



wwPDB EM Validation Summary Report ⓘ

Nov 11, 2025 – 01:10 AM JST

PDB ID : 8X9Z / pdb_00008x9z
EMDB ID : EMD-38189
Title : P-hexon capsomer of the VZV C-Capsid
Authors : Nan, W.; Lei, C.; Xiangxi, W.
Deposited on : 2023-12-01
Resolution : 3.10 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.dev129
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
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) : 2.46

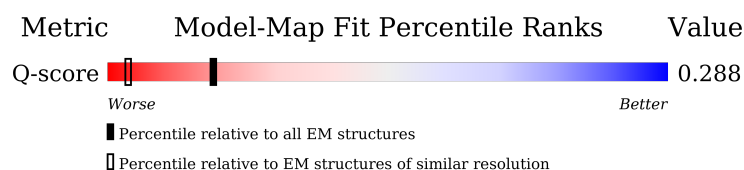
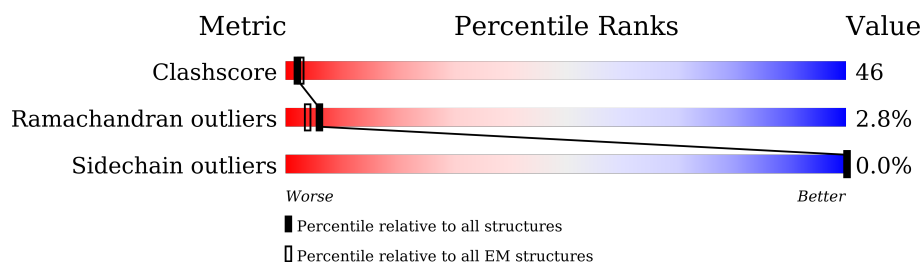
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.10 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.






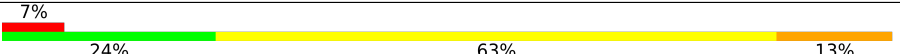
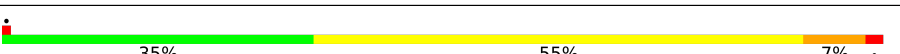
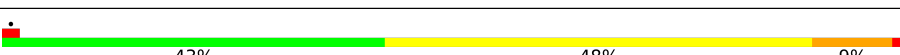
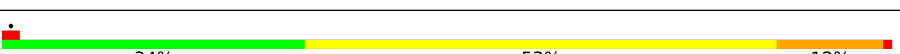
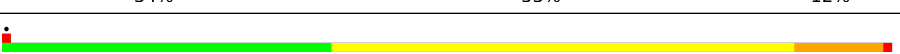
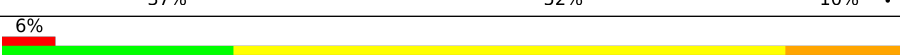

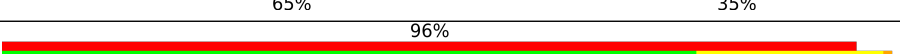
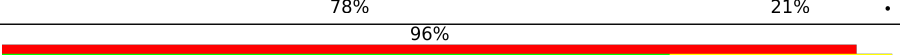
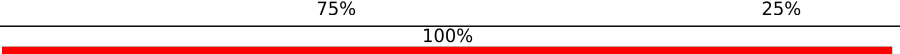
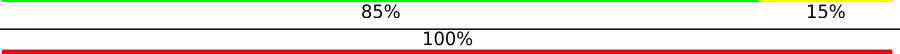





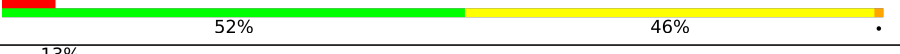
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
Q-score	-	25397	14724 (2.60 - 3.60)

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	A	1369	
1	F	1369	
1	G	1369	
1	H	1369	

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Mol	Chain	Length	Quality of chain
1	I	1369	
2	E	1370	
3	J	1371	
4	L	94	
4	R	94	
4	X	94	
4	d	94	
4	e	94	
4	f	94	
5	k	550	
6	l	94	
7	m	80	
8	n	47	
8	o	47	
9	P	256	
9	a	256	
10	V	263	
10	b	263	
11	c	286	
11	h	286	

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 93092 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	A	1309	Total	C	N	O	S	0	0
			10163	6438	1780	1881	64		
1	F	1331	Total	C	N	O	S	0	0
			10325	6541	1808	1910	66		
1	G	1331	Total	C	N	O	S	0	0
			10325	6541	1808	1910	66		
1	H	1331	Total	C	N	O	S	0	0
			10330	6543	1811	1910	66		
1	I	1331	Total	C	N	O	S	0	0
			10325	6541	1808	1910	66		

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	814	ALA	GLY	conflict	UNP P09245
F	814	ALA	GLY	conflict	UNP P09245
G	814	ALA	GLY	conflict	UNP P09245
H	814	ALA	GLY	conflict	UNP P09245
I	814	ALA	GLY	conflict	UNP P09245

- Molecule 2 is a protein called Major capsid protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	1297	Total	C	N	O	S	0	0
			10033	6354	1760	1856	63		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	185	SER	LEU	conflict	UNP P09245
E	814	ALA	GLY	conflict	UNP P09245

- Molecule 3 is a protein called Major capsid protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	J	1155	Total	C	N	O	S	0	0
			8917	5660	1575	1628	54		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	185	SER	LEU	conflict	UNP P09245
J	814	ALA	GLY	conflict	UNP P09245

- Molecule 4 is a protein called Small capsomere-interacting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	L	94	Total	C	N	O	S	0	0
			699	437	135	125	2		
4	R	94	Total	C	N	O	S	0	0
			699	437	135	125	2		
4	X	94	Total	C	N	O	S	0	0
			699	437	135	125	2		
4	d	94	Total	C	N	O	S	0	0
			699	437	135	125	2		
4	e	94	Total	C	N	O	S	0	0
			699	437	135	125	2		
4	f	94	Total	C	N	O	S	0	0
			699	437	135	125	2		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	95	ARG	LYS	conflict	UNP U5NQG6
R	95	ARG	LYS	conflict	UNP U5NQG6
X	95	ARG	LYS	conflict	UNP U5NQG6
d	95	ARG	LYS	conflict	UNP U5NQG6
e	95	ARG	LYS	conflict	UNP U5NQG6
f	95	ARG	LYS	conflict	UNP U5NQG6

- Molecule 5 is a protein called CVC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	k	550	Total	C	N	O	S	0	0
			4206	2674	764	747	21		

- Molecule 6 is a protein called Capsid vertex component 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	l	94	Total	C	N	O	S	0	0
			766	486	138	138	4		

- Molecule 7 is a protein called Capsid vertex component 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	m	80	Total	C	N	O	S	0	0
			654	413	124	115	2		

- Molecule 8 is a protein called Large tegument protein deneddylase.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	n	47	Total	C	N	O	S	0	0
			384	237	84	61	2		
8	o	47	Total	C	N	O	S	0	0
			384	237	84	61	2		

- Molecule 9 is a protein called Tri2A.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	P	256	Total	C	N	O	S	0	0
			1847	1191	315	333	8		
9	a	256	Total	C	N	O	S	0	0
			1847	1191	315	333	8		

- Molecule 10 is a protein called Tri2A.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	V	263	Total	C	N	O	S	0	0
			1975	1269	339	358	9		
10	b	263	Total	C	N	O	S	0	0
			1975	1269	339	358	9		

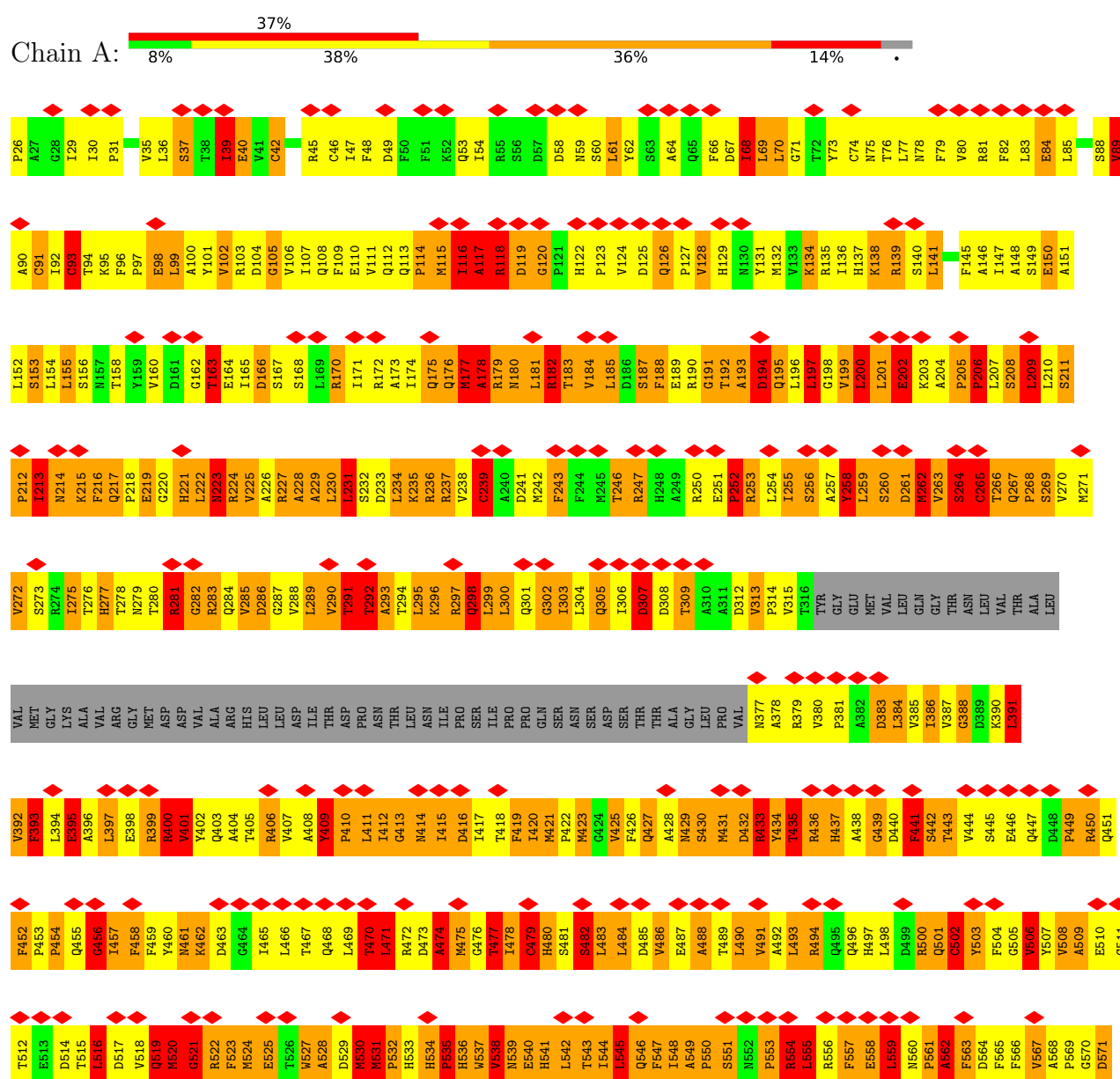
- Molecule 11 is a protein called Tri1.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	c	286	Total	C	N	O	S	0	0
			2221	1408	411	389	13		
11	h	286	Total	C	N	O	S	0	0
			2221	1408	411	389	13		

3 Residue-property plots

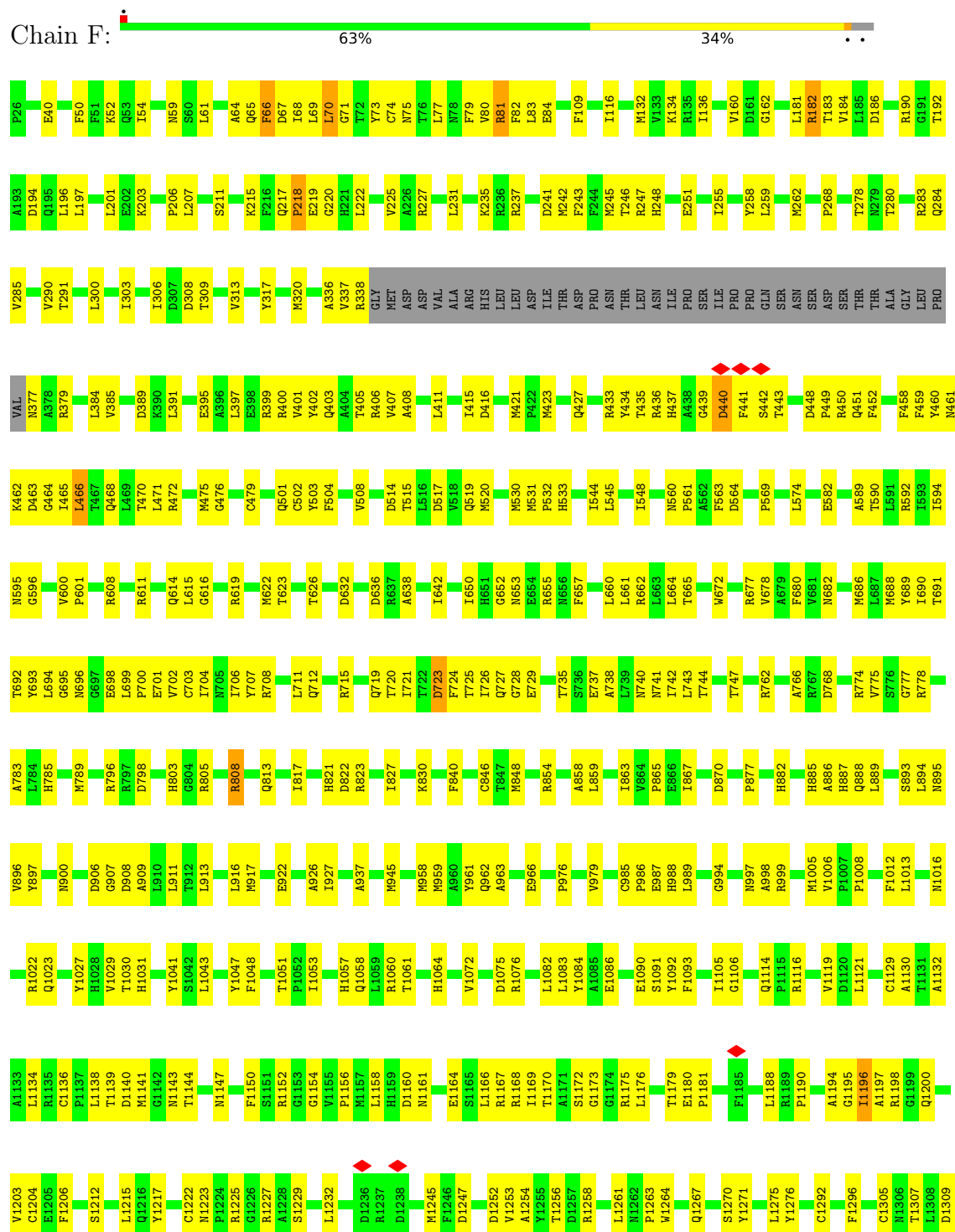
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

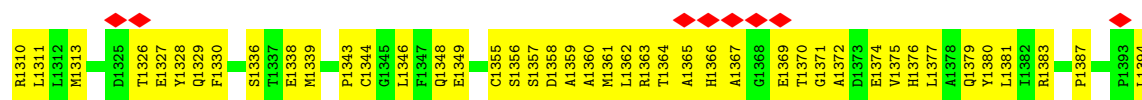
• Molecule 1: Major capsid protein



K1294	M1234	G1174	Q1114	S1054	G994	D934	A873	Q813	I752	T692	D632	V572
F1295	G1235	R1175	P1115	L1055	M995	A935	P874	A814	I753	Y693	T633	D573
F1296	R1236	L1176	R1116	T1056	T996	G936	T875	P816	W754	L694	F634	L574
T1297	D1237	M1177	A1117	Q1057	N997	A937	T876	P817	D755	G695	E635	P575
P1298	D1238	P1178	H1118	Q1058	A998	A938	T877	T818	C756	N696	D636	G576
A1299	A1239	T1179	V1119	L1059	R999	T939	P877	P819	D757	G697	R637	P577
E1300	D1240	E1180	D1120	R1060	R1000	A940	E878	H820	A758	E698	A638	Q578
V1301	L1241	E1181	L1121	T1061	V1001	T941	D879	H821	L759	E699	P640	R579
R1302	I1242	P1181	G1122	G1062	L1002	R943	P880	D822	I760	R620	T641	P580
T1303	E1243	L1182	V1123	F1063	A1003	R944	H881	E823	Y761	P700	E642	P581
M1304	A1244	P1183	G1124	P1064	K1004	N945	H882	E824	E762	V702	I642	E582
C1305	I1245	Y1125	Y1125	P1065	M1005	P846	P883	W825	E764	D703	F643	A583
M1306	M1246	F1185	T1126	G1066	Y1006	T947	H884	I827	Y644	T705	M584	M584
T1307	F1247	G1186	A1127	I1067	P1007	Y948	A886	I828	A765	I706	M645	P585
D1308	D1248	G1187	C1129	F1069	P1008	Y949	H887	L828	A766	Y707	E647	T586
D1309	H1249	L1188	A1130	T1070	P1010	G950	Q888	S829	R767	R708	A648	V587
R1310	T1249	R1189	T1131	V1071	P1011	A951	L889	K830	D768	L710	V649	N588
L1311	A1132	P1190	A1132	Y1072	F1012	L952	V690	Y832	R769	L711	I650	A589
L1312	A1133	A1191	A1133	Q1073	L1013	Y953	P891	Y833	P771	Q712	H651	T590
E1314	T1192	S1193	L1134	D1074	A1015	G955	N892	Y834	A772	H713	N652	L591
A1315	R1135	A1194	C1136	D1075	M1016	P1076	L894	I835	I773	W714	E654	R592
K1316	P1137	I1196	R1137	F1077	H1017	R1077	N895	Y836	I774	R715	R655	I593
A1317	T1138	T1197	T1139	A1078	H1018	A958	Y896	P838	W775	A716	N656	I594
V1318	D1250	R1198	D1140	T1079	A1019	N959	Y897	A839	S776	L717	F657	N595
A1319	A1251	L1199	M1141	E1080	I1021	A960	F698	F940	S777	R718	C588	N597
S1320	A1252	Q1200	G1142	L1081	R1022	Y961	H899	R842	N779	Q719	L660	I598
Q1321	D1253	A1201	N1143	L1082	Q1023	Q962	N900	R843	I721	L661	T665	P589
S1322	N1262	S1202	T1144	L1083	P1024	A963	A901	G844	G780	R662	Q666	V600
T1324	P1263	V1203	A1145	Y1084	V1025	Y964	H902	S844	W781	L663	C667	P601
D1325	W1264	C1204	A1146	A1085	A1026	D965	L903	C945	Q782	L664	T665	L602
T1326	A1265	E1205	Q1147	E1086	Y1027	E966	T904	C946	L784	T665	C603	C604
E1327	S1266	L1206	L1148	R1087	Y1028	T967	V905	T847	H785	T726	P604	I605
Y1328	Q1267	A1208	F1149	A1088	H1028	Y968	D908	M848	Q727	I725	C604	I606
K1329	H1268	M1209	F1150	S1089	Y1029	A969	A909	G849	G728	Q670	C605	F607
F1330	S1151	P1210	S1151	E1090	T1030	T970	L910	V850	T729	S675	I608	R608
K1331	R1152	V1211	R1152	S1091	H1031	G971	L911	Y852	R789	Q670	D609	D609
P1332	G1153	S1212	G1153	Y1092	S1032	T972	T912	D853	Y671	Y671	C610	R611
P1333	T1154	T1213	G1154	F1093	S1033	F973	L913	R854	W672	W672	R611	G612
P1334	V1155	D1214	V1155	Y1094	D1035	F974	Q914	L855	E673	E673	G612	T613
G1335	P1156	L1215	P1156	Q1095	F1036	Y975	E915	Y856	Q674	Q674	T614	Q614
S1336	M1157	Q1216	M1157	T1097	N1037	P976	L916	P857	H792	S675	L615	L616
T1337	L1158	L1217	L1158	Q1098	T1038	V977	N917	A858	N793	H676	G616	G616
E1338	H1159	F1218	H1159	V1099	L1038	P978	D918	L859	Q795	R677	V678	L617
M1339	D1160	R1219	D1160	H1100	L1039	Y979	M920	Q860	R796	V678	A679	G618
T1340	N1161	T1220	N1161	H1101	T1040	N980	A921	Q861	L739	A679	R619	R619
Q1341	V1162	A1221	V1162	H1102	S1042	P981	E922	V862	Y797	F680	H620	T621
D1342	T1163	C1222	T1163	D1103	L1043	F983	R923	L863	N740	N682	M622	M622
P1343	E1164	M1223	E1164	A1104	L1044	A984	T924	V864	N741	N683	F684	T623
C1344	S1165	P1224	S1165	I1105	G1045	C985	T925	P865	I742	E681	M622	T624
G1345	L1166	G1225	L1166	G1107	G1046	P986	A926	E866	T744	F684	M622	A625
S1346	R1167	G1226	R1167	G1108	Y1047	E987	I927	I867	D745	M685	P624	A625
F1347	A1228	R1227	A1228	V1108	F1048	H988	L928	P868	D746	M686	P624	T626
T1348	P1287	R1168	P1287	F1109	K1049	L989	V929	A869	T747	L687	A625	T627
Q1349	T1169	T1170	T1169	F1110	F1050	A990	S930	D870	F748	M688	A625	T628
A1350	S1290	G1230	S1290	T1111	P1051	S991	S931	E871	I749	Y689	A625	T629
Y1351	L1112	L1112	L1112	T1111	P1052	L992	A932	E872	D810	I690	K628	A629
P1352	S1172	Y1233	S1172	L1113	I1053	R993	P933	E872	T811	P751	V630	K631
P1353	G1173		G1173						G812			

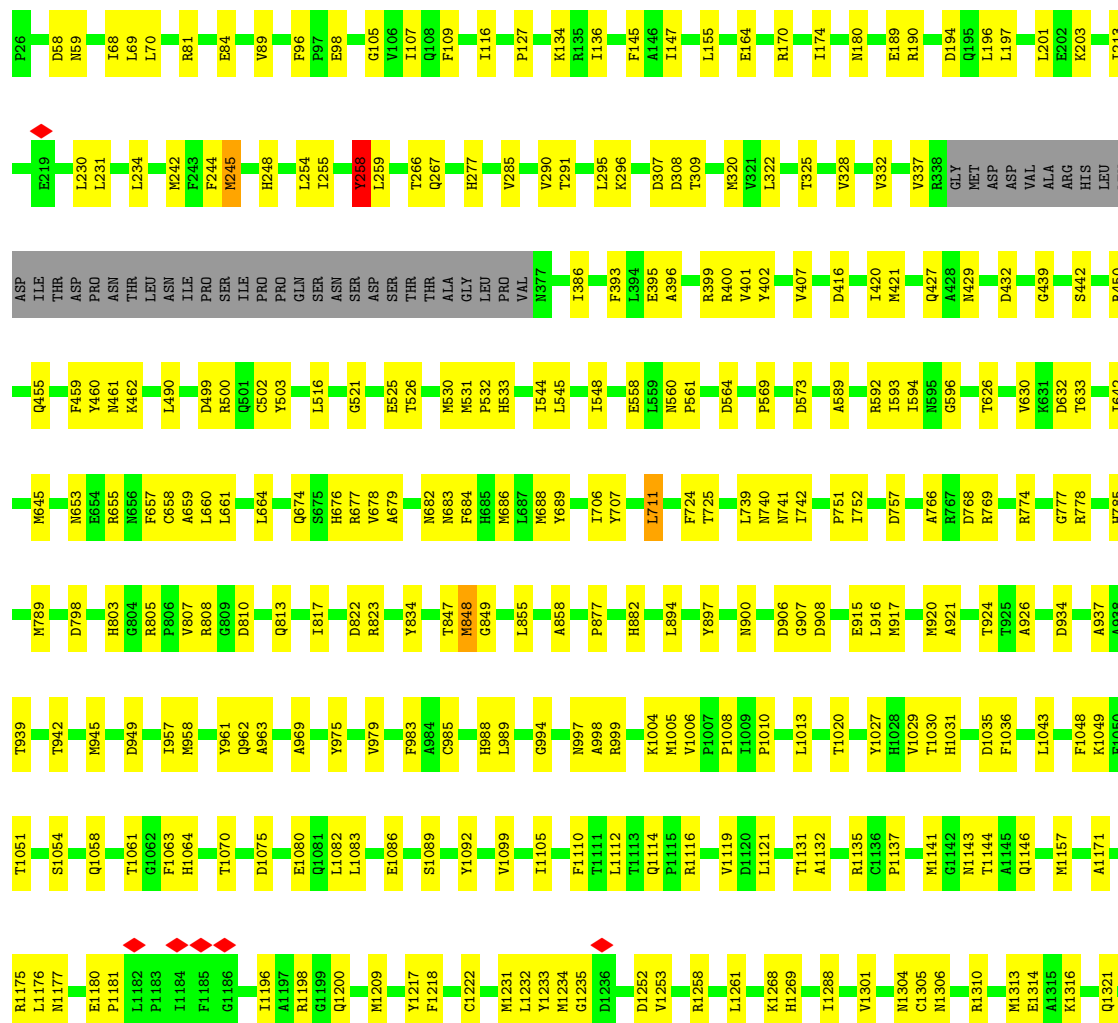
- Molecule 1: Major capsid protein





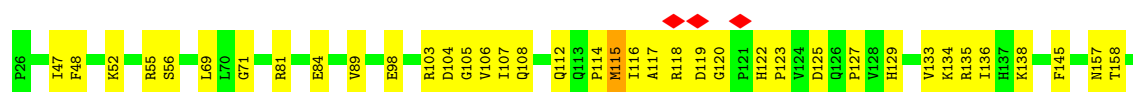
• Molecule 1: Major capsid protein

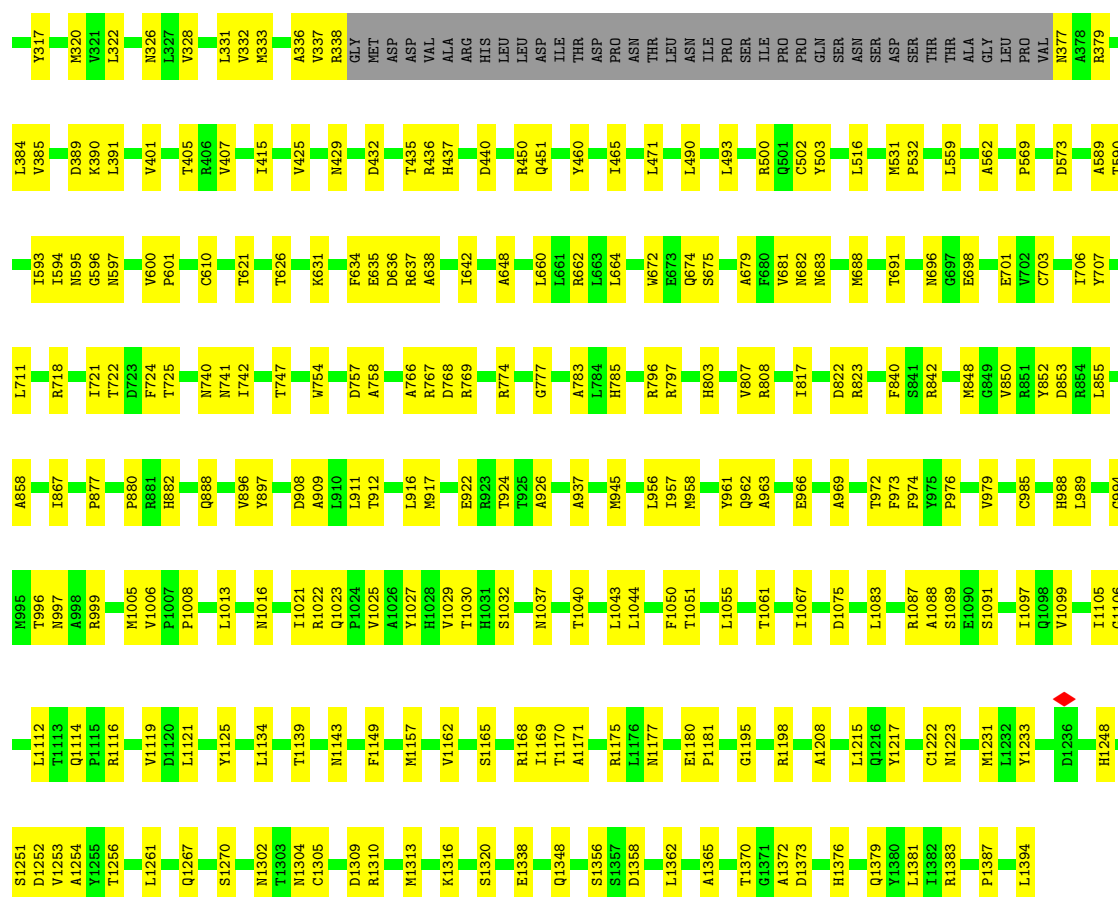
Chain G: 75% 22%



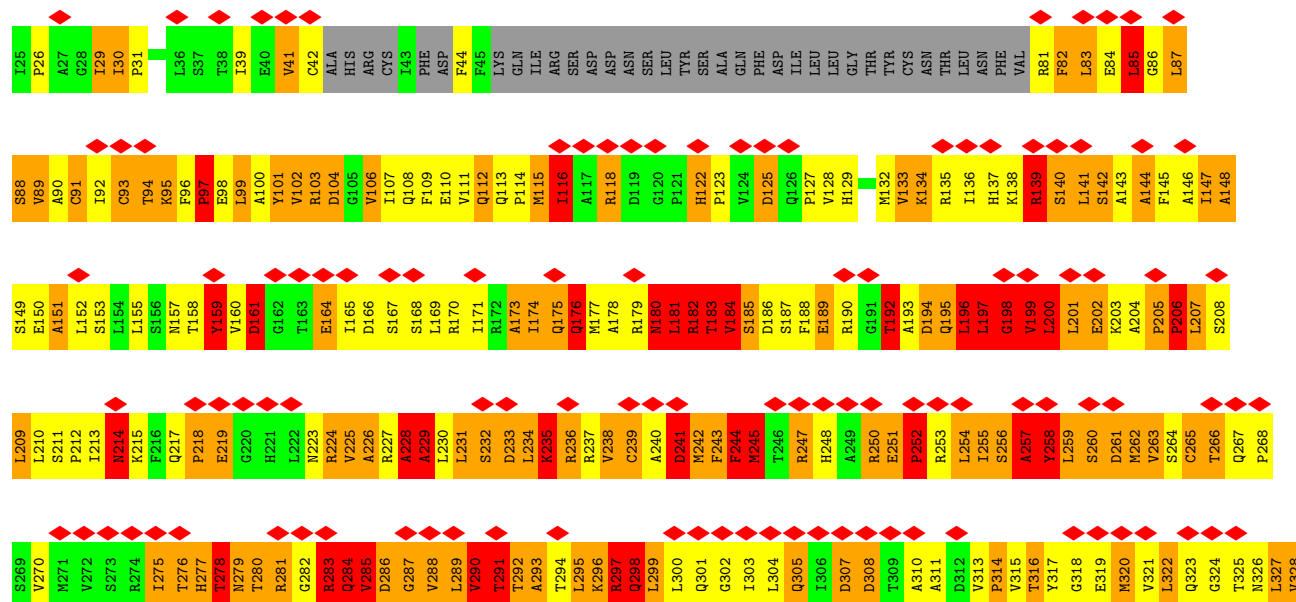
• Molecule 1: Major capsid protein

Chain H: 62% 34%

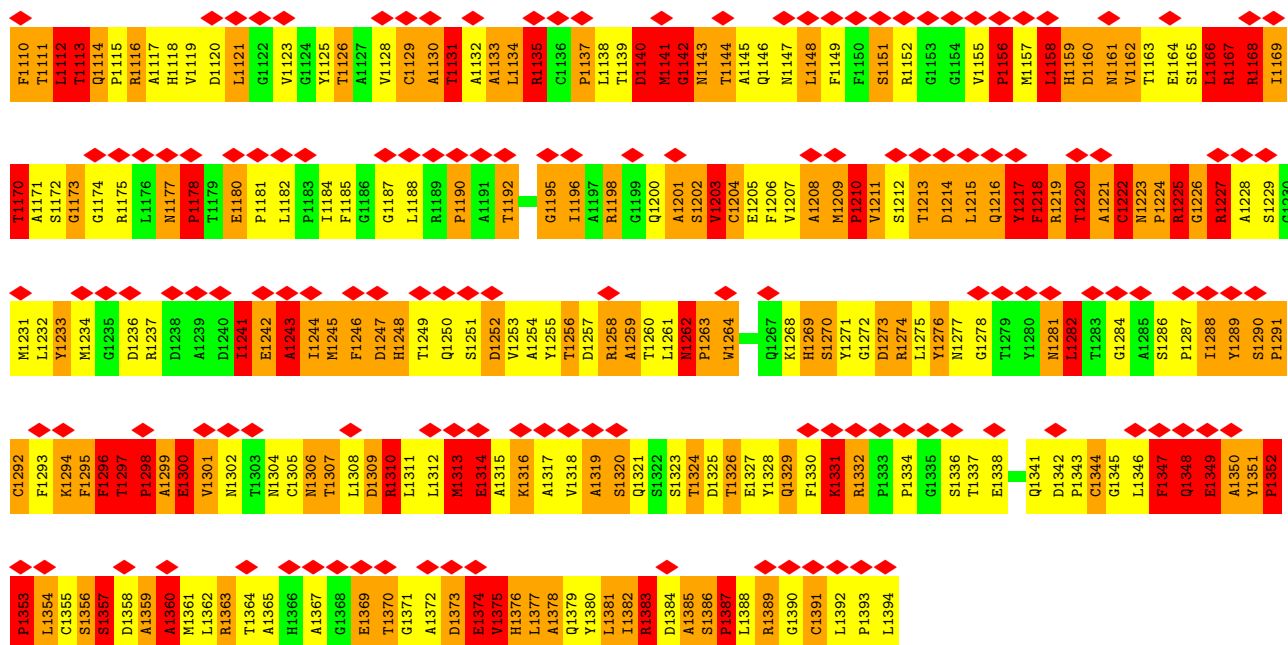




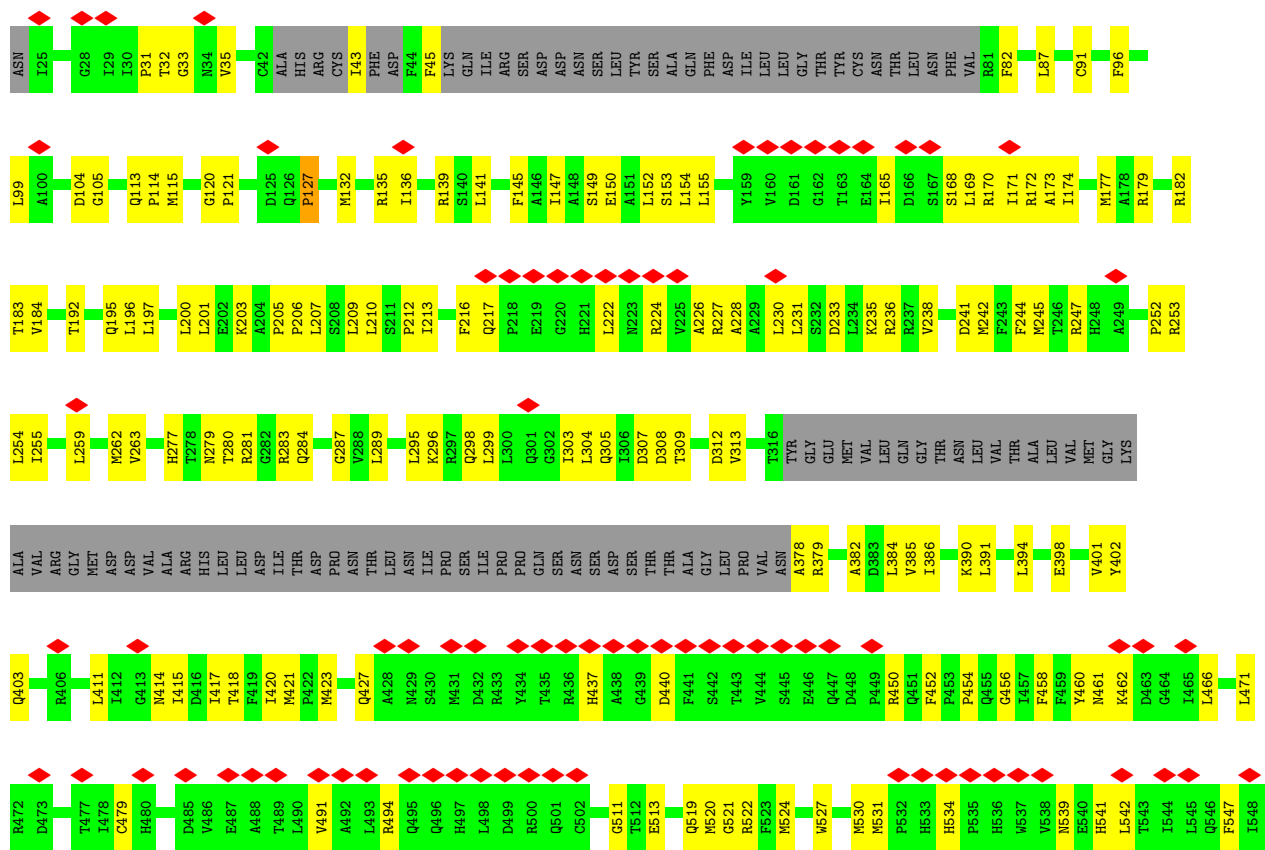
• Molecule 2: Major capsid protein

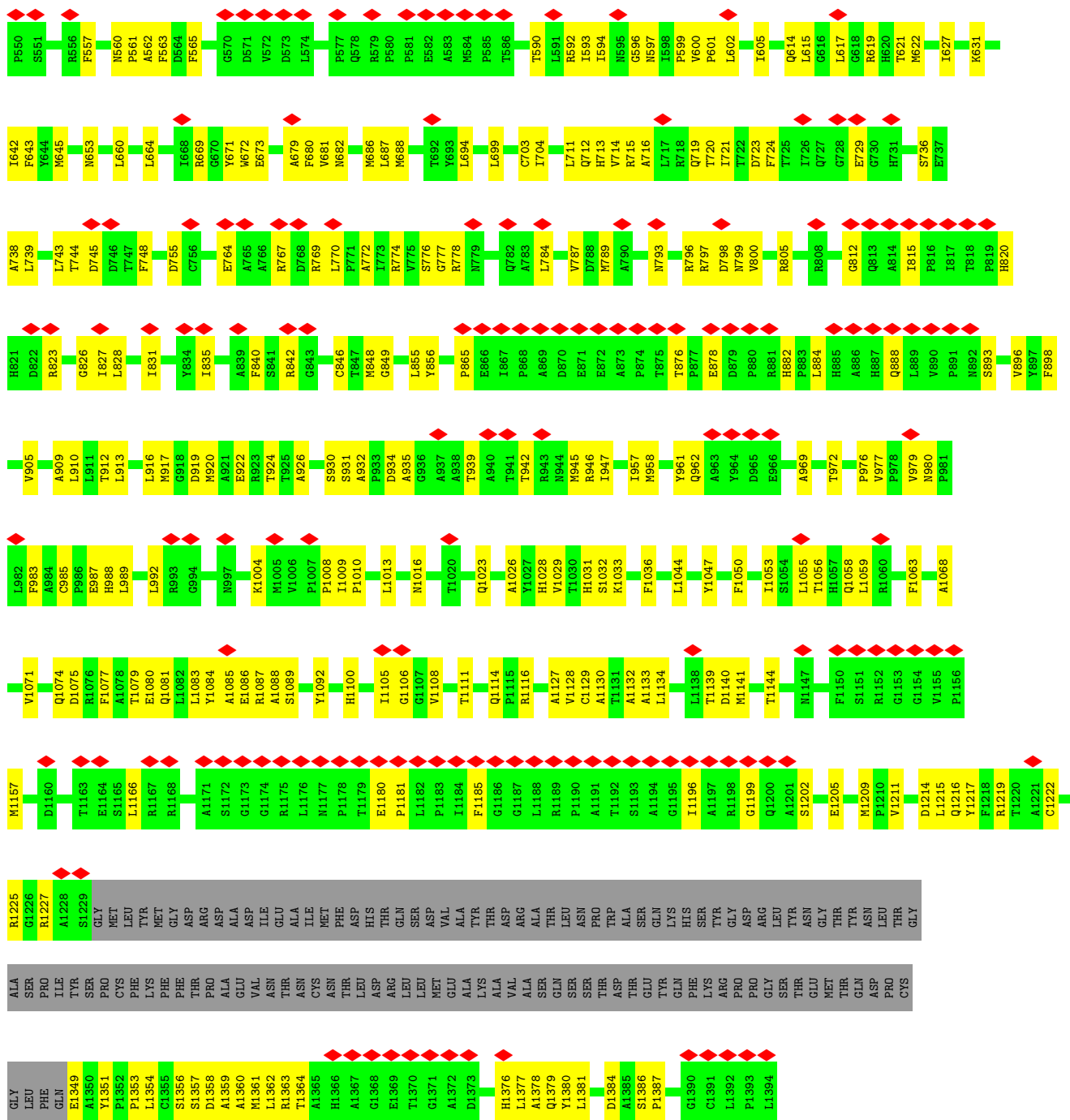


F1050	T1051	P1052	I1053	S1054	L1055	T1056	L1057	Q1058	R1059	R1060	T1061	G1062	F1063	H1064	P1065	G1066	I1067	A1068	V1069	F1070	T1071	I1072	R1073	Q1074	D1075	R1076	F1077	H1078	T1079	E1080	Q1081	L1082	L1083	Y1084	A1085	E1086	R1087	A1088	S1089	E1090	S1091	F1092	F1093	V1094	G1095	Q1096	I1097	G1098	V1099	H1100	H1101	H1102	D1103	A1104	L1105	G1106	G1107	V1108	M1109		
A990	S991	L992	P993	D994	M995	T996	N997	Q998	R999	R1000	V1001	L1002	A1003	M1004	K1005	V1006	P1007	P1008	I1009	P1010	F1011	F1012	L1013	G1014	A1015	N1016	H1017	T1018	H1019	A1020	Q1021	R1022	Q1023	P1024	V1025	A1026	Y1027	E1028	V1029	T1030	H1031	S1032	K1033	S1034	D1035	F1036	N1037	T1038	L1039	Y1040	Y1041	S1042	L1043	L1044	G1045	G1046	Y1047	F1048	K1049		
G809	D810	T811	G812	Q813	R814	R815	R816	R817	R818	R819	R820	H821	R822	R823	E824	R825	G826	L827	R828	S829	R830	R831	R832	R833	R834	R835	R836	R837	R838	R839	R840	R841	R842	R843	R844	R845	R846	R847	R848	R849	R850	R851	R852	R853	R854	R855	R856	R857	R858	R859	R860	R861	R862	R863	R864	R865	R866	R867	R868		
E871	E872	A873	P874	T875	T876	T877	E878	D879	P880	R881	H882	P883	L884	R885	A886	H887	O888	L889	V890	P891	N892	S893	L894	N895	V896	R897	R898	R899	A900	H901	H902	L903	T904	V905	D906	G907	D908	A909	L910	L911	T912	L913	D914	E915	L916	R917	G918	D919	H920	A921	E922	T923	T924	T925	F983	A984	C985	P986	E987	H988	L989
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G809	D810	T811	G812	Q813	R814	R815	R816	R817	R818	R819	R820	H821	R822	R823	E824	R825	G826	L827	R828	S829	R830	R831	R832	R833	R834	R835	R836	R837	R838	R839	R840	R841	R842	R843	R844	R845	R846	R847	R848	R849	R850	R851	R852	R853	R854	R855	R856	R857	R858	R859	R860	R861	R862	R863	R864	R865	R866	R867	R868		
E871	E872	A873	P874	T875	T876	T877	E878	D879	P880	R881	H882	P883	L884	R885	A886	H887	O888	L889	V890	P891	N892	S893	L894	N895	V896	R897	R898	R899	A900	H901	H902	L903	T904	V905	D906	G907	D908	A909	L910	L911	T912	L913	D914	E915	L916	R917	G918	D919	H920	A921	E922	T923	T924	T925	F983	A984	C985	P986	E987	H988	L989
S930	S931	A932	P933	D934	A935	G936	A937	A938	T939	A940	T941	T942	R943	R944	R945	R946	R947	Y948	D949	G950	A951	L952	R953	H954	G955	L956	T957	N958	N959	A960	Y961	Q962	A963	Y964	D965	E966	T967	L968	A969	T970	G971	T972	F973	F974	Y975	F976	Y977	F978	R979	P980	L981	L982	F983	A984	C985	P986	E987	H988	L989		
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A990	S991	L992	P993	D994	M995	T996	N997	Q998	R999	R1000	V1001	L1002	A1003	M1004	K1005	V1006	P1007	P1008	I1009	P1010	F1011	F1012	L1013	G1014	A1015	N1016	H1017	T1018	H1019	A1020	Q1021	R1022	Q1023	P1024	V1025	A1026	Y1027	E1028	V1029	T1030	H1031	S1032	K1033	S1034	D1035	F1036	N1037	T1038	L1039	Y1040	Y1041	S1042	L1043	L1044	G1045	G1046	Y1047	F1048	K1049		
P449	R450	Q451	F452	P453	P454	Q455	G456	I457	F458	E459	Y460	N461	K462	D463	Q464	A465	T466	R467	Q468	L469	T470	P471	L472	D473	A474	M475	G476	T477	I478	C479	H480	S481	S482	L483	L484	D485	G486	V487	A488	T489	L490	V491	A492	L493	R494	Q495	Q496	L497	L498	D499	R500	Q501	C502	Y503	F504	G505	V506	Y507	V508		
A509	E510	G511	T512	E513	D514	T515	L516	D517	V518	Q519	M520	G521	R522	F523	M524	E525	T526	W527	Q528	A529	D529	M530	M531	P532	D533	H534	P535	H536	W537	I538	N539	E540	H541	L542	T543	I544	L545	Q546	F547	A548	A549	P550	S551	N552	P553	Q554	L555	R556	F557	E558	L559	N560	P561	A562	F563	D564	F565	G566	A567	A568	
P569	G570	V571	D572	D573	L574	P575	G576	P577	Q578	R579	M580	P581	E582	A583	M584	P585	T586	W587	N588	A589	D589	G590	L591	R592	I593	I594	N595	G596	N597	I598	P599	V600	L602	C603	P604	L605	S606	F607	R608	D609	C610	R611	G612	T613	Q614	L615	G616	L617	G618	R619	H620	T621	M622	F623	D624	A625	T626	I627	G628		
A629	V630	K631	D632	T633	F634	E635	D636	R637	A638	Y639	P640	T641	I642	F643	Y644	M645	L646	E647	A648	V649	I650	H651	G652	N653	E654	R655	V714	N656	F657	C658	A659	L660	R662	L663	L664	T665	Q666	C667	I668	R669	G670	Y671	R672	E673	Q674	S675	H676	R677	V678	A679	F680	V681	N682	N683	F684	H685	L686	L687	M688		
Y689	L690	T691	P692	V693	L694	G695	N696	G697	E698	L699	P700	E701	V702	C703	I704	N705	I706	Y707	R708	L709	L710	L711	Q712	H713	V714	R715	A716	L717	R718	Q719	T720	T722	D723	L724	Q666	C667	I668	R669	G670	Y671	R672	E673	Q674	S675	H676	R677	V678	A679	F680	V681	N682	N683	F684	H685	L686	L687	M688				
L749	A750	P751	L752	L753	W754	D755	C756	D757	A758	L759	I760	R761	R762	D763	E764	A765	A766	R767	D768	R769	L770	P771	A772	I773	R774	V775	S776	G777	R778	N779	T780	Y781	Q782	A783	C845	C846	T847	R848	G849	R850	R851	Y852	D853	R854	L855	Y856	P857	L858	L859	Q860	A861	R862	L863	Y864	R865	F866	L867	P868			
G809	D810	T811	G812	Q813	R814	R815	R816	R817	R818	R819	R820	H821	R822	R823	E824	R825	G826	L827	R828	S829	R830	R831	R832	R833	R834	R835	R836	R837	R838	R839	R840	R841	R842	R843	R844	R845	R846	R847	R848	R849	R850	R851	R852	R853	R854	R855	R856	R857	R858	R859	R860	R861	R862	R863	R864	R865	R866	R867	R868		
E871	E872	A873	P874	T875	T876	T877	E878	D879	P880	R881	H882	P883	L884	R885	A886	H887	O888	L889	V890	P891	N892	S893	L894	N895	V896	R897	R898	R899	A900	H901	H902	L903	T904	V905	D906	G907	D908	A909	L910	L911	T912	L913	D914	E915	L916	R917	G918	D919	H920	A921	E922	T923	T924	T925	F983	A984	C985	P986	E987	H988	L989
S930	S931	A932	P933	D934	A935	G936	A937	A938	T939	A940	T941	T942	R943	R944	R945	R946	R947	Y948	D949	G950	A951	L952	R953	H954	G955	L956	T957	N958	N959	A960	Y961	Q962	A963	Y964	D965	E966	T967	L968	A969	T970	G971	T972	F973	F974	Y975	F976	Y977	F978	R979	P980	L981	L982	F983	A984	C985	P986	E987	H988	L989		
F1050	T1051	P1052	I1053	S1054	L1055	T1056	L1057	Q1058	R1059	R1060	T1061	G1062	F1063	H1064	P1065	G1066	I1067	A1068	V1069	F1070	T1071	I1072	R1073	Q1074	D1075	R1076	F1077	H1078	T1079	E1080	Q1081	L1082	L1083	Y1084	A1085	E1086	R1087	A1088	S1089	E1090	S1091	F1092	F1093	V1094	G1095	Q1096	I1097	G1098	V1099	H1100	H1101	H1102	D1103	A1104	L1105	G1106	G1107	V1108	M1109		
A990	S991	L992	P993	D994	M995	T996	N997	Q998	R999	R1000	V1001	L1002	A1003	M1004	K1005	V1006	P1007	P1008	I1009	P1010	F1011	F1012	L1013	G1014	A1015	N1016	H1017	T1018	H1019	A1020	Q1021	R1022	Q1023	P1024	V1025	A1026	Y1027	E1028	V1029	T1030	H1031	S1032	K1033	S1034	D1035	F1036	N1037	T1038	L1039	Y1040	Y1041	S1042	L1043	L1044	G1045	G1046	Y1047	F1048	K1049		
P449	R450	Q451	F452	P453	P454	Q455	G456	I457	F458	E459	Y460	N461	K462	D463	Q464	A465	T466	R467	Q468	L469	T470	P471	L472	D473	A474	M475	G476	T477	I478	C479	H480	S481	S482	L483	L484	D485	G486	V487	A488	T489	L490	V491	A492	L493	R494	Q495	Q496	L497	L498	D499	R500	Q501	C502	Y503	F504	G505	V506	Y507	V508		
A509	E510	G511	T512	E513	D514	T515	L516	D517	V518	Q519	M520	G521	R522	F523	M524	E525	T526	W527	Q528	A529	D529	M530	M531	P532	D533	H534	P535	H536	W537	I538	N539	E540	H541	L542	T543	I544	L545	Q546	F547	A548	A549	P550	S551	N552	P553	Q554	L555	R556	F557	E558	L559	N560	P561	A562	F563	D564	F565	G566	A567	A568	
P569	G570	V571	D572	D573	L574	P575	G576	P577	Q578	R579	M580	P581	E582	A583	M584	P585	T586	W587	N588	A589	D589	G590	L591	R592	I593	I594	N595	G596	N597	I598	P599	V600	L602	C603	P604	L605	S606	F607	R608	D609	C610	R611	G612	T613	Q614	L615	G616	L617	G618	R619	H620	T621	M622	F623	D624	A625	T626	I627	G628		
A629	V630	K631	D632	T633	F634	E635	D636	R637	A638	Y639	P640	T641	I642	F643	Y644	M645	L646																																												

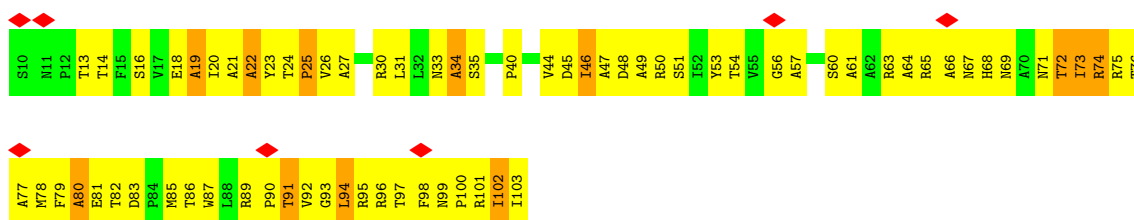


• Molecule 3: Major capsid protein

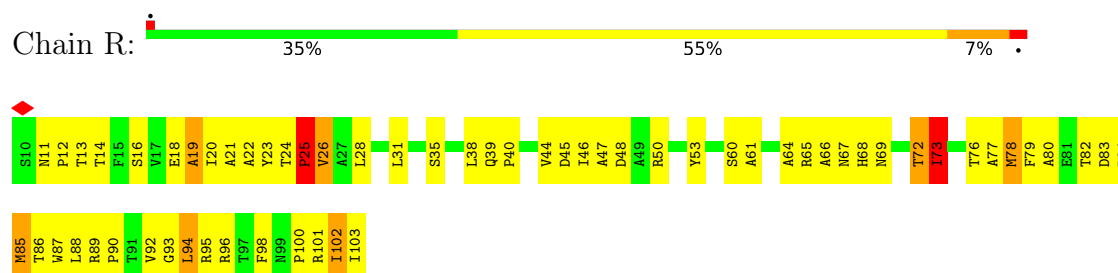




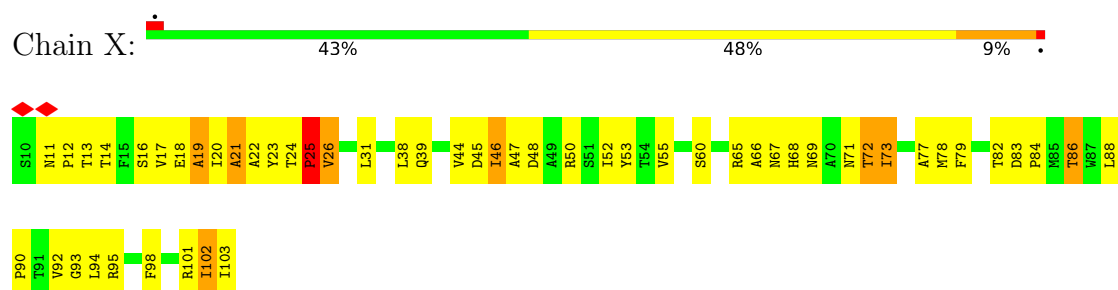
• Molecule 4: Small capsomere-interacting protein



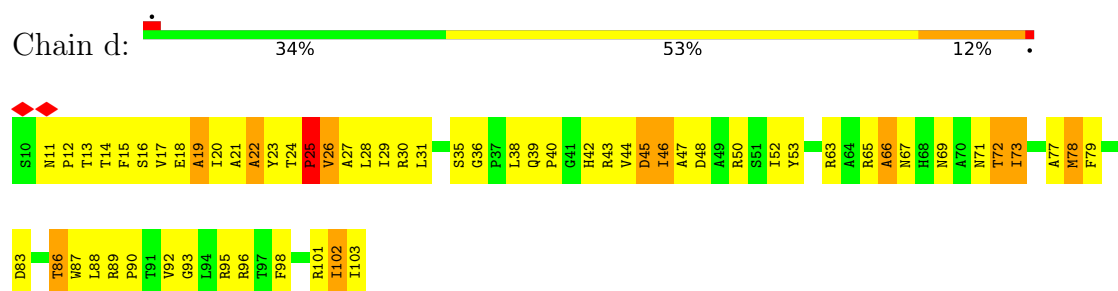
- Molecule 4: Small capsomere-interacting protein



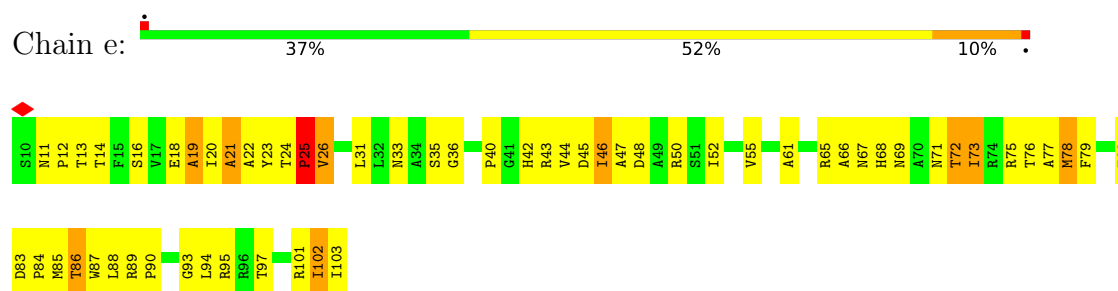
- Molecule 4: Small capsomere-interacting protein



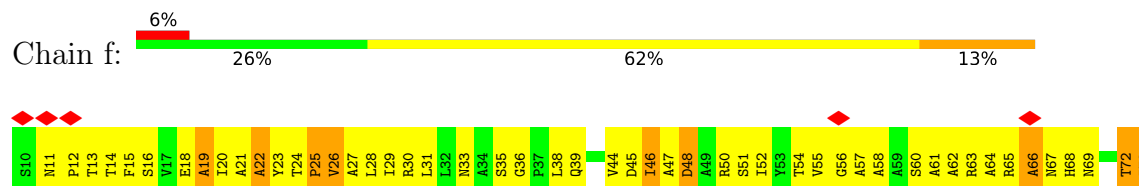
- Molecule 4: Small capsomere-interacting protein

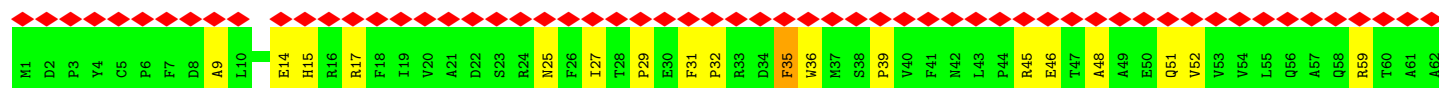


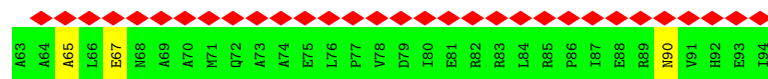
- Molecule 4: Small capsomere-interacting protein



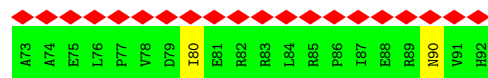
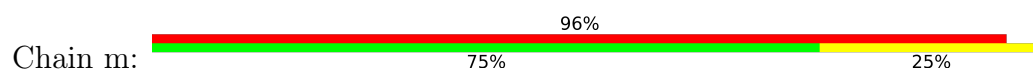
- Molecule 4: Small capsomere-interacting protein



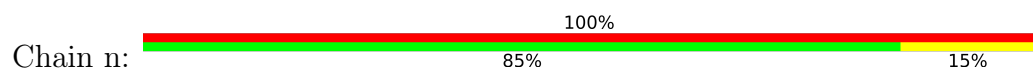




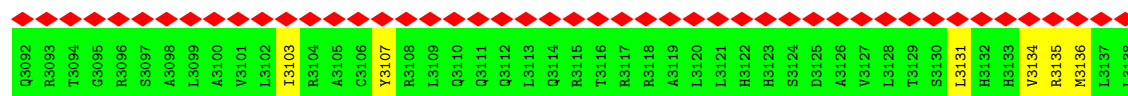
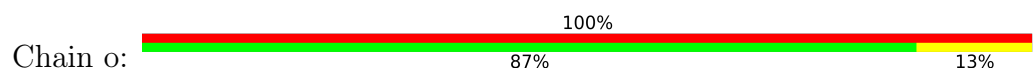
- Molecule 7: Capsid vertex component 2



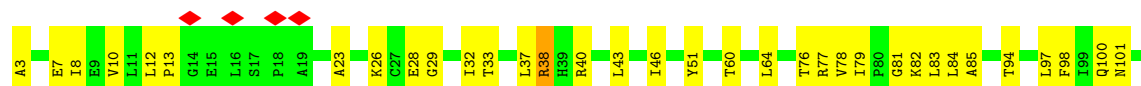
- Molecule 8: Large tegument protein deneddylase



- Molecule 8: Large tegument protein deneddylase

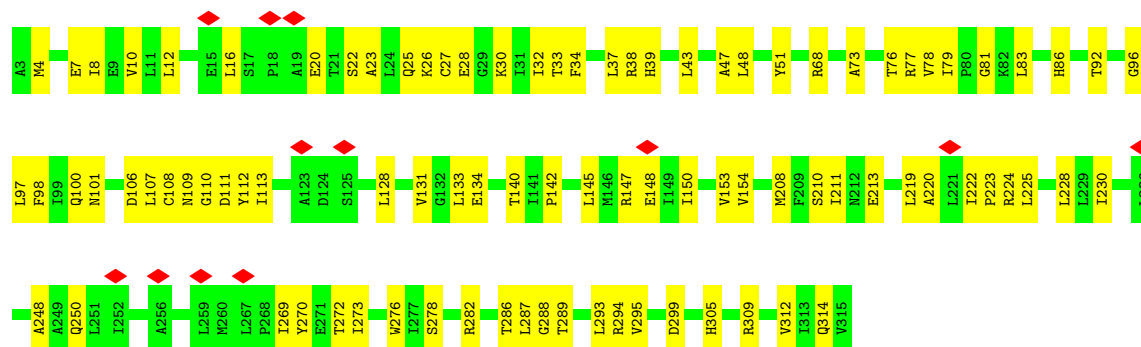


- Molecule 9: Tri2A



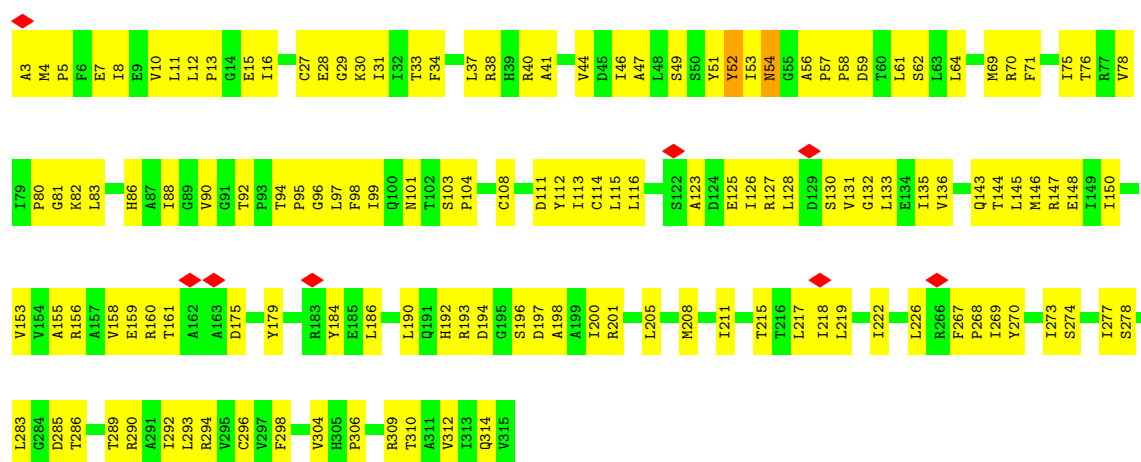
- Molecule 9: Tri2A





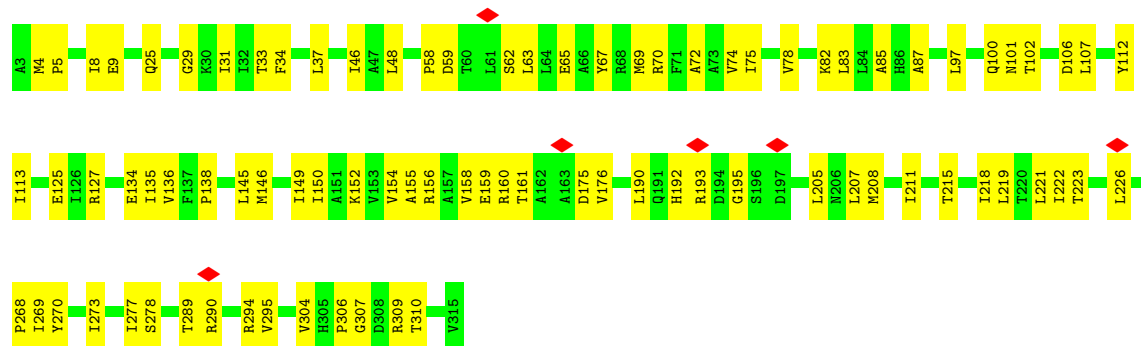
• Molecule 10: Tri2A

Chain V: 48% 52%



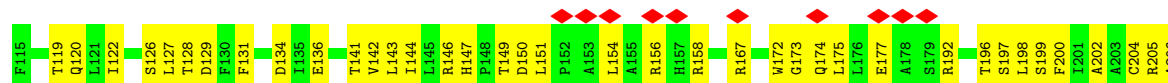
• Molecule 10: Tri2A

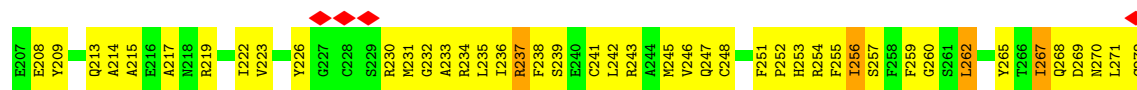
Chain b: 67% 33%



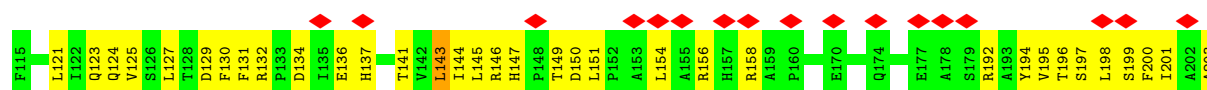
• Molecule 11: Tri1

Chain c: 6% 52% 46%





• Molecule 11: Tri1



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	1671456	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TECNAI F30	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 BASE (4k x 4k)	Depositor
Maximum map value	0.063	Depositor
Minimum map value	-0.039	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.004	Depositor
Map size (Å)	378.0, 378.0, 378.0	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.35, 1.35, 1.35	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	2.07	287/10412 (2.8%)	2.68	961/14195 (6.8%)
1	F	0.37	0/10575	0.58	7/14415 (0.0%)
1	G	0.29	0/10575	0.43	5/14415 (0.0%)
1	H	0.38	3/10580 (0.0%)	0.56	10/14421 (0.1%)
1	I	0.27	0/10575	0.42	0/14415
2	E	2.12	365/10275 (3.6%)	2.73	1019/14009 (7.3%)
3	J	0.16	0/9132	0.40	1/12452 (0.0%)
4	L	0.52	0/714	1.20	3/978 (0.3%)
4	R	0.44	0/714	1.16	6/978 (0.6%)
4	X	0.33	0/714	1.05	5/978 (0.5%)
4	d	0.32	0/714	1.06	7/978 (0.7%)
4	e	0.32	0/714	1.03	4/978 (0.4%)
4	f	0.53	0/714	1.26	5/978 (0.5%)
5	k	0.21	0/4307	0.45	2/5866 (0.0%)
6	l	0.32	0/786	0.53	0/1072
7	m	0.14	0/670	0.33	0/912
8	n	0.18	0/388	0.42	0/521
8	o	0.09	0/388	0.29	0/521
9	P	0.20	0/1878	0.42	0/2568
9	a	0.19	0/1878	0.43	1/2568 (0.0%)
10	V	0.22	0/2010	0.46	0/2743
10	b	0.22	0/2010	0.39	0/2743
11	c	0.23	0/2269	0.55	0/3078
11	h	0.29	0/2269	0.56	2/3078 (0.1%)
All	All	1.01	655/95261 (0.7%)	1.35	2038/129860 (1.6%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	1	334

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	F	0	6
1	G	0	1
1	H	0	4
2	E	1	337
4	L	0	5
4	R	0	1
4	X	0	1
4	d	0	1
4	e	0	1
4	f	0	3
6	l	0	1
10	V	0	1
11	c	0	1
All	All	2	697

The worst 5 of 655 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	857	PRO	CB-CG	46.64	3.82	1.49
2	E	1350	ALA	C-N	24.07	1.66	1.32
1	A	632	ASP	C-N	23.30	1.66	1.33
1	A	703	CYS	C-N	21.73	1.63	1.33
1	A	704	ILE	N-CA	21.69	1.73	1.46

The worst 5 of 2038 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	857	PRO	CA-CB-CG	-19.80	66.89	104.50
2	E	1243	ALA	CA-C-N	18.01	142.19	121.84
2	E	1243	ALA	C-N-CA	18.01	142.19	121.84
1	A	1029	VAL	CG1-CB-CG2	-17.96	71.28	110.80
2	E	415	ILE	CG1-CB-CG2	-17.48	58.27	110.70

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	1244	ILE	CB
2	E	773	ILE	CB

5 of 697 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	35	VAL	Peptide
1	A	36	LEU	Peptide
1	A	42	CYS	Peptide
1	A	45	ARG	Peptide
1	A	47	ILE	Peptide

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	A	10163	0	9929	3130	0
1	F	10325	0	10104	598	0
1	G	10325	0	10104	250	0
1	H	10330	0	10113	532	0
1	I	10325	0	10104	248	0
2	E	10033	0	9817	2876	0
3	J	8917	0	8748	315	0
4	L	699	0	696	144	0
4	R	699	0	696	87	0
4	X	699	0	696	63	0
4	d	699	0	696	64	0
4	e	699	0	696	56	0
4	f	699	0	696	138	0
5	k	4206	0	4190	192	0
6	l	766	0	745	33	0
7	m	654	0	642	25	0
8	n	384	0	410	16	0
8	o	384	0	410	5	0
9	P	1847	0	1851	76	0
9	a	1847	0	1851	74	0
10	V	1975	0	2031	131	0
10	b	1975	0	2031	69	0
11	c	2221	0	2184	142	0
11	h	2221	0	2184	148	0
All	All	93092	0	91624	8569	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 46.

The worst 5 of 8569 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:A:857:PRO:CA	1:A:857:PRO:C	1.74	1.58
1:A:1024:PRO:CA	1:A:1024:PRO:C	1.74	1.58
1:A:897:TYR:CA	1:A:897:TYR:C	1.76	1.55
1:A:632:ASP:C	1:A:632:ASP:CA	1.75	1.55
2:E:199:VAL:CA	2:E:199:VAL:C	1.75	1.55

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	A	1305/1369 (95%)	581 (44%)	589 (45%)	135 (10%)	0	3
1	F	1327/1369 (97%)	1209 (91%)	117 (9%)	1 (0%)	48	79
1	G	1327/1369 (97%)	1233 (93%)	93 (7%)	1 (0%)	48	79
1	H	1327/1369 (97%)	1198 (90%)	129 (10%)	0	100	100
1	I	1327/1369 (97%)	1219 (92%)	108 (8%)	0	100	100
2	E	1291/1370 (94%)	599 (46%)	562 (44%)	130 (10%)	0	3
3	J	1145/1371 (84%)	1062 (93%)	81 (7%)	2 (0%)	44	74
4	L	92/94 (98%)	57 (62%)	28 (30%)	7 (8%)	1	4
4	R	92/94 (98%)	59 (64%)	24 (26%)	9 (10%)	0	3
4	X	92/94 (98%)	58 (63%)	25 (27%)	9 (10%)	0	3
4	d	92/94 (98%)	57 (62%)	25 (27%)	10 (11%)	0	2
4	e	92/94 (98%)	57 (62%)	25 (27%)	10 (11%)	0	2
4	f	92/94 (98%)	52 (56%)	33 (36%)	7 (8%)	1	4
5	k	534/550 (97%)	509 (95%)	25 (5%)	0	100	100
6	l	92/94 (98%)	83 (90%)	9 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	m	78/80 (98%)	78 (100%)	0	0	100	100
8	n	45/47 (96%)	44 (98%)	1 (2%)	0	100	100
8	o	45/47 (96%)	44 (98%)	1 (2%)	0	100	100
9	P	248/256 (97%)	235 (95%)	11 (4%)	2 (1%)	16	48
9	a	248/256 (97%)	233 (94%)	14 (6%)	1 (0%)	30	63
10	V	257/263 (98%)	230 (90%)	26 (10%)	1 (0%)	30	63
10	b	257/263 (98%)	236 (92%)	20 (8%)	1 (0%)	30	63
11	c	280/286 (98%)	240 (86%)	35 (12%)	5 (2%)	7	29
11	h	280/286 (98%)	232 (83%)	44 (16%)	4 (1%)	9	34
All	All	11965/12578 (95%)	9605 (80%)	2025 (17%)	335 (3%)	6	20

5 of 335 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	99	LEU
1	A	139	ARG
1	A	164	GLU
1	A	221	HIS
1	A	252	PRO

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	A	1089/1158 (94%)	1086 (100%)	3 (0%)	91	95
1	F	1106/1158 (96%)	1106 (100%)	0	100	100
1	G	1106/1158 (96%)	1106 (100%)	0	100	100
1	H	1107/1158 (96%)	1107 (100%)	0	100	100
1	I	1106/1158 (96%)	1106 (100%)	0	100	100
2	E	1072/1159 (92%)	1072 (100%)	0	100	100
3	J	947/1160 (82%)	947 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	L	69/73 (94%)	69 (100%)	0	100	100
4	R	69/73 (94%)	69 (100%)	0	100	100
4	X	69/73 (94%)	69 (100%)	0	100	100
4	d	69/73 (94%)	69 (100%)	0	100	100
4	e	69/73 (94%)	69 (100%)	0	100	100
4	f	69/73 (94%)	69 (100%)	0	100	100
5	k	429/429 (100%)	429 (100%)	0	100	100
6	l	80/80 (100%)	80 (100%)	0	100	100
7	m	67/67 (100%)	67 (100%)	0	100	100
8	n	41/41 (100%)	41 (100%)	0	100	100
8	o	41/41 (100%)	41 (100%)	0	100	100
9	P	188/218 (86%)	188 (100%)	0	100	100
9	a	188/218 (86%)	188 (100%)	0	100	100
10	V	214/224 (96%)	213 (100%)	1 (0%)	86	92
10	b	214/224 (96%)	214 (100%)	0	100	100
11	c	225/238 (94%)	225 (100%)	0	100	100
11	h	225/238 (94%)	225 (100%)	0	100	100
All	All	9859/10565 (93%)	9855 (100%)	4 (0%)	100	100

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	836	VAL
1	A	916	LEU
1	A	1006	VAL
10	V	54	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 159 such sidechains are listed below:

Mol	Chain	Res	Type
1	I	1016	ASN
9	P	100	GLN
3	J	176	GLN
3	J	1031	HIS
11	c	120	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 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
5	k	7
9	a	3
9	P	3
1	A	3
10	b	2
10	V	2
11	h	2
11	c	2
2	E	2
3	J	1

The worst 5 of 27 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	k	266:ARG	C	355:ARG	N	38.97
1	b	226:LEU	C	266:ARG	N	28.86

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	V	226:LEU	C	266:ARG	N	28.60
1	a	236:LEU	C	244:VAL	N	20.40
1	P	236:LEU	C	244:VAL	N	20.38

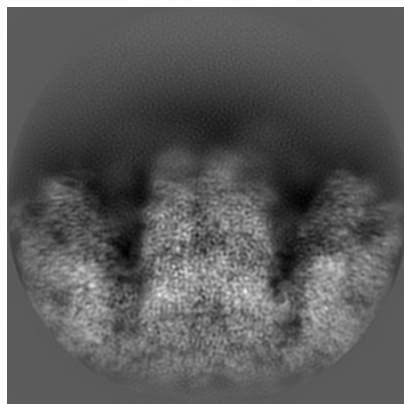
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-38189. These allow visual inspection of the internal detail of the map and identification of artifacts.

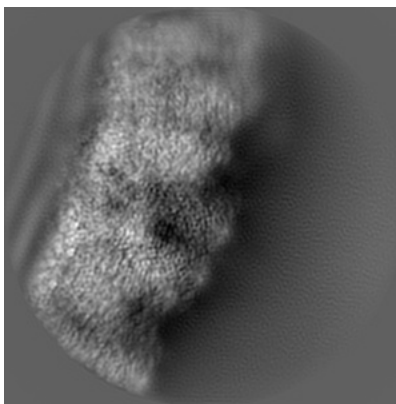
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

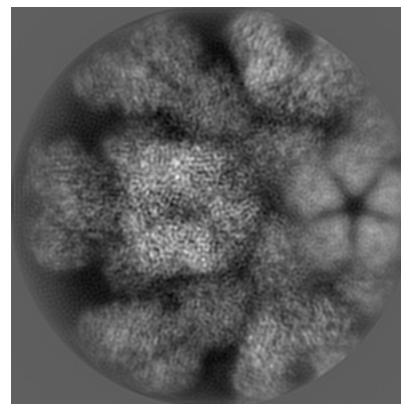
6.1.1 Primary map



X

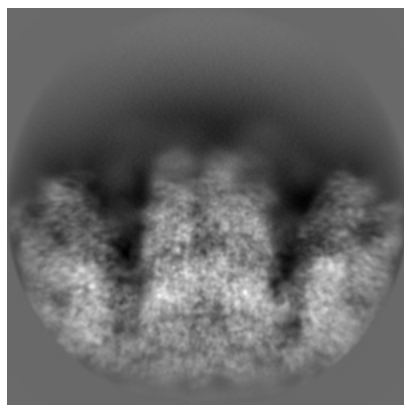


Y

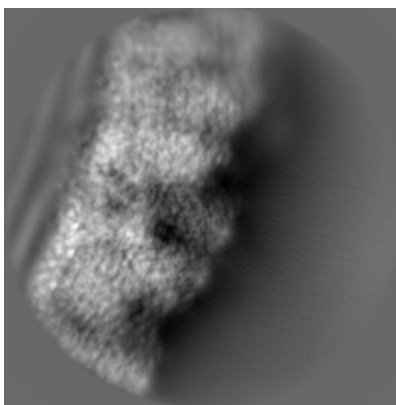


Z

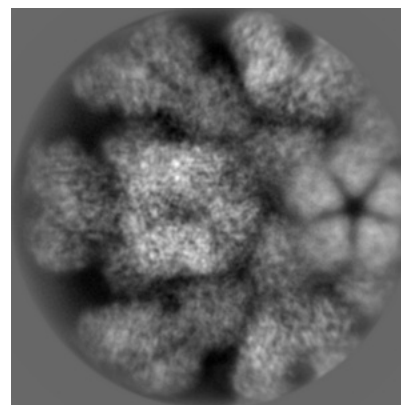
6.1.2 Raw map



X



Y

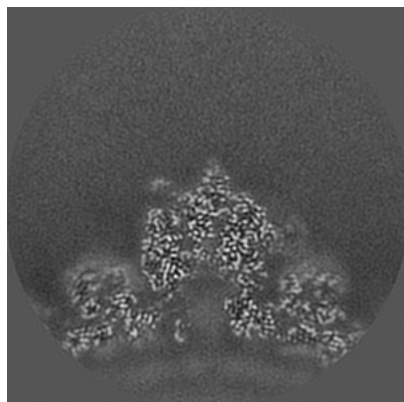


Z

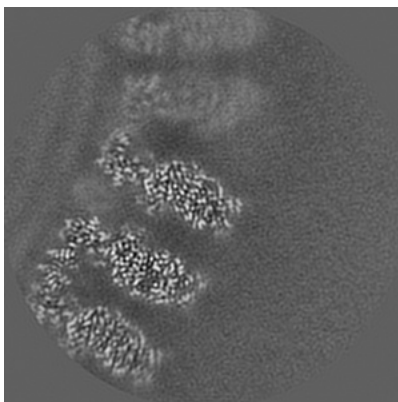
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

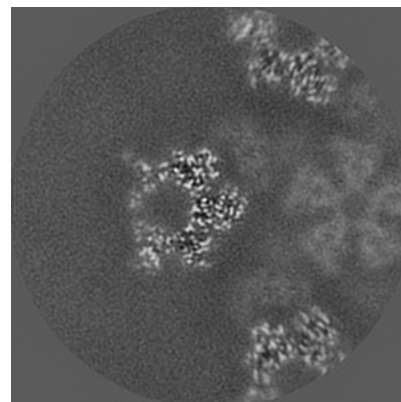
6.2.1 Primary map



X Index: 140

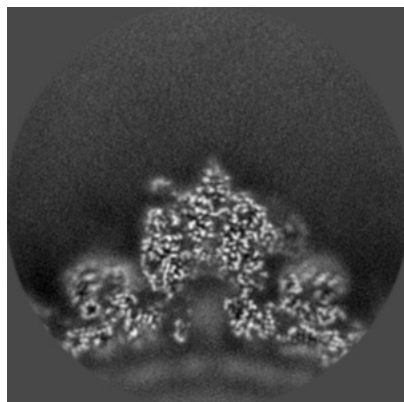


Y Index: 140

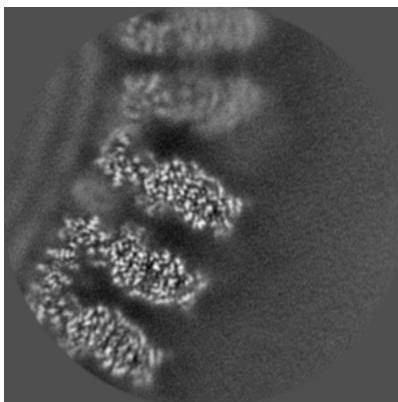


Z Index: 140

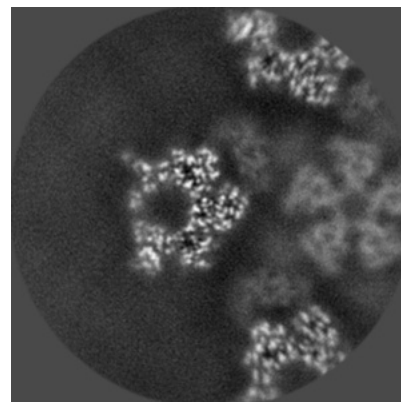
6.2.2 Raw map



X Index: 140



Y Index: 140

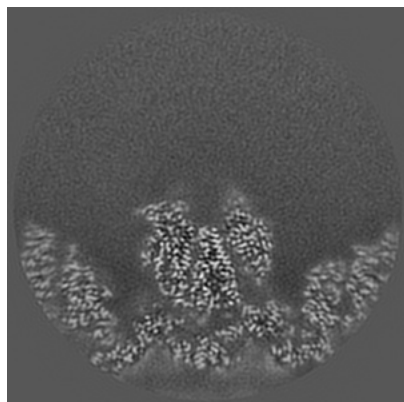


Z Index: 140

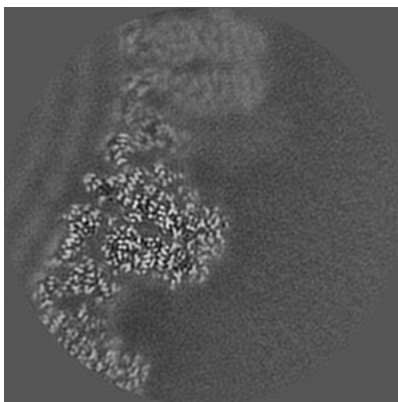
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

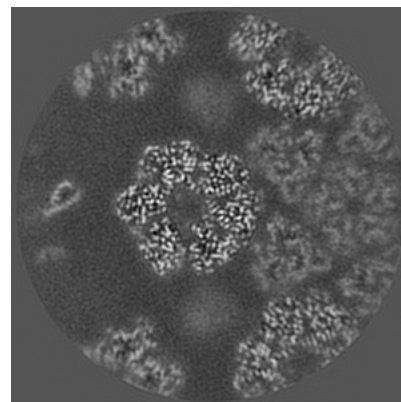
6.3.1 Primary map



X Index: 101

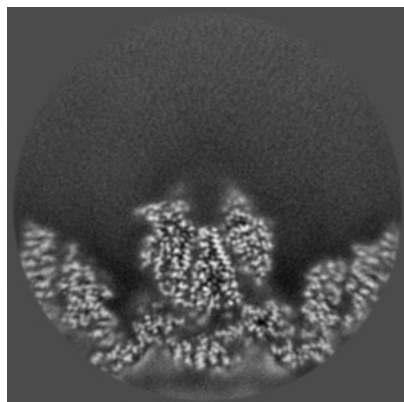


Y Index: 118

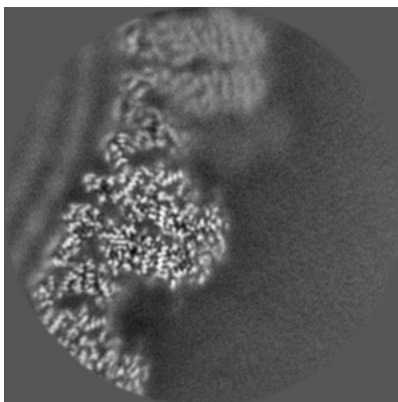


Z Index: 104

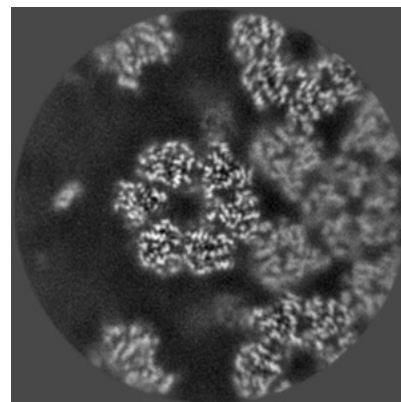
6.3.2 Raw map



X Index: 101



Y Index: 119

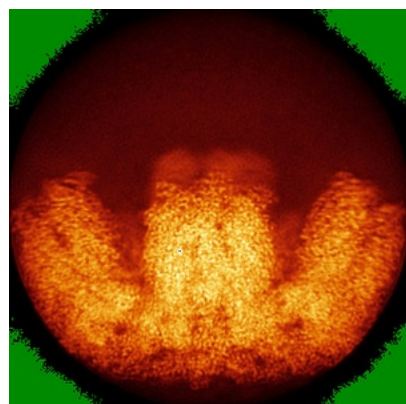


Z Index: 109

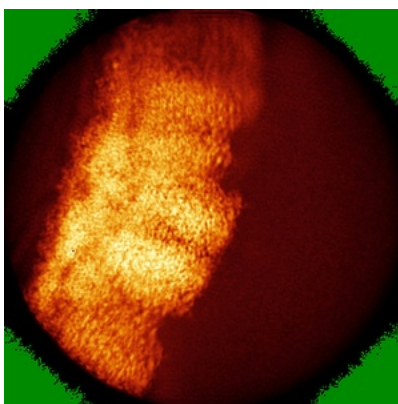
The images above show the largest variance slices of the map in three orthogonal directions.

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

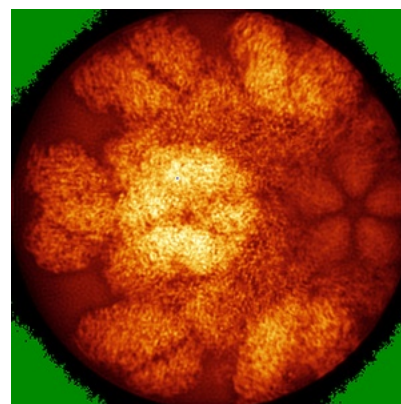
6.4.1 Primary map



X

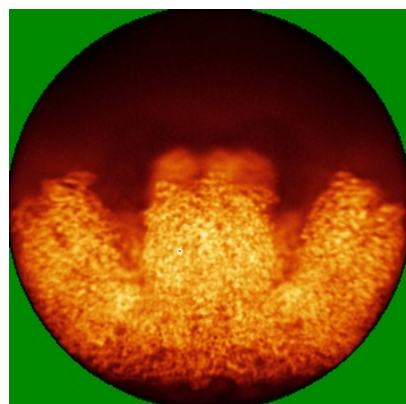


Y

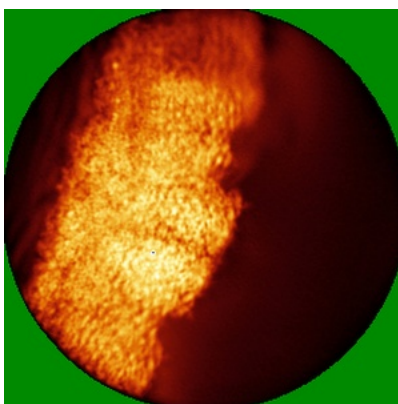


Z

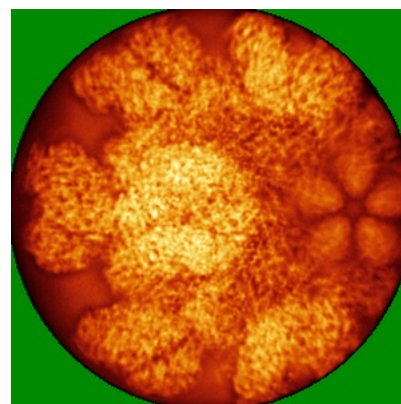
6.4.2 Raw map



X



Y

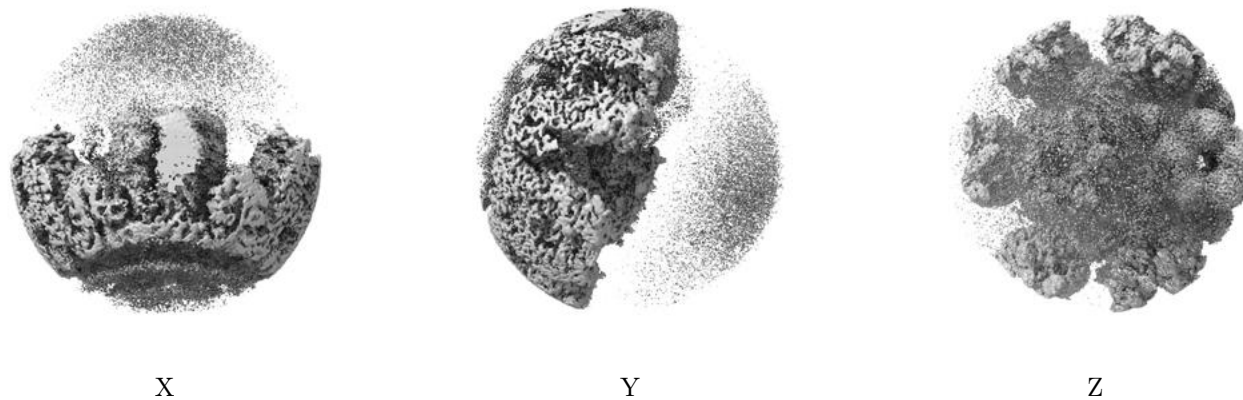


Z

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 0.004. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

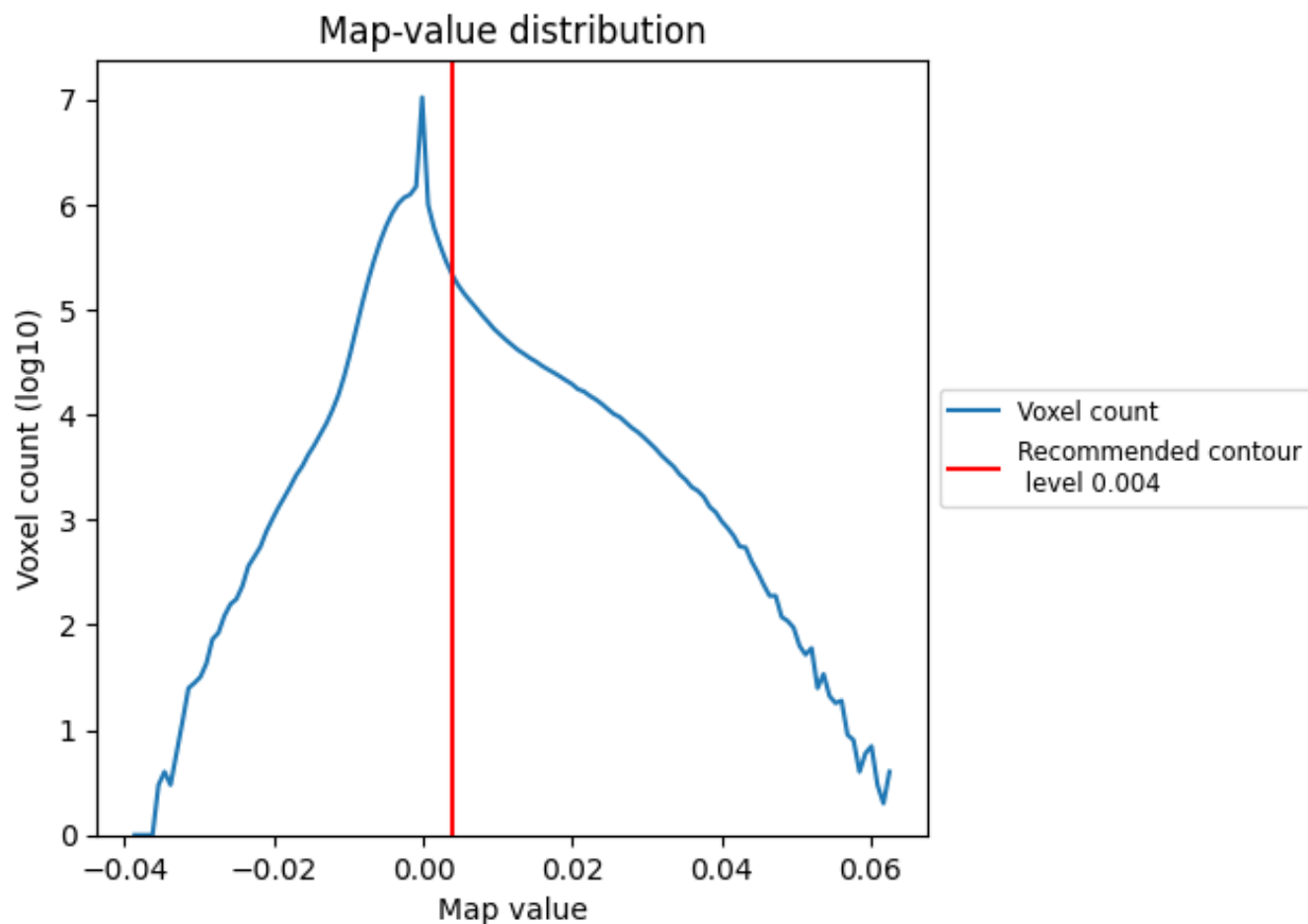
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

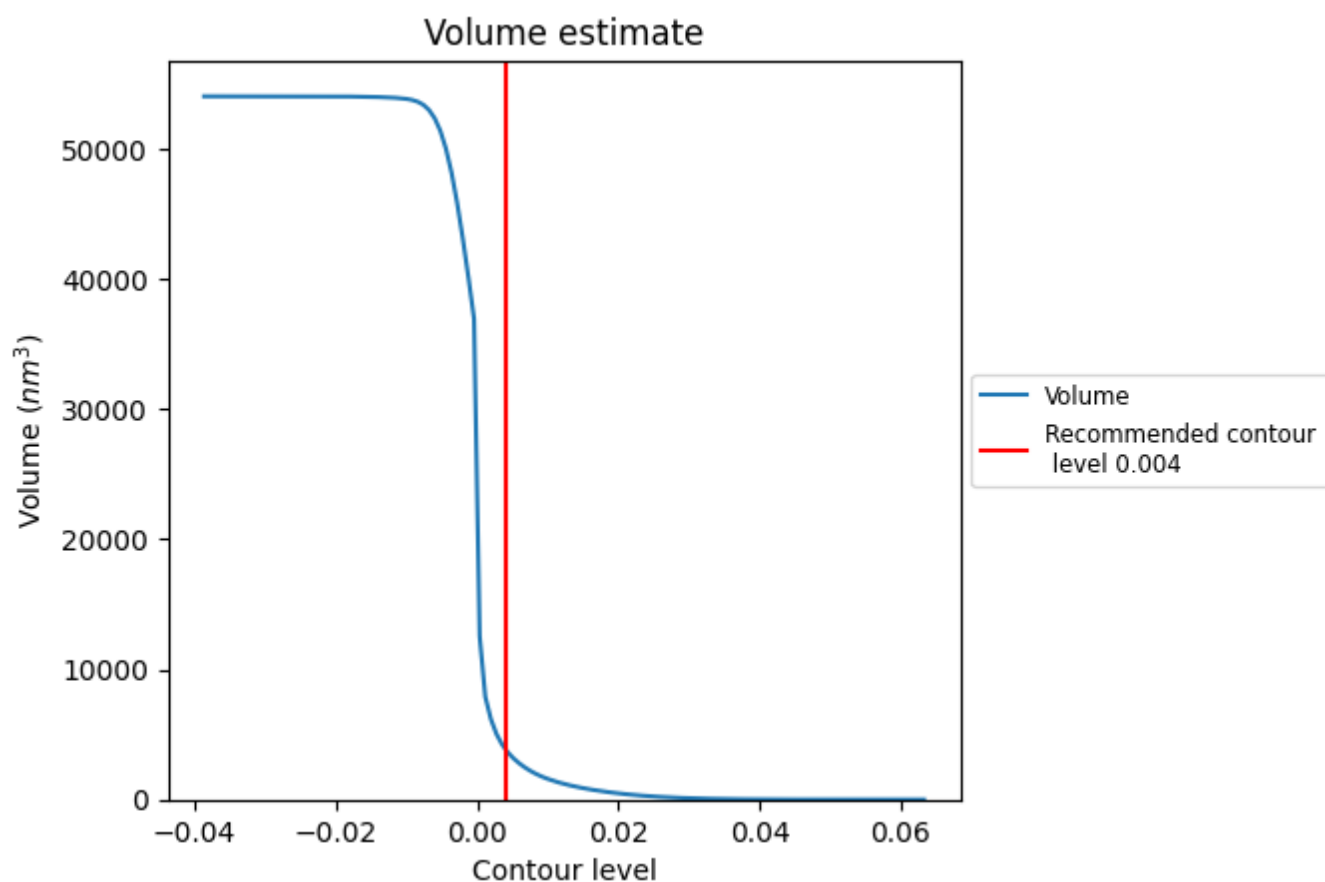
This section contains the results of statistical analysis of the map.

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.

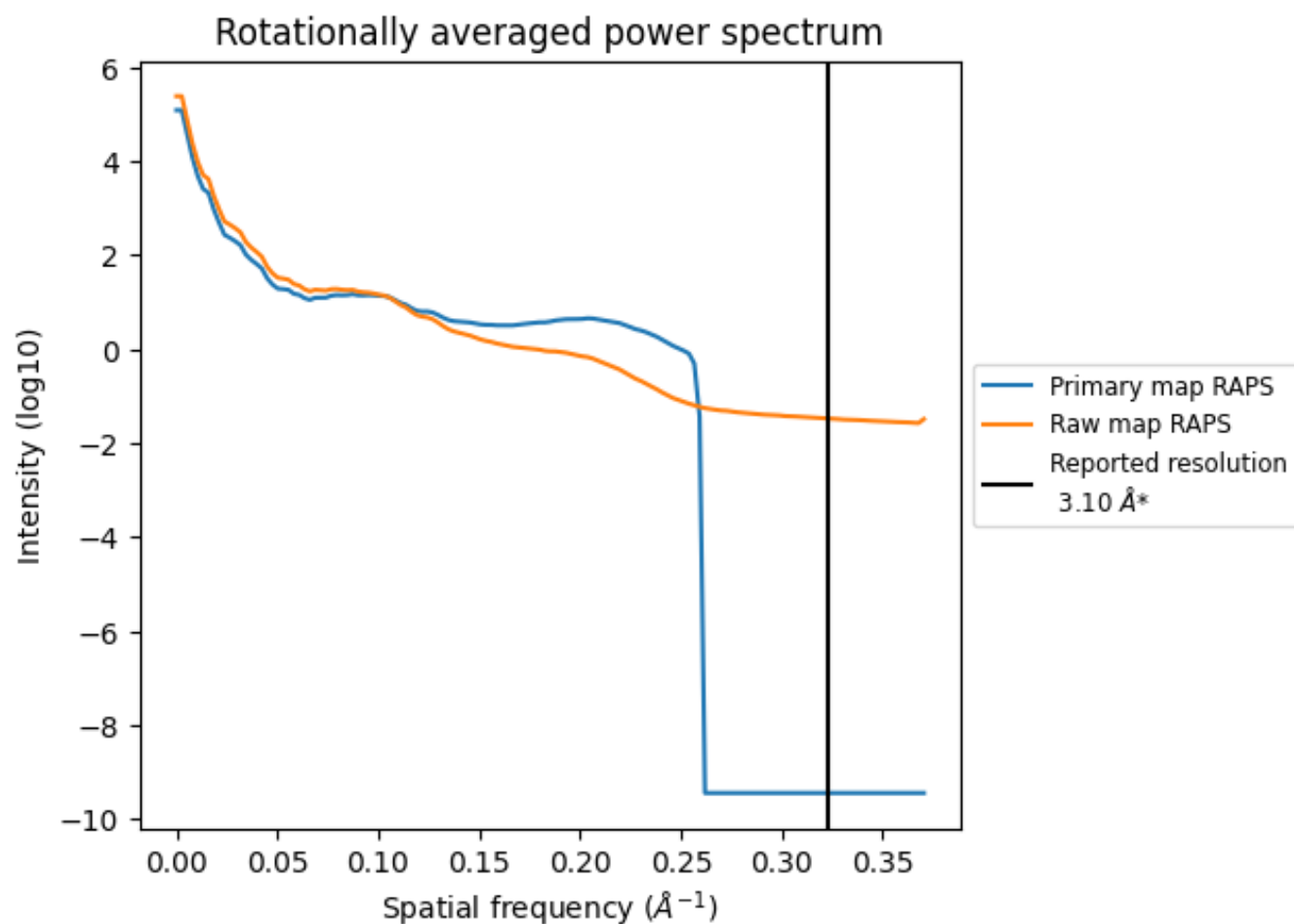
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 3897 nm³; this corresponds to an approximate mass of 3520 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 ⓘ

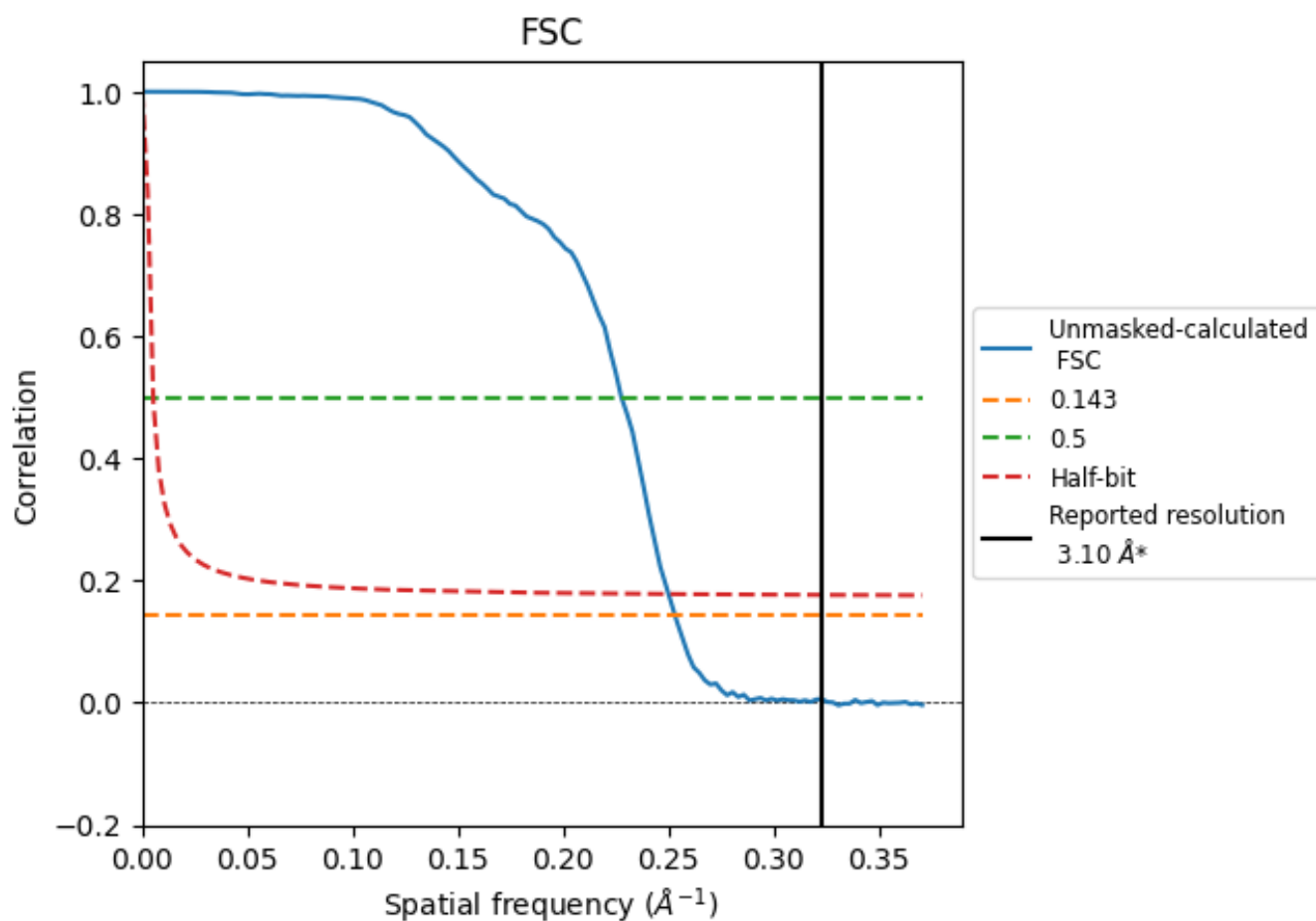


*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

8.2 Resolution estimates [i](#)

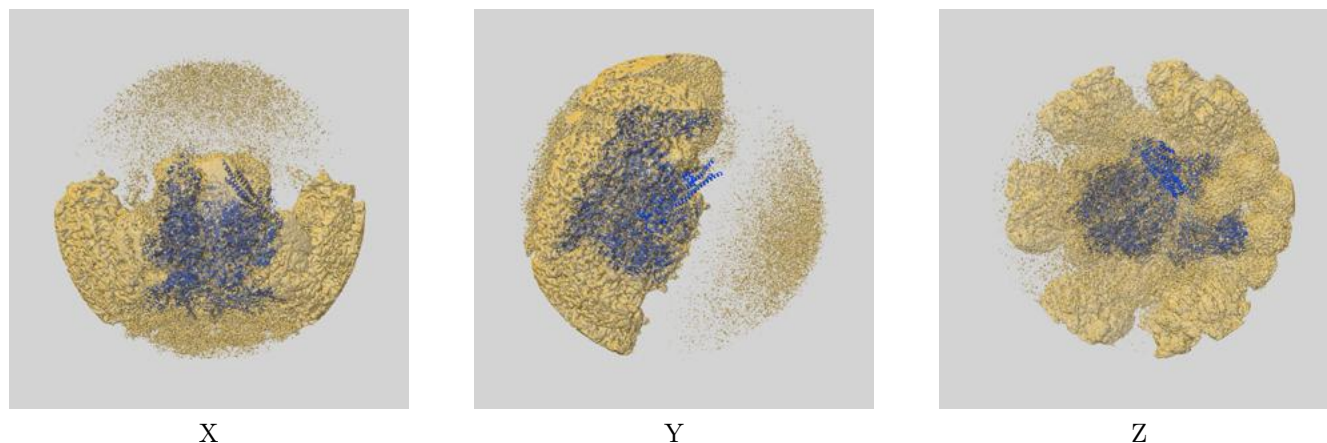
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.95	4.39	4.00

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.95 differs from the reported value 3.1 by more than 10 %

9 Map-model fit [i](#)

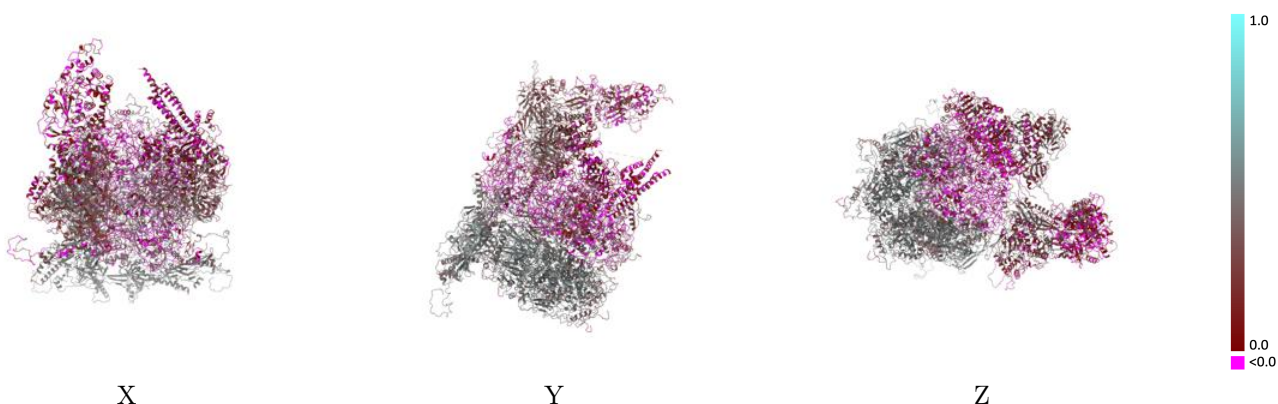
This section contains information regarding the fit between EMDB map EMD-38189 and PDB model 8X9Z. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



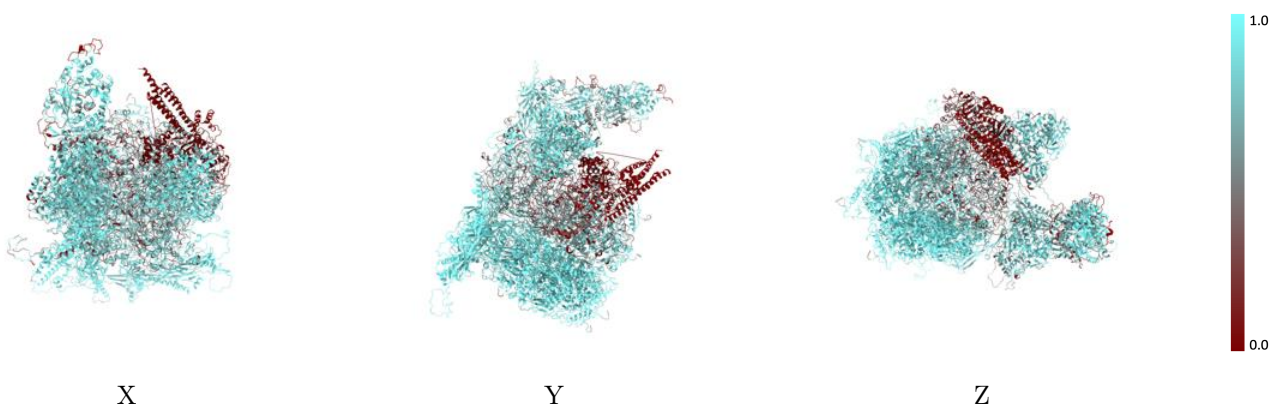
The images above show the 3D surface view of the map at the recommended contour level 0.004 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



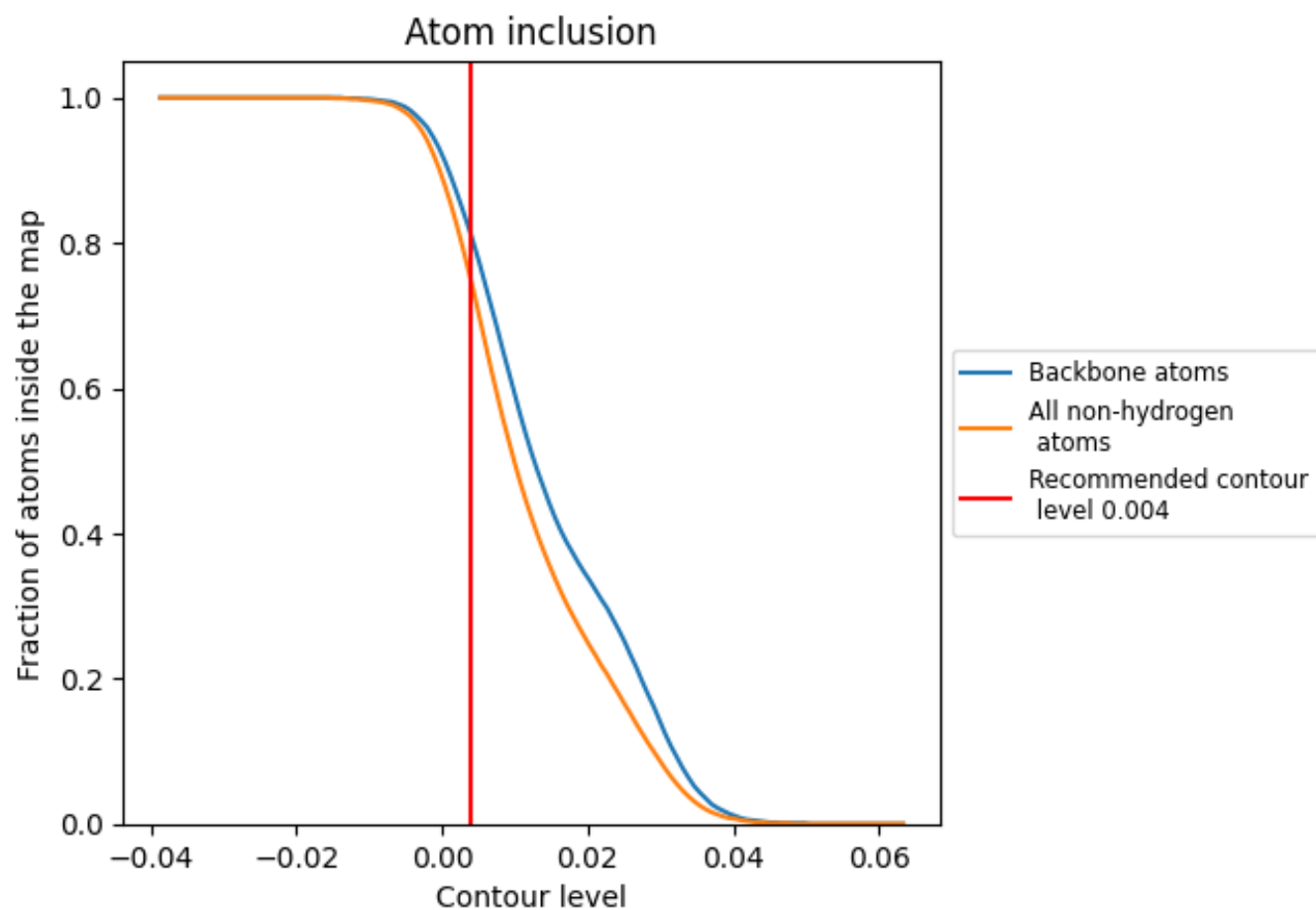
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.004).



















































9.4 Atom inclusion [i](#)



At the recommended contour level, 81% of all backbone atoms, 75% 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 (0.004) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7480	 0.2880
A	 0.5140	 0.0380
E	 0.4810	 0.0340
F	 0.9440	 0.4560
G	 0.9510	 0.4760
H	 0.9400	 0.4580
I	 0.9560	 0.4750
J	 0.6830	 0.1430
L	 0.8400	 0.2850
P	 0.8320	 0.2910
R	 0.9360	 0.3630
V	 0.8310	 0.3250
X	 0.9530	 0.4050
a	 0.8340	 0.2420
b	 0.8450	 0.3140
c	 0.7930	 0.2920
d	 0.9380	 0.4060
e	 0.9500	 0.4160
f	 0.8700	 0.3110
h	 0.7320	 0.2240
k	 0.1280	 0.1200
l	 0.0630	 0.1060
m	 0.0760	 0.0540
n	 0.0270	 0.1090
o	 0.0410	 0.0470

