



wwPDB EM Validation Summary Report ⓘ

Mar 9, 2026 – 02:39 PM UTC

PDB ID : 6W2E / pdb_00006w2e
EMDB ID : EMD-21526
Title : Structures of Capsid and Capsid-Associated Tegument Complex inside the Epstein-Barr Virus
Authors : Liu, W.; Cui, Y.X.; Wang, C.Y.; Li, Z.H.; Gong, D.Y.; Dai, X.H.; Bi, G.Q.; Sun, R.; Zhou, Z.H.
Deposited on : 2020-03-05
Resolution : 4.40 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:

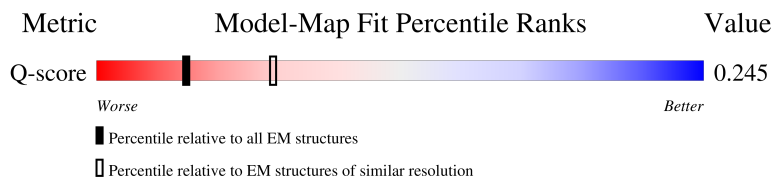
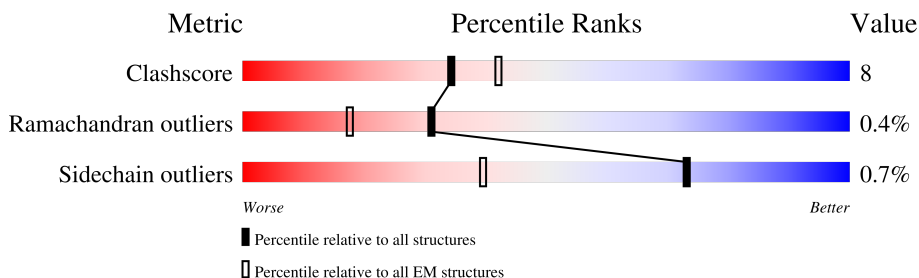
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 4.40 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	3132 (3.91 - 4.90)

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	J	1381	
1	K	1381	
1	N	1381	
1	O	1381	

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Mol	Chain	Length	Quality of chain
2	v	507	
3	w	570	
3	x	570	
4	y	3149	
4	z	3149	
5	Z	176	
5	a	176	
5	d	176	
5	e	176	
6	f	364	
6	h	364	
7	k	301	
7	m	301	
7	p	301	
7	r	301	

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 62525 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
1	J	1305	Total	C	N	O	S	0	0
			10252	6507	1779	1908	58		
1	K	1381	Total	C	N	O	S	0	0
			10832	6868	1884	2018	62		
1	N	1362	Total	C	N	O	S	0	0
			10683	6777	1854	1991	61		
1	O	1299	Total	C	N	O	S	0	0
			10194	6468	1771	1895	60		

- Molecule 2 is a protein called Capsid vertex component 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	v	293	Total	C	N	O	S	0	0
			2288	1472	398	407	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	w	68	Total	C	N	O	S	0	0
			549	332	106	108	3		
3	x	68	Total	C	N	O	S	0	0
			549	332	106	108	3		

- Molecule 4 is a protein called Large tegument protein deneddylase.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	y	37	Total	C	N	O	0	0
			317	200	64	53		
4	z	37	Total	C	N	O	0	0
			317	200	64	53		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	Z	77	Total	C	N	O	S	0	0
			649	411	121	115	2		
5	a	77	Total	C	N	O	S	0	0
			649	411	121	115	2		
5	d	77	Total	C	N	O	S	0	0
			649	411	121	115	2		
5	e	77	Total	C	N	O	S	0	0
			649	411	121	115	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	f	253	Total	C	N	O	S	0	0
			1992	1291	333	361	7		
6	h	336	Total	C	N	O	S	0	0
			2604	1667	458	471	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	k	299	Total	C	N	O	S	0	0
			2338	1500	386	434	18		
7	m	299	Total	C	N	O	S	0	0
			2338	1500	386	434	18		
7	p	299	Total	C	N	O	S	0	0
			2338	1500	386	434	18		
7	r	299	Total	C	N	O	S	0	0
			2338	1500	386	434	18		

3 Residue-property plots

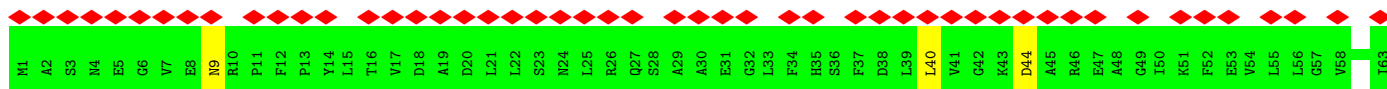
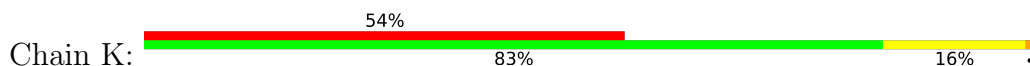
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

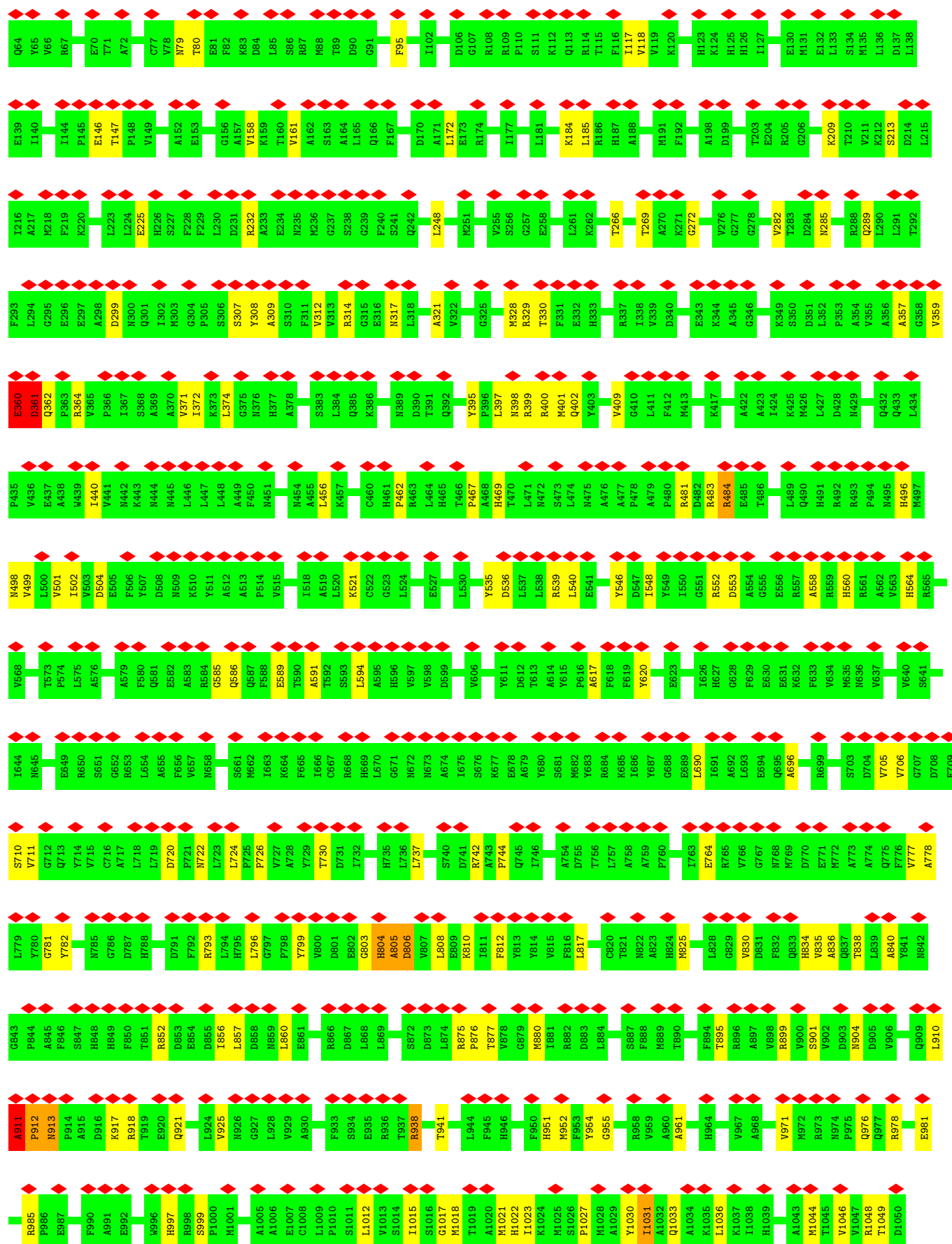
• Molecule 1: Major capsid protein

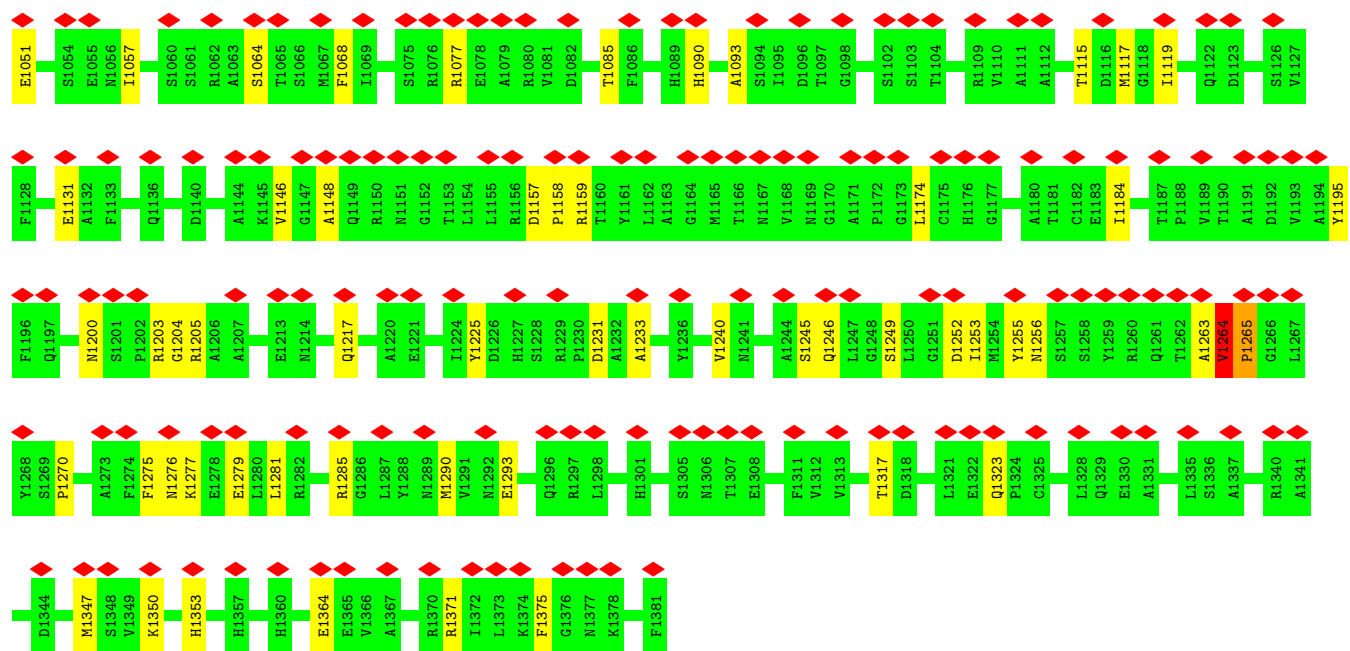




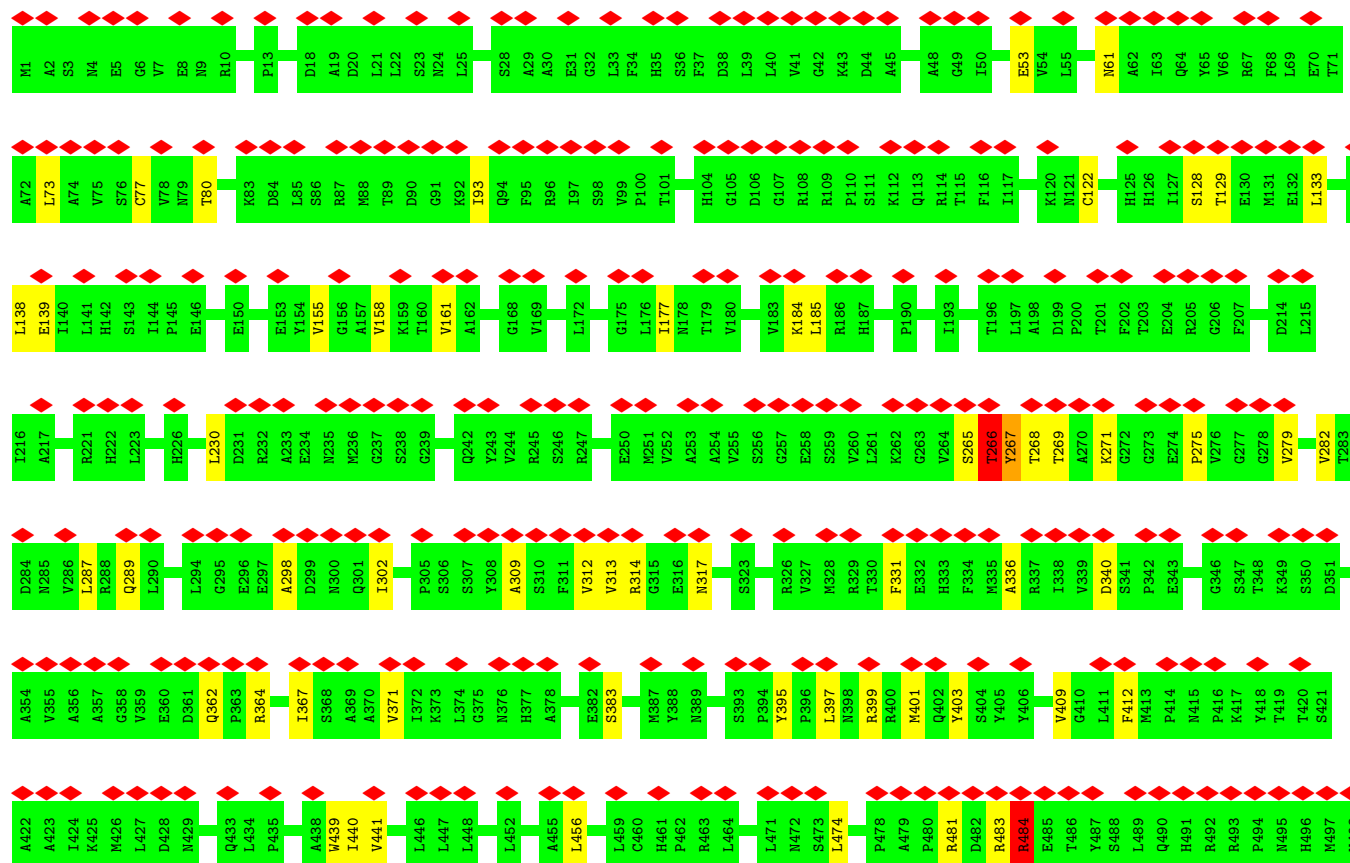
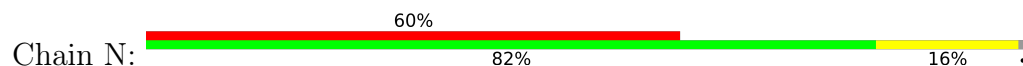
• Molecule 1: Major capsid protein



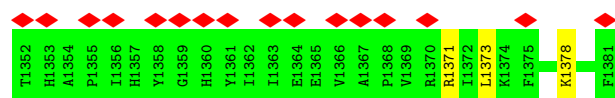




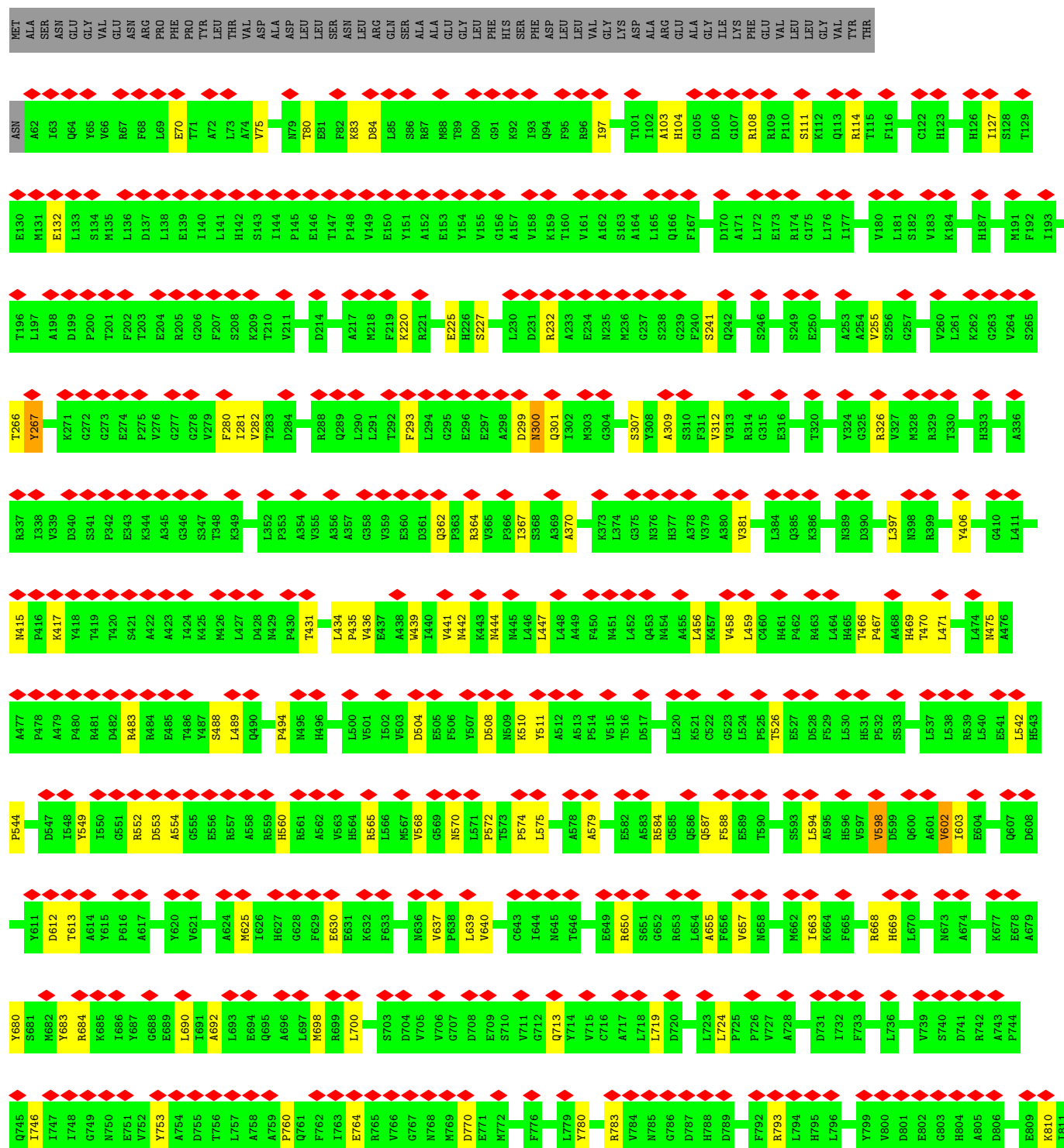
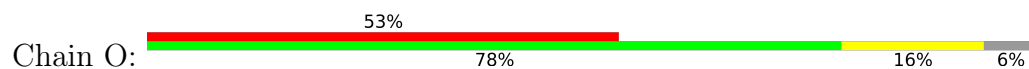
• Molecule 1: Major capsid protein

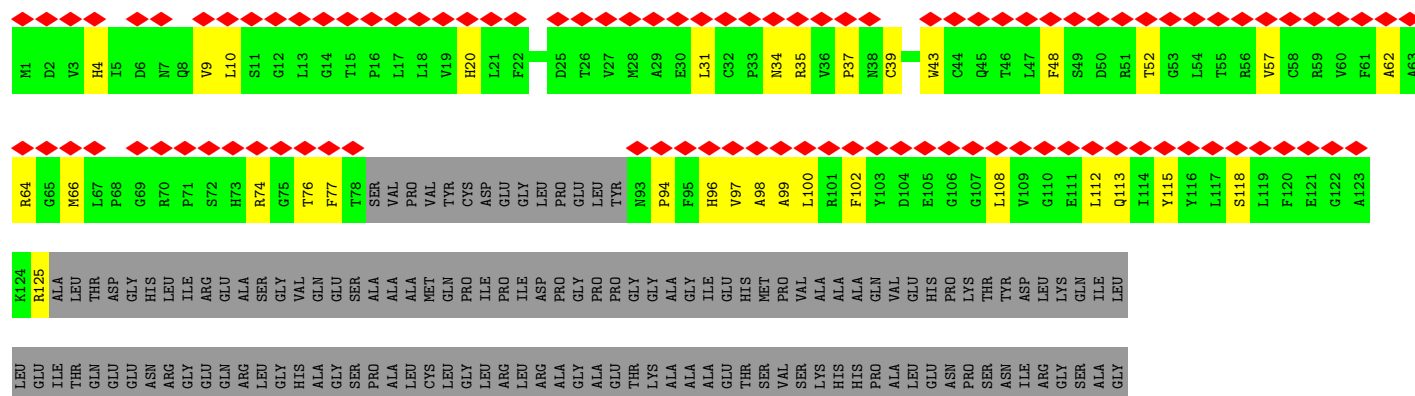
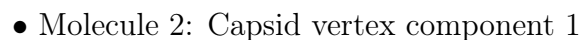


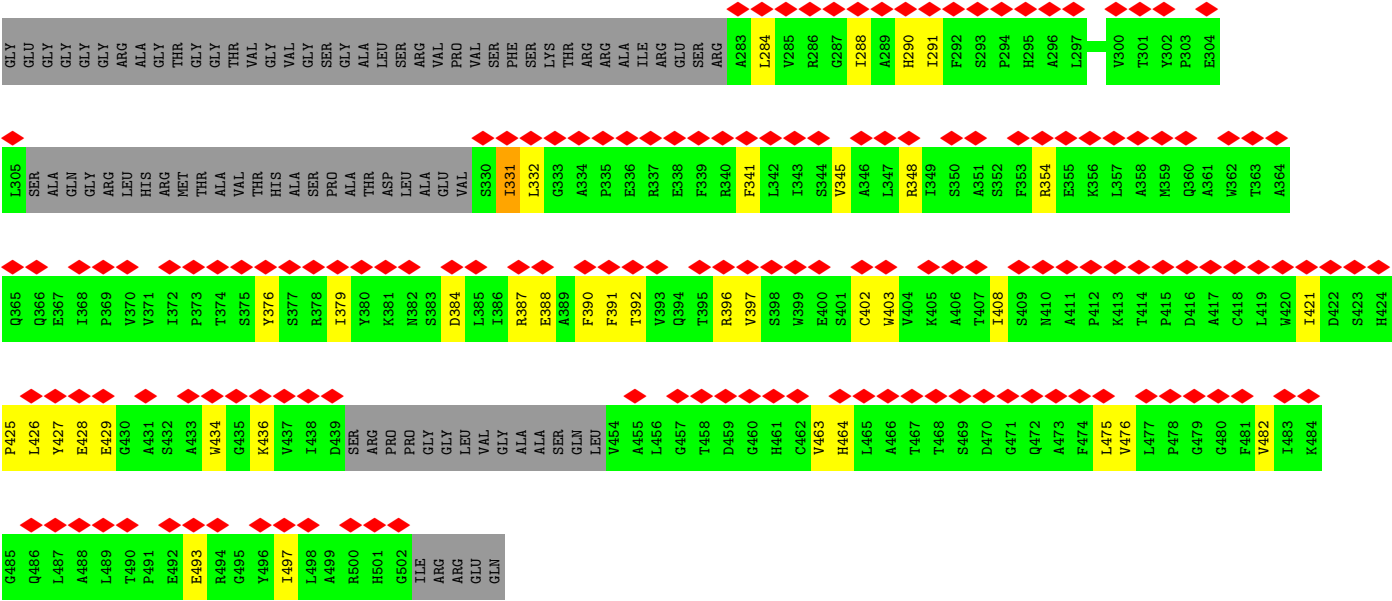
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F1086	E1087	V1088	H1089	H1090	E1091	M1092	A1093	S1094	I1095	D1096	L1099	S1100	Y1101	S1102	A1108	R1109	V1110	A1111	A1112	T1115	D1116	M1117	G1118	I1119	H1120	D1123	F1124	F1125	S1126	V1127	F1128	P1129	A1130	E1131	A1132	F1133	G1134	N1135	V1138	N1139	D1140	Y1141	I1142	K1143	A1144	K1145	V1146	G1147	A1148	Q1149	ARG	ASN	GLY	THR				
LEU	LEU	ARG	ASP	PRO	ARG	ARG	THR	TYR	LEU	ALA	GLY	MET	THR	ASN	VAL	M1169	G1170	A1171	L1174	C1175	H1176	G1177	Q1178	Q1179	A1180	E1183	I1184	I1185	V1186	T1187	P1188	V1189	T1190	A1191	D1192	V1193	A1194	Y1195	S1199	M1200	S1201	P1202	R1203	G1204	R1205	A1206	A1207	C1208	V1209	V1210	S1211	C1212	E1213	M1214	Y1215	M1216	Q1217	
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Y499	L500	V501	I502	E505	F506	Y507	D508	N509	K510	Y511	A512	A513	P514	V515	T516	D517	I518	A519	L520	K521	C522	G523	L524	P525	T526	E527	D528	F529	P532	D536	L537	L538	R539	L540	E541	L542	H543	Y546	D547	I548	Y549	I550	G551	R552	D553	A554	G555	E556	R557	A558	R559	H560	R561	H564				
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M636	V637	P638	L639	V640	S641	L642	C643	I644	Y647	W648	E649	R650	S651	G652	R653	L654	A655	F656	V657	N658	S659	F660	S661	M662	I663	K664	F665	R668	H669	L670	G671	N672	N673	A674	I675	S676	K677	E678	A679	M682	Y683	R684	K685	I686	Y687	G688	E689	L693	E694	Q695	A696	L697	M698	R699	L700			
A701	G702	S703	D704	V705	V706	G707	D708	C643	I644	Y647	W648	E649	R650	S651	G652	R653	L654	A655	F656	V657	N658	S659	F660	S661	M662	I663	K664	F665	R668	H669	L670	G671	N672	N673	A674	I675	S676	K677	E678	A679	M682	Y683	R684	K685	I686	Y687	G688	E689	L693	E694	Q695	A696	L697	M698	R699	L700		
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G829	V830	D831	F832	Q833	H834	V835	A836	Q837	T838	L839	A840	Y841	N842	G843	P844	A845	F846	S847	H848	H849	F850	T851	D852	D853	E854	D855	L856	L857	D858	N859	L860	E861	N862	G863	T864	L865	R866	D867	L868	L869	E870	T871	S872	D873	L874	S875	P876	T877	V878	G879	N880	T881	R882	L884	S885	A886	S887	F888
M889	T890	T893	F894	T895	R896	A897	V898	R899	V900	S901	Y902	D903	N904	D905	V906	T907	N913	P914	A915	D916	K917	R918	T919	E920	Q921	T922	V923	L924	V925	N926	G927	L928	V929	A930	F931	A932	F933	S934	E935	R936	T937	R938	A939	V940	T941	Q942	C943	L944	F945	H946	A947	I948	P949	F950	H951	N952	F953	
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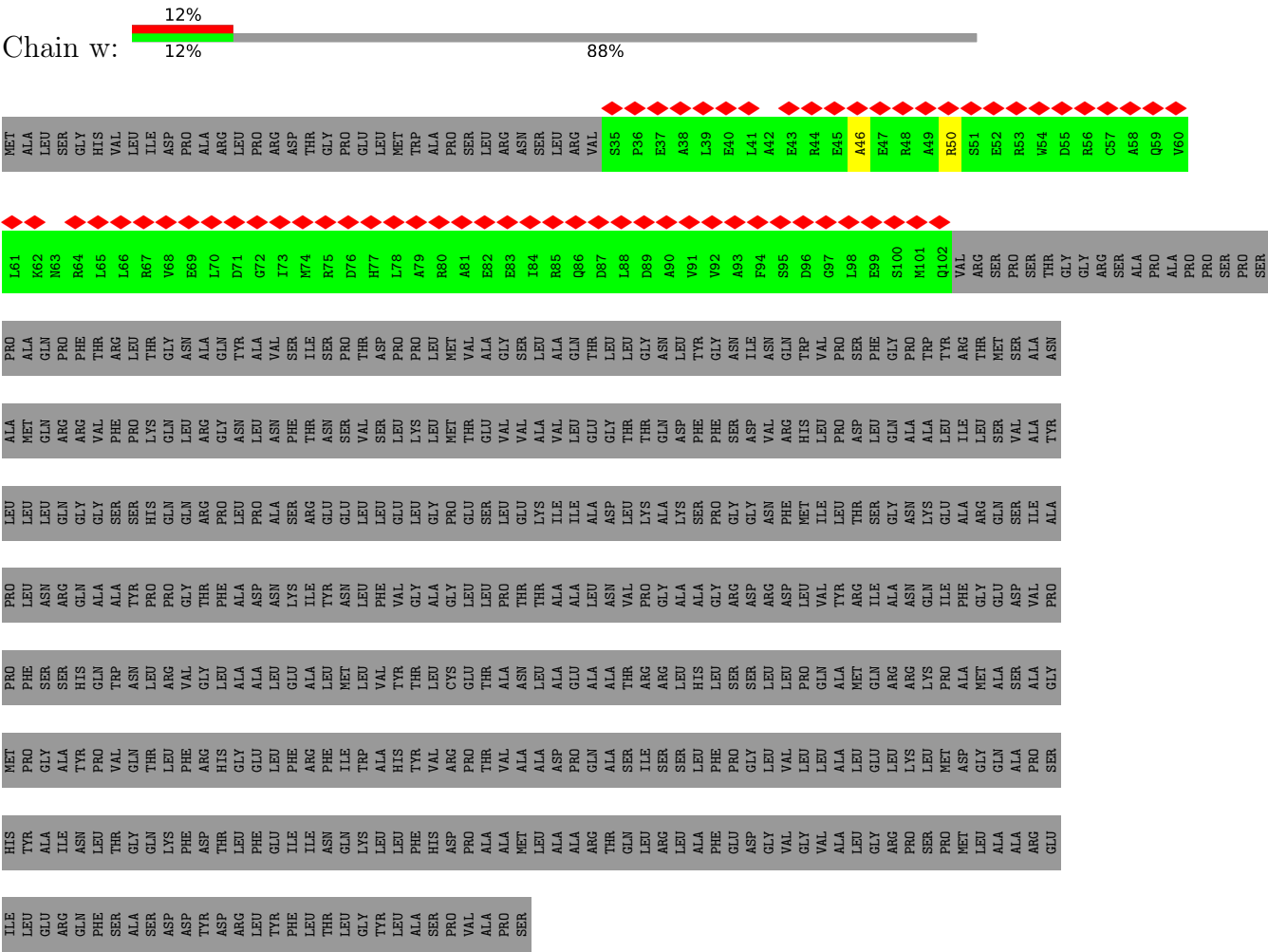
• Molecule 1: Major capsid protein



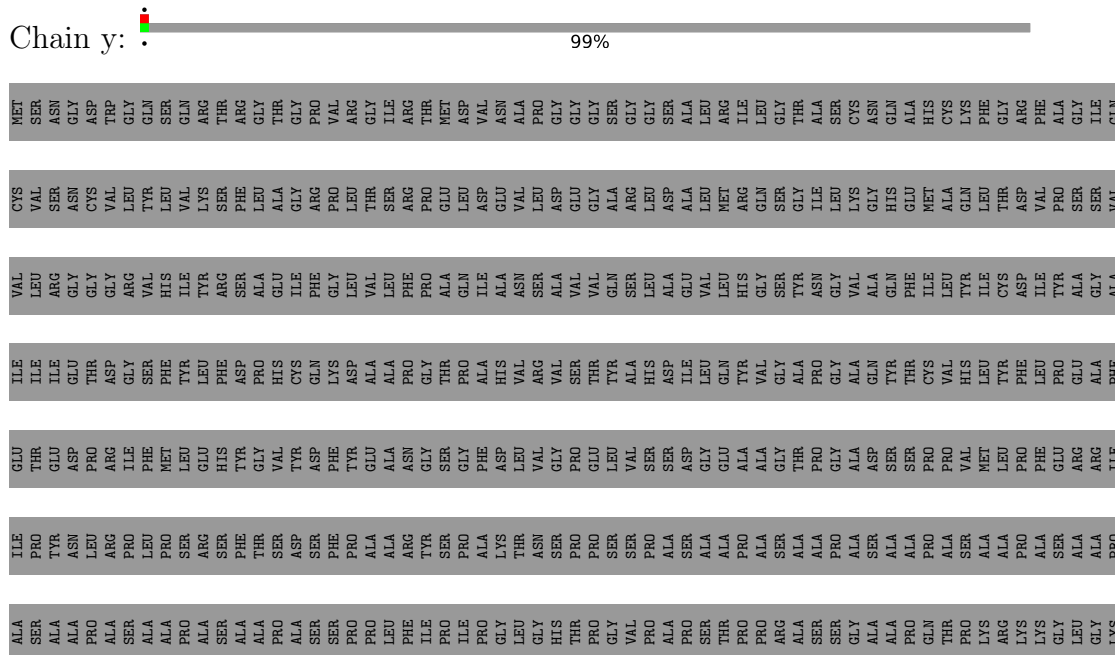




• Molecule 3: Capsid vertex component 2



• Molecule 3: Capsid vertex component 2







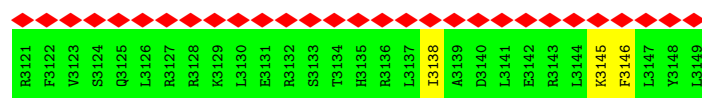
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Chain z: 99%

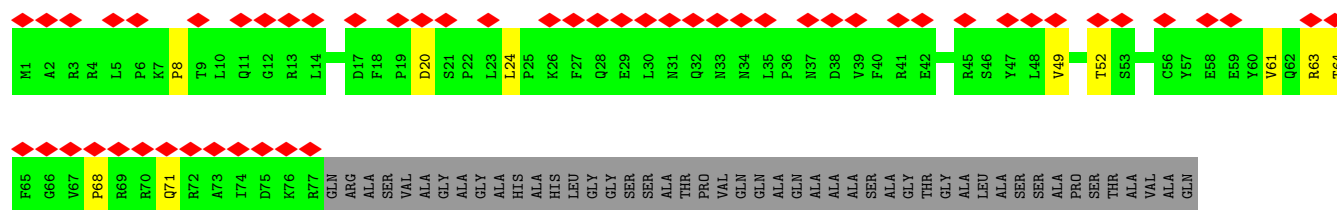
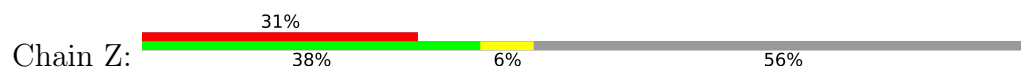
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GLU	PRO	GLN	PRO	HIS	PRO	ASN	ASP	GLY	GLY	ASN	GLY
PRO	PRO	PRO	VAL	LYS	ALA	LEU	PRO	THR	GLY	VAL	TRP
PHE	ALA	GLN	SER	PRO	SER	ARG	ILE	ASP	ARG	LEU	GLN
LEU	GLN	SER	ILE	THR	ALA	PRO	PHE	SER	VAL	TYR	GLY
MET	GLN	ALA	ALA	SER	ALA	PRO	MET	PHE	HIS	LEU	GLN
GLU	LEU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



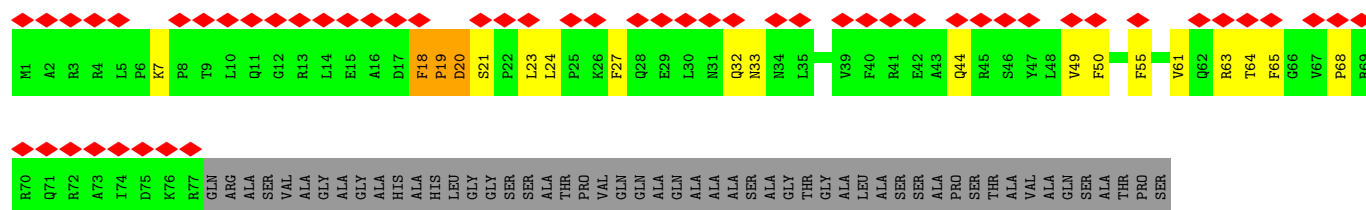
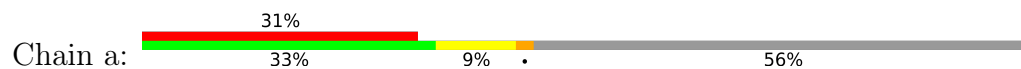




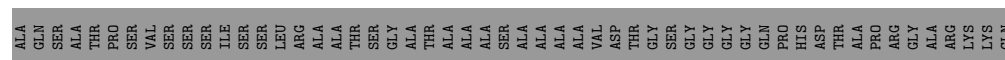
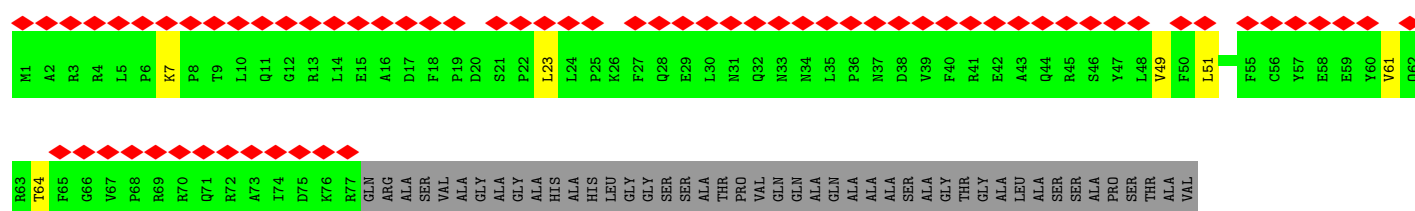
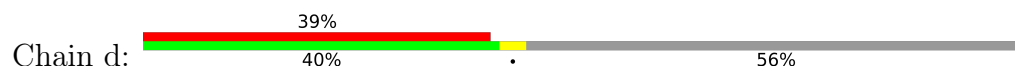
• Molecule 5: Small capsomere-interacting protein



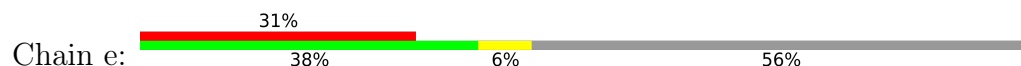
• Molecule 5: Small capsomere-interacting protein



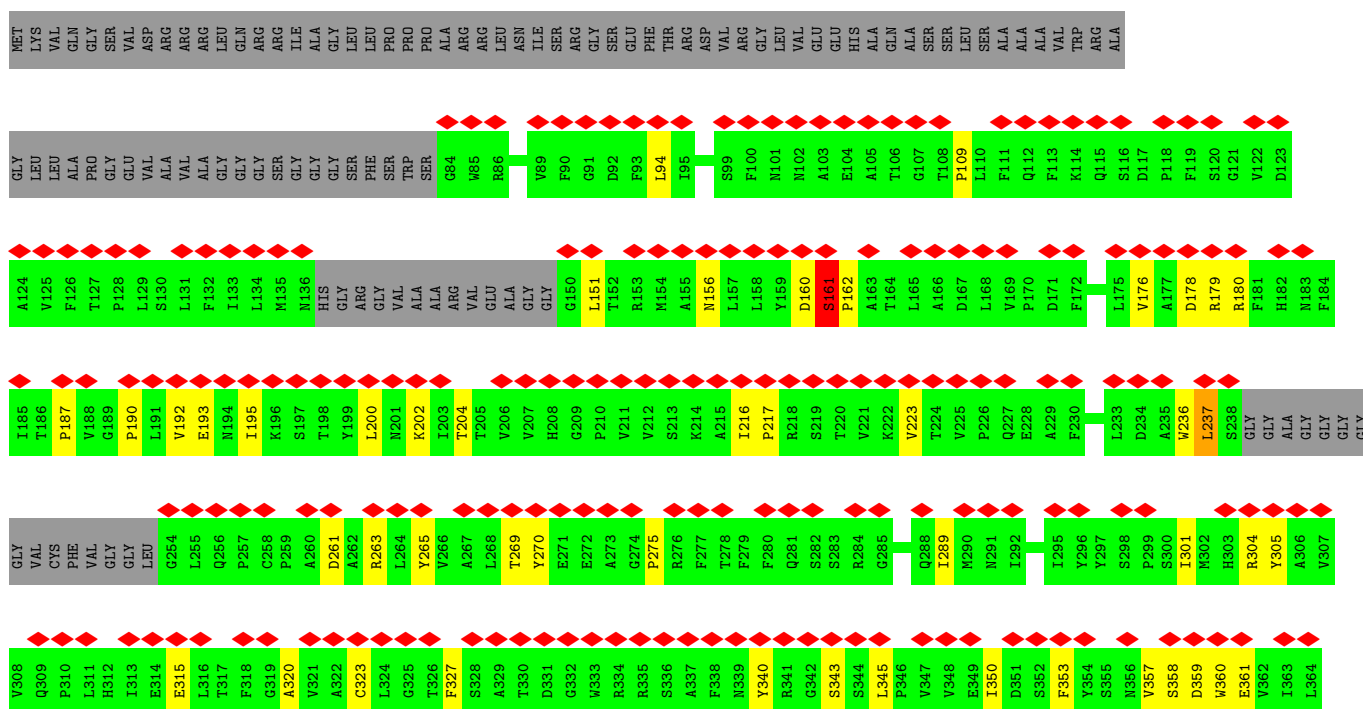
• Molecule 5: Small capsomere-interacting protein



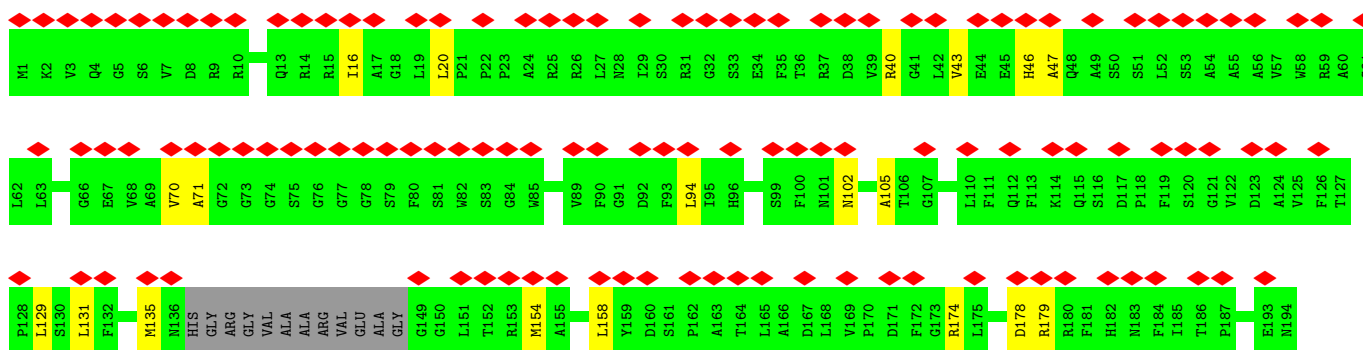
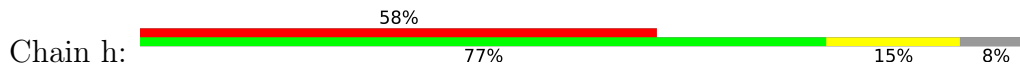
• Molecule 5: Small capsomere-interacting protein

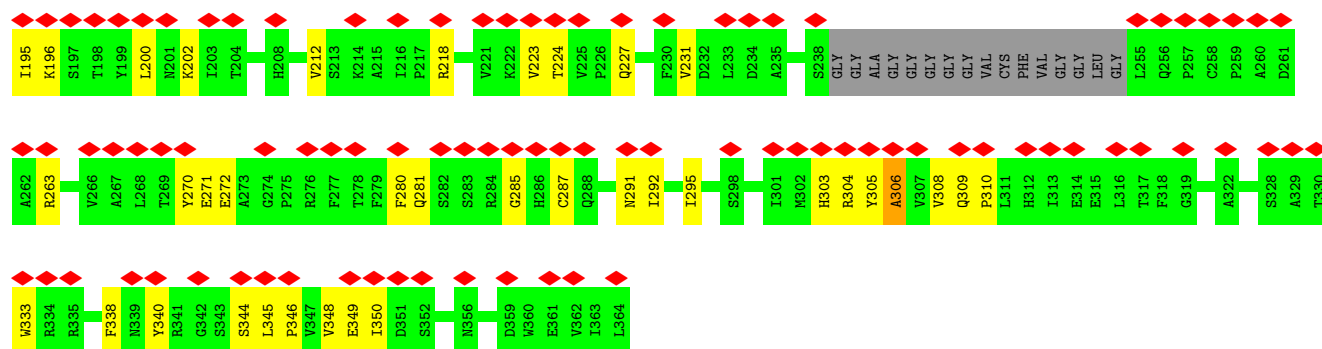


- Molecule 6: Triplex capsid protein 1

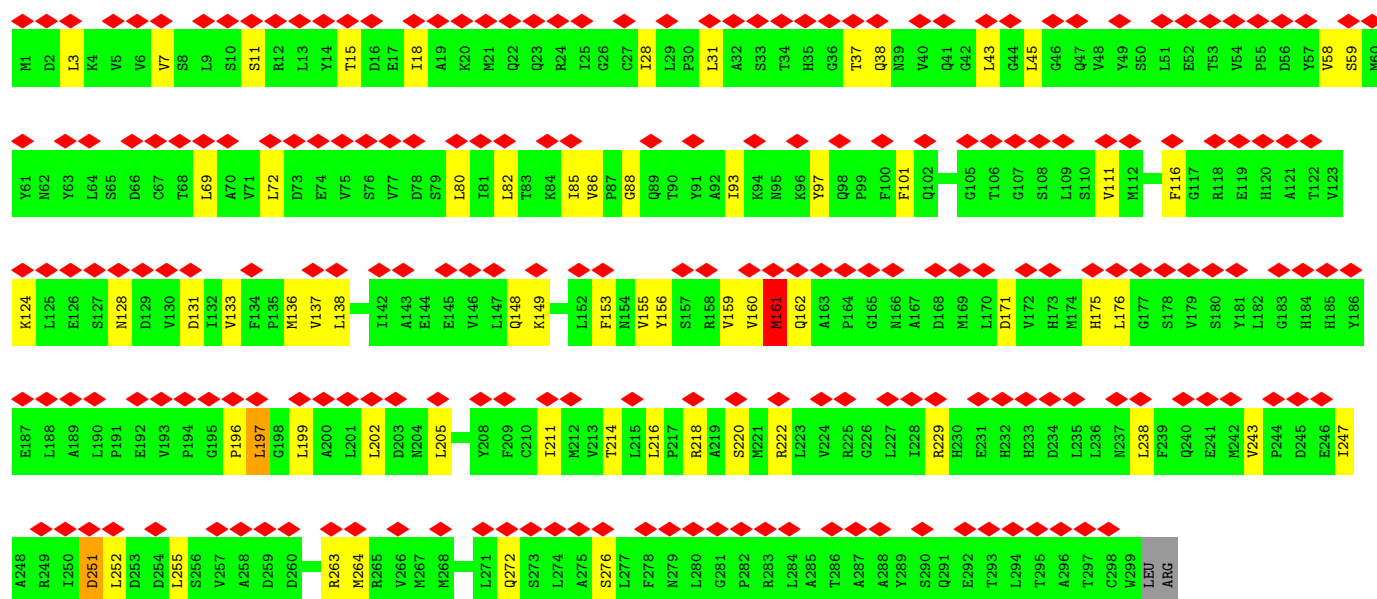
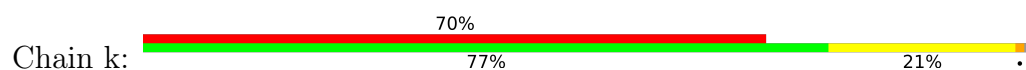


- Molecule 6: Triplex capsid protein 1

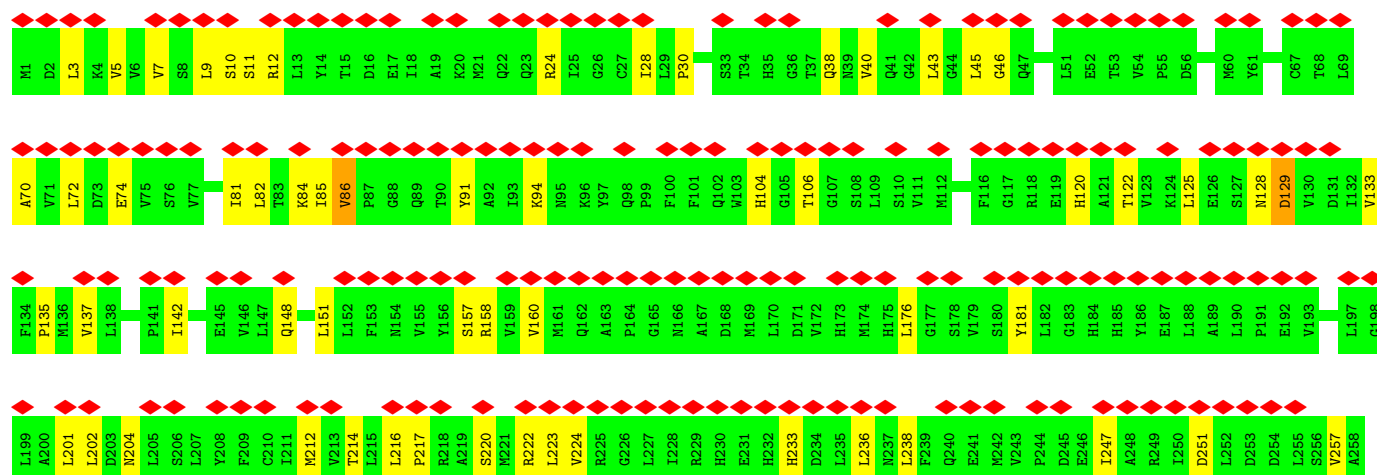
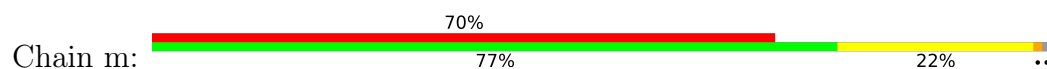


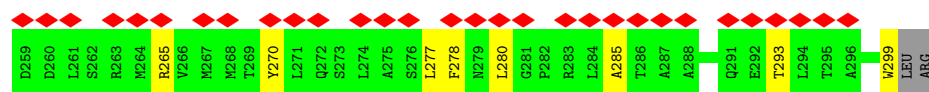


• Molecule 7: Triplex capsid protein 2

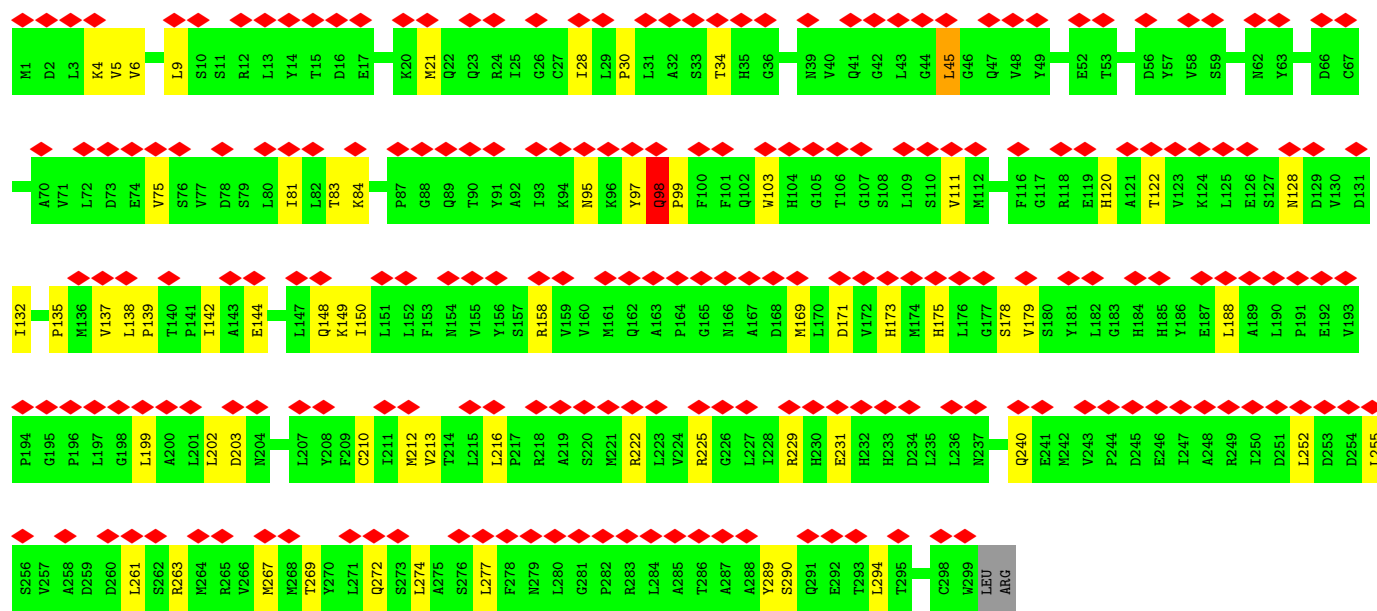
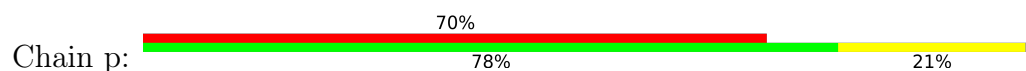


• Molecule 7: Triplex capsid protein 2

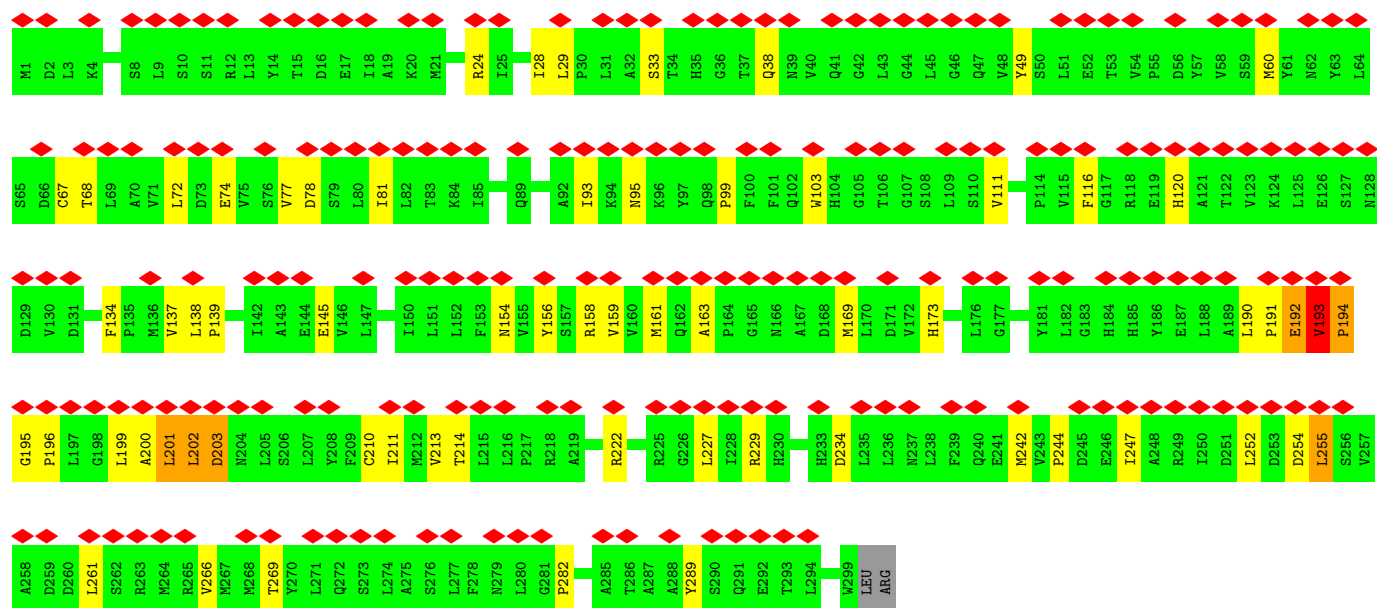
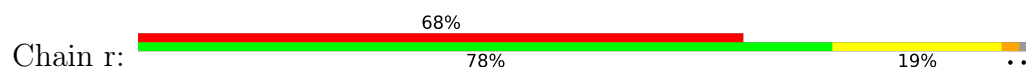




• Molecule 7: Triplex capsid protein 2



• Molecule 7: Triplex capsid protein 2



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	2305	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 ($e^-/\text{\AA}^2$)	28	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.040	Depositor
Minimum map value	-0.027	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.012	Depositor
Map size (Å)	435.2, 435.2, 435.2	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.36, 1.36, 1.36	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	J	0.27	0/10492	0.61	6/14259 (0.0%)
1	K	0.28	0/11085	0.63	6/15066 (0.0%)
1	N	0.28	0/10933	0.59	1/14858 (0.0%)
1	O	0.28	0/10435	0.60	2/14183 (0.0%)
2	v	0.31	0/2346	0.70	1/3190 (0.0%)
3	w	0.32	0/553	0.61	0/741
3	x	0.30	0/553	0.56	0/741
4	y	0.27	0/320	0.60	0/424
4	z	0.27	0/320	0.56	0/424
5	Z	0.31	0/664	0.67	0/896
5	a	0.29	0/664	1.04	2/896 (0.2%)
5	d	0.32	0/664	0.60	0/896
5	e	0.26	0/664	0.59	0/896
6	f	0.29	0/2049	0.88	2/2795 (0.1%)
6	h	0.28	0/2672	0.67	2/3635 (0.1%)
7	k	0.28	0/2388	0.60	2/3254 (0.1%)
7	m	0.29	0/2388	0.62	0/3254
7	p	0.27	0/2388	0.63	1/3254 (0.0%)
7	r	0.28	0/2388	0.64	1/3254 (0.0%)
All	All	0.28	0/63966	0.63	26/86916 (0.0%)

There are no bond length outliers.

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	f	161	SER	CA-C-N	-23.18	90.86	119.84
6	f	161	SER	C-N-CA	-23.18	90.86	119.84
5	a	18	PHE	CA-C-N	-16.47	99.25	119.84
5	a	18	PHE	C-N-CA	-16.47	99.25	119.84
1	N	483	ARG	N-CA-C	9.12	120.82	111.07

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	J	10252	0	10074	165	0
1	K	10832	0	10655	186	0
1	N	10683	0	10500	153	0
1	O	10194	0	10022	147	0
2	v	2288	0	2273	60	0
3	w	549	0	540	5	0
3	x	549	0	540	23	0
4	y	317	0	341	6	0
4	z	317	0	341	5	0
5	Z	649	0	649	6	0
5	a	649	0	649	23	0
5	d	649	0	649	4	0
5	e	649	0	649	6	0
6	f	1992	0	1953	32	0
6	h	2604	0	2577	33	0
7	k	2338	0	2364	67	0
7	m	2338	0	2364	50	0
7	p	2338	0	2364	72	0
7	r	2338	0	2364	74	0
All	All	62525	0	61868	1008	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 1008 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:857:LEU:HD12	1:K:875:ARG:CD	1.20	1.58
1:J:1264:VAL:CG1	1:J:1265:PRO:HD2	1.34	1.52
1:K:1264:VAL:HB	1:K:1265:PRO:CD	1.09	1.44
7:r:193:VAL:HB	7:r:194:PRO:CD	1.33	1.43
1:K:1264:VAL:CB	1:K:1265:PRO:HD2	1.45	1.42

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	J	1299/1381 (94%)	1225 (94%)	73 (6%)	1 (0%)	48	83
1	K	1379/1381 (100%)	1313 (95%)	56 (4%)	10 (1%)	18	55
1	N	1358/1381 (98%)	1305 (96%)	49 (4%)	4 (0%)	36	71
1	O	1295/1381 (94%)	1239 (96%)	52 (4%)	4 (0%)	36	71
2	v	283/507 (56%)	260 (92%)	22 (8%)	1 (0%)	30	66
3	w	66/570 (12%)	65 (98%)	1 (2%)	0	100	100
3	x	66/570 (12%)	66 (100%)	0	0	100	100
4	y	35/3149 (1%)	35 (100%)	0	0	100	100
4	z	35/3149 (1%)	34 (97%)	1 (3%)	0	100	100
5	Z	75/176 (43%)	71 (95%)	4 (5%)	0	100	100
5	a	75/176 (43%)	71 (95%)	3 (4%)	1 (1%)	9	41
5	d	75/176 (43%)	73 (97%)	2 (3%)	0	100	100
5	e	75/176 (43%)	73 (97%)	1 (1%)	1 (1%)	9	41
6	f	247/364 (68%)	224 (91%)	21 (8%)	2 (1%)	16	52
6	h	330/364 (91%)	308 (93%)	20 (6%)	2 (1%)	21	58
7	k	297/301 (99%)	282 (95%)	14 (5%)	1 (0%)	36	71
7	m	297/301 (99%)	281 (95%)	15 (5%)	1 (0%)	36	71
7	p	297/301 (99%)	285 (96%)	11 (4%)	1 (0%)	36	71
7	r	297/301 (99%)	282 (95%)	10 (3%)	5 (2%)	7	35
All	All	7881/16105 (49%)	7492 (95%)	355 (4%)	34 (0%)	31	66

5 of 34 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	J	556	GLU
1	K	360	GLU
1	K	911	ALA
1	K	912	PRO
1	K	1264	VAL

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	J	1110/1171 (95%)	1105 (100%)	5 (0%)	81	81
1	K	1171/1171 (100%)	1163 (99%)	8 (1%)	76	79
1	N	1155/1171 (99%)	1146 (99%)	9 (1%)	73	77
1	O	1103/1171 (94%)	1096 (99%)	7 (1%)	78	80
2	v	243/400 (61%)	239 (98%)	4 (2%)	55	69
3	w	57/465 (12%)	57 (100%)	0	100	100
3	x	57/465 (12%)	57 (100%)	0	100	100
4	y	35/2539 (1%)	35 (100%)	0	100	100
4	z	35/2539 (1%)	35 (100%)	0	100	100
5	Z	71/128 (56%)	71 (100%)	0	100	100
5	a	71/128 (56%)	70 (99%)	1 (1%)	59	71
5	d	71/128 (56%)	71 (100%)	0	100	100
5	e	71/128 (56%)	71 (100%)	0	100	100
6	f	218/289 (75%)	217 (100%)	1 (0%)	81	81
6	h	278/289 (96%)	278 (100%)	0	100	100
7	k	265/267 (99%)	263 (99%)	2 (1%)	73	77
7	m	265/267 (99%)	263 (99%)	2 (1%)	73	77
7	p	265/267 (99%)	263 (99%)	2 (1%)	73	77
7	r	265/267 (99%)	260 (98%)	5 (2%)	50	66
All	All	6806/13250 (51%)	6760 (99%)	46 (1%)	73	79

5 of 46 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	O	1369	VAL
7	k	161	MET
2	v	52	THR
2	v	397	VAL
7	m	86	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 132 such sidechains are listed below:

Mol	Chain	Res	Type
7	k	204	ASN
7	m	128	ASN
7	r	204	ASN
1	N	125	HIS
1	N	123	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no 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 ⓘ

There are no chain breaks in this entry.

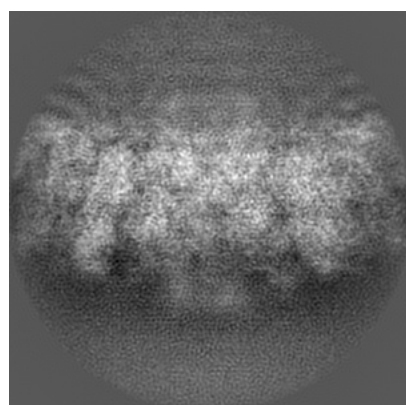
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-21526. These allow visual inspection of the internal detail of the map and identification of artifacts.

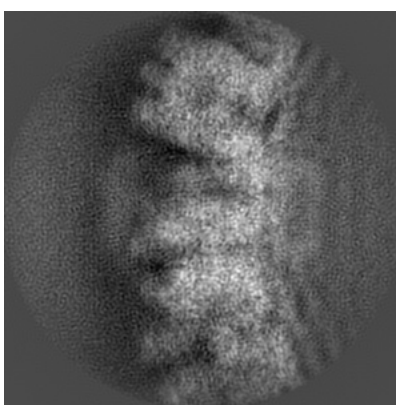
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

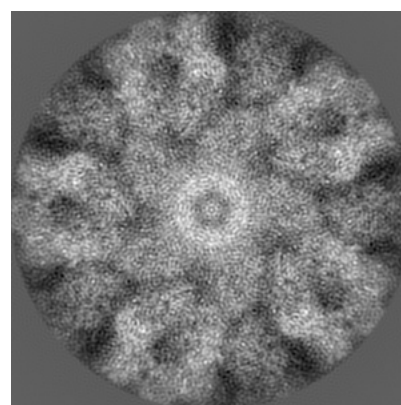
6.1.1 Primary map



X



Y

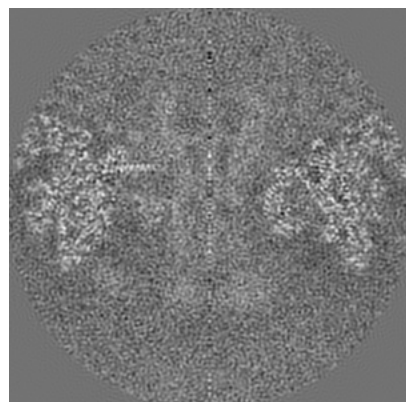


Z

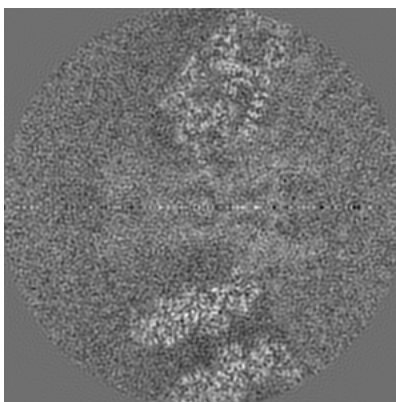
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

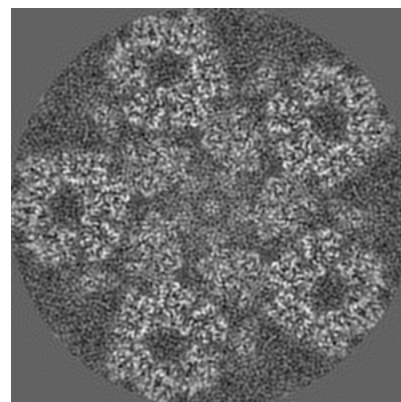
6.2.1 Primary map



X Index: 160



Y Index: 160

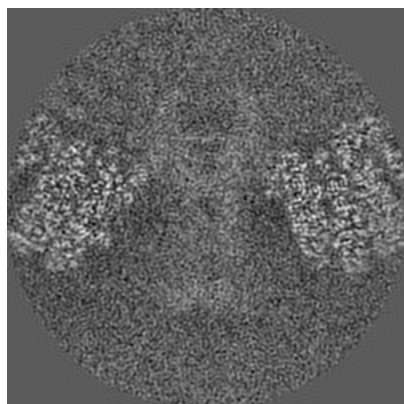


Z Index: 160

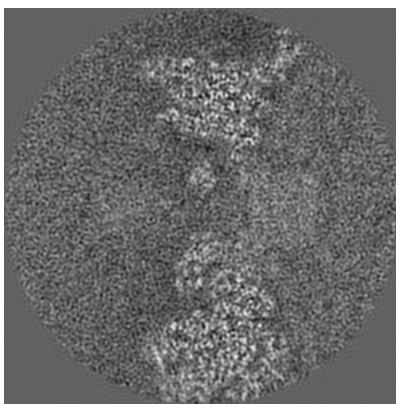
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

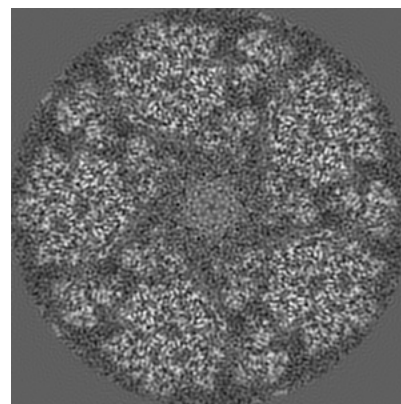
6.3.1 Primary map



X Index: 147



Y Index: 193

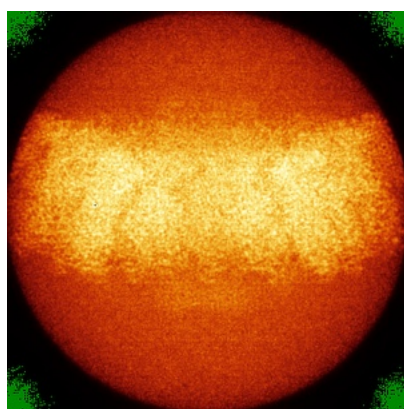


Z Index: 175

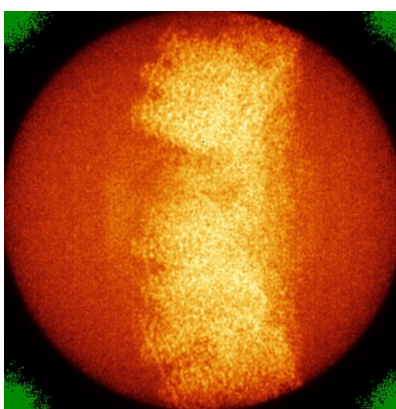
The images above show the largest variance slices of the map in three orthogonal directions.

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

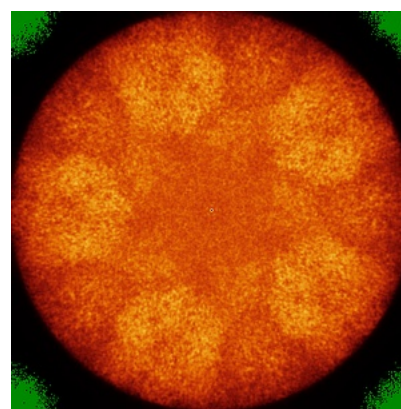
6.4.1 Primary map



X



Y



Z

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

This section was not generated.

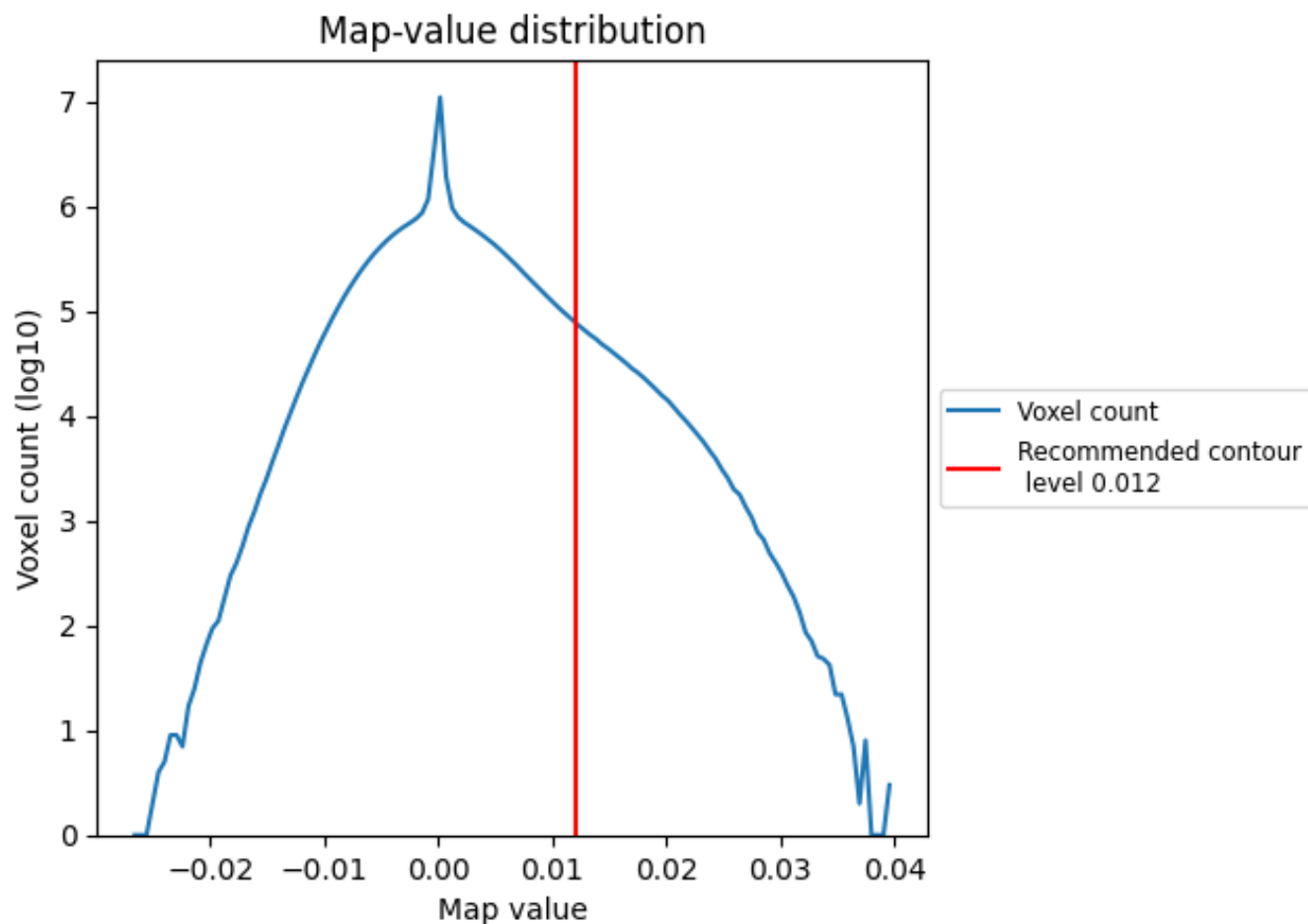
6.6 Mask visualisation

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

7 Map analysis [i](#)

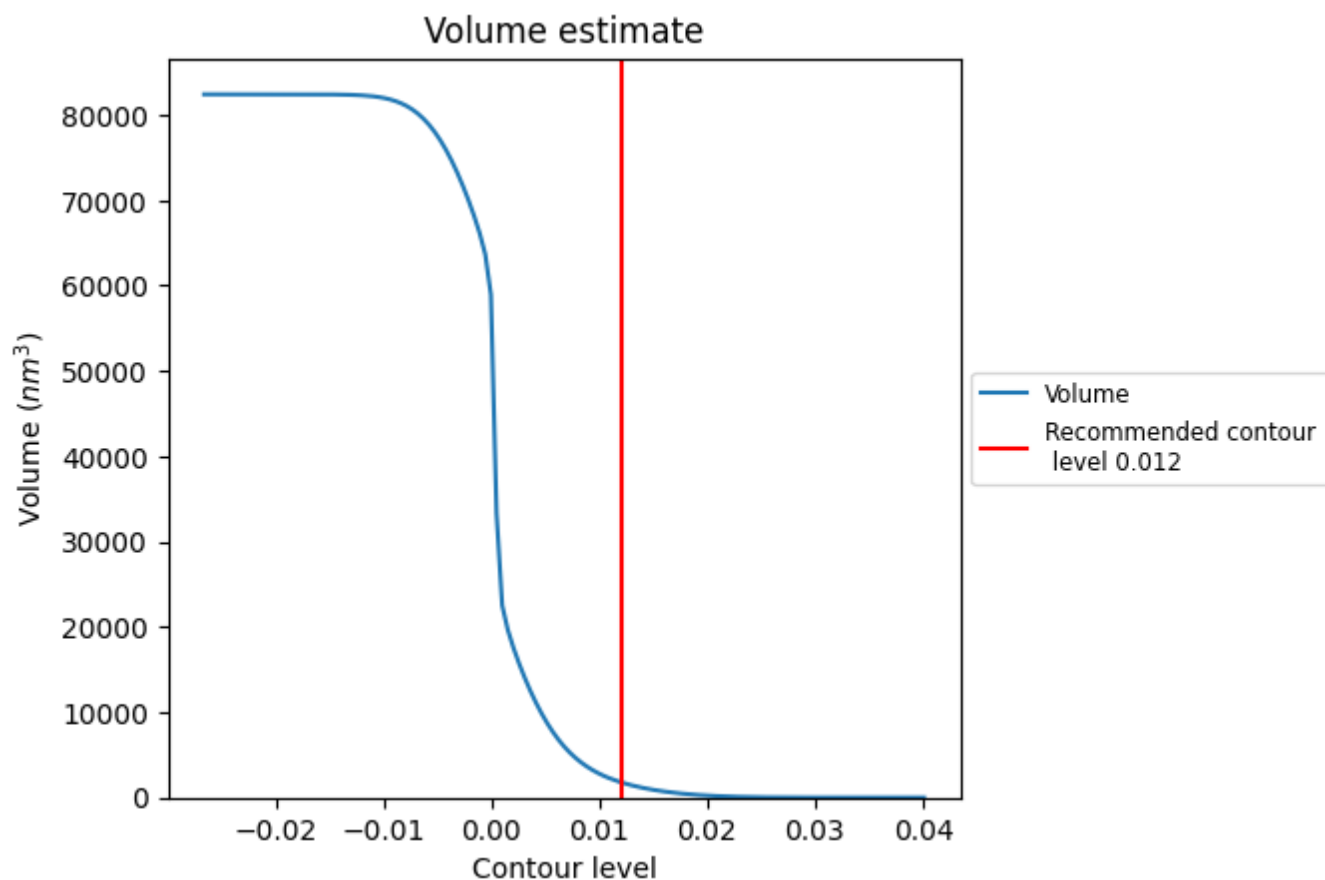
This section contains the results of statistical analysis of the map.

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.

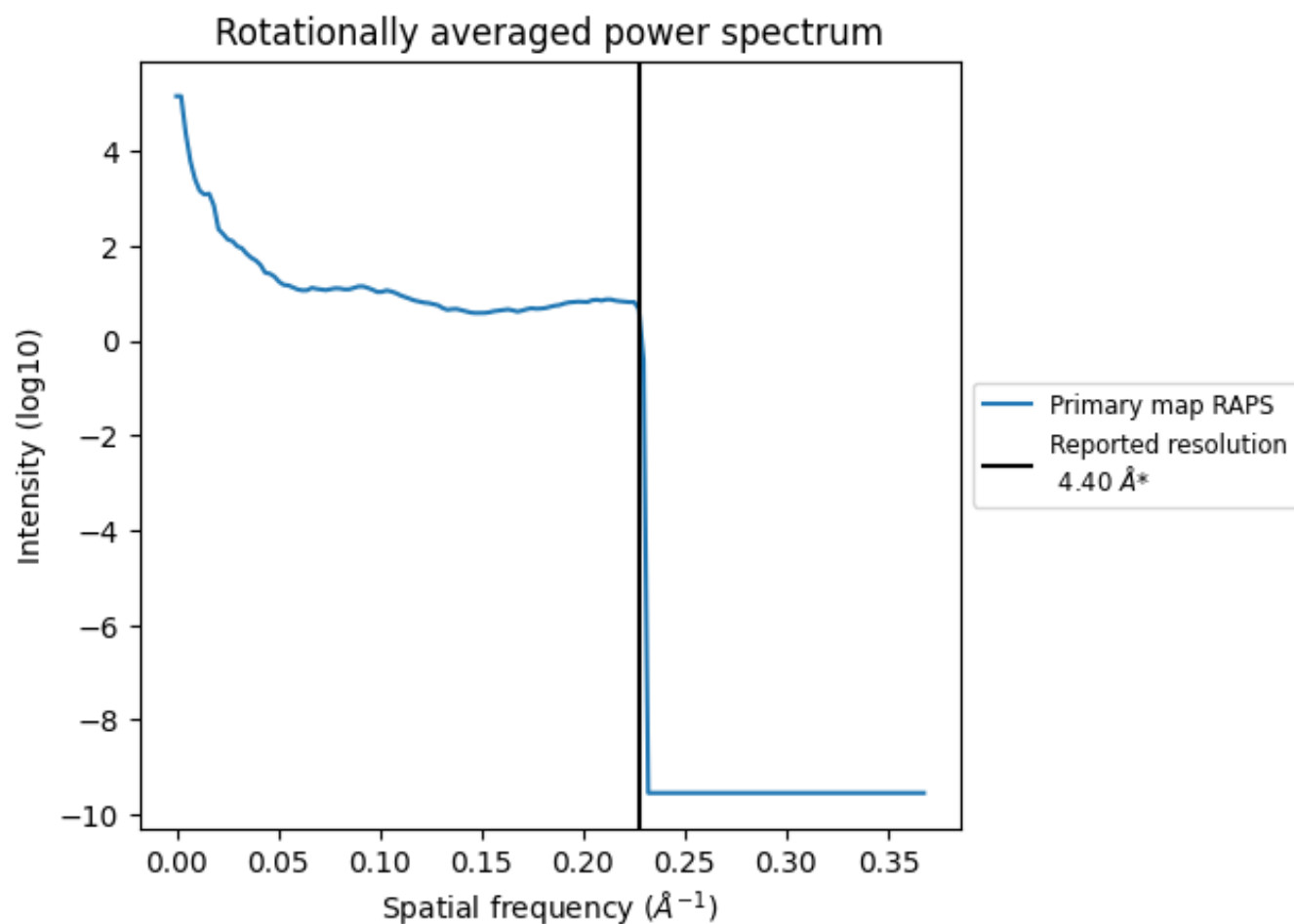
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1798 nm³; this corresponds to an approximate mass of 1624 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 0.227 $\text{\AA}^{-1}$

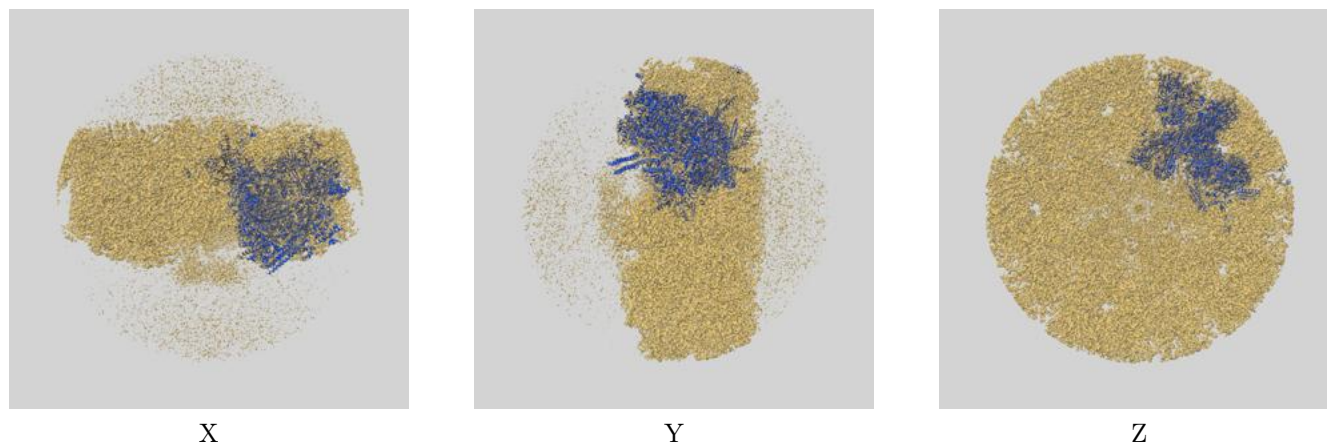
8 Fourier-Shell correlation

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-21526 and PDB model 6W2E. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

9.1 Map-model overlay [i](#)



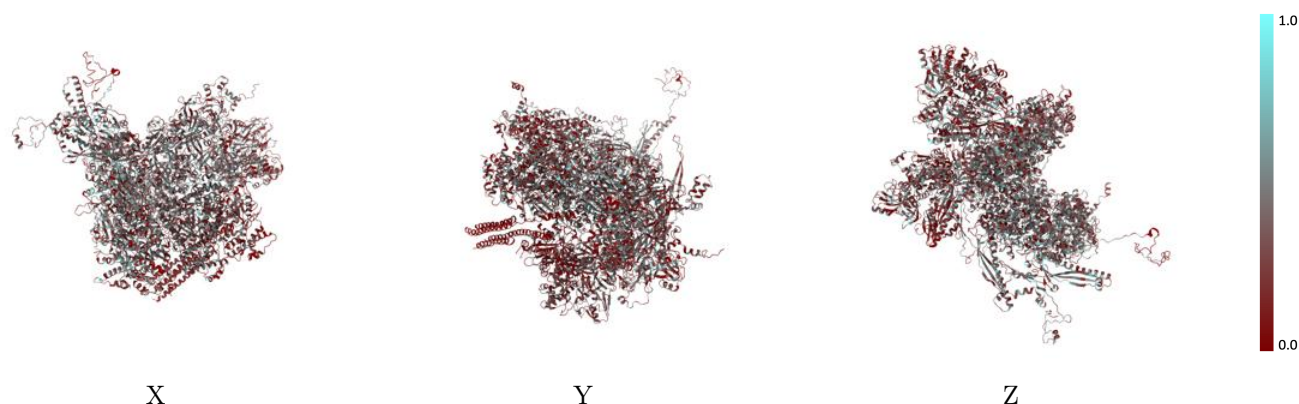
The images above show the 3D surface view of the map at the recommended contour level 0.012 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



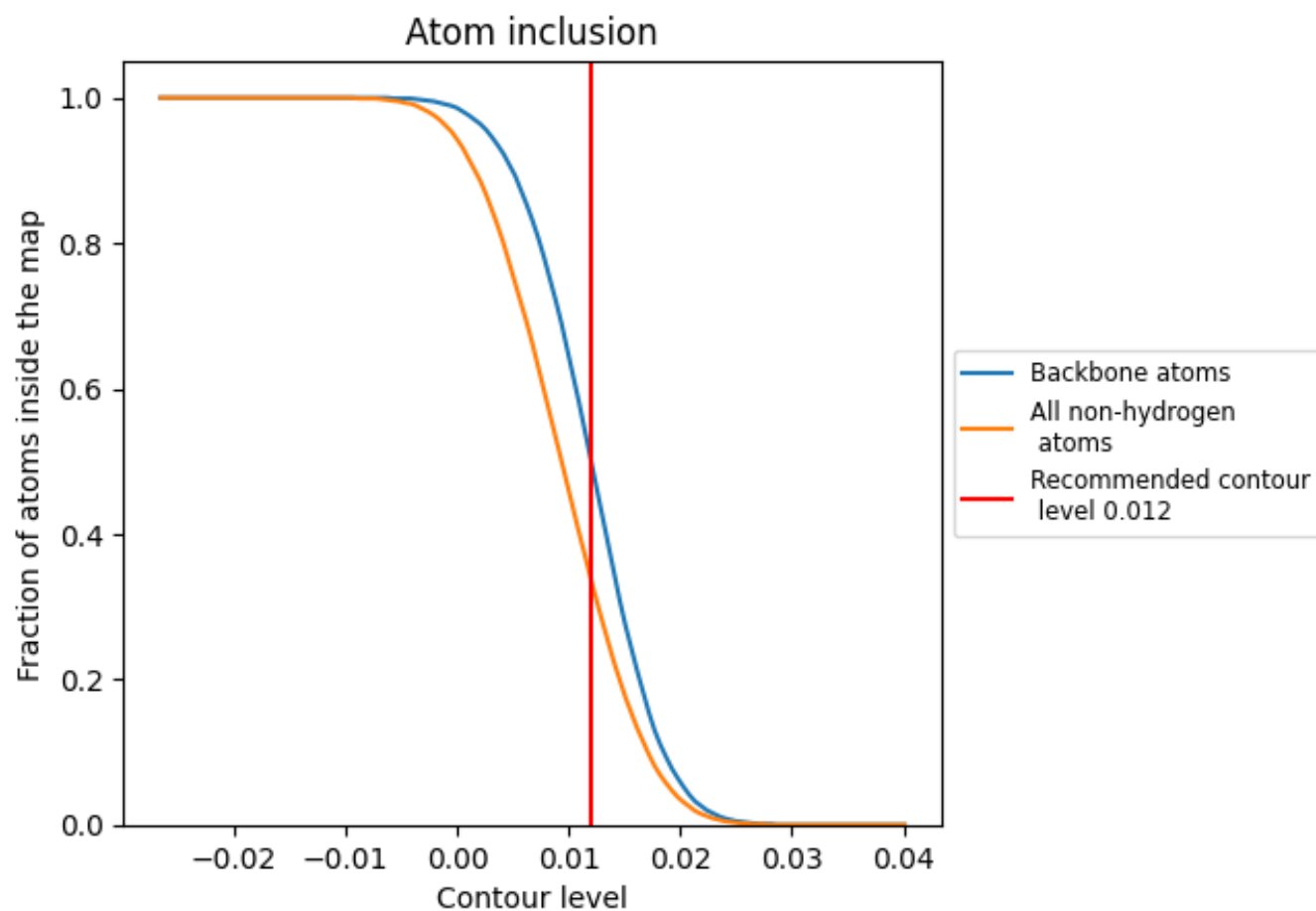
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.012).

9.4 Atom inclusion [i](#)



At the recommended contour level, 50% of all backbone atoms, 34% 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 (0.012) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.3360	 0.2450
J	 0.3910	 0.2500
K	 0.3870	 0.2640
N	 0.3500	 0.2590
O	 0.3700	 0.2460
Z	 0.3000	 0.2300
a	 0.3100	 0.2180
d	 0.1720	 0.1880
e	 0.2860	 0.2230
f	 0.2490	 0.2260
h	 0.3450	 0.2610
k	 0.2780	 0.2310
m	 0.2860	 0.2490
p	 0.2910	 0.2330
r	 0.2990	 0.2550
v	 0.1690	 0.1870
w	 0.0720	 0.1710
x	 0.1170	 0.1700
y	 0.0630	 0.1150
z	 0.0500	 0.1040

