



## wwPDB EM Validation Summary Report ⓘ

Nov 12, 2022 – 12:23 PM EST

PDB ID : 6PPD  
EMDB ID : EMD-20433  
Title : Kaposi's sarcoma-associated herpesvirus (KSHV), C1 penton vertex register, CATC-absent structure  
Authors : Gong, D.; Dai, X.; Jih, J.; Liu, Y.T.; Bi, G.Q.; Sun, R.; Zhou, Z.H.  
Deposited on : 2019-07-06  
Resolution : 3.70 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

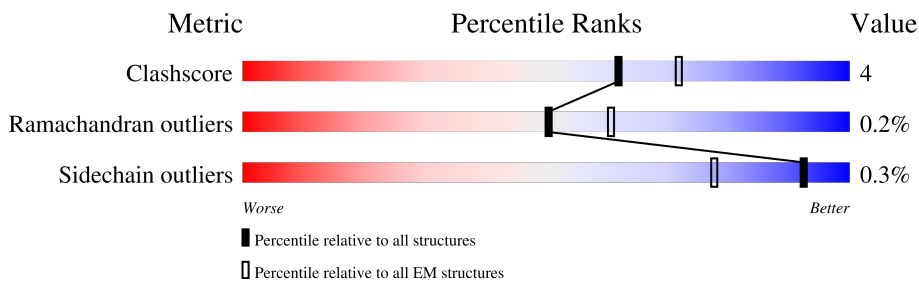
EMDB validation analysis : 0.0.1.dev43  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 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 3.70 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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	0	170	
1	1	170	
1	2	170	
1	3	170	
1	A	170	
2	4	1376	
2	S	1376	
2	T	1376	

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Mol	Chain	Length	Quality of chain
2	W	1376	 15% 84% 14% .
2	X	1376	 6% 85% 13% .
3	5	331	 18% 86% 9% 5%
3	b	331	 16% 96% . .
4	6	305	 23% 84% 13% .
4	7	305	 46% 87% 8% . 5%
4	c	305	 29% 96% .
4	d	305	 34% 98% .

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 68769 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 Small capsomere-interacting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	0	78	Total 666	C 418	N 130	O 115	S 3	0	0
1	2	78	Total 666	C 418	N 130	O 115	S 3	0	0
1	3	78	Total 666	C 418	N 130	O 115	S 3	0	0
1	A	44	Total 380	C 244	N 72	O 62	S 2	0	0
1	1	78	Total 666	C 418	N 130	O 115	S 3	0	0

- Molecule 2 is a protein called Major capsid protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	W	1354	Total 10622	C 6748	N 1842	O 1960	S 72	0	0
2	S	1281	Total 10061	C 6401	N 1739	O 1852	S 69	0	0
2	T	1360	Total 10667	C 6776	N 1851	O 1967	S 73	0	0
2	4	1222	Total 9634	C 6133	N 1673	O 1757	S 71	0	0
2	X	1341	Total 10519	C 6685	N 1824	O 1939	S 71	0	0

- Molecule 3 is a protein called Triplex capsid protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	5	314	Total 2425	C 1554	N 416	O 441	S 14	0	0
3	b	321	Total 2478	C 1586	N 424	O 453	S 15	0	0

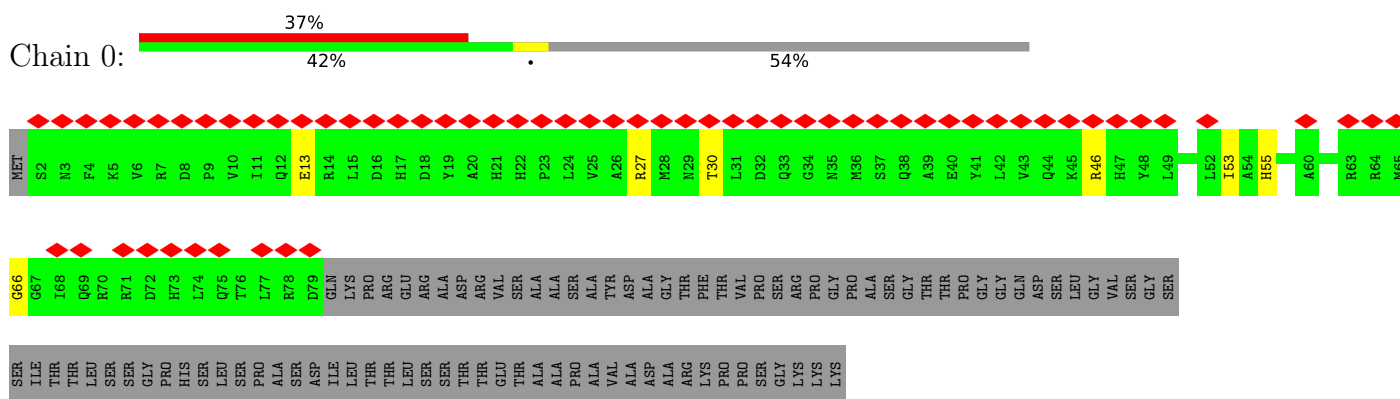
- Molecule 4 is a protein called Triplex capsid protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	6	294	Total 2330	1485	397	434	14	0	0
4	7	291	Total 2294	1465	388	426	15	0	0
4	c	294	Total 2330	1485	397	434	14	0	0
4	d	300	Total 2365	1505	401	444	15	0	0

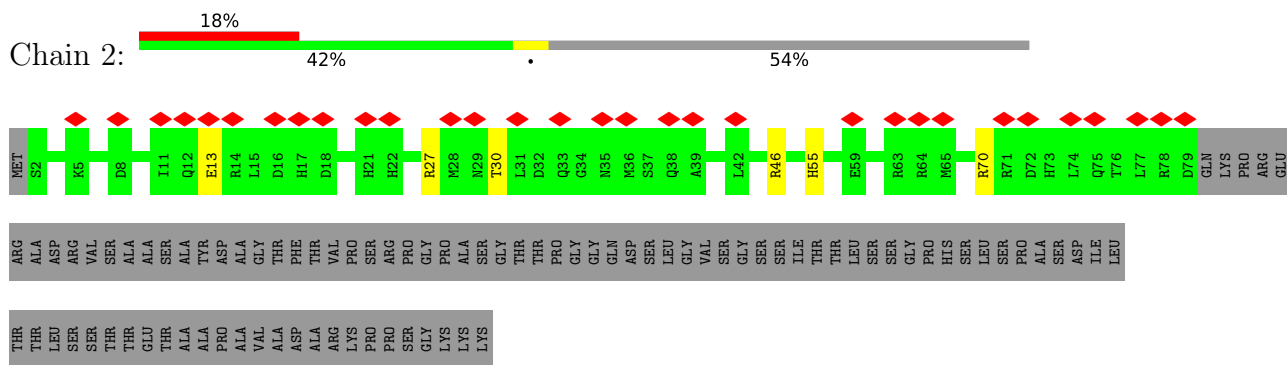
### 3 Residue-property plots i

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.

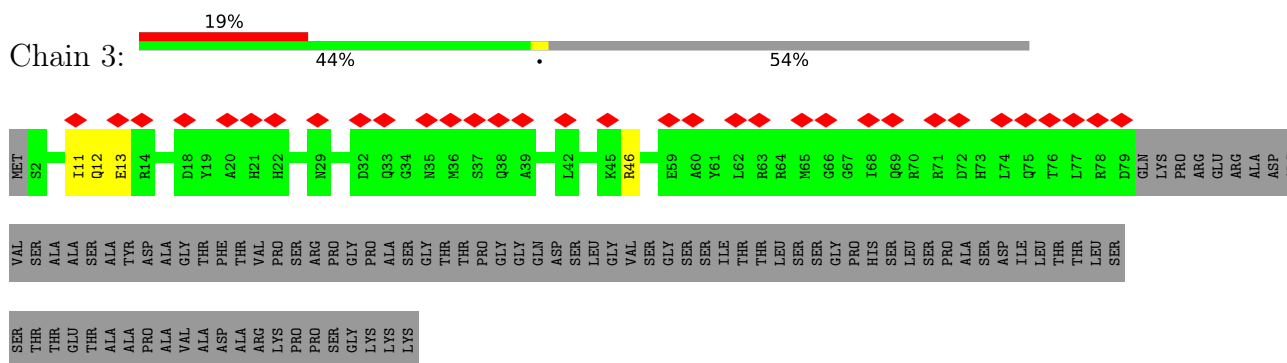
- Molecule 1: Small capsomere-interacting protein



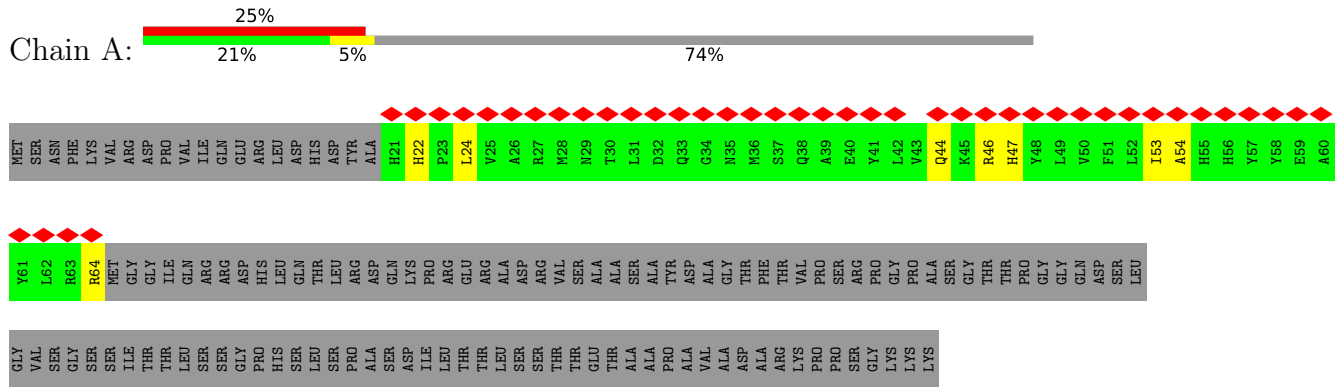
- Molecule 1: Small capsomere-interacting protein



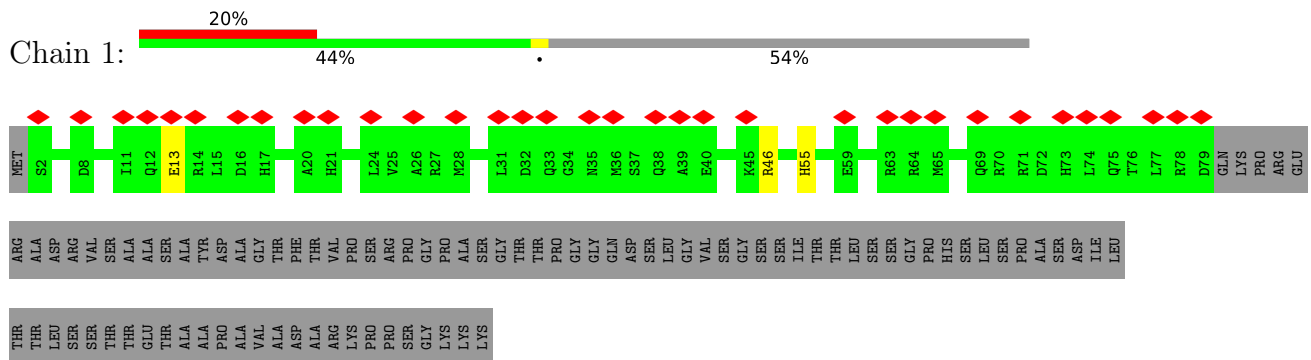
- Molecule 1: Small capsomere-interacting protein



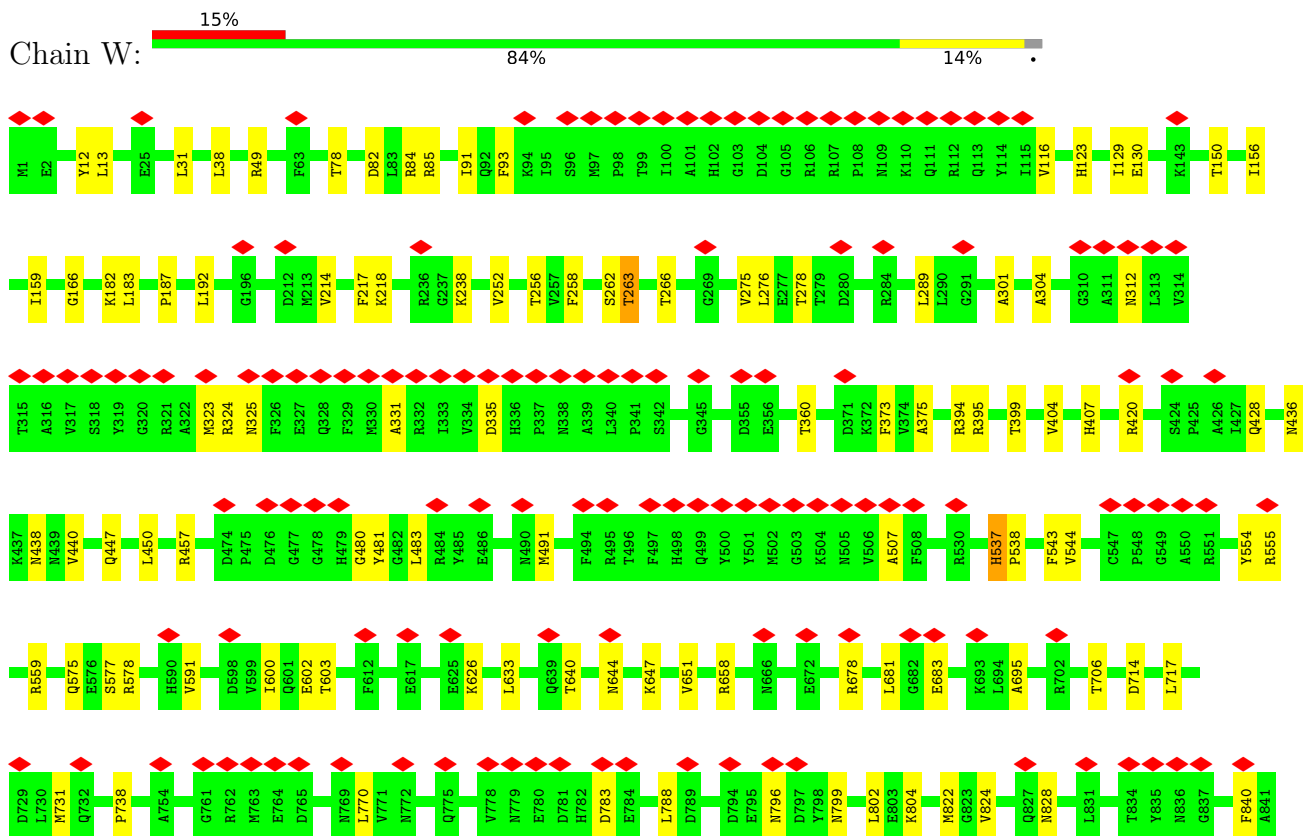
• Molecule 1: Small capsomere-interacting protein

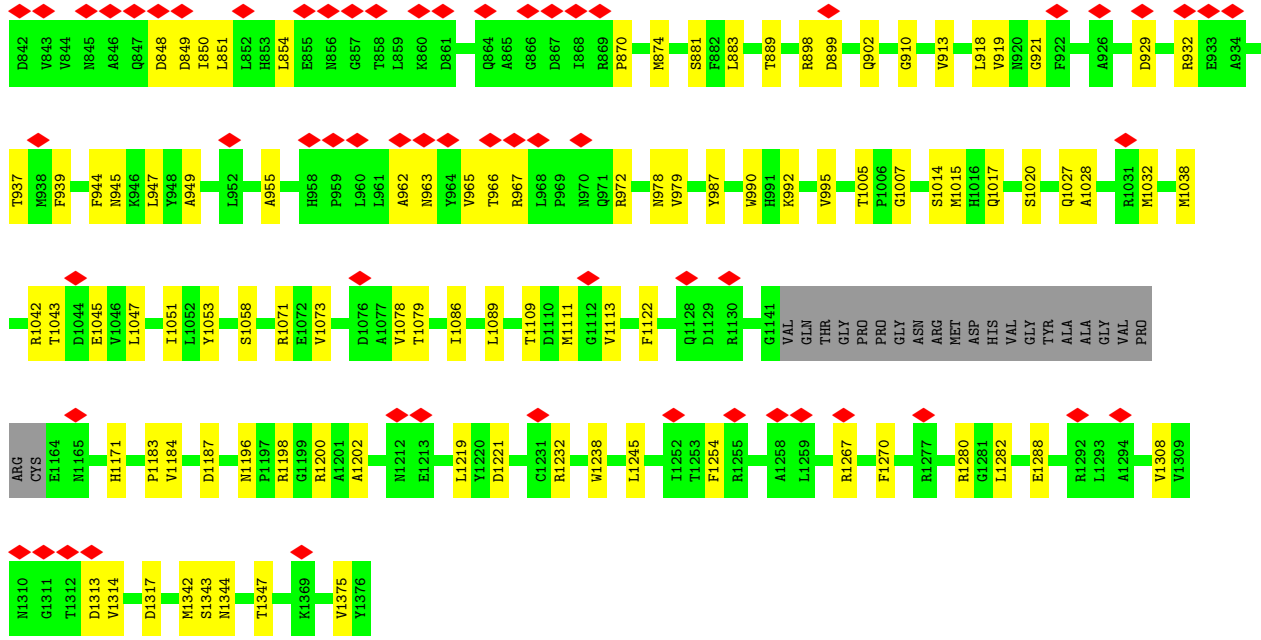


• Molecule 1: Small capsomere-interacting protein

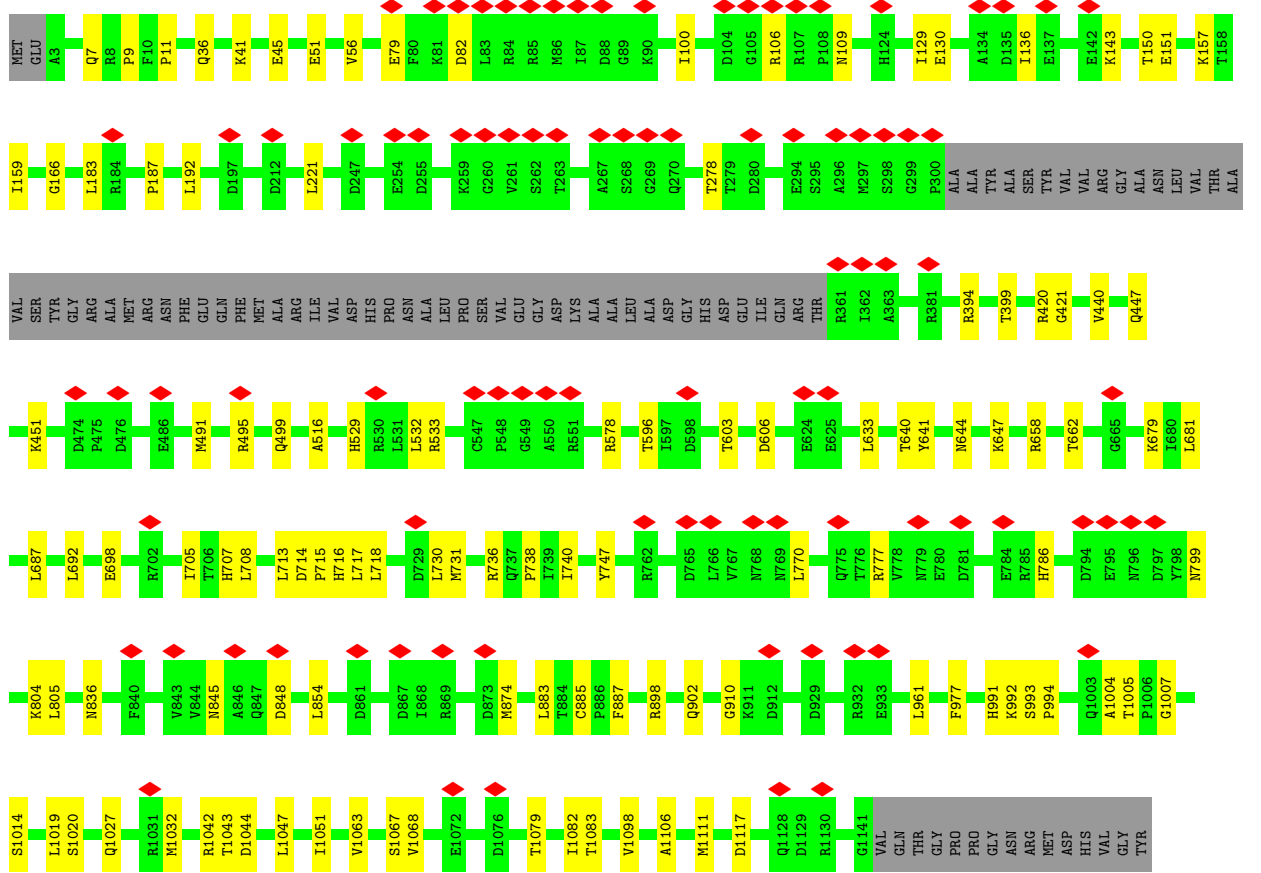
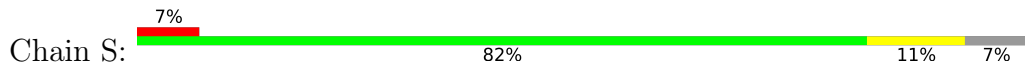


• Molecule 2: Major capsid protein

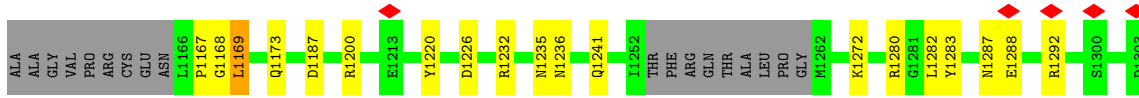




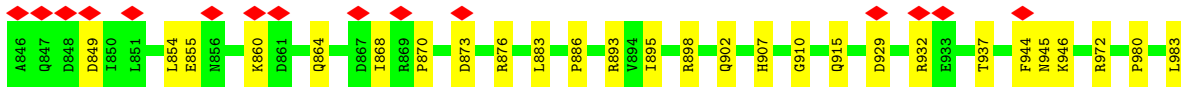
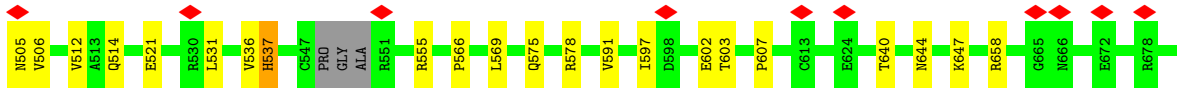
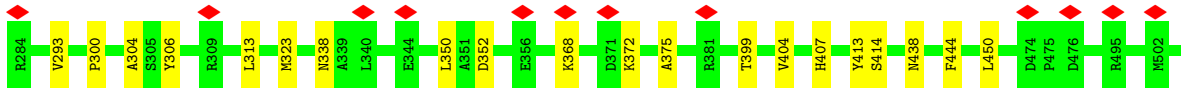
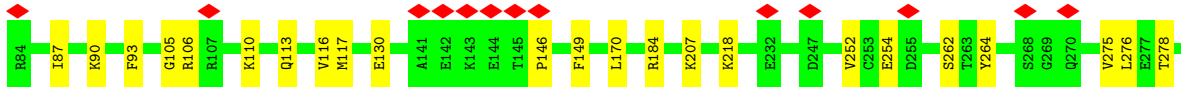
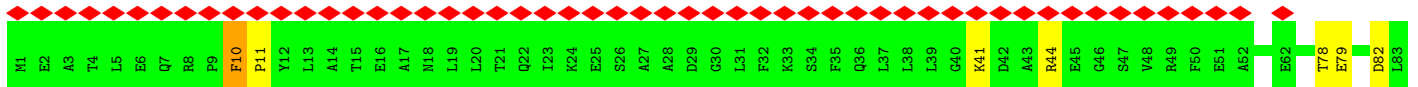
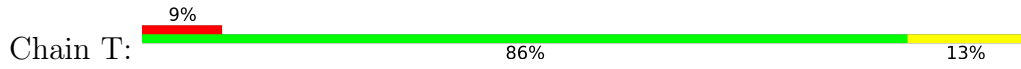
• Molecule 2: Major capsid protein



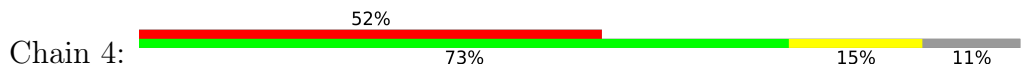




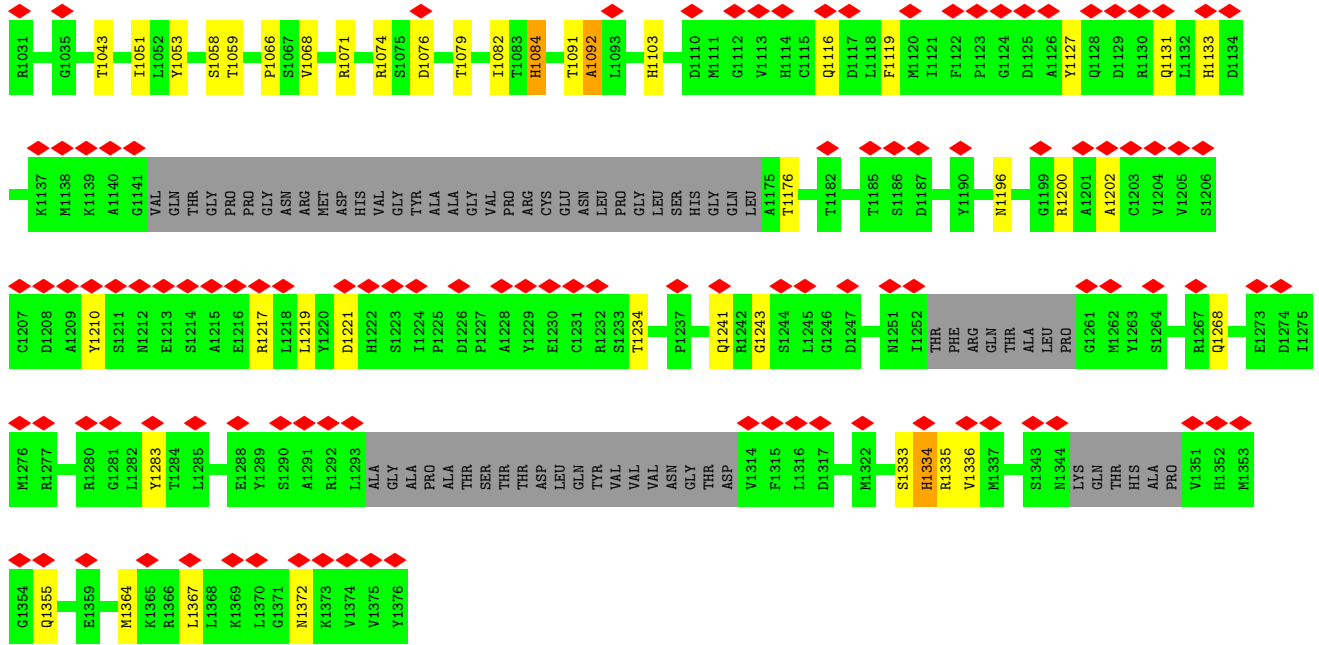
• Molecule 2: Major capsid protein



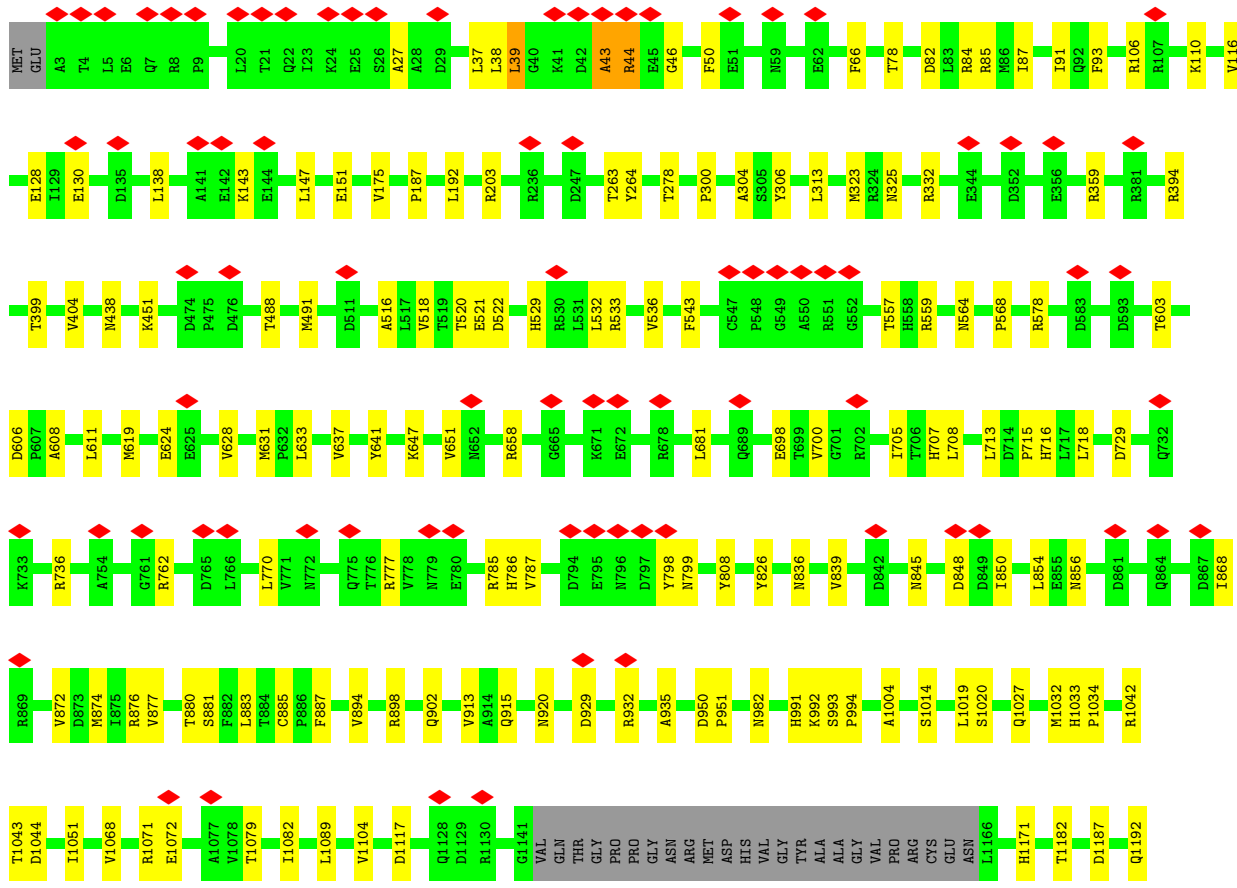
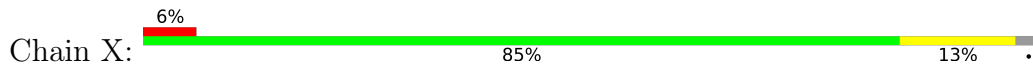
• Molecule 2: Major capsid protein

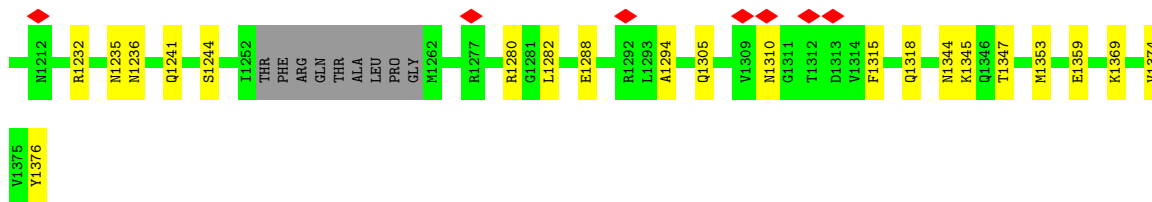


MET	GLU	ALA	THR	LEU	GLY	GLN	ARG	PRO	PHE	PRO	TYR	LEU	ALA	THR	GLU	ALA	ASN	ASP	LEU	LEU	THR	THR	ILE	LYS	GLY	GLU	SER	ALA	ALA	ASP	ASP	GLY	PHE	PHE	LYS	SER	PHE	GLN	LEU	LEU	LEU	LEU	GLY	ASP	LYS	ASP	ALA	ALA	ARG	GLU	GLY	S47	V48	E52	A70	E79	D82	L83	R84	R85	M86																																																																																																																																																																																																																																																																																																																																																																																																																																																																
I87	D88	G89	K90	H102	G103	D104	G105	R106	R107	P108	N109	K110	Q111	R112	Q113	Y114	H124	E128	I129	E130	A134	D135	I136	E137	F140	A141	E142	K143	E144	D148	E151	L163	K182	L183	G196	D197	S201	E202	R203	G204	K206	K207	A208	V209	K210	S211	D212	M213	V214	K218	F226	F227	L228	L233	R236	D247	C253	GLU	ASP	THR	VAL	PHE	LYS	GLY	VAL	SER	T263	S268	G269	V275	Q358	L276	E277	T278	V282	R285	G291	Q292	V293	E294	S295	A296	M297	S298	A301	Y306	R309	G310	A311	N312	L313	V314	T315	K306	A316	R321	R324	E327	R332	D335	L340	P341	SER	GLU	GLY	ASP	VAL	ALA	ALA	LEU	ALA	ALA	ASP	GLY	HIS	ASP	GLU	I357	Q452	R359	T360	R361	K368	D371	K372	V374	A375	I376	E377	R381	R394	T399	L406	H407	L408	P409	VAL	PRO	ARG	TYR	SER	THR	G477	G478	H479	G480	Y481	G482	L483	R484	Y485	E486	Q487	T488	P489	M490	M491	M492	L493	F494	R495	T496	F497	H498	Q499	Y500	Y501	M502	G503	K504	M505	A507	F508	V509	P510	D511	V512	A513	Q514	K515	A516	L517	V518	T519	T520	E521	D522	L523	L524	H525	P526	T527	H529	R530	L531	L532	R533	L534	E535	V536	H537	P538	F543	V544	H545	P546	C547	P548	G549	A550	R551	G552	S553	Y554	R555	R559	T560	M561	M564	F566	Q567	P568	L569	A570	F571	R572	E573	F574	L575	Q576	E577	R578	G579	A580	Q581	F582	D583	A584	V585	T586	N587	H588	T589	H590	V591	I592	D593	Q594	L595	T596	L597	D598	V599	I600	Q601	E602	T603	A604	F605	D606	P607	A608	Y609	P610	L611	F612	C613	Y614	V615	I616	E617	A618	M619	L620	H621	G622	Q623	E624	L625	K626	F627	V628	H629	N630	H631	P632	L633	L634	A635	E636	S637	R638	Q639	T640	Y641	V642	V643	H644	S645	G646	K647	L648	A649	F650	V651	H652	S653	H654	H655	H656	V657	R658	F659	L660	C661	T662	H663	H664	G665	H666	G667	S668	I669	P670	K671	E672	A673	H674	G675	H676	Y677	R678	K679	L680	L681	G682	E683	L684	L685	A686	L687	E688	Q689	A690	L691	L692	K693	L694	A695	A696	G697	H698	E699	H818	H819	C820	G821	M822	G823	H824	D825	L766	V767	N768	V769	L770	V771	N772	L773	Y774	Q775	T776	L777	V778	M779	E780	D781	A841	D842	V843	V844	N845	H846	Q847	D848	D849	I850	L851	L852	H853	L854	E855	N856	G857	T858	L859	K860	D861	L862	L863	Q864	A865	G866	D867	T868	R869	D870	N871	H872	D873	H874	A875	T876	R877	L878	C879	T880	S881	F882	L883	T884	C885	P886	F887	V888	T889	Q890	A891	A892	R893	V894	A895	A896	T896	K897	R898	D899	P900	L960	L961	Q902	S903	F904	A905	T906	H907	E908	Y909	G910	K911	D912	V913	A914	Q915	Y916	F977	N978	V979	P980	S981	N982	L983	L984	A985	E986	Y987	E988	E989	A990	H991	K992	S993	P994	Y995	A996	A997	Y998	A999	A1000	S1001	C1002	Q1003	A1004	T1005	P1006	G1007	A1008	I1009	S1010	A1011	M1012	V1013	S1014	M1015	H1016	Q1017	K1018	L1019	S1020	A1021	P1022	S1023	F1024	I1025	C1026	Q1027	A1028	K1029	H1030

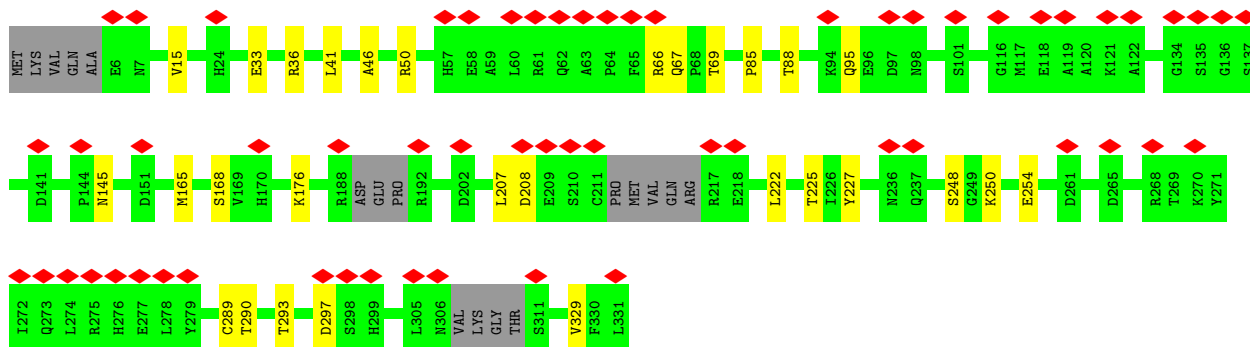
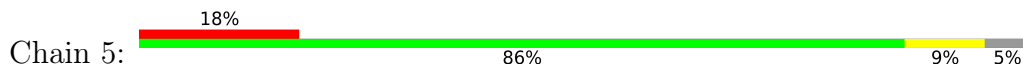


• Molecule 2: Major capsid protein

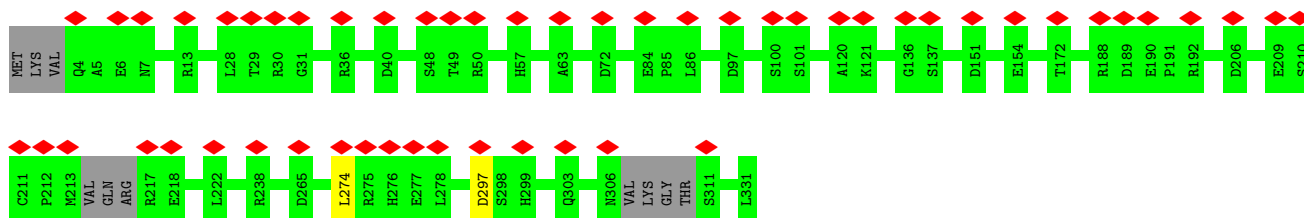




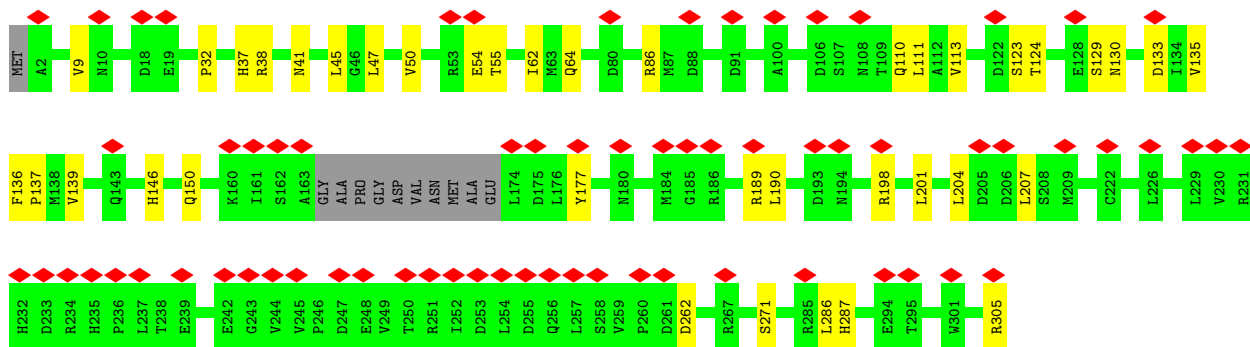
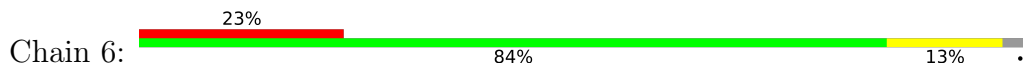
• Molecule 3: Triplex capsid protein 1




• Molecule 3: Triplex capsid protein 1

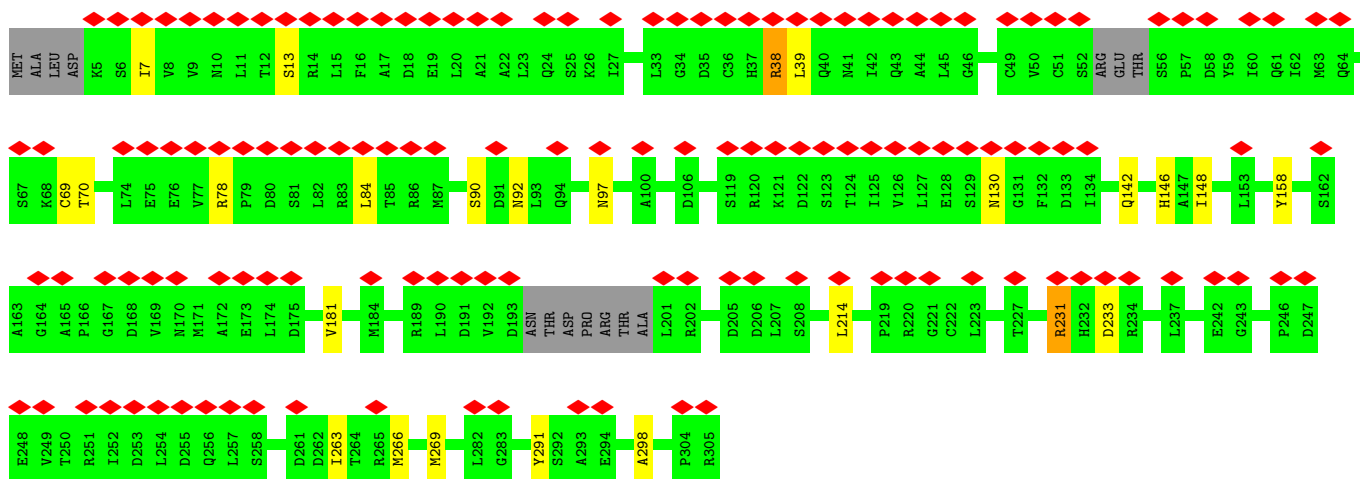


• Molecule 4: Triplex capsid protein 2

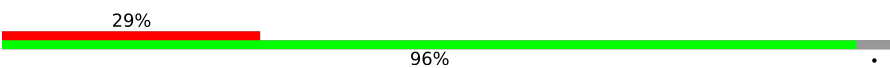


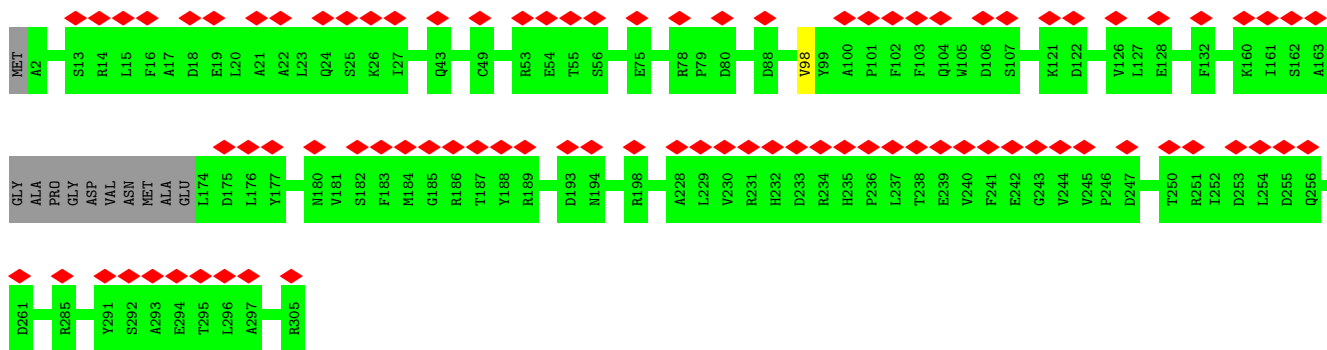
• Molecule 4: Triplex capsid protein 2

Chain 7: 



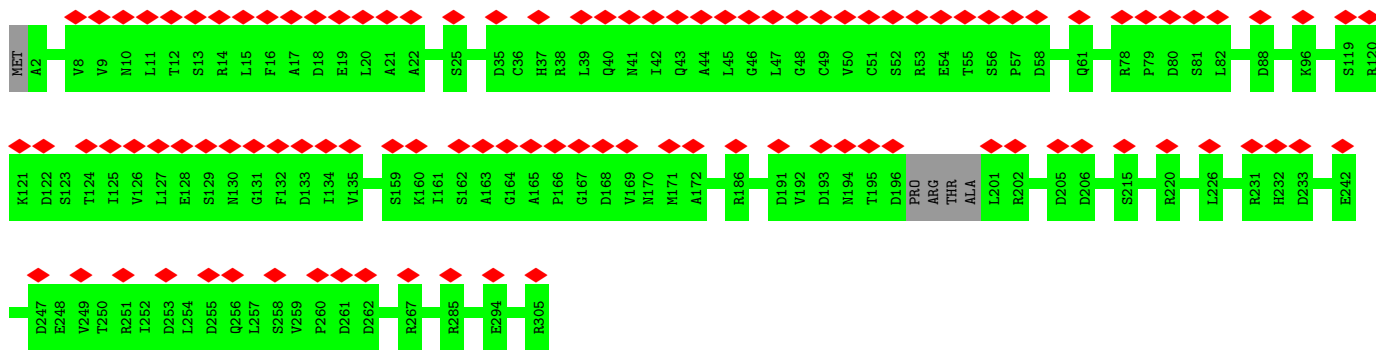
• Molecule 4: Triplex capsid protein 2

Chain c: 



• Molecule 4: Triplex capsid protein 2

Chain d: 



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	1521505	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 ( $e^-/\text{\AA}^2$ )	25	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	24271	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.117	Depositor
Minimum map value	-0.074	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	395.52, 395.52, 395.52	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.03, 1.03, 1.03	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	0	0.29	0/682	0.49	0/919
1	1	0.29	0/682	0.49	0/919
1	2	0.29	0/682	0.49	0/919
1	3	0.29	0/682	0.49	0/919
1	A	0.24	0/391	0.46	0/528
2	4	0.34	0/9861	0.61	4/13391 (0.0%)
2	S	0.39	0/10300	0.62	5/13998 (0.0%)
2	T	0.42	0/10919	0.64	2/14839 (0.0%)
2	W	0.40	0/10874	0.62	2/14780 (0.0%)
2	X	0.39	0/10768	0.61	6/14635 (0.0%)
3	5	0.34	0/2484	0.58	1/3373 (0.0%)
3	b	0.37	0/2540	0.63	2/3452 (0.1%)
4	6	0.35	0/2376	0.63	1/3234 (0.0%)
4	7	0.31	0/2339	0.58	1/3181 (0.0%)
4	c	0.33	0/2376	0.61	0/3234
4	d	0.35	0/2411	0.60	0/3281
All	All	0.38	0/70367	0.61	24/95602 (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
2	4	0	12
2	S	0	1
2	T	0	7
2	W	0	5
2	X	0	2
All	All	0	27

There are no bond length outliers.

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	S	1004	ALA	C-N-CA	9.52	145.49	121.70
2	X	1004	ALA	C-N-CA	8.30	142.46	121.70
3	b	297	ASP	CB-CG-OD1	7.52	125.07	118.30
2	S	708	LEU	CA-CB-CG	7.13	131.69	115.30
2	X	708	LEU	CA-CB-CG	7.11	131.64	115.30

There are no chirality outliers.

5 of 27 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	W	262	SER	Peptide
2	W	263	THR	Mainchain
2	W	537	HIS	Peptide
2	W	848	ASP	Peptide
2	W	849	ASP	Peptide

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	666	0	647	5	0
1	1	666	0	647	2	0
1	2	666	0	647	5	0
1	3	666	0	647	3	0
1	A	380	0	369	6	0
2	4	9634	0	9527	124	0
2	S	10061	0	9955	83	0
2	T	10667	0	10543	101	0
2	W	10622	0	10500	118	0
2	X	10519	0	10398	103	0
3	5	2425	0	2419	20	0
3	b	2478	0	2466	0	0
4	6	2330	0	2354	24	0
4	7	2294	0	2315	15	0
4	c	2330	0	2354	0	0
4	d	2365	0	2379	0	0
All	All	68769	0	68167	546	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 4.

The worst 5 of 546 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:T:536:VAL:HG13	2:T:1244:SER:HA	1.72	0.72
1:2:70:ARG:NH2	1:3:12:GLN:O	2.26	0.68
2:S:770:LEU:HD21	2:S:883:LEU:HD22	1.75	0.67
1:1:55:HIS:HD2	2:X:770:LEU:HD22	1.59	0.67
2:W:799:ASN:HD21	2:W:802:LEU:HD12	1.61	0.66

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	0	76/170 (45%)	74 (97%)	2 (3%)	0	100	100
1	1	76/170 (45%)	74 (97%)	2 (3%)	0	100	100
1	2	76/170 (45%)	74 (97%)	2 (3%)	0	100	100
1	3	76/170 (45%)	74 (97%)	2 (3%)	0	100	100
1	A	42/170 (25%)	42 (100%)	0	0	100	100
2	4	1206/1376 (88%)	1120 (93%)	80 (7%)	6 (0%)	29	66
2	S	1273/1376 (92%)	1188 (93%)	83 (6%)	2 (0%)	47	78
2	T	1354/1376 (98%)	1276 (94%)	74 (6%)	4 (0%)	41	74
2	W	1350/1376 (98%)	1282 (95%)	66 (5%)	2 (0%)	51	83
2	X	1335/1376 (97%)	1246 (93%)	86 (6%)	3 (0%)	47	78
3	5	306/331 (92%)	293 (96%)	13 (4%)	0	100	100
3	b	315/331 (95%)	307 (98%)	8 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	6	290/305 (95%)	273 (94%)	17 (6%)	0	100	100
4	7	285/305 (93%)	268 (94%)	17 (6%)	0	100	100
4	c	290/305 (95%)	277 (96%)	13 (4%)	0	100	100
4	d	296/305 (97%)	292 (99%)	4 (1%)	0	100	100
All	All	8646/9612 (90%)	8160 (94%)	469 (5%)	17 (0%)	50	78

5 of 17 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	W	263	THR
2	4	843	VAL
2	S	992	LYS
2	T	10	PHE
2	X	992	LYS

### 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	0	70/141 (50%)	70 (100%)	0	100	100
1	1	70/141 (50%)	70 (100%)	0	100	100
1	2	70/141 (50%)	70 (100%)	0	100	100
1	3	70/141 (50%)	70 (100%)	0	100	100
1	A	39/141 (28%)	38 (97%)	1 (3%)	46	69
2	4	1044/1166 (90%)	1041 (100%)	3 (0%)	92	96
2	S	1094/1166 (94%)	1088 (100%)	6 (0%)	88	94
2	T	1154/1166 (99%)	1154 (100%)	0	100	100
2	W	1150/1166 (99%)	1149 (100%)	1 (0%)	93	98
2	X	1139/1166 (98%)	1131 (99%)	8 (1%)	84	91
3	5	266/281 (95%)	266 (100%)	0	100	100
3	b	272/281 (97%)	272 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	6	267/274 (97%)	265 (99%)	2 (1%)	84	91
4	7	262/274 (96%)	258 (98%)	4 (2%)	65	81
4	c	267/274 (97%)	266 (100%)	1 (0%)	91	95
4	d	270/274 (98%)	270 (100%)	0	100	100
All	All	7504/8193 (92%)	7478 (100%)	26 (0%)	92	96

5 of 26 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	7	78	ARG
4	c	98	VAL
2	X	1104	VAL
4	7	231	ARG
2	X	106	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 98 such sidechains are listed below:

Mol	Chain	Res	Type
3	5	67	GLN
3	b	124	GLN
4	6	64	GLN
4	6	235	HIS
4	c	130	ASN

### 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 [i](#)

There are no chain breaks in this entry.

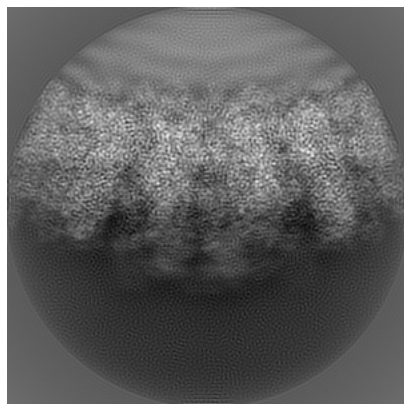
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-20433. These allow visual inspection of the internal detail of the map and identification of artifacts.

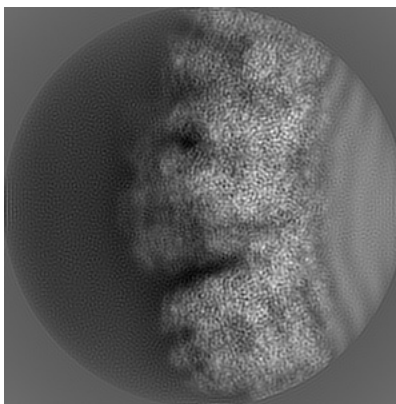
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

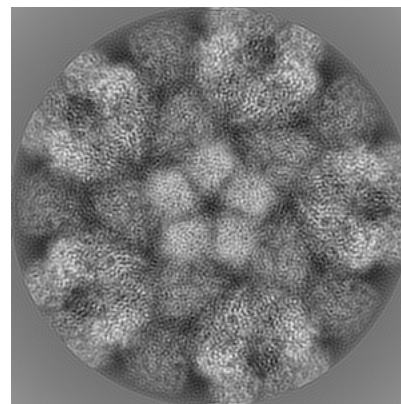
#### 6.1.1 Primary map



X

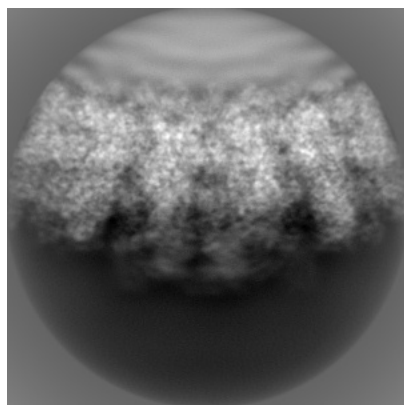


Y

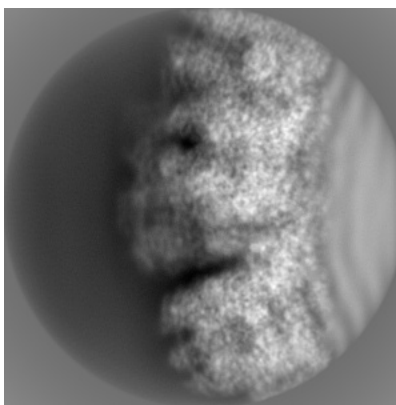


Z

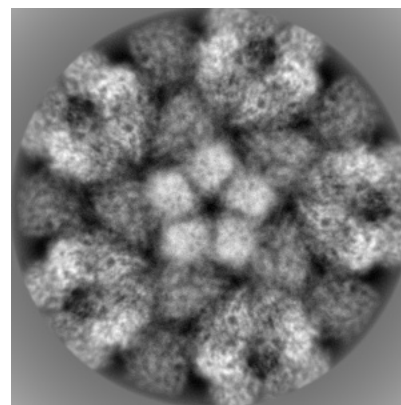
#### 6.1.2 Raw map



X



Y

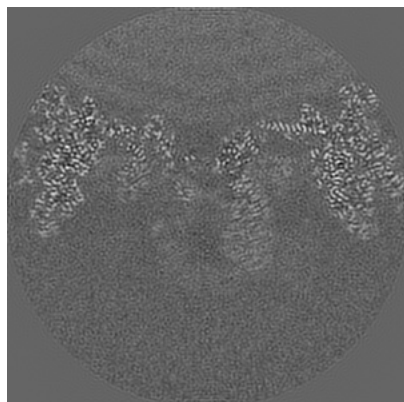


Z

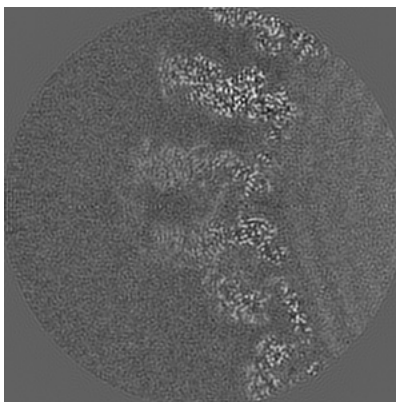
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

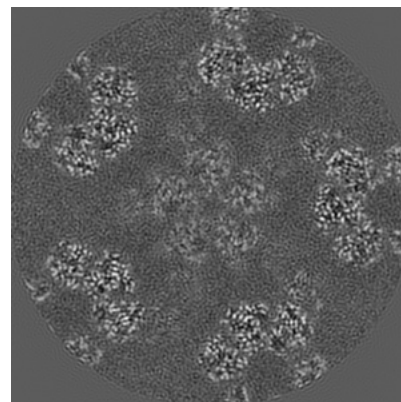
### 6.2.1 Primary map



X Index: 192

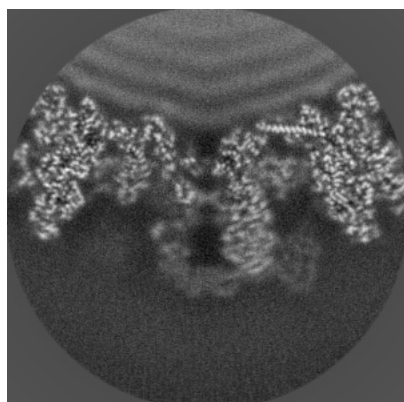


Y Index: 192

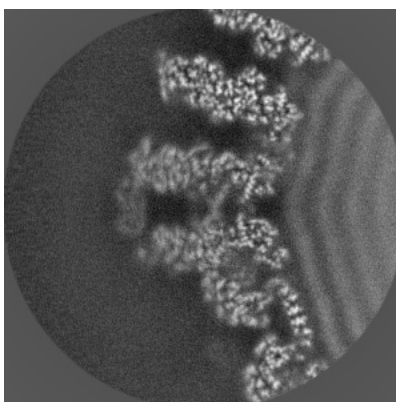


Z Index: 192

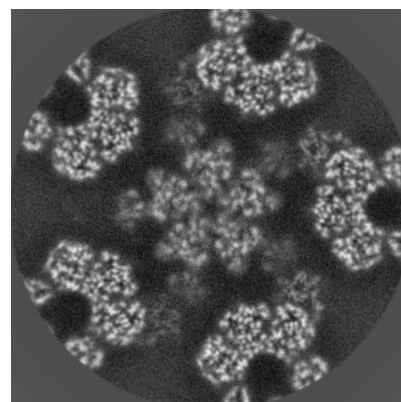
### 6.2.2 Raw map



X Index: 192



Y Index: 192

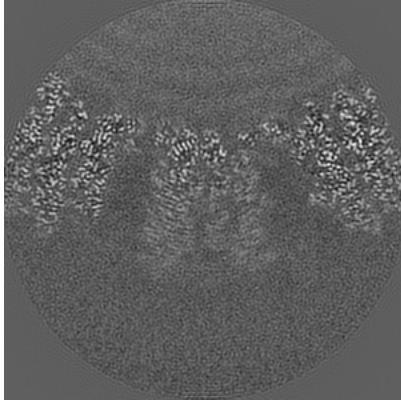


Z Index: 192

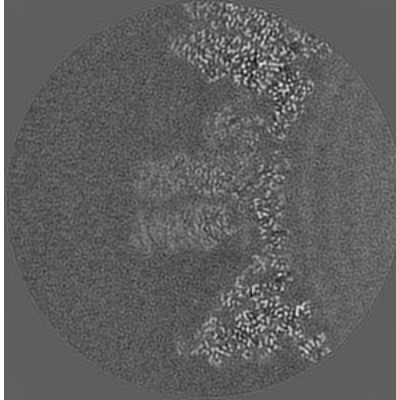
The images above show central slices of the map in three orthogonal directions.

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

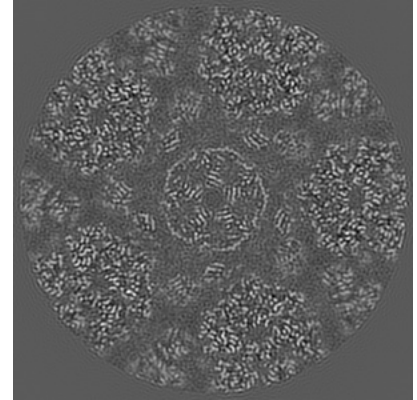
### 6.3.1 Primary map



X Index: 208

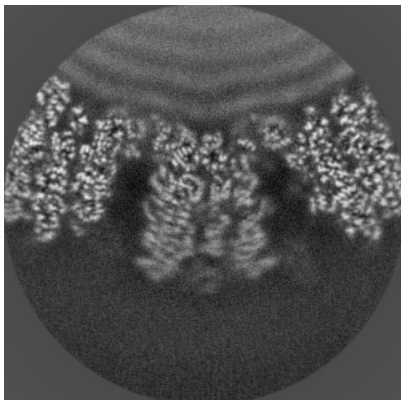


Y Index: 155

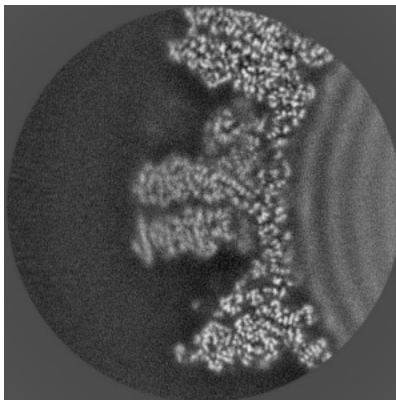


Z Index: 246

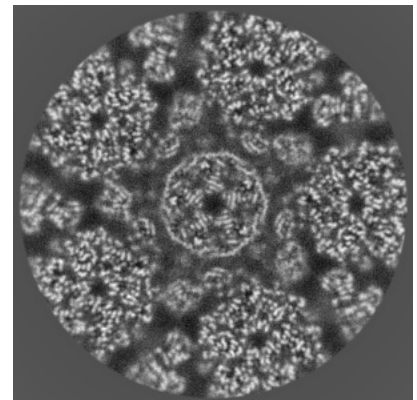
### 6.3.2 Raw map



X Index: 209



Y Index: 154

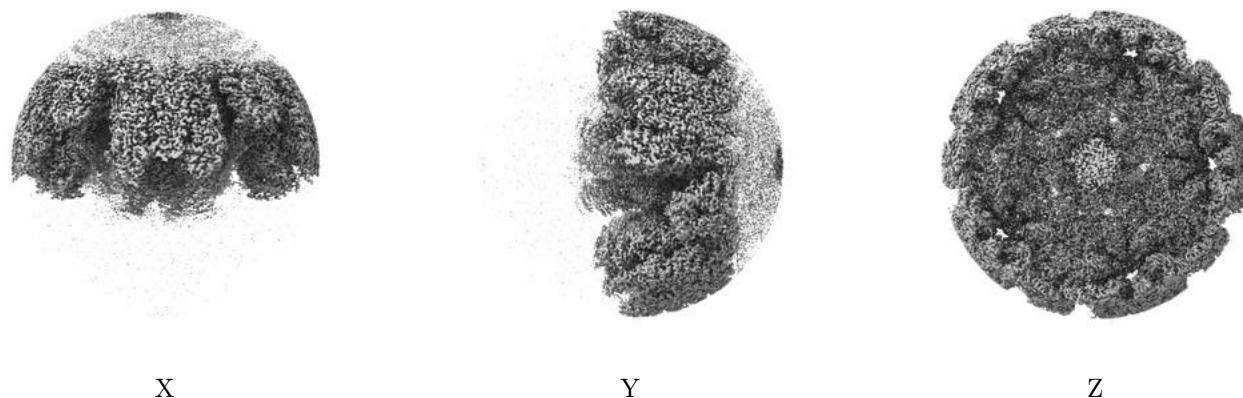


Z Index: 246

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

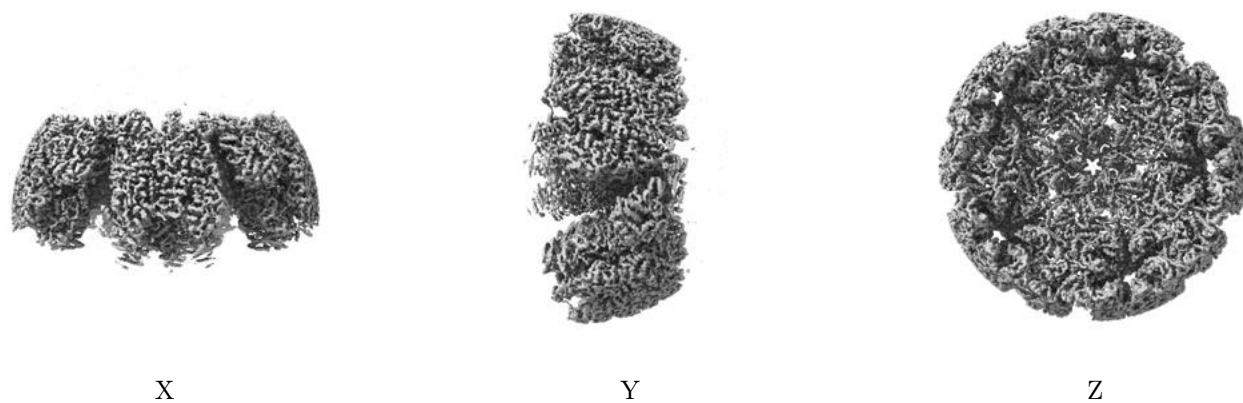
## 6.4 Orthogonal surface views [i](#)

### 6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.02. 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.



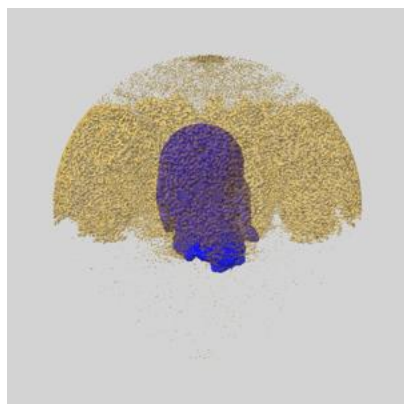
## 6.5 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

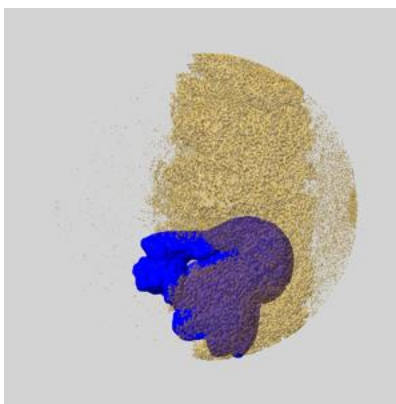
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

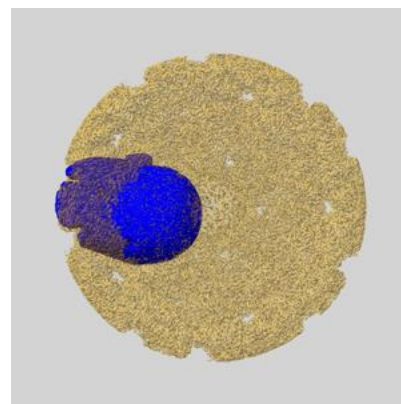
### 6.5.1 emd\_20433\_msk\_1.map [i](#)



X



Y

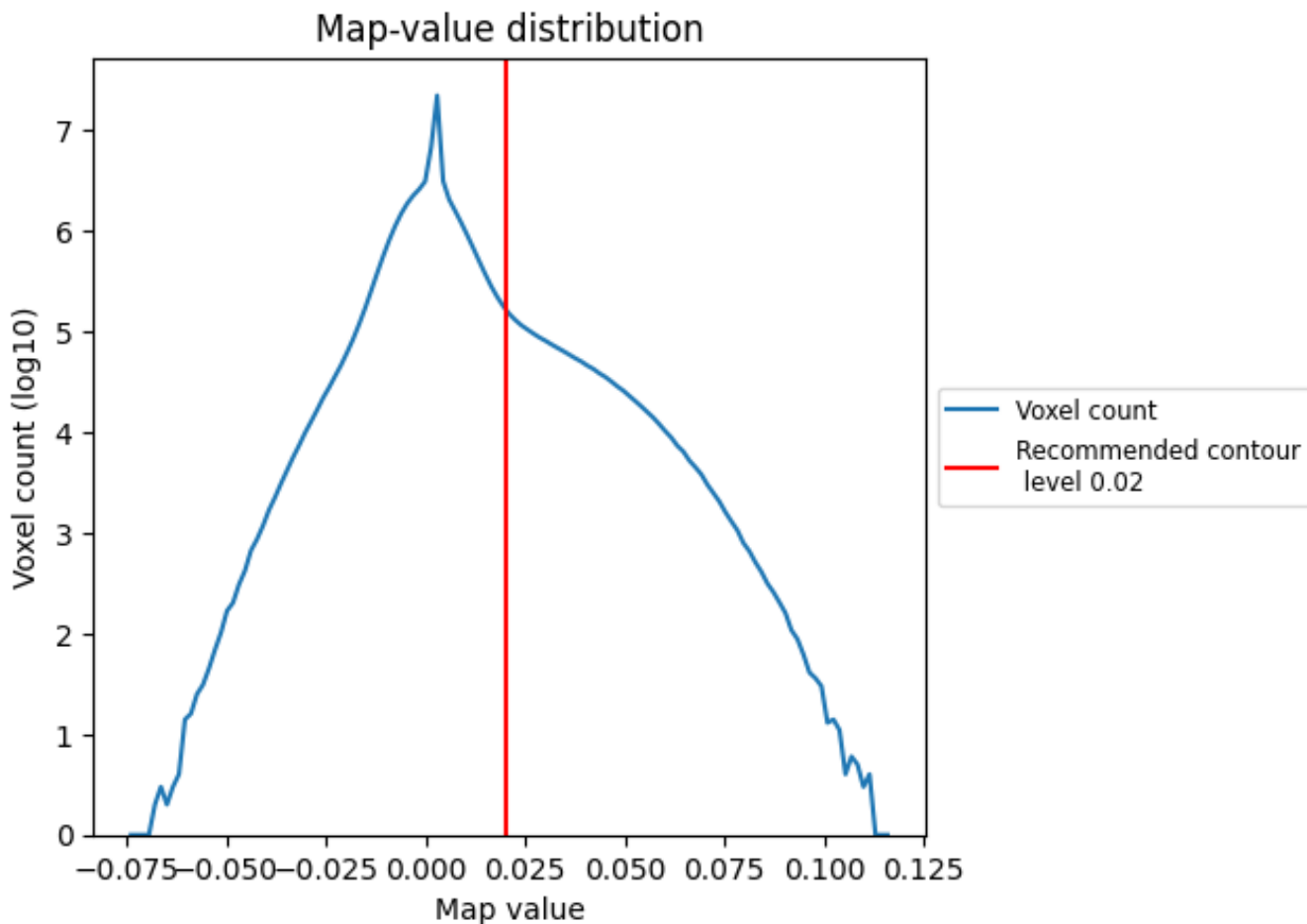


Z

## 7 Map analysis [i](#)

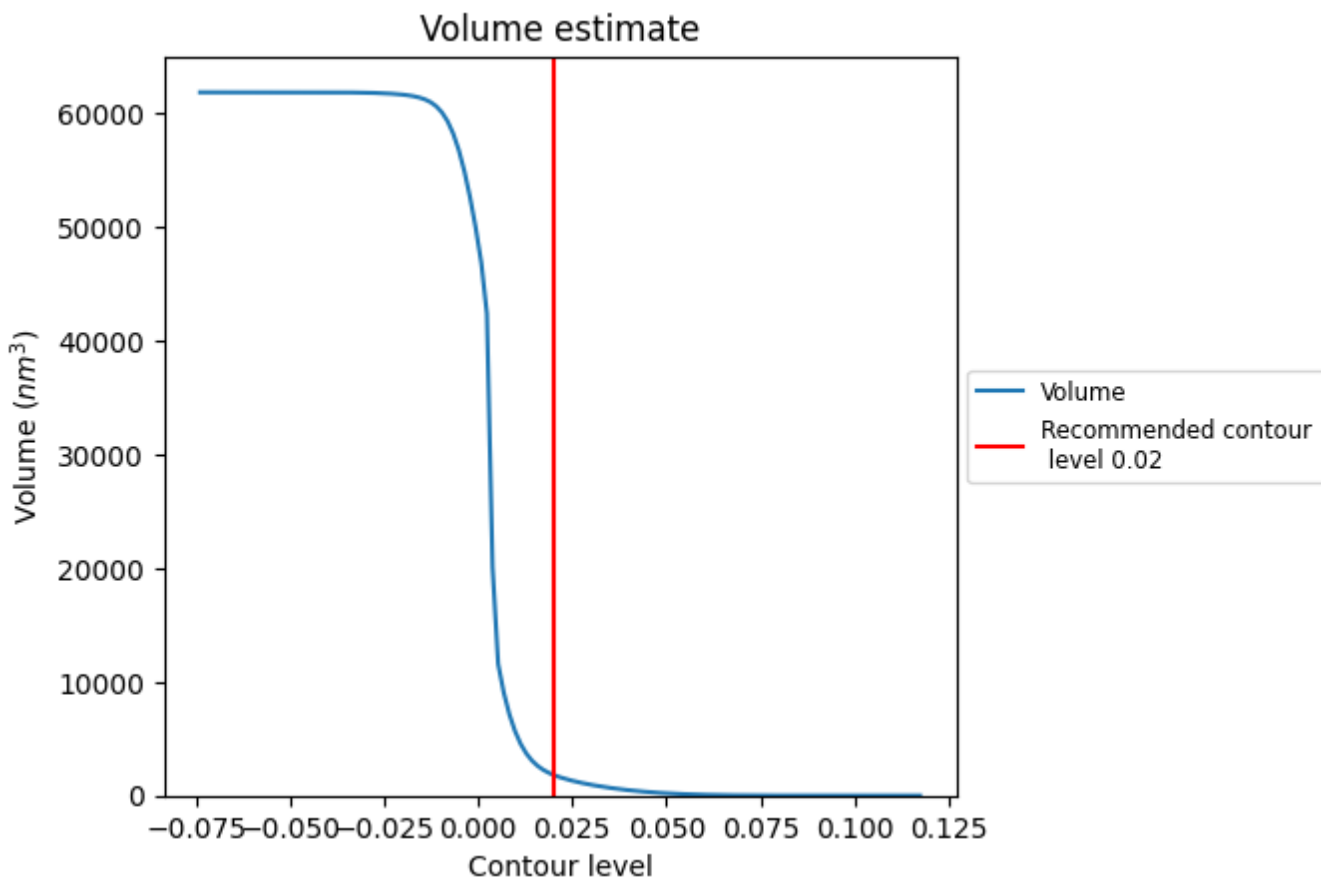
This section contains the results of statistical analysis of the map.

### 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.

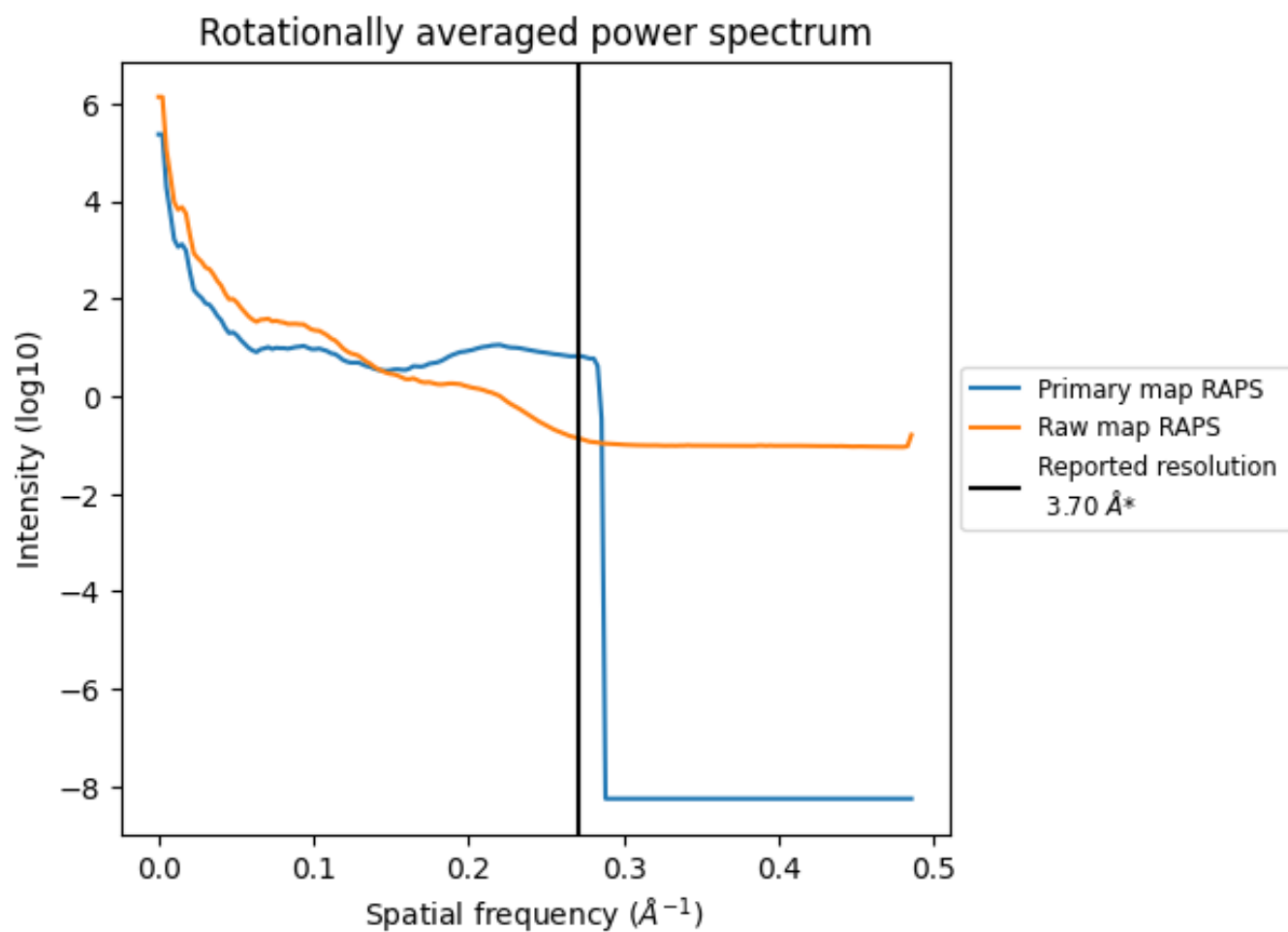
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1827 nm<sup>3</sup>; this corresponds to an approximate mass of 1651 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

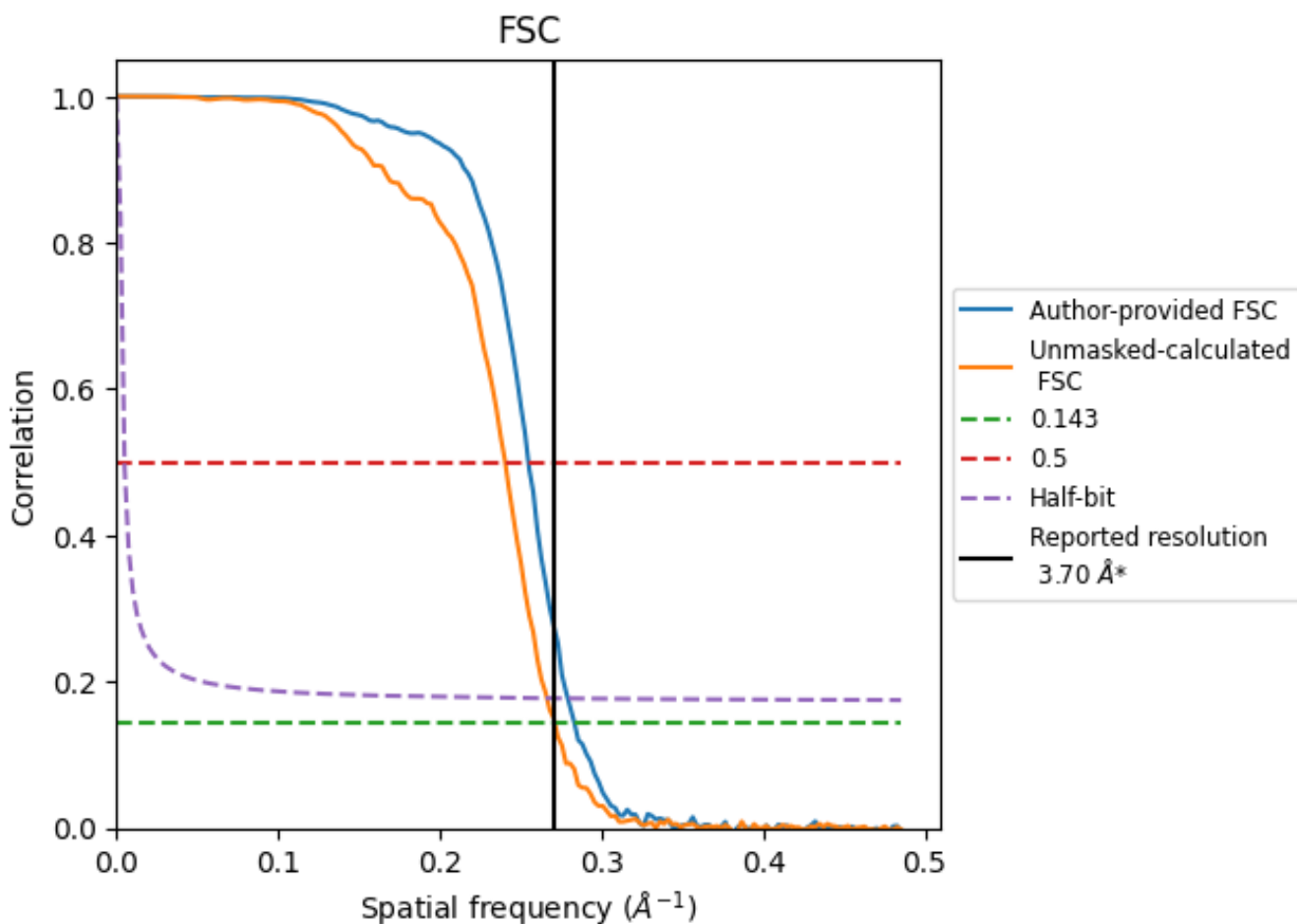


\*Reported resolution corresponds to spatial frequency of 0.270 Å<sup>-1</sup>

## 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 0.270 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

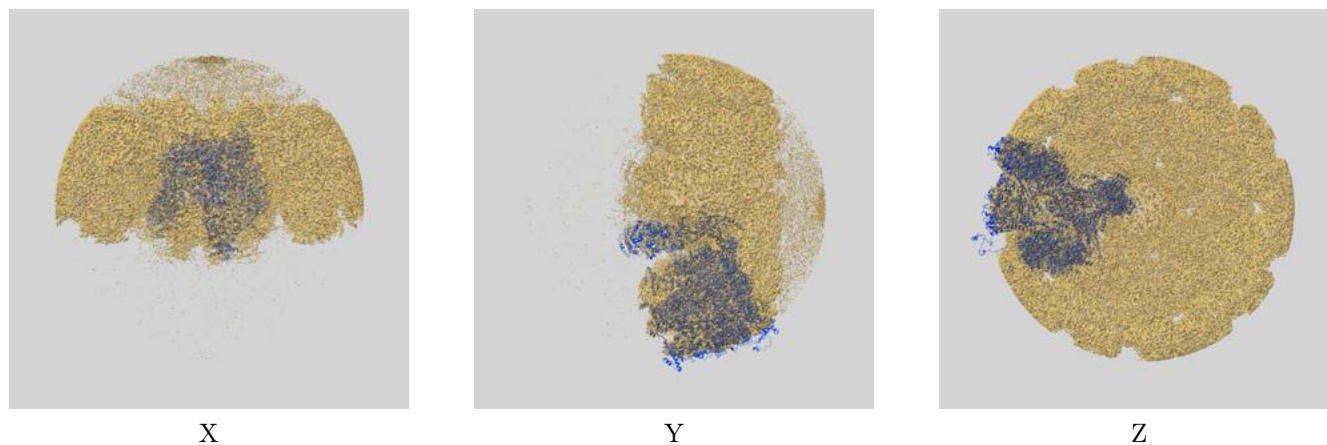
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	3.53	3.92	3.58
Unmasked-calculated*	3.69	4.16	3.76

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

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

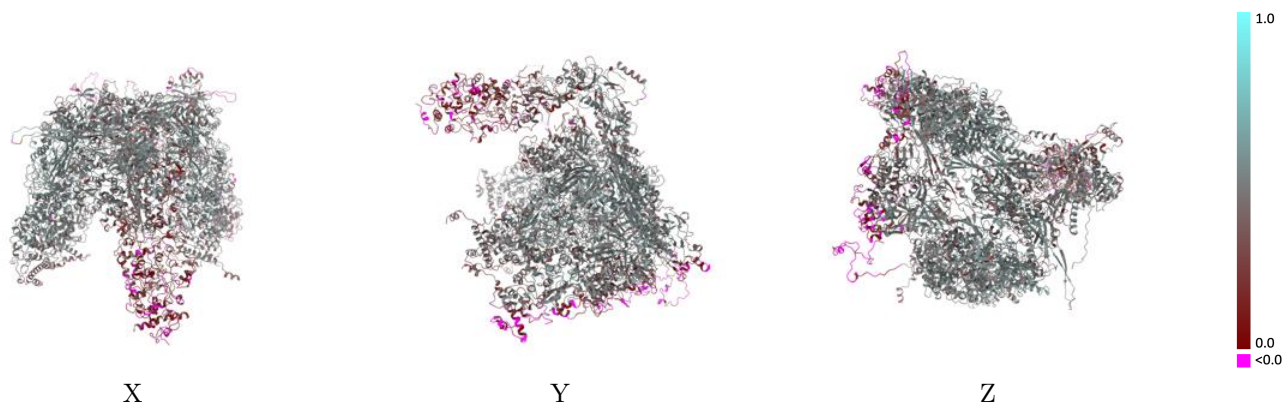
This section contains information regarding the fit between EMDB map EMD-20433 and PDB model 6PPD. Per-residue inclusion information can be found in section 3 on page 6.

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



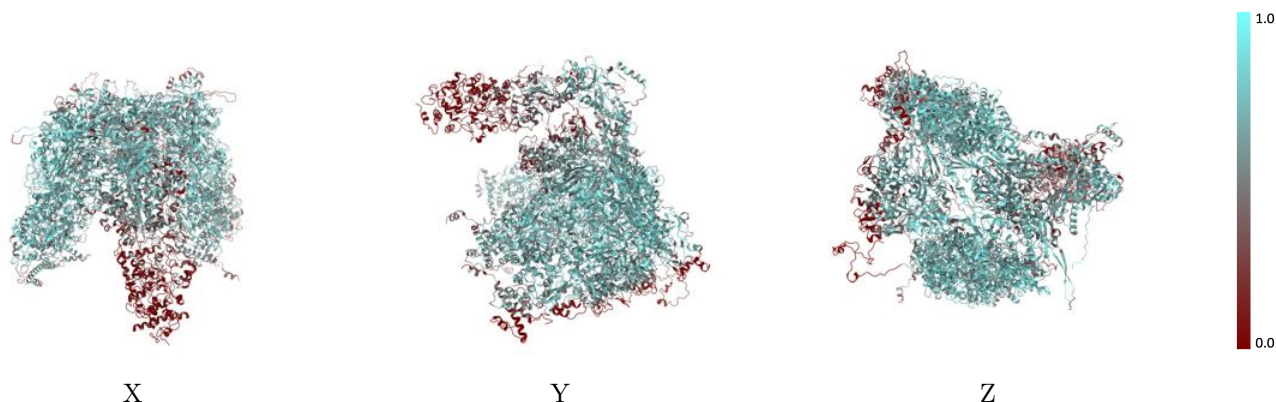
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 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.

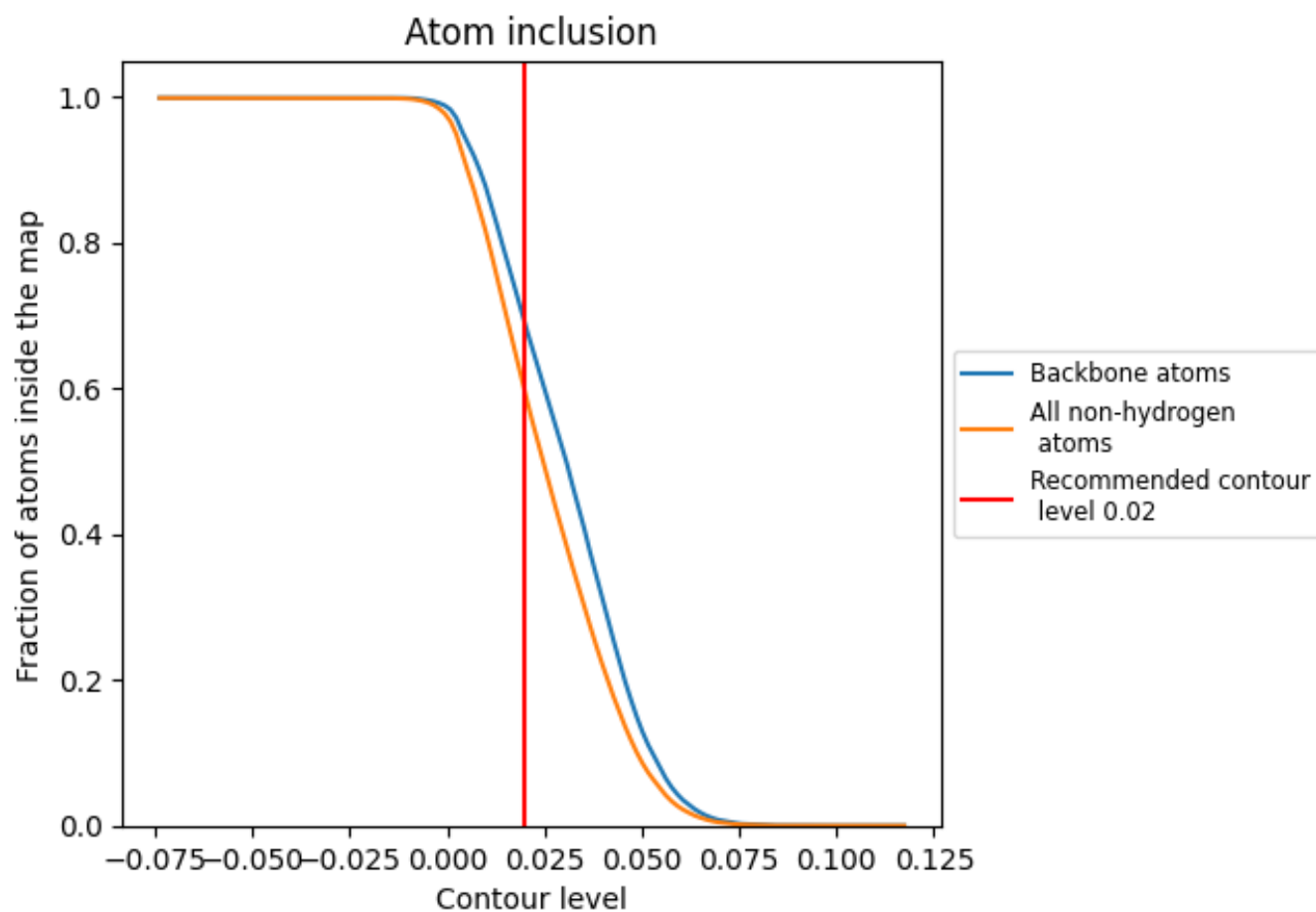
## 9.3 Atom inclusion mapped to coordinate model [i](#)



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 (0.02).





































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 69% of all backbone atoms, 59% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5946	 0.4260
0	 0.1791	 0.1420
1	 0.4720	 0.3820
2	 0.5187	 0.3700
3	 0.4844	 0.3680
4	 0.3502	 0.3030
5	 0.5737	 0.4690
6	 0.5677	 0.4580
7	 0.4140	 0.3970
A	 0.0763	 0.1380
S	 0.7146	 0.5000
T	 0.6915	 0.4580
W	 0.6382	 0.4310
X	 0.7140	 0.4930
b	 0.6163	 0.4330
c	 0.5031	 0.3550
d	 0.4881	 0.3290

