



wwPDB EM Validation Summary Report ⓘ

Mar 6, 2026 – 08:46 AM UTC

PDB ID : 8TEP / pdb_00008tep
EMDB ID : EMD-41194
Title : Human cytomegalovirus portal vertex, virion configuration 1 (VC1)
Authors : Jih, J.; Liu, Y.T.; Liu, W.; Zhou, H.
Deposited on : 2023-07-06
Resolution : 3.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

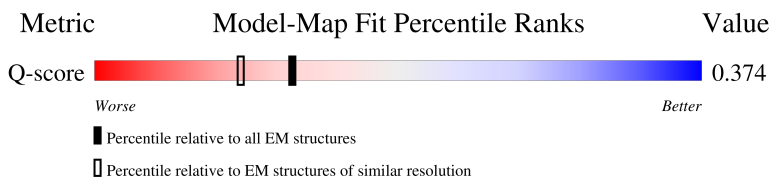
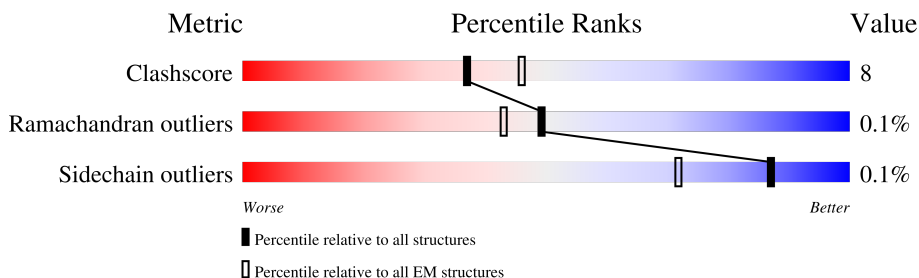
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.50 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13950 (3.00 - 4.00)

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	19% 23% 10% 68%
1	C	2241	28% 23% 8% 69%
2	B	983	26% 33% 17% 50%
2	D	983	43% 32% 14% 54%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	E	642	
3	F	642	
4	G	594	
5	H	1370	
5	I	1370	
5	J	1370	
5	K	1370	
5	L	1370	
5	M	1370	
6	N	75	
6	O	75	
6	P	75	
6	Q	75	
6	R	75	
6	S	75	
7	T	290	
7	W	290	
8	U	306	
8	V	306	
8	X	306	
8	Y	306	
9	Z	1048	

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 112987 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	723	Total	C	N	O	S	0	0
			5833	3733	1026	1052	22		
1	C	699	Total	C	N	O	S	0	0
			5651	3626	997	1006	22		

- Molecule 2 is a protein called Inner tegument protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	492	Total	C	N	O	S	0	0
			3993	2535	709	734	15		
2	D	453	Total	C	N	O	S	0	0
			3685	2349	645	676	15		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	482	Total	C	N	O	S	0	0
			3915	2516	688	699	12		
3	F	492	Total	C	N	O	S	0	0
			3986	2562	705	708	11		

- Molecule 4 is a protein called Capsid vertex component 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	G	472	Total	C	N	O	S	0	0
			3873	2422	744	693	14		

- Molecule 5 is a protein called Major capsid protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	H	1311	Total	C	N	O	S	0	0
			10406	6630	1802	1913	61		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	1350	Total	C	N	O	S	0	0
			10693	6809	1853	1970	61		
5	J	1317	Total	C	N	O	S	0	0
			10433	6641	1814	1919	59		
5	K	1298	Total	C	N	O	S	0	0
			10282	6544	1792	1887	59		
5	L	1350	Total	C	N	O	S	0	0
			10693	6809	1853	1970	61		
5	M	1350	Total	C	N	O	S	0	0
			10693	6809	1853	1970	61		

- Molecule 6 is a protein called Small capsomere-interacting protein.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	T	240	Total	C	N	O	S	0	0
			1919	1235	335	338	11		
7	W	290	Total	C	N	O	S	0	0
			2325	1485	411	417	12		

- Molecule 8 is a protein called Triplex capsid protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	U	292	Total	C	N	O	S	0	0
			2317	1489	399	411	18		
8	V	288	Total	C	N	O	S	0	0
			2292	1471	397	407	17		

Continued on next page...

Continued from previous page...

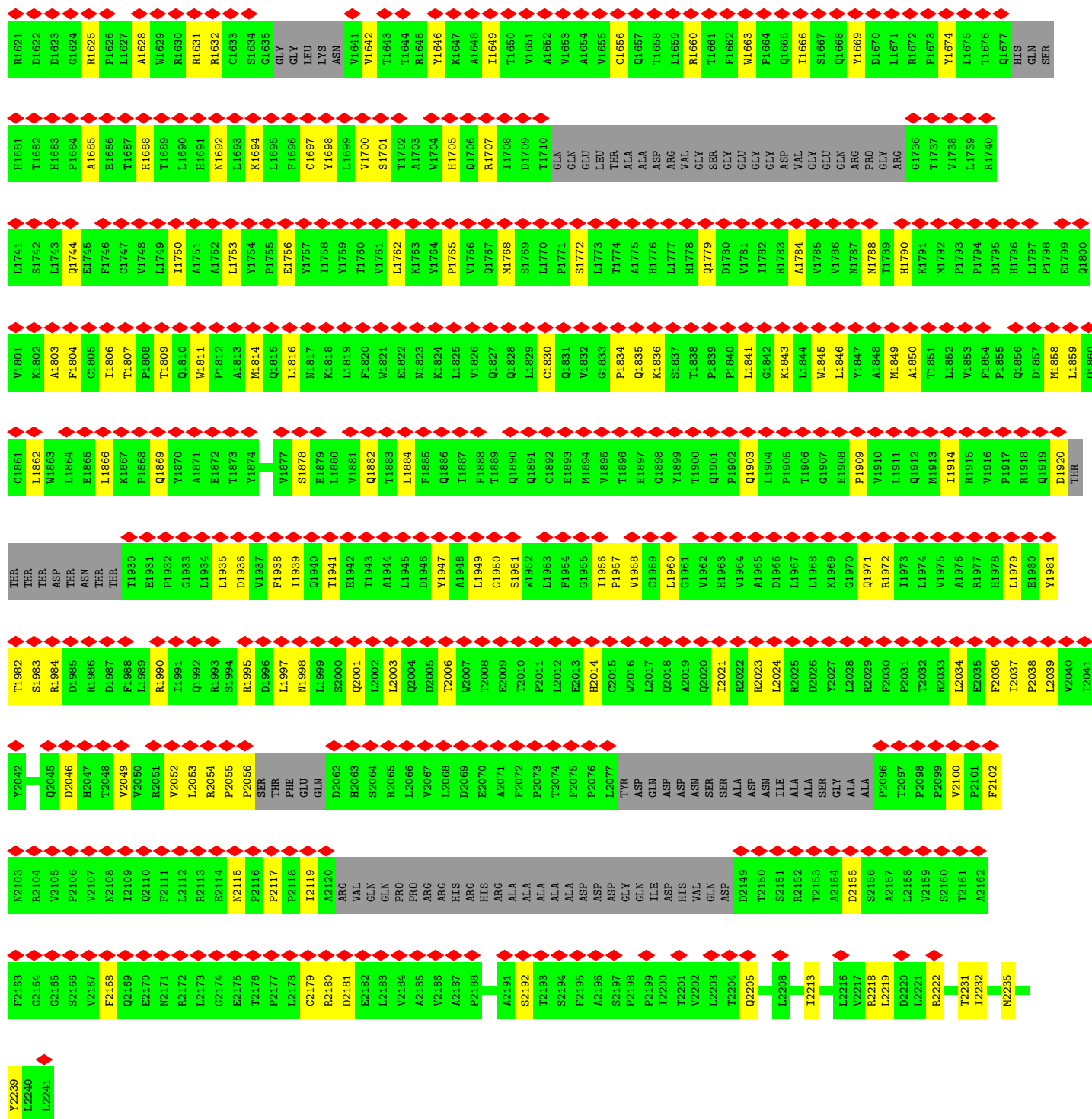
Mol	Chain	Residues	Atoms					AltConf	Trace
8	X	295	Total	C	N	O	S	0	0
			2334	1501	402	412	19		
8	Y	285	Total	C	N	O	S	0	0
			2266	1456	387	405	18		

- Molecule 9 is a protein called Large structural phosphoprotein.

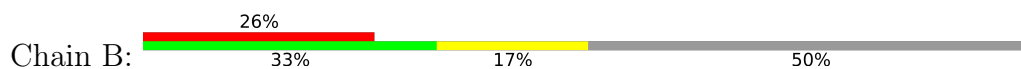
Mol	Chain	Residues	Atoms					AltConf	Trace
9	Z	284	Total	C	N	O	S	0	0
			2320	1463	425	420	12		

Y1757	F1696	R1630	R1569	GLN	ASN	GLN	LYS	ASP	GLN	LEU	VAL	GLY	LYS	ARG	LEU	MET
I1758	C1697	R1631	D1570	THR	ALA	THR	VAL	PRO	ALA	ASP	ILE	ASP	LYS	ARG	ARG	GLY
Y1759	Y1698	R1632	R1571	G1444	ALA	LEU	THR	TYR	ALA	GLY	GLN	THR	THR	PHE	ARG	LYS
T1760	L1699	C1633	R1572	D1445	ASN	LEU	GLN	CYS	THR	ILE	ASP	THR	THR	ALA	ALA	GLN
Y1761	V1700	S1634	R1573	L1446	ASN	ALA	ALA	VAL	SER	GLY	VAL	THR	THR	ASP	GLU	ASP
L1762	S1701	G1635	R1574	E1447	PHE	GLU	ALA	THR	VAL	LYS	VAL	THR	THR	ARG	GLU	GLY
K1763	S1702	GLY	L1575	L1448	ILE	ALA	GLN	ARG	THR	CYS	VAL	VAL	VAL	ARG	GLU	SER
Y1764	A1703	LEU	C1576	L1449	ALA	THR	THR	VAL	VAL	GLN	ASP	VAL	GLU	LEU	PRO	LEU
P1765	W1704	LYS	F1577	Q1449	GLN	THR	ASP	GLY	GLN	GLY	ASP	GLY	TYR	VAL	ARG	PRO
V1766	H1705	Q1706	A1578	E1450	HIS	VAL	GLN	VAL	ASP	GLY	ALA	ASP	GLY	TYR	ARG	PRO
Q1767	R1707	G1516	R1579	T1451	GLU	ARG	GLN	GLY	GLY	ASP	VAL	VAL	GLN	PHE	THR	THR
M1768	I1708	H1580	H1581	L1452	ALA	MET	SER	PRO	LYS	THR	GLY	VAL	VAL	ARG	PHE	PHE
S1769	P1771	T1643	H1584	E1455	THR	ALA	THR	GLY	PHE	THR	THR	GLY	GLY	ASP	ASP	ASP
L1770	T1710	T1644	F1584	E1456	ALA	ALA	ALA	GLY	GLY	THR	THR	ALA	ALA	VAL	VAL	VAL
P1771	GLN	R1645	L1585	Y1456	GLY	PHE	ASN	LEU	GLN	THR	THR	ALA	TYR	GLY	SER	SER
S1772	GLN	Y1646	L1586	F1457	ALA	GLU	ALA	GLU	GLU	ILE	THR	THR	PRO	GLY	PHE	LEU
T1773	GLU	E1586	E1586	A1458	SER	ALA	SER	LEU	LEU	GLY	ARG	ARG	CYS	ARG	PHE	LEU
L1774	LEU	V1587	V1587	L1459	THR	ALA	THR	ALA	ALA	PHE	HIS	HIS	HIS	GLN	PHE	LEU
A1775	THR	V1588	V1588	L1460	PRO	LEU	PRO	GLY	GLY	GLY	GLN	VAL	VAL	GLN	MET	GLN
H1776	ALA	D1589	D1589	H1461	VAL	ALA	VAL	ILE	ILE	ASP	PRO	PRO	GLY	GLY	GLY	LEU
L1777	ALA	V1590	V1590	I1463	ASP	VAL	ASP	THR	THR	GLY	THR	THR	GLN	GLN	PRO	PRO
H1778	ALA	F1591	F1591	Q1464	MET	GLY	VAL	ALA	PRO	ALA	ALA	ALA	GLY	GLY	ARG	ARG
Q1779	ASP	G1592	G1592	T1465	GLN	ASP	THR	ASP	PRO	ARG	THR	THR	GLN	GLN	GLY	SER
D1780	VAL	M1593	M1593	F1466	ALA	PRO	ALA	MET	ALA	TYR	ALA	VAL	VAL	VAL	VAL	GLN
Y1781	GLY	R1594	R1594	S1467	VAL	GLY	VAL	GLY	ASP	ARG	GLY	GLY	THR	GLY	GLY	GLY
V1785	SER	Q1595	Q1595	Y1468	ALA	PRO	ALA	GLY	PHE	SER	SER	THR	GLN	PRO	PRO	ARG
H1788	GLY	L1596	I1596	G1469	VAL	HIS	HIS	LEU	GLN	GLN	GLN	ALA	VAL	VAL	VAL	ASP
T1789	GLY	V1597	V1597	L1470	THR	GLY	GLY	ASP	PRO	GLN	GLN	GLY	THR	THR	THR	LEU
M1790	ASP	T1598	T1598	D1471	GLY	VAL	VAL	VAL	VAL	LYS	LYS	MET	GLY	GLY	GLY	ARG
K1791	VAL	Q1599	Q1599	F1472	ARG	SER	SER	THR	PHE	ASN	ASN	GLN	GLN	ASN	ALA	ALA
F1792	GLY	A1600	A1600	R1473	LEU	GLU	GLU	THR	THR	GLY	GLY	ASP	ASP	TYR	GLY	ASN
V1795	GLN	G1601	G1601	S1474	PRO	GLY	PRO	HIS	LEU	GLN	GLN	LEU	GLN	GLY	VAL	VAL
E1799	ARG	E1602	E1602	Q1475	GLY	THR	THR	TYR	LEU	GLN	GLN	ASP	GLY	GLY	GLY	ASP
H1796	PRO	P1603	P1603	L1476	VAL	ARG	ARG	ARG	LEU	GLN	GLN	ILE	ASP	TYR	THR	THR
L1797	GLY	I1604	I1604	E1477	ALA	VAL	VAL	GLY	ASN	GLY	GLY	LEU	GLY	HIS	ALA	ALA
E1798	ARG	H1605	H1605	K1478	ALA	LEU	LEU	LEU	GLN	THR	THR	ASP	LYS	GLY	MET	MET
E1799	G1736	L1606	L1606	D1481	GLY	GLN	GLN	GLN	ASP	GLN	GLN	LYS	LYS	VAL	VAL	VAL
T1797	T1737	Y1674	Y1674	L1482	ALA	GLN	GLN	ALA	ALA	GLN	GLN	GLY	GLY	GLY	GLY	GLY
Q1800	V1738	L1675	Y1546	L1483	ALA	ALA	ALA	ALA	ALA	MET	LEU	LEU	GLN	GLN	GLN	LYS
V1801	L1739	T1676	T1608	T1484	ARG	VAL	VAL	VAL	ARG	THR	THR	THR	GLY	GLY	GLY	LYS
K1802	R1740	Q1677	D1609	R1548	HIS	GLU	GLU	GLU	LYS	GLY	GLY	GLY	GLN	GLN	GLN	GLY
A1803	L1743	H1677	G1611	T1485	GLN	SER	SER	SER	ALA	THR	THR	THR	GLY	GLY	GLY	GLY
F1804	Q1744	H1678	N1612	E1488	LYS	ALA	ALA	VAL	LEU	SER	THR	THR	ARG	ARG	ILE	ILE
T1807	E1745	Q1679	V1613	E1489	VAL	THR	THR	THR	SER	GLY	GLY	GLY	GLN	GLY	GLY	GLY
P1808	F1746	S1680	A1614	L1489	GLN	GLU	GLU	GLU	ASP	GLY	GLY	GLY	GLN	LEU	LEU	LYS
T1809	T1747	H1681	F1615	A1490	LEU	LEU	LEU	LEU	ALA	ALA	ALA	ALA	GLY	ALA	ALA	ALA
Q1810	V1748	T1682	K1616	K1491	LEU	LEU	LEU	LEU	ALA	ASP	ASP	ASP	GLY	GLY	GLY	THR
W1811	L1749	H1683	Y1617	R1492	GLN	GLN	GLN	GLN	LYS	ARG	ARG	ARG	GLY	GLY	GLY	GLY
M1814	I1750	P1684	L1618	R1493	GLY	GLY	GLY	GLY	ALA	GLY	GLY	GLY	GLY	GLY	GLY	GLY
Q1815	A1751	A1685	A1619	G1494	LYS	ALA	ALA	ALA	LEU	THR	THR	THR	GLY	GLY	GLY	GLY
K1818	A1752	E1686	L1620	T1495	VAL	VAL	VAL	VAL	LEU	ARG	ARG	ARG	GLN	GLN	GLN	GLN
L1819	L1753	T1687	R1621	R1496	GLN	THR	THR	THR	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
E1822	Y1754	H1688	D1622	L1497	GLY	GLU	GLU	GLU	ASP	GLY	GLY	GLY	GLY	GLY	GLY	GLY
N1823	P1755	H1691	G1624	S1498	LEU	LEU	LEU	LEU	ALA	ASP	ASP	ASP	GLY	GLY	GLY	GLY
K1824	E1756	L1693	D1625	N1499	ALA	ALA	ALA	ALA	ALA	ASP	ASP	ASP	GLY	GLY	GLY	GLY
		K1694	P1626	E1500	LYS	LYS	LYS	LYS	LYS	ASP	ASP	ASP	GLY	GLY	GLY	GLY
		L1695	L1627	G1501	GLY	GLY	GLY	GLY	GLY	ASN	ASN	ASN	GLY	GLY	GLY	GLY
			A1628	V1502	GLY	GLY	GLY	GLY	GLY	GLN	GLN	GLN	GLY	GLY	GLY	GLY
			W1629	L1503												





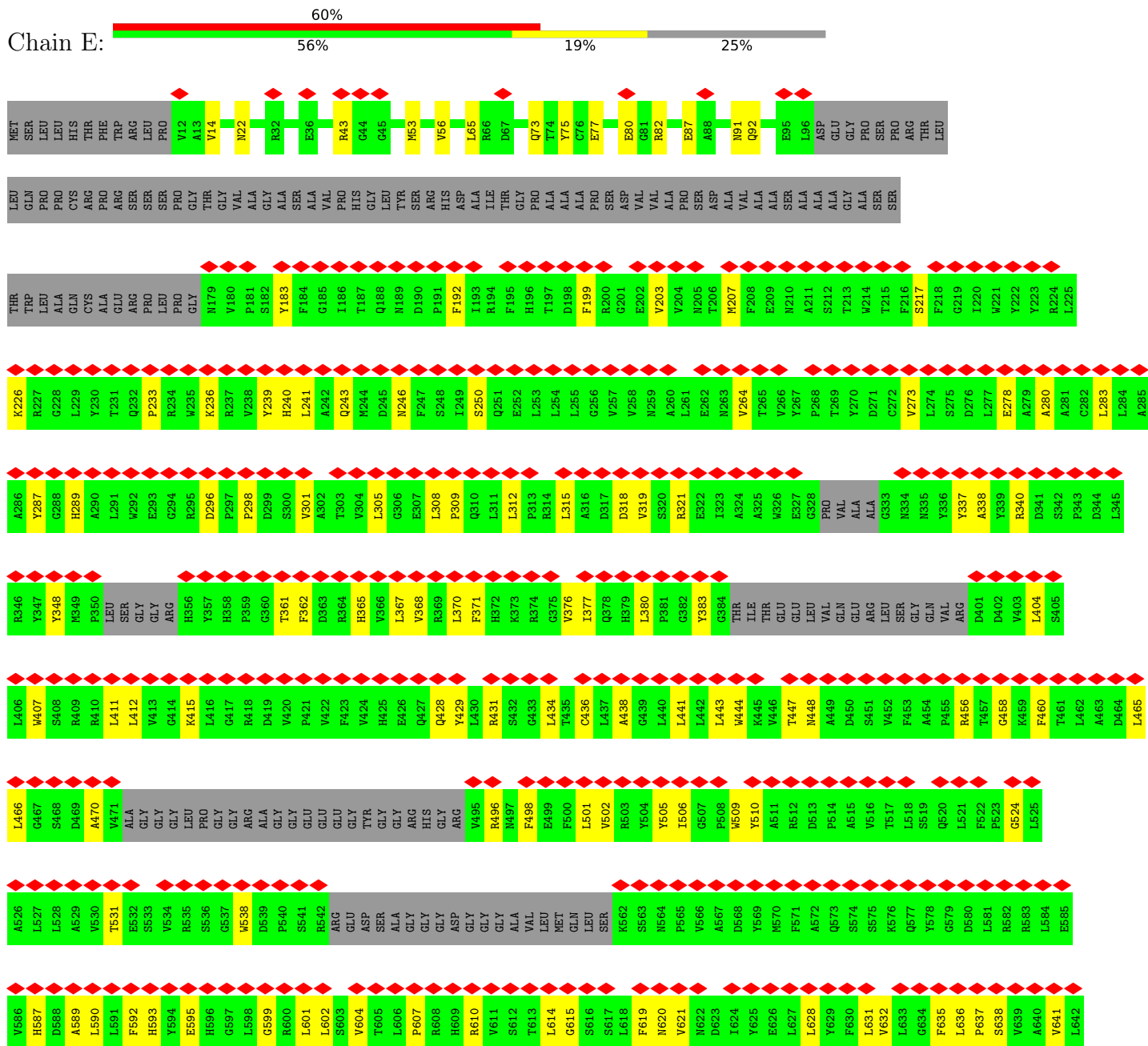
• Molecule 2: Inner tegument protein



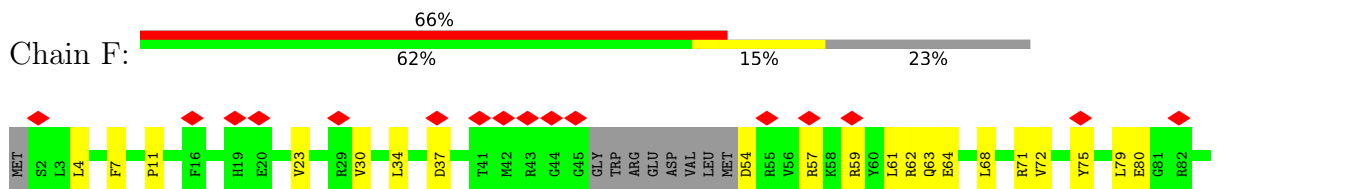


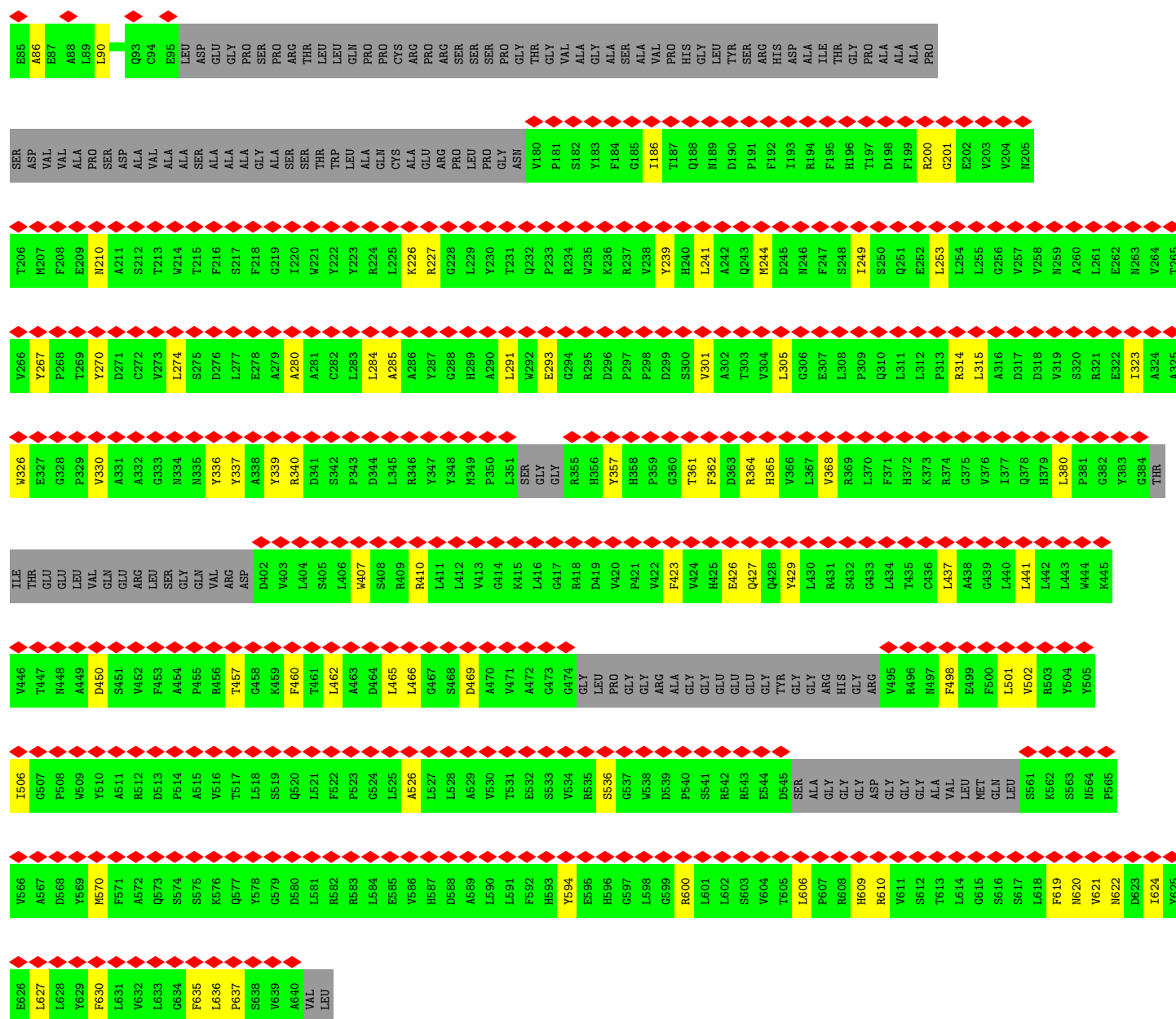


- Molecule 3: Capsid vertex component 2

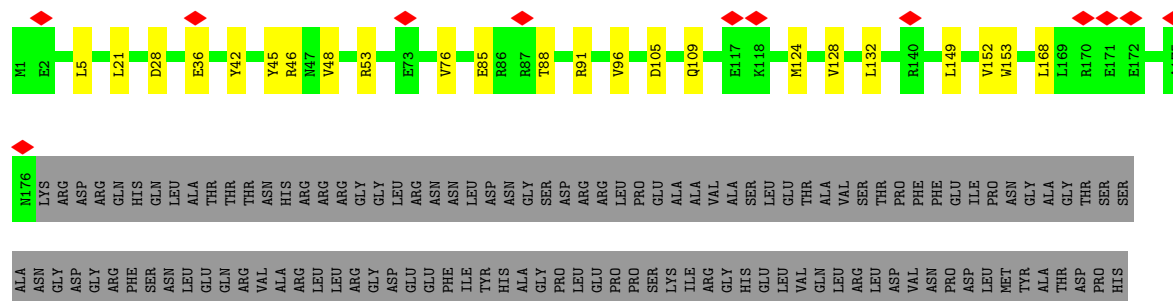


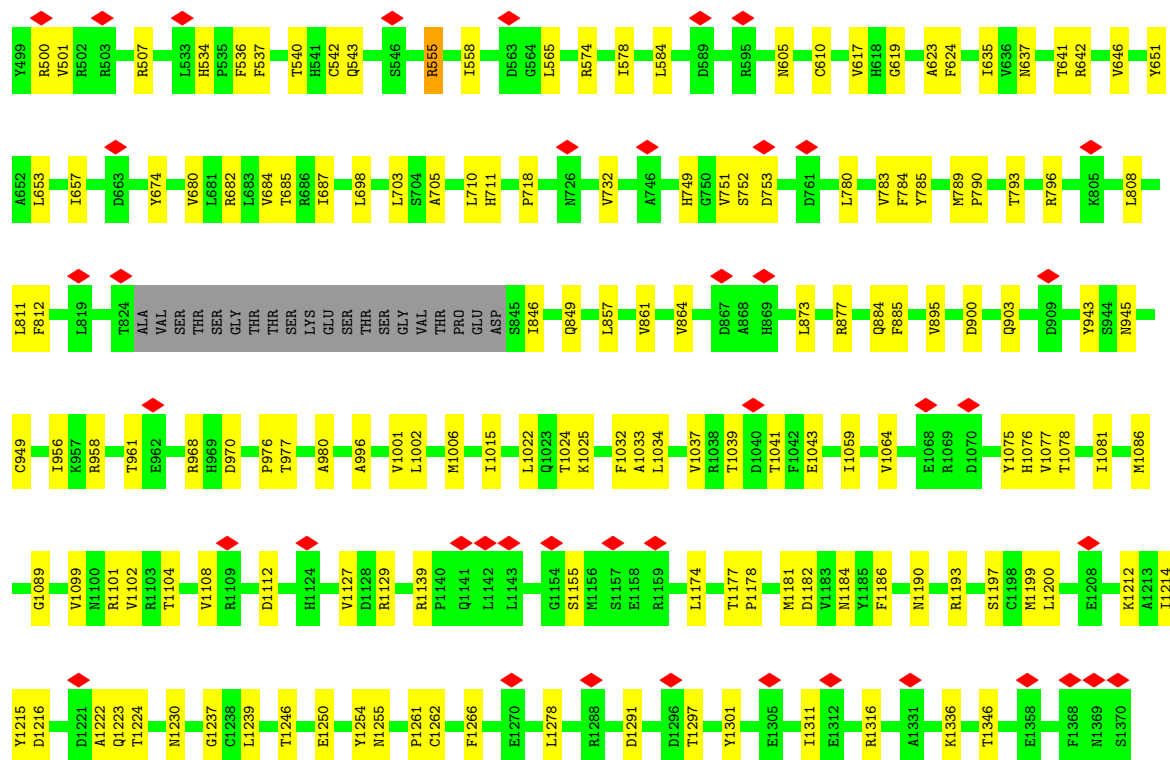
- Molecule 3: Capsid vertex component 2



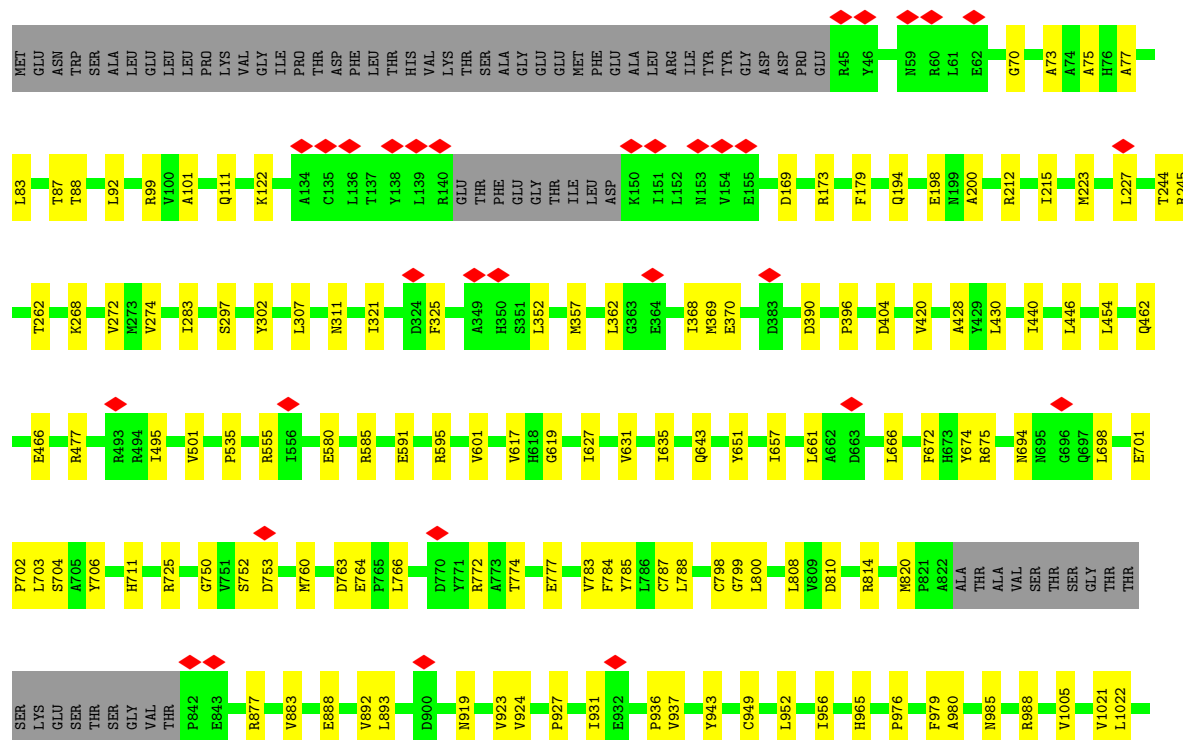
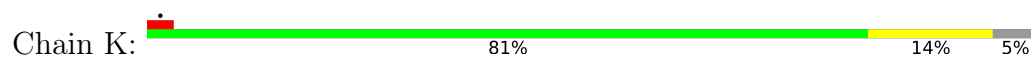


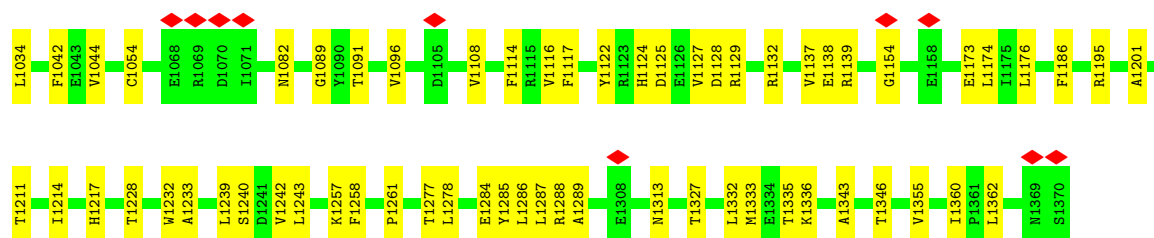
• Molecule 4: Capsid vertex component 1





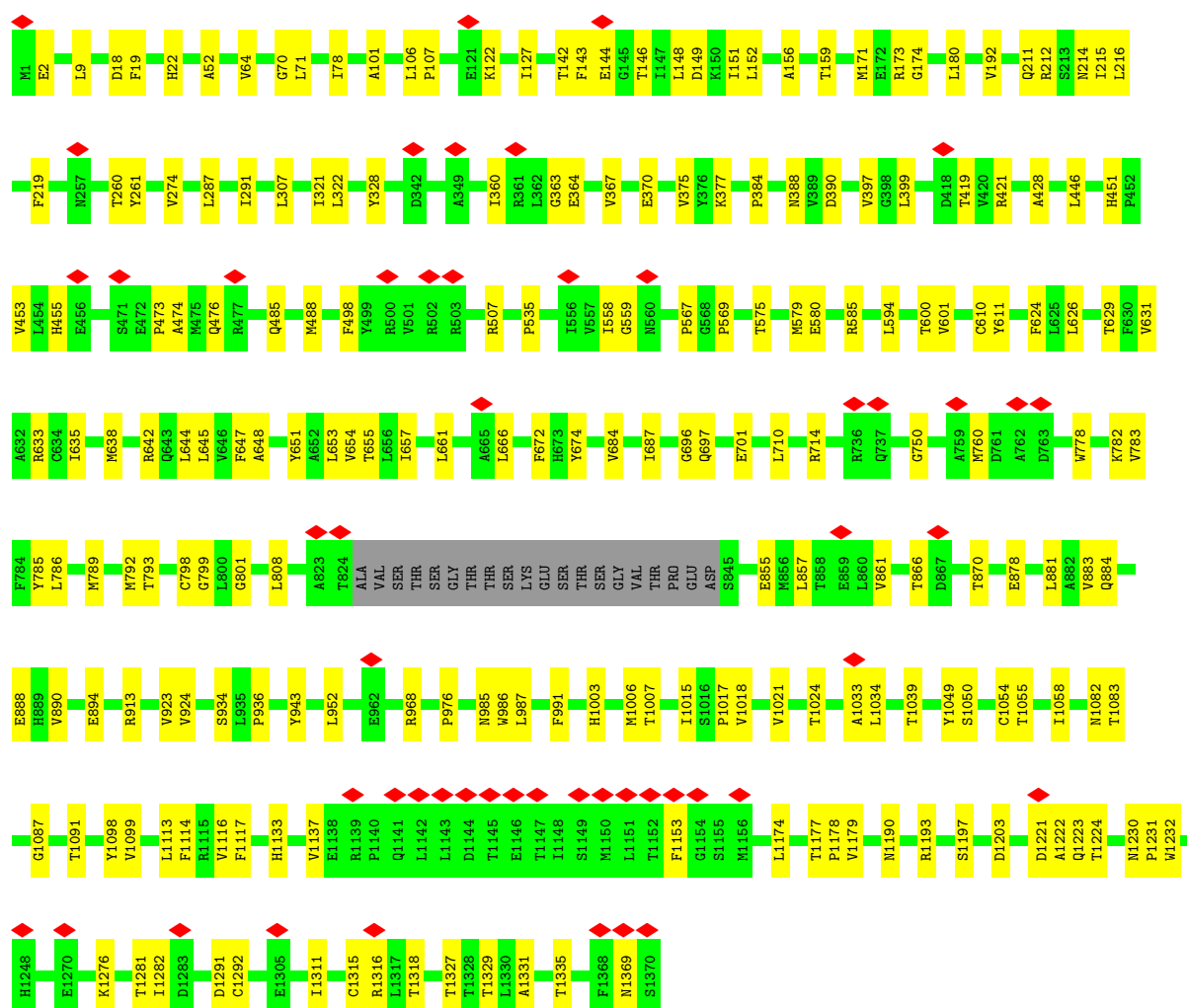
• Molecule 5: Major capsid protein





• Molecule 5: Major capsid protein

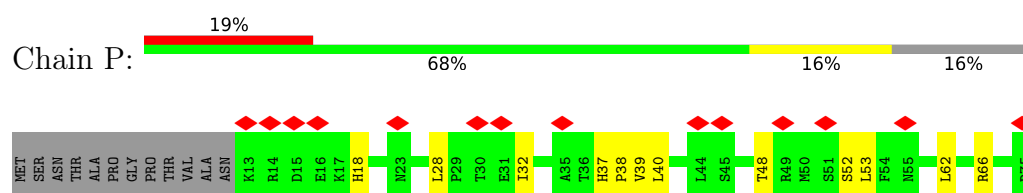
Chain L: 83% 15%



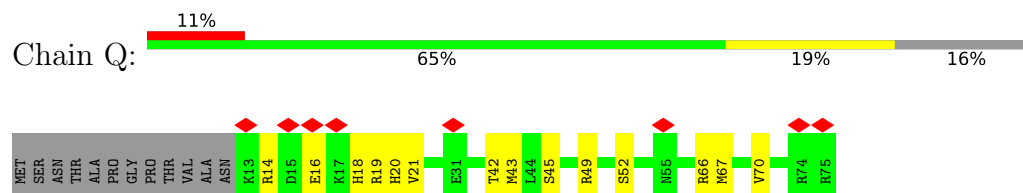
• Molecule 5: Major capsid protein

Chain M: 6% 82% 17%

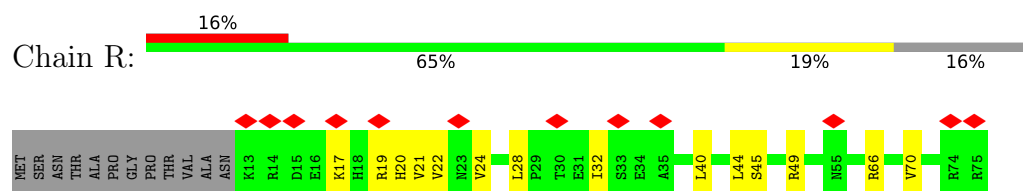




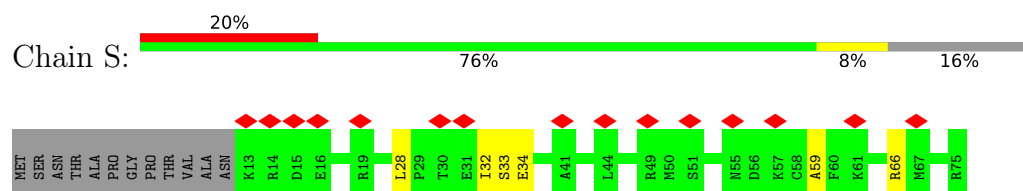
- Molecule 6: Small capsomere-interacting protein



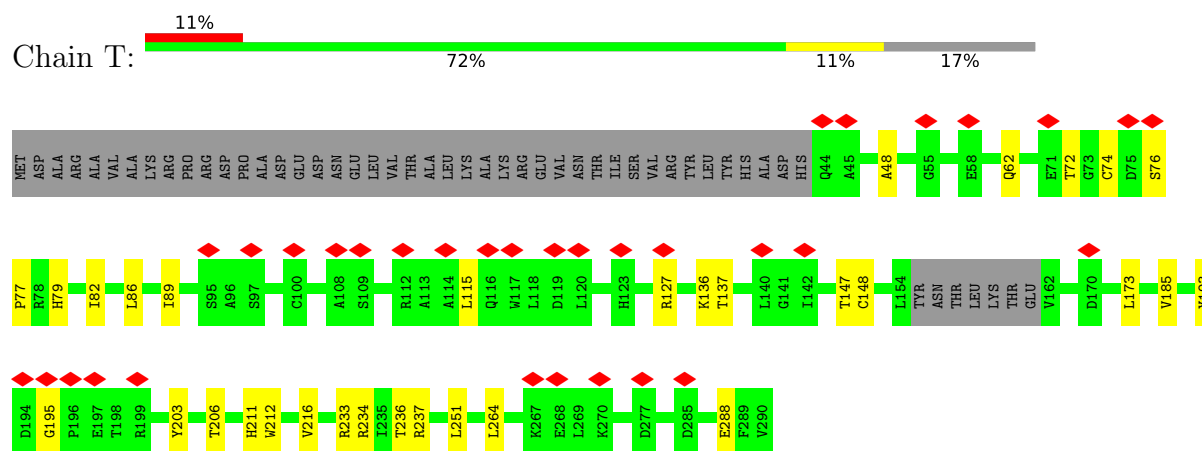
- Molecule 6: Small capsomere-interacting protein



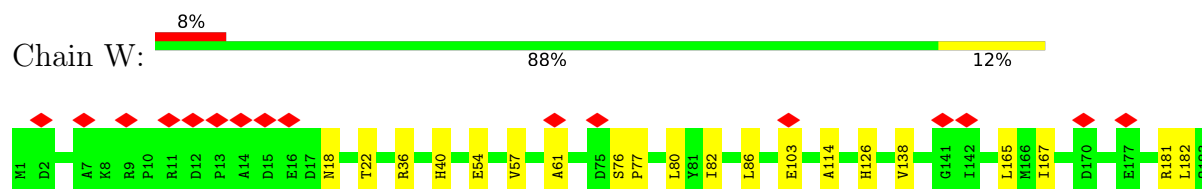
- Molecule 6: Small capsomere-interacting protein



- Molecule 7: Triplex capsid protein 1

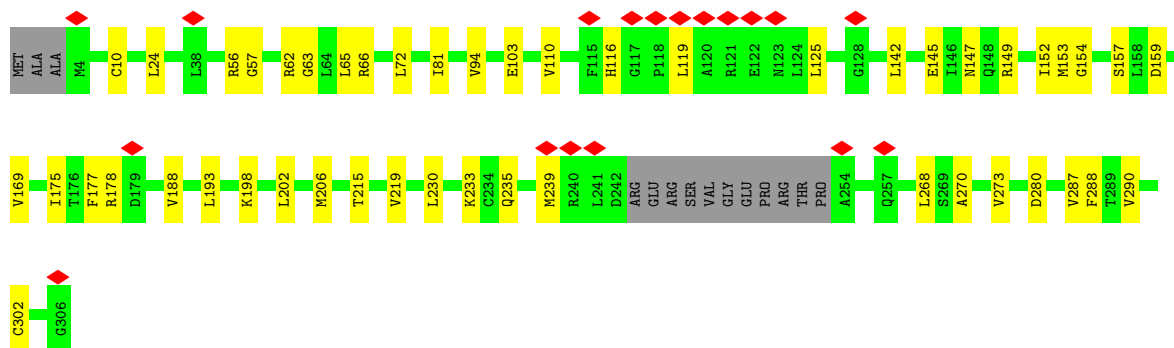
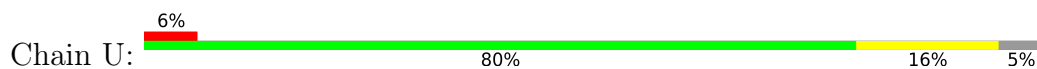


- Molecule 7: Triplex capsid protein 1

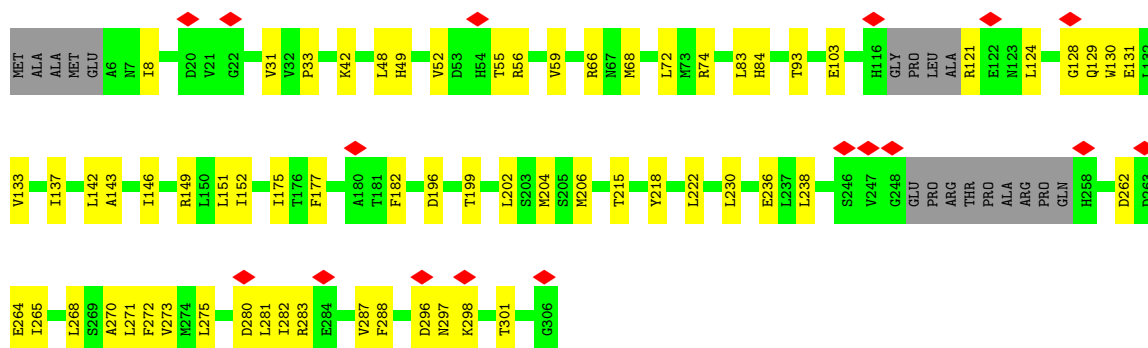
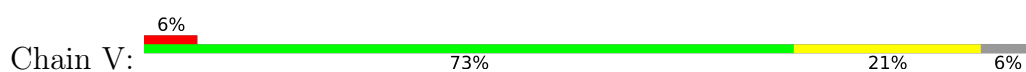




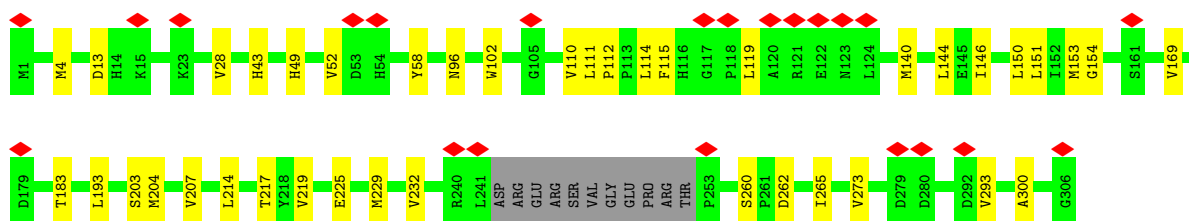
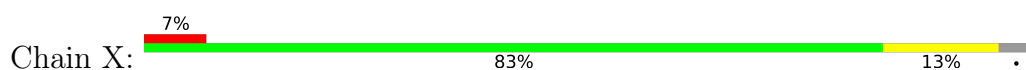
- Molecule 8: Triplex capsid protein 2



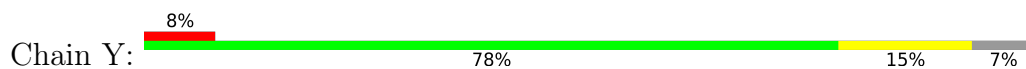
- Molecule 8: Triplex capsid protein 2



- Molecule 8: Triplex capsid protein 2



- Molecule 8: Triplex capsid protein 2



[illegible]

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C5	Depositor
Number of particles used	35055	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	0.035	Depositor
Minimum map value	-0.023	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.005	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	0.14	0/5975	0.41	0/8149
1	C	0.18	0/5787	0.48	1/7885 (0.0%)
2	B	0.15	0/4082	0.45	1/5535 (0.0%)
2	D	0.19	0/3768	0.46	0/5111
3	E	0.14	0/4015	0.42	0/5453
3	F	0.13	0/4090	0.42	0/5557
4	G	0.17	0/3962	0.55	0/5371
5	H	0.30	0/10653	0.65	8/14508 (0.1%)
5	I	0.27	0/10949	0.61	6/14916 (0.0%)
5	J	0.23	0/10682	0.54	1/14553 (0.0%)
5	K	0.25	0/10527	0.58	7/14339 (0.0%)
5	L	0.21	0/10949	0.54	4/14916 (0.0%)
5	M	0.15	0/10949	0.46	2/14916 (0.0%)
6	N	0.14	0/520	0.46	0/697
6	O	0.12	0/520	0.45	0/697
6	P	0.15	0/520	0.48	0/697
6	Q	0.16	0/520	0.50	0/697
6	R	0.16	0/520	0.51	0/697
6	S	0.15	0/520	0.49	0/697
7	T	0.15	0/1960	0.50	0/2658
7	W	0.31	0/2374	0.66	0/3221
8	U	0.16	0/2361	0.45	0/3206
8	V	0.18	0/2333	0.52	0/3164
8	X	0.18	0/2379	0.48	0/3230
8	Y	0.20	0/2305	0.55	0/3126
9	Z	0.16	0/2358	0.49	0/3182
All	All	0.21	0/115578	0.53	30/157178 (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
5	H	0	1
5	J	0	1
All	All	0	2

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	555	ARG	NE-CZ-NH2	7.03	125.53	119.20
5	H	1195	ARG	NE-CZ-NH2	6.81	125.33	119.20
5	H	1215	TYR	N-CA-C	6.50	121.41	112.90
5	I	1244	TYR	N-CA-C	6.15	119.98	112.23
5	L	18	ASP	CA-CB-CG	5.80	118.40	112.60

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	H	611	TYR	Sidechain
5	J	555	ARG	Sidechain

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	5833	0	5848	155	0
1	C	5651	0	5691	131	0
2	B	3993	0	3925	124	0
2	D	3685	0	3611	101	0
3	E	3915	0	3838	85	0
3	F	3986	0	3912	70	0
4	G	3873	0	3792	49	0
5	H	10406	0	10362	139	0
5	I	10693	0	10635	168	0
5	J	10433	0	10379	139	0
5	K	10282	0	10238	124	0
5	L	10693	0	10635	140	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	M	10693	0	10635	151	0
6	N	513	0	539	9	0
6	O	513	0	539	9	0
6	P	513	0	539	11	0
6	Q	513	0	539	11	0
6	R	513	0	539	9	0
6	S	513	0	539	5	0
7	T	1919	0	1957	21	0
7	W	2325	0	2363	25	0
8	U	2317	0	2405	37	0
8	V	2292	0	2379	44	0
8	X	2334	0	2431	28	0
8	Y	2266	0	2355	28	0
9	Z	2320	0	2351	26	0
All	All	112987	0	112976	1709	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

The worst 5 of 1709 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)
5:K:1327:THR:HG21	5:K:1333:MET:HB2	1.58	0.83
5:M:446:LEU:HD21	5:M:1024:THR:HG21	1.61	0.83
1:A:1553:PRO:HB3	2:B:402:ILE:HA	1.62	0.80
5:H:446:LEU:HD11	5:H:1021:VAL:HG23	1.64	0.80
9:Z:57:MET:HE1	9:Z:272:ILE:HD11	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	711/2241 (32%)	685 (96%)	26 (4%)	0	100	100
1	C	681/2241 (30%)	657 (96%)	24 (4%)	0	100	100
2	B	488/983 (50%)	476 (98%)	12 (2%)	0	100	100
2	D	445/983 (45%)	436 (98%)	9 (2%)	0	100	100
3	E	468/642 (73%)	461 (98%)	7 (2%)	0	100	100
3	F	478/642 (74%)	467 (98%)	11 (2%)	0	100	100
4	G	468/594 (79%)	446 (95%)	22 (5%)	0	100	100
5	H	1305/1370 (95%)	1255 (96%)	47 (4%)	3 (0%)	43	74
5	I	1346/1370 (98%)	1291 (96%)	55 (4%)	0	100	100
5	J	1313/1370 (96%)	1245 (95%)	66 (5%)	2 (0%)	43	74
5	K	1292/1370 (94%)	1238 (96%)	53 (4%)	1 (0%)	48	79
5	L	1346/1370 (98%)	1280 (95%)	65 (5%)	1 (0%)	48	79
5	M	1346/1370 (98%)	1284 (95%)	61 (4%)	1 (0%)	48	79
6	N	61/75 (81%)	59 (97%)	2 (3%)	0	100	100
6	O	61/75 (81%)	58 (95%)	3 (5%)	0	100	100
6	P	61/75 (81%)	60 (98%)	1 (2%)	0	100	100
6	Q	61/75 (81%)	59 (97%)	2 (3%)	0	100	100
6	R	61/75 (81%)	61 (100%)	0	0	100	100
6	S	61/75 (81%)	57 (93%)	4 (7%)	0	100	100
7	T	236/290 (81%)	228 (97%)	8 (3%)	0	100	100
7	W	288/290 (99%)	274 (95%)	14 (5%)	0	100	100
8	U	288/306 (94%)	281 (98%)	7 (2%)	0	100	100
8	V	282/306 (92%)	262 (93%)	18 (6%)	2 (1%)	18	51
8	X	291/306 (95%)	281 (97%)	10 (3%)	0	100	100
8	Y	279/306 (91%)	266 (95%)	11 (4%)	2 (1%)	18	51
9	Z	282/1048 (27%)	270 (96%)	12 (4%)	0	100	100
All	All	13999/19848 (70%)	13437 (96%)	550 (4%)	12 (0%)	49	79

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	H	764	GLU
8	Y	297	ASN
5	J	377	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	L	377	LYS
8	V	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%)	647 (100%)	0	100	100
1	C	626/1941 (32%)	626 (100%)	0	100	100
2	B	431/837 (52%)	431 (100%)	0	100	100
2	D	400/837 (48%)	399 (100%)	1 (0%)	86	83
3	E	417/526 (79%)	417 (100%)	0	100	100
3	F	423/526 (80%)	423 (100%)	0	100	100
4	G	398/500 (80%)	398 (100%)	0	100	100
5	H	1144/1192 (96%)	1140 (100%)	4 (0%)	86	83
5	I	1175/1192 (99%)	1174 (100%)	1 (0%)	88	87
5	J	1146/1192 (96%)	1145 (100%)	1 (0%)	88	87
5	K	1131/1192 (95%)	1130 (100%)	1 (0%)	88	87
5	L	1175/1192 (99%)	1175 (100%)	0	100	100
5	M	1175/1192 (99%)	1175 (100%)	0	100	100
6	N	59/68 (87%)	59 (100%)	0	100	100
6	O	59/68 (87%)	59 (100%)	0	100	100
6	P	59/68 (87%)	59 (100%)	0	100	100
6	Q	59/68 (87%)	59 (100%)	0	100	100
6	R	59/68 (87%)	59 (100%)	0	100	100
6	S	59/68 (87%)	59 (100%)	0	100	100
7	T	209/252 (83%)	209 (100%)	0	100	100
7	W	252/252 (100%)	251 (100%)	1 (0%)	84	81
8	U	262/273 (96%)	262 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	V	260/273 (95%)	260 (100%)	0	100	100
8	X	263/273 (96%)	263 (100%)	0	100	100
8	Y	257/273 (94%)	257 (100%)	0	100	100
9	Z	255/883 (29%)	255 (100%)	0	100	100
All	All	12400/17147 (72%)	12391 (100%)	9 (0%)	87	87

5 of 9 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	K	1228	THR
7	W	40	HIS
5	H	1228	THR
5	H	1239	LEU
5	I	861	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 130 such sidechains are listed below:

Mol	Chain	Res	Type
5	M	1133	HIS
8	U	209	ASN
5	H	1264	GLN
5	H	1184	ASN
8	V	147	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

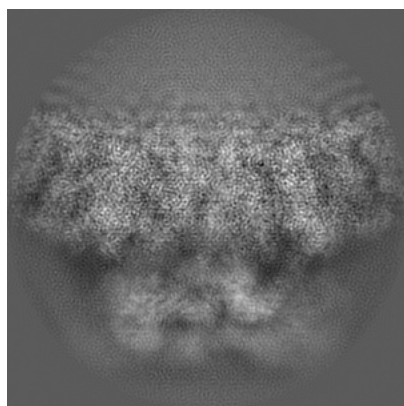
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-41194. These allow visual inspection of the internal detail of the map and identification of artifacts.

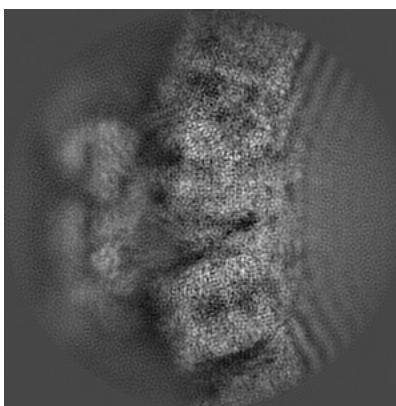
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

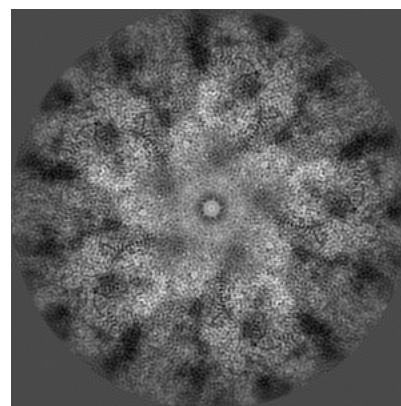
6.1.1 Primary map



X

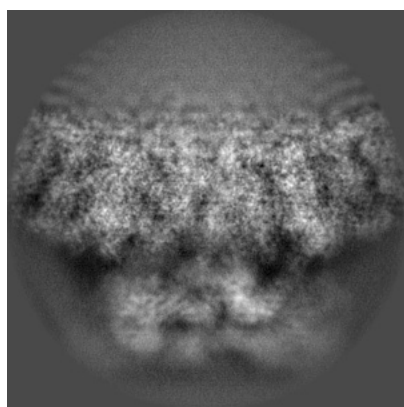


Y

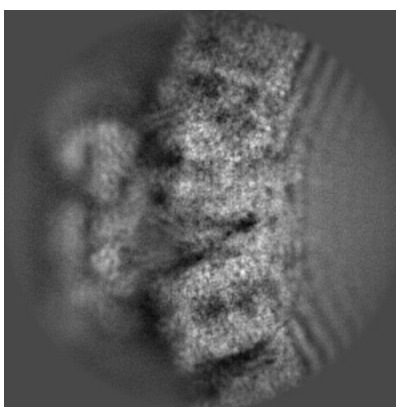


Z

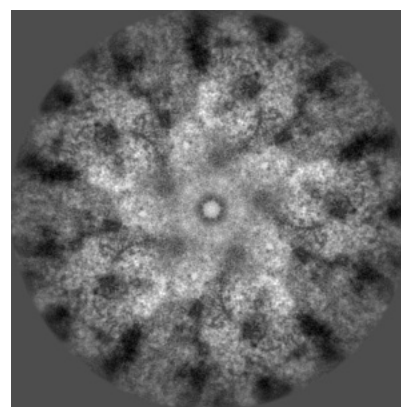
6.1.2 Raw map



X



Y

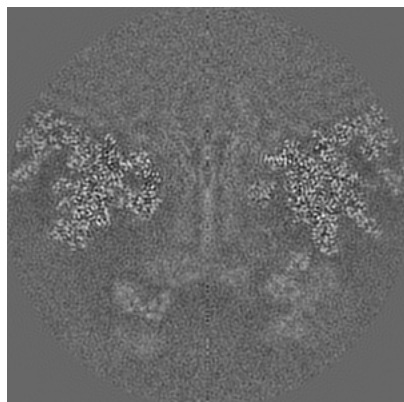


Z

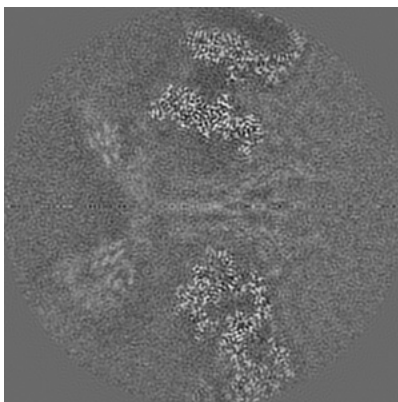
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

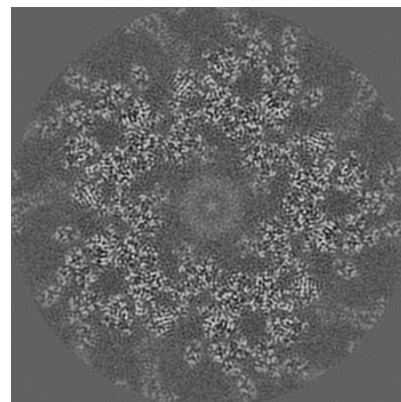
6.2.1 Primary map



X Index: 180

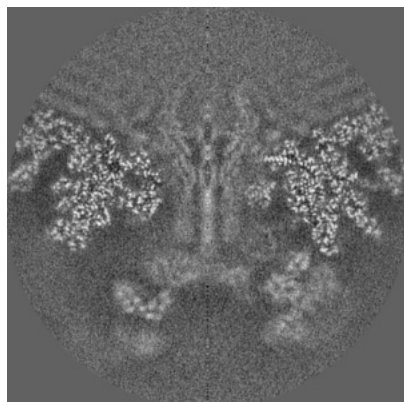


Y Index: 180

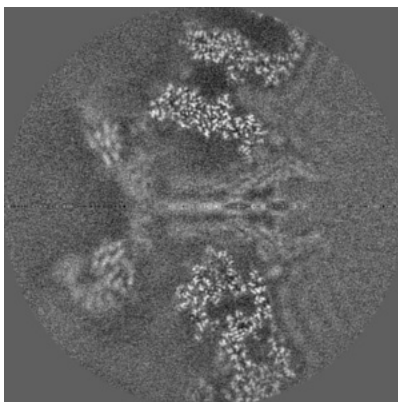


Z Index: 180

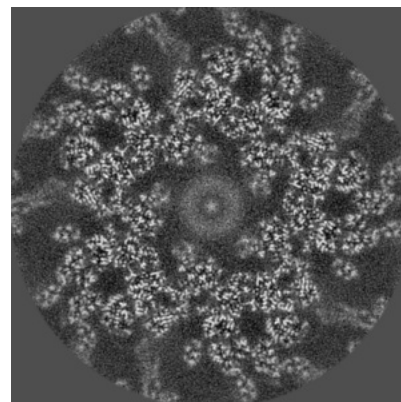
6.2.2 Raw map



X Index: 180



Y Index: 180



Z Index: 180

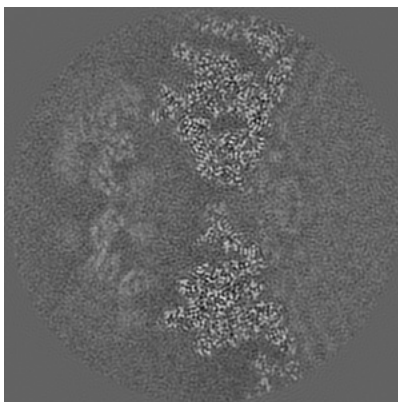
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

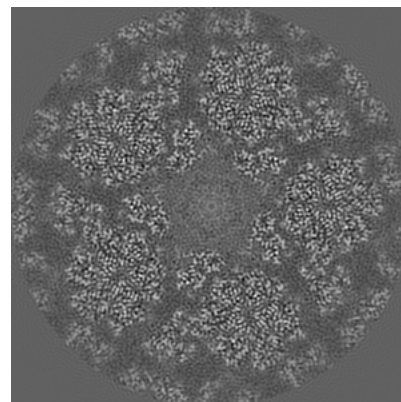
6.3.1 Primary map



X Index: 235

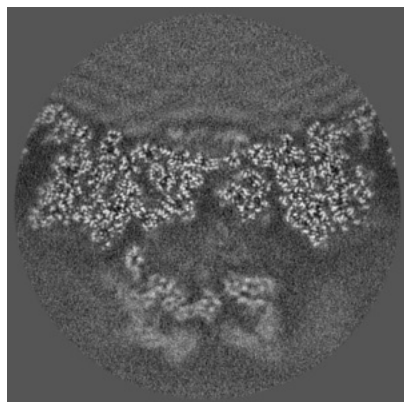


Y Index: 218

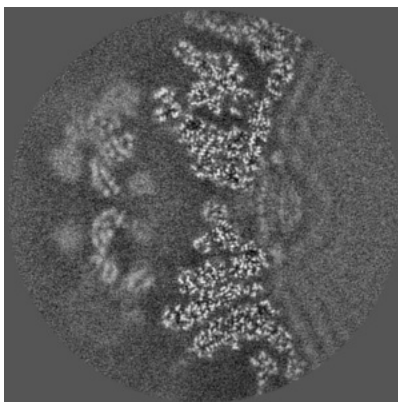


Z Index: 203

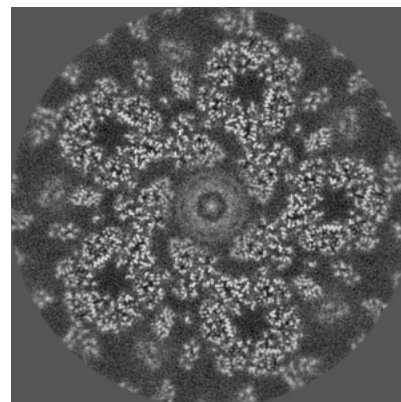
6.3.2 Raw map



X Index: 233



Y Index: 221

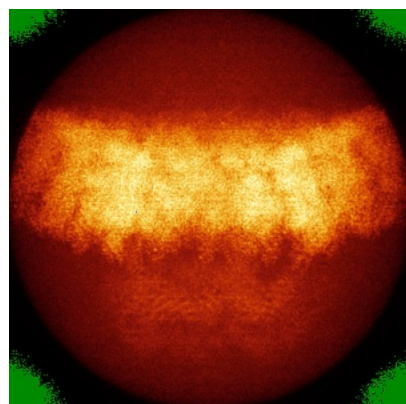


Z Index: 189

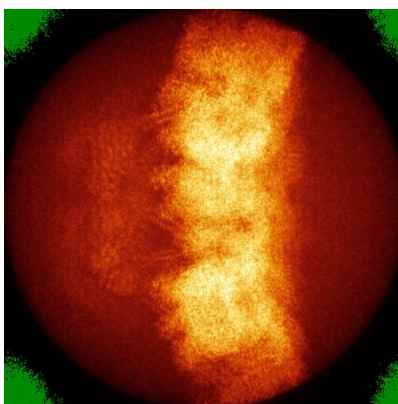
The images above show the largest variance slices of the map in three orthogonal directions.

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

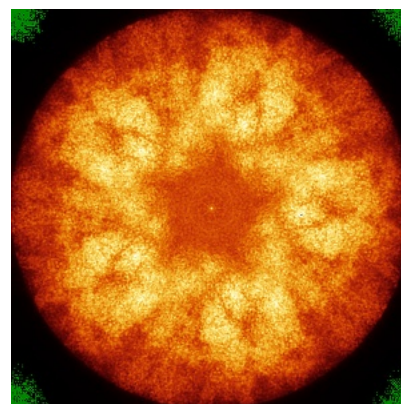
6.4.1 Primary map



X

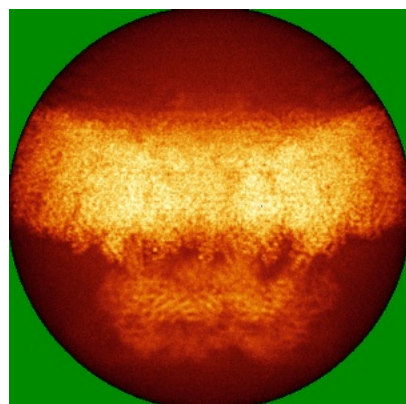


Y

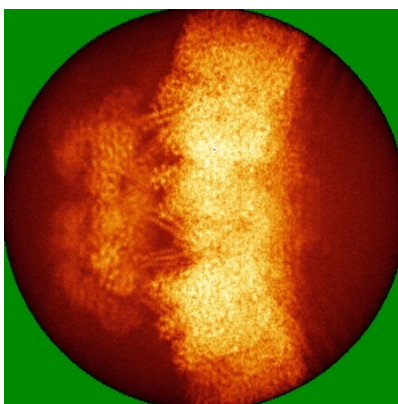


Z

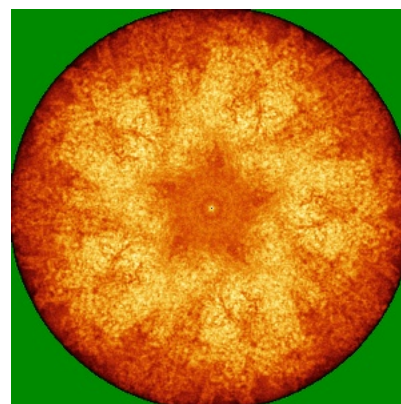
6.4.2 Raw map



X



Y

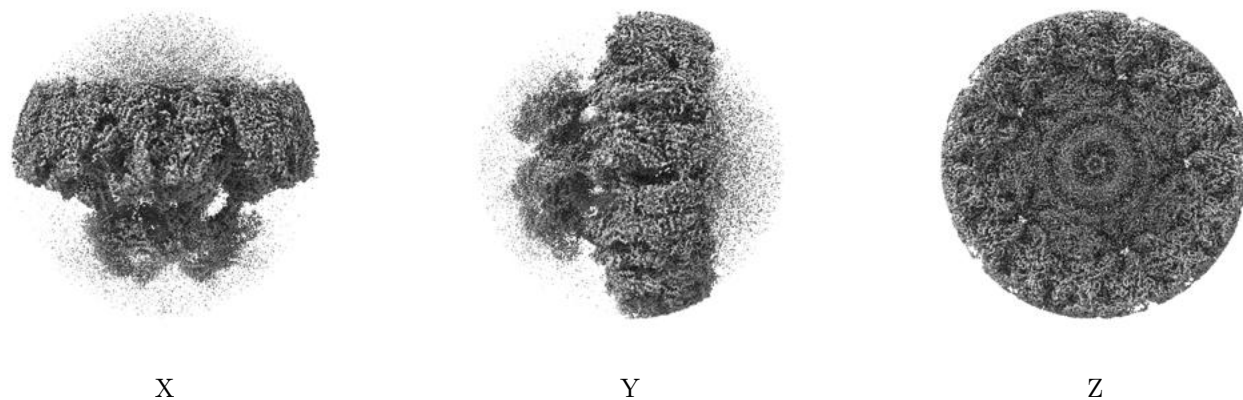


Z

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.

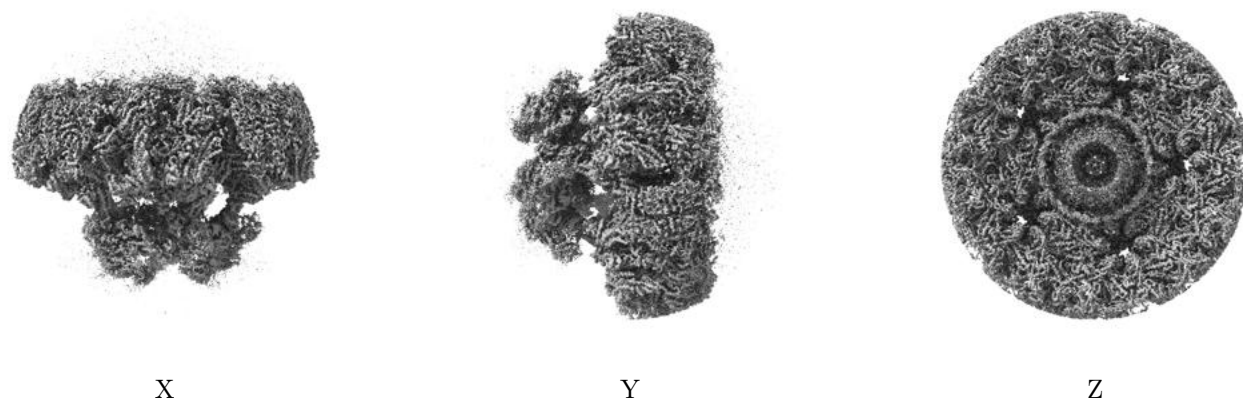
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.005. 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.

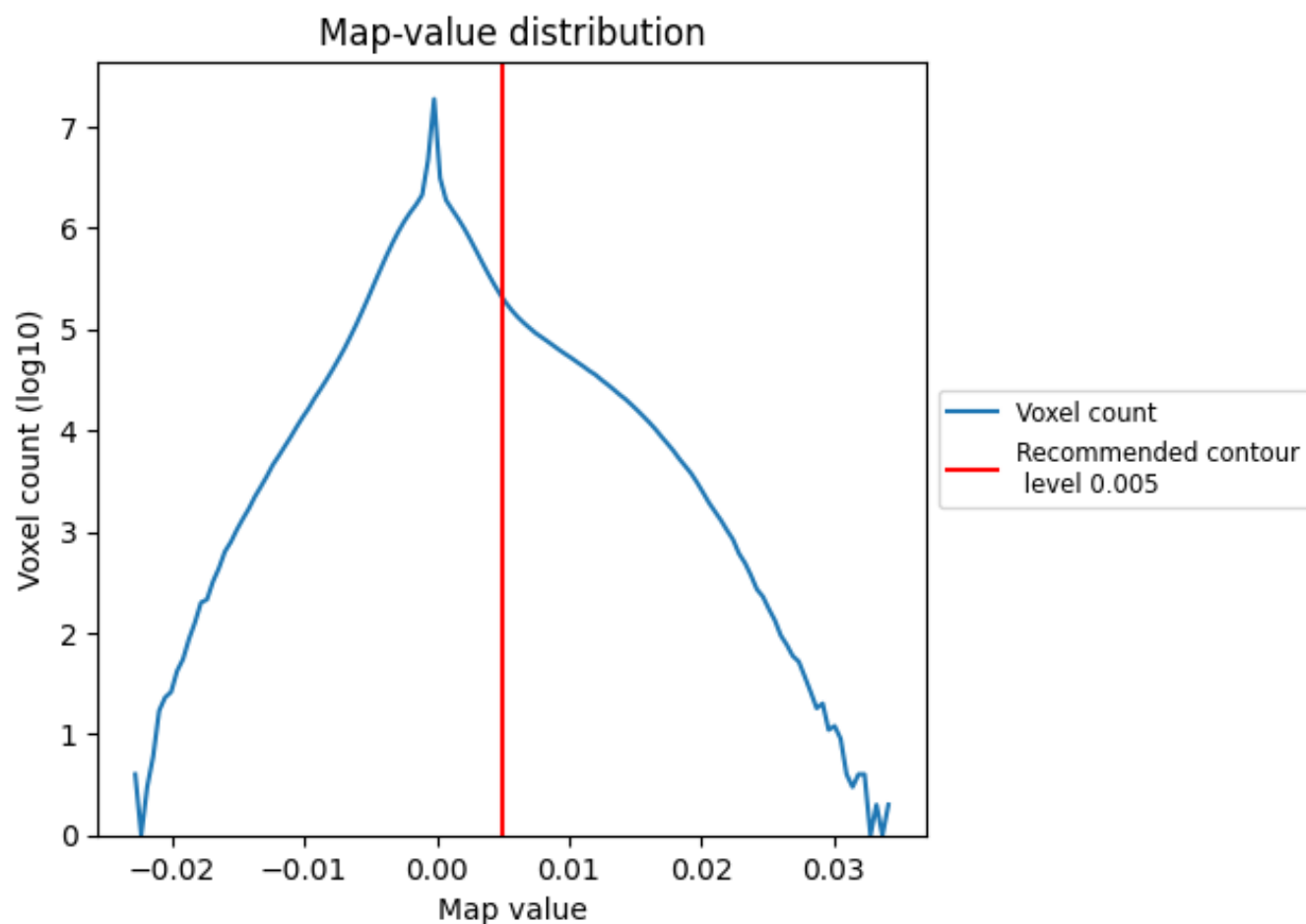
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

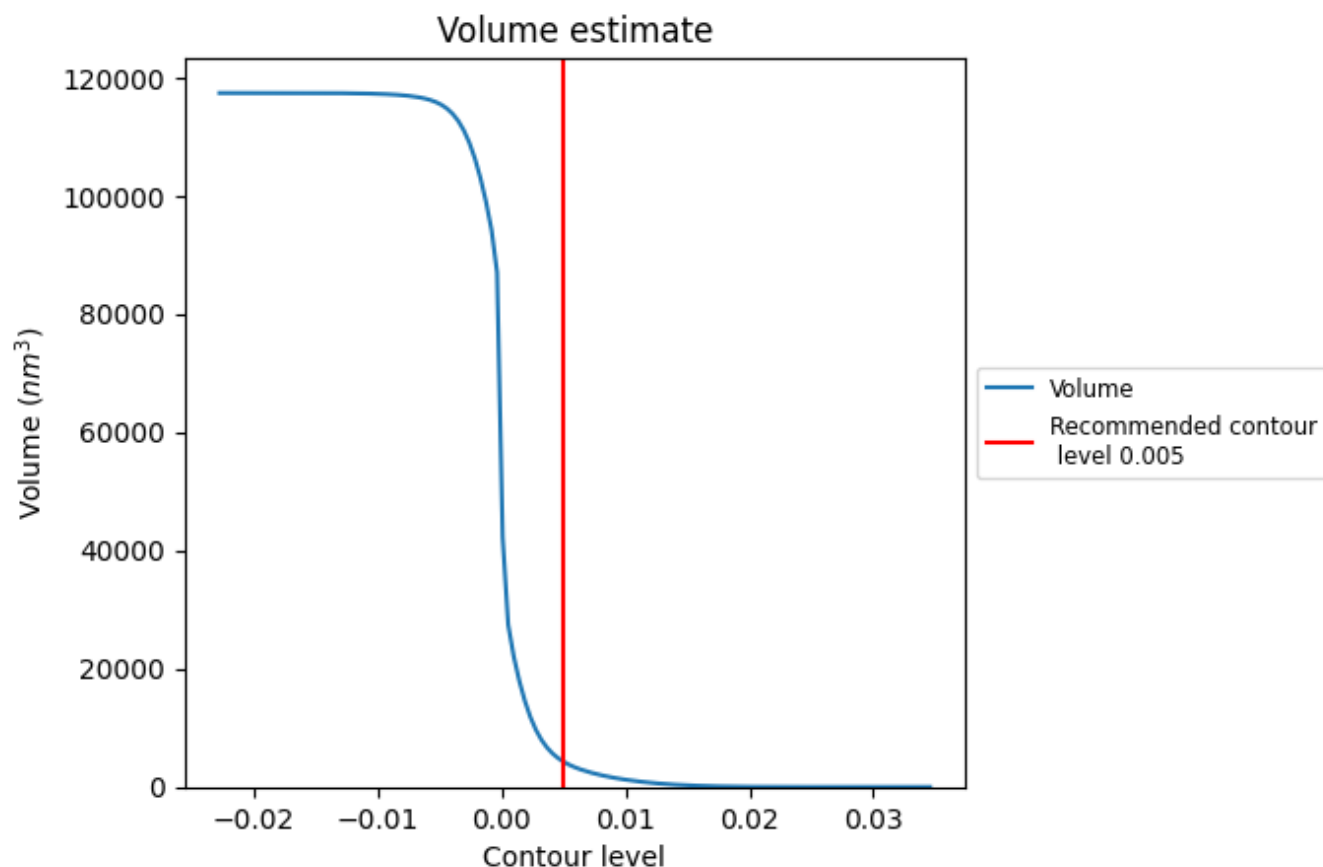
This section contains the results of statistical analysis of the map.

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.

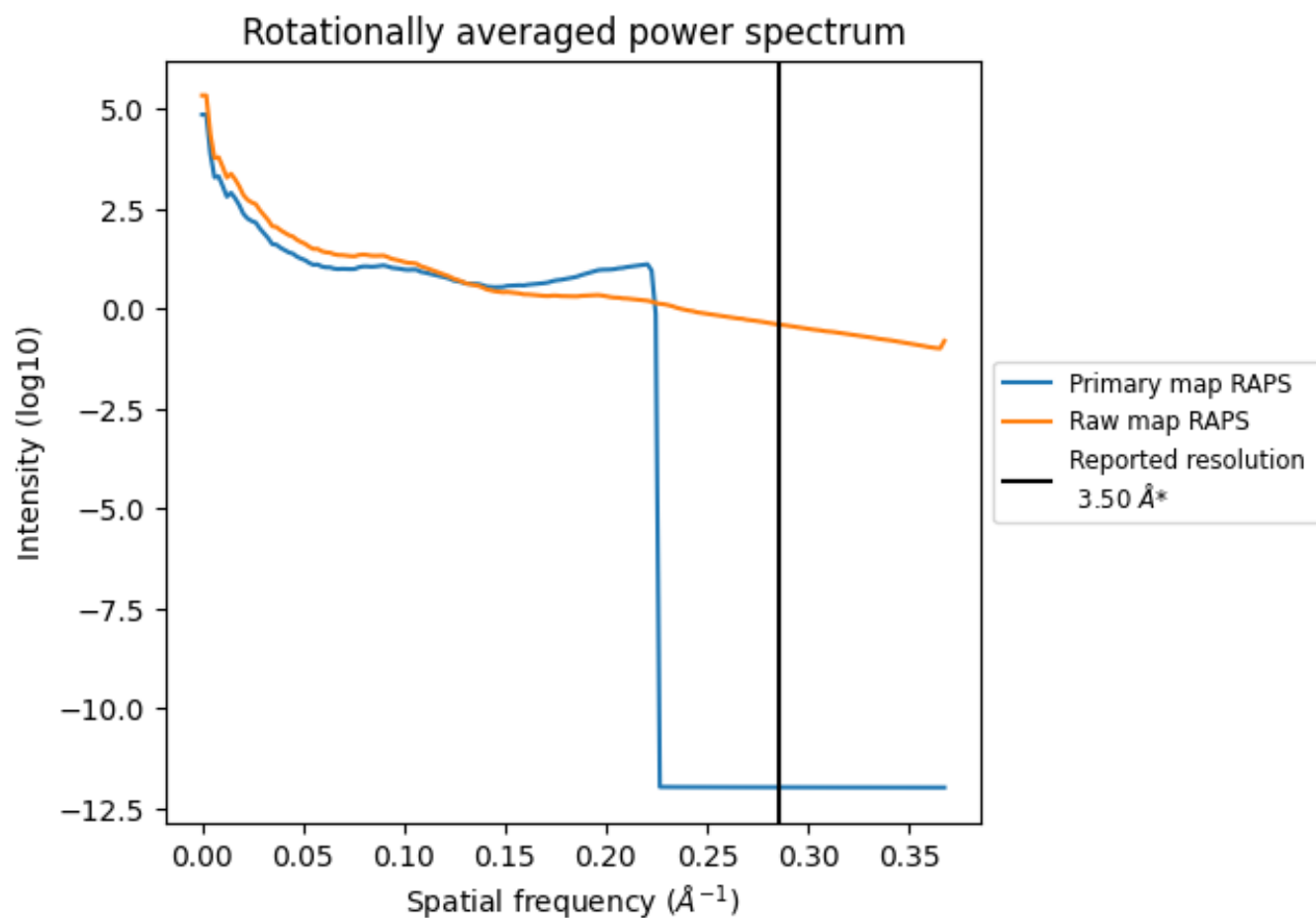
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 4271 nm³; this corresponds to an approximate mass of 3858 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 ⓘ

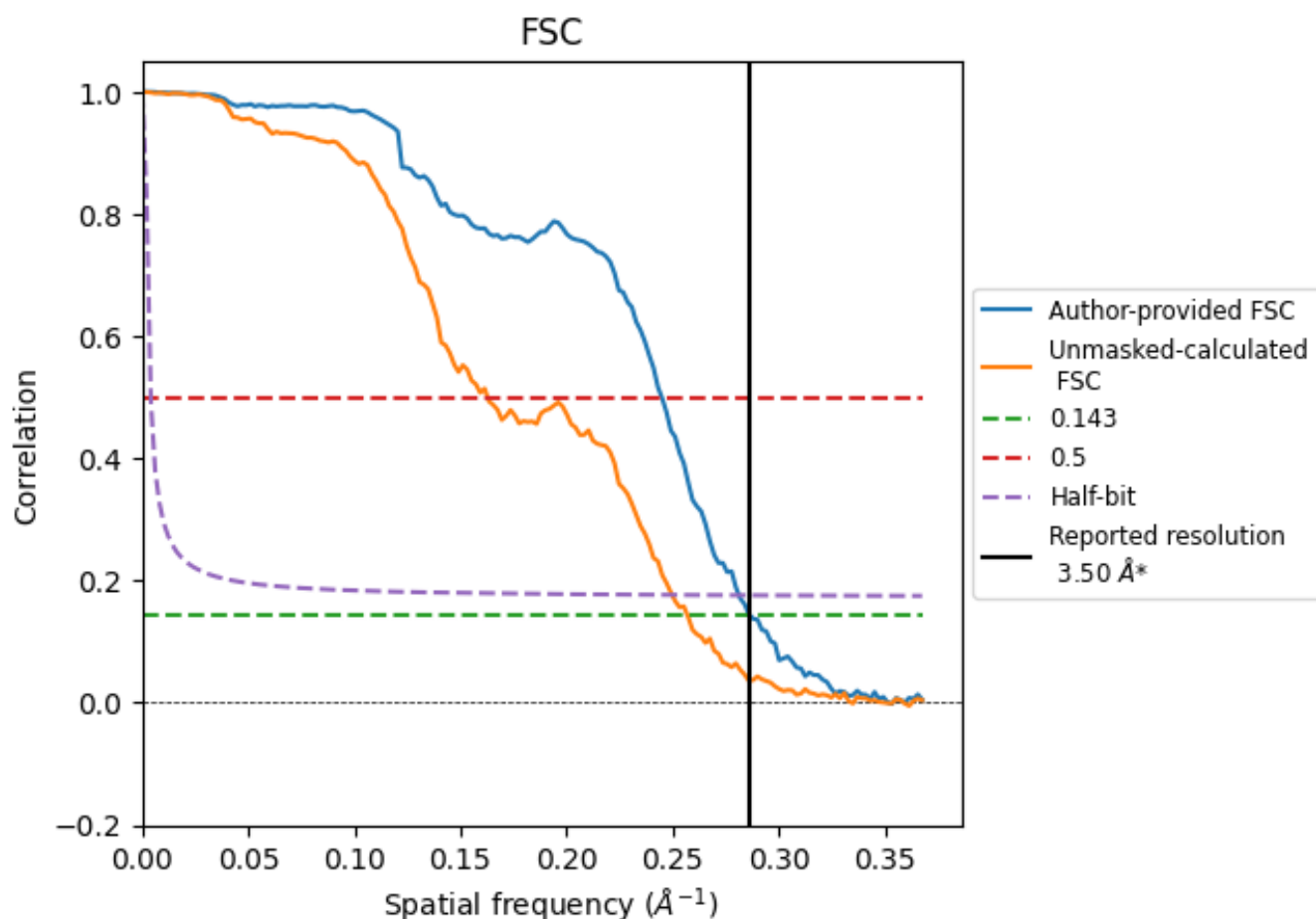


*Reported resolution corresponds to spatial frequency of 0.286 $\text{\AA}^{-1}$

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 0.286 Å⁻¹

8.2 Resolution estimates [i](#)

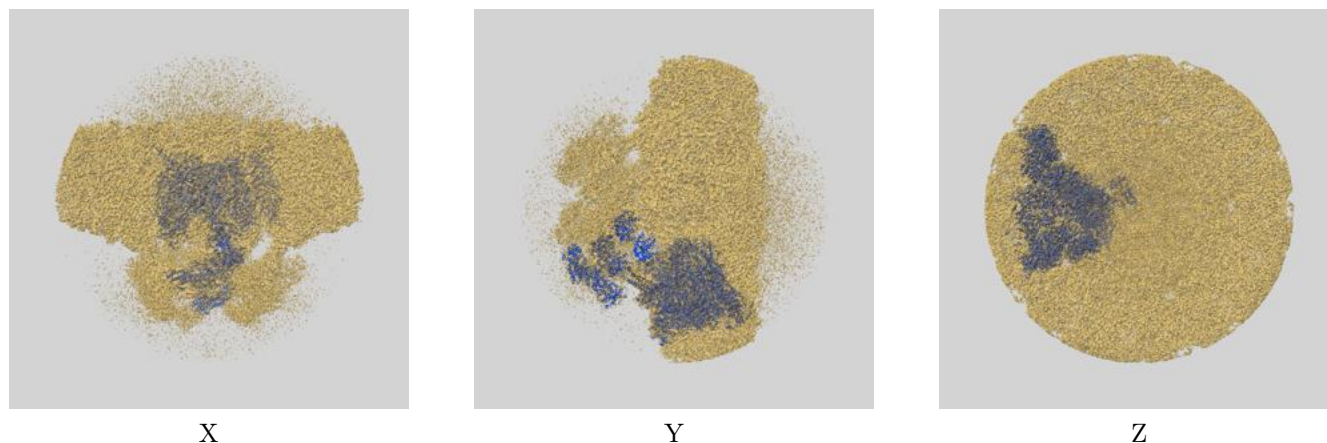
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	3.49	4.08	3.55
Unmasked-calculated*	3.89	6.15	4.00

*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 3.89 differs from the reported value 3.5 by more than 10 %

9 Map-model fit [i](#)

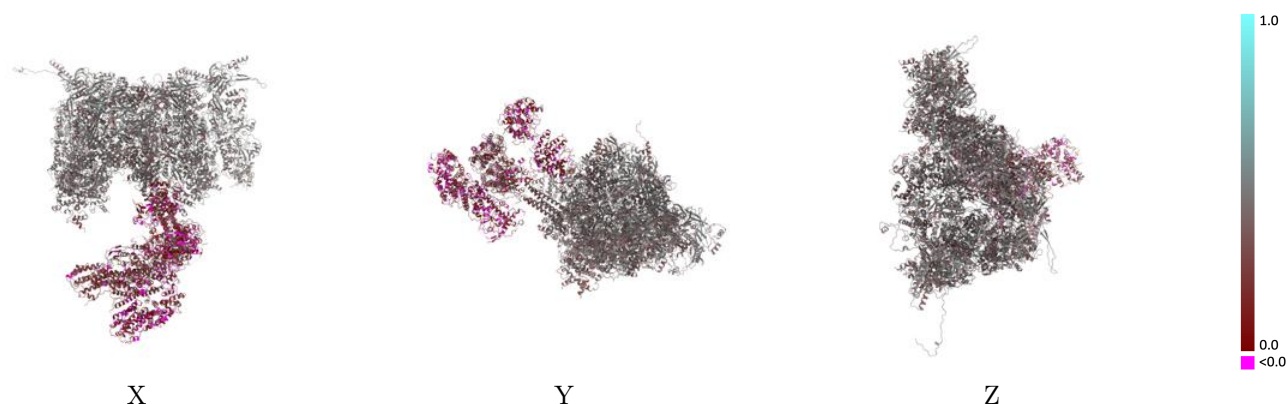
This section contains information regarding the fit between EMDB map EMD-41194 and PDB model 8TEP. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



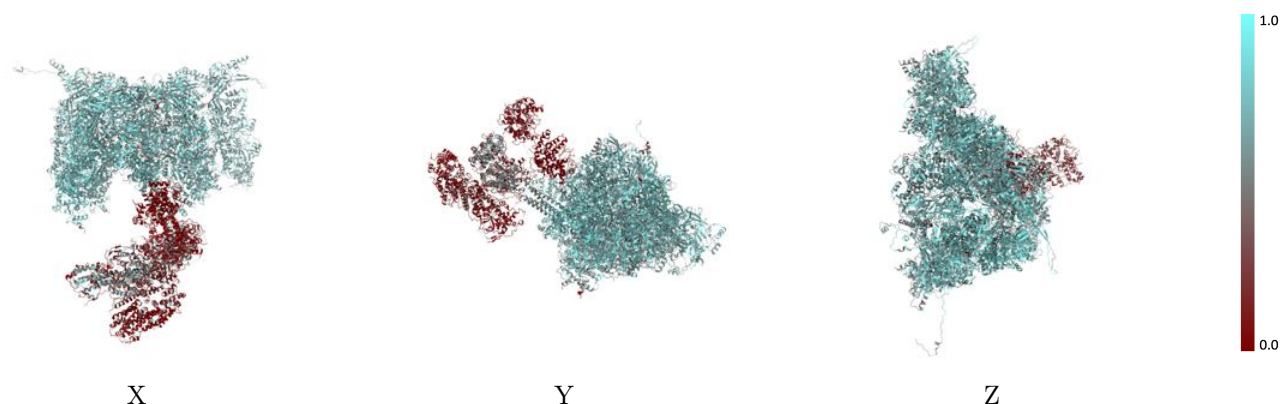
The images above show the 3D surface view of the map at the recommended contour level 0.005 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



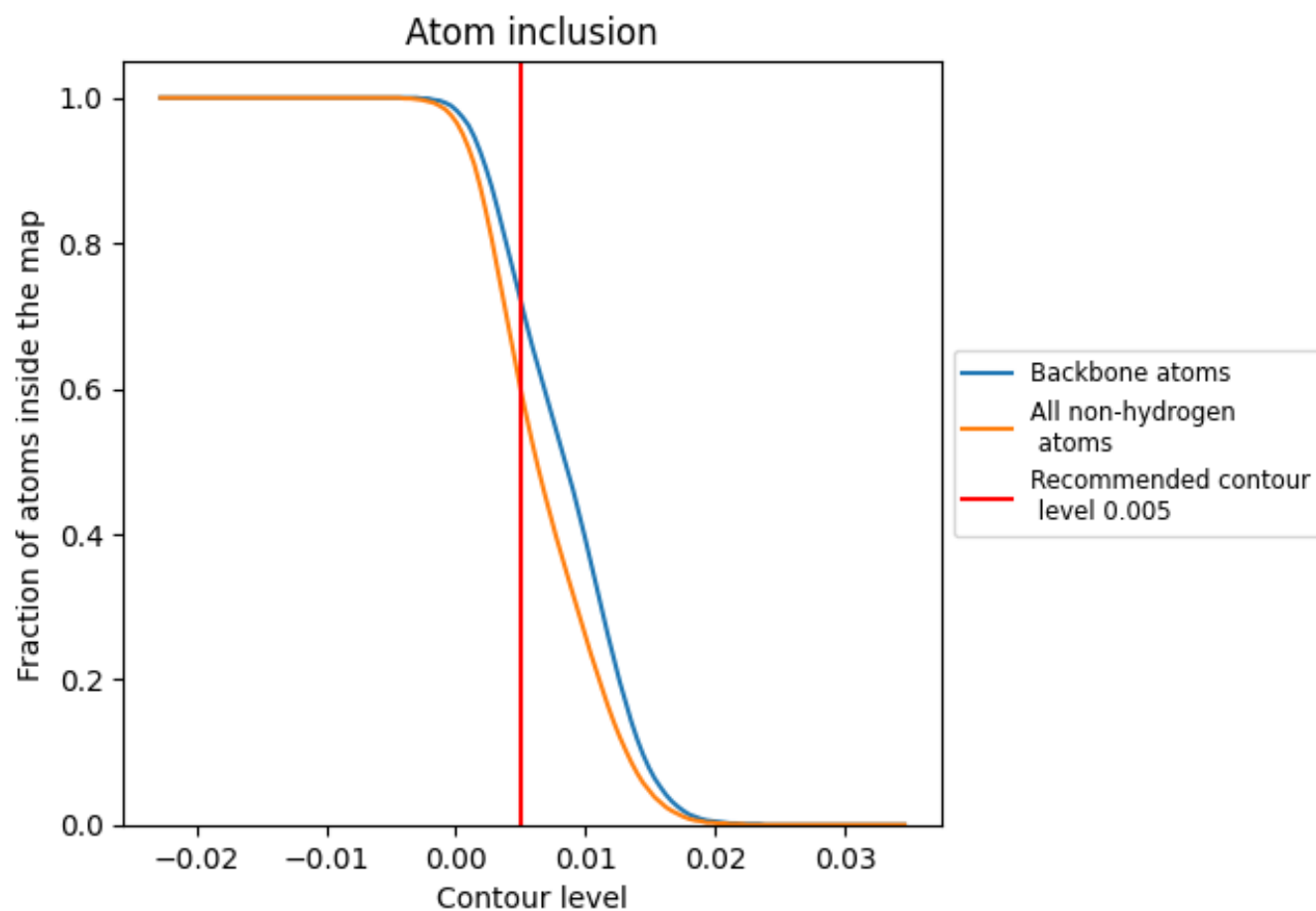
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.005).

9.4 Atom inclusion [i](#)



At the recommended contour level, 72% of all backbone atoms, 60% 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 (0.005) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5980	 0.3740
A	 0.3660	 0.2590
B	 0.3970	 0.2380
C	 0.1390	 0.1570
D	 0.1140	 0.1200
E	 0.2180	 0.2180
F	 0.1150	 0.1960
G	 0.7370	 0.4310
H	 0.7570	 0.4380
I	 0.7440	 0.4340
J	 0.6960	 0.4280
K	 0.7470	 0.4340
L	 0.7190	 0.4320
M	 0.6800	 0.4260
N	 0.6930	 0.3750
O	 0.7210	 0.4110
P	 0.5840	 0.3640
Q	 0.6730	 0.3730
R	 0.5940	 0.3800
S	 0.5120	 0.3750
T	 0.6480	 0.4150
U	 0.7190	 0.4300
V	 0.7250	 0.4310
W	 0.7210	 0.4410
X	 0.6620	 0.4320
Y	 0.6510	 0.4240
Z	 0.6320	 0.4060

