



wwPDB EM Validation Summary Report ⓘ

Nov 6, 2022 – 03:25 PM EST

PDB ID : 6B43
EMDB ID : EMD-7047
Title : CryoEM structure and atomic model of the Kaposi's sarcoma-associated herpesvirus capsid
Authors : Dai, X.H.; Gong, D.Y.; Sun, R.; Zhou, Z.H.
Deposited on : 2017-09-25
Resolution : 4.20 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:

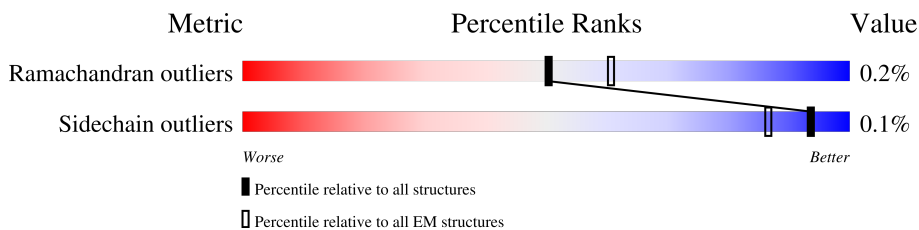
EMDB validation analysis : 0.0.1.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

1 Overall quality at a glance

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

The reported resolution of this entry is 4.20 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)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	4	1376	58% 87% 12%
1	A	1376	9% 98% ..
1	B	1376	10% 98% ..
1	C	1376	11% 97% ..
1	D	1376	11% 97% ..
1	E	1376	10% 98% ..
1	F	1376	10% 97% ..
1	M	1376	9% 98% ..
1	N	1376	9% 98% ..

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	O	1376	9% 97% ..
1	S	1376	19% 92% 7%
1	T	1376	14% 98% ..
1	U	1376	12% 98% ..
1	V	1376	13% 97% ..
1	W	1376	16% 98% ..
1	X	1376	20% 97% ..
2	0	170	22% 46% 54%
2	1	170	20% 46% 54%
2	2	170	28% 46% 54%
2	3	170	29% 46% 54%
2	G	170	16% 46% 54%
2	H	170	26% 46% 54%
2	I	170	14% 46% 54%
2	J	170	18% 46% 54%
2	K	170	15% 46% 54%
2	L	170	13% 46% 54%
2	P	170	15% 46% 54%
2	Q	170	20% 46% 54%
2	R	170	15% 46% 54%
2	Y	170	28% 46% 54%
2	Z	170	31% 46% 54%
3	5	331	59% 95% ..
3	8	331	11% 97% .
3	b	331	12% 97% .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	e	331	14% 96%
3	h	331	13% 96%
4	6	305	55% 96%
4	7	305	81% 98%
4	9	305	12% 95%
4	a	305	11% 97%
4	c	305	7% 95%
4	d	305	9% 98%
4	f	305	22% 96%
4	g	305	17% 97%
4	i	305	9% 96%
4	j	305	11% 97%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 214334 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Major capsid protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1363	10682	6786	1854	1969	73	0	0
1	B	1355	10627	6751	1843	1960	73	0	0
1	C	1354	10621	6748	1842	1959	72	0	0
1	D	1355	10627	6751	1843	1960	73	0	0
1	E	1363	10682	6786	1854	1969	73	0	0
1	F	1356	10638	6757	1847	1961	73	0	0
1	M	1355	10627	6751	1843	1960	73	0	0
1	N	1363	10682	6786	1854	1969	73	0	0
1	O	1355	10627	6751	1843	1960	73	0	0
1	S	1281	10060	6397	1737	1855	71	0	0
1	T	1360	10666	6776	1851	1966	73	0	0
1	U	1355	10627	6751	1843	1960	73	0	0
1	V	1352	10604	6739	1839	1954	72	0	0
1	W	1354	10621	6748	1842	1959	72	0	0
1	X	1345	10548	6701	1829	1946	72	0	0
1	4	1216	9586	6102	1665	1748	71	0	0

- Molecule 2 is a protein called Small capsomere-interacting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	G	78	Total 666	C 418	N 130	O 115	S 3	0	0
2	H	78	Total 666	C 418	N 130	O 115	S 3	0	0
2	I	78	Total 666	C 418	N 130	O 115	S 3	0	0
2	J	78	Total 666	C 418	N 130	O 115	S 3	0	0
2	K	78	Total 666	C 418	N 130	O 115	S 3	0	0
2	L	78	Total 666	C 418	N 130	O 115	S 3	0	0
2	P	78	Total 666	C 418	N 130	O 115	S 3	0	0
2	Q	78	Total 666	C 418	N 130	O 115	S 3	0	0
2	R	78	Total 666	C 418	N 130	O 115	S 3	0	0
2	Y	78	Total 666	C 418	N 130	O 115	S 3	0	0
2	Z	78	Total 666	C 418	N 130	O 115	S 3	0	0
2	0	78	Total 666	C 418	N 130	O 115	S 3	0	0
2	1	78	Total 666	C 418	N 130	O 115	S 3	0	0
2	2	78	Total 666	C 418	N 130	O 115	S 3	0	0
2	3	78	Total 666	C 418	N 130	O 115	S 3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	5	319	Total 2463	C 1578	N 421	O 449	S 15	0	0
3	8	321	Total 2477	C 1586	N 424	O 452	S 15	0	0
3	b	321	Total 2477	C 1586	N 424	O 452	S 15	0	0
3	e	319	Total 2460	C 1575	N 422	O 448	S 15	0	0
3	h	321	Total 2477	C 1586	N 424	O 452	S 15	0	0

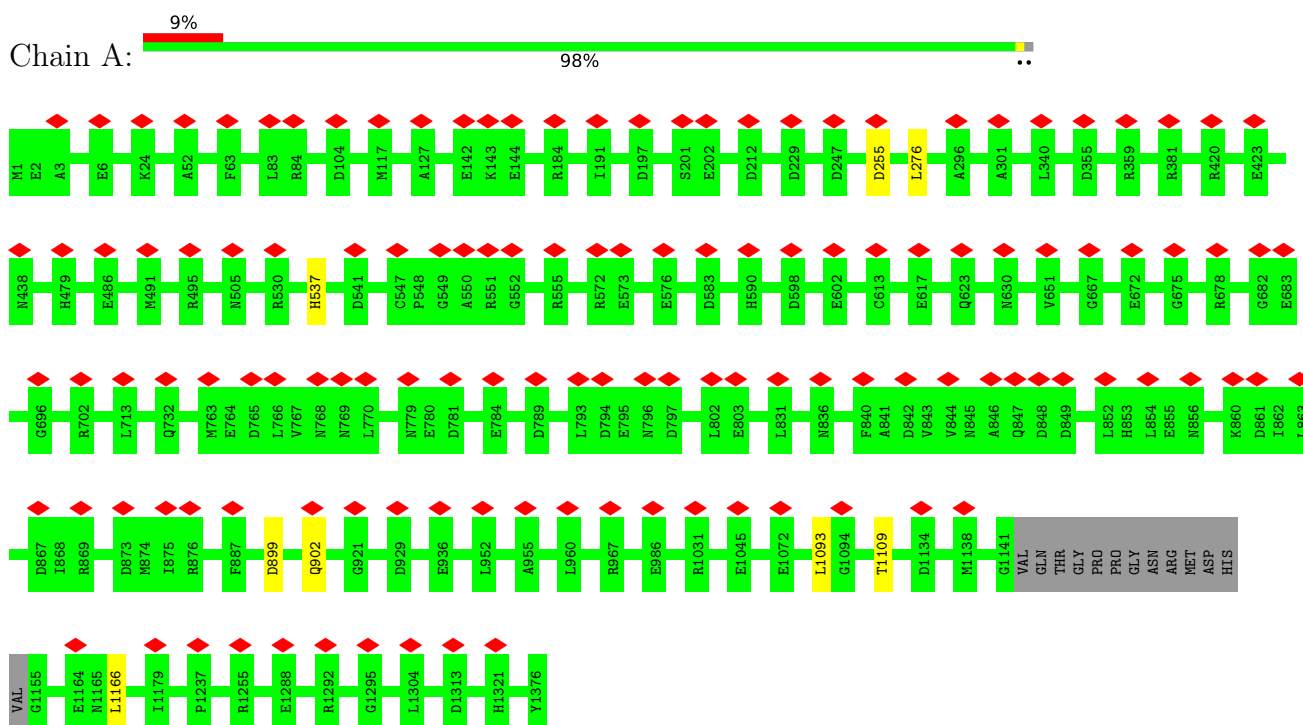
- Molecule 4 is a protein called Triplex capsid protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	6	294	Total	C	N	O	S	0	0
			2329	1485	397	433	14		
4	7	300	Total	C	N	O	S	0	0
			2364	1505	401	443	15		
4	9	294	Total	C	N	O	S	0	0
			2329	1485	397	433	14		
4	a	300	Total	C	N	O	S	0	0
			2364	1505	401	443	15		
4	c	294	Total	C	N	O	S	0	0
			2329	1485	397	433	14		
4	d	300	Total	C	N	O	S	0	0
			2364	1505	401	443	15		
4	f	294	Total	C	N	O	S	0	0
			2329	1485	397	433	14		
4	g	300	Total	C	N	O	S	0	0
			2364	1505	401	443	15		
4	i	294	Total	C	N	O	S	0	0
			2329	1485	397	433	14		
4	j	300	Total	C	N	O	S	0	0
			2364	1505	401	443	15		

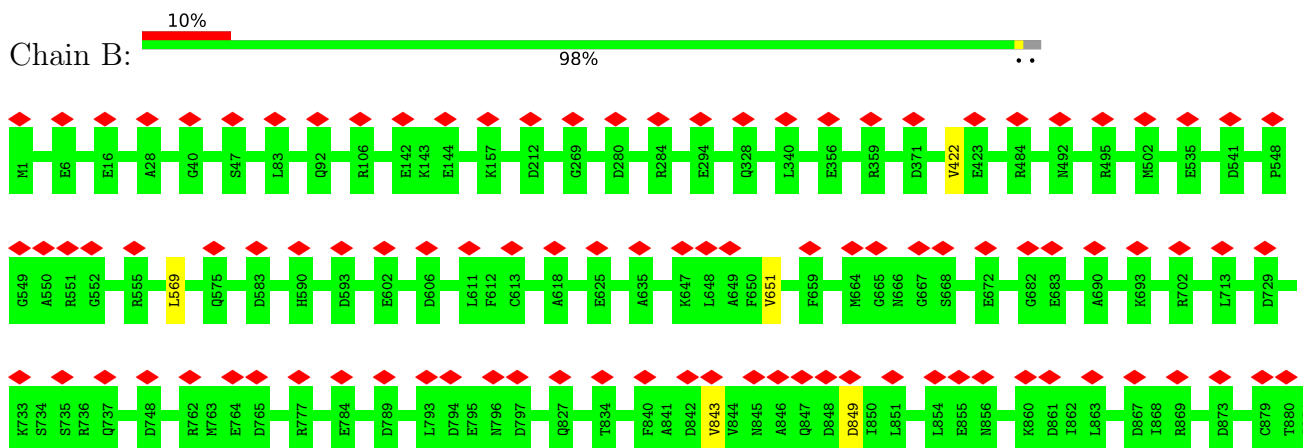
3 Residue-property plots [i](#)

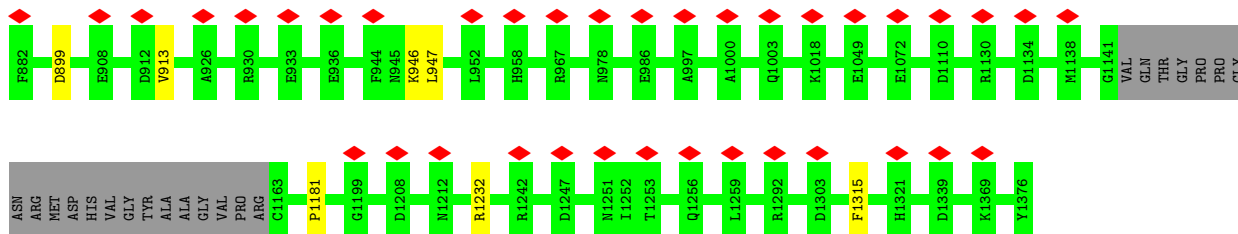
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Major capsid protein

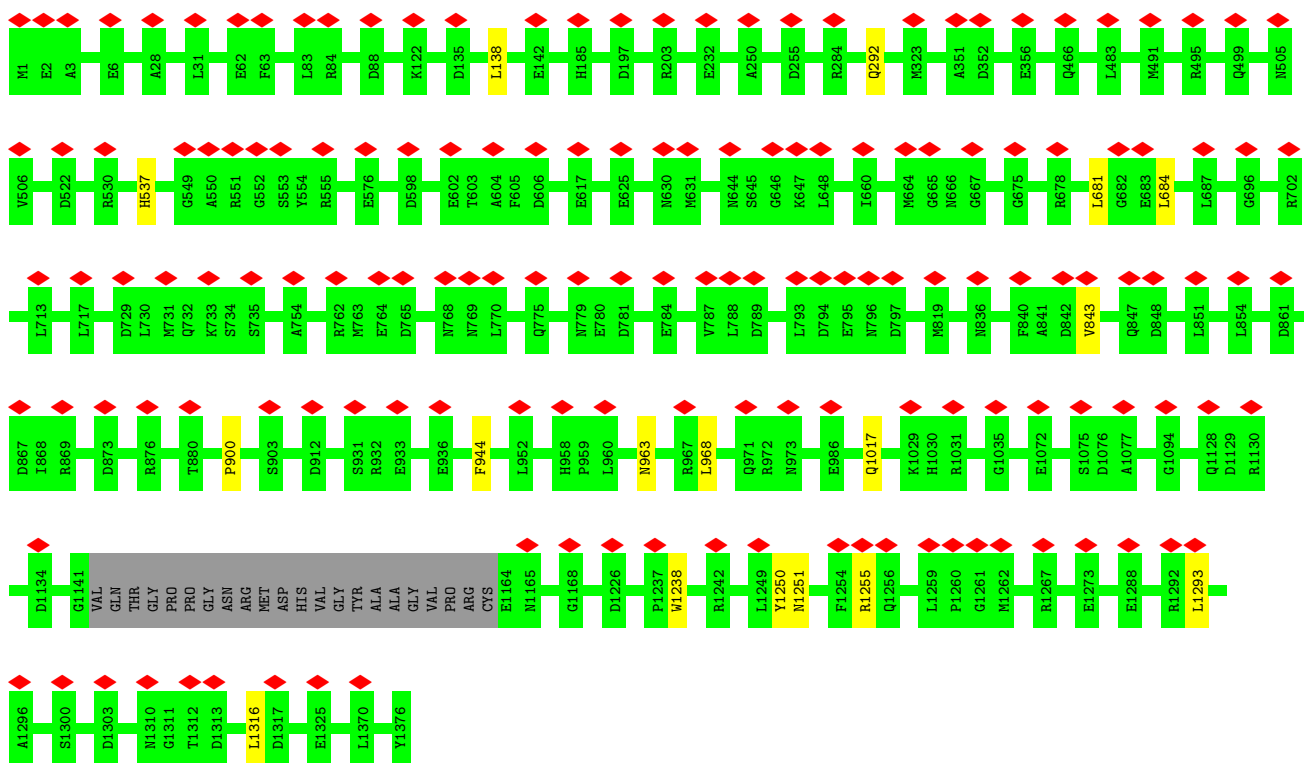


- Molecule 1: Major capsid protein

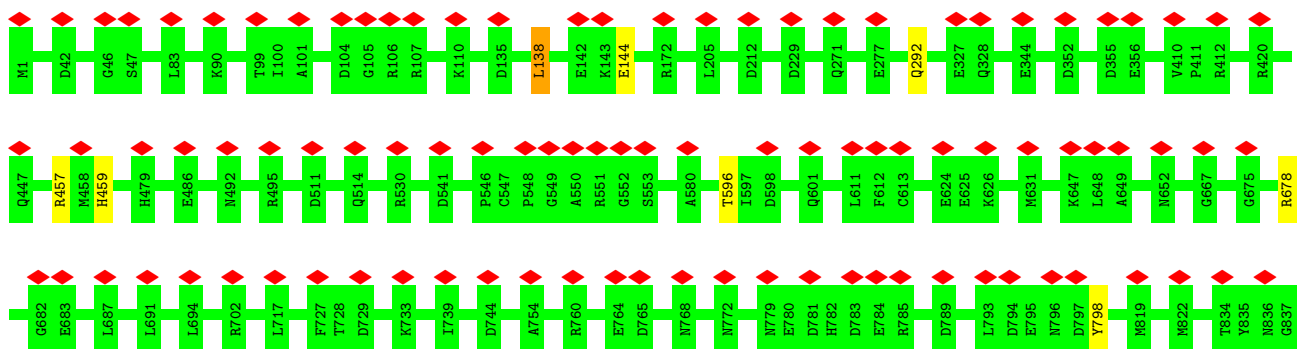


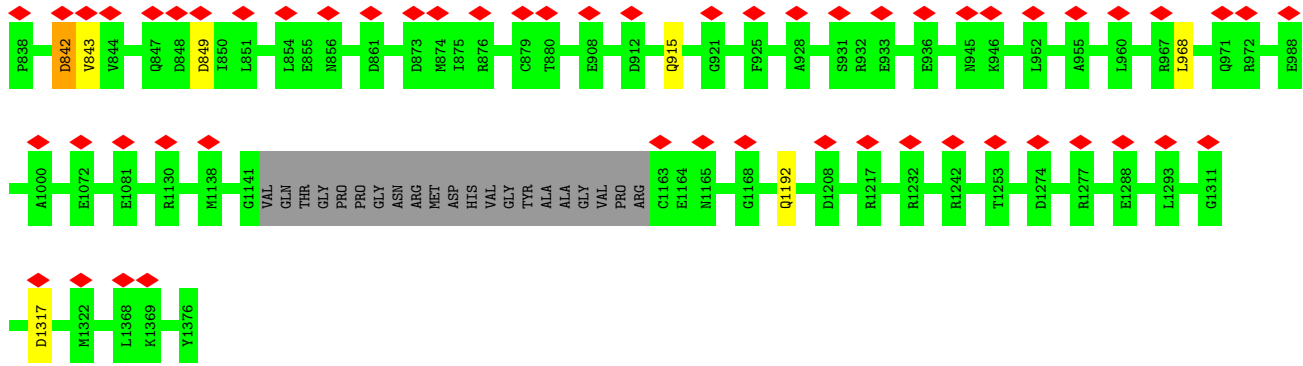


• Molecule 1: Major capsid protein



• Molecule 1: Major capsid protein

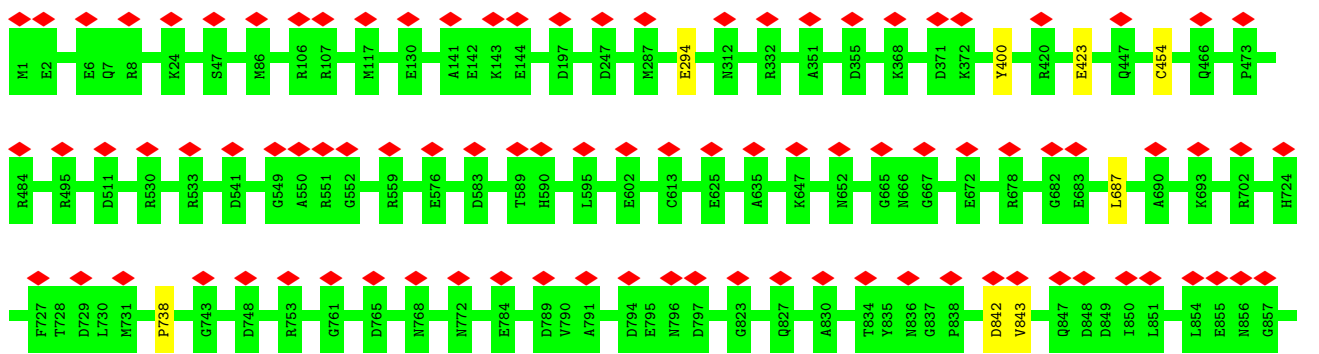


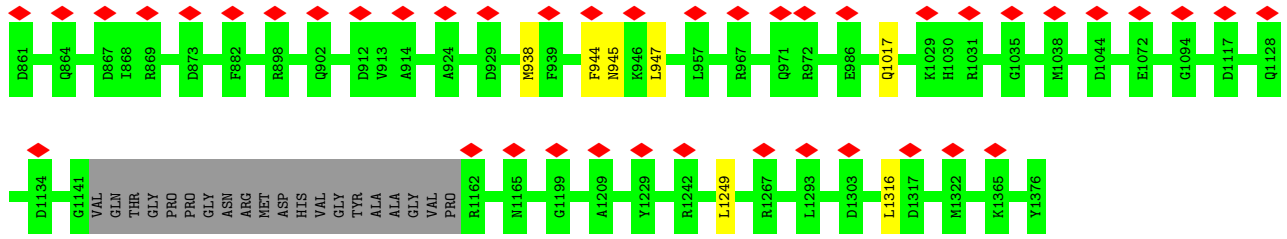


• Molecule 1: Major capsid protein

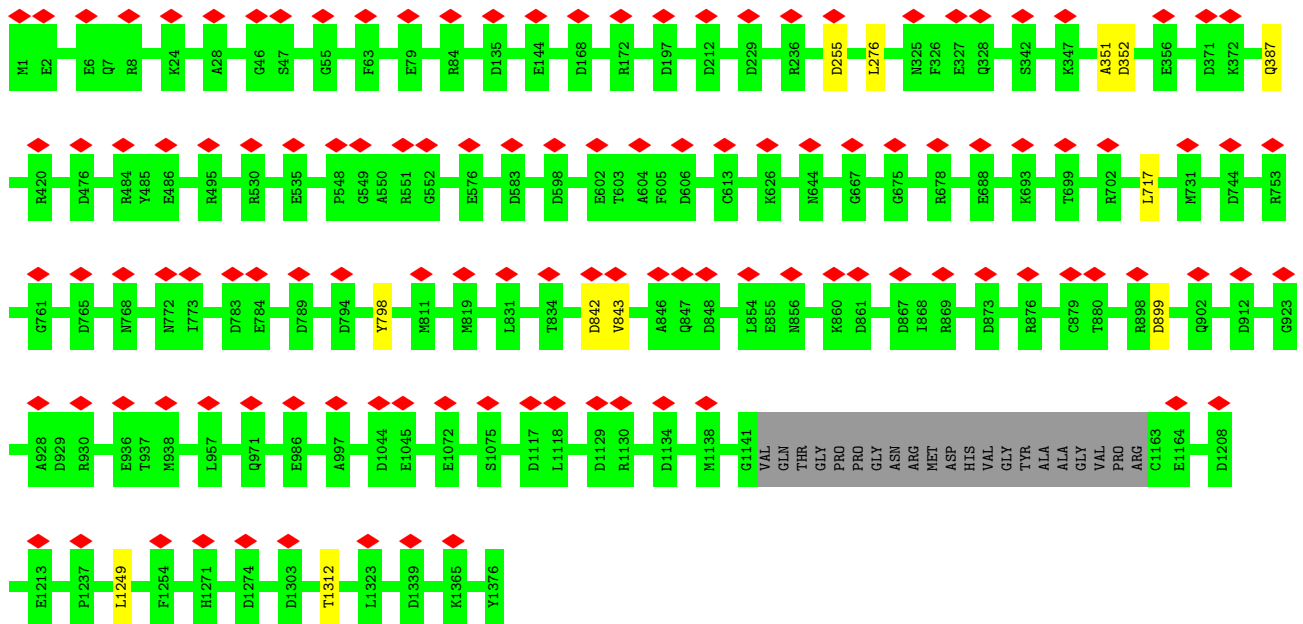


• Molecule 1: Major capsid protein

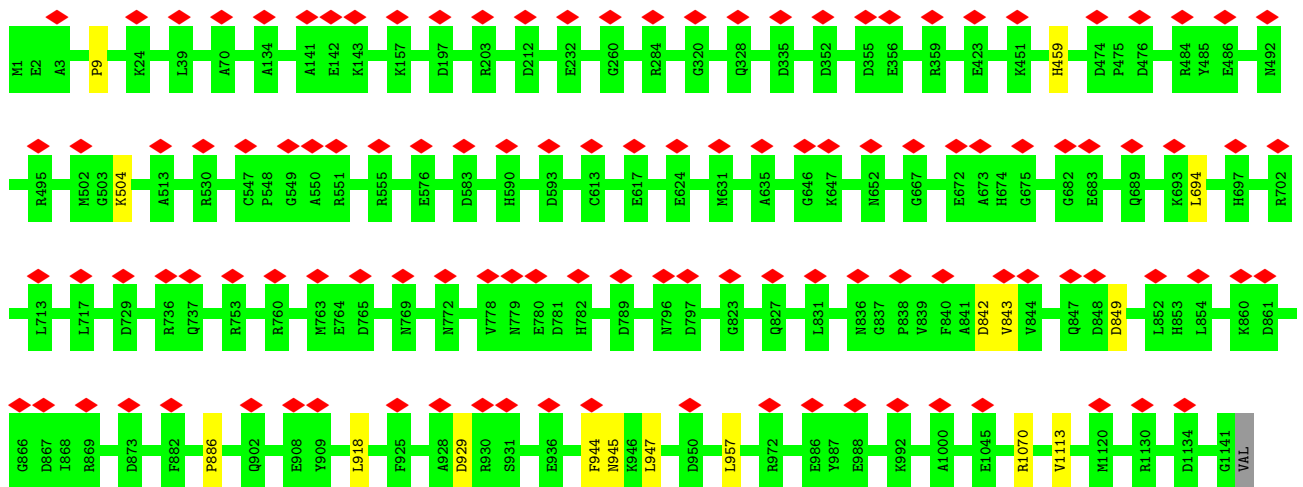


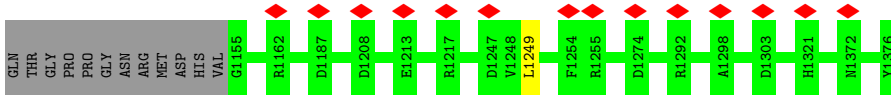


• Molecule 1: Major capsid protein

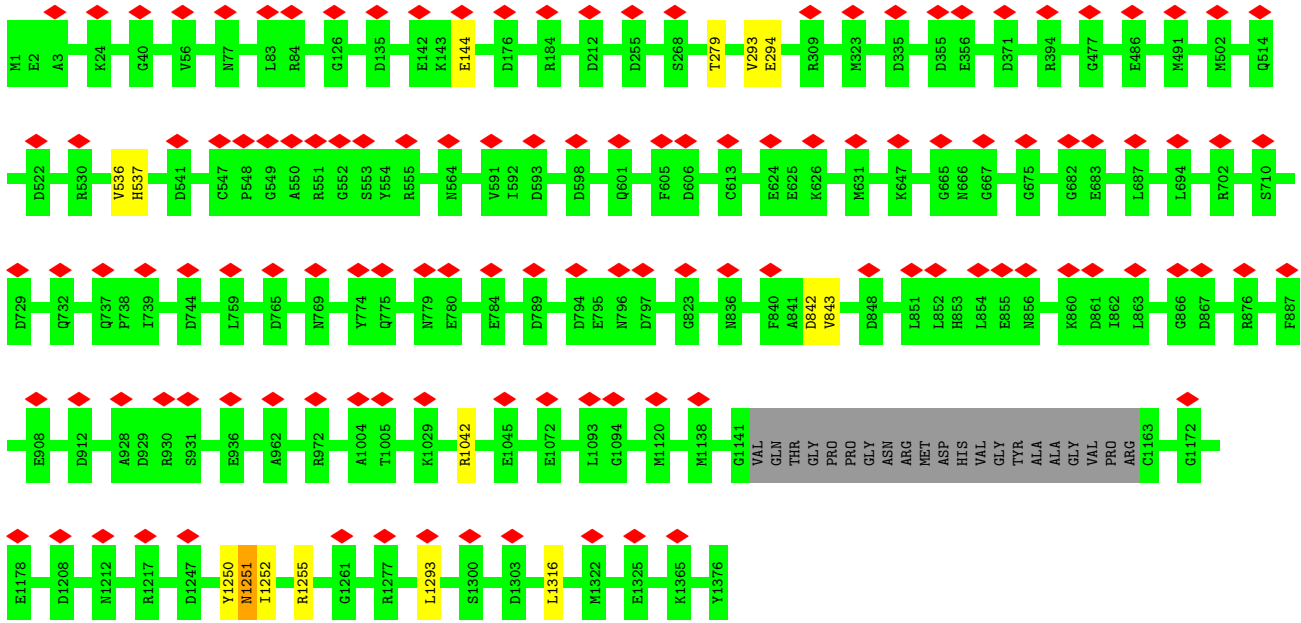


• Molecule 1: Major capsid protein

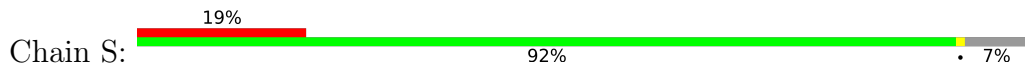


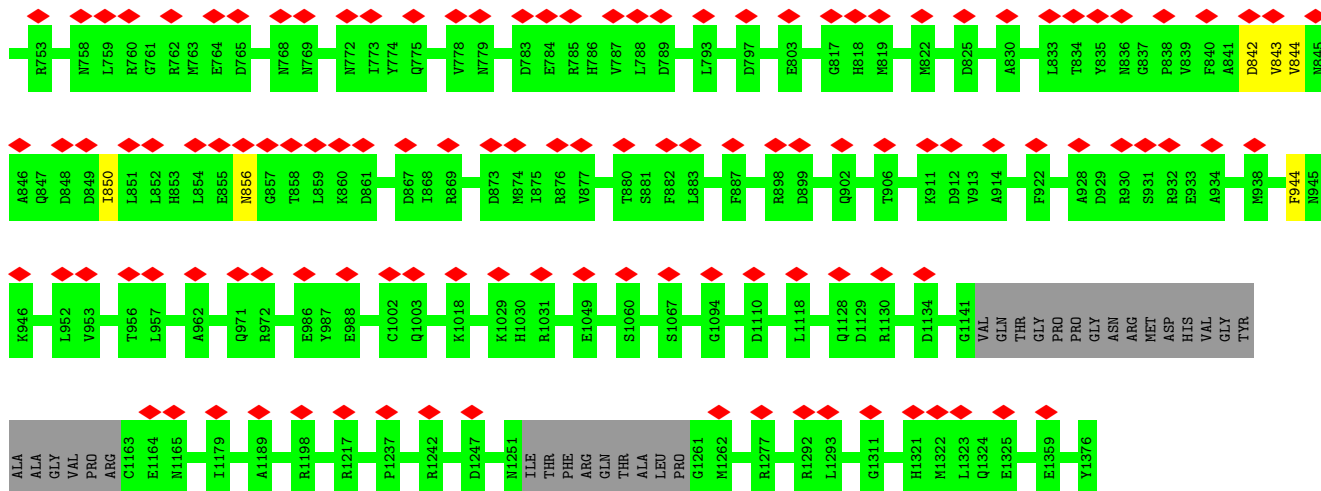


● Molecule 1: Major capsid protein

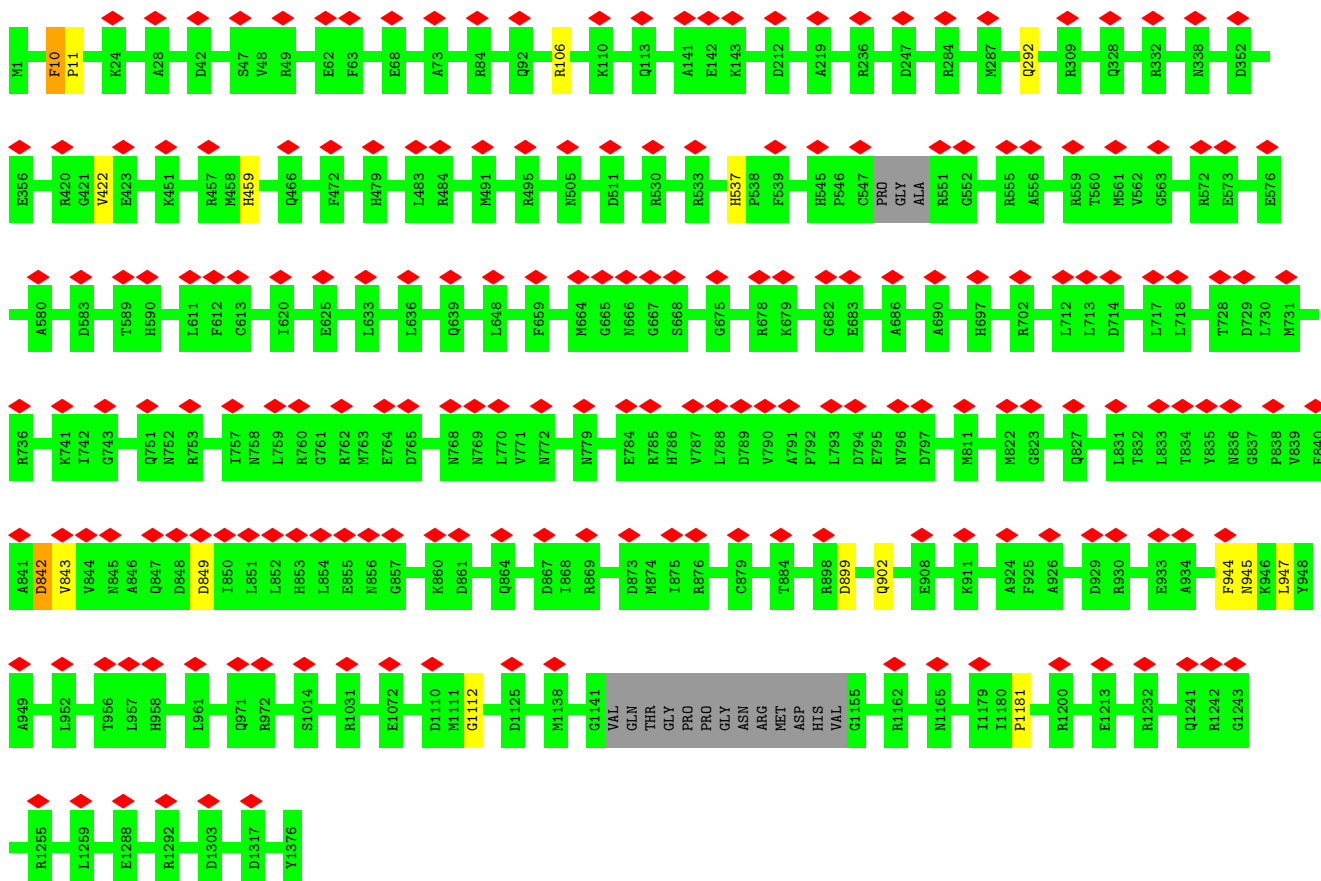


● Molecule 1: Major capsid protein



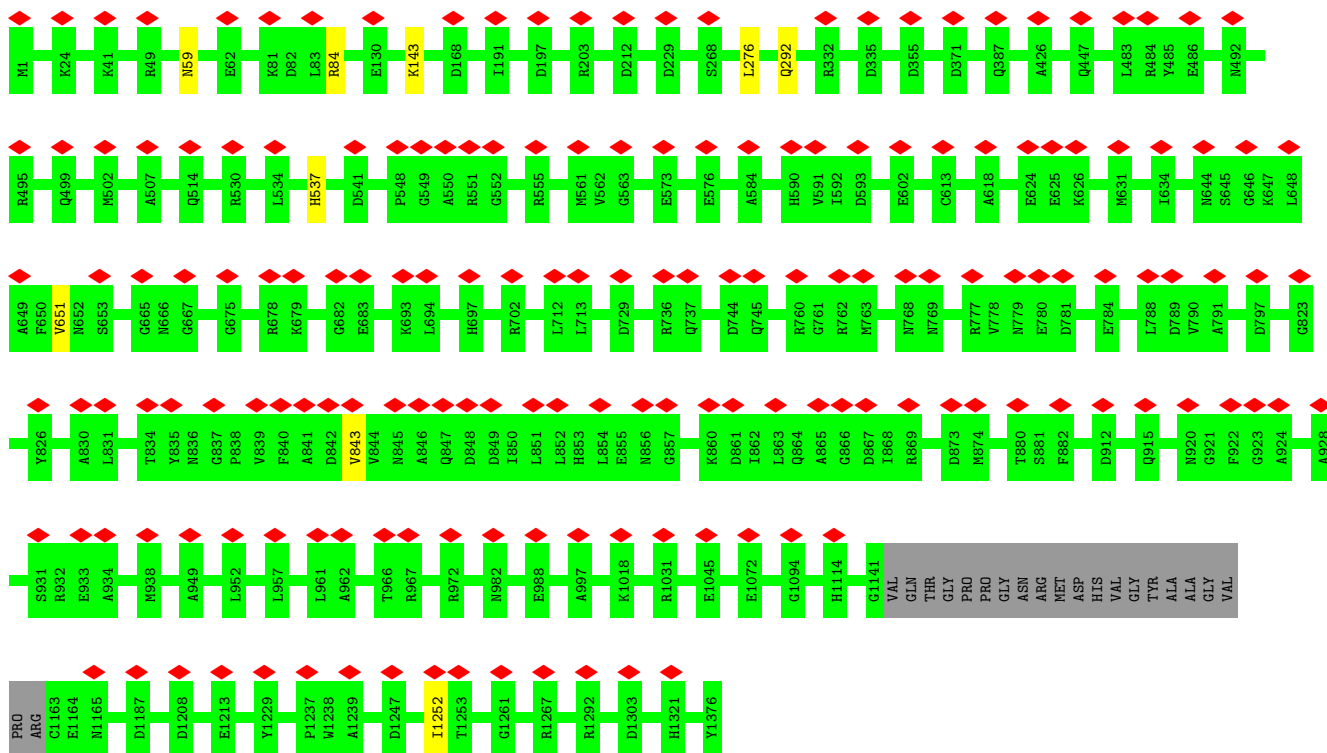


• Molecule 1: Major capsid protein

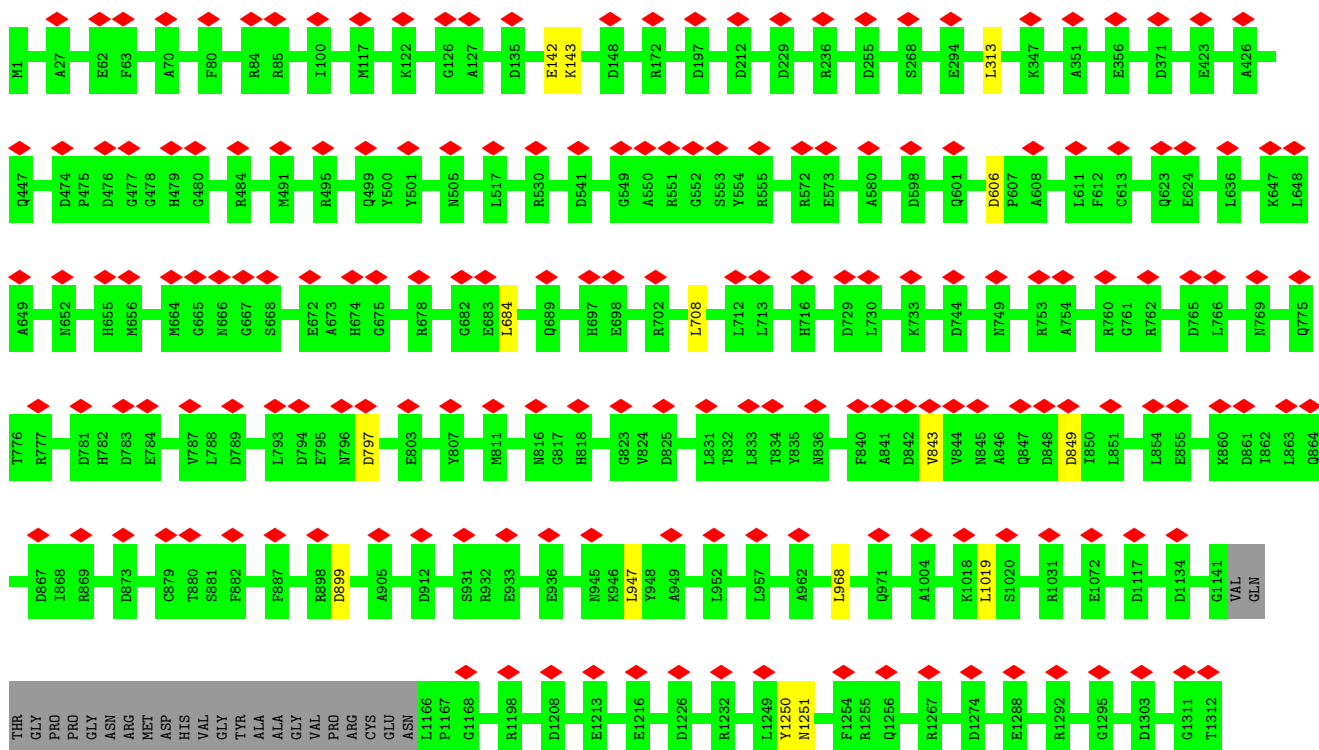


• Molecule 1: Major capsid protein



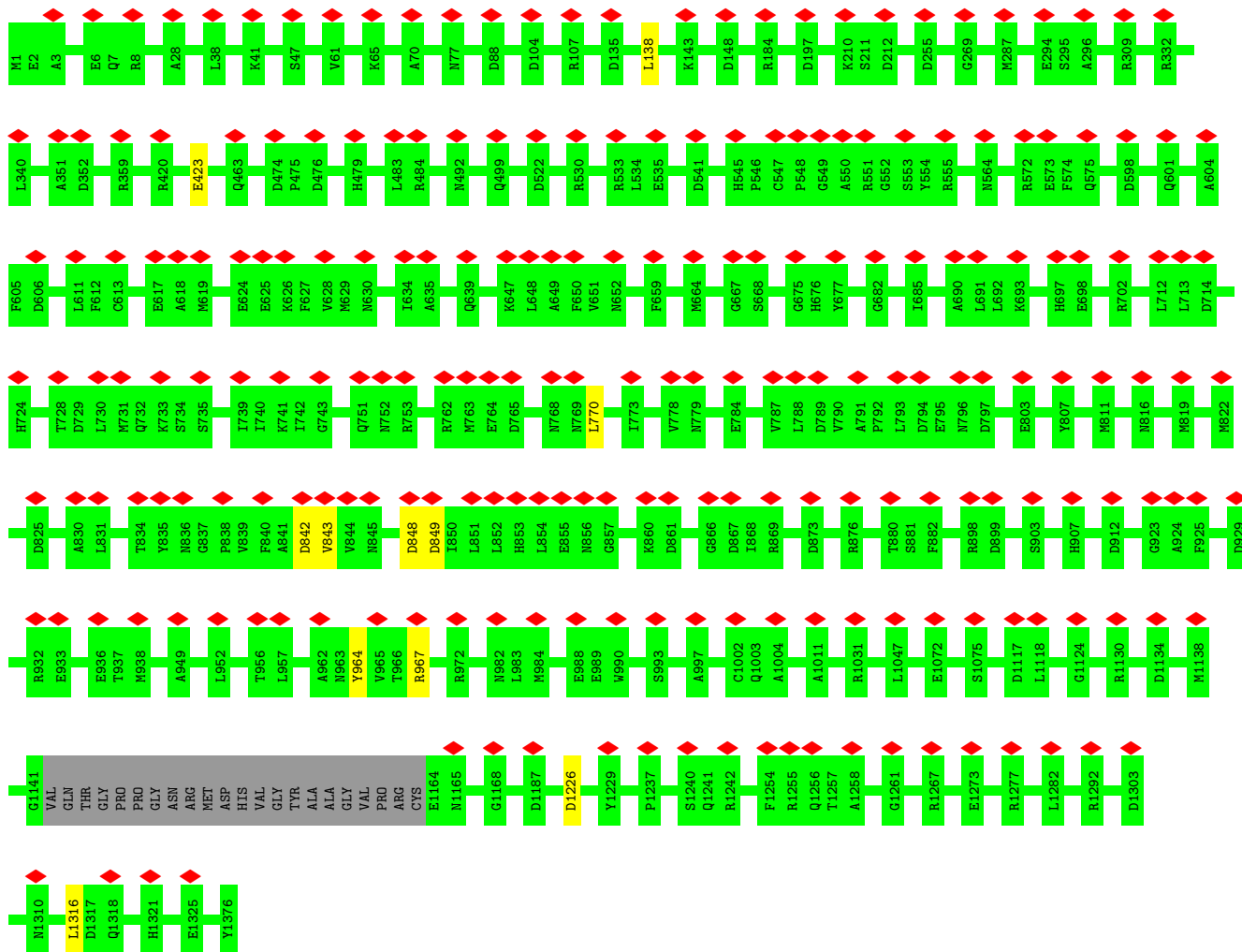


• Molecule 1: Major capsid protein

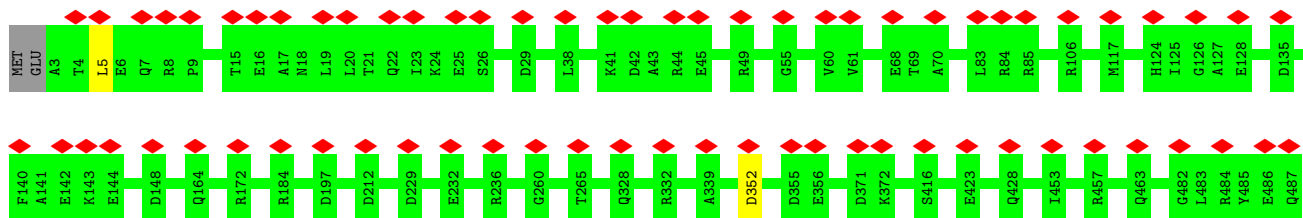


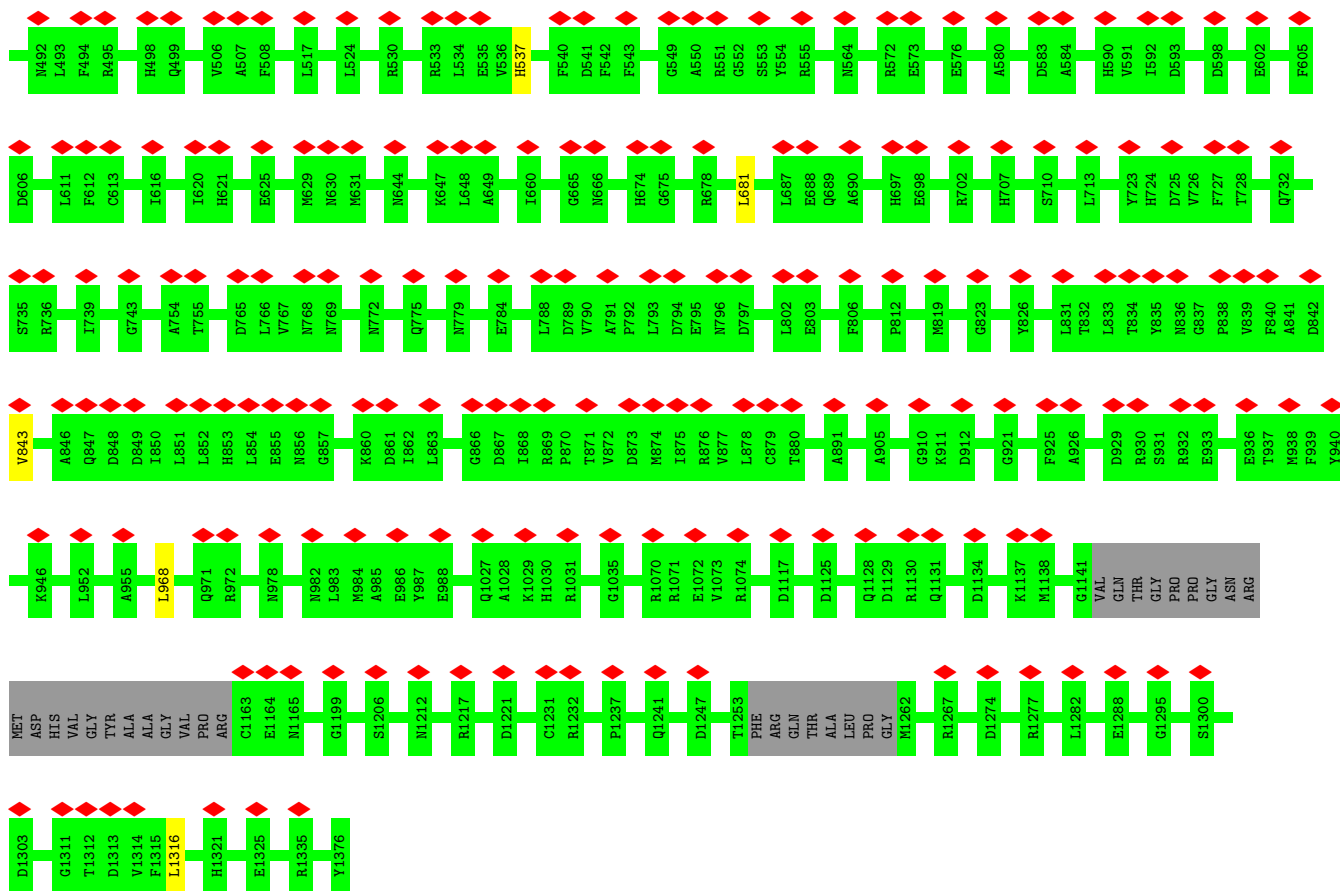


• Molecule 1: Major capsid protein

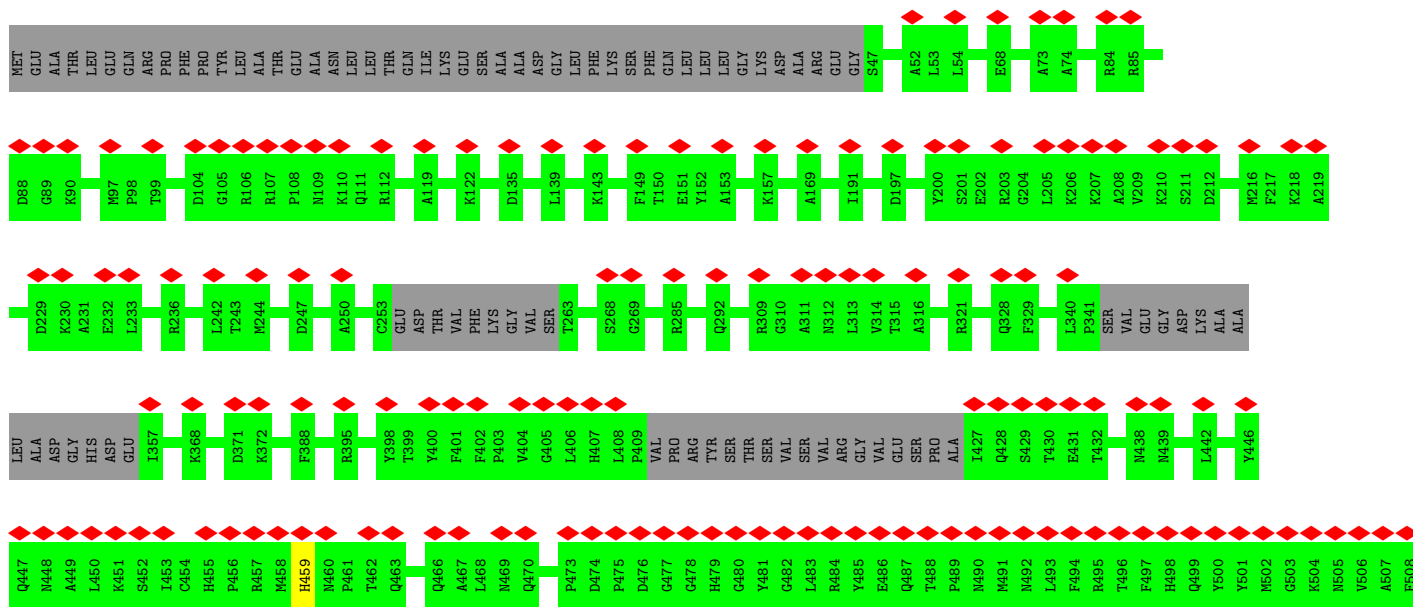
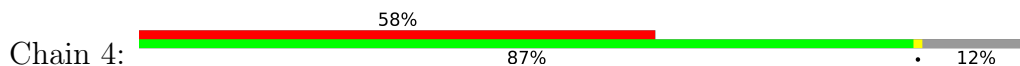


• Molecule 1: Major capsid protein

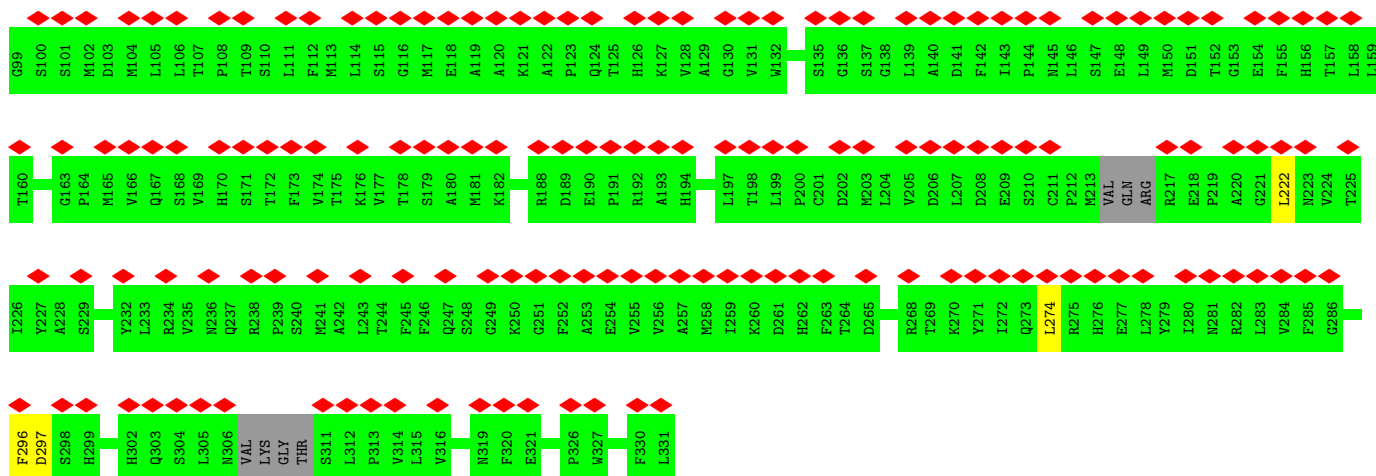




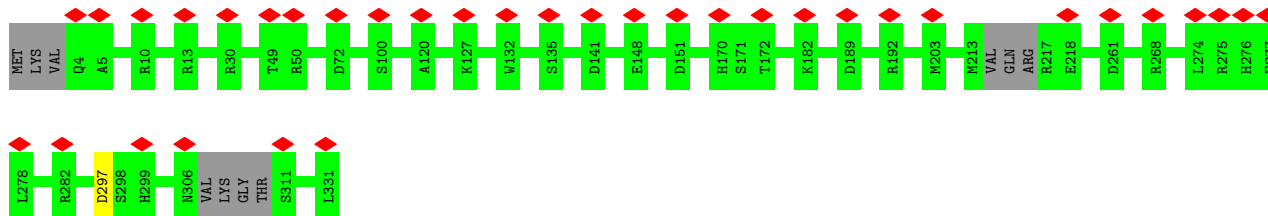
• Molecule 1: Major capsid protein



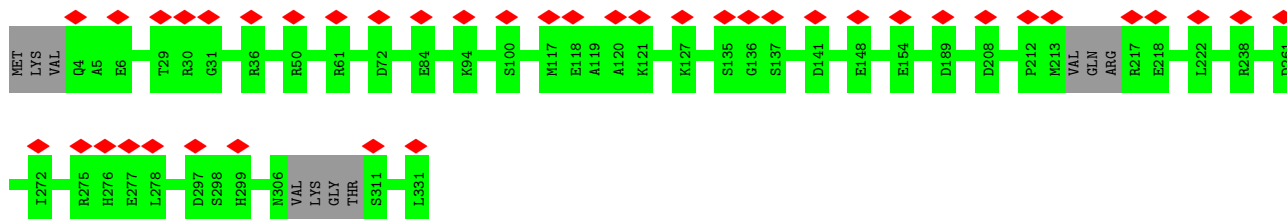
ASN	THR	S1233	LEU	E989	V809	N749	Q889	M629	L869	V509
LYS	SER	T1234	PRO	W990	L810	P750	A690	M630	A570	P610
VAL	THR	M1235	GLY	H991	M811	Q751	A691	M631	P571	D511
TYR	THR	N1236	LEU	K992	P812	N752	L692	P632	E572	V612
	ASP	M1237	SER	S993	V813	R753	K693	L633	E573	A513
	LEU	P1238	HIS	P994	C814	A754	L694	I634	F574	Q614
	GLY	M1111	GLY	V995	S815	R755	A695	A635	Q575	K515
	GLN	G1112	LEU	A996	N816	F756	G696	L636	E576	A616
	LEU	H1113	VAL	A997	H817	I757	H697	V637	S577	L517
	LEU	V1114	HIS	Y998	G818	N758	E698	I638	R578	V618
		D1117	LEU	A999	M819	L759	T699	Q639	G579	T519
		L1118	I1180	A1000	C820	R760	V700	T640	A580	T520
		F1119	P941	S1001	G821	G761	G701	Y641	Q581	E521
		M1120	P942	C1002	M822	R762	R702	W642	F582	D522
		T1185	P943	Q1003	G823	M763	T703	V643	D583	L523
		S1186	F944	A1004	V824	E764	F704	N644	A584	L524
		D1187	N945	T1005	D825	D765	I705	S645	V585	H525
		Y1190	K946	P1006	Y826	L766	T706	G646	T586	P526
		F1191	L947	G1007	Q827	V767	H707	K647	N587	T527
		Q1192	Y948	A1008	N828	N768	L708	L648	M588	S528
		S1195	A949	I1009	V829	M769	V709	A649	T589	H529
		N1196	D950	S1010	A830	L770	S710	F650	H590	R530
		P1197	P951	A1011	L831	V771	A711	V651	V591	L531
		R1198	L952	M1012	T832	N772	L712	N652	I592	L532
		R1199	Y953	V1013	L833	I773	L713	S653	D593	R533
		R1200	A954	H1016	T834	V774	D714	Y654	Q594	L534
		A1201	A955	Q1017	Y835	Q775	P715	H555	L595	E535
		A1202	T956	K1018	N836	T776	H716	M656	T596	V536
		C1203	L957	L1019	G837	R777	L717	V657	I597	H537
		S1206	H958	S1020	P838	V778	L718	R658	D598	P538
		C1207	P959	A1021	V839	N779	P719	F659	V599	F539
		D1208	L960	P1022	F940	E780	P720	I660	I600	F540
		A1209	L961	S1023	A941	D781	F721	Q661	Q601	D541
		Y1210	N963	F1024	D842	H782	A722	T662	E602	F542
		N1211	Y964	I1025	V843	D783	T723	H663	T603	F543
		N1212	Y965	C1026	N845	E784	H724	M664	A604	V444
		E1213	T966	Q1027	A846	R785	D725	G665	F605	H545
		S1214	T967	Q1028	Q847	H786	V726	G666	D606	P546
		A1215	L968	K1029	Q848	V787	T727	G667	P607	C547
		E1216	P969	H1030	D848	L788	D729	S668	A608	P548
		R1217	P970	R1031	D849	V789	L730	I669	Y609	G549
		L1218	Q971	M1032	I850	V790	M731	P670	P610	A550
		Y1283	R972	H1033	L851	A791	Q732	K671	L611	R551
		T1284	N973	C1034	L852	P792	K733	E672	F612	S552
		H1288	Y975	F1036	H853	L793	E673	A673	C613	S553
		S1290	V976	A1037	L854	D794	H734	H674	Y614	Y554
		A1291	V977	M1038	E855	E795	R736	G675	V615	R555
		L1292	F978	R1042	N856	N796	Q737	I616	I616	A556
		L1293	N978	T1043	G857	D797	P738	Y677	E617	T557
		ALA	R979	D1044	L859	V798	I739	R678	A618	H558
		GLY	P980	E1045	L859	N799	I740	K679	M619	R559
		ALA	S981	L1065	K960	P900	I741	I680	I620	T560
		PRO	N982	L1072	D861	V801	I742	L681	H621	V562
		ALA	L983	E1073	I862	L802	I743	G682	G622	G563
		ALA	M984	R1074	L863	E803	D744	E683	Q623	N564
			A985		Q864	K904	G745	L684	E624	I565
			E986		A865	L805	N746	I685	E625	P566
			Y987		G866	F906	Y747	A686	K626	Q667
			E988		D867	Y807	D748	L687	F627	P568
					I868	Y808		E688	V628	



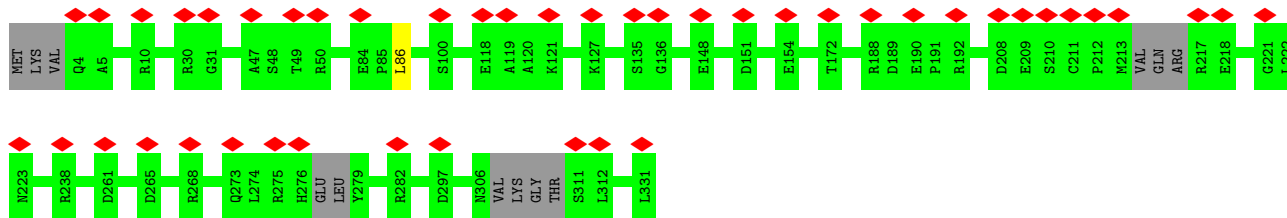
• Molecule 3: Triplex capsid protein 1



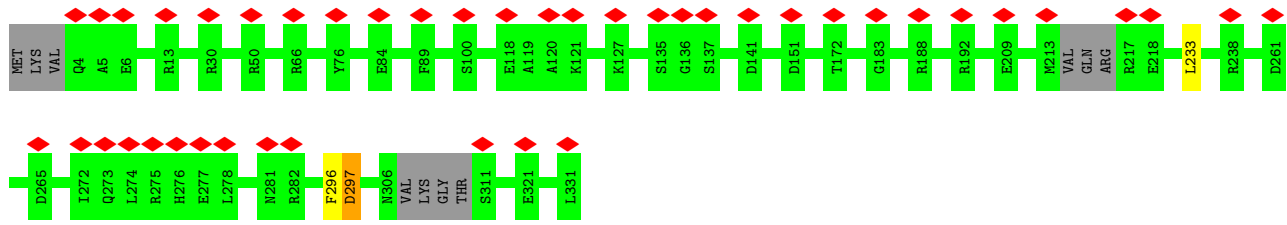
• Molecule 3: Triplex capsid protein 1



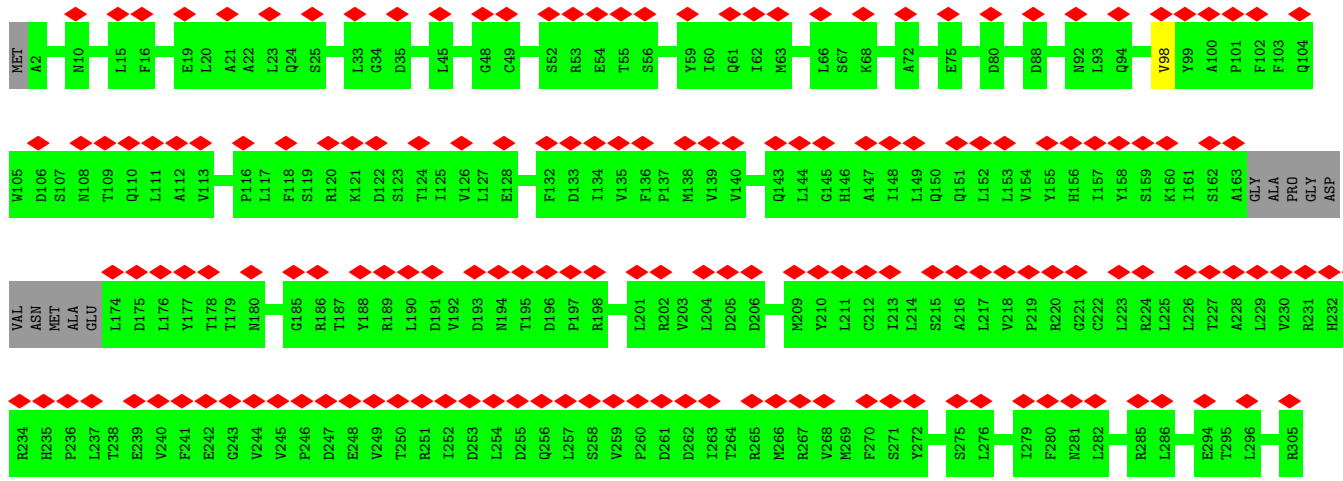
• Molecule 3: Triplex capsid protein 1



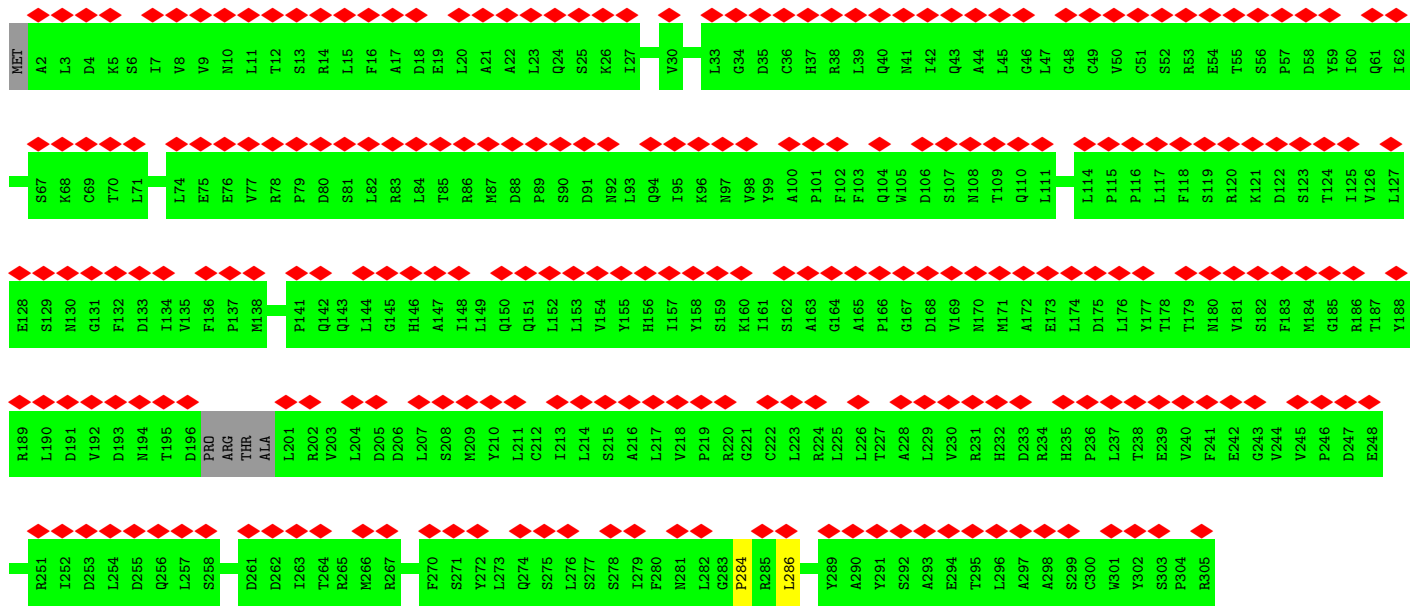
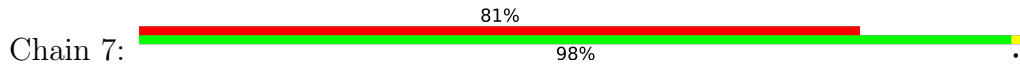
• Molecule 3: Triplex capsid protein 1



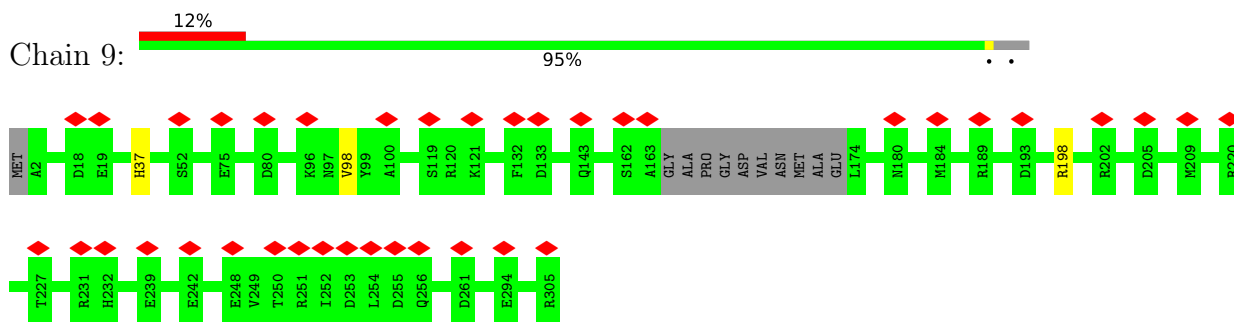
• Molecule 4: Triplex capsid protein 2



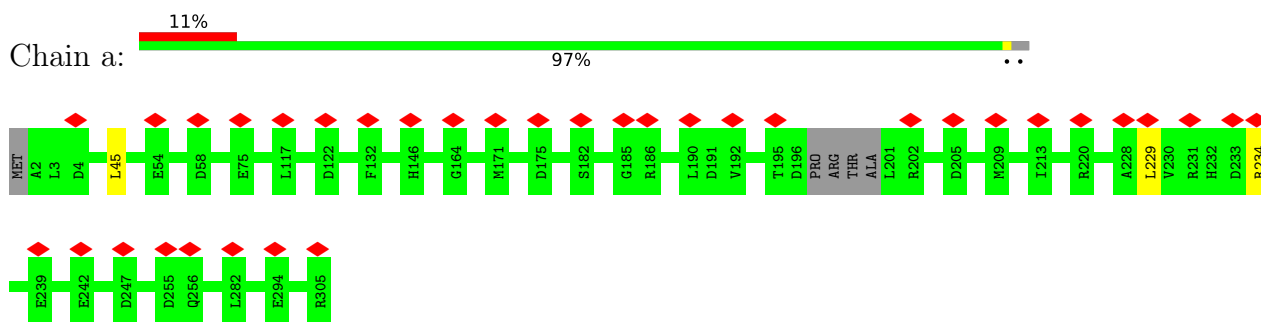
• Molecule 4: Triplex capsid protein 2



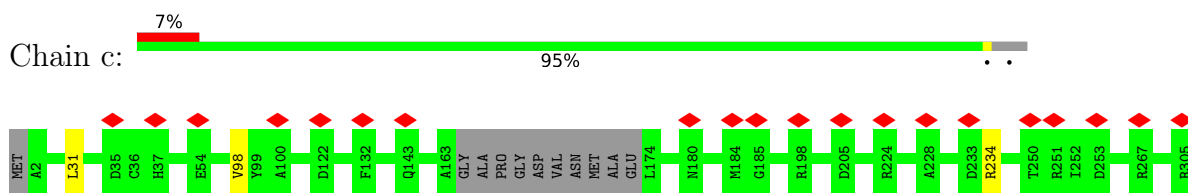
• Molecule 4: Triplex capsid protein 2



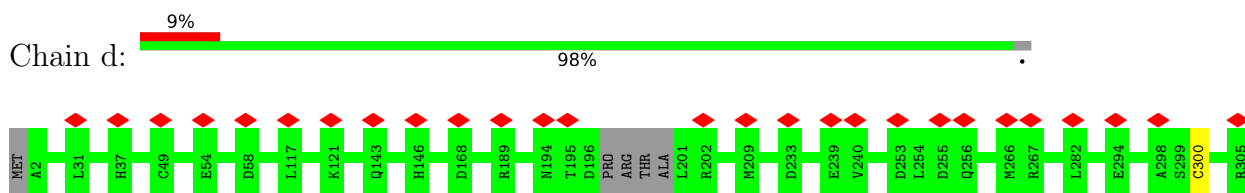
• Molecule 4: Triplex capsid protein 2



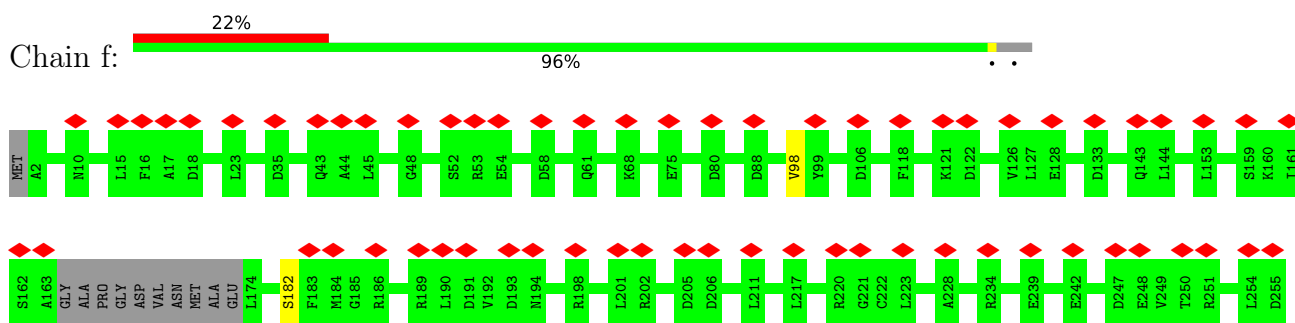
• Molecule 4: Triplex capsid protein 2

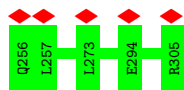


• Molecule 4: Triplex capsid protein 2

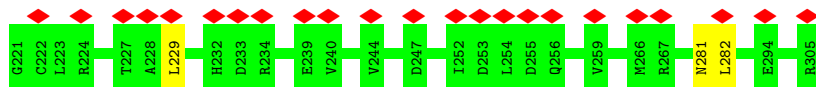
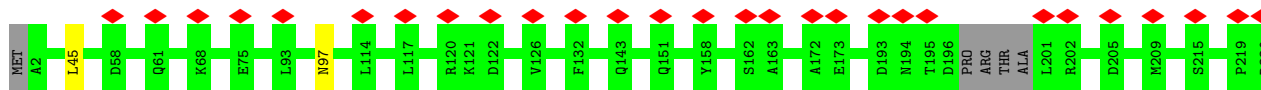


• Molecule 4: Triplex capsid protein 2

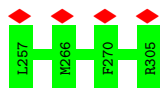
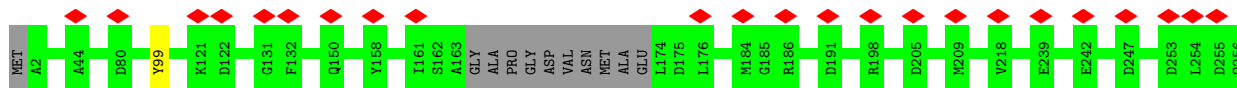




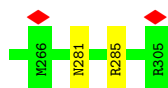
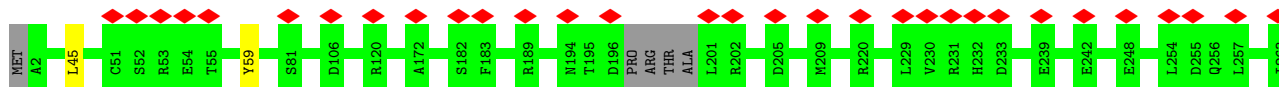
• Molecule 4: Triplex capsid protein 2



• Molecule 4: Triplex capsid protein 2



• Molecule 4: Triplex capsid protein 2



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	25315	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)	2000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	24271	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	15.720	Depositor
Minimum map value	-11.596	Depositor
Average map value	0.008	Depositor
Map value standard deviation	1.070	Depositor
Recommended contour level	2.5	Depositor
Map size (Å)	1318.3999, 1318.3999, 1318.3999	wwPDB
Map dimensions	1280, 1280, 1280	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.03, 1.03, 1.03	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	4	0.34	0/9812	0.62	3/13326 (0.0%)
1	A	0.42	0/10936	0.64	4/14866 (0.0%)
1	B	0.44	0/10879	0.67	4/14788 (0.0%)
1	C	0.43	0/10873	0.64	7/14780 (0.0%)
1	D	0.43	1/10879 (0.0%)	0.66	4/14788 (0.0%)
1	E	0.45	1/10936 (0.0%)	0.66	3/14866 (0.0%)
1	F	0.44	1/10890 (0.0%)	0.66	4/14802 (0.0%)
1	M	0.44	0/10879	0.66	3/14788 (0.0%)
1	N	0.45	1/10936 (0.0%)	0.67	5/14866 (0.0%)
1	O	0.44	0/10879	0.66	3/14788 (0.0%)
1	S	0.40	0/10298	0.64	3/13995 (0.0%)
1	T	0.42	0/10918	0.65	2/14839 (0.0%)
1	U	0.44	0/10879	0.65	1/14788 (0.0%)
1	V	0.43	0/10856	0.66	5/14757 (0.0%)
1	W	0.43	3/10873 (0.0%)	0.65	7/14780 (0.0%)
1	X	0.40	0/10797	0.64	5/14676 (0.0%)
2	0	0.37	0/682	0.52	0/919
2	1	0.38	0/682	0.52	0/919
2	2	0.37	0/682	0.52	0/919
2	3	0.37	0/682	0.52	0/919
2	G	0.38	0/682	0.52	0/919
2	H	0.37	0/682	0.52	0/919
2	I	0.37	0/682	0.52	0/919
2	J	0.37	0/682	0.52	0/919
2	K	0.38	0/682	0.52	0/919
2	L	0.37	0/682	0.52	0/919
2	P	0.37	0/682	0.52	0/919
2	Q	0.37	0/682	0.52	0/919
2	R	0.38	0/682	0.52	0/919
2	Y	0.37	0/682	0.52	0/919
2	Z	0.37	0/682	0.52	0/919
3	5	0.33	0/2525	0.62	4/3433 (0.1%)
3	8	0.41	0/2539	0.63	1/3452 (0.0%)
3	b	0.41	0/2539	0.63	0/3452

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
3	e	0.40	0/2521	0.62	1/3426 (0.0%)
3	h	0.41	0/2539	0.64	2/3452 (0.1%)
4	6	0.34	0/2375	0.65	0/3234
4	7	0.33	0/2410	0.61	1/3281 (0.0%)
4	9	0.43	0/2375	0.66	0/3234
4	a	0.45	1/2410 (0.0%)	0.65	1/3281 (0.0%)
4	c	0.43	0/2375	0.67	1/3234 (0.0%)
4	d	0.44	0/2410	0.64	0/3281
4	f	0.38	0/2375	0.65	0/3234
4	g	0.41	0/2410	0.66	2/3281 (0.1%)
4	i	0.42	0/2375	0.65	0/3234
4	j	0.43	0/2410	0.66	2/3281 (0.1%)
All	All	0.42	8/219338 (0.0%)	0.65	78/298068 (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
1	4	0	9
1	A	0	4
1	B	0	7
1	C	0	8
1	D	0	10
1	E	0	5
1	F	0	4
1	M	0	6
1	N	0	7
1	O	0	6
1	S	0	6
1	T	0	11
1	U	0	4
1	V	0	6
1	W	0	2
1	X	0	1
3	h	0	1
4	6	0	1
4	7	0	1
4	9	0	2
4	a	0	1
4	c	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
4	d	0	1
4	f	0	2
4	g	0	2
4	i	0	1
4	j	0	2
All	All	0	111

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	454	CYS	C-N	-7.03	1.17	1.34
4	a	234	ARG	CZ-NH2	-6.59	1.24	1.33
1	W	964	TYR	CD1-CE1	-6.35	1.29	1.39
1	N	9	PRO	C-N	-6.01	1.20	1.34
1	E	1192	GLN	C-N	-5.61	1.21	1.34

The worst 5 of 78 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1181	PRO	C-N-CA	10.87	148.86	121.70
1	B	1232	ARG	NE-CZ-NH1	9.29	124.94	120.30
1	X	5	LEU	CA-CB-CG	8.38	134.58	115.30
1	B	1232	ARG	NE-CZ-NH2	-8.22	116.19	120.30
1	F	454	CYS	C-N-CA	8.04	141.80	121.70

There are no chirality outliers.

5 of 111 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1109	THR	Peptide
1	A	255	ASP	Peptide
1	A	537	HIS	Peptide
1	A	899	ASP	Peptide
1	B	422	VAL	Peptide

5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles

5.3.1 Protein backbone

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	4	1200/1376 (87%)	1061 (88%)	136 (11%)	3 (0%)	41	76
1	A	1359/1376 (99%)	1204 (89%)	155 (11%)	0	100	100
1	B	1351/1376 (98%)	1192 (88%)	158 (12%)	1 (0%)	51	85
1	C	1350/1376 (98%)	1200 (89%)	148 (11%)	2 (0%)	51	85
1	D	1351/1376 (98%)	1186 (88%)	163 (12%)	2 (0%)	51	85
1	E	1359/1376 (99%)	1203 (88%)	155 (11%)	1 (0%)	51	85
1	F	1352/1376 (98%)	1197 (88%)	149 (11%)	6 (0%)	34	72
1	M	1351/1376 (98%)	1185 (88%)	163 (12%)	3 (0%)	47	80
1	N	1359/1376 (99%)	1189 (88%)	168 (12%)	2 (0%)	51	85
1	O	1351/1376 (98%)	1191 (88%)	155 (12%)	5 (0%)	34	72
1	S	1273/1376 (92%)	1126 (88%)	145 (11%)	2 (0%)	47	80
1	T	1354/1376 (98%)	1195 (88%)	154 (11%)	5 (0%)	34	72
1	U	1351/1376 (98%)	1199 (89%)	150 (11%)	2 (0%)	51	85
1	V	1348/1376 (98%)	1200 (89%)	146 (11%)	2 (0%)	51	85
1	W	1350/1376 (98%)	1211 (90%)	136 (10%)	3 (0%)	47	80
1	X	1339/1376 (97%)	1198 (90%)	140 (10%)	1 (0%)	51	85
2	0	76/170 (45%)	73 (96%)	3 (4%)	0	100	100
2	1	76/170 (45%)	73 (96%)	3 (4%)	0	100	100
2	2	76/170 (45%)	73 (96%)	3 (4%)	0	100	100
2	3	76/170 (45%)	73 (96%)	3 (4%)	0	100	100
2	G	76/170 (45%)	73 (96%)	3 (4%)	0	100	100
2	H	76/170 (45%)	73 (96%)	3 (4%)	0	100	100
2	I	76/170 (45%)	73 (96%)	3 (4%)	0	100	100
2	J	76/170 (45%)	73 (96%)	3 (4%)	0	100	100
2	K	76/170 (45%)	73 (96%)	3 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	L	76/170 (45%)	73 (96%)	3 (4%)	0	100	100
2	P	76/170 (45%)	73 (96%)	3 (4%)	0	100	100
2	Q	76/170 (45%)	73 (96%)	3 (4%)	0	100	100
2	R	76/170 (45%)	73 (96%)	3 (4%)	0	100	100
2	Y	76/170 (45%)	73 (96%)	3 (4%)	0	100	100
2	Z	76/170 (45%)	73 (96%)	3 (4%)	0	100	100
3	5	313/331 (95%)	279 (89%)	34 (11%)	0	100	100
3	8	315/331 (95%)	293 (93%)	22 (7%)	0	100	100
3	b	315/331 (95%)	288 (91%)	27 (9%)	0	100	100
3	e	311/331 (94%)	288 (93%)	23 (7%)	0	100	100
3	h	315/331 (95%)	288 (91%)	26 (8%)	1 (0%)	41	76
4	6	290/305 (95%)	263 (91%)	27 (9%)	0	100	100
4	7	296/305 (97%)	261 (88%)	35 (12%)	0	100	100
4	9	290/305 (95%)	264 (91%)	26 (9%)	0	100	100
4	a	296/305 (97%)	270 (91%)	26 (9%)	0	100	100
4	c	290/305 (95%)	265 (91%)	25 (9%)	0	100	100
4	d	296/305 (97%)	277 (94%)	19 (6%)	0	100	100
4	f	290/305 (95%)	263 (91%)	27 (9%)	0	100	100
4	g	296/305 (97%)	269 (91%)	27 (9%)	0	100	100
4	i	290/305 (95%)	264 (91%)	26 (9%)	0	100	100
4	j	296/305 (97%)	272 (92%)	24 (8%)	0	100	100
All	All	27037/29271 (92%)	24136 (89%)	2860 (11%)	41 (0%)	50	80

5 of 41 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	1251	ASN
1	O	144	GLU
1	T	10	PHE
1	V	1251	ASN
1	B	843	VAL

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	4	1039/1166 (89%)	1038 (100%)	1 (0%)	93	97
1	A	1155/1166 (99%)	1155 (100%)	0	100	100
1	B	1151/1166 (99%)	1150 (100%)	1 (0%)	93	97
1	C	1150/1166 (99%)	1150 (100%)	0	100	100
1	D	1151/1166 (99%)	1151 (100%)	0	100	100
1	E	1155/1166 (99%)	1155 (100%)	0	100	100
1	F	1152/1166 (99%)	1151 (100%)	1 (0%)	93	97
1	M	1151/1166 (99%)	1151 (100%)	0	100	100
1	N	1155/1166 (99%)	1153 (100%)	2 (0%)	93	96
1	O	1151/1166 (99%)	1149 (100%)	2 (0%)	93	96
1	S	1094/1166 (94%)	1094 (100%)	0	100	100
1	T	1154/1166 (99%)	1153 (100%)	1 (0%)	93	97
1	U	1151/1166 (99%)	1149 (100%)	2 (0%)	93	96
1	V	1148/1166 (98%)	1146 (100%)	2 (0%)	93	96
1	W	1150/1166 (99%)	1150 (100%)	0	100	100
1	X	1143/1166 (98%)	1143 (100%)	0	100	100
2	0	70/141 (50%)	70 (100%)	0	100	100
2	1	70/141 (50%)	70 (100%)	0	100	100
2	2	70/141 (50%)	70 (100%)	0	100	100
2	3	70/141 (50%)	70 (100%)	0	100	100
2	G	70/141 (50%)	70 (100%)	0	100	100
2	H	70/141 (50%)	70 (100%)	0	100	100
2	I	70/141 (50%)	70 (100%)	0	100	100
2	J	70/141 (50%)	70 (100%)	0	100	100
2	K	70/141 (50%)	70 (100%)	0	100	100
2	L	70/141 (50%)	70 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	P	70/141 (50%)	70 (100%)	0	100	100
2	Q	70/141 (50%)	70 (100%)	0	100	100
2	R	70/141 (50%)	70 (100%)	0	100	100
2	Y	70/141 (50%)	70 (100%)	0	100	100
2	Z	70/141 (50%)	70 (100%)	0	100	100
3	5	271/281 (96%)	271 (100%)	0	100	100
3	8	272/281 (97%)	272 (100%)	0	100	100
3	b	272/281 (97%)	272 (100%)	0	100	100
3	e	270/281 (96%)	270 (100%)	0	100	100
3	h	272/281 (97%)	272 (100%)	0	100	100
4	6	267/274 (97%)	267 (100%)	0	100	100
4	7	270/274 (98%)	270 (100%)	0	100	100
4	9	267/274 (97%)	266 (100%)	1 (0%)	91	94
4	a	270/274 (98%)	270 (100%)	0	100	100
4	c	267/274 (97%)	266 (100%)	1 (0%)	91	94
4	d	270/274 (98%)	270 (100%)	0	100	100
4	f	267/274 (97%)	267 (100%)	0	100	100
4	g	270/274 (98%)	269 (100%)	1 (0%)	91	94
4	i	267/274 (97%)	267 (100%)	0	100	100
4	j	270/274 (98%)	270 (100%)	0	100	100
All	All	23342/24916 (94%)	23327 (100%)	15 (0%)	93	97

5 of 15 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	U	84	ARG
4	c	234	ARG
1	U	143	LYS
4	g	281	ASN
1	4	947	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 354 such sidechains are listed below:

Mol	Chain	Res	Type
1	W	102	HIS
2	2	73	HIS
1	W	498	HIS
1	X	354	HIS
1	4	920	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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	N	1
1	F	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	N	9:PRO	C	10:PHE	N	1.20
1	F	454:CYS	C	455:HIS	N	1.17

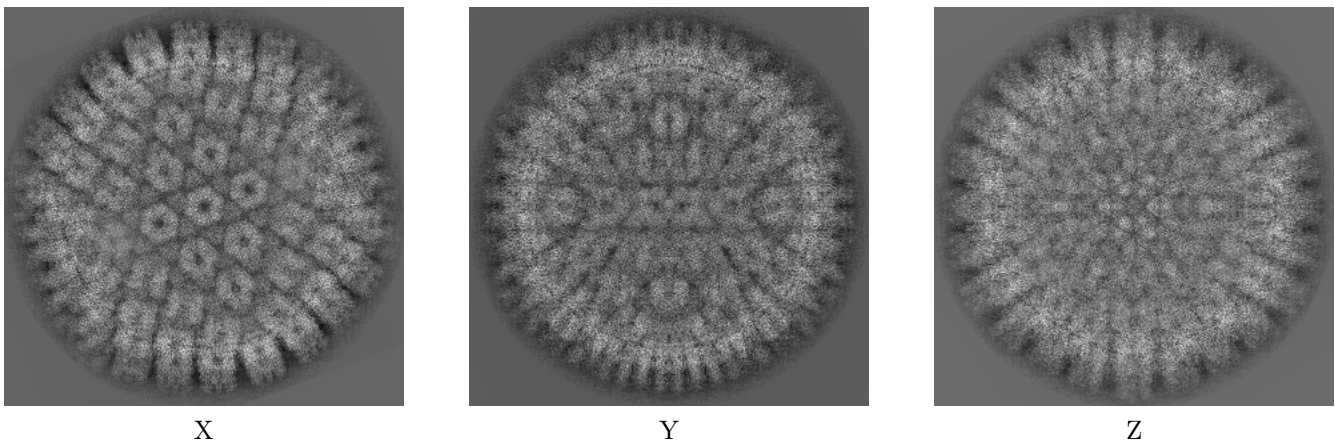
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-7047. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1 Orthogonal projections [i](#)

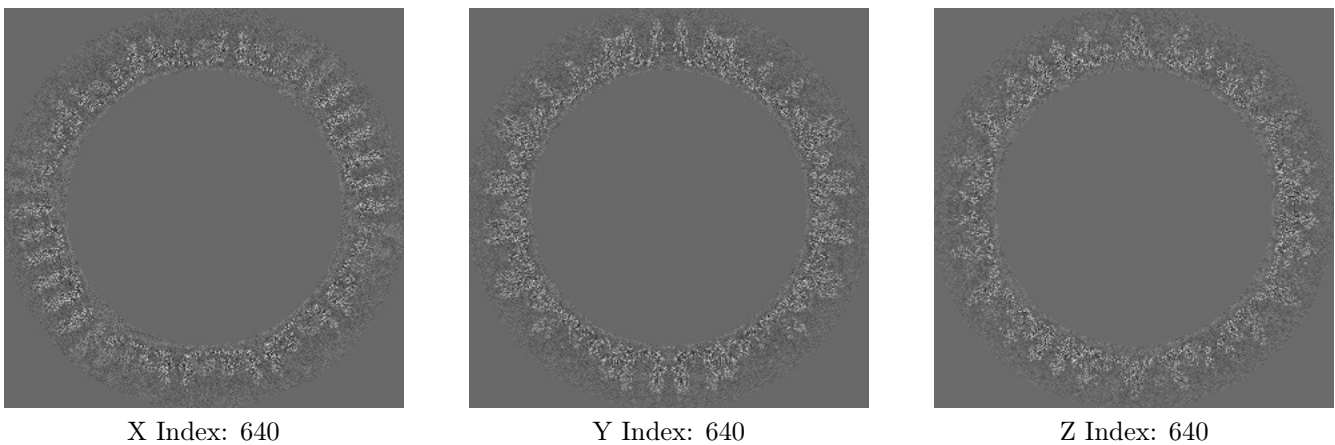
6.1.1 Primary map



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

6.2 Central slices [i](#)

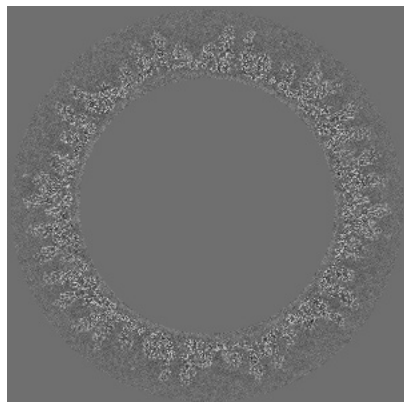
6.2.1 Primary map



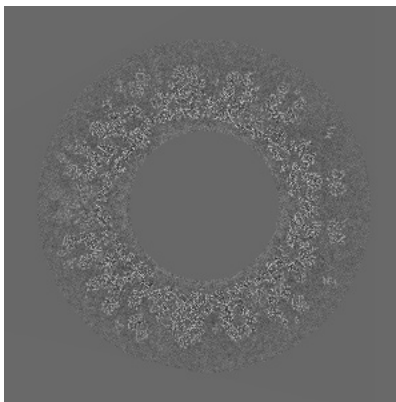
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

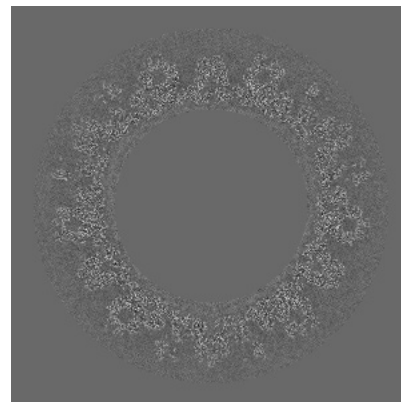
6.3.1 Primary map



X Index: 475



Y Index: 270



Z Index: 326

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

6.4 Orthogonal surface views [i](#)

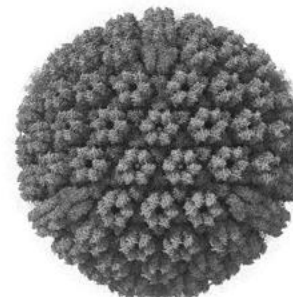
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 2.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

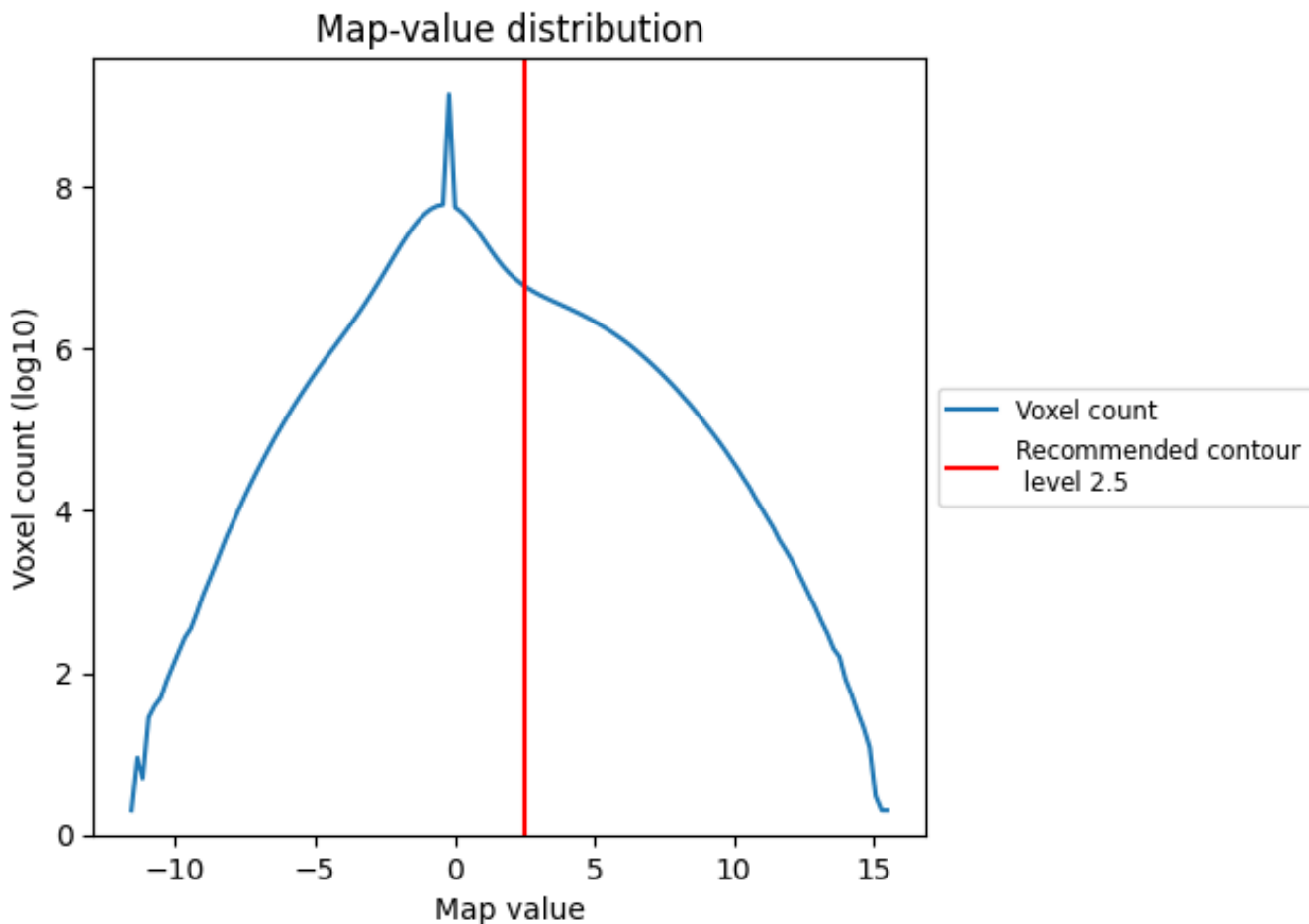
6.5 Mask visualisation

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

7 Map analysis [i](#)

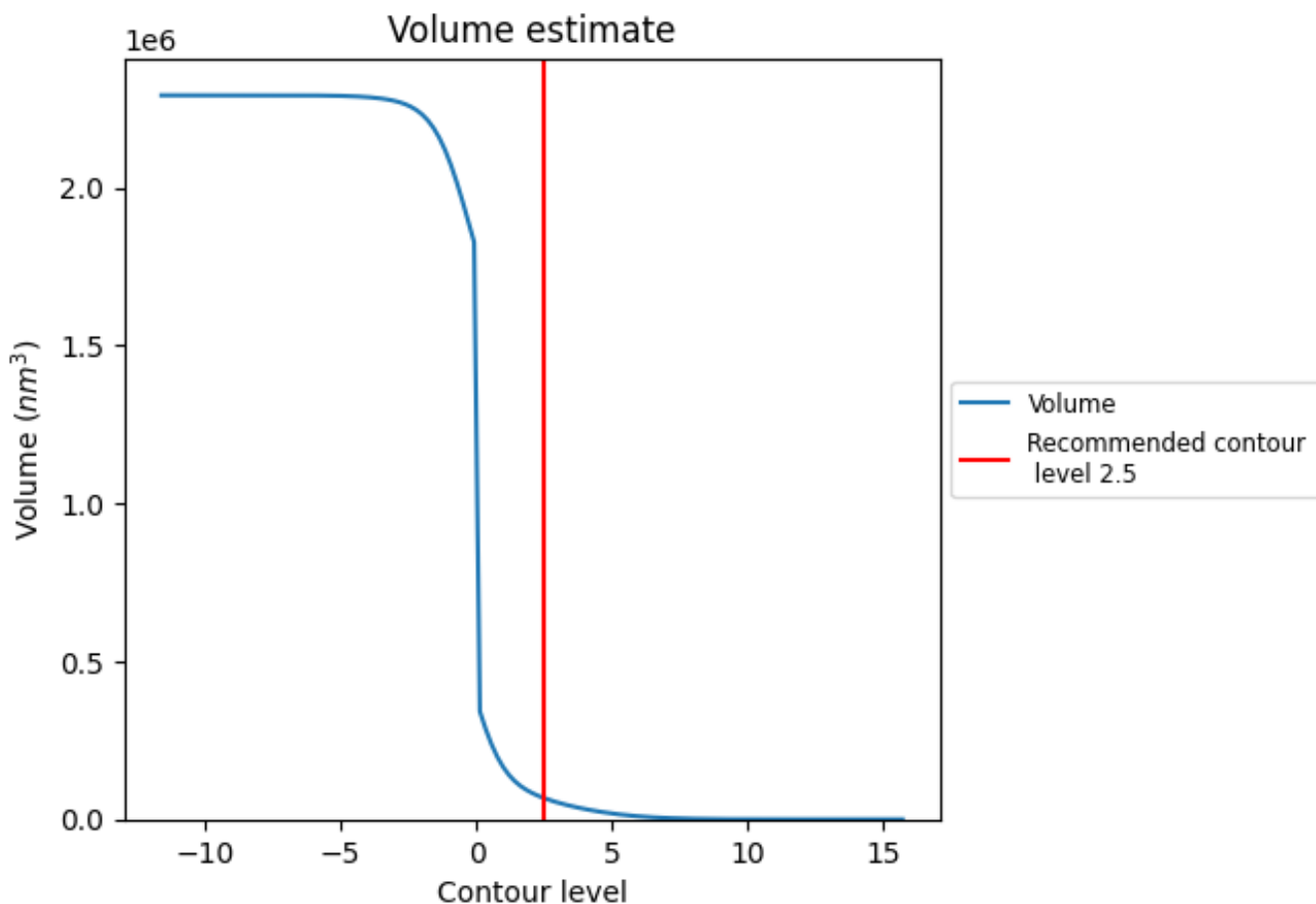
This section contains the results of statistical analysis of the map.

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.

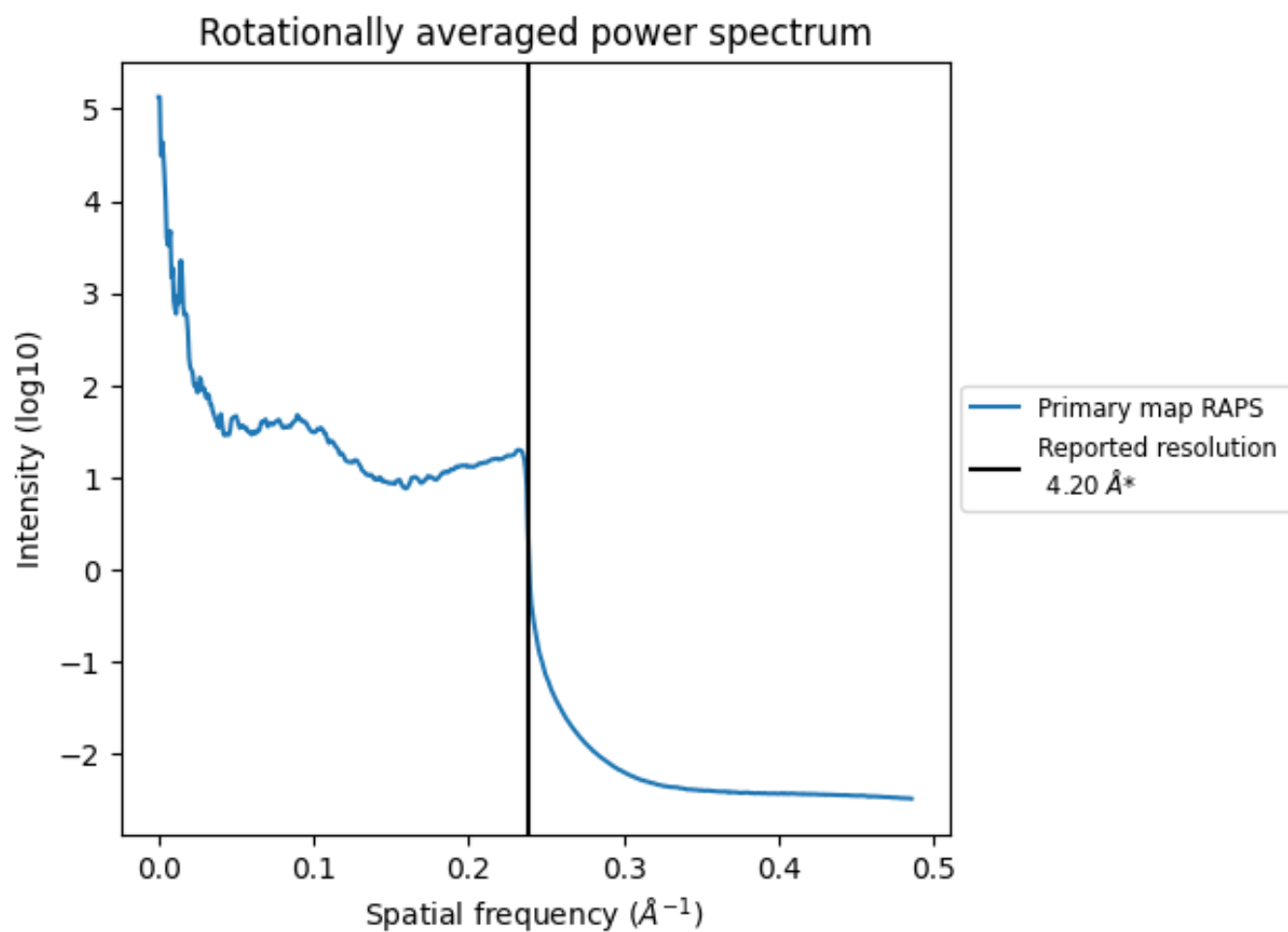
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 67318 nm³; this corresponds to an approximate mass of 60810 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 0.238\AA^{-1}

8 Fourier-Shell correlation

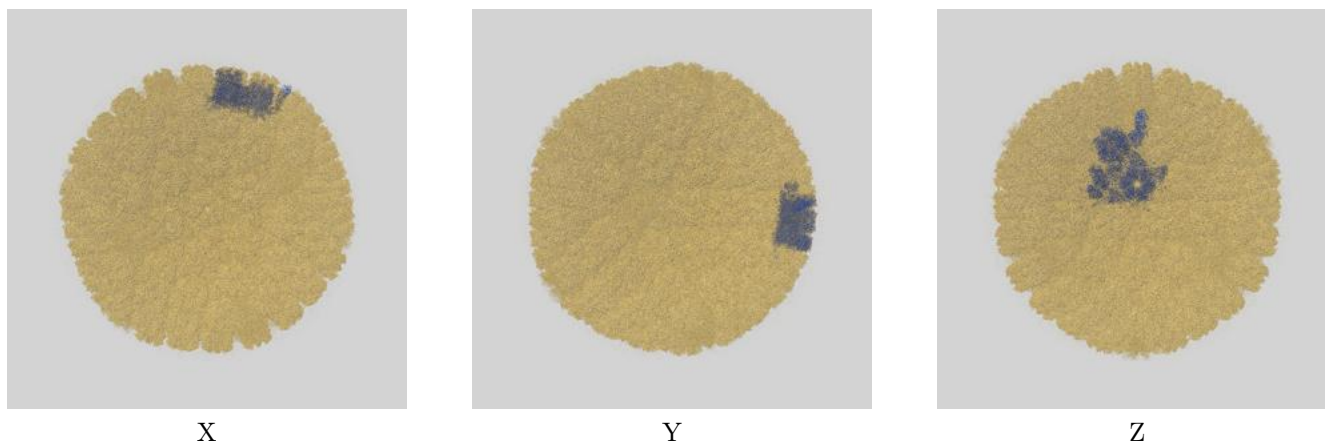
This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

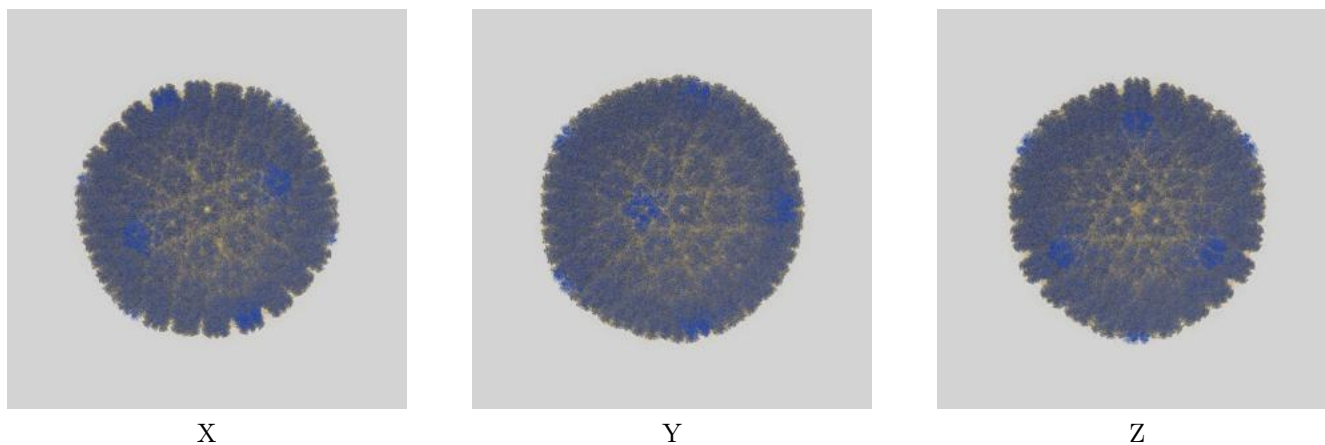
This section contains information regarding the fit between EMDB map EMD-7047 and PDB model 6B43. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlays

9.1.1 Map-model overlay [i](#)

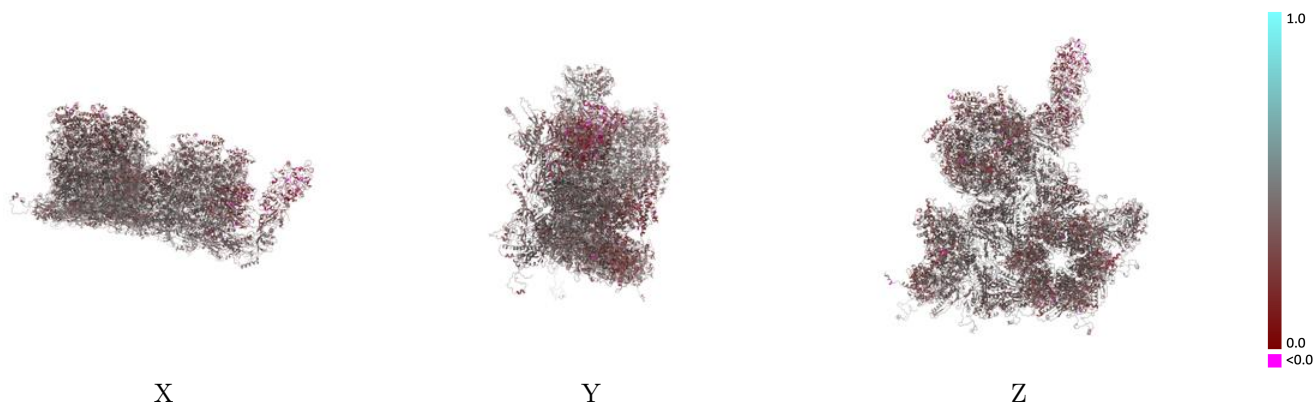


9.1.2 Map-model assembly overlay [i](#)



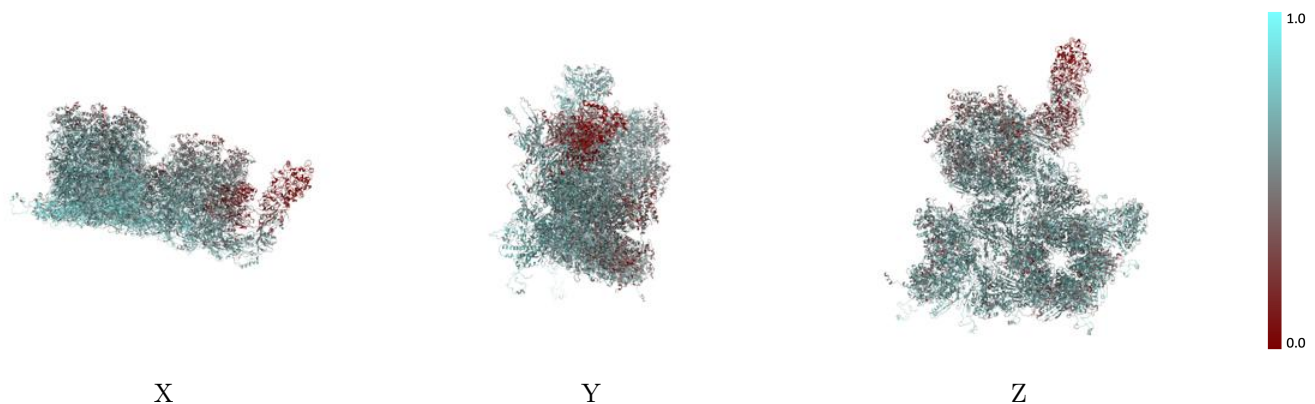
The images above show the 3D surface view of the map at the recommended contour level 2.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



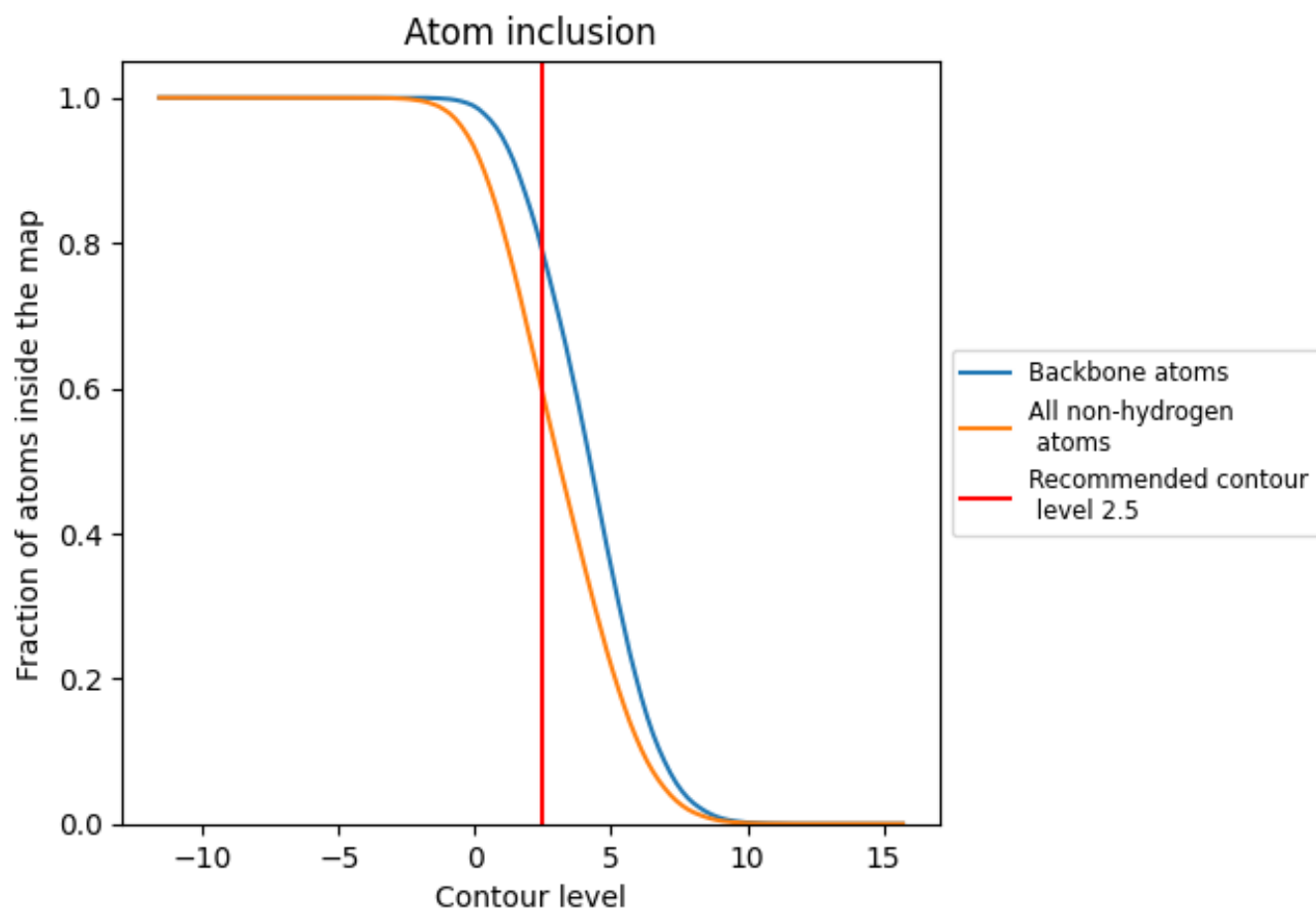
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (2.5).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 79% 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 (2.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5906	 0.3760
0	 0.4377	 0.2910
1	 0.4517	 0.3070
2	 0.3660	 0.2610
3	 0.3598	 0.2470
4	 0.2802	 0.2860
5	 0.3307	 0.3130
6	 0.3455	 0.2850
7	 0.1933	 0.2500
8	 0.6515	 0.3990
9	 0.6273	 0.3870
A	 0.6422	 0.3980
B	 0.6386	 0.3880
C	 0.6270	 0.3870
D	 0.6327	 0.3840
E	 0.6453	 0.3990
F	 0.6419	 0.3960
G	 0.4829	 0.3050
H	 0.4019	 0.2270
I	 0.5031	 0.3280
J	 0.4735	 0.2980
K	 0.4829	 0.2990
L	 0.4844	 0.3170
M	 0.6514	 0.3990
N	 0.6495	 0.3980
O	 0.6498	 0.3960
P	 0.5000	 0.3220
Q	 0.4844	 0.2840
R	 0.4953	 0.2980
S	 0.5690	 0.3780
T	 0.6079	 0.3870
U	 0.6238	 0.3890
V	 0.6213	 0.3830
W	 0.5952	 0.3780
X	 0.5732	 0.3720



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
Y	 0.3894	 0.2760
Z	 0.3520	 0.2410
a	 0.6354	 0.3950
b	 0.6457	 0.4070
c	 0.6563	 0.3980
d	 0.6505	 0.3980
e	 0.6142	 0.3910
f	 0.5618	 0.3680
g	 0.5926	 0.3790
h	 0.6379	 0.3950
i	 0.6422	 0.3950
j	 0.6410	 0.3940