



wwPDB EM Validation Summary Report ⓘ

Nov 14, 2022 – 06:54 PM EST

PDB ID : 6W2E
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.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

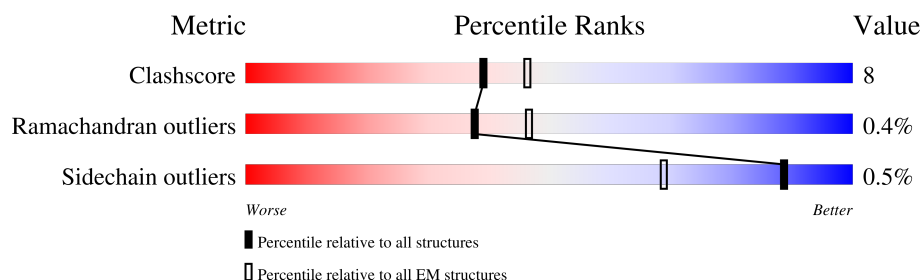
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.40 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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 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	<div> <div>50%</div> <div>78% 17% 6%</div> </div>
1	K	1381	<div> <div>54%</div> <div>84% 15% .</div> </div>
1	N	1381	<div> <div>60%</div> <div>84% 15% .</div> </div>
1	O	1381	<div> <div>53%</div> <div>79% 15% 6%</div> </div>
2	v	507	<div> <div>50%</div> <div>58% 42%</div> </div>
3	w	570	<div> <div>12%</div> <div>12% 88%</div> </div>
3	x	570	<div> <div>11%</div> <div>12% 88%</div> </div>
4	y	3149	<div> <div>.</div> <div>99%</div> </div>

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Mol	Chain	Length	Quality of chain
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		

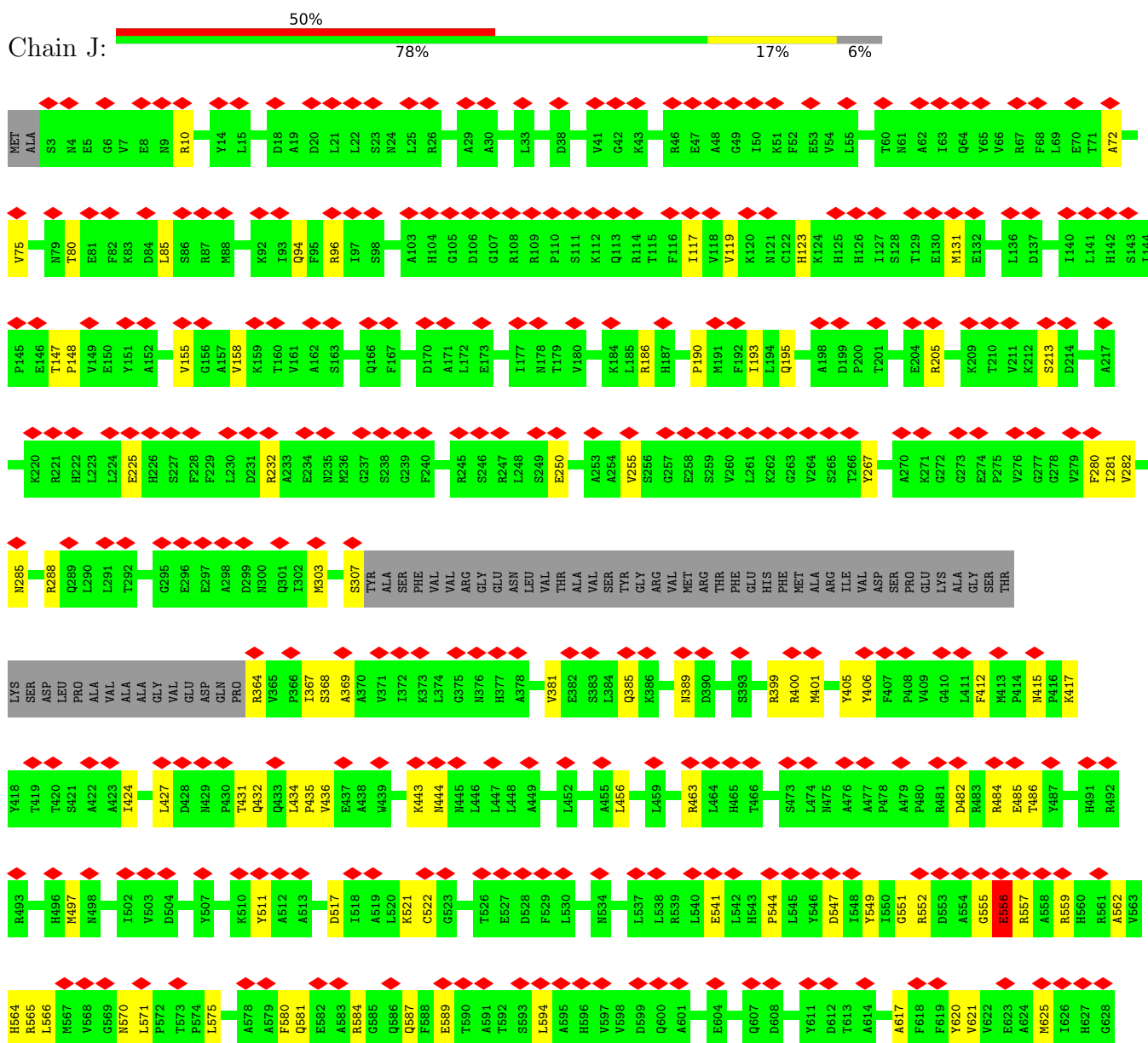
- Molecule 7 is a protein called Triplex capsid protein 2.

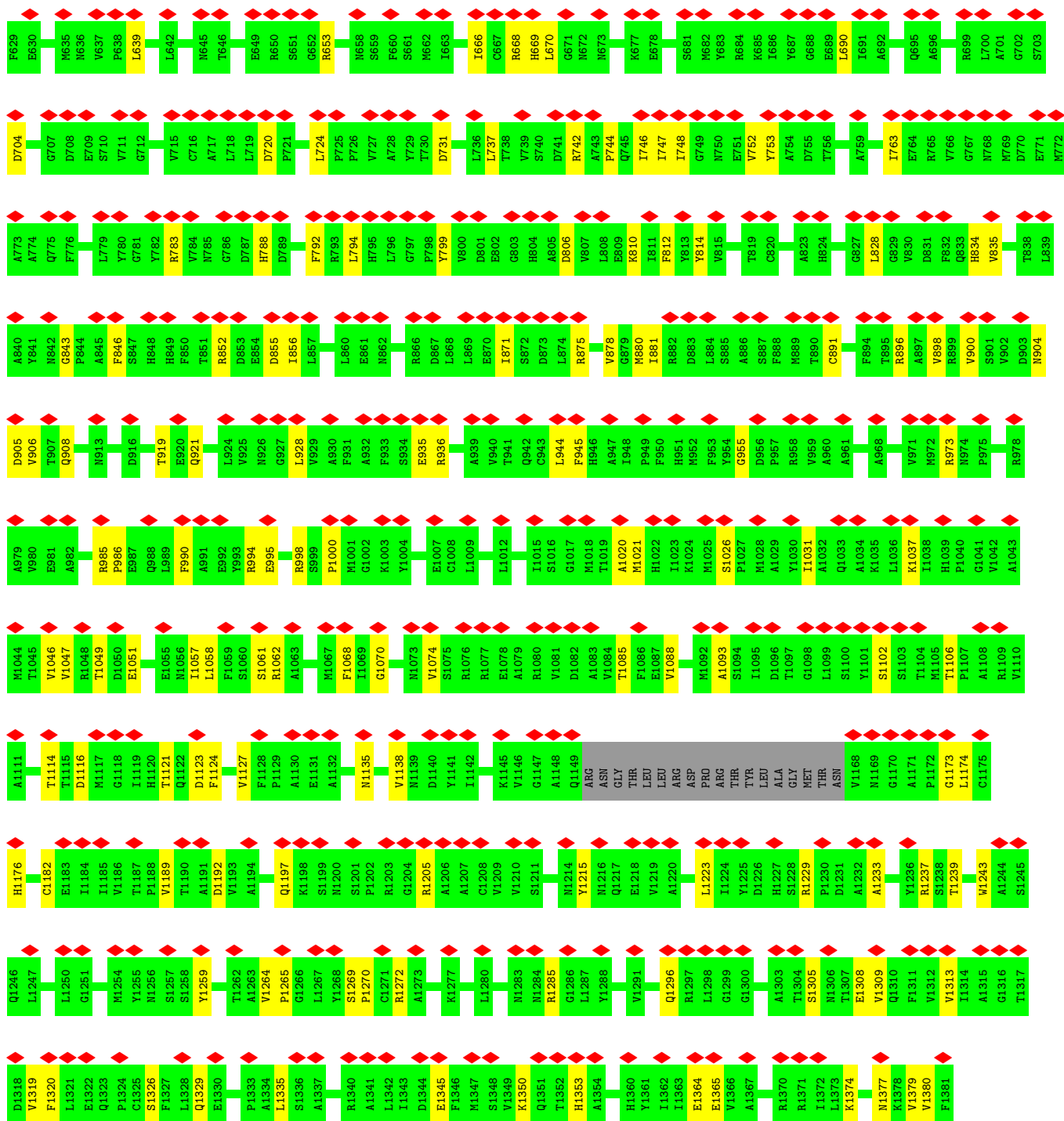
Mol	Chain	Residues	Atoms					AltConf	Trace
7	k	299	Total	C	N	O	S	0	0
			2338	1500	386	434	18		
7	m	299	Total	C	N	O	S	0	0
			2338	1500	386	434	18		
7	p	299	Total	C	N	O	S	0	0
			2338	1500	386	434	18		
7	r	299	Total	C	N	O	S	0	0
			2338	1500	386	434	18		

3 Residue-property plots

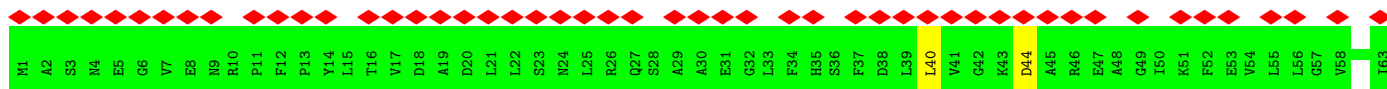
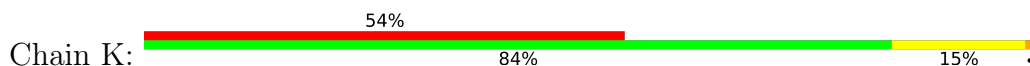
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

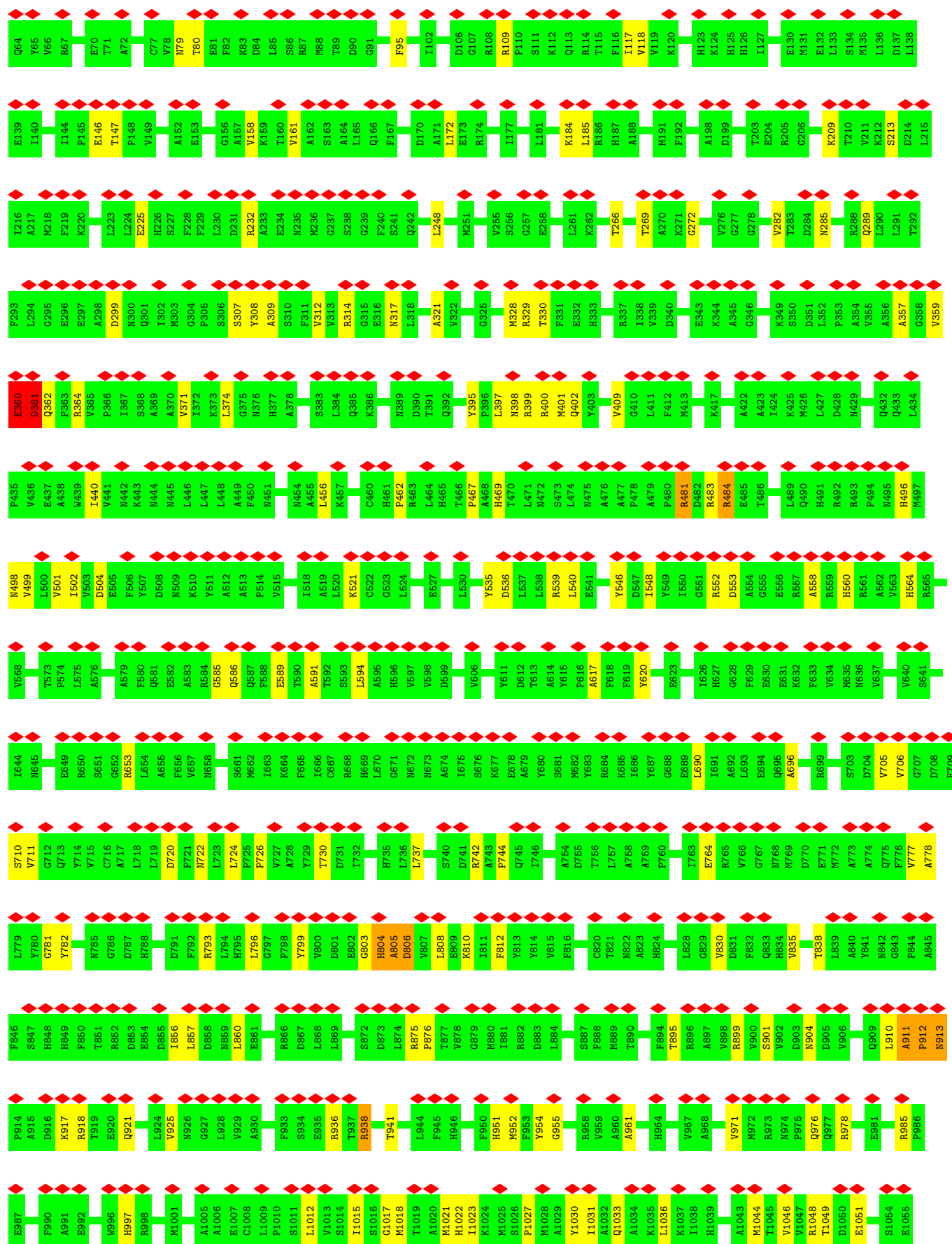
- Molecule 1: Major capsid protein

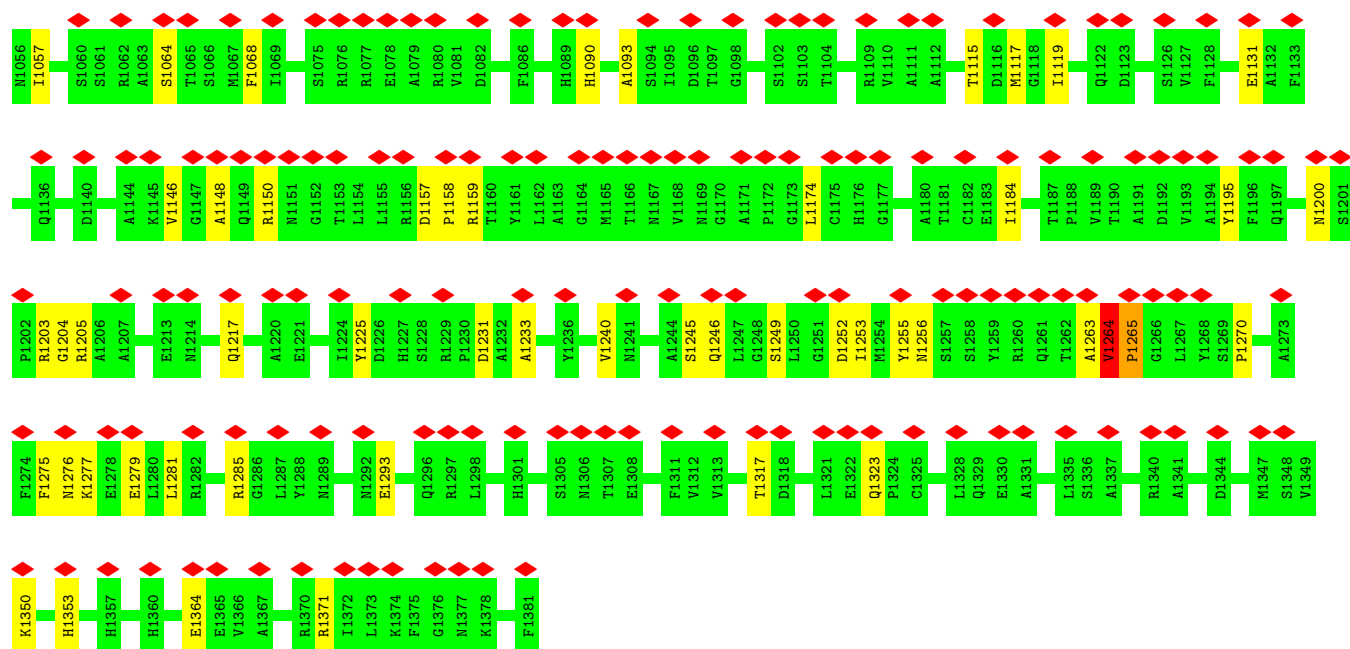




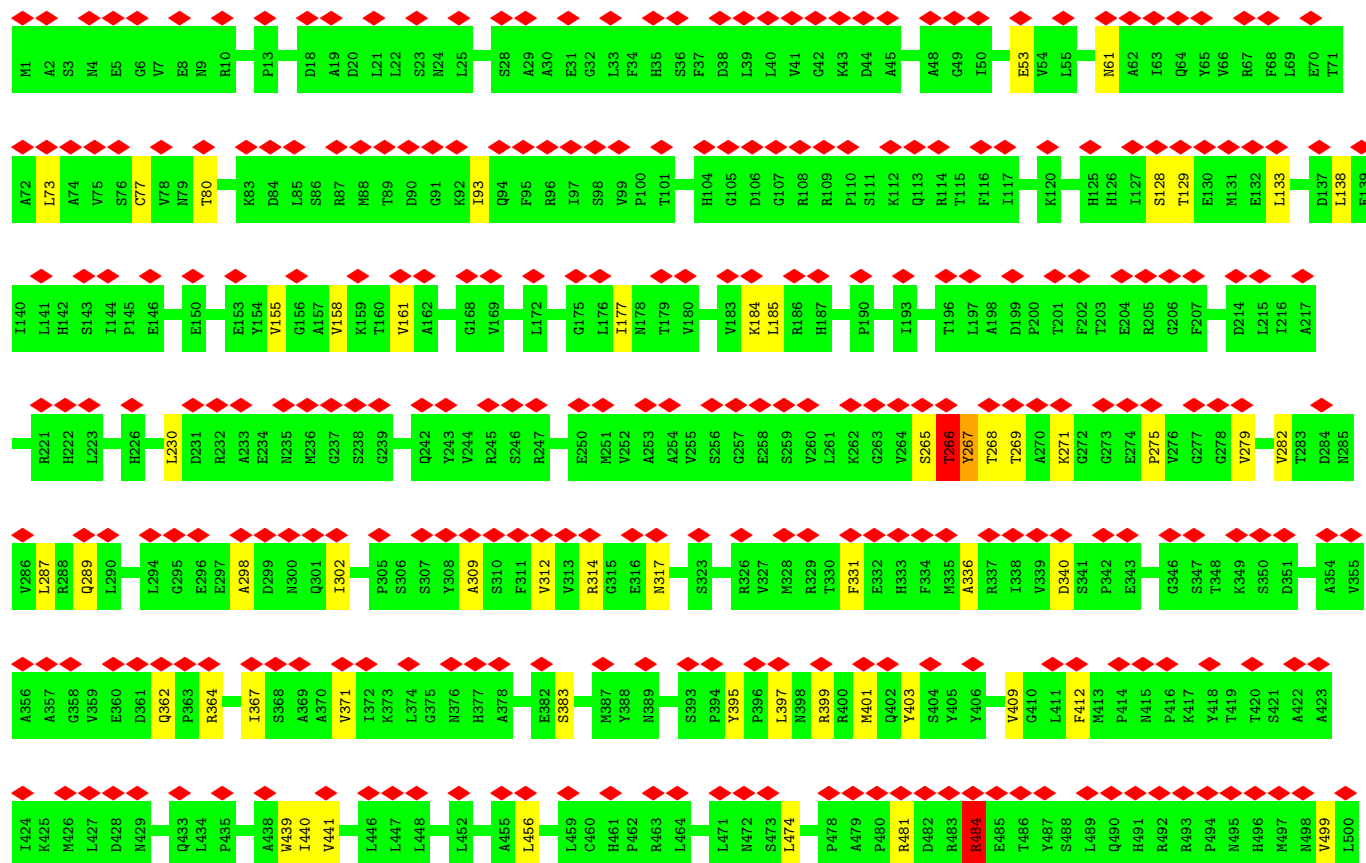
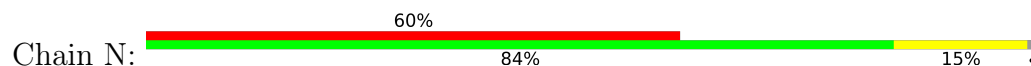
• Molecule 1: Major capsid protein



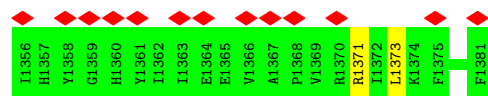




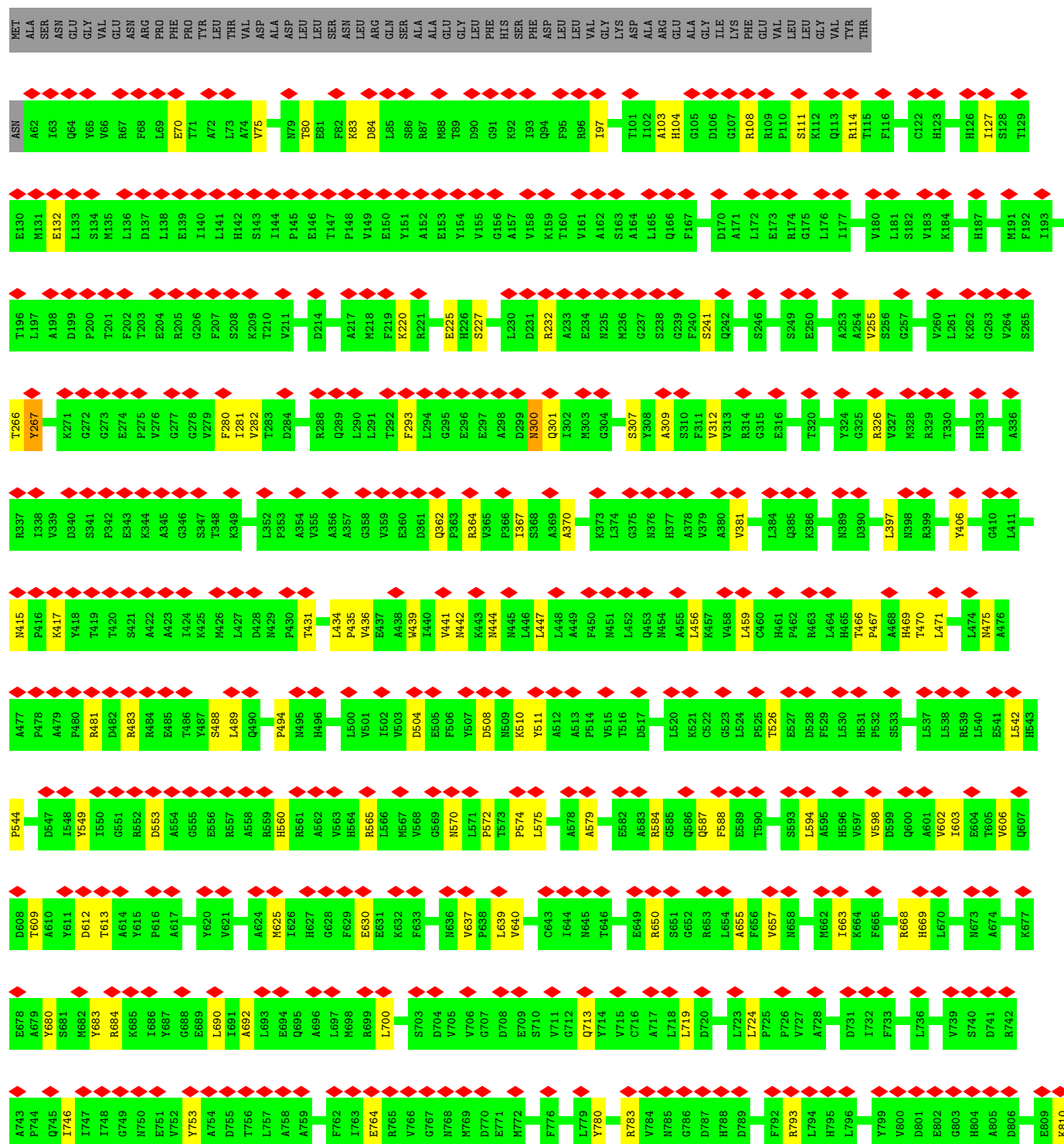
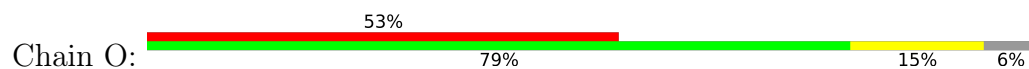
• Molecule 1: Major capsid protein

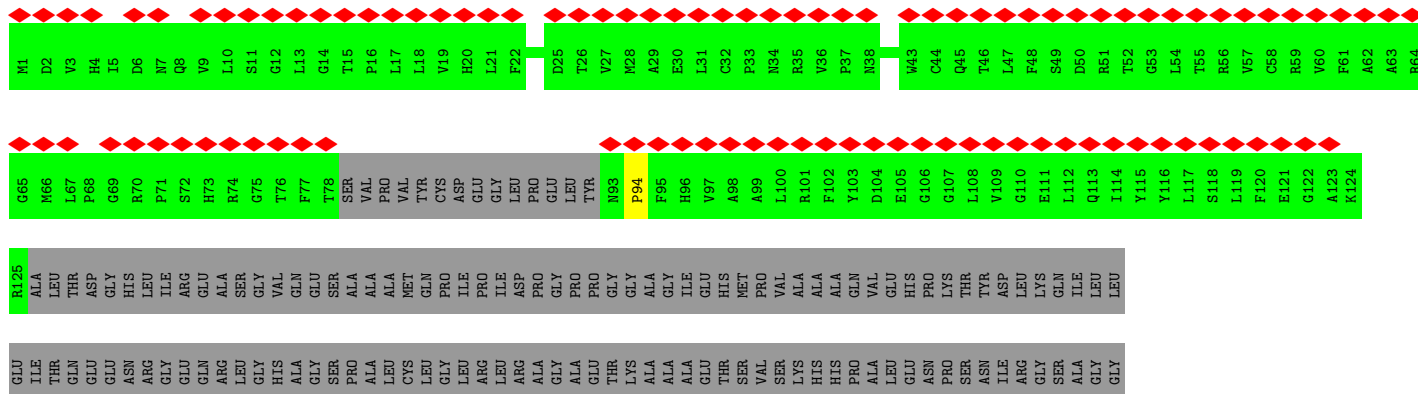
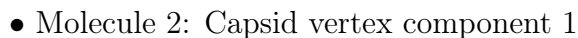


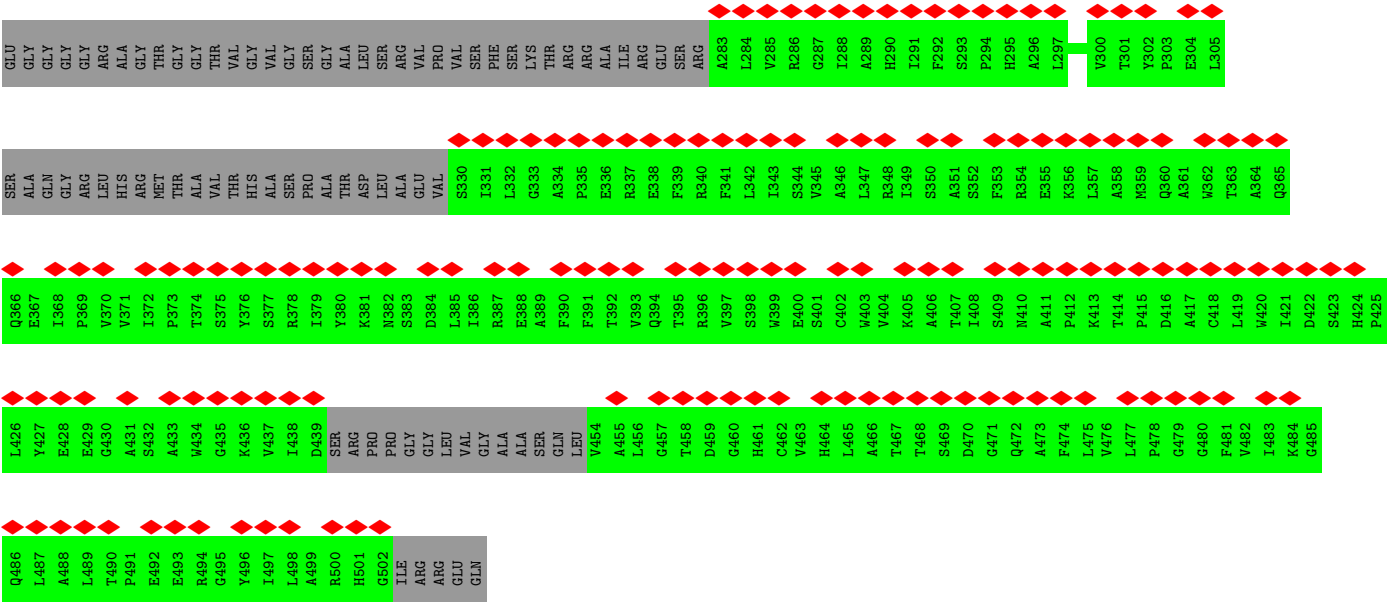
Y1288	M1289	V1291	M1292	E1293	Y1294	S1295	Q1296	L1297	L1298	G1299	G1300	H1301	P1302	A1303	T1304	S1305	N1306	Q1310	F1311	T1314	A1315	G1316	T1317	D1318	V1319	F1320	L1321	A1322	Q1323	F1327	L1328	Q1329	E1330	A1331	S1336	A1337	S1338	S1339	L1342	I1343	D1344	E1345	F1346	M1347	S1348	V1349	K1350	Q1351	T1352	H1353	A1354	P1355							
G1222	L1223	I1224	Y1225	D1226	H1227	S1228	R1229	D1231	A1232	A1233	Y1234	E1235	Y1236	R1237	S1238	P1242	W1243	A1244	S1245	Q1246	L1247	G1248	S1249	L1250	G1251	D1252	I1253	S1257	S1258	Y1259	L1260	Q1261	T1262	A1263	V1264	G1266	L1267	Y1268	S1269	P1270	C1271	R1272	A1273	F1274	F1275	N1276	K1277	E1278	E1279	L1280	L1281	R1282	N1283	N1284	R1285				
PRO	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	F1128	F1129	A1130	E1131	A1132	F1133	G1134	M1067	F1068	I1069	G1070	T1071	P1072	N1073	V1074	S1075	A1076	R1077	E1078	A1079	R1080	V1081	D1082	A1083	F1086	E1087	V1088	H1089
H1090	E1091	M1092	A1093	S1094	I1095	D1096	L1099	S1100	Y1101	S1102	A1108	M1109	V1110	A1111	A1112	T1115	D1116	G1117	G1118	I1119	H1120	D1123	F1124	F1125	S1126	V1127	F1128	F1129	A1130	E1131	A1132	F1133	G1134	M1135	V1138	N1139	D1140	Y1141	I1142	K1143	A1144	K1145	V1146	G1147	A1148	Q1149	ARG	ASN	GLY	THR	LEU	LEU	ARG	ASP					
I1023	K1024	P1027	T1030	Q1033	A1034	K1035	L1036	K1037	I1038	H1039	P1040	G1041	V1042	A1043	M1044	T1045	T1049	D1050	E1051	I1052	L1053	S1054	E1055	M1056	I1057	L1058	F1059	S1060	A1063	S1064	A1065	F1066	M1067	F1068	I1069	G1070	T1071	P1072	N1073	V1074	S1075	A1076	R1077	E1078	A1079	R1080	V1081	D1082	A1083	F1086	E1087	V1088	H1089						
P957	R958	V959	A960	A961	T962	M963	H964	Q965	D966	V967	A968	T969	F970	V971	M972	R973	N974	P975	Q976	Q977	R978	A979	V980	E981	A982	F983	N984	R985	R986	E987	Q988	F990	A991	E992	Y993	W996	H997	R998	S999	G1002	K1003	A1006	E1007	C1008	L1009	V1013	S1014	G1017	M1018	T1019	A1020	M1021	H1022						
T893	F894	T895	R896	A897	R898	R899	V900	S901	V902	D903	N904	D905	V906	T907	N913	P914	A915	D916	K917	R918	T919	E920	Q921	T922	V923	L924	V925	N926	Q927	L928	A930	F931	A932	R933	S934	E935	R936	T937	R938	A939	V940	T941	Q942	C943	L944	F945	H946	A947	L948	P949	F950	H951	N952	F953	Y954	G955	D956		
F832	Q833	H834	R835	A836	Q837	T838	L839	A840	Y841	N842	G843	P844	A845	F846	S847	H848	H849	F850	T851	R852	D853	E854	D855	L856	L857	D858	N859	E861	N862	G863	T864	L865	R866	D867	L868	L869	E870	L871	S872	D873	L874	R875	P876	T877	G879	M880	L881	D882	D883	L884	S885	A886	S887	F888	N889	T890			
E771	M772	A773	Q775	F776	V777	A778	L779	Y780	G781	Y782	R783	F784	N785	G786	D787	H788	D789	T790	D791	F792	Y729	I663	K664	F665	R668	H669	G671	N672	N673	A674	Y611	D612	T613	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	S710	V711	G712	Q713	Y714	V715	C716	A717	L718	L719	D720	F721	N722	L723	L724	A728	Y729	I663	K664	F665	R668	H669	G671	N672	N673	A674	Y611	D612	T613	S676	K677	E678	A679	M682	Y683	R684	K685	I686	Y687	G688	E689	L693	E694	Q695	A696	L697	M698	R699	L700	A701	G702	S703			
M567	V568	G569	N570	P572	L575	A579	F580	R584	G585	Q586	Q587	F588	E589	T590	A591	L594	I603	E604	Q607	D608	T609	A610	Y611	D612	T613	A614	Y615	P616	A617	F618	F619	Y620	V621	A624	M625	I626	H627	G628	F629	E630	F633	V634	M635	N636	V637	P638													
V501	I502	E505	F506	F507	D508	N509	K510	Y511	A512	A513	P514	V515	T516	D517	I518	A519	L520	K521	G522	G523	L524	P525	T526	E527	D528	F529	P532	D536	L537	L538	R539	L540	E541	L542	H543	Y546	D547	I548	Y549	G551	R552	D553	A554	G555	E556	R557	A558	R559	H560	R561	H564	R565	L566						



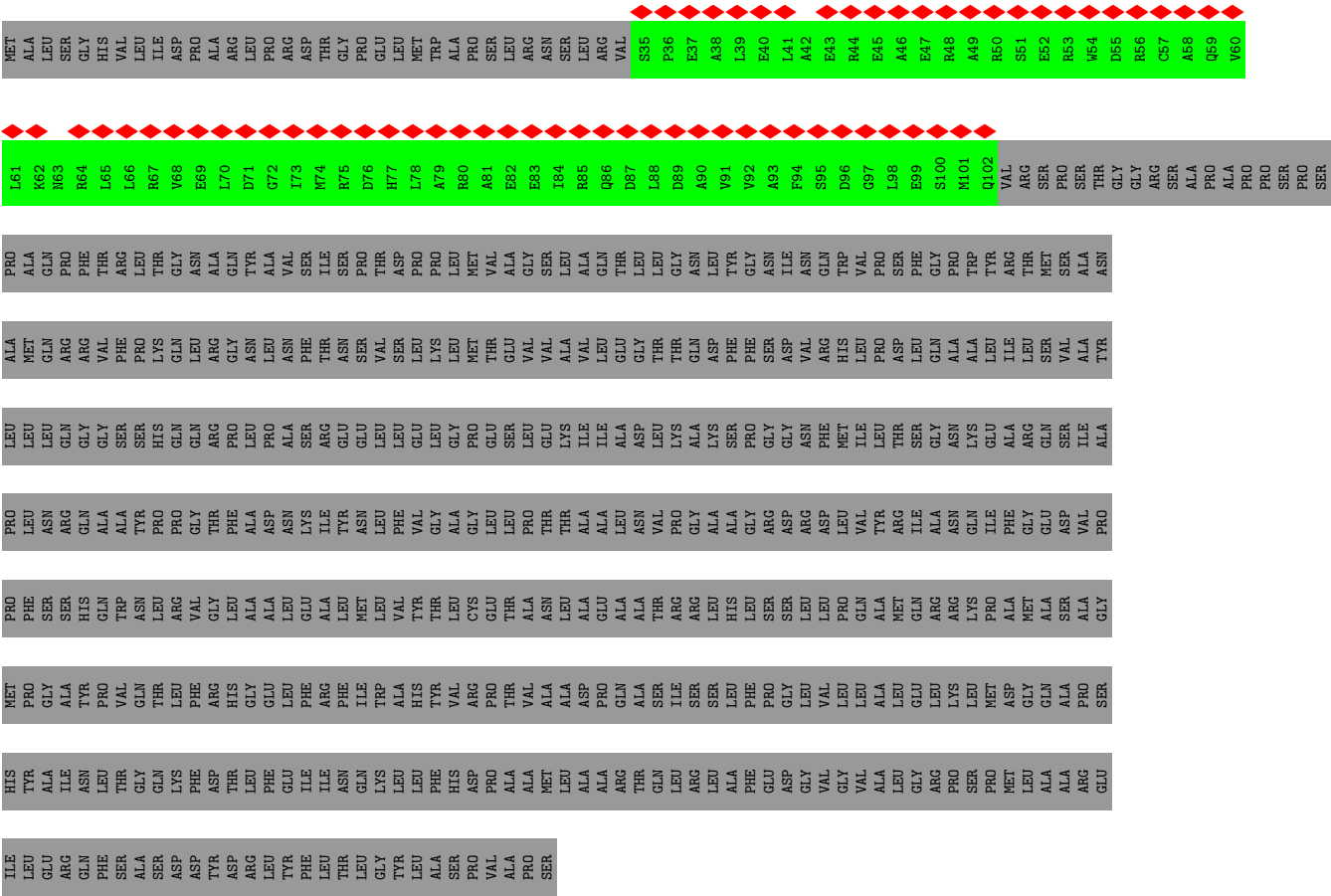
● Molecule 1: Major capsid protein







• Molecule 3: Capsid vertex component 2



• Molecule 3: Capsid vertex component 2





R3121	PRO	LYS	THR	LEU	GLY
F3122	SER	GLU	ALA	ALA	ARG
V3123	VAL	ALA	ALA	ALA	GLU
S3124	VAL	PRO	PRO	PRO	GLU
Q3125	THR	PRO	SER	HIS	GLU
R3126	GLN	SER	ALA	THR	ALA
R3127	PHE	ALA	ALA	PRO	ILE
R3128	ILE	SER	SER	VAL	ARG
K3129	ILE	GLN	PRO	GLY	PRO
L3130	ASP	LEU	PRO	SER	ALA
E3131	ILE	LYS	VAL	THR	ALA
R3132	ILE	MET	SER	PRO	ARG
S3133	ARG	PRO	LEU	ARG	LEU
T3134	GLU	LYS	PRO	GLN	THR
H3135	VAL	CYS	VAL	LYS	ALA
H3136	VAL	ASP	SER	THR	VAL
R3136	THR	SER	ARG	GLN	GLY
L3137	GLY	MET	GLN	ALA	LEU
I3138	SER	TYR	GLN	GLN	ARG
A3139	THR	TYR	SER	PRO	ARG
D3140	SER	PRO	PRO	GLN	ALA
L3141	ASP	SER	ALA	ASP	PRO
E3142	LEU	GLY	ILE	ALA	VAL
R3143	VAL	SER	PRO	ALA	VAL
L3144	VAL	ALA	LEU	ALA	ALA
K3145	PRO	ARG	PRO	LEU	GLY
F3146	SER	TYR	PRO	PRO	ALA
L3147	GLY	PRO	MET	THR	ALA
Y3148	SER	ALA	HIS	PRO	ALA
L3149	PRO	PRO	SER	THR	ALA
	SER	PHE	GLY	GLY	ALA
	LEU	SER	ALA	ALA	PHE
	ALA	SER	ARG	ARG	ASP
	PRO	GLN	PRO	PRO	PRO
	GLU	SER	GLU	VAL	GLY
	GLN	VAL	VAL	PRO	GLU
	ASP	ALA	ARG	LYS	ALA
	LEU	SER	LEU	ALA	PRO
	ARG	PRO	SER	THR	SER
	TYR	ALA	GLN	GLY	GLY
	SER	PRO	TYR	ALA	PHE
	LEU	SER	ARG	LEU	PRO
	THR	SER	HIS	ALA	ILE
	LEU	ASP	ALA	ALA	PRO
	S3113	GLN	GLY	GLY	GLN
Q3114	THR	THR	PRO	ALA	ALA
A3115	THR	THR	GLN	ARG	PRO
S3116	LEU	LEU	THR	PRO	ALA
R3117	LEU	LEU	TYR	ARG	LEU
V3118	ASP	ASN	THR	VAL	GLY
L3119	THR	THR	ARG	PRO	SER
S3120					GLY

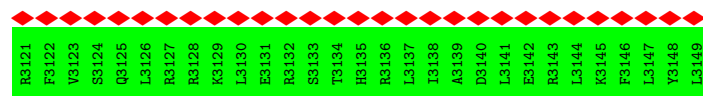
- Molecule 4: Large tegument protein deneddylase

Chain z: 

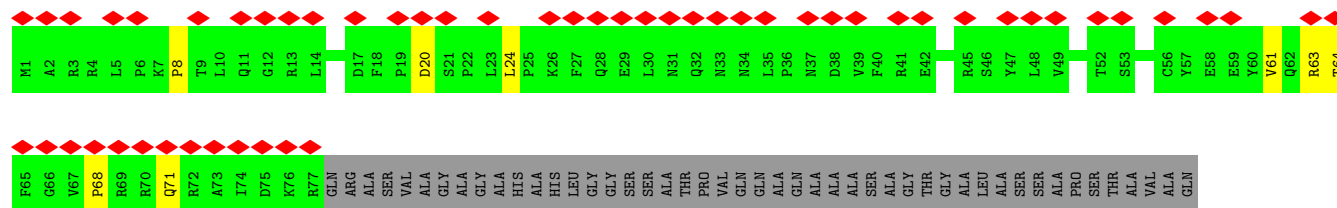
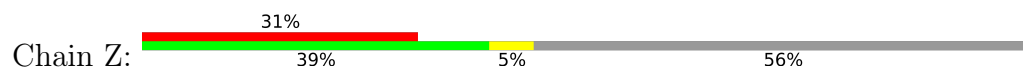
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ASP	PRO	GLN	PRO	SER	SER	PRO	THR	ILE	LEU	VAL	SER
LEU	ALA	GLN	ALA	PRO	ALA	TYR	GLU	ILE	ARG	SER	ASN
GLU	PRO	GLN	PRO	HIS	PRO	ASN	ASP	GLY	GLY	CYS	ASP
PRO	PRO	PRO	VAL	LYS	ALA	LEU	ARG	ASP	GLY	VAL	TRP
PHE	ALA	GLN	SER	PRO	SER	ARG	ILE	GLY	ARG	LEU	GLN
LEU	GLN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



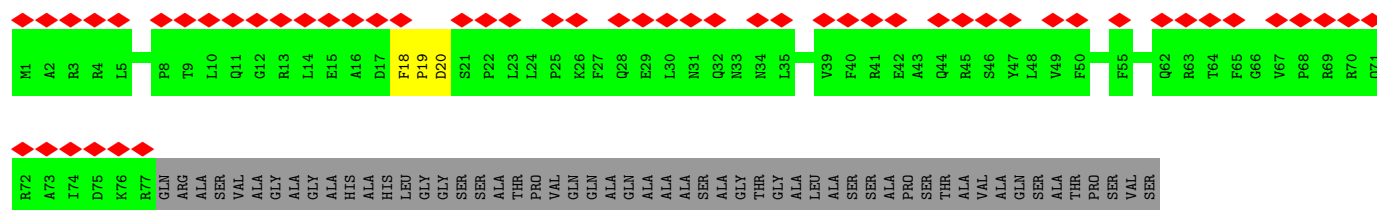




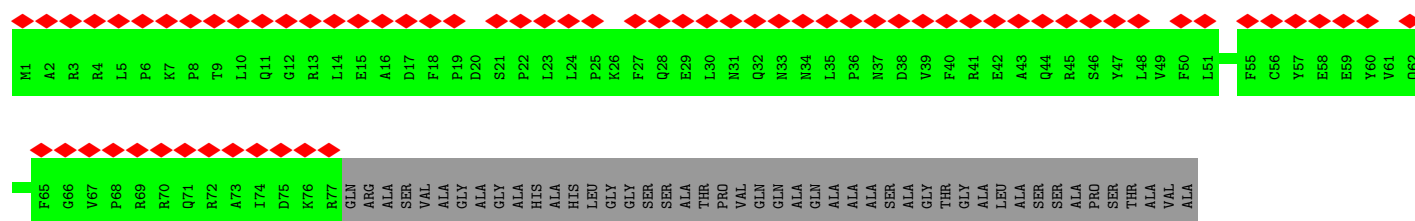
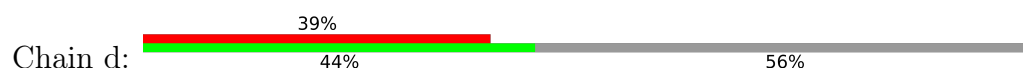
• Molecule 5: Small capsomere-interacting protein



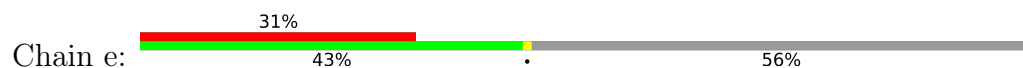
• Molecule 5: Small capsomere-interacting protein



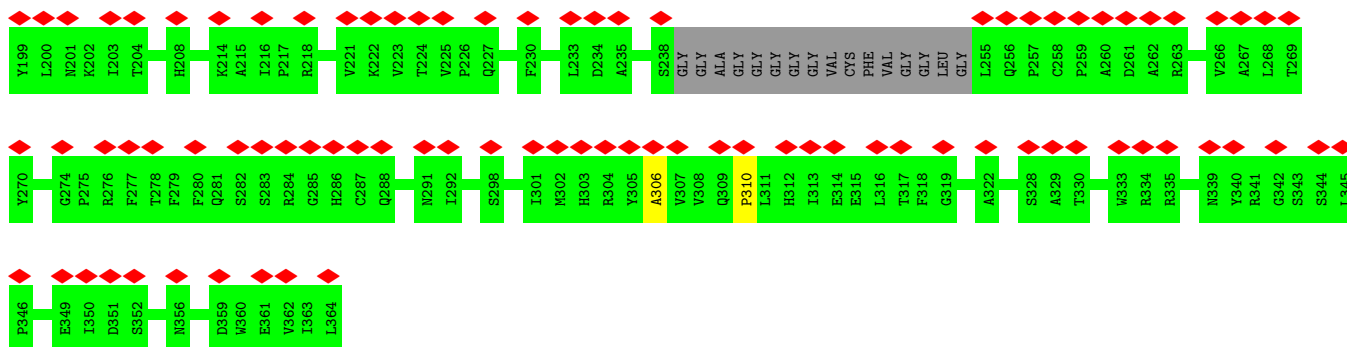
• Molecule 5: Small capsomere-interacting protein



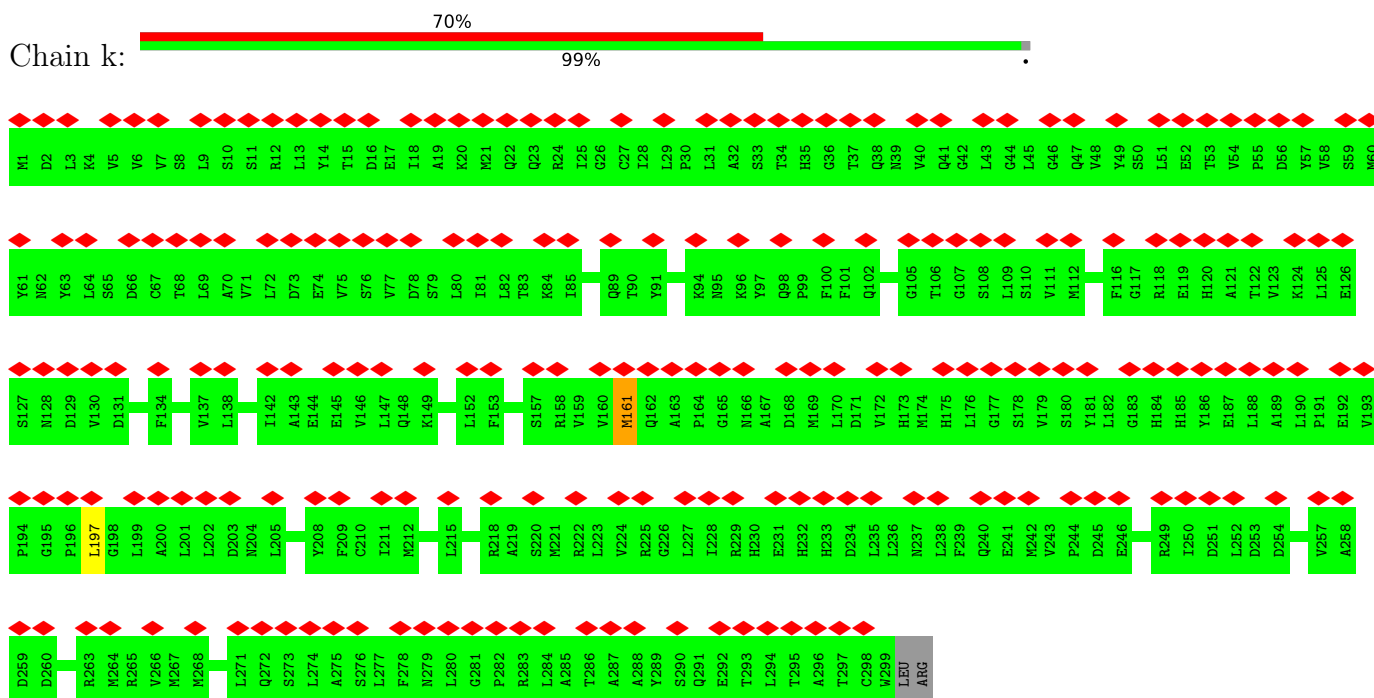
• Molecule 5: Small capsomere-interacting protein



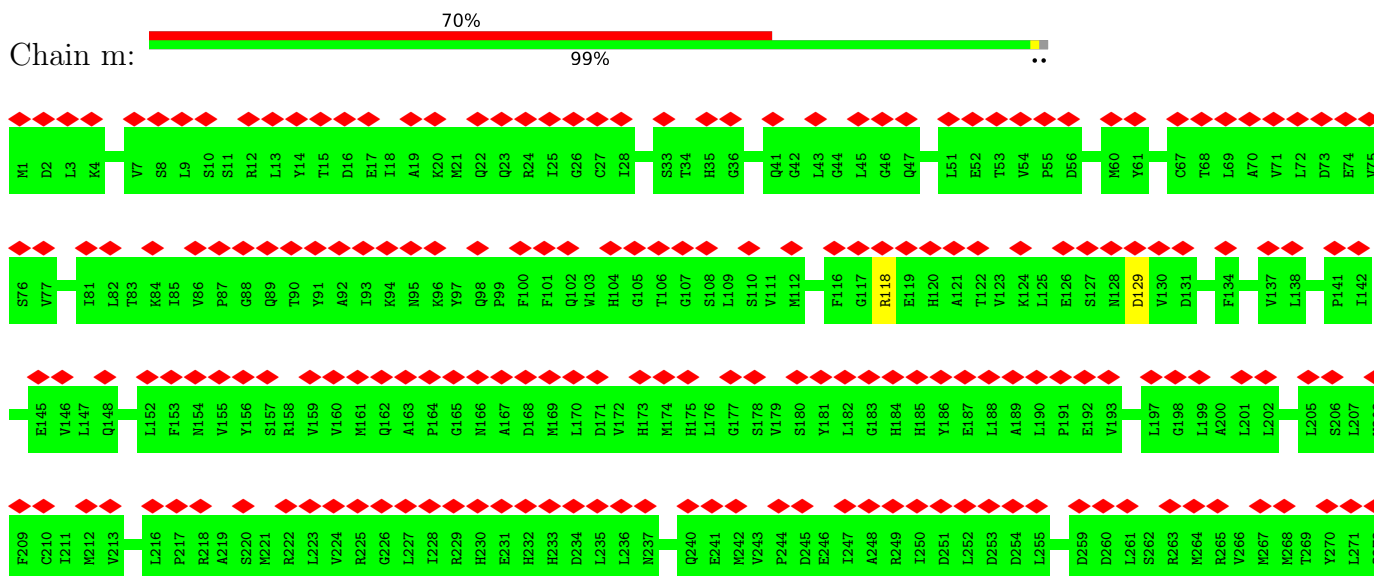


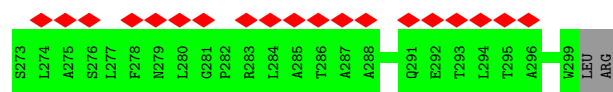


• Molecule 7: Triplex capsid protein 2



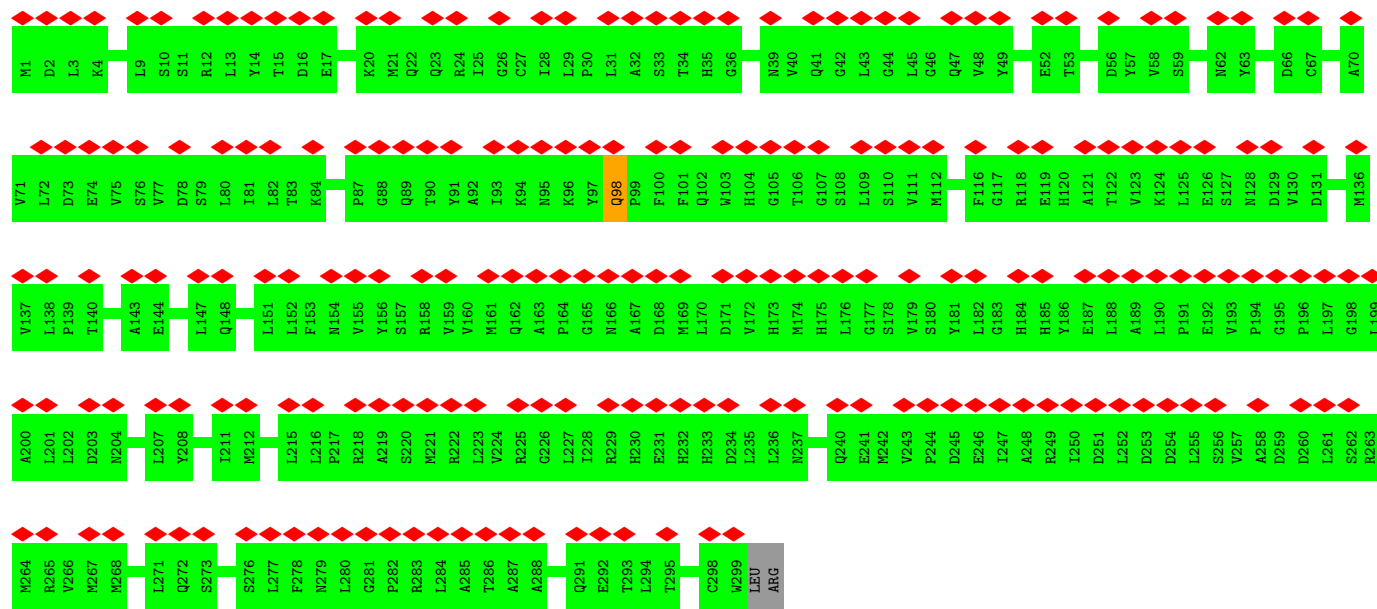
• Molecule 7: Triplex capsid protein 2





• Molecule 7: Triplex capsid protein 2

Chain p: 70% 99%



• Molecule 7: Triplex capsid protein 2

Chain r: 68% 97%



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	0.34	0/10492	0.57	0/14259
1	K	0.34	0/11085	0.58	0/15066
1	N	0.34	0/10933	0.57	0/14858
1	O	0.35	0/10435	0.57	0/14183
2	v	0.36	0/2346	0.61	0/3190
3	w	0.32	0/553	0.58	0/741
3	x	0.32	0/553	0.50	0/741
4	y	0.31	0/320	0.58	0/424
4	z	0.30	0/320	0.57	0/424
5	Z	0.35	0/664	0.58	0/896
5	a	0.34	0/664	0.60	1/896 (0.1%)
5	d	0.34	0/664	0.57	0/896
5	e	0.31	0/664	0.51	0/896
6	f	0.34	0/2049	0.63	2/2795 (0.1%)
6	h	0.34	0/2672	0.60	0/3635
7	k	0.34	0/2388	0.61	0/3254
7	m	0.35	0/2388	0.62	0/3254
7	p	0.32	0/2388	0.61	0/3254
7	r	0.33	0/2388	0.65	2/3254 (0.1%)
All	All	0.34	0/63966	0.59	5/86916 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	r	203	ASP	CB-CG-OD1	9.93	127.24	118.30
6	f	161	SER	C-N-CA	-7.42	90.86	122.00
7	r	203	ASP	CB-CG-OD2	-5.82	113.07	118.30
5	a	18	PHE	C-N-CA	-5.42	99.25	122.00
6	f	160	ASP	CB-CG-OD2	5.23	123.00	118.30

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	154	0
1	K	10832	0	10655	174	0
1	N	10683	0	10500	144	0
1	O	10194	0	10022	135	0
2	v	2288	0	2273	0	0
3	w	549	0	540	0	0
3	x	549	0	540	0	0
4	y	317	0	341	0	0
4	z	317	0	341	0	0
5	Z	649	0	649	5	0
5	a	649	0	649	0	0
5	d	649	0	649	0	0
5	e	649	0	649	0	0
6	f	1992	0	1953	0	0
6	h	2604	0	2577	0	0
7	k	2338	0	2364	0	0
7	m	2338	0	2364	0	0
7	p	2338	0	2364	0	0
7	r	2338	0	2364	0	0
All	All	62525	0	61868	587	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 587 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
1:K:1264:VAL:CB	1:K:1265:PRO:HD2	1.45	1.42
1:K:467:PRO:CG	1:K:912:PRO:HG3	1.59	1.33

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%)	51	85
1	K	1379/1381 (100%)	1313 (95%)	56 (4%)	10 (1%)	22	62
1	N	1358/1381 (98%)	1305 (96%)	49 (4%)	4 (0%)	41	76
1	O	1295/1381 (94%)	1239 (96%)	52 (4%)	4 (0%)	41	76
2	v	283/507 (56%)	260 (92%)	22 (8%)	1 (0%)	34	72
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%)	12	48
5	d	75/176 (43%)	73 (97%)	2 (3%)	0	100	100
5	e	75/176 (43%)	73 (97%)	1 (1%)	1 (1%)	12	48
6	f	247/364 (68%)	224 (91%)	21 (8%)	2 (1%)	19	60
6	h	330/364 (91%)	308 (93%)	20 (6%)	2 (1%)	25	65
7	k	297/301 (99%)	282 (95%)	14 (5%)	1 (0%)	41	76
7	m	297/301 (99%)	281 (95%)	15 (5%)	1 (0%)	41	76
7	p	297/301 (99%)	285 (96%)	11 (4%)	1 (0%)	41	76
7	r	297/301 (99%)	282 (95%)	10 (3%)	5 (2%)	9	43
All	All	7881/16105 (49%)	7492 (95%)	355 (4%)	34 (0%)	38	72

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%)	1107 (100%)	3 (0%)	92	95
1	K	1171/1171 (100%)	1160 (99%)	11 (1%)	78	88
1	N	1155/1171 (99%)	1148 (99%)	7 (1%)	86	92
1	O	1103/1171 (94%)	1098 (100%)	5 (0%)	88	93
2	v	243/400 (61%)	243 (100%)	0	100	100
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%)	67	81
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%)	216 (99%)	2 (1%)	78	88
6	h	278/289 (96%)	278 (100%)	0	100	100
7	k	265/267 (99%)	263 (99%)	2 (1%)	81	89
7	m	265/267 (99%)	264 (100%)	1 (0%)	91	94
7	p	265/267 (99%)	264 (100%)	1 (0%)	91	94
7	r	265/267 (99%)	261 (98%)	4 (2%)	65	80
All	All	6806/13250 (51%)	6769 (100%)	37 (0%)	89	93

5 of 37 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	f	294	ARG
7	r	202	LEU
7	k	161	MET
7	p	98	GLN
1	K	1150	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 81 such sidechains are listed below:

Mol	Chain	Res	Type
1	O	587	GLN
7	m	128	ASN
1	O	977	GLN
3	w	77	HIS
7	m	291	GLN

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

There are no chain breaks in this entry.

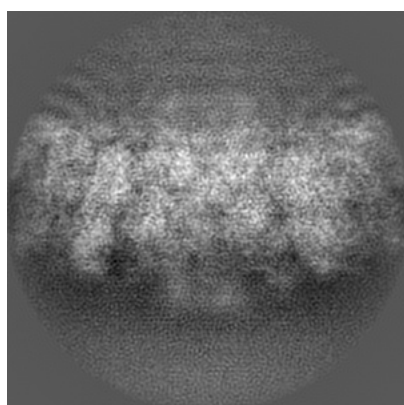
6 Map visualisation [i](#)

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.

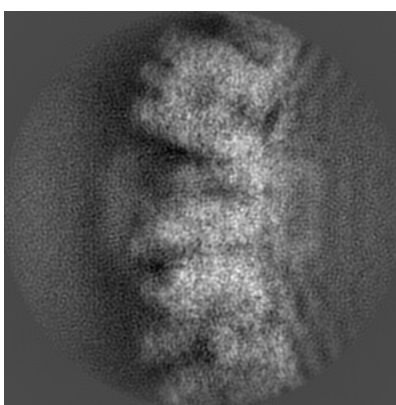
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

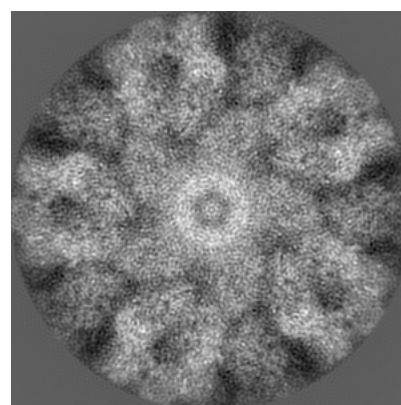
6.1.1 Primary map



X



Y

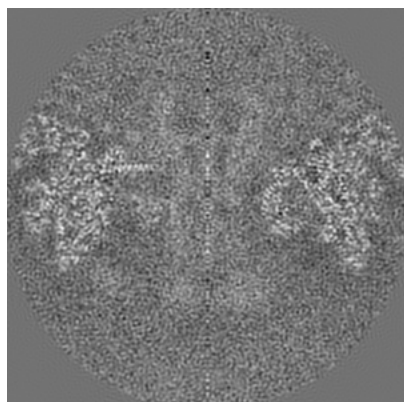


Z

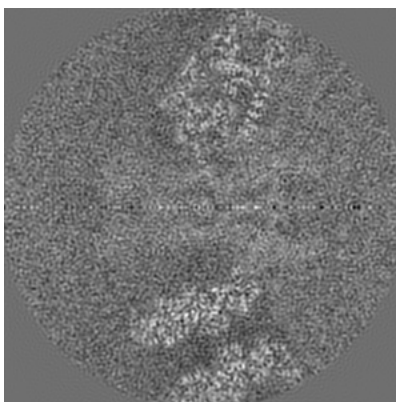
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

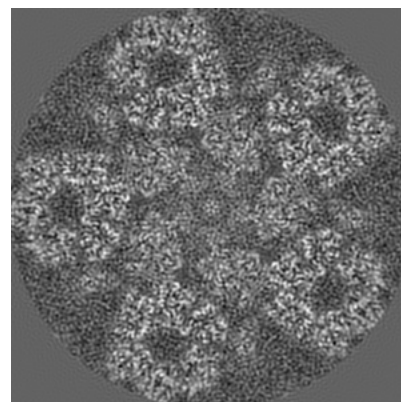
6.2.1 Primary map



X Index: 160



Y Index: 160

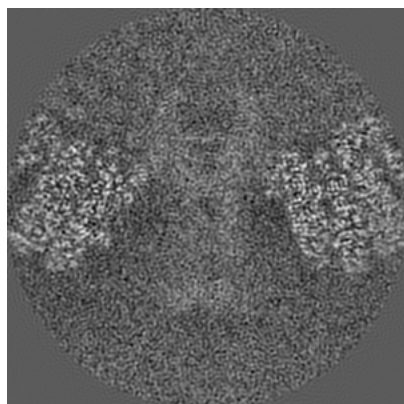


Z Index: 160

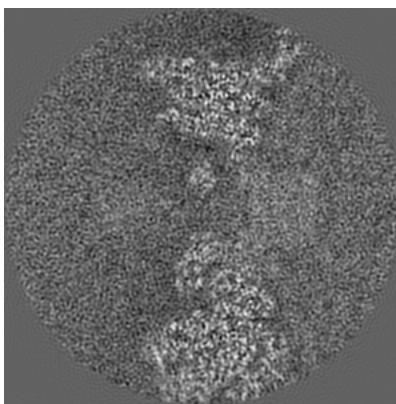
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

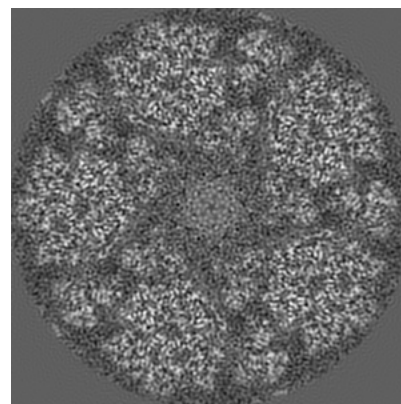
6.3.1 Primary map



X Index: 147



Y Index: 193

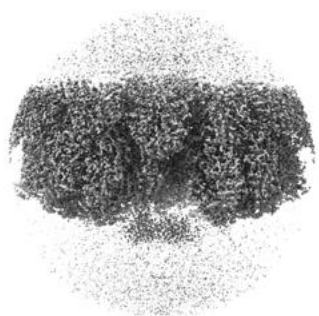


Z Index: 175

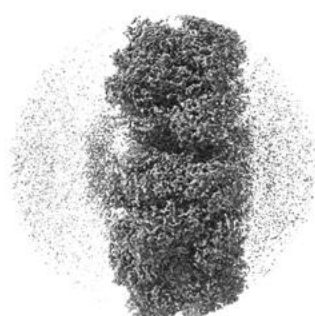
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

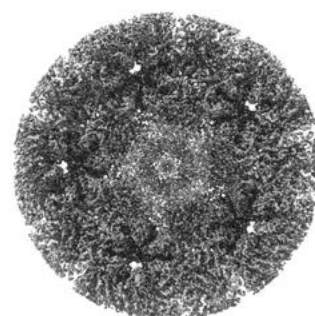
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.012. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

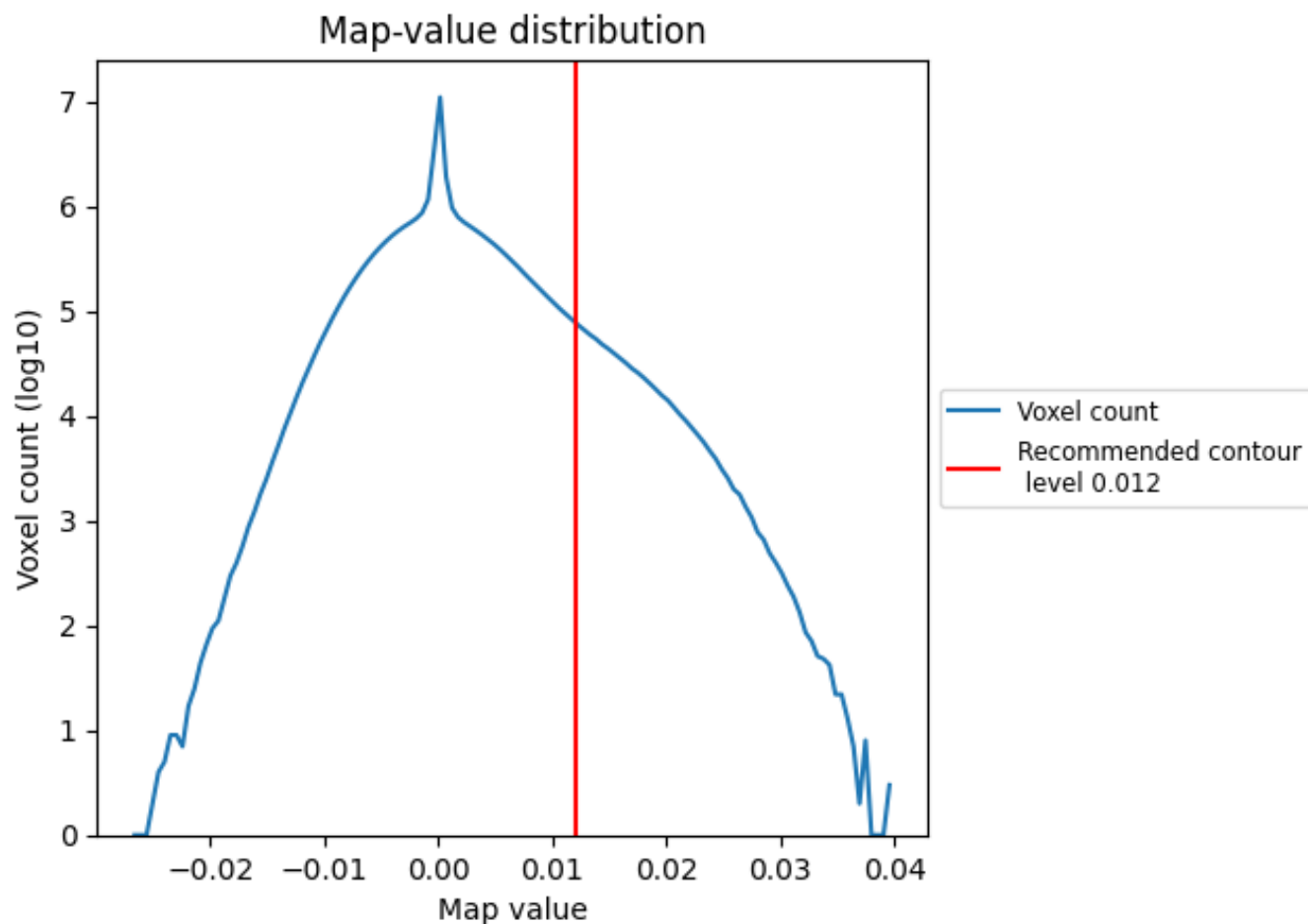
6.5 Mask visualisation

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

7 Map analysis [i](#)

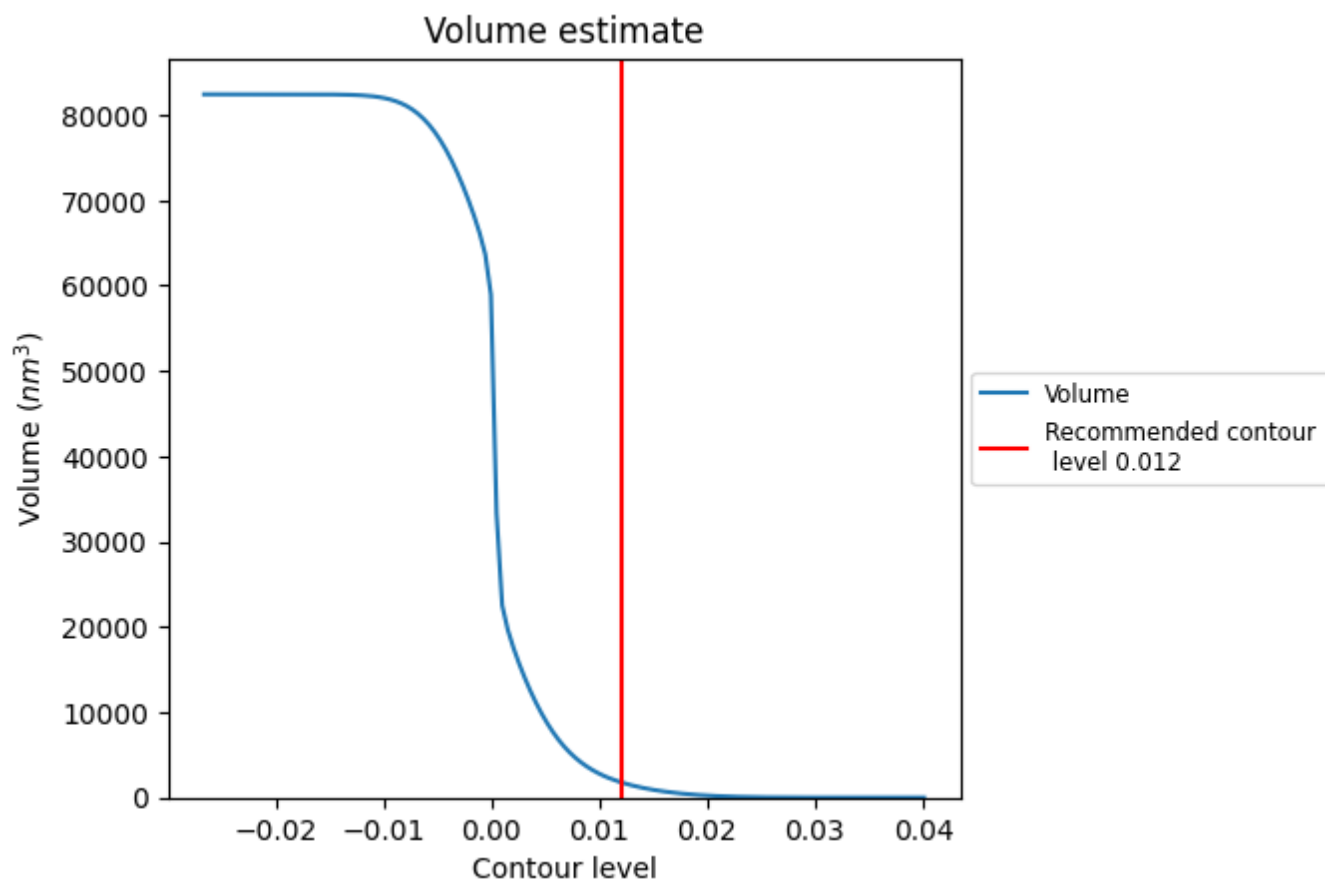
This section contains the results of statistical analysis of the map.

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.

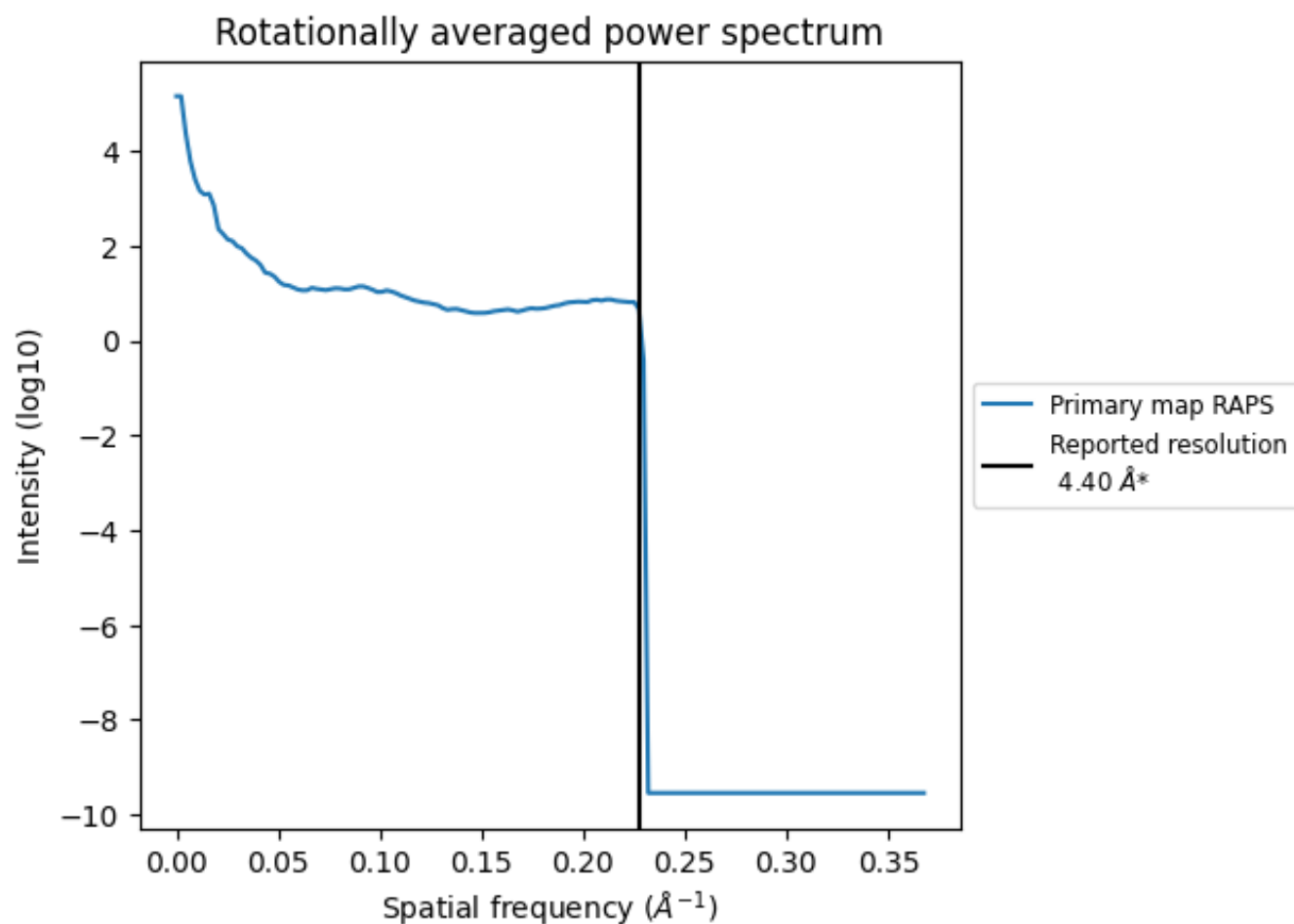
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 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 Å⁻¹

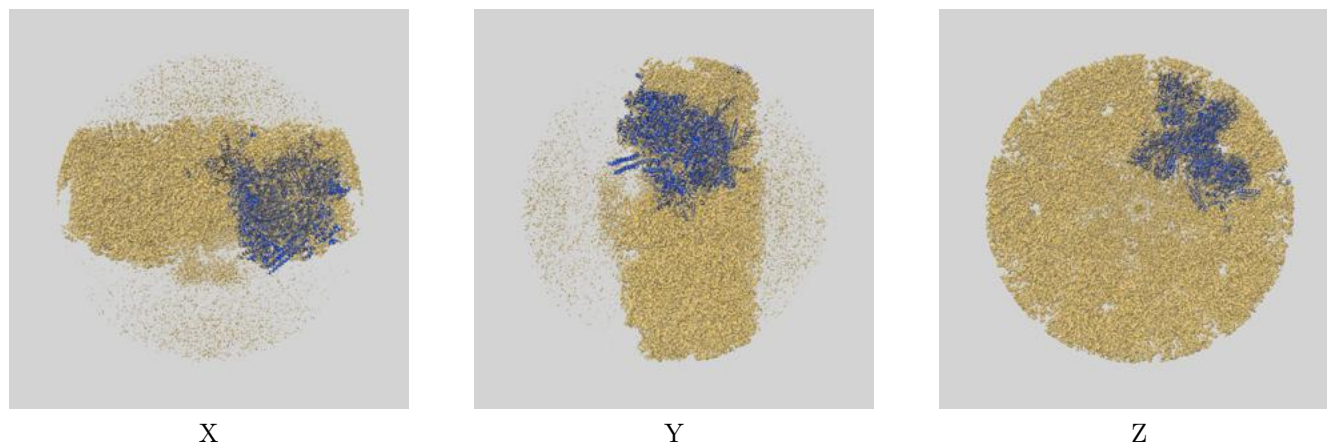
8 Fourier-Shell correlation

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

9.1 Map-model overlay [i](#)



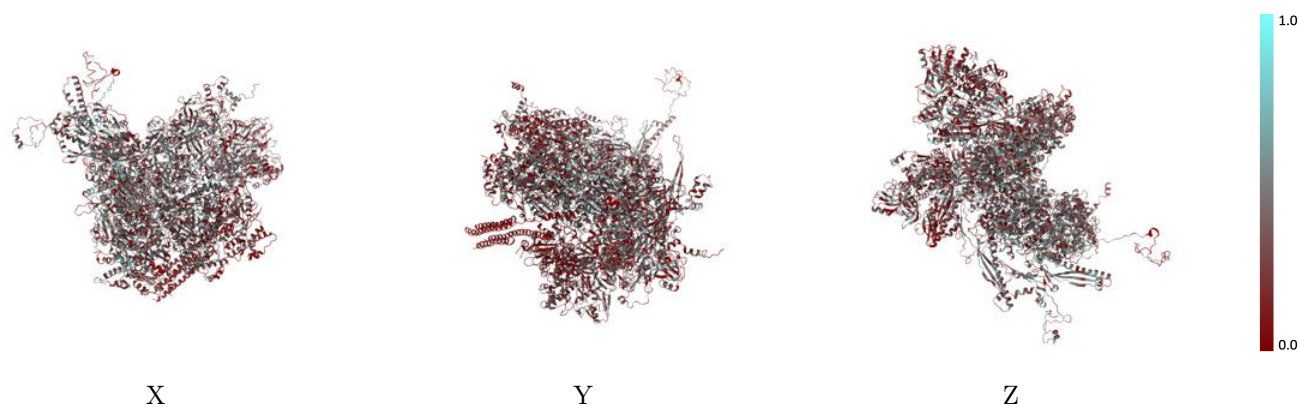
The images above show the 3D surface view of the map at the recommended contour level 0.012 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



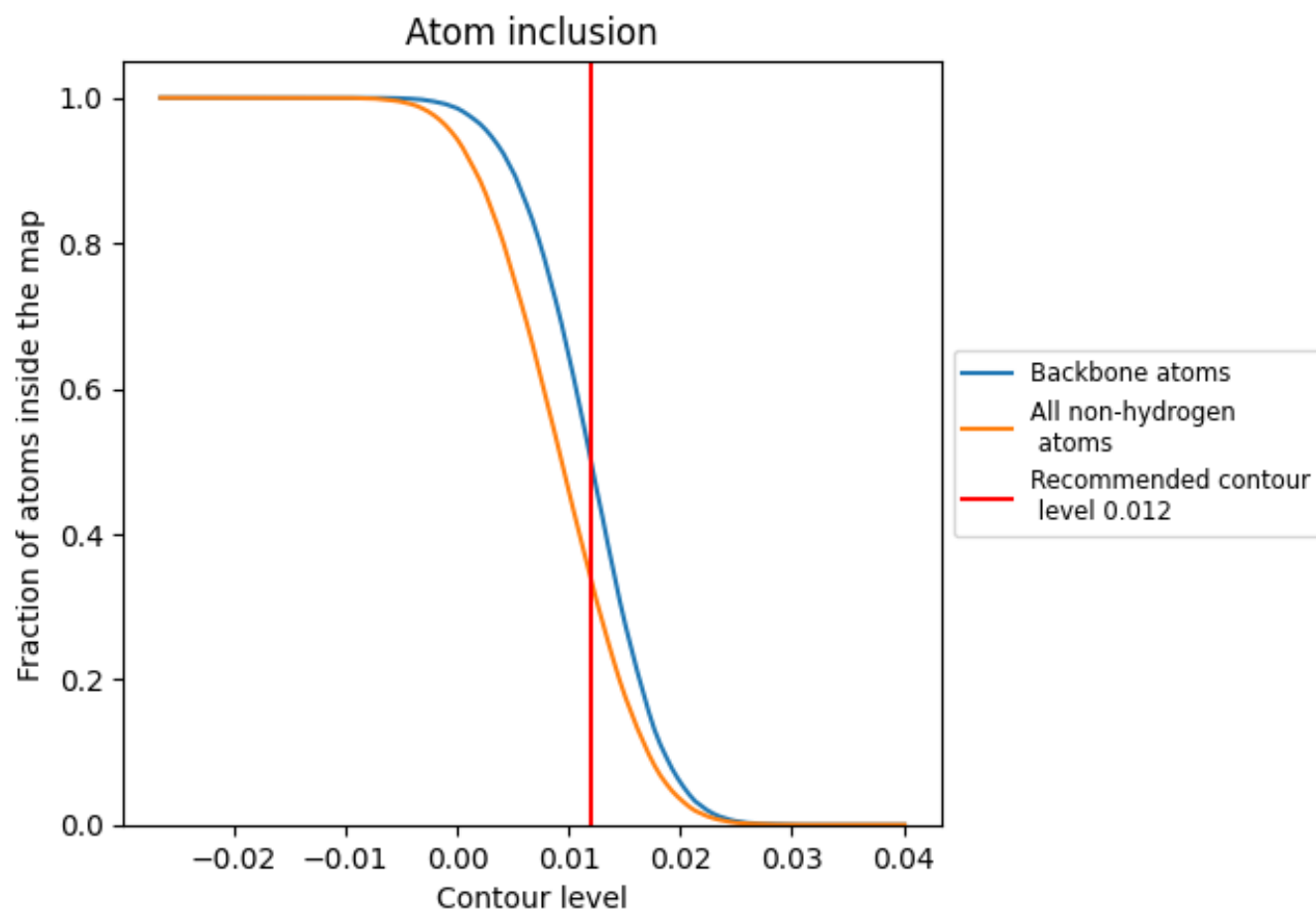
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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	 0.3364	 0.2450
J	 0.3909	 0.2500
K	 0.3873	 0.2640
N	 0.3498	 0.2590
O	 0.3698	 0.2460
Z	 0.3003	 0.2310
a	 0.3099	 0.2180
d	 0.1725	 0.1880
e	 0.2859	 0.2230
f	 0.2491	 0.2260
h	 0.3450	 0.2610
k	 0.2775	 0.2310
m	 0.2858	 0.2490
p	 0.2914	 0.2330
r	 0.2993	 0.2550
v	 0.1691	 0.1870
w	 0.0720	 0.1710
x	 0.1174	 0.1700
y	 0.0629	 0.1150
z	 0.0497	 0.1040

