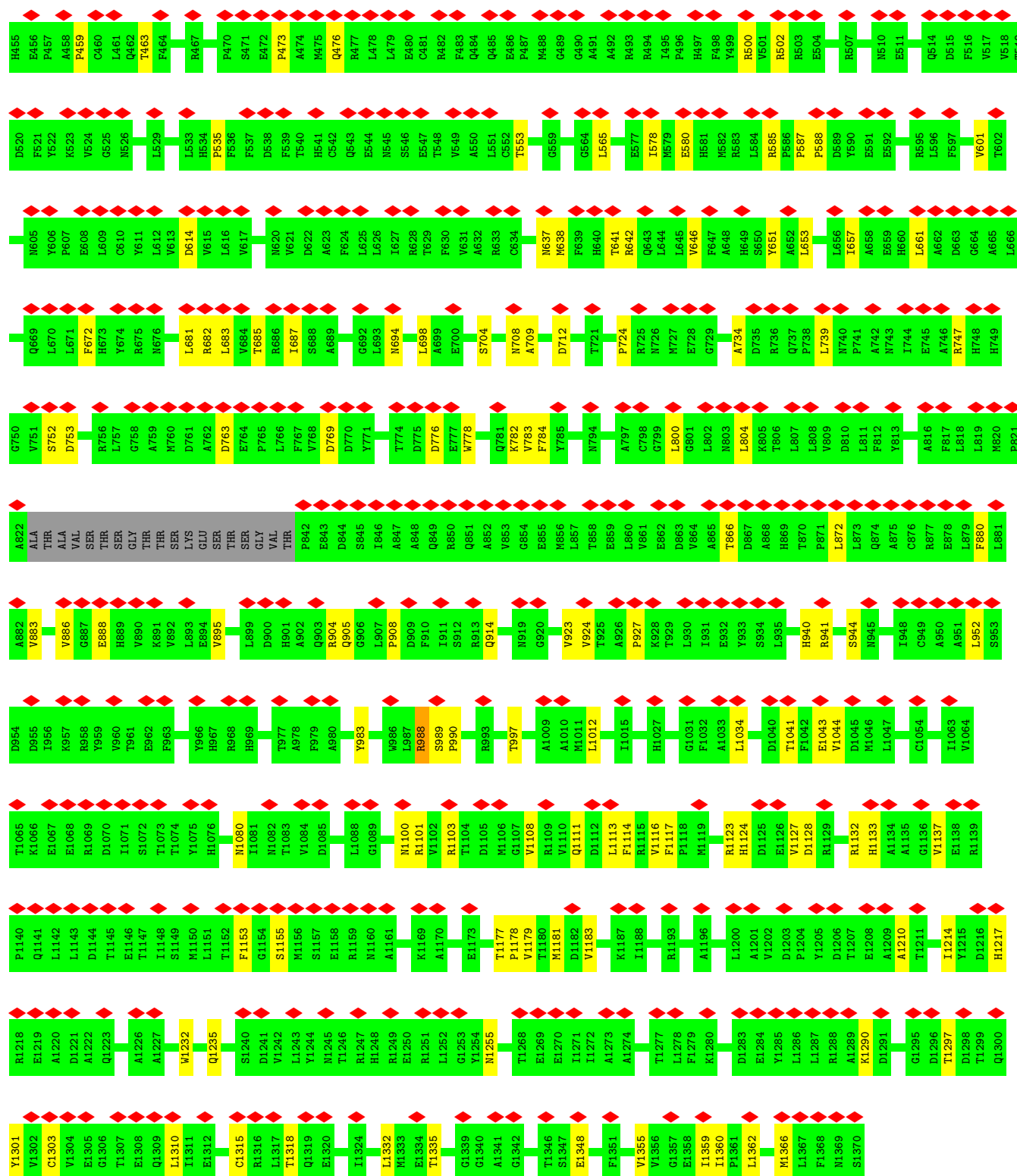


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F938	G758	L818	L818	H638	L578	E503	V443	R361	L287	K222	I151	
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C949	D769	GLY	D769	H649	F589	F516	H455		N304	D236	M166	
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R896	F776	GLY	F776	L656	F597	K523	F464		A312	T244	G174	T108
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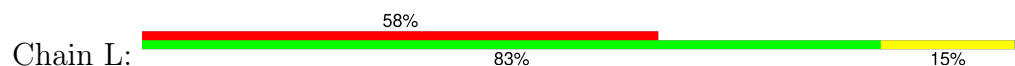


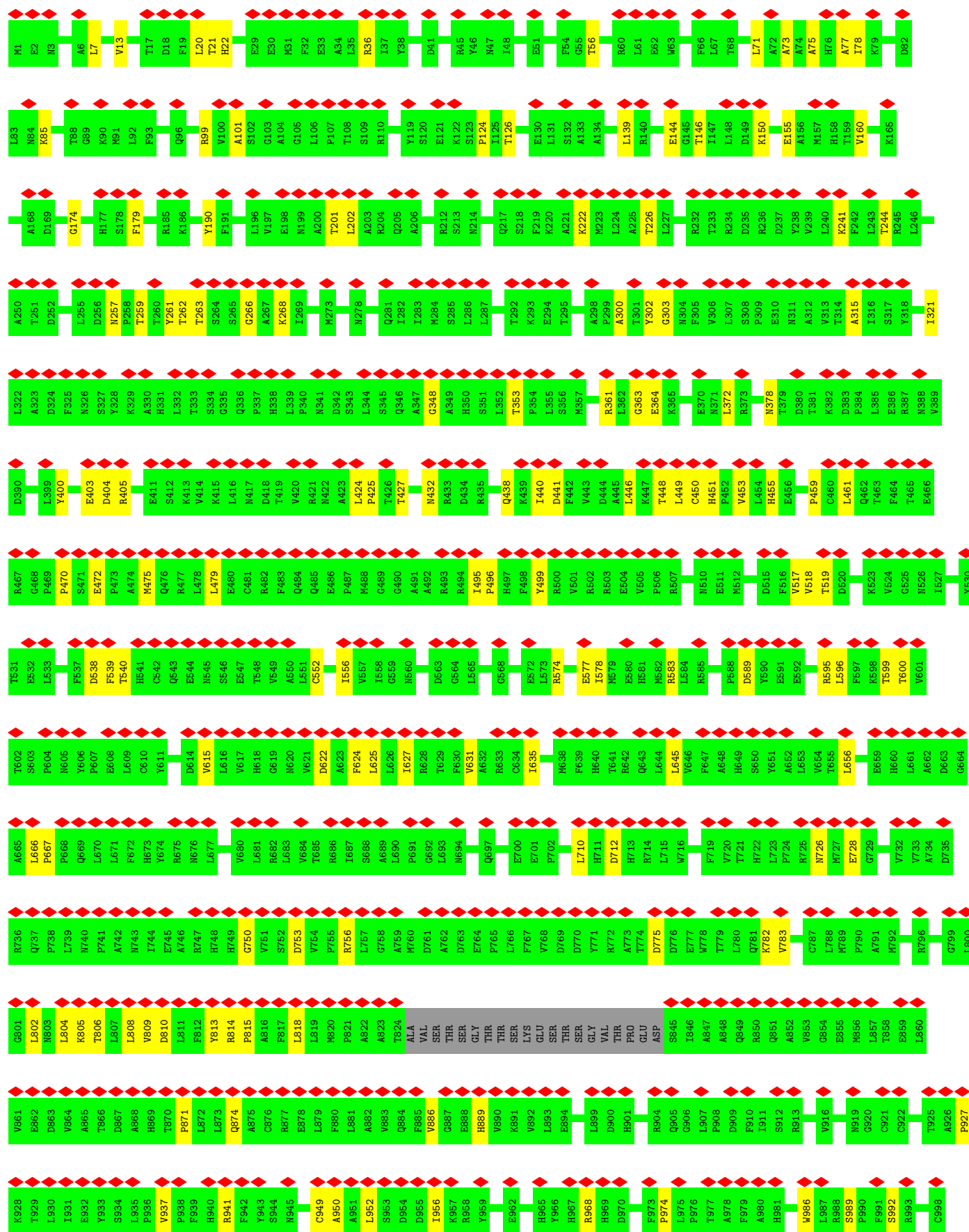
• Molecule 4: Major capsid protein





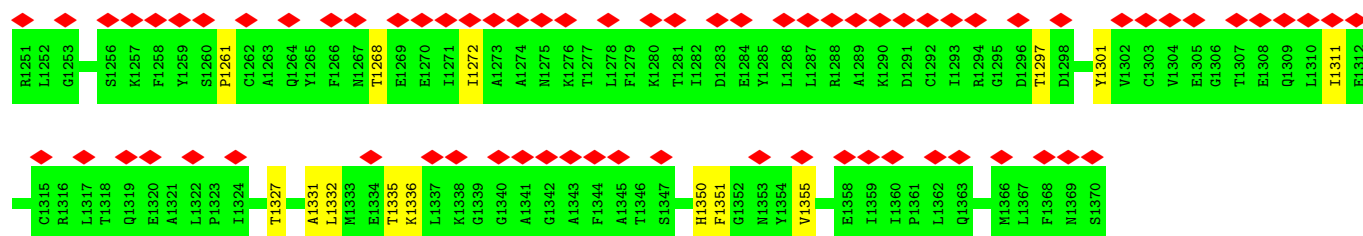
• Molecule 4: Major capsid protein



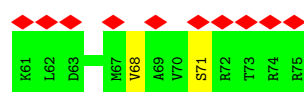
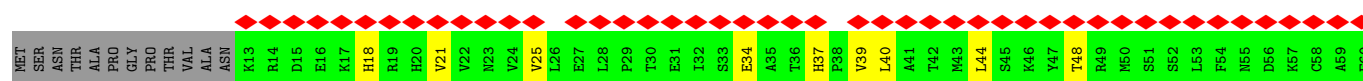
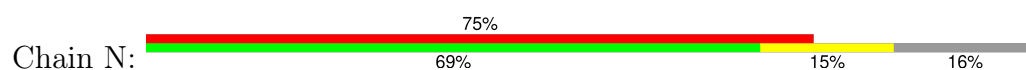




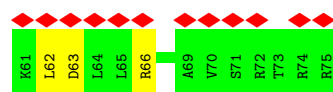
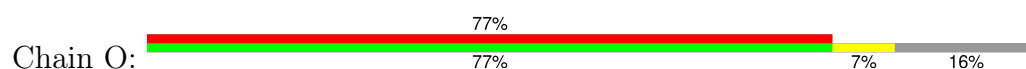
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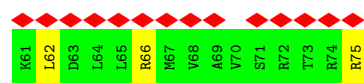
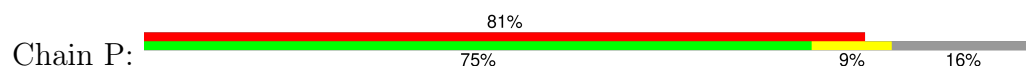
• Molecule 5: Small capsomere-interacting protein



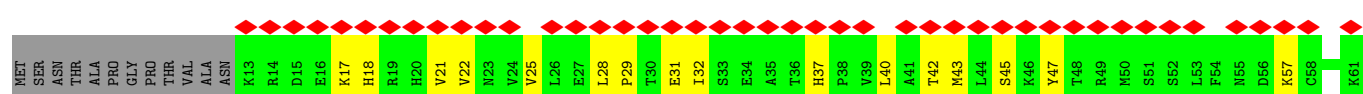
• Molecule 5: Small capsomere-interacting protein

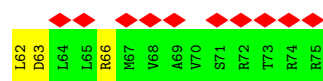


• Molecule 5: Small capsomere-interacting protein

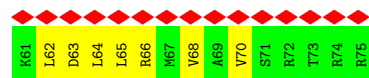
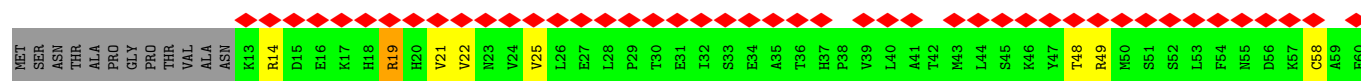
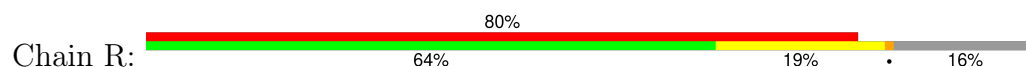


• Molecule 5: Small capsomere-interacting protein

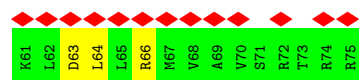
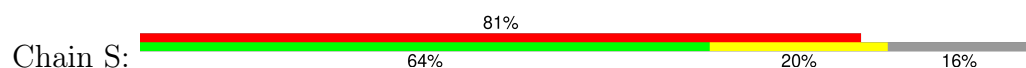




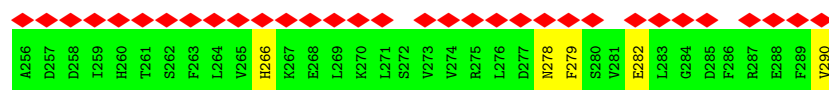
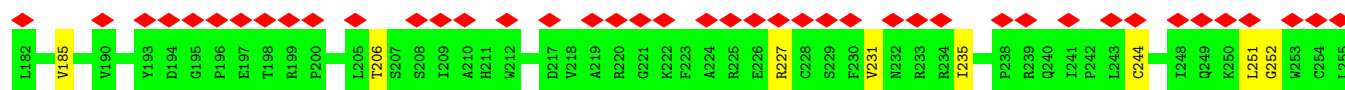
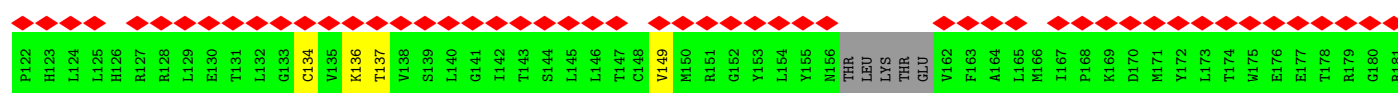
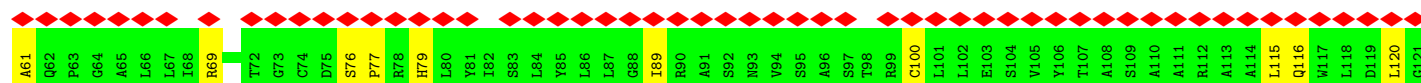
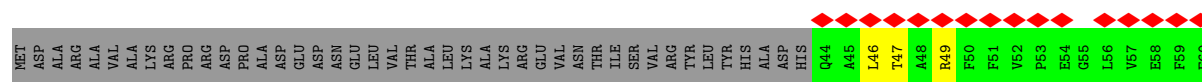
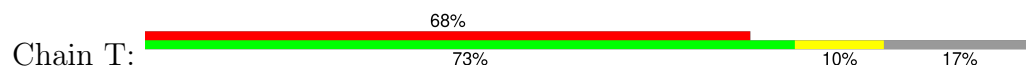
• Molecule 5: Small capsomere-interacting protein



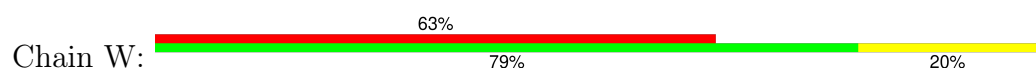
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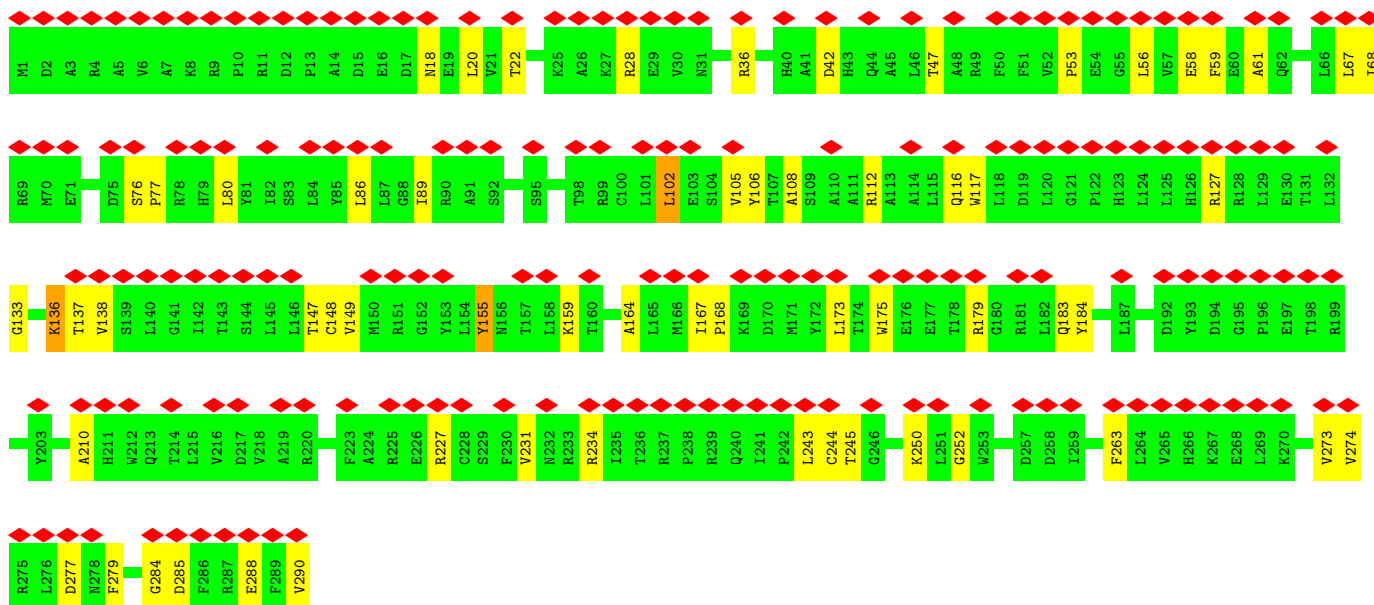


• Molecule 6: Triplex capsid protein 1

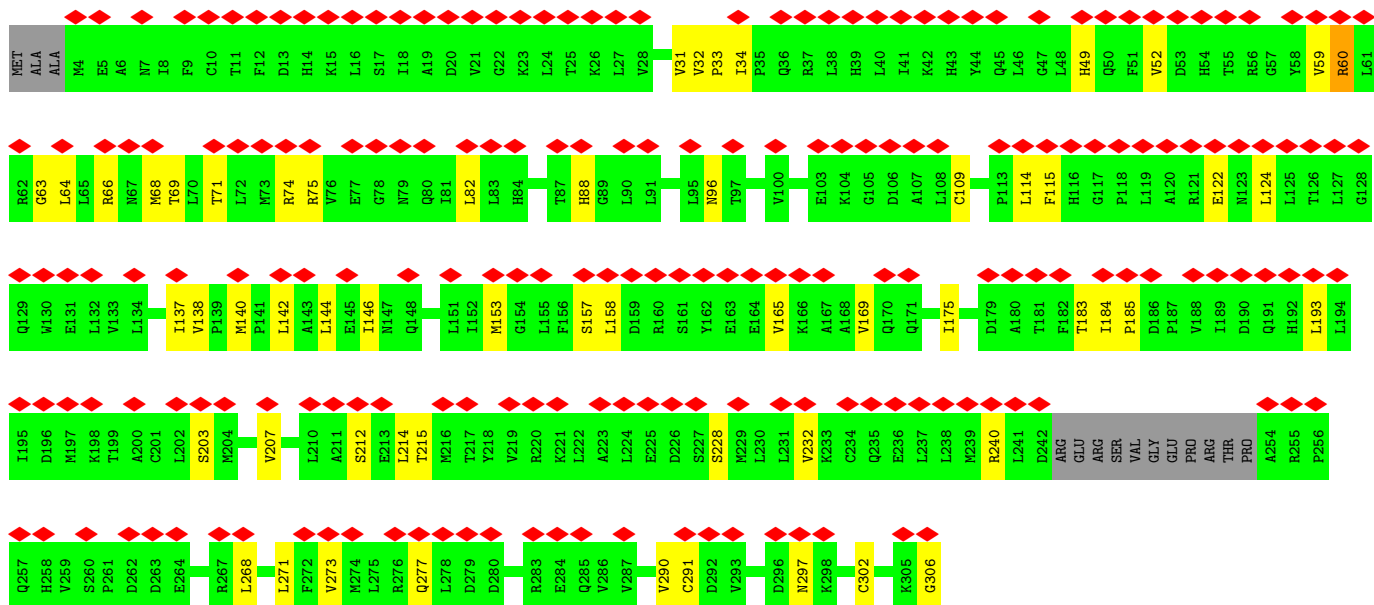
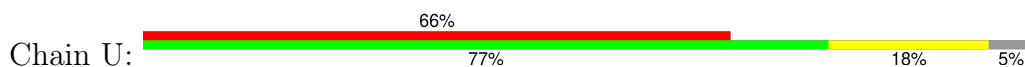


• Molecule 6: Triplex capsid protein 1

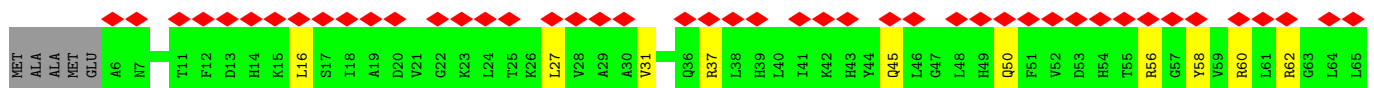
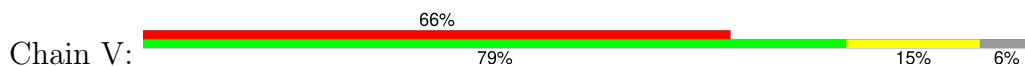


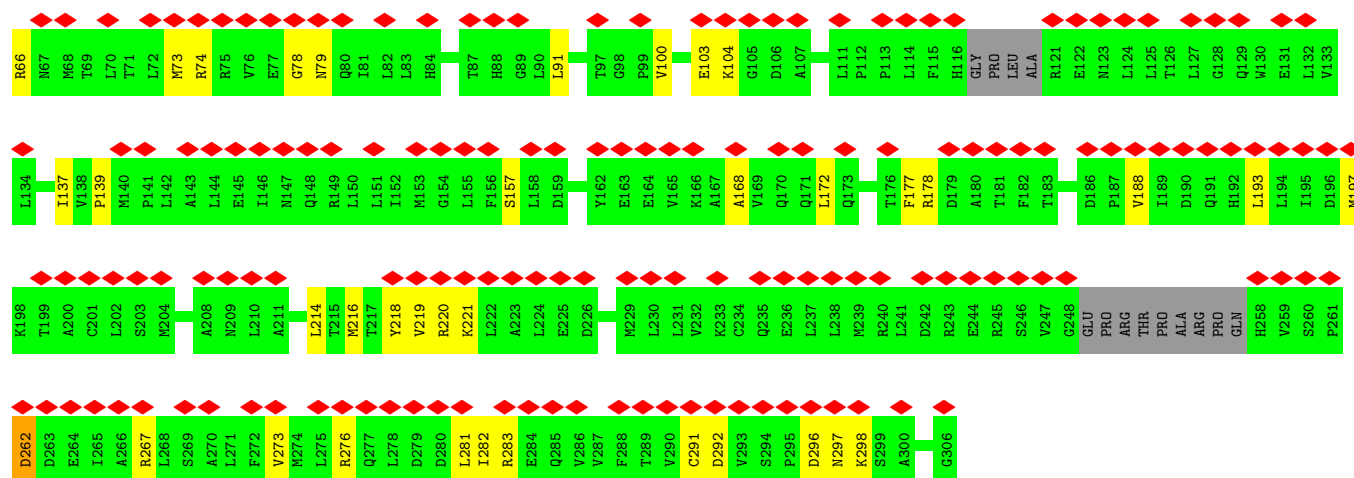


- Molecule 7: Triplex capsid protein 2

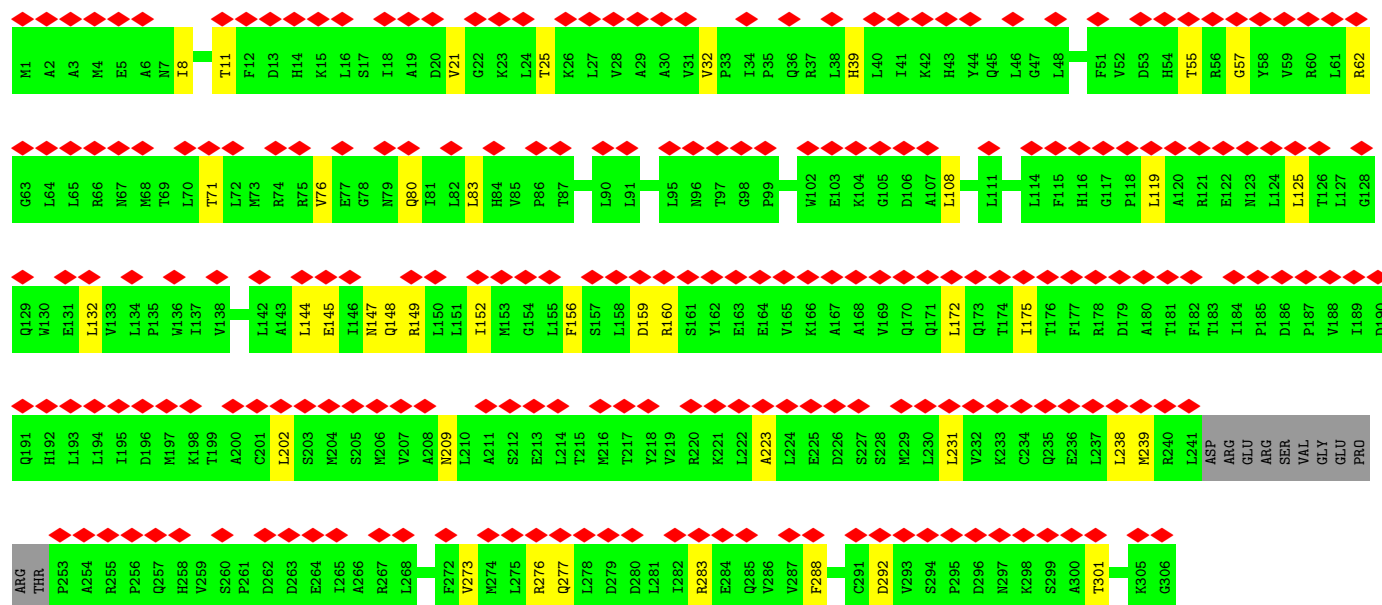
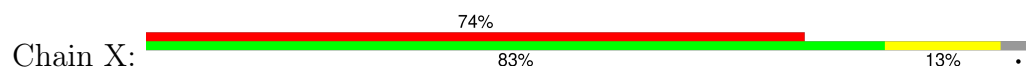


- Molecule 7: Triplex capsid protein 2

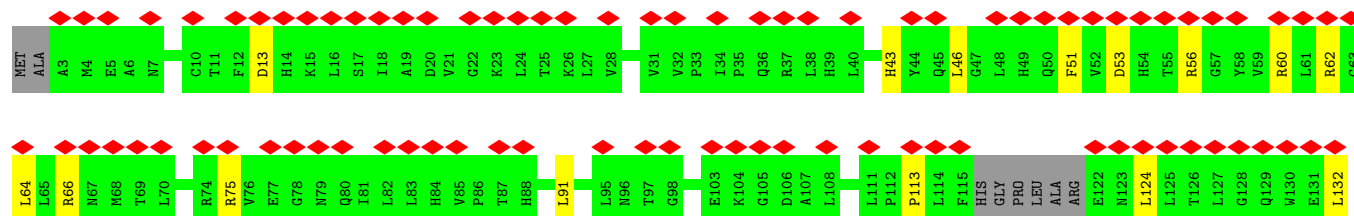
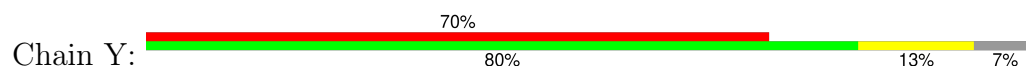


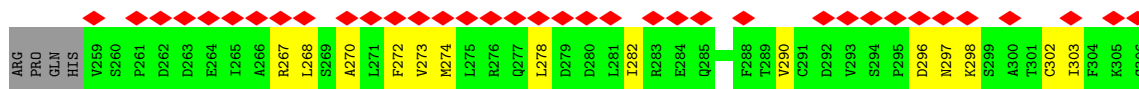
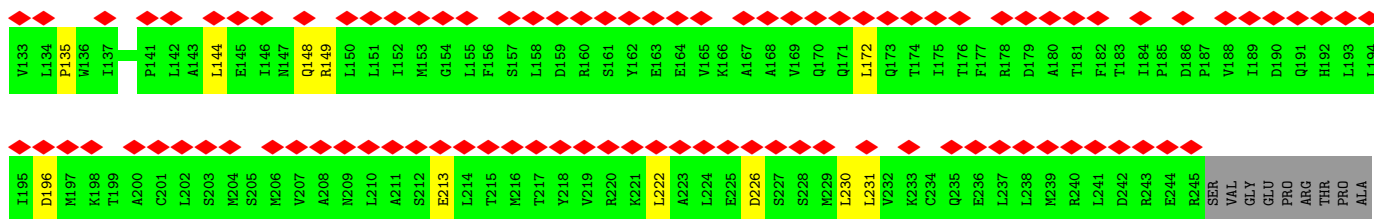


• Molecule 7: Triplex capsid protein 2

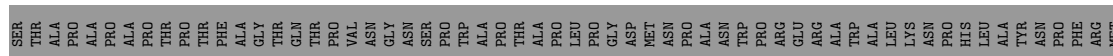
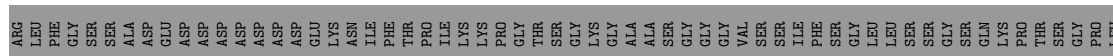
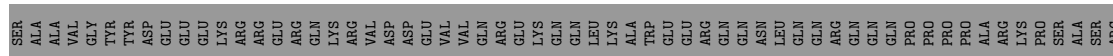
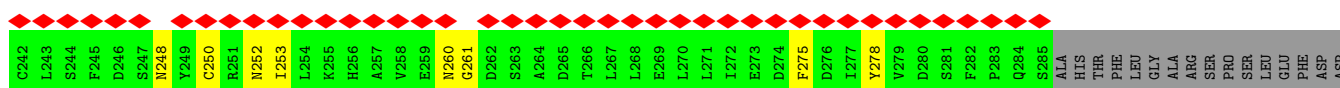
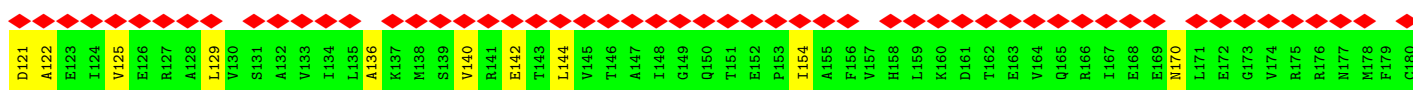
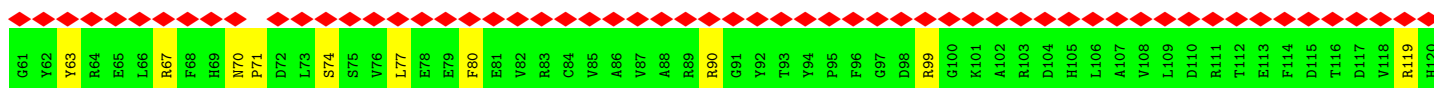
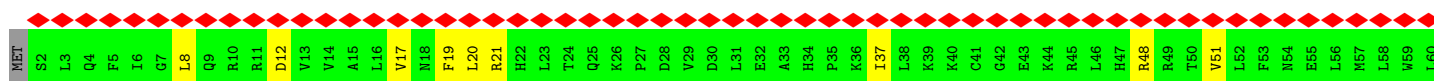


• Molecule 7: Triplex capsid protein 2





• Molecule 8: Large structural phosphoprotein



GLY	PRO	LEU	SER	VAL	ASP
MET	PRO	LYS	ALA	ALA	THR
GLY	VAL	PRO	SER	THR	GLY
ALA	ALA	THR	SER	PRO	SER
LYS	SER	GLY	ALA	HIS	VAL
THR	SER	GLY	GLN	ALA	SER
PRO	ILE	LYS	PRO	ALA	LEU
SER	LEU	VAL	SER	ARG	GLY
ASP	LYS	ALA	ALA	ALA	HIS
ALA	PRO	VAL	SER	GLN	THR
VAL	GLY	GLY	ALA	THR	THR
GLN	ALA	ARG	SER	VAL	PRO
ASN	SER	PRO	VAL	THR	SER
ILE	ALA	PRO	VAL	THR	SER
LYS	LEU	VAL	SER	THR	ASP
GLN	LEU	VAL	PRO	PRO	TVR
LYS	GLN	VAL	THR	VAL	ASN
ILE	SER	VAL	GLY	GLN	ASN
GLY	ARG	SER	ASP	GLY	ASP
LYS	ARG	GLY	VAL	LEU	VAL
ILE	SER	SER	VAL	LEU	ILE
LYS	THR	ALA	VAL	GLY	SER
ASN	GLY	PRO	SER	LYS	PRO
THR	THR	GLY	PRO	GLN	PRO
GLY	ALA	ARG	ALA	VAL	SER
GLU	VAL	LEU	THR	SER	GLN
	VAL	GLY	SER	GLY	THR
	GLY	GLY	PRO	THR	PRO
	SER	SER	LEU	PRO	GLY
	PRO	SER	SER	SER	GLN
	VAL	ARG	MET	THR	SER
	LYS	ALA	LEU	VAL	THR
	SER	ALA	SER	PRO	PRO
	THR	SER	SER	ALA	SER
	THR	THR	ALA	THR	ARG
	GLY	THR	SER	LEU	ILE
	MET	PRO	PRO	LEU	ARG
	LYS	THR	SER	GLN	LYS
	THR	TVR	PRO	PRO	ALA
	VAL	PRO	ALA	GLN	LYS
	ALA	ALA	LYS	PRO	LEU
	PHE	VAL	SER	ALA	SER
	ASP	THR	ALA	SER	SER
	LEU	THR	PRO	SER	PRO
	SER	VAL	PRO	LYS	MET
	SER	TVR	SER	THR	THR
	PRO	PRO	PRO	THR	THR
	GLN	PRO	VAL	SER	THR
	LYS	SER	LYS	ARG	THR
	THR	SER	GLY	ASN	SER
	THR	ALA	GLY	VAL	GLN
	GLY	LYS	SER	THR	LYS
	PRO	SER	ARG	THR	PRO
	GLN	SER	VAL	SER	VAL
	PRO	VAL	GLY	ALA	LEU
	GLY	SER	VAL	GLY	GLY
	PRO	ASN	PRO	THR	THR
	ALA	ALA	SER	SER	ARG

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C5	Depositor
Number of particles used	16225	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 ($e^-/\text{\AA}^2$)	47.2	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.063	Depositor
Minimum map value	-0.049	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.019	Depositor
Map size (Å)	489.6, 489.6, 489.6	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.36, 1.36, 1.36	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.25	0/5969	0.53	0/8139
1	C	0.25	0/334	0.53	0/450
2	E	0.26	0/4094	0.53	1/5558 (0.0%)
2	F	0.25	0/721	0.58	0/969
3	G	0.24	0/3951	0.58	0/5357
4	H	0.25	0/10638	0.52	0/14487
4	I	0.25	0/10949	0.51	0/14916
4	J	0.24	0/10682	0.51	0/14553
4	K	0.25	0/10503	0.51	1/14307 (0.0%)
4	L	0.25	0/10949	0.51	0/14916
4	M	0.24	0/10949	0.50	0/14916
5	N	0.23	0/520	0.53	0/697
5	O	0.23	0/520	0.51	0/697
5	P	0.23	0/520	0.54	0/697
5	Q	0.24	0/520	0.54	0/697
5	R	0.24	0/520	0.55	0/697
5	S	0.23	0/520	0.53	0/697
6	T	0.25	0/1981	0.56	0/2687
6	W	0.25	0/2374	0.55	0/3221
7	U	0.24	0/2361	0.53	0/3206
7	V	0.26	0/2333	0.56	0/3164
7	X	0.24	0/2379	0.52	0/3230
7	Y	0.25	0/2305	0.52	0/3126
8	Z	0.25	0/2358	0.56	0/3182
All	All	0.25	0/98950	0.52	2/134566 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	G	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
4	H	0	2
4	I	0	1
4	J	0	1
4	K	0	2
4	M	0	1
6	W	0	1
All	All	0	9

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	606	LEU	CA-CB-CG	5.55	128.06	115.30
4	K	753	ASP	CB-CG-OD2	5.13	122.92	118.30

There are no chirality outliers.

5 of 9 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	G	312	SER	Peptide
4	H	1100	ASN	Peptide
4	H	265	SER	Peptide
4	I	1143	LEU	Peptide
4	J	794	ASN	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5830	0	5830	158	0
1	C	332	0	358	14	0
2	E	3992	0	3913	138	0
2	F	710	0	711	12	0
3	G	3862	0	3779	43	0
4	H	10391	0	10342	127	0
4	I	10693	0	10635	149	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	J	10433	0	10379	102	0
4	K	10259	0	10216	98	0
4	L	10693	0	10635	127	0
4	M	10693	0	10635	119	0
5	N	513	0	539	7	0
5	O	513	0	539	3	0
5	P	513	0	539	5	0
5	Q	513	0	539	12	0
5	R	513	0	539	10	0
5	S	513	0	539	11	0
6	T	1939	0	1972	19	0
6	W	2325	0	2363	42	0
7	U	2317	0	2405	32	0
7	V	2292	0	2379	26	0
7	X	2334	0	2431	26	0
7	Y	2266	0	2355	23	0
8	Z	2320	0	2351	28	0
All	All	96759	0	96923	1238	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 6.

The worst 5 of 1238 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)
2:E:267:TYR:HE1	2:E:270:TYR:HB3	1.35	0.90
4:J:795:ASN:ND2	4:J:969:HIS:O	2.09	0.84
7:U:240:ARG:HB2	7:V:267:ARG:HH21	1.43	0.84
2:E:267:TYR:CE1	2:E:270:TYR:HB3	2.15	0.81
2:E:371:PHE:HB3	2:E:376:VAL:HB	1.64	0.80

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	A	710/2241 (32%)	695 (98%)	15 (2%)	0	100	100
1	C	38/2241 (2%)	38 (100%)	0	0	100	100
2	E	483/642 (75%)	459 (95%)	22 (5%)	2 (0%)	30	66
2	F	81/642 (13%)	80 (99%)	1 (1%)	0	100	100
3	G	467/594 (79%)	451 (97%)	16 (3%)	0	100	100
4	H	1303/1370 (95%)	1241 (95%)	61 (5%)	1 (0%)	48	81
4	I	1346/1370 (98%)	1281 (95%)	64 (5%)	1 (0%)	48	81
4	J	1313/1370 (96%)	1251 (95%)	61 (5%)	1 (0%)	48	81
4	K	1290/1370 (94%)	1235 (96%)	55 (4%)	0	100	100
4	L	1346/1370 (98%)	1290 (96%)	55 (4%)	1 (0%)	48	81
4	M	1346/1370 (98%)	1288 (96%)	55 (4%)	3 (0%)	44	76
5	N	61/75 (81%)	60 (98%)	1 (2%)	0	100	100
5	O	61/75 (81%)	59 (97%)	2 (3%)	0	100	100
5	P	61/75 (81%)	60 (98%)	1 (2%)	0	100	100
5	Q	61/75 (81%)	60 (98%)	1 (2%)	0	100	100
5	R	61/75 (81%)	60 (98%)	1 (2%)	0	100	100
5	S	61/75 (81%)	61 (100%)	0	0	100	100
6	T	238/290 (82%)	228 (96%)	10 (4%)	0	100	100
6	W	288/290 (99%)	277 (96%)	11 (4%)	0	100	100
7	U	288/306 (94%)	270 (94%)	17 (6%)	1 (0%)	37	71
7	V	282/306 (92%)	265 (94%)	15 (5%)	2 (1%)	19	55
7	X	291/306 (95%)	275 (94%)	16 (6%)	0	100	100
7	Y	279/306 (91%)	268 (96%)	10 (4%)	1 (0%)	30	66
8	Z	282/1048 (27%)	275 (98%)	6 (2%)	1 (0%)	30	66
All	All	12037/17882 (67%)	11527 (96%)	496 (4%)	14 (0%)	50	81

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	H	266	GLY
4	I	266	GLY
4	M	760	MET

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Mol	Chain	Res	Type
4	M	886	VAL
7	Y	297	ASN

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	647/1941 (33%)	643 (99%)	4 (1%)	84	88
1	C	38/1941 (2%)	38 (100%)	0	100	100
2	E	422/526 (80%)	414 (98%)	8 (2%)	52	70
2	F	76/526 (14%)	73 (96%)	3 (4%)	27	50
3	G	397/500 (79%)	388 (98%)	9 (2%)	45	64
4	H	1142/1192 (96%)	1132 (99%)	10 (1%)	75	83
4	I	1175/1192 (99%)	1169 (100%)	6 (0%)	86	90
4	J	1146/1192 (96%)	1138 (99%)	8 (1%)	81	86
4	K	1129/1192 (95%)	1121 (99%)	8 (1%)	81	86
4	L	1175/1192 (99%)	1165 (99%)	10 (1%)	75	83
4	M	1175/1192 (99%)	1167 (99%)	8 (1%)	81	86
5	N	59/68 (87%)	59 (100%)	0	100	100
5	O	59/68 (87%)	59 (100%)	0	100	100
5	P	59/68 (87%)	58 (98%)	1 (2%)	56	73
5	Q	59/68 (87%)	59 (100%)	0	100	100
5	R	59/68 (87%)	58 (98%)	1 (2%)	56	73
5	S	59/68 (87%)	59 (100%)	0	100	100
6	T	211/252 (84%)	209 (99%)	2 (1%)	75	83
6	W	252/252 (100%)	246 (98%)	6 (2%)	44	63
7	U	262/273 (96%)	260 (99%)	2 (1%)	79	84
7	V	260/273 (95%)	254 (98%)	6 (2%)	45	64
7	X	263/273 (96%)	261 (99%)	2 (1%)	79	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	Y	257/273 (94%)	254 (99%)	3 (1%)	67	79
8	Z	255/883 (29%)	252 (99%)	3 (1%)	67	79
All	All	10636/15473 (69%)	10536 (99%)	100 (1%)	74	83

5 of 100 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	L	99	ARG
4	M	441	ASP
8	Z	144	LEU
4	L	589	ASP
4	L	1368	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
4	J	438	GLN
4	M	965	HIS
4	J	1166	HIS
5	N	18	HIS
4	M	697	GLN

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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

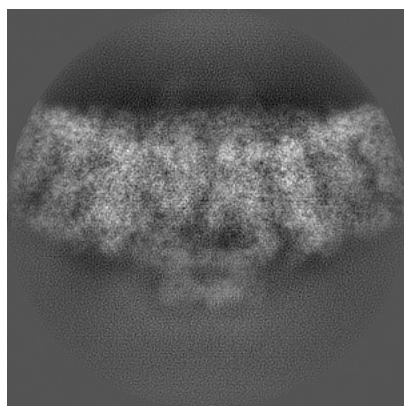
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-41202. These allow visual inspection of the internal detail of the map and identification of artifacts.

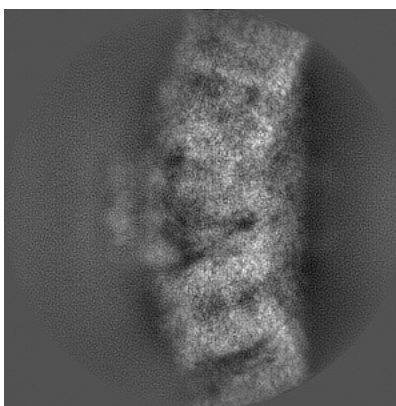
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

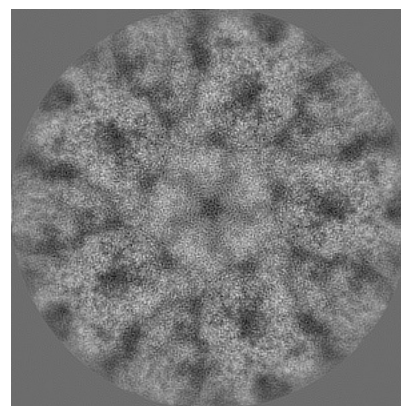
6.1.1 Primary map



X

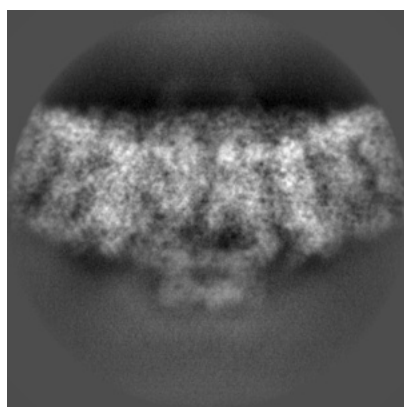


Y

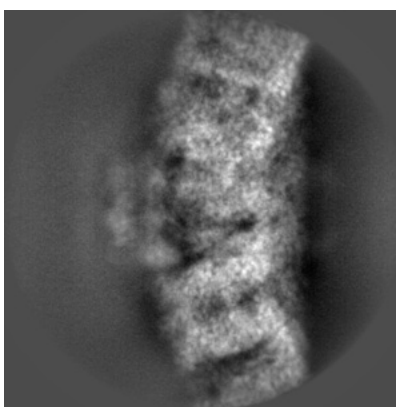


Z

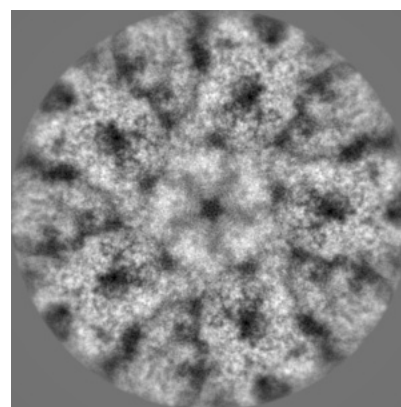
6.1.2 Raw map



X



Y

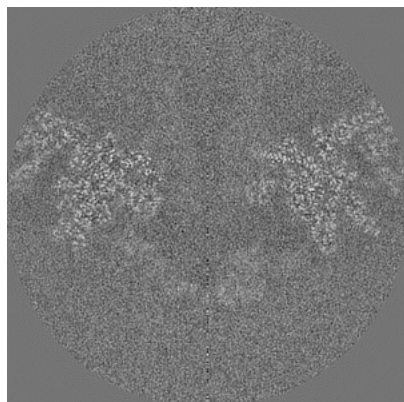


Z

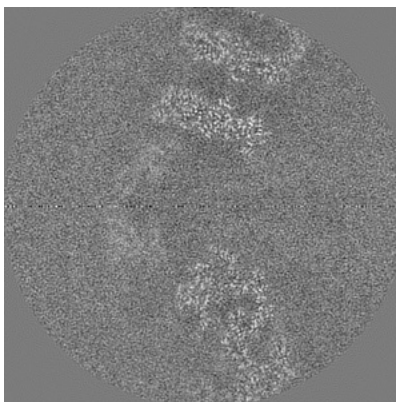
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

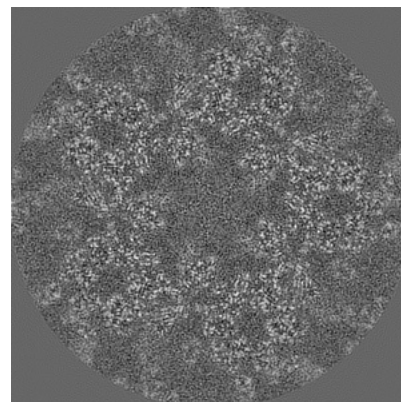
6.2.1 Primary map



X Index: 180

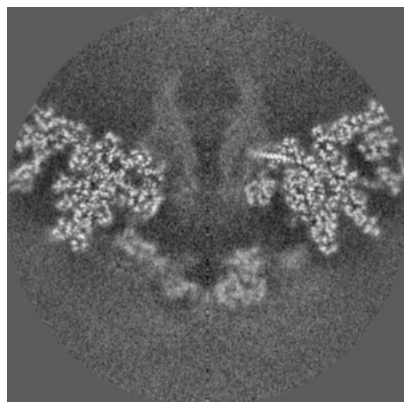


Y Index: 180

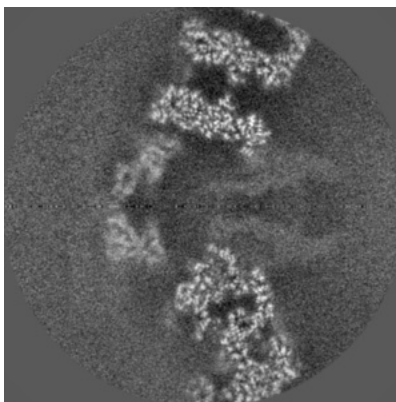


Z Index: 180

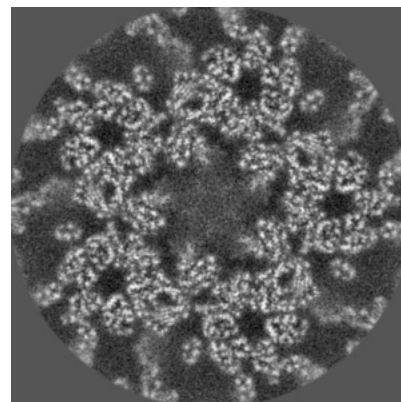
6.2.2 Raw map



X Index: 180



Y Index: 180

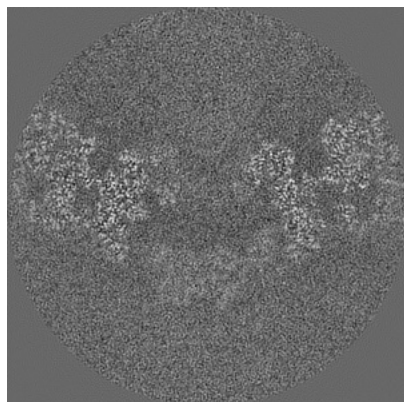


Z Index: 180

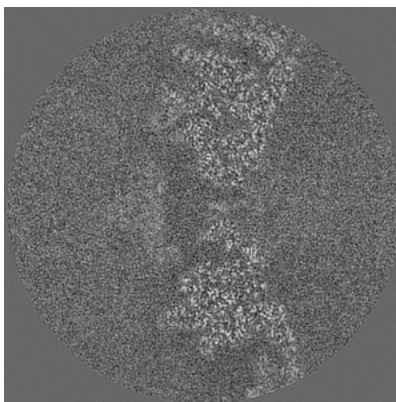
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

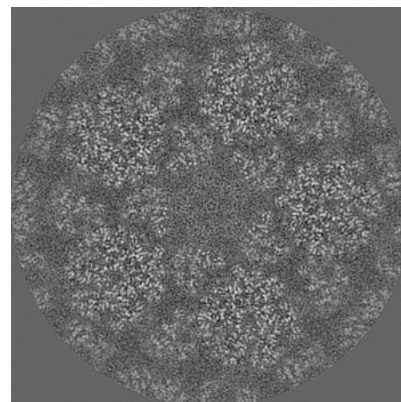
6.3.1 Primary map



X Index: 204

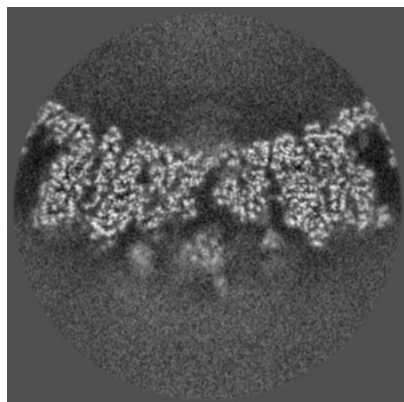


Y Index: 217

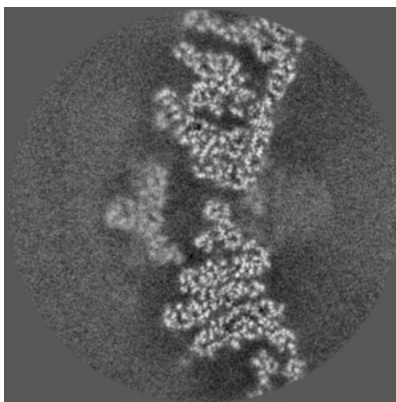


Z Index: 203

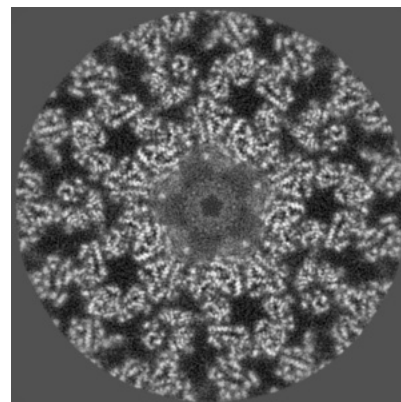
6.3.2 Raw map



X Index: 230



Y Index: 220

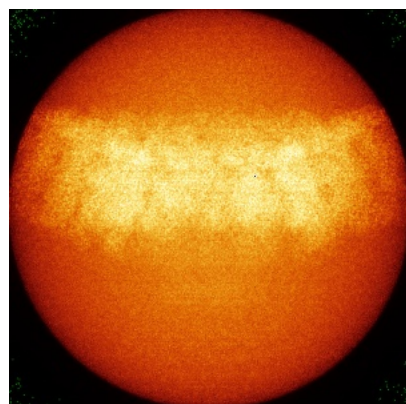


Z Index: 223

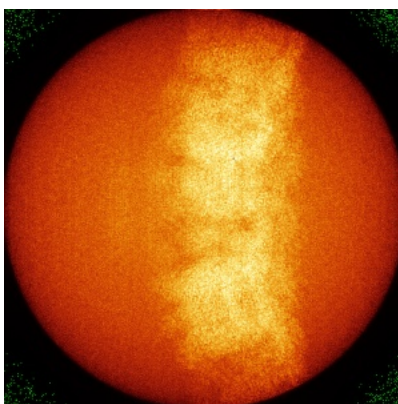
The images above show the largest variance slices of the map in three orthogonal directions.

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

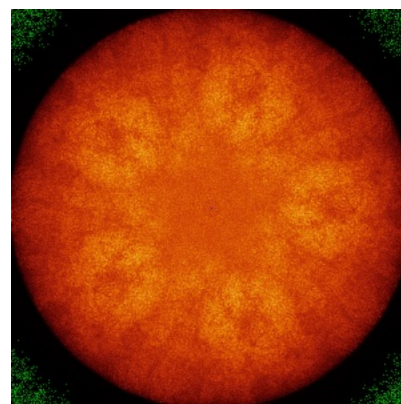
6.4.1 Primary map



X

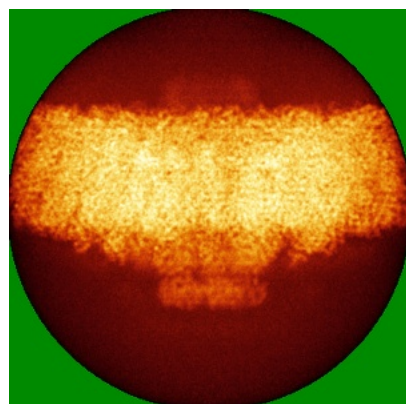


Y

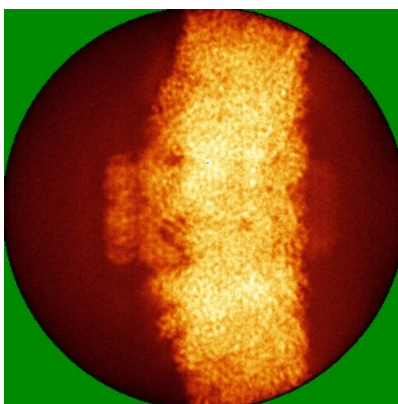


Z

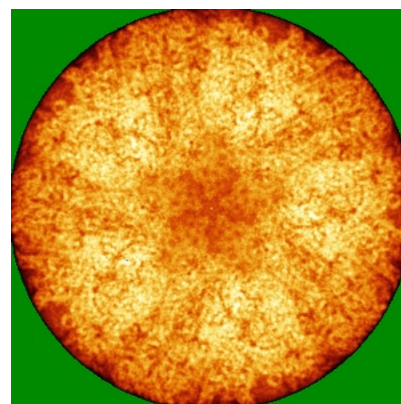
6.4.2 Raw map



X



Y

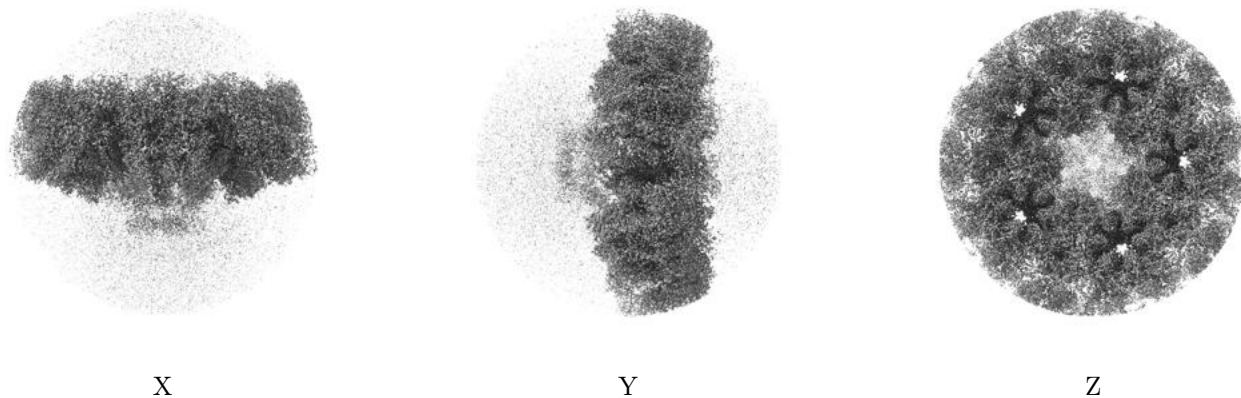


Z

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

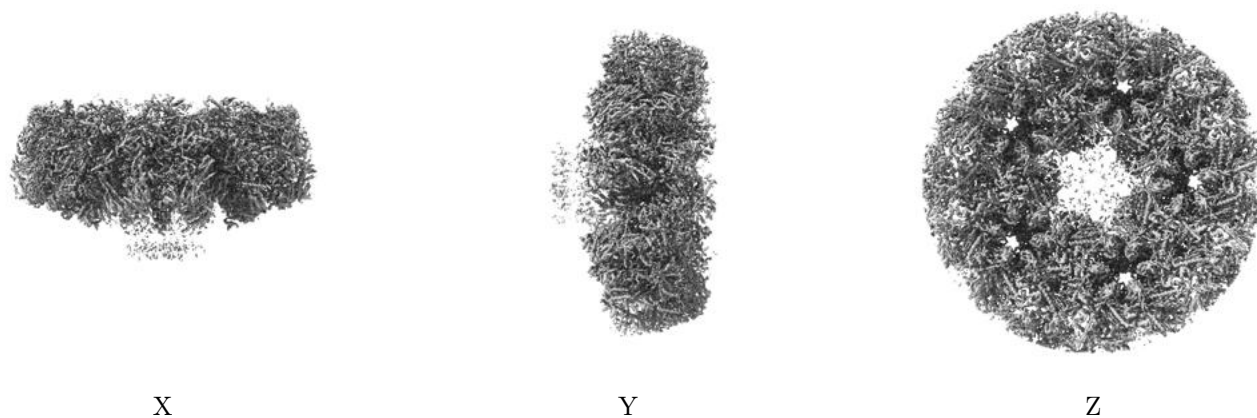
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.019. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 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.

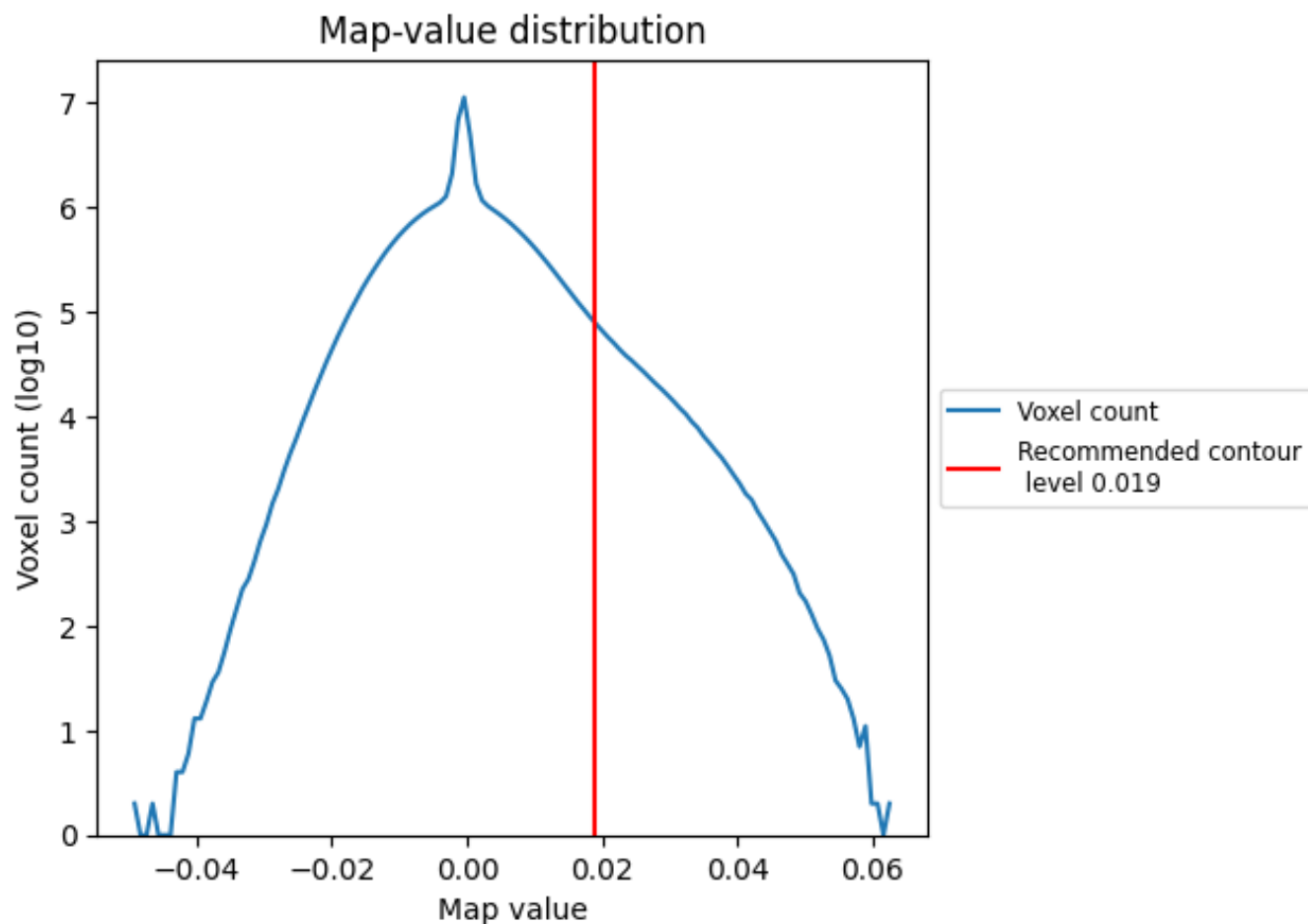
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

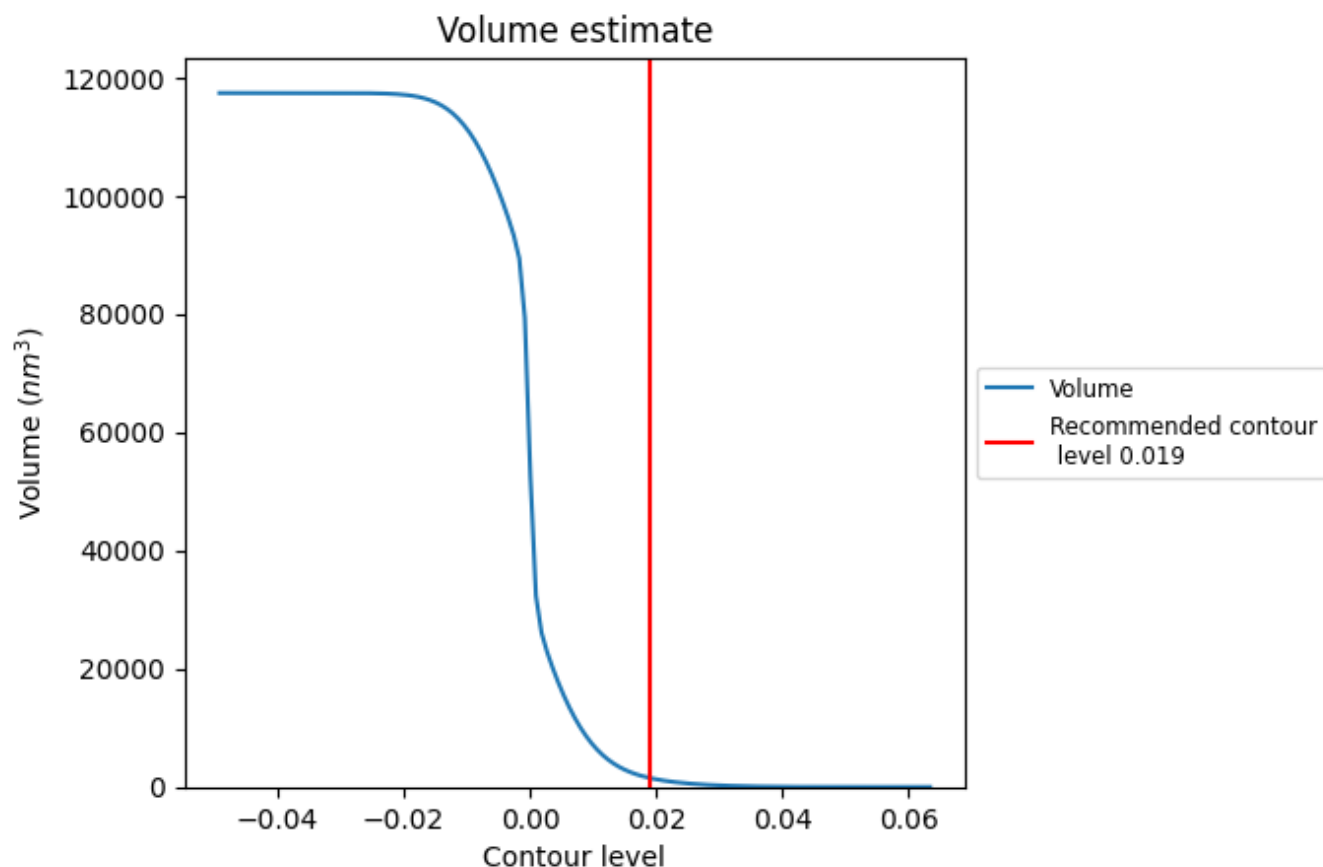
This section contains the results of statistical analysis of the map.

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.

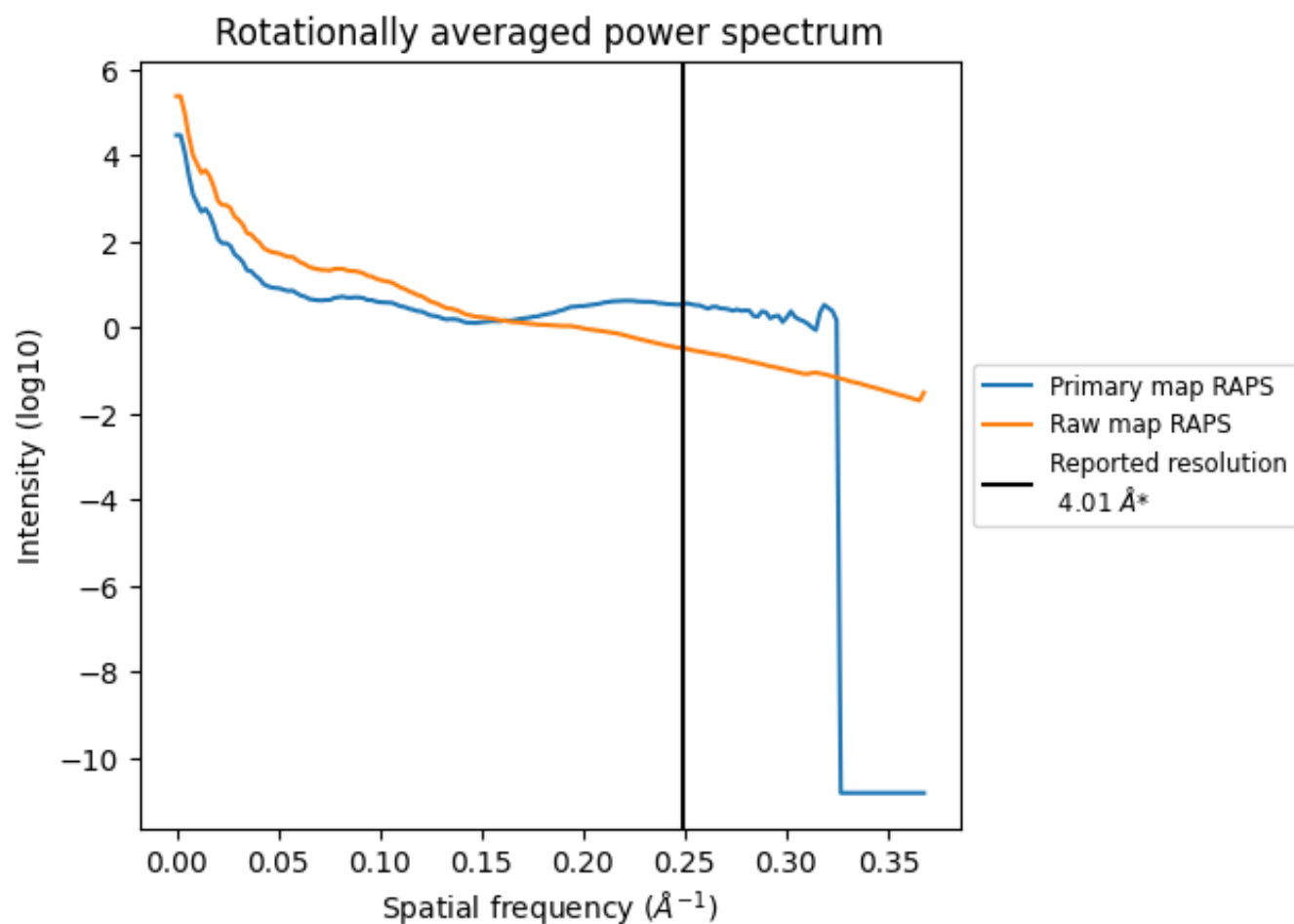
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1523 nm^3 ; this corresponds to an approximate mass of 1376 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 ⓘ

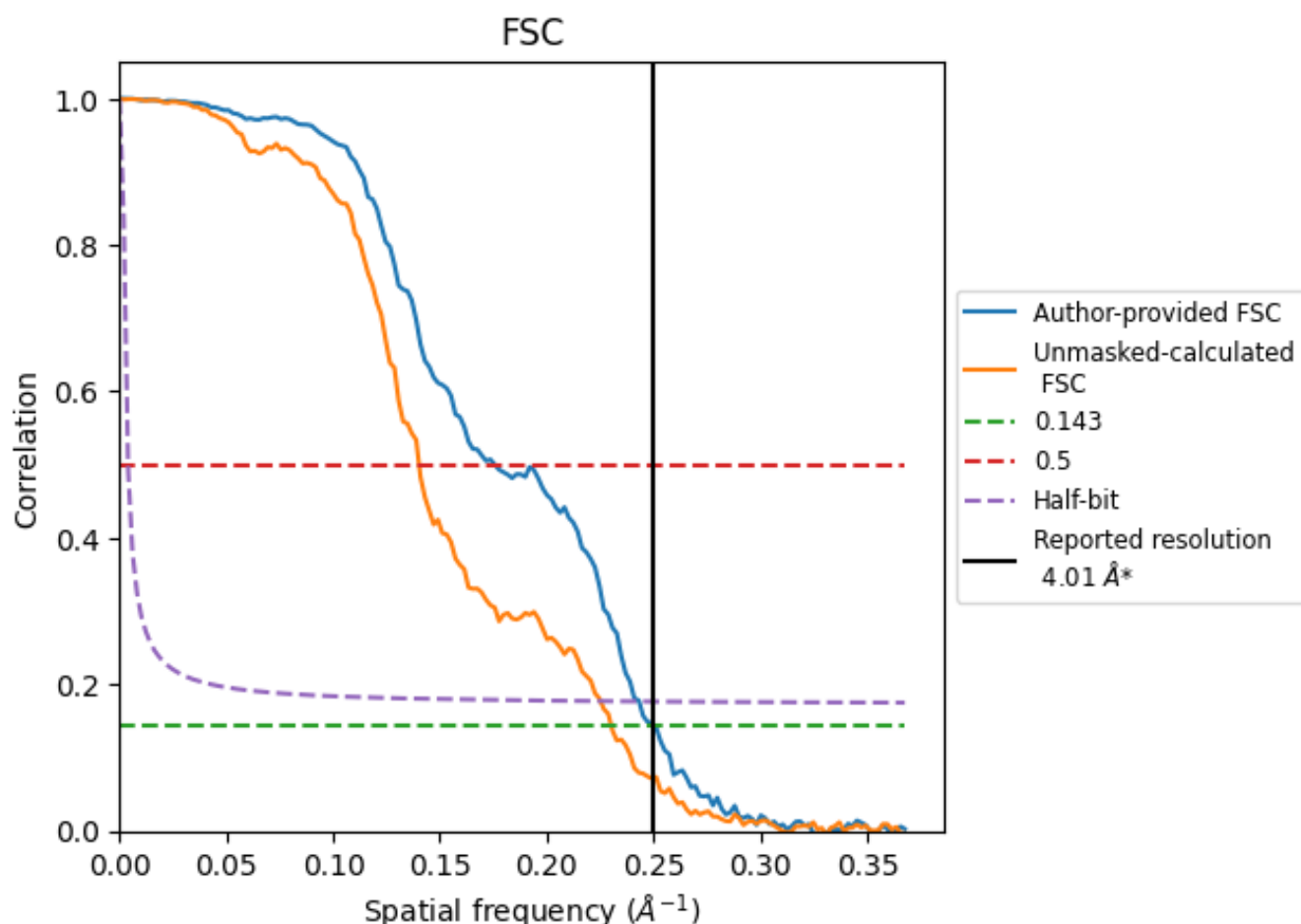


*Reported resolution corresponds to spatial frequency of 0.249 Å⁻¹

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 0.249 Å⁻¹

8.2 Resolution estimates [i](#)

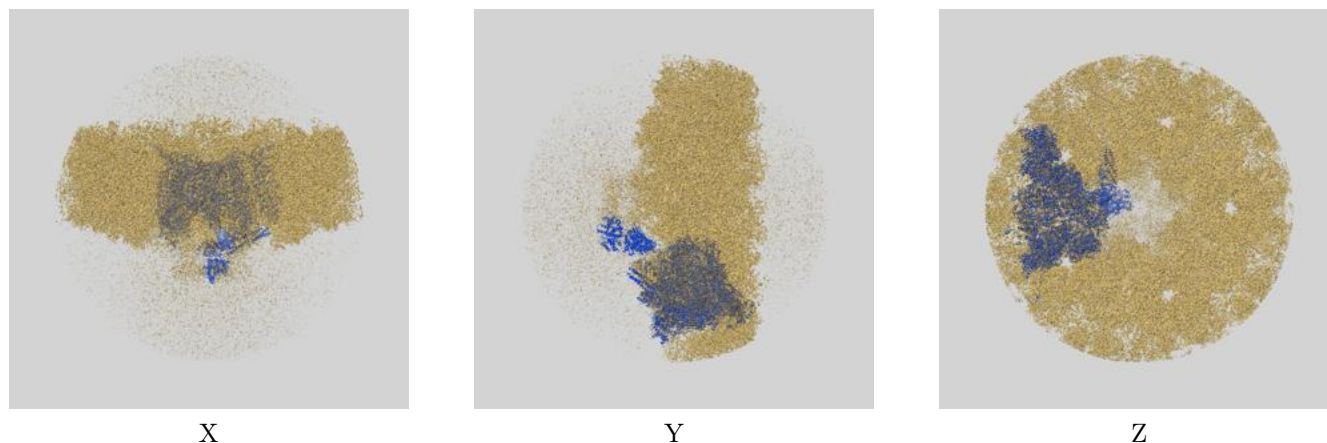
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.01	-	-
Author-provided FSC curve	3.99	5.69	4.11
Unmasked-calculated*	4.34	7.13	4.44

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

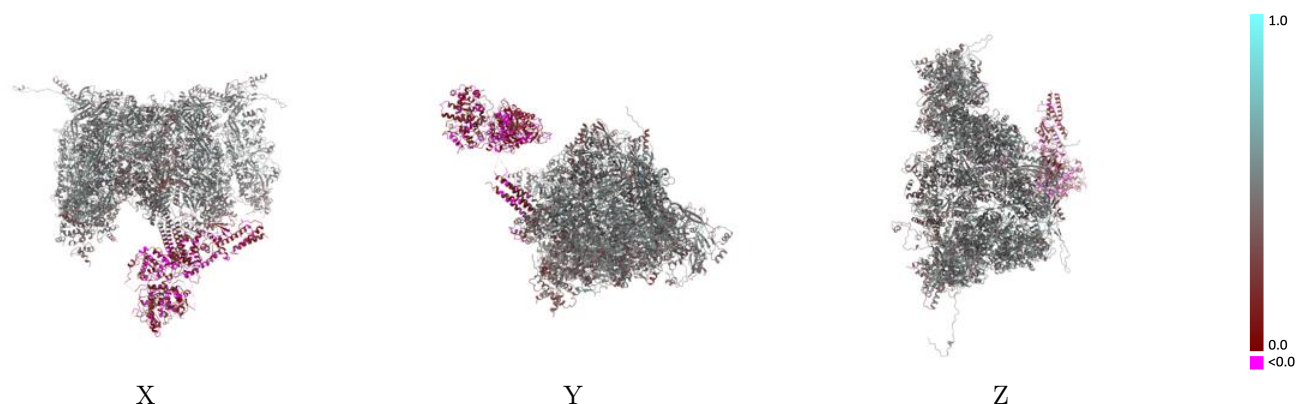
This section contains information regarding the fit between EMDB map EMD-41202 and PDB model 8TEU. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



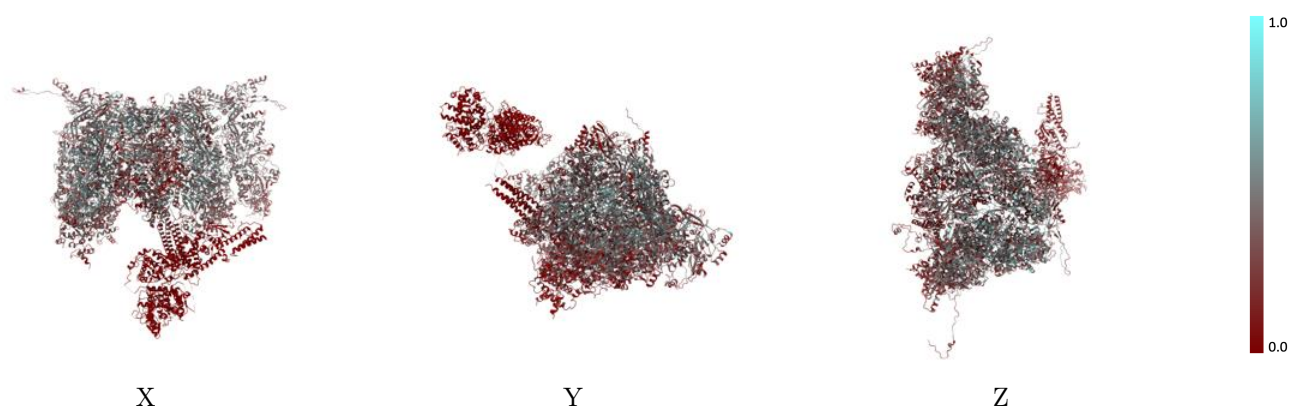
The images above show the 3D surface view of the map at the recommended contour level 0.019 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



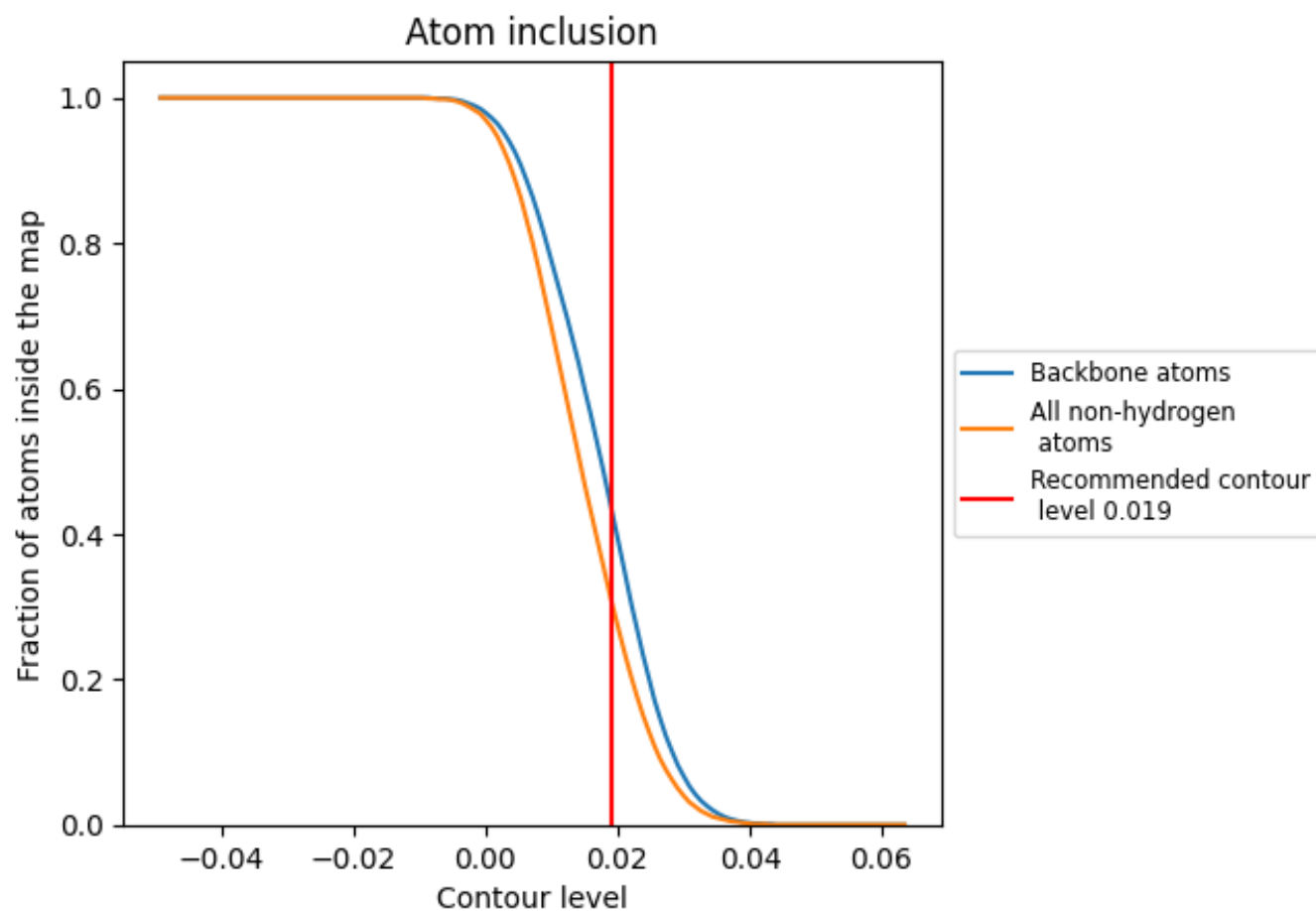
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.019).



















































9.4 Atom inclusion [i](#)



At the recommended contour level, 44% of all backbone atoms, 31% 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 (0.019) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.3100	 0.4300
A	 0.0170	 0.1030
C	 0.0190	 0.1850
E	 0.0350	 0.1650
F	 0.1000	 0.3010
G	 0.3070	 0.4630
H	 0.4230	 0.4860
I	 0.4030	 0.4820
J	 0.3360	 0.4690
K	 0.4120	 0.4810
L	 0.3660	 0.4750
M	 0.3180	 0.4690
N	 0.1870	 0.3950
O	 0.1990	 0.3710
P	 0.1270	 0.3470
Q	 0.1950	 0.3570
R	 0.1290	 0.3740
S	 0.1120	 0.3710
T	 0.2090	 0.4150
U	 0.3140	 0.4590
V	 0.3100	 0.4470
W	 0.3340	 0.4730
X	 0.2610	 0.4490
Y	 0.2850	 0.4550
Z	 0.1620	 0.4000

