



wwPDB EM Validation Summary Report ⓘ

Mar 12, 2026 – 02:15 AM UTC

PDB ID : 6W2D / pdb_00006w2d
EMDB ID : EMD-21525
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 : 4.00 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

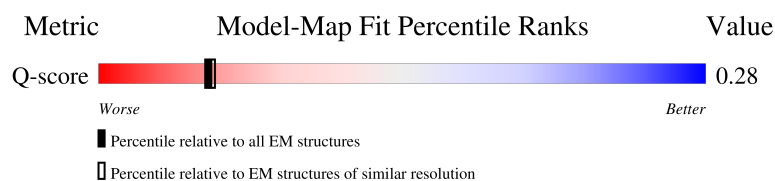
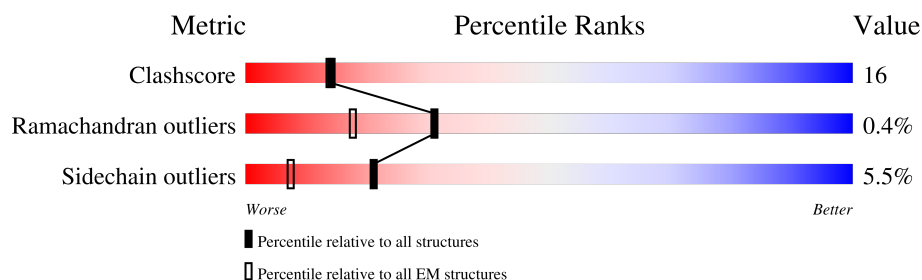
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.00 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	7587 (3.50 - 4.50)

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	40% 62% 33% ..
1	K	1381	42% 68% 31% .
1	N	1381	51% 66% 30% ..
1	O	1381	43% 64% 30% ..

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Mol	Chain	Length	Quality of chain
1	P	1381	
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	
5	u	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 74272 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	1352	Total	C	N	O	S	0	0
			10628	6744	1849	1974	61		
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	1332	Total	C	N	O	S	0	0
			10447	6633	1812	1942	60		
1	P	1283	Total	C	N	O	S	0	0
			10113	6429	1754	1871	59		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	v	292	Total	C	N	O	S	0	0
			2283	1469	397	406	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		
5	u	63	Total	C	N	O	S	0	0
			528	339	90	98	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	f	315	Total	C	N	O	S	0	0
			2474	1586	436	444	8		
6	h	336	Total	C	N	O	S	0	0
			2604	1667	458	471	8		

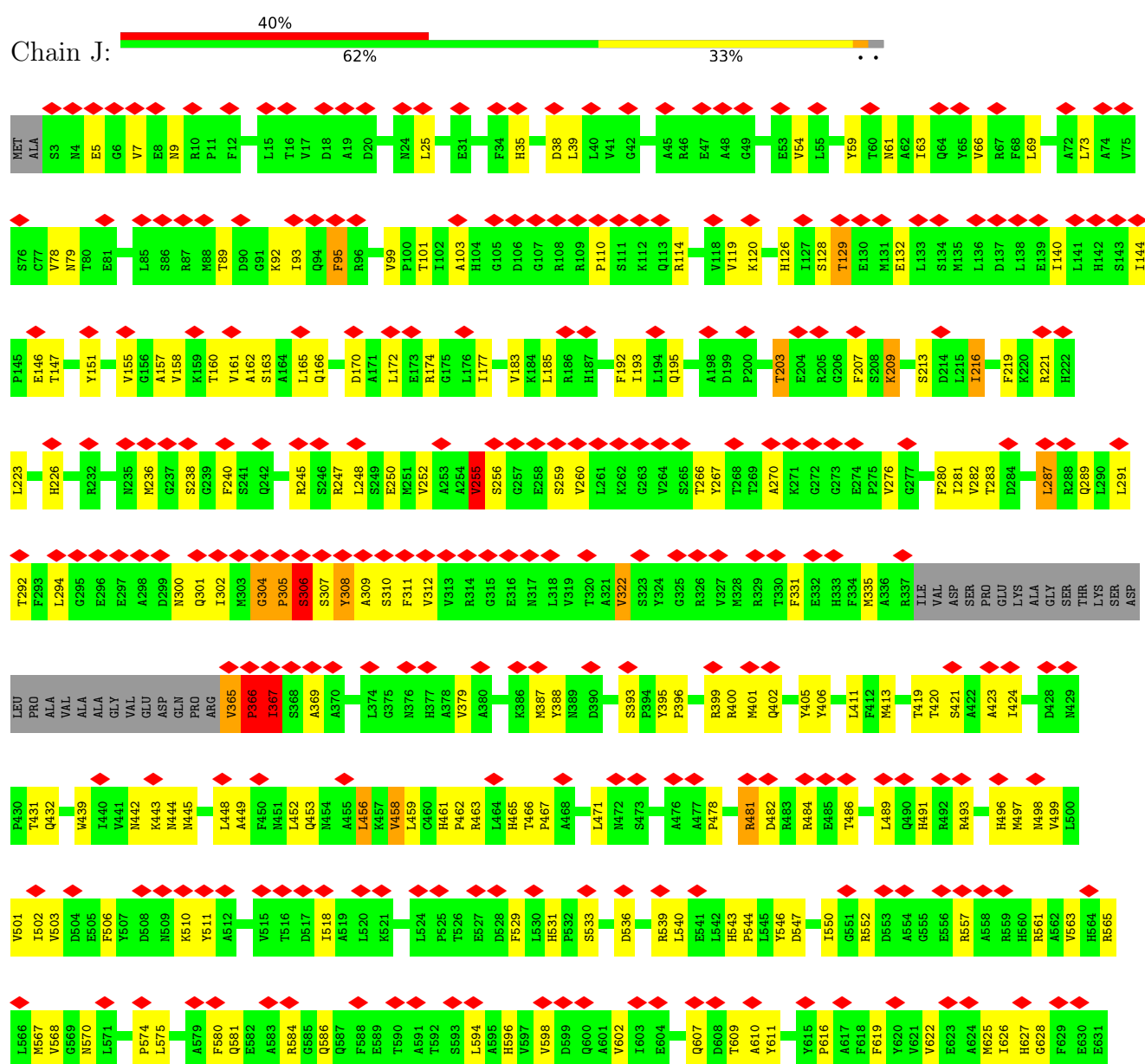
- Molecule 7 is a protein called Triplex capsid protein 2.

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

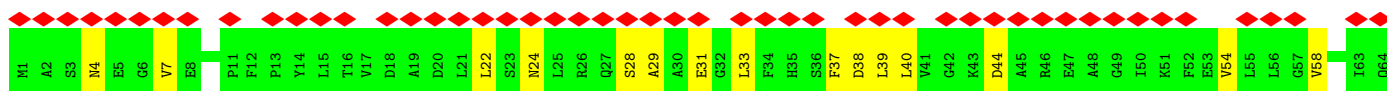
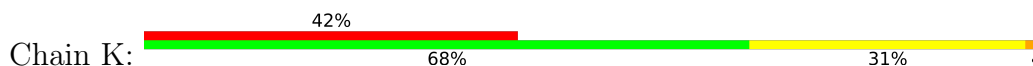
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

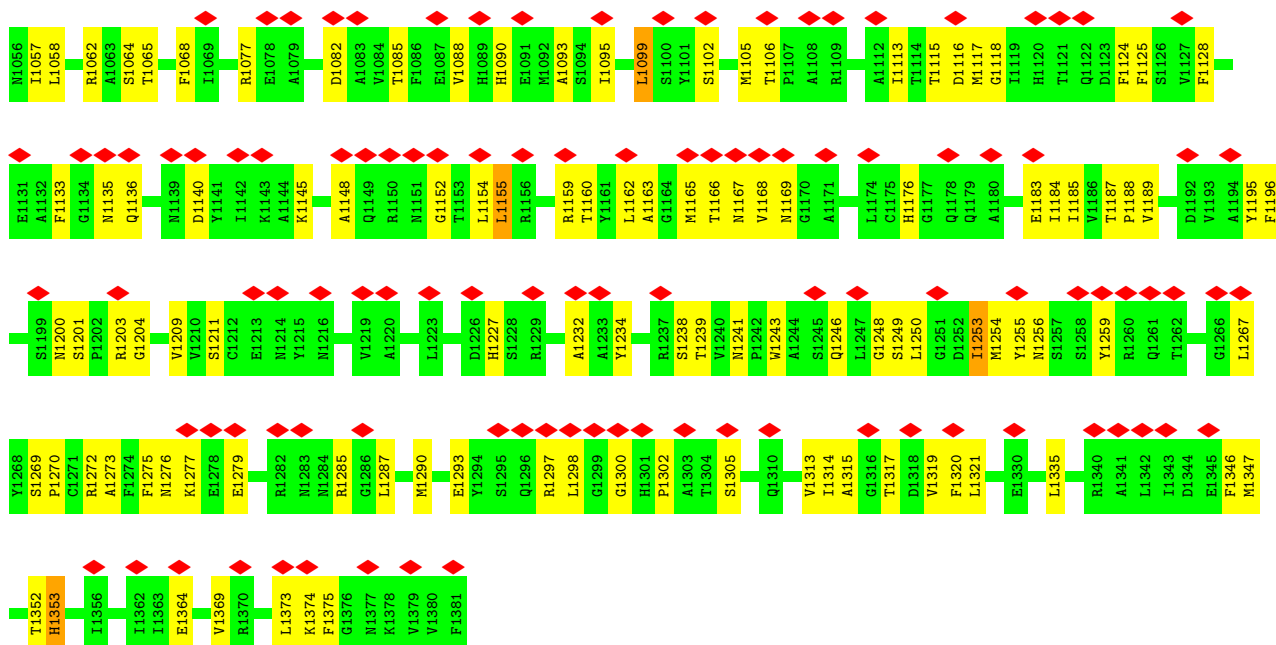




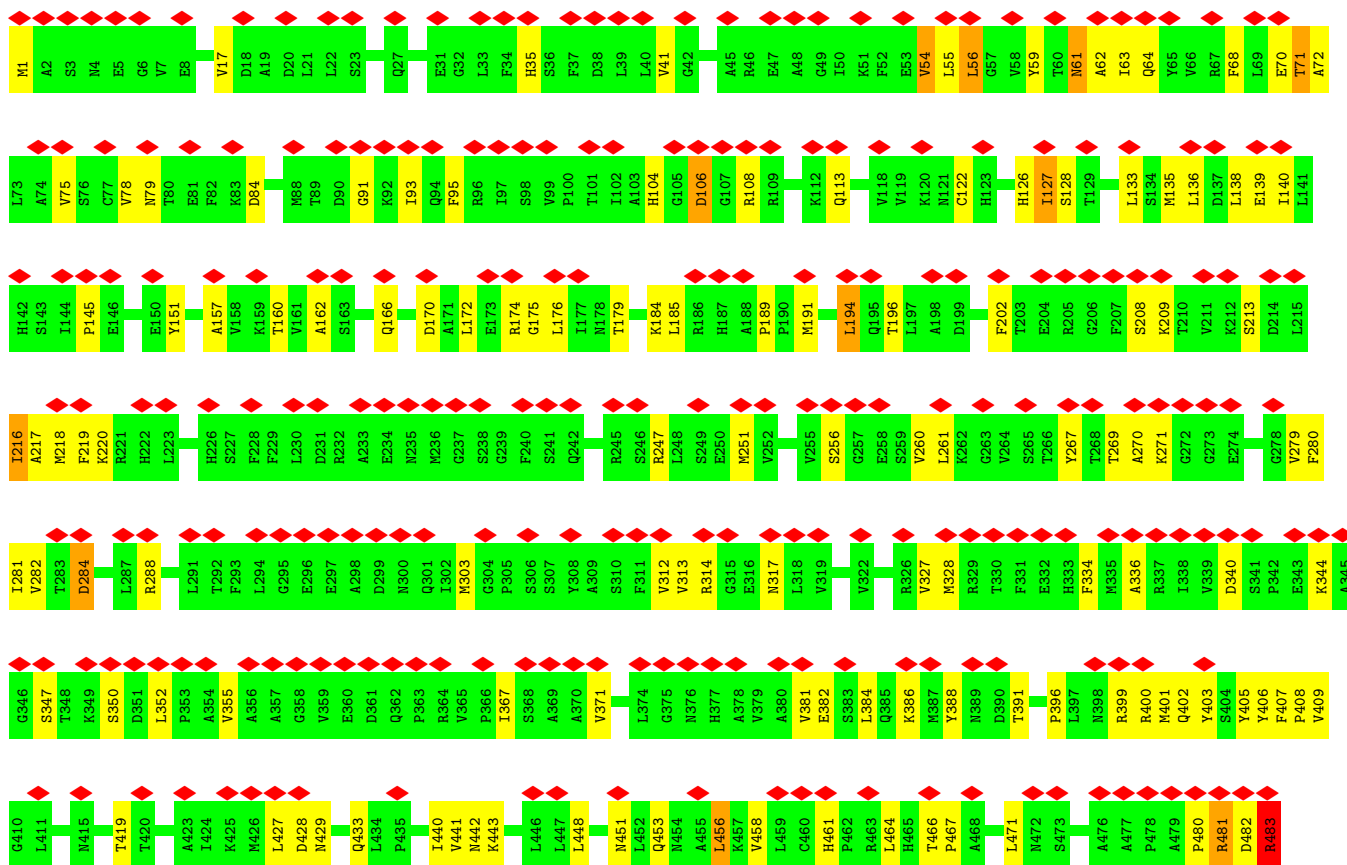
• Molecule 1: Major capsid protein



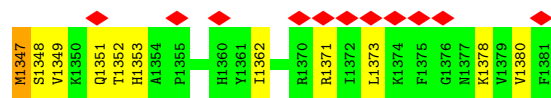
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L910	A911	P912	N913	D916	K917	R918	T919	R920	Q921	T922	V923	L924	V925	N926	G927	L928	V929	N930	F931	A932	P933	E934	E935	R936	T937	R938	A939	V940	T941	L944	F945	H946	A947	L948	P949	F950	H951	M952	F953	Y954	G955	P956	P957	R958	T959	F959	R959	Y900	M903	H904	G965	D966	V967	M972	R973		
A845	F846	S847	H848	H849	F850	T851	R852	D853	E854	D855	I856	L857	D858	N859	L860	E861	V862	G863	T864	L865	R866	D867	L868	L869	E870	I871	S872	D873	L874	V878	G879	M880	F881	R882	D883	L884	S885	A886	S887	F888	P892	T893	F894	T895	R896	A897	R898	R899	Y900	S901	N904	D905	V906	T907	G843	P844	Q909
D708	E709	S710	V711	T714	V715	C716	L717	L719	D720	L723	L724	T730	D731	I732	F733	T734	H735	L736	L737	S740	D741	R742	A743	P744	Q745	I746	T747	I748	G749	N750	E751	V752	Y753	A754	L757	A758	A759	F762	T763	E764	R765	V766	G767	N768	M769	D770	E771	M772	Q775	F776	V777	A778					
L779	Y780	R783	V784	H785	G786	D787	H788	D789	H790	R793	L794	H795	L796	V799	V800	D801	E802	G803	H804	A805	D806	V807	L808	E809	R810	I811	F812	Y813	H814	R815	F816	L817	P818	T819	C820	T821	N822	M825	L828	G829	V830	D831	F832	V835	A836	Q837	T838	L839	A840	T841	D905	V906	T907	G843	P844	Q909	
M567	V568	L571	P572	T573	P574	A579	A583	S584	G585	D586	E589	T590	A591	L594	A596	H596	V597	V598	D599	Q600	A601	V602	L603	E604	D608	T609	A610	V611	D612	T613	P616	A617	F618	F619	E623	A624	H625	T626	H627	Q628	F629	E630	F633	V634	M635	H636	V637	V640	S641								
T431	Q432	Q433	E437	A438	V439	I440	V441	M442	K443	L447	L448	A449	F450	M451	K452	Q453	M454	L455	L456	K457	V458	L459	C460	H461	P462	R463	L464	H465	T466	P467	A468	H469	T470	L474	A477	P478	A479	M480	L481	D482	R483	R484	E485	T486	Y487	S488	L489	Q490	H491	R492	R493	H496	M497	M498			
A356	A357	G358	V359	E360	D361	R364	V365	P366	L367	S368	A369	A370	V371	K372	K373	L374	G375	N376	H377	A378	V379	A380	V381	E382	S383	L384	Q385	K386	M387	D390	S393	P394	Y395	P396	L397	N398	R399	R400	M401	Q402	P408	L411	T420	S421	A422	A423	L424	K425	M426	L427	D428	N429	P430				
R288	Q289	L290	T292	F293	L294	G295	E296	E297	A298	D299	N300	Q301	T302	M303	G304	F305	S306	S307	Y308	A309	S310	V312	V313	R314	G315	E316	Y324	V327	M328	R329	T330	F331	E332	H333	F334	M335	A336	R337	I338	V339	D340	E343	K344	A345	G346	S347	T348	K349	S350	D351	L352	P353	A354	V355			
L215	I216	F219	K220	R221	E222	T223	L224	F229	L230	D231	R232	A233	E234	N235	M236	G237	S238	G239	F240	S241	R245	S246	R247	L248	S249	E250	A253	A254	V255	G257	V260	L261	K262	H263	V264	S265	A270	K271	G272	G273	E274	G277	G278	V279	V282	T283	D284	N285	V286	L287							
L141	H142	S143	I144	P145	E146	T147	P148	V149	E150	Y151	A152	V155	G156	A157	V158	K159	A162	S163	A164	L165	Q166	V169	R171	L172	E173	R174	A253	A254	N177	T179	K184	L185	R186	H187	A188	P189	M191	F192	I193	L194	A198	D199	E204	F207	S208	K209	T210	S213	D214								
Y65	V66	R67	F68	L69	E70	T71	A72	L73	A74	N79	T80	E81	K83	D84	S86	R87	M88	T89	K92	I93	Q94	F95	R96	I102	H104	G105	D106	R109	P110	S111	K112	Q113	R114	T115	F116	I117	H123	I127	S128	T129	E132	L133	S134	L136	D137	L138	E139	I140									



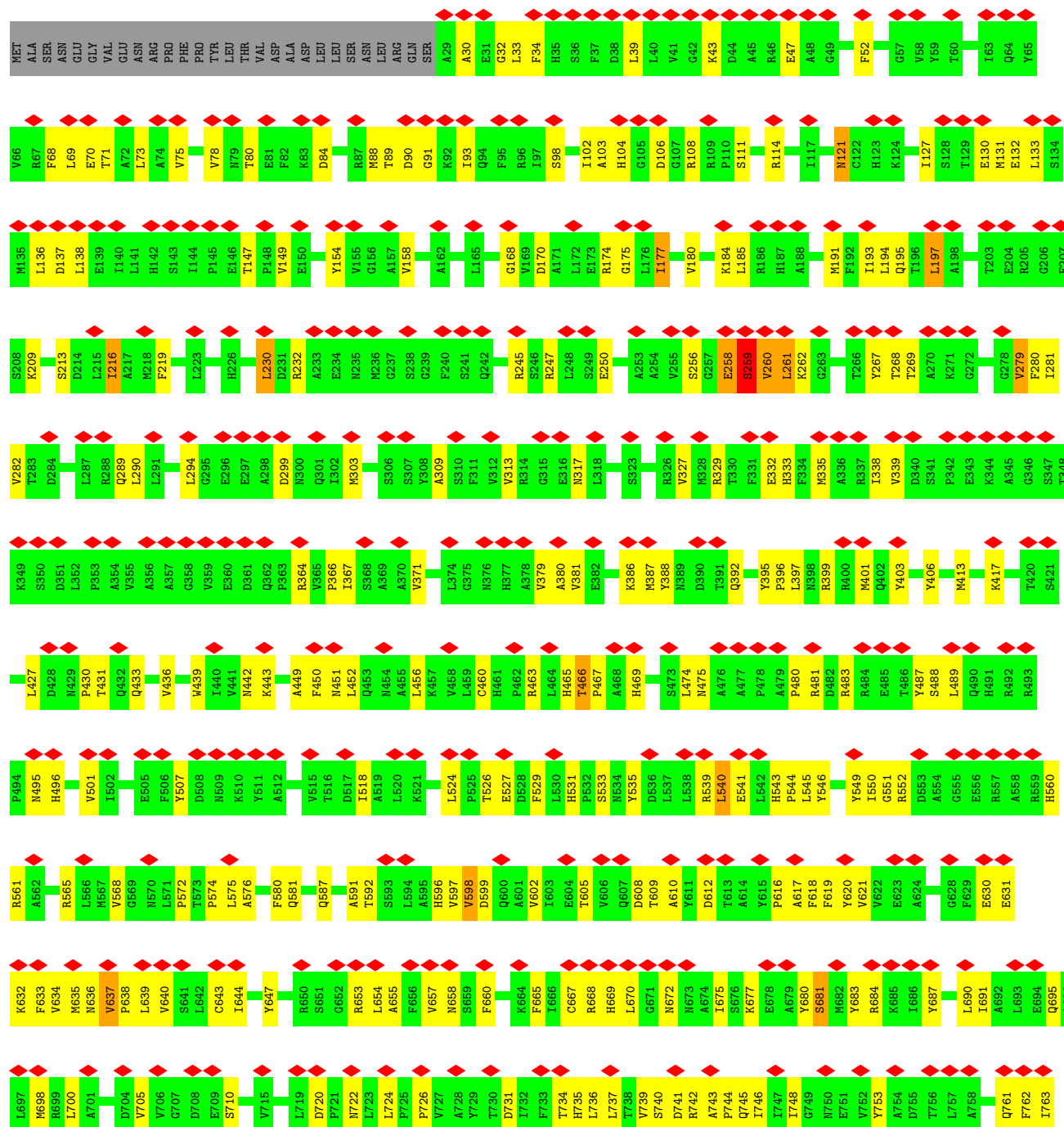
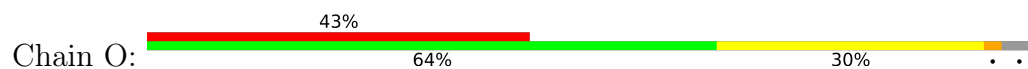
• Molecule 1: Major capsid protein

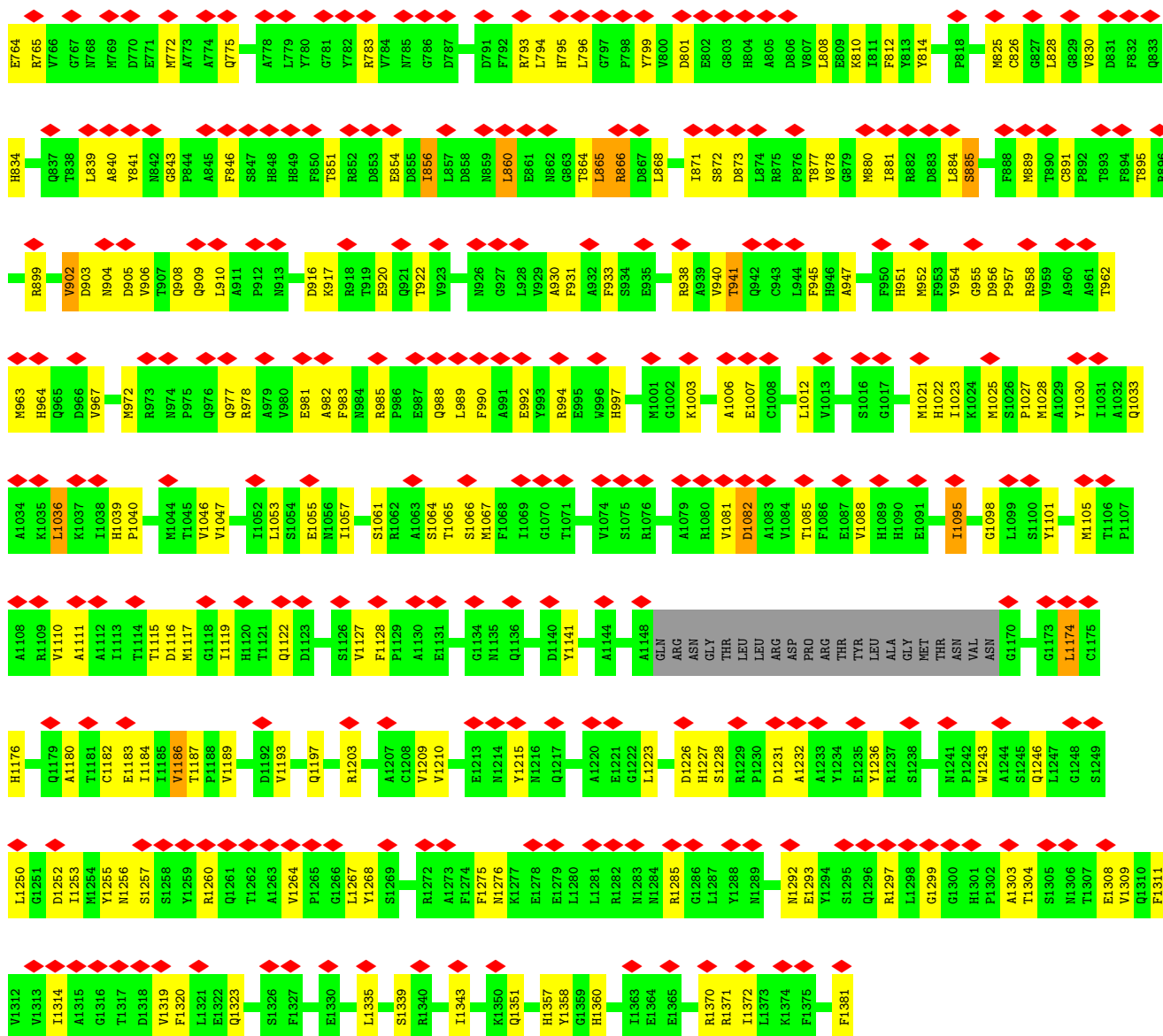


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K1145	V1146	G1147	A1148	Q1149	ARG	ASN	GLY	THR	LEU	ARG	ASP	PRO	THR	TYR	LEU	ALA	GLY	MET	THR	ASN	VAL	M1169	G1170	A1171	P1172	G1173	L1174	C1175	H1176	G1177	Q1178	Q1179	A1180	T1181	I1184	T1187	P1188	A1191	D1192	Y1195	F1196	S1199	M1200	S1201	F1202	R1203	G1204	H1205	A1206	A1207	C1208	V1209									
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E556	R557	A558	R559	H560	R561	A562	R565	L566	M567	V568	C569	N570	L571	P574	L575	F580	Q581	E582	A583	R584	Q587	A591	A595	H596	V597	V598	D599	G523	A601	V602	I603	V606	Q607	D608	T609	A610	Y611	D612	T613	A614	H643	P644	L645	A617	F618	F619	Y620	V621	V622	E623	A624	I626									
R484	E485	T486	Y487	S488	L489	Q490	H491	R492	R493	P494	N495	H496	M497	M498	V501	I502	E505	M509	K510	Y511	A512	A513	P514	D517	I518	K521	C522	G523	L524	F525	T526	E527	N534	Y535	D536	L537	L538	R539	L540	H543	P544	L545	Y546	D547	I548	Y549	I550	G551	R552	D553	A554	G555									

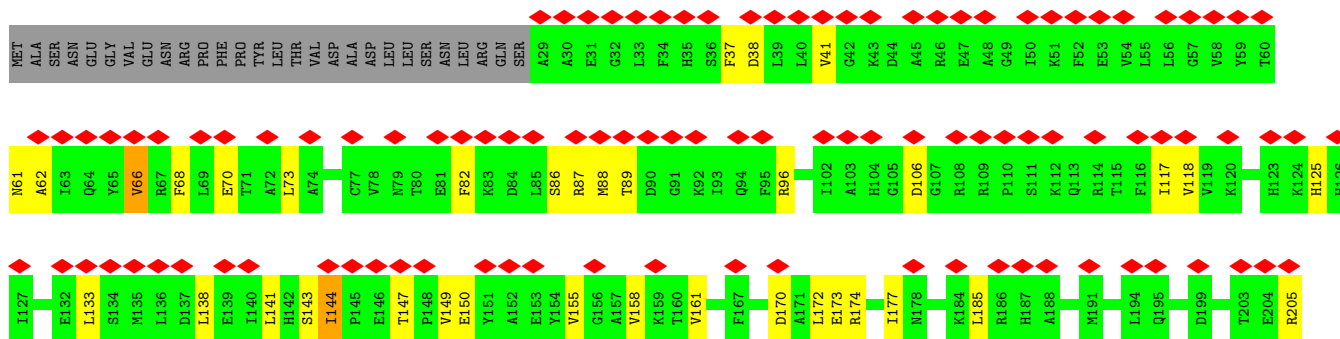


• Molecule 1: Major capsid protein

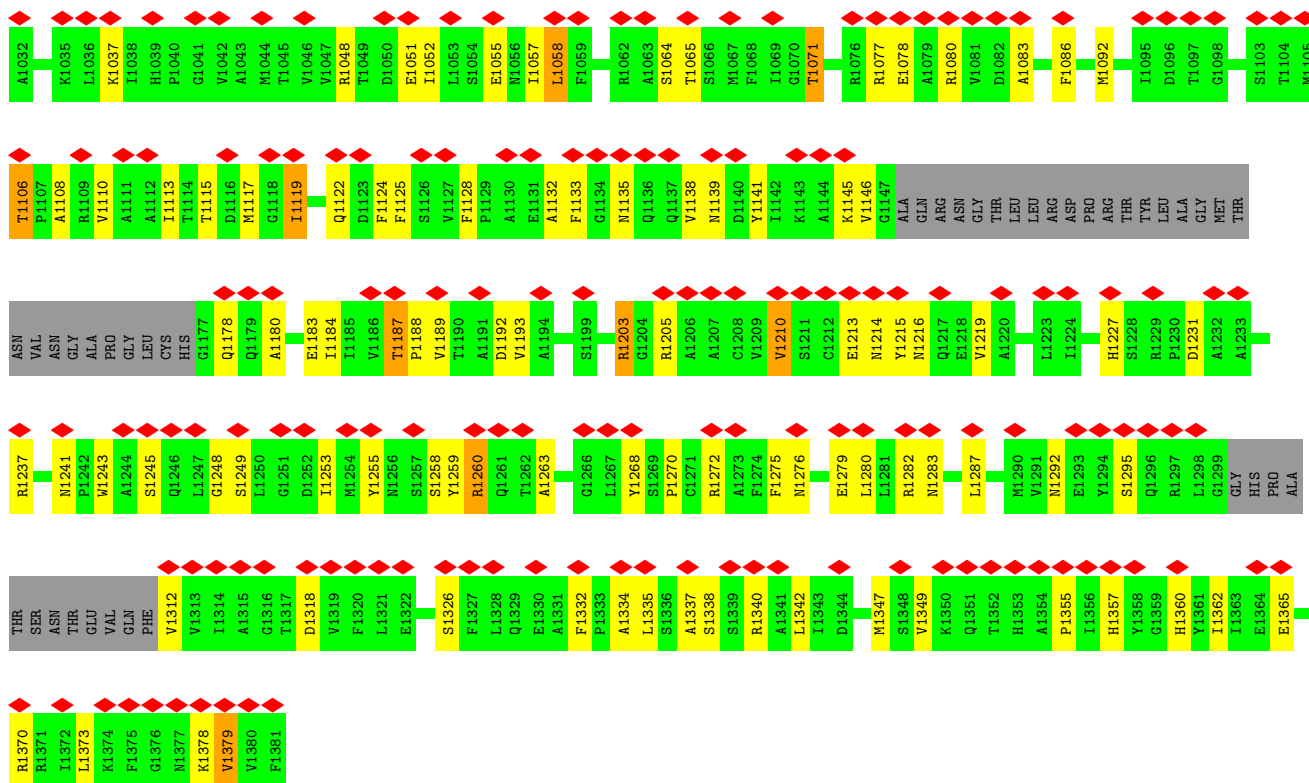




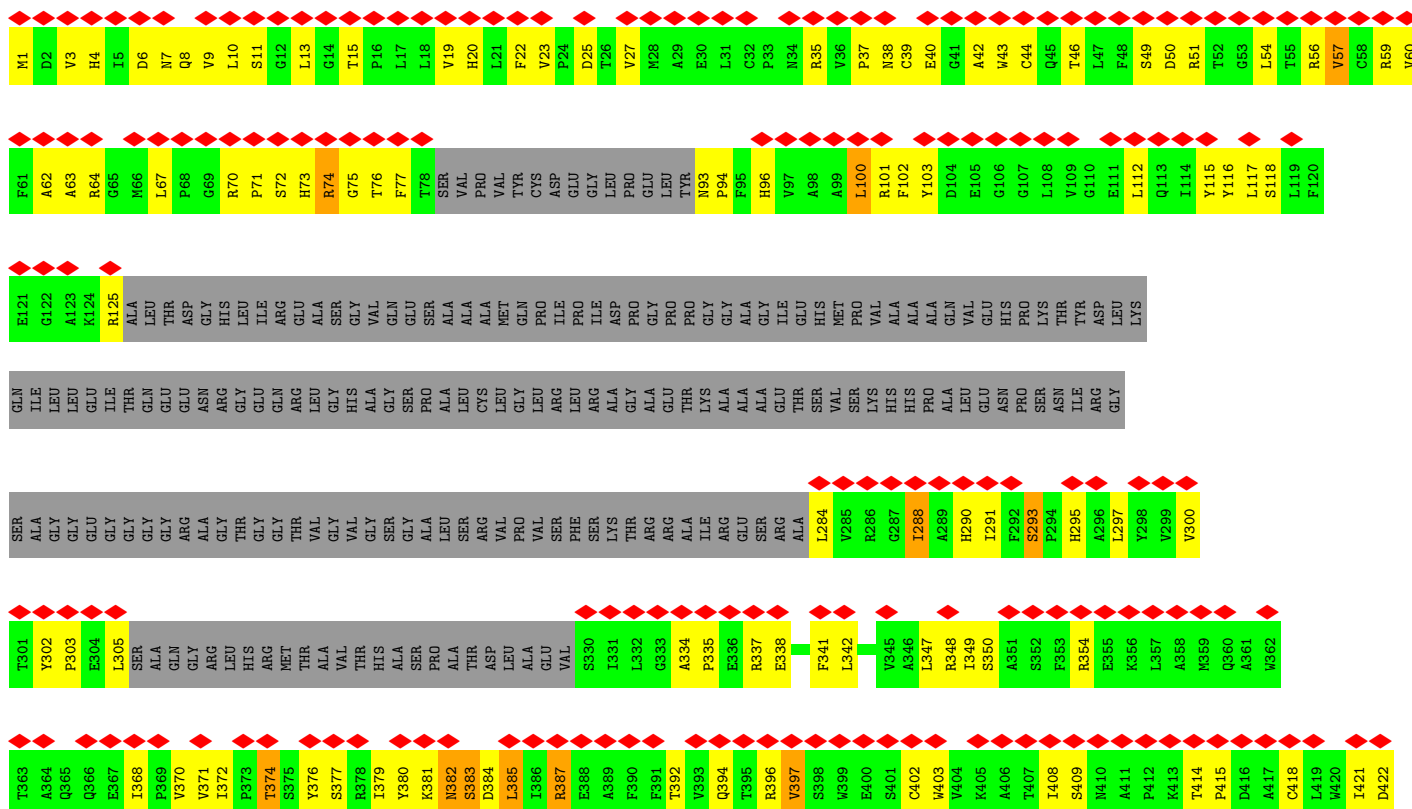
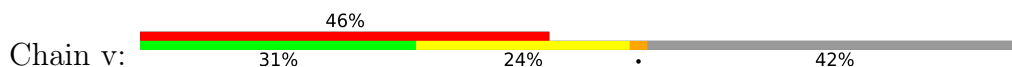
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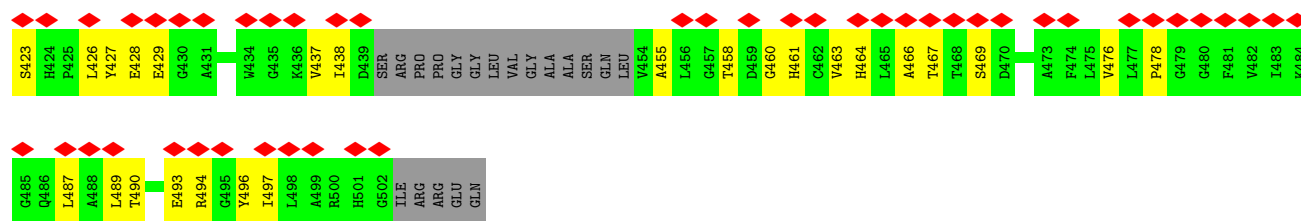


T969	Q909	H849	T666	V606	P544	R483	K417	LYS	G372	G206
F970	L910	F850	C667	Q607	L545	R484	Y418	ALA	G273	F207
R973	A911	T851	R668	D608	Y546	E485	T419	SER	E274	S208
Q976	N913	D853	H669	T609	D547	E486	T420	THR	T381	K209
Q977	N914	D854	L670	A610	T548	S488	S421	LYS	V282	T210
R978	A915	D855	F733	Y611	Y549	S489	A422	SER	V283	V211
A979	D916	L856	T734	D612	Y550	A490	A423	ASP	D284	K212
V980	K917	L857	H672	T613	R551	H491	I424	PRO	N285	S213
E981	R918	D858	H673	A614	R552	H492	K425	ALA	V286	D214
E982	T919	F798	H674	T615	D553	R492	M426	VAL	L287	L215
F983	E920	S676	L675	P616	A554	R493	L427	ALA	R288	I216
N984	N921	K677	E678	F618	E555	P494	D428	GLY	A217	A217
R985	Q921	E679	E680	P619	E556	H495	N429	VAL	L291	M218
F986	T922	H681	H682	Y620	R557	H496	N430	GLU	T292	F219
Q987	N923	A743	H683	V621	A558	H497	P430	ASP	F293	K220
Q988	L924	H744	H684	V622	H560	N498	T431	ASP	L294	R221
L989	V925	H745	H685	E623	A562	N499	Q432	ASP	G295	H222
F990	G927	I747	H686	A624	V563	V499	Q433	ASP	E296	E225
A991	V929	I748	H687	T626	H564	S503	L434	ASP	E297	H226
Y993	A930	H749	H688	H627	R565	E505	P435	ASP	A298	F228
R994	E932	H750	H689	H628	L566	F506	E437	ASP	D299	F229
Y996	F931	E751	L690	F629	H567	Y507	A438	ASP	M303	L230
H997	A932	H752	L691	E630	V568	D508	N444	ASP	S306	D231
R998	S934	H753	L692	E631	G569	N509	N445	ASP	S307	R232
S999	E935	H754	L693	E632	N570	K510	L446	ASP	Y308	A233
P1000	R936	H755	E694	F633	L571	Y511	L447	ASP	E309	E234
M1001	T937	H756	H695	V634	P572	A512	L448	ASP	S310	N235
G1002	R938	H757	L697	H635	L575	A513	F450	ASP	F311	M236
K1003	A939	H758	H698	H636	A576	V515	N451	ASP	V312	G237
Y1004	Y940	H759	H699	H637	P577	T516	L452	ASP	G315	S238
A1005	T941	H760	L700	P638	A578	D517	Q453	ASP	N317	G239
A1006	R822	H762	H823	L639	A579	I518	N454	ASP	L318	F240
E1007	D823	H763	H824	H640	F580	A519	K457	ASP	Y319	Y243
C1008	H825	H764	H826	S641	R584	L520	V458	ASP	R245	R244
L1009	S825	H765	H827	L642	G585	K521	L459	ASP	S246	R246
L1010	A826	H766	H828	C643	Q586	G523	C460	ASP	R247	L248
V1013	S827	H767	H829	T644	Q587	L524	H461	ASP	A321	S249
S1014	F888	H768	H830	N645	F588	P525	P462	ASP	V322	E250
I1015	H889	H769	H831	T646	E589	T526	R463	ASP	Y324	M251
S1016	T890	H770	D831	H648	T590	E527	L464	ASP	G325	V255
G1017	C891	H771	H832	E649	A591	L530	H465	ASP	S326	SER
M1018	P892	H772	H833	H650	T592	H531	T466	ASP	Y327	GLY
T1019	F893	H773	H834	S651	S593	P532	P467	ASP	M328	GLU
A1020	Y954	H774	H835	G652	L594	S333	A468	ASP	R329	SER
M1021	T895	H775	H836	H653	A595	N534	H469	ASP	T330	VAL
D956	R896	H776	H837	L654	H596	N535	S473	ASP	E332	GLY
P957	A897	H777	H838	A655	V597	D536	N475	ASP	H333	S265
I1023	H898	H778	H839	F656	V598	L537	A476	ASP	R337	T269
K1024	R899	H779	H840	H657	D599	L538	A477	ASP	D340	A270
M1025	Y841	H780	H841	H658	Q600	R539	P478	ASP	S341	K271
S1026	N842	H781	H842	S659	A601	L540	A479	ASP	PRO	
P1027	G843	H782	H843	F660	V602	E541	L542	ASP	GLU	
M1028	P844	H783	H844	S661	I603	L543	H481	ASP		
A1029	A845	H784	H845	H662	E604	H543	D482	ASP		
Y1030	F846	H785	H846	T663	T605			ASP		
I1031	G786	H786	H847	K664				ASP		
	D787	H787	H848	F665				ASP		

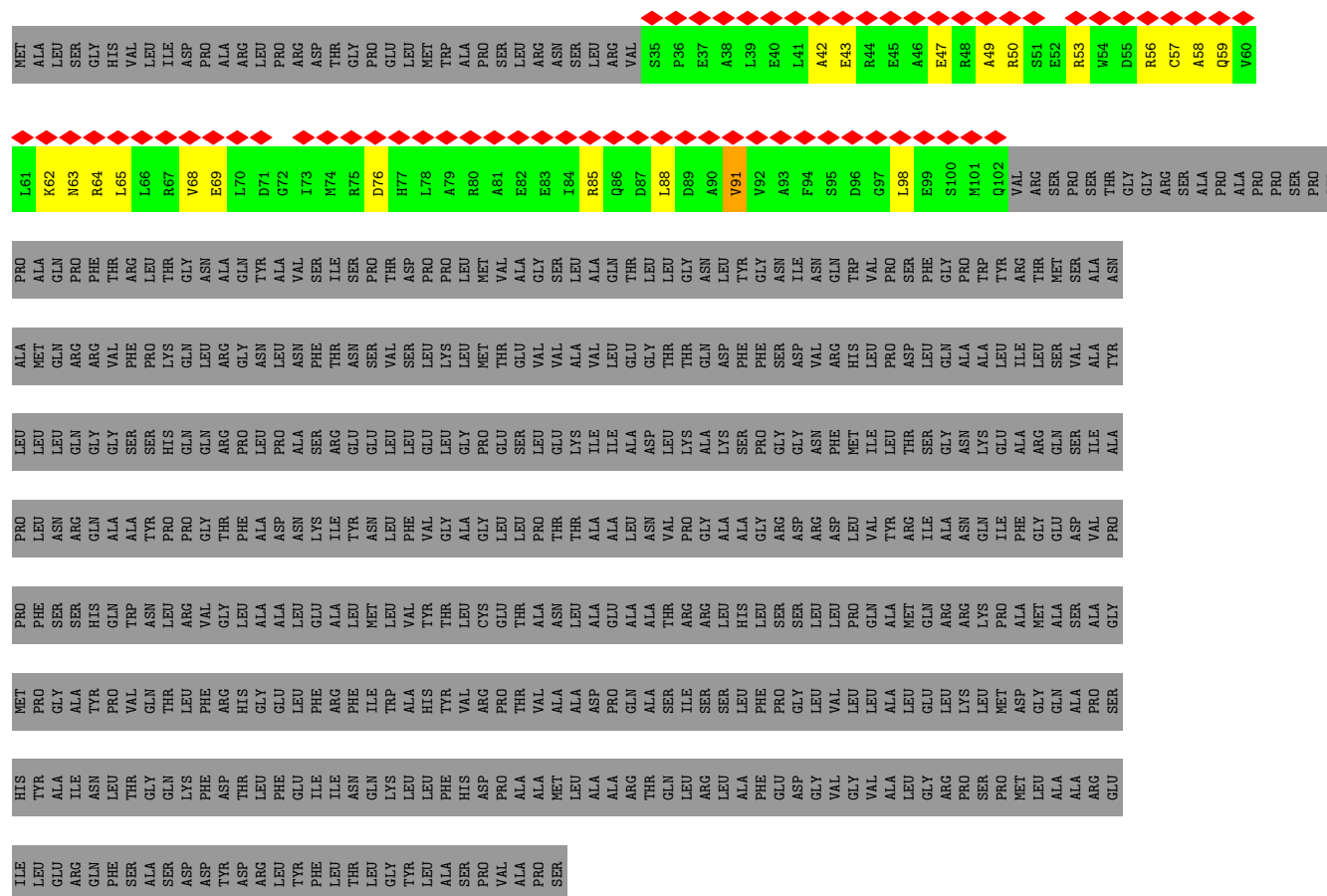


• Molecule 2: Capsid vertex component 1

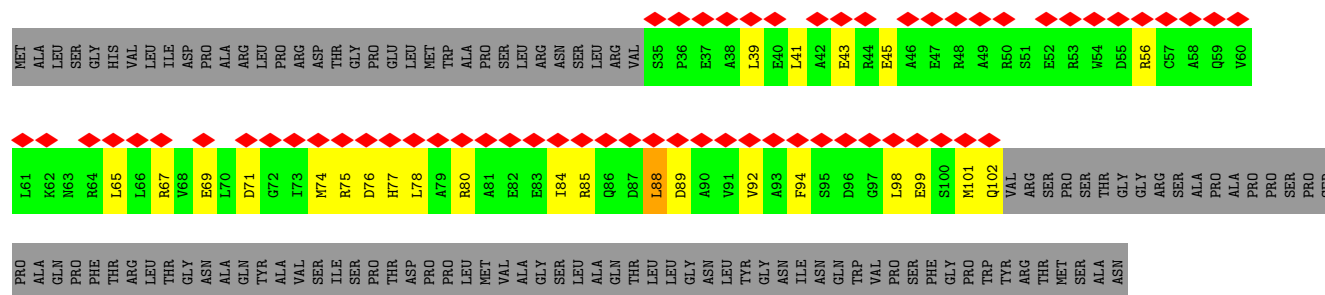




• Molecule 3: Capsid vertex component 2



• Molecule 3: Capsid vertex component 2



[illegible]

- Molecule 4: Large tegument protein deneddylase

Chain y: 99%

[illegible]

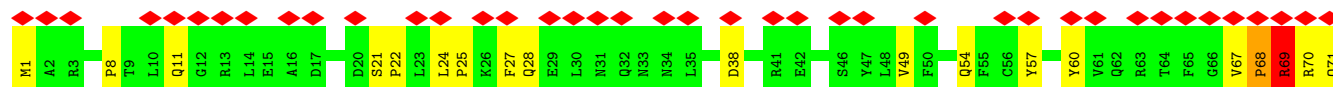




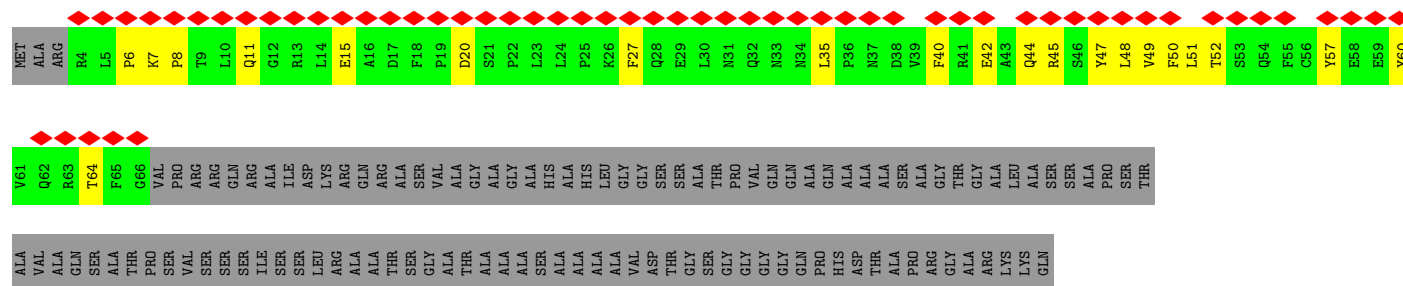




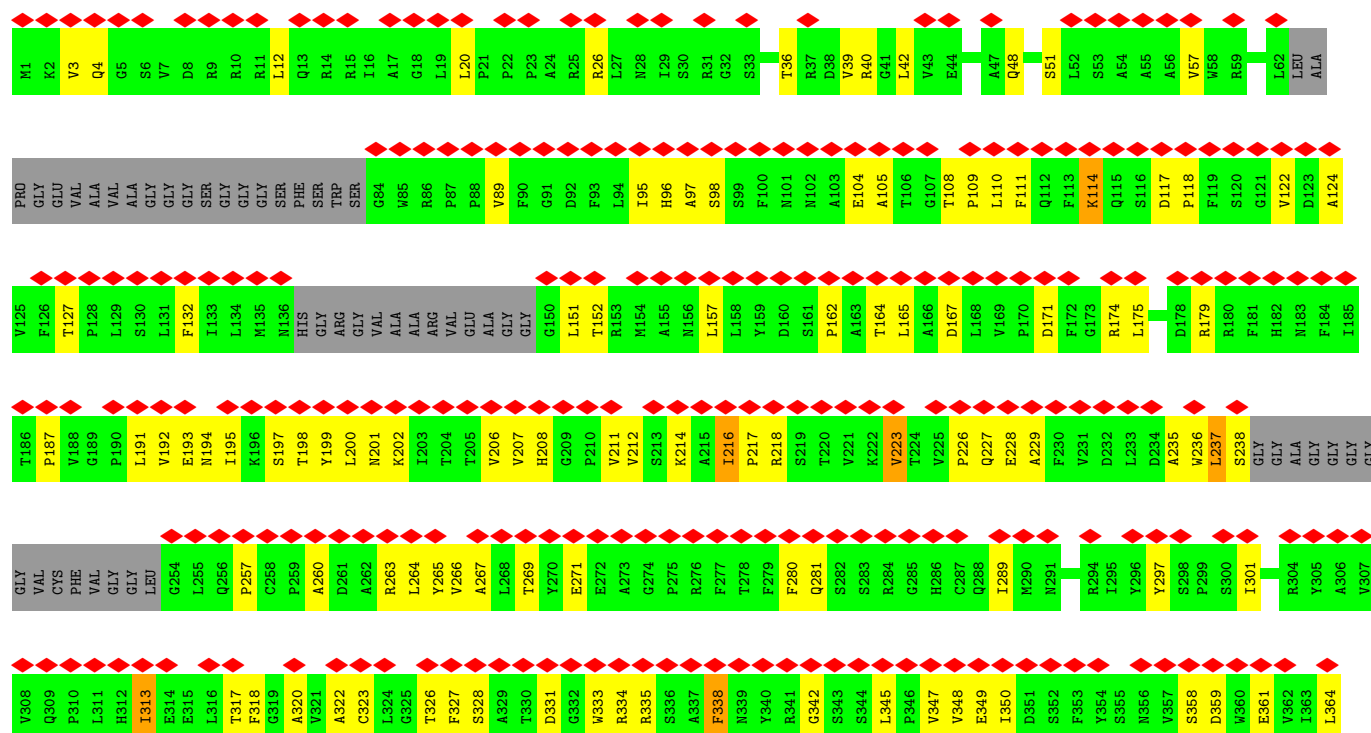
Chain Z: 26% 32% 11% .. 56%



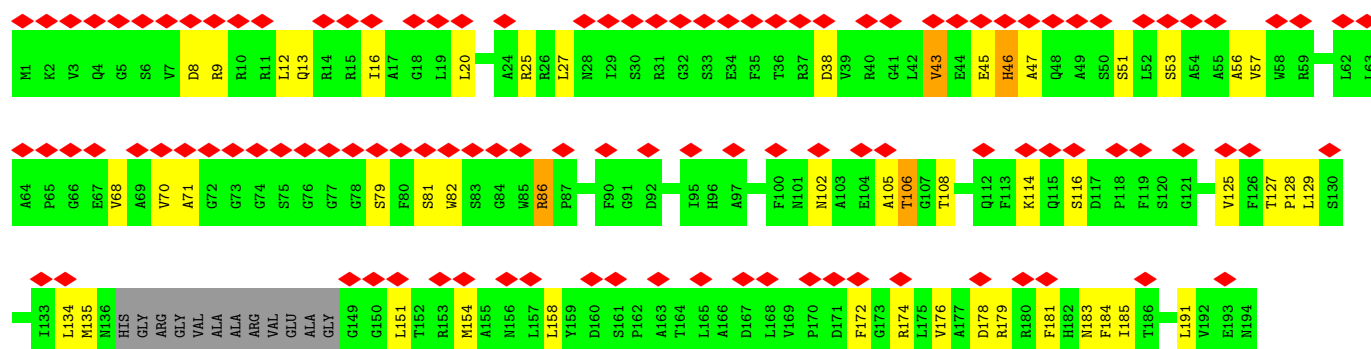


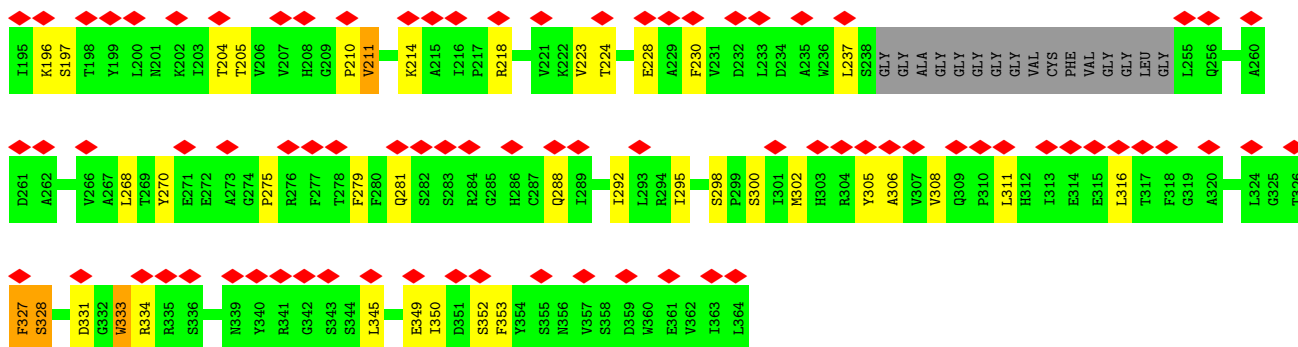


• Molecule 6: Triplex capsid protein 1

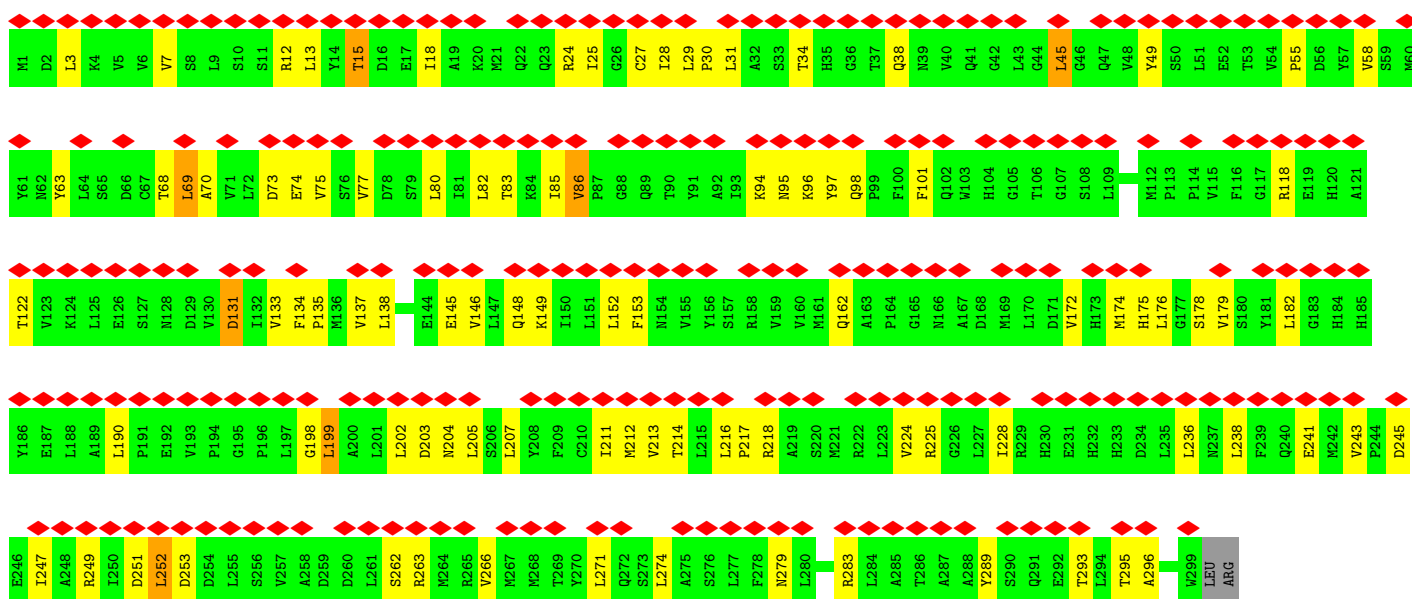
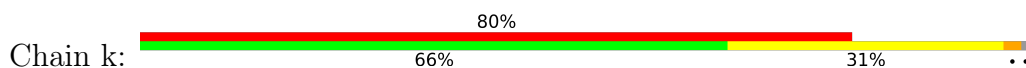


• Molecule 6: Triplex capsid protein 1

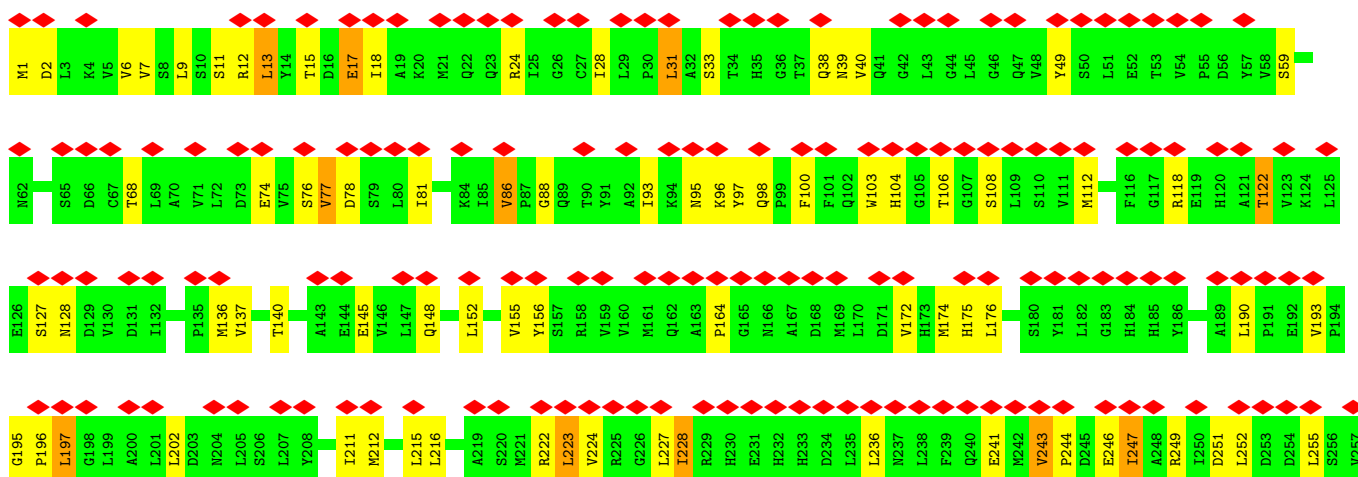


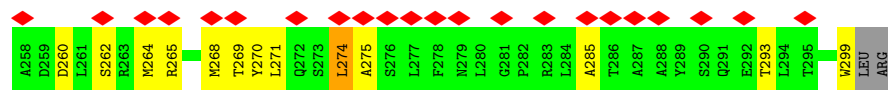


• Molecule 7: Triplex capsid protein 2

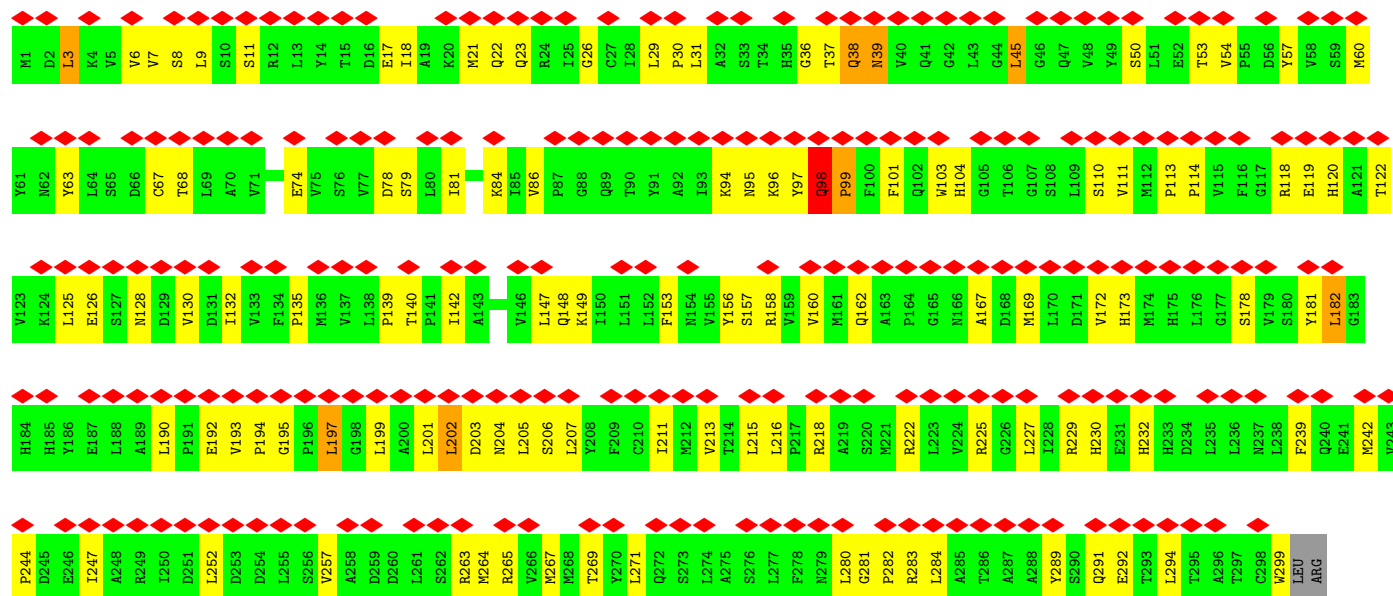
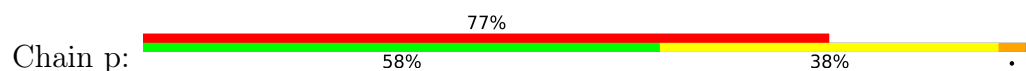


• Molecule 7: Triplex capsid protein 2

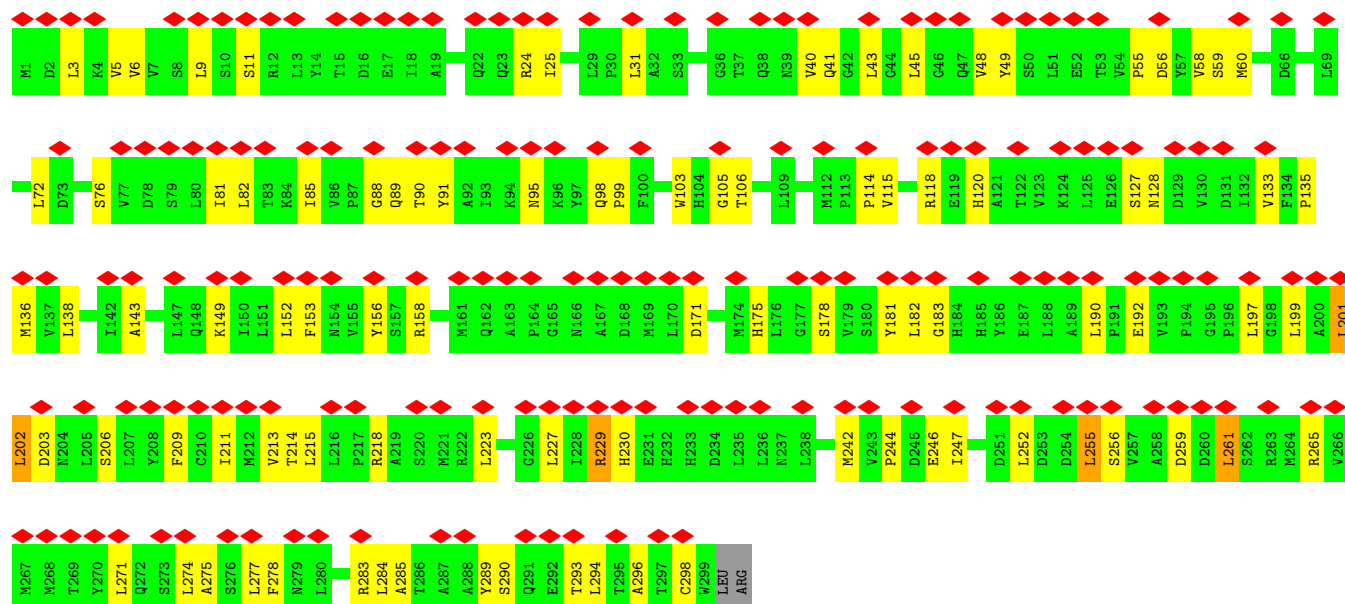




• Molecule 7: Triplex capsid protein 2



• 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	21085	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	0.058	Depositor
Minimum map value	-0.035	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.015	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	0.28	0/10877	0.47	3/14781 (0.0%)
1	K	0.27	0/11085	0.44	1/15066 (0.0%)
1	N	0.26	0/10933	0.42	0/14858
1	O	0.26	0/10693	0.42	0/14531
1	P	0.23	0/10349	0.43	1/14057 (0.0%)
2	v	0.23	0/2341	0.43	0/3183
3	w	0.19	0/553	0.39	0/741
3	x	0.22	0/553	0.44	0/741
4	y	0.21	0/320	0.45	0/424
4	z	0.22	0/320	0.42	0/424
5	Z	0.20	0/664	0.44	0/896
5	a	0.22	0/664	0.43	0/896
5	d	0.21	0/664	0.51	0/896
5	e	0.21	0/664	0.42	0/896
5	u	0.20	0/542	0.44	0/735
6	f	0.22	0/2537	0.45	0/3450
6	h	0.26	0/2672	0.46	0/3635
7	k	0.22	0/2388	0.44	0/3254
7	m	0.24	0/2388	0.45	0/3254
7	p	0.21	0/2388	0.45	0/3254
7	r	0.24	0/2388	0.42	0/3254
All	All	0.25	0/75983	0.44	5/103226 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	304	GLY	CA-C-N	7.65	129.40	119.84
1	J	304	GLY	C-N-CA	7.65	129.40	119.84
1	P	319	VAL	N-CA-C	-5.84	107.60	113.20
1	J	366	PRO	N-CA-C	-5.58	100.97	112.47
1	K	299	ASP	N-CA-C	-5.36	105.44	111.28

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	10628	0	10448	366	0
1	K	10832	0	10655	323	0
1	N	10683	0	10500	379	0
1	O	10447	0	10273	357	0
1	P	10113	0	9949	290	0
2	v	2283	0	2268	132	0
3	w	549	0	540	19	0
3	x	549	0	540	32	0
4	y	317	0	341	17	0
4	z	317	0	341	16	0
5	Z	649	0	649	51	0
5	a	649	0	649	19	0
5	d	649	0	649	32	0
5	e	649	0	649	28	0
5	u	528	0	510	27	0
6	f	2474	0	2459	78	0
6	h	2604	0	2577	62	0
7	k	2338	0	2364	75	0
7	m	2338	0	2364	65	0
7	p	2338	0	2364	110	0
7	r	2338	0	2364	70	0
All	All	74272	0	73453	2308	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 16.

The worst 5 of 2308 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:O:258:GLU:CG	1:O:262:LYS:CD	1.74	1.55
1:O:258:GLU:HG2	1:O:262:LYS:CD	1.28	1.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:483:ARG:NH1	1:N:485:GLU:HG2	1.25	1.40
1:O:743:ALA:HB2	2:v:73:HIS:NE2	1.21	1.40
1:O:258:GLU:CG	1:O:262:LYS:HD2	0.91	1.39

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	1348/1381 (98%)	1269 (94%)	72 (5%)	7 (0%)	24	60
1	K	1379/1381 (100%)	1310 (95%)	67 (5%)	2 (0%)	48	81
1	N	1358/1381 (98%)	1288 (95%)	62 (5%)	8 (1%)	21	57
1	O	1328/1381 (96%)	1259 (95%)	68 (5%)	1 (0%)	48	81
1	P	1273/1381 (92%)	1202 (94%)	69 (5%)	2 (0%)	43	75
2	v	282/507 (56%)	262 (93%)	19 (7%)	1 (0%)	30	65
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%)	34 (97%)	1 (3%)	0	100	100
4	z	35/3149 (1%)	34 (97%)	1 (3%)	0	100	100
5	Z	75/176 (43%)	67 (89%)	6 (8%)	2 (3%)	4	28
5	a	75/176 (43%)	70 (93%)	5 (7%)	0	100	100
5	d	75/176 (43%)	69 (92%)	4 (5%)	2 (3%)	4	28
5	e	75/176 (43%)	72 (96%)	3 (4%)	0	100	100
5	u	61/176 (35%)	56 (92%)	5 (8%)	0	100	100
6	f	307/364 (84%)	289 (94%)	18 (6%)	0	100	100
6	h	330/364 (91%)	305 (92%)	25 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	k	297/301 (99%)	282 (95%)	14 (5%)	1 (0%)	36	70
7	m	297/301 (99%)	282 (95%)	13 (4%)	2 (1%)	18	54
7	p	297/301 (99%)	282 (95%)	10 (3%)	5 (2%)	7	36
7	r	297/301 (99%)	288 (97%)	8 (3%)	1 (0%)	36	70
All	All	9356/17662 (53%)	8851 (95%)	471 (5%)	34 (0%)	31	65

5 of 34 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	J	305	PRO
1	J	366	PRO
1	K	298	ALA
1	K	805	ALA
1	N	483	ARG

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	1149/1171 (98%)	1073 (93%)	76 (7%)	15	40
1	K	1171/1171 (100%)	1100 (94%)	71 (6%)	17	41
1	N	1155/1171 (99%)	1080 (94%)	75 (6%)	15	40
1	O	1128/1171 (96%)	1064 (94%)	64 (6%)	18	43
1	P	1093/1171 (93%)	1047 (96%)	46 (4%)	26	49
2	v	243/400 (61%)	222 (91%)	21 (9%)	10	33
3	w	57/465 (12%)	56 (98%)	1 (2%)	51	68
3	x	57/465 (12%)	56 (98%)	1 (2%)	51	68
4	y	35/2539 (1%)	34 (97%)	1 (3%)	37	58
4	z	35/2539 (1%)	35 (100%)	0	100	100
5	Z	71/128 (56%)	70 (99%)	1 (1%)	59	71
5	a	71/128 (56%)	70 (99%)	1 (1%)	59	71

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	d	71/128 (56%)	70 (99%)	1 (1%)	59	71
5	e	71/128 (56%)	70 (99%)	1 (1%)	59	71
5	u	59/128 (46%)	59 (100%)	0	100	100
6	f	267/289 (92%)	255 (96%)	12 (4%)	24	47
6	h	278/289 (96%)	257 (92%)	21 (8%)	12	36
7	k	265/267 (99%)	254 (96%)	11 (4%)	26	49
7	m	265/267 (99%)	246 (93%)	19 (7%)	13	37
7	p	265/267 (99%)	253 (96%)	12 (4%)	24	47
7	r	265/267 (99%)	255 (96%)	10 (4%)	29	51
All	All	8071/14549 (56%)	7626 (94%)	445 (6%)	21	44

5 of 445 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	O	147	THR
7	r	261	LEU
1	P	66	VAL
7	r	115	VAL
7	k	199	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 195 such sidechains are listed below:

Mol	Chain	Res	Type
1	O	1033	GLN
1	P	1283	ASN
1	P	226	HIS
1	P	750	ASN
2	v	295	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [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 [i](#)

There are no chain breaks in this entry.

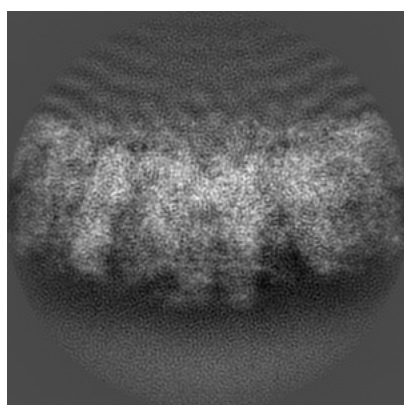
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-21525. These allow visual inspection of the internal detail of the map and identification of artifacts.

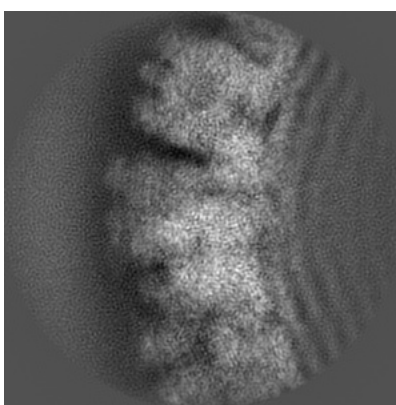
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

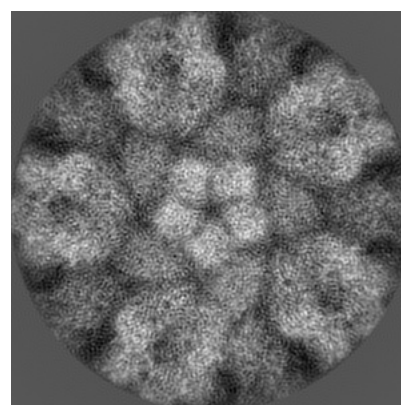
6.1.1 Primary map



X



Y

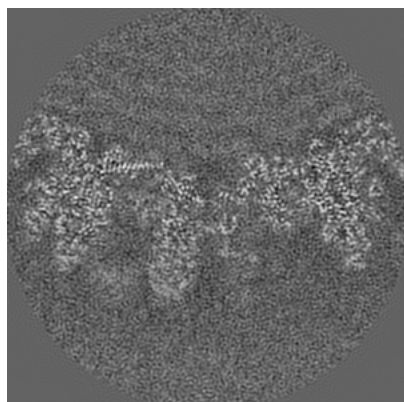


Z

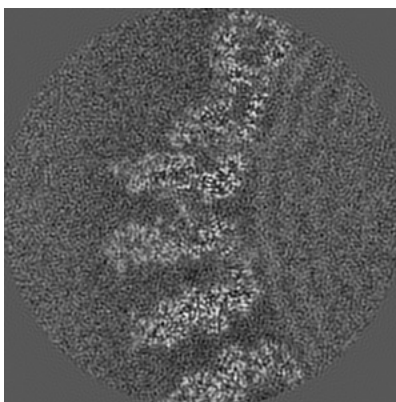
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

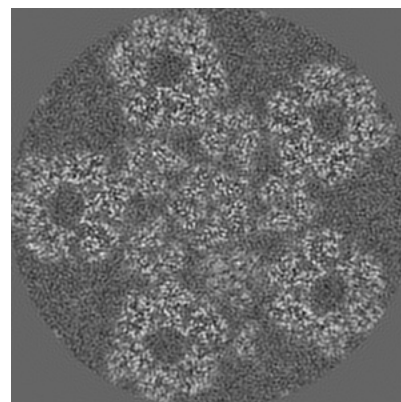
6.2.1 Primary map



X Index: 160



Y Index: 160

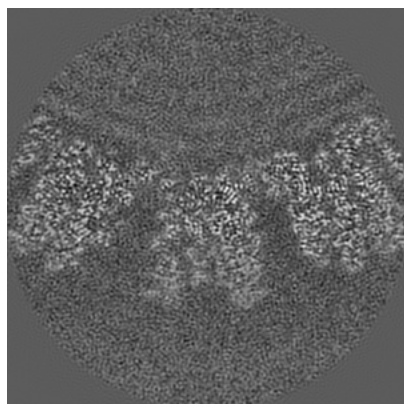


Z Index: 160

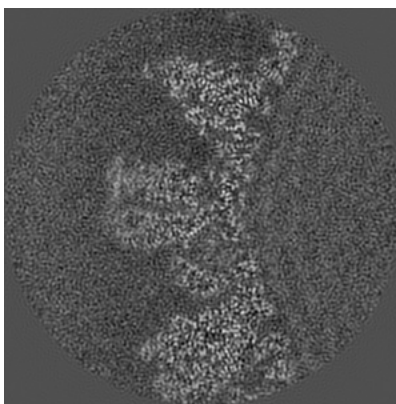
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

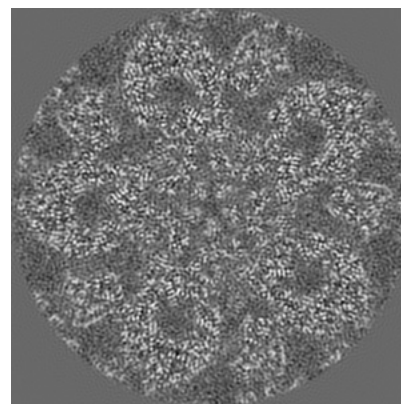
6.3.1 Primary map



X Index: 147



Y Index: 189

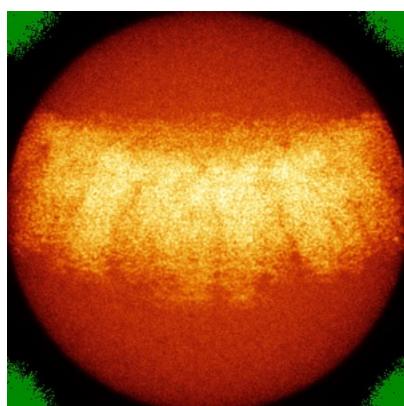


Z Index: 185

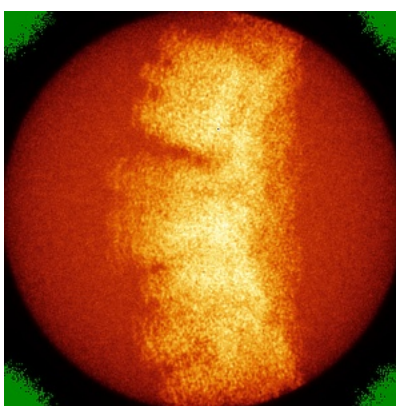
The images above show the largest variance slices of the map in three orthogonal directions.

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

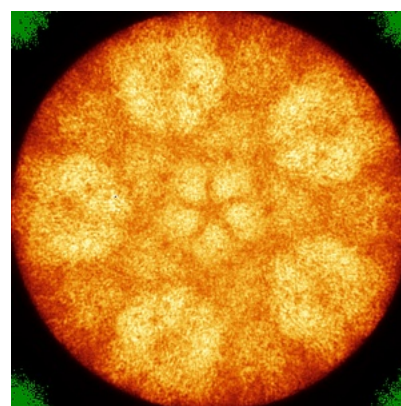
6.4.1 Primary map



X



Y

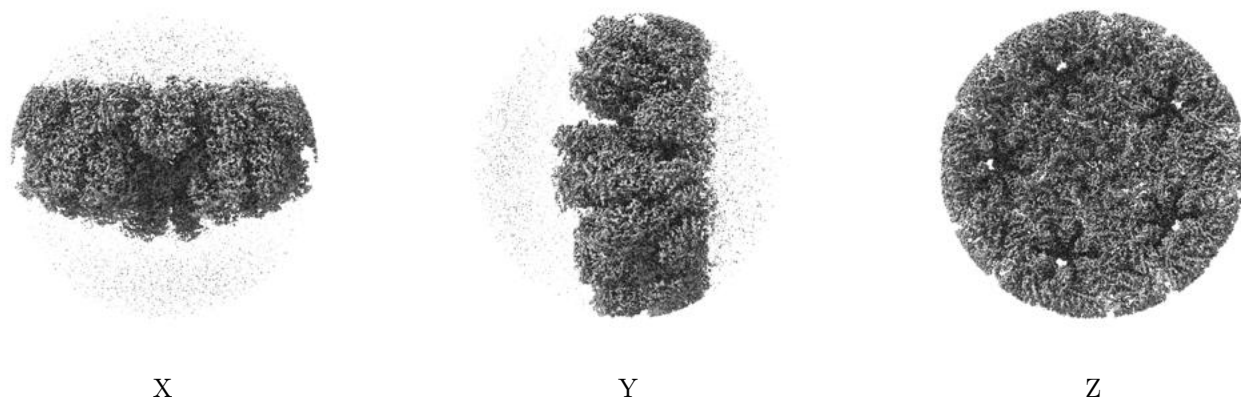


Z

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 [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.015. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

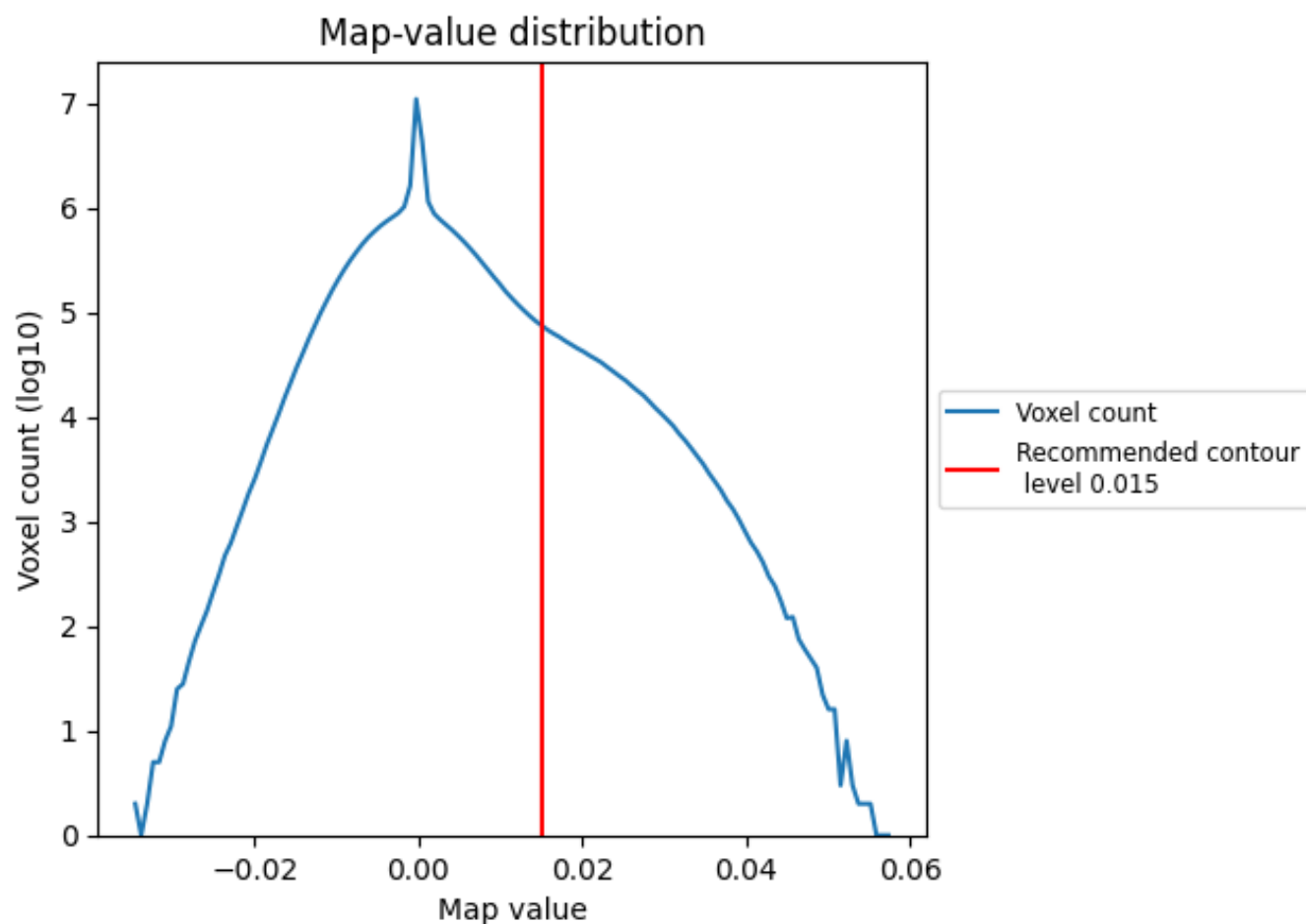
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

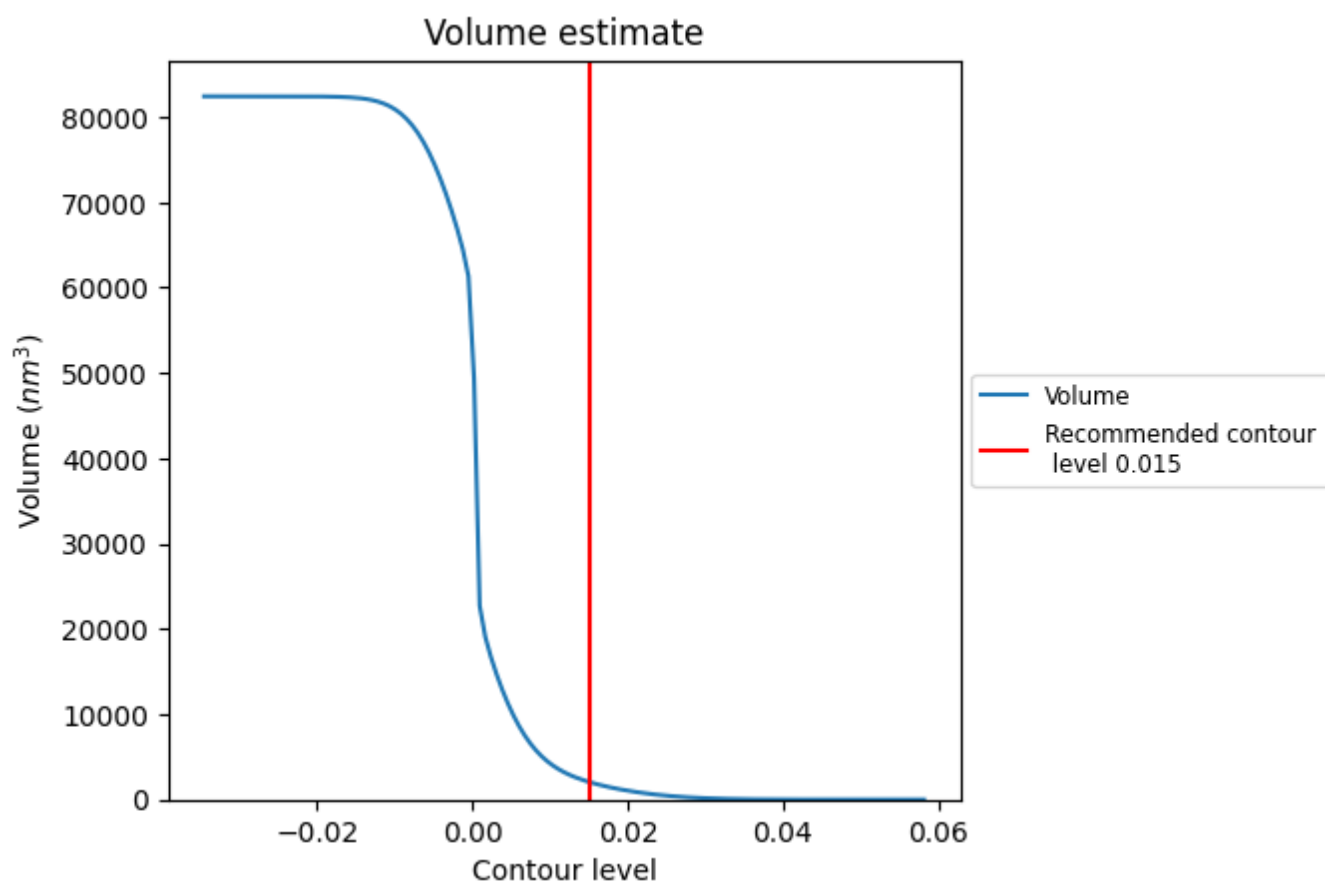
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

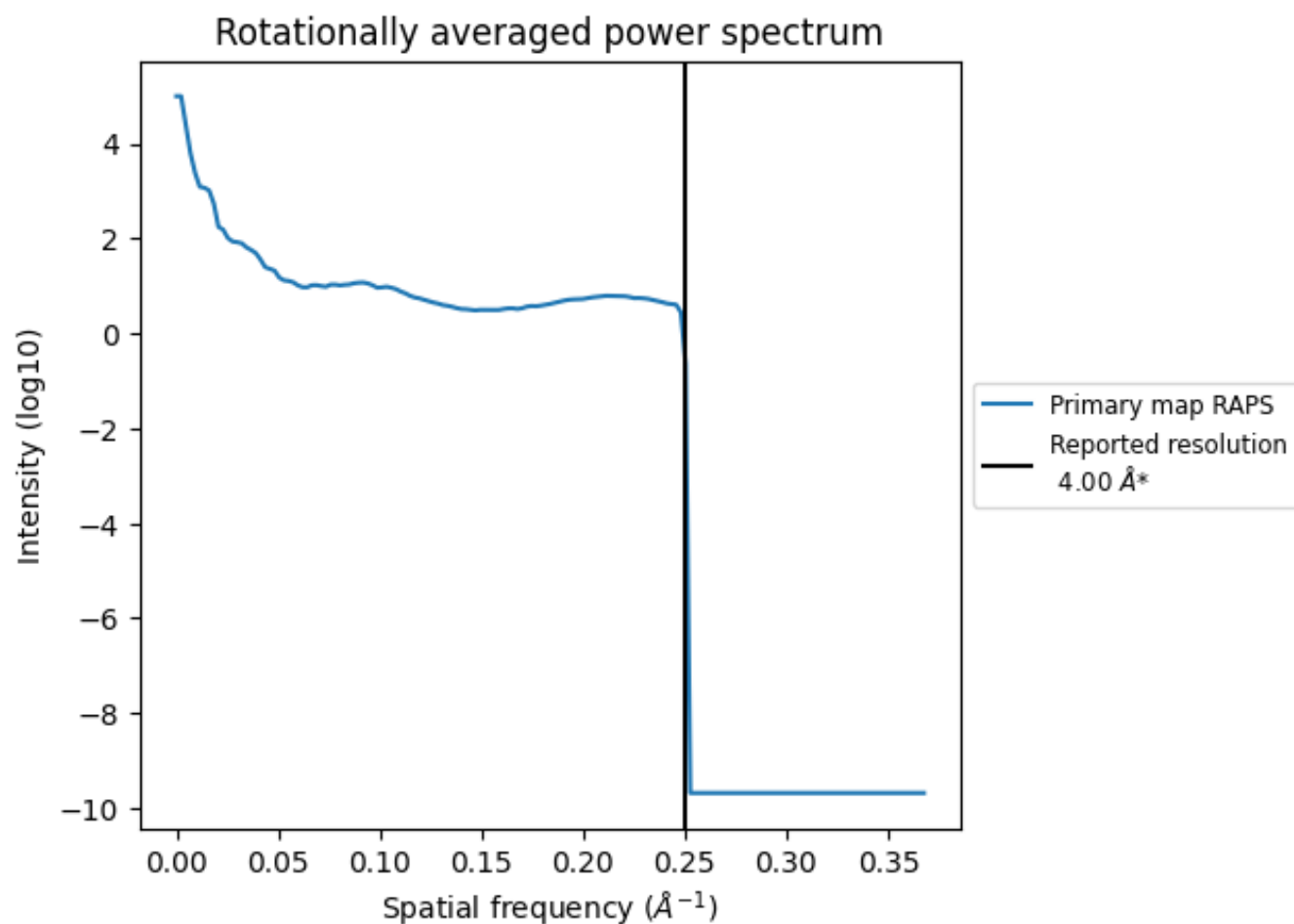
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2067 nm³; this corresponds to an approximate mass of 1867 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 0.250 Å⁻¹

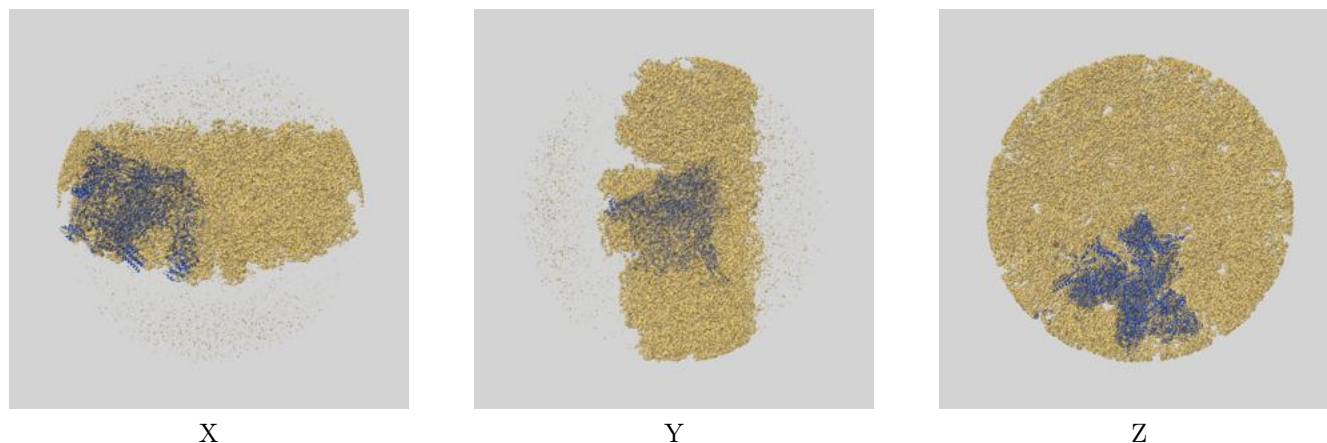
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

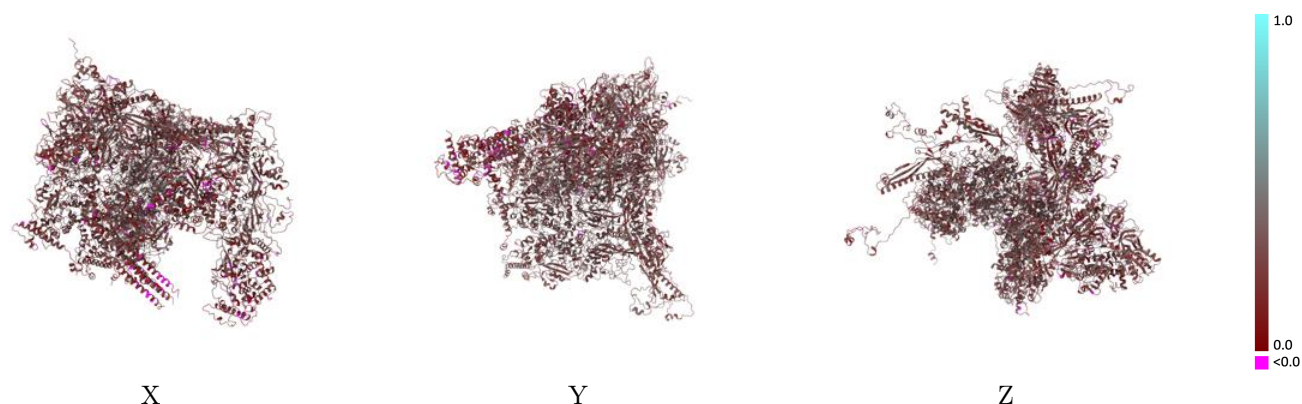
This section contains information regarding the fit between EMDB map EMD-21525 and PDB model 6W2D. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

9.1 Map-model overlay [i](#)



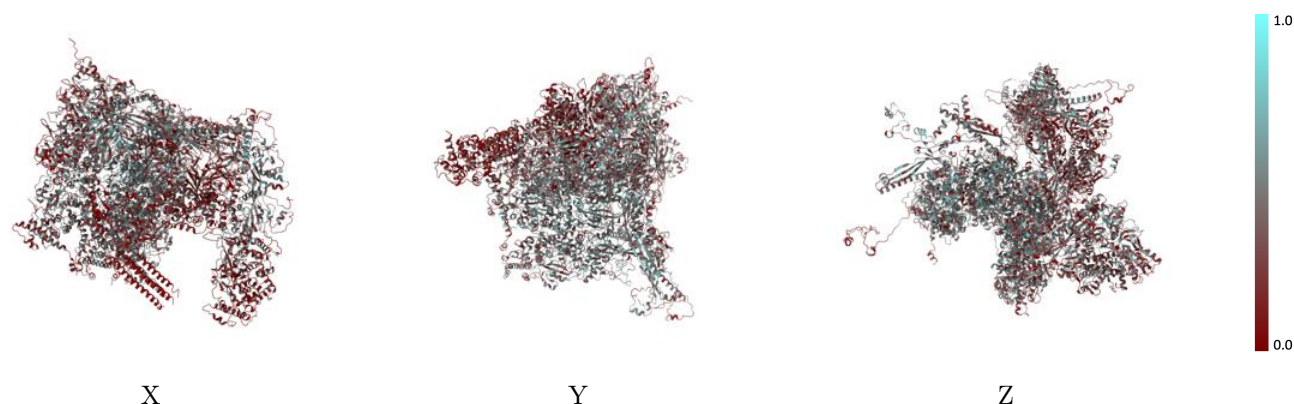
The images above show the 3D surface view of the map at the recommended contour level 0.015 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



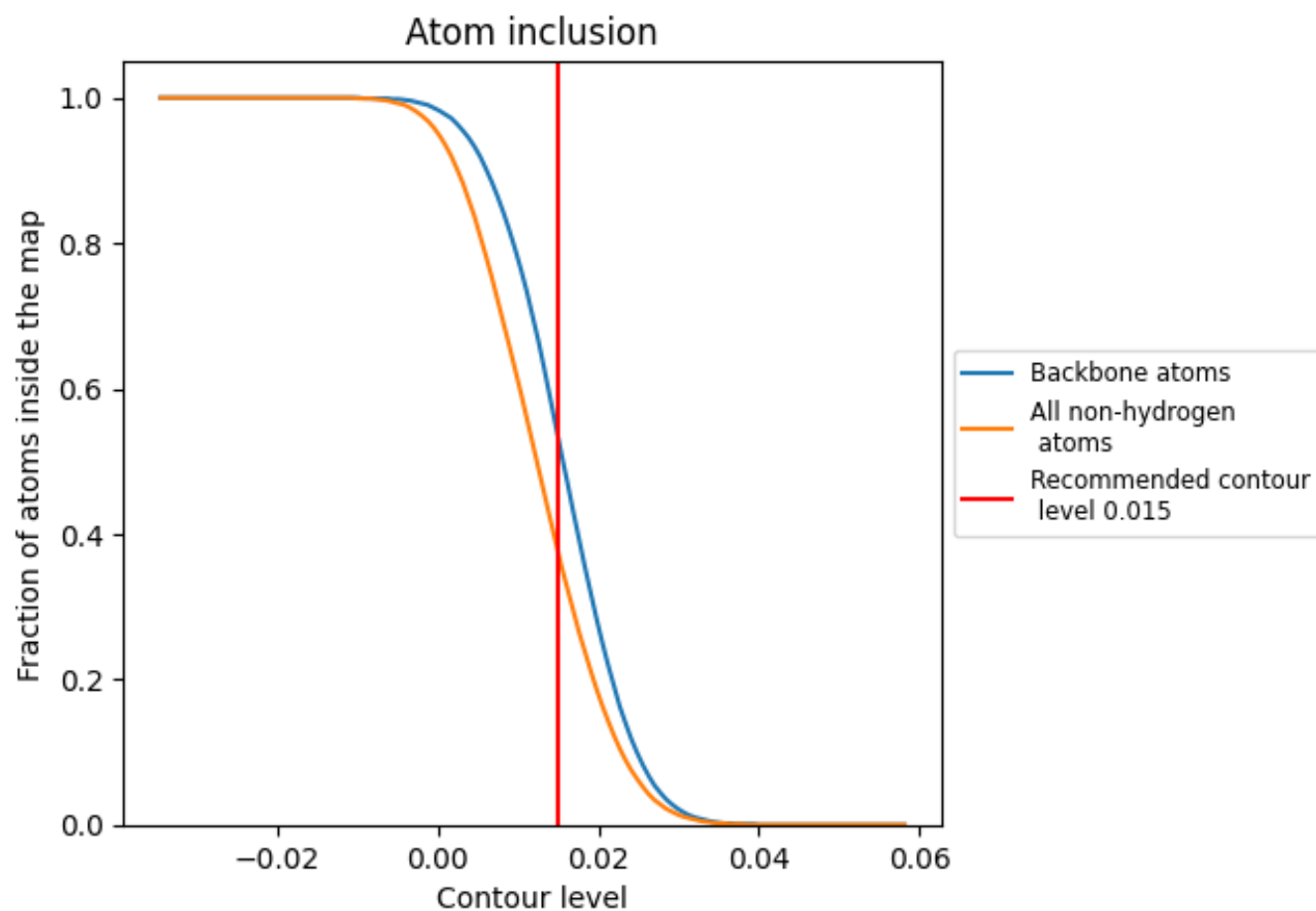
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.015).

9.4 Atom inclusion [i](#)



At the recommended contour level, 53% of all backbone atoms, 37% 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 (0.015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.3740	 0.2800
J	 0.4580	 0.3060
K	 0.4470	 0.3030
N	 0.4050	 0.2910
O	 0.4400	 0.3030
P	 0.3240	 0.2580
Z	 0.3450	 0.2420
a	 0.3080	 0.2810
d	 0.2430	 0.2360
e	 0.2950	 0.2580
f	 0.2000	 0.2340
h	 0.3770	 0.2720
k	 0.2460	 0.2530
m	 0.3430	 0.2700
p	 0.2390	 0.2550
r	 0.3660	 0.2810
u	 0.1380	 0.1670
v	 0.2220	 0.2410
w	 0.1000	 0.1630
x	 0.1880	 0.1900
y	 0.1090	 0.1880
z	 0.0960	 0.1620

