



wwPDB EM Validation Summary Report ⓘ

Mar 5, 2026 – 08:57 PM UTC

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.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

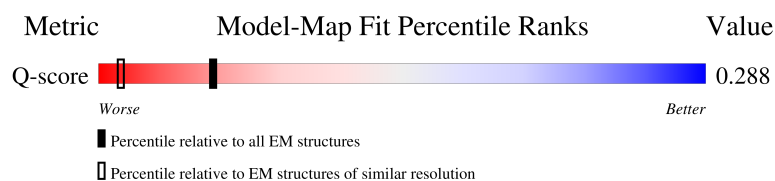
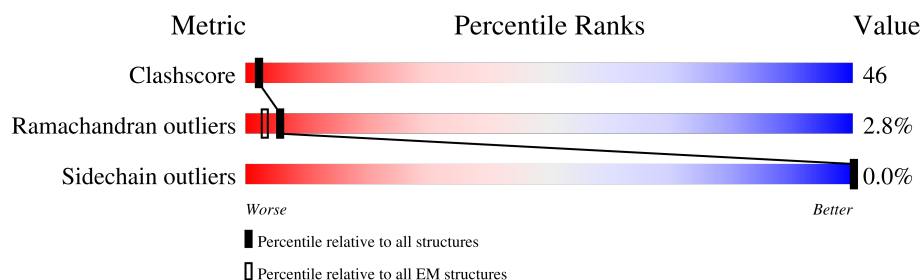
1 Overall quality at a glance i

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.



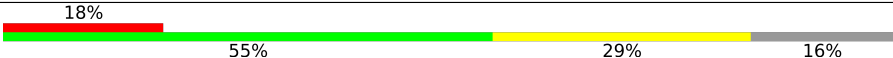
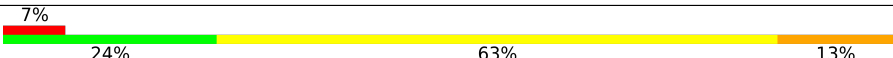
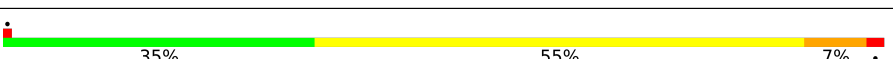
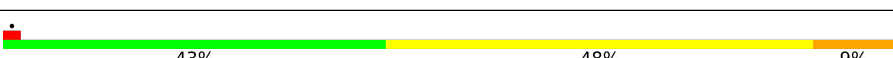
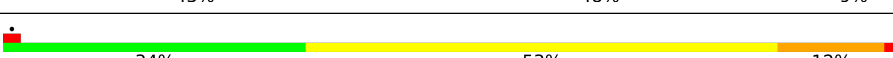
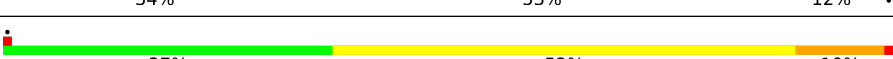
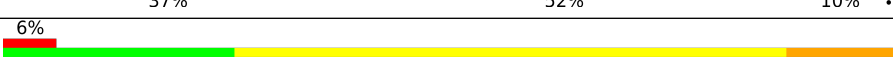
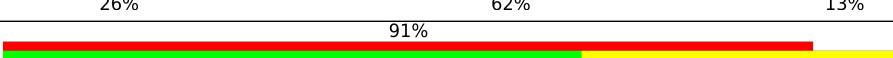
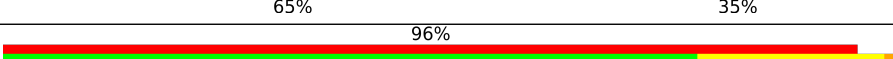
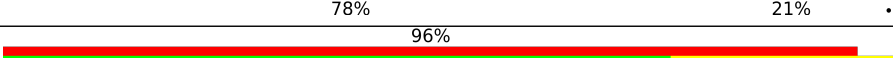
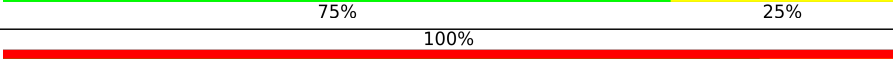
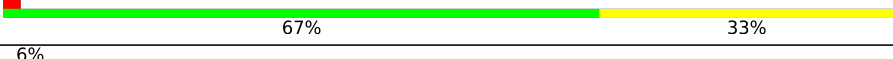
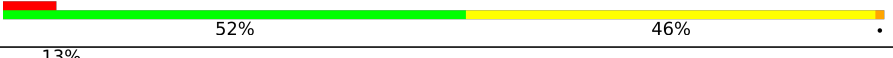
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14724 (2.60 - 3.60)

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	37% 8% 38% 36% 14% .
1	F	1369	63% 34% ..
1	G	1369	75% 22% .
1	H	1369	62% 34% ..

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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 [i](#)

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		

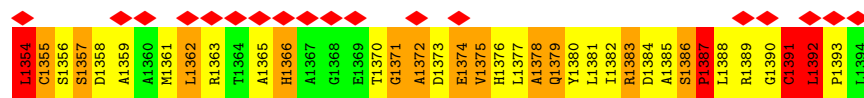
- Molecule 10 is a protein called Tri2A.

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		

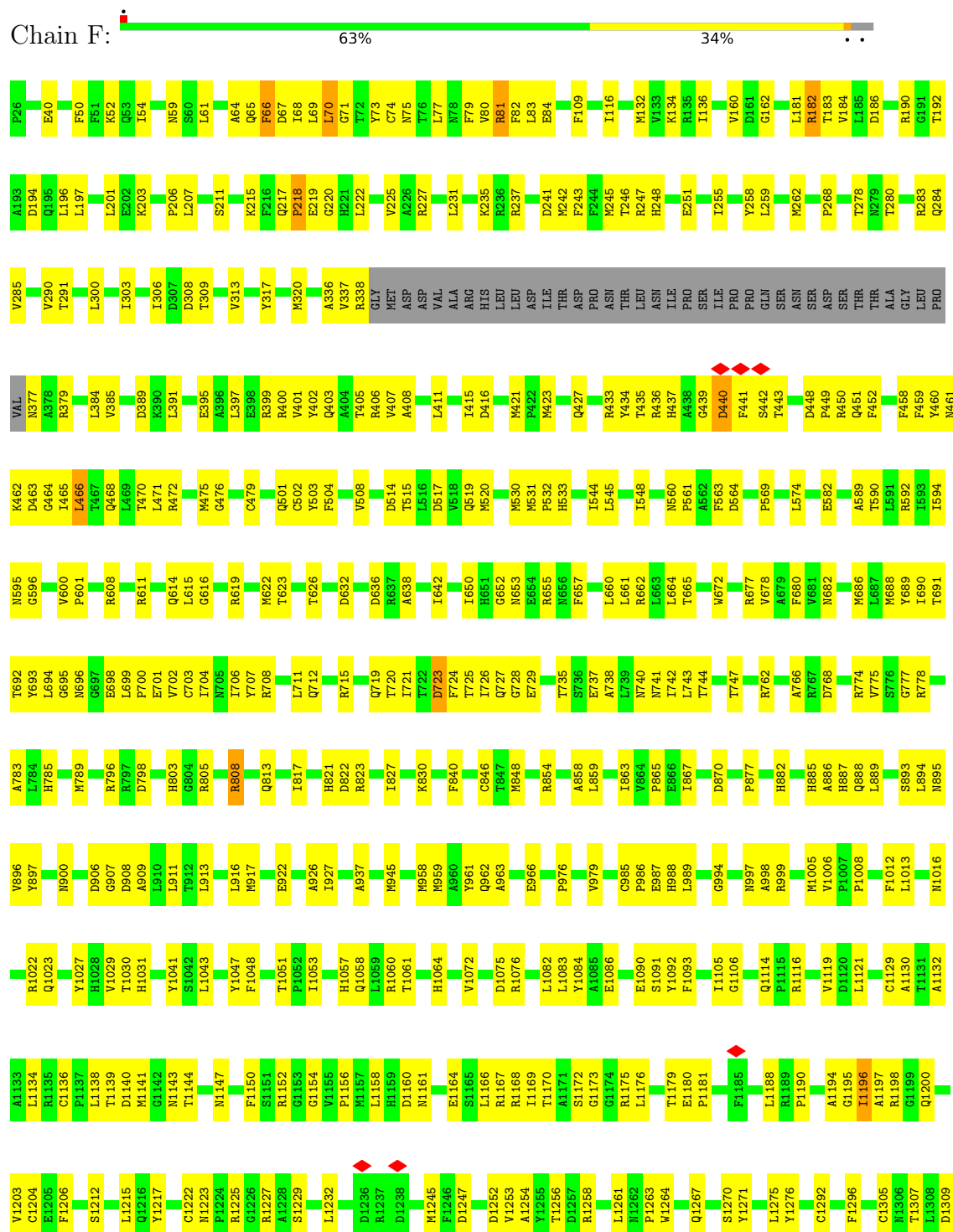
- Molecule 11 is a protein called Tri1.

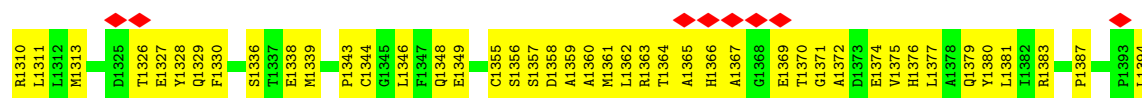
Mol	Chain	Residues	Atoms					AltConf	Trace
11	c	286	Total	C	N	O	S	0	0
			2221	1408	411	389	13		
11	h	286	Total	C	N	O	S	0	0
			2221	1408	411	389	13		

K1294	F1295	F1296	T1297	P1298	A1299	E1300	V1301	R1302	T1303	M1304	C1305	M1306	T1307	L1308	D1309	R1310	L1311	L1312	M1313	E1314	A1315	K1316	A1317	V1318	A1319	S1320	Q1321	S1322	S1323	T1324	D1325	T1326	E1327	Y1328	K1329	F1330	K1331	R1332	P1333	P1334	G1335	S1336	T1337	E1338	M1339	T1340	Q1341	D1342	P1343	C1344	G1345	L1346	F1347	Q1348	E1349	A1350	V1351	P1352	P1353	
M1234	G1235	D1236	R1237	D1238	A1239	D1240	I1241	E1242	A1243	I1244	M1245	H1246	F1247	D1248	H1249	T1250	S1251	D1252	V1253	A1254	T1255	T1256	D1257	R1258	A1259	T1260	G1261	L1262	N1263	N1264	A1265	S1266	Q1267	H1268	H1269	F1270	S1271	Y1272	G1273	D1274	R1275	L1276	Y1277	N1278	G1279	T1280	M1281	T1282	T1283	G1284	A1285	S1286	P1287	T1288	S1289	A1290	P1291	C1292	F1293	
Q1114	P1115	R1116	A1117	H1118	V1119	D1120	L1121	G1122	V1123	G1124	Y1125	T1126	A1127	C1129	A1130	A1132	A1133	L1134	C1136	P1137	L1138	T1139	D1140	M1141	G1142	N1143	T1144	A1145	Q1146	N1147	L1148	F1149	F1150	S1151	R1152	G1153	G1154	V1155	P1156	M1157	L1158	H1159	D1160	N1161	V1162	T1163	E1164	S1165	L1166	R1167	R1168	T1169	T1170	A1171	S1172	G1173				
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G1174	L1175	M1176	N1177	P1178	T1179	E1180	P1181	L1182	P1183	Y1184	F1185	G1186	G1187	L1188	R1189	P1190	A1191	T1192	D1193	S1193	A1194	Y1255	T1256	D1257	R1258	A1259	T1260	G1261	L1262	N1263	N1264	A1265	S1266	Q1267	H1268	H1269	F1270	S1271	Y1272	G1273	D1274	R1275	L1276	Y1277	N1278	G1279	T1280	M1281	T1282	T1283	G1284	A1285	S1286	P1287	T1288	S1289	A1290	P1291	C1292	F1293
K1294	F1295	F1296	T1297	P1298	A1299	E1300	V1301	R1302	T1303	M1304	C1305	M1306	T1307	L1308	D1309	R1310	L1311	L1312	M1313	E1314	A1315	K1316	A1317	V1318	A1319	S1320	Q1321	S1322	S1323	T1324	D1325	T1326	E1327	Y1328	K1329	F1330	K1331	R1332	P1333	P1334	G1335	S1336	T1337	E1338	M1339	T1340	Q1341	D1342	P1343	C1344	G1345	L1346	F1347	Q1348	E1349	A1350	V1351	P1352	P1353	



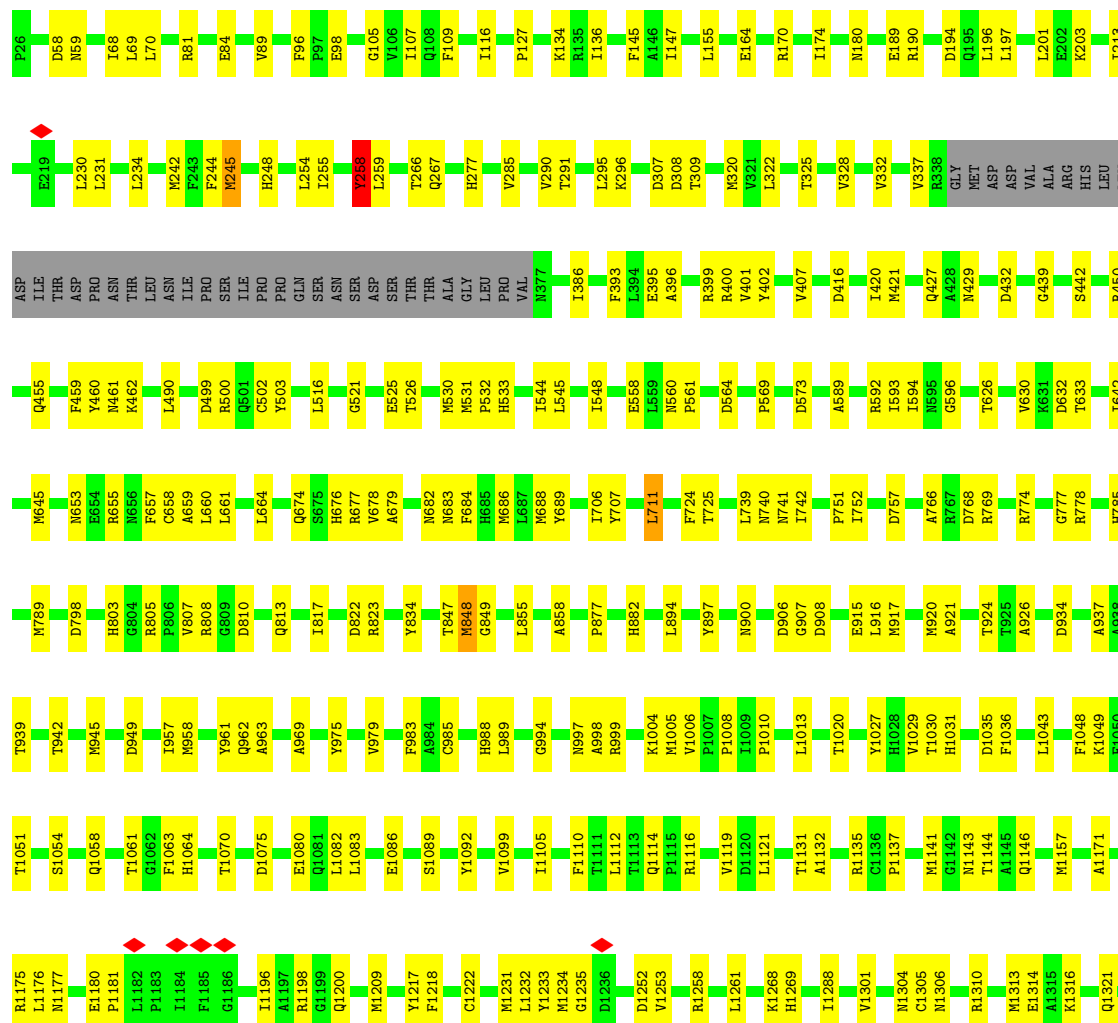
• Molecule 1: Major capsid protein





• Molecule 1: Major capsid protein

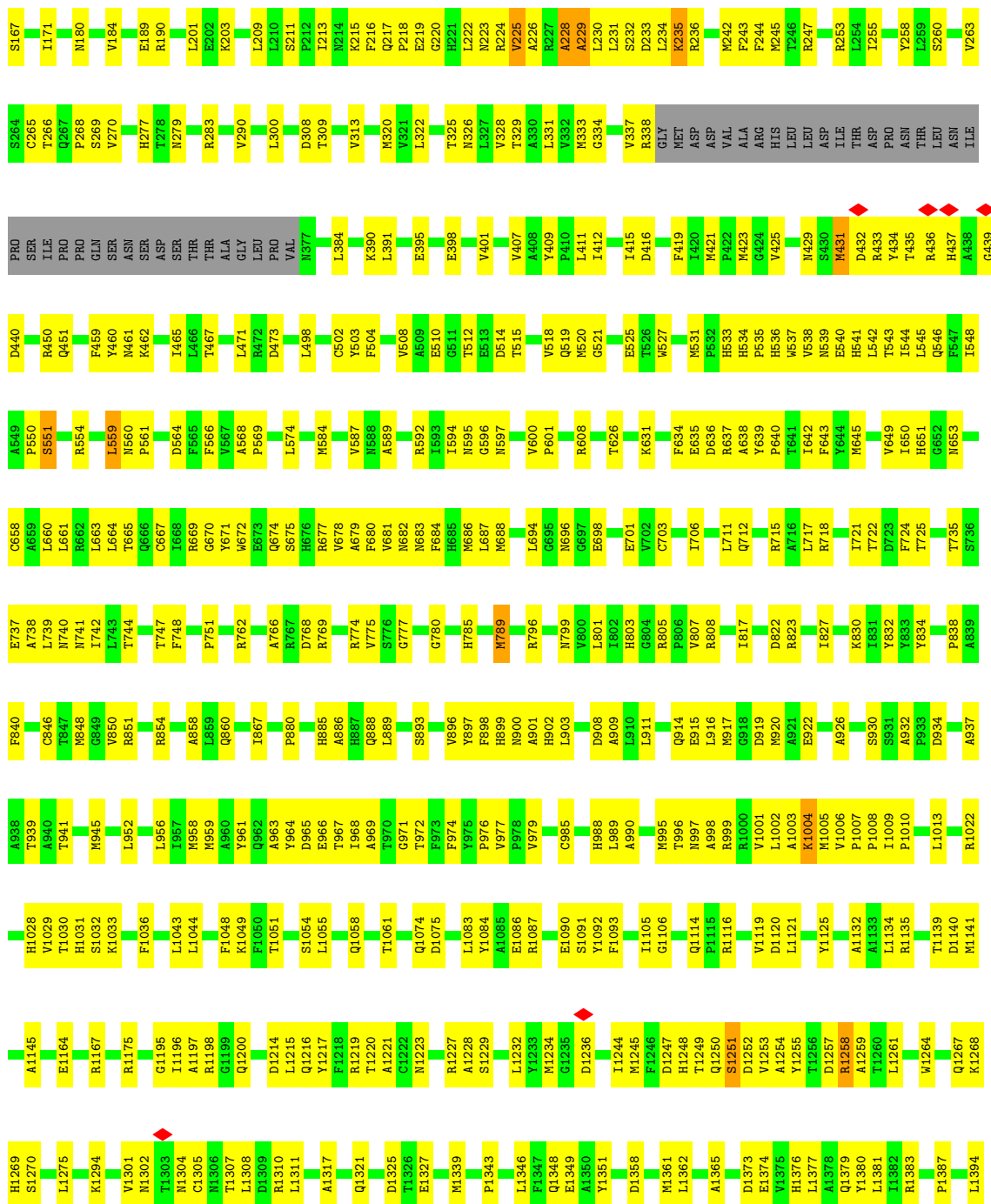
Chain G: 75% 22%



• Molecule 1: Major capsid protein

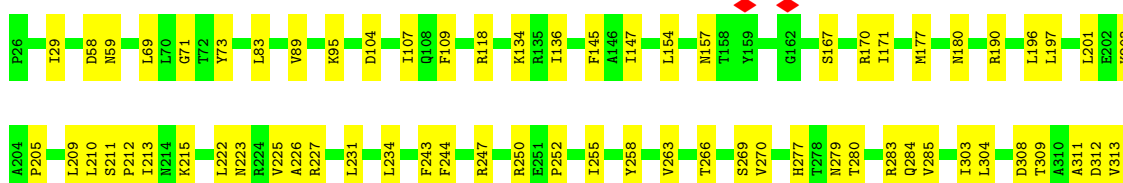
Chain H: 62% 34%

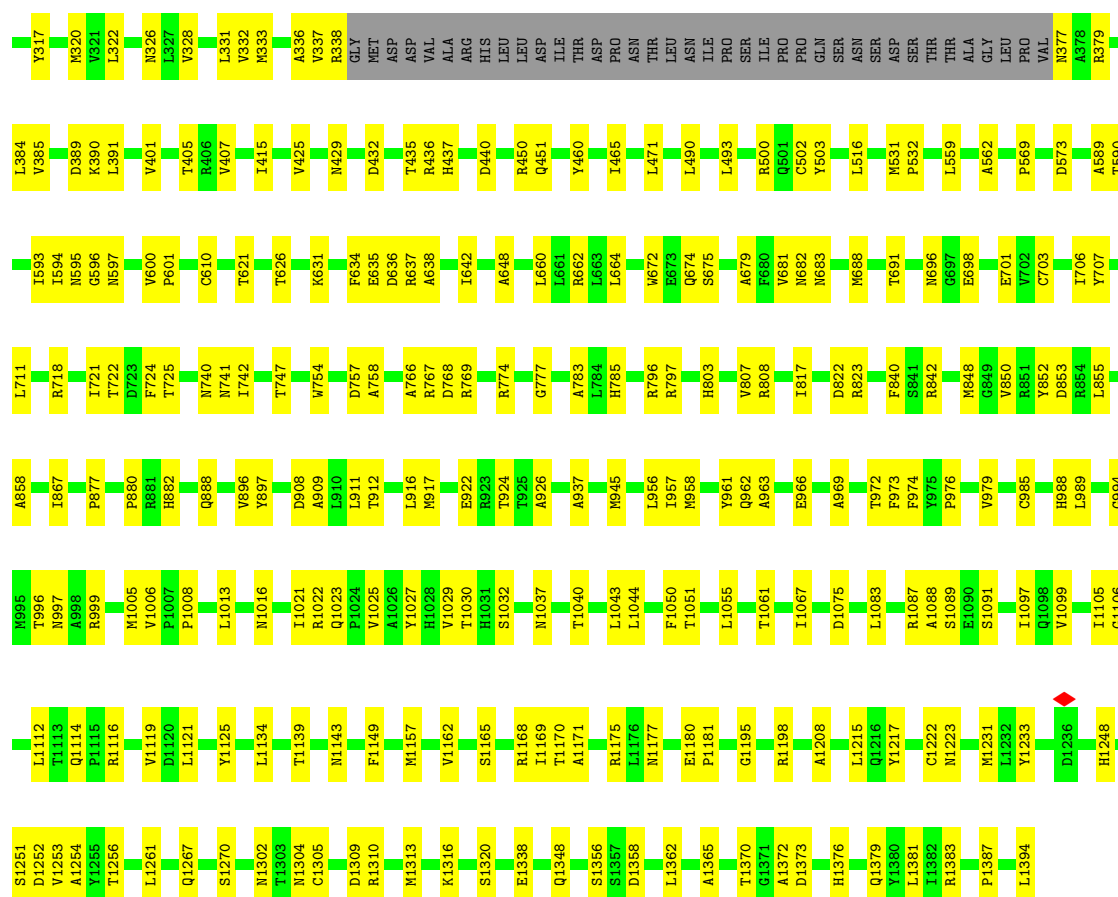




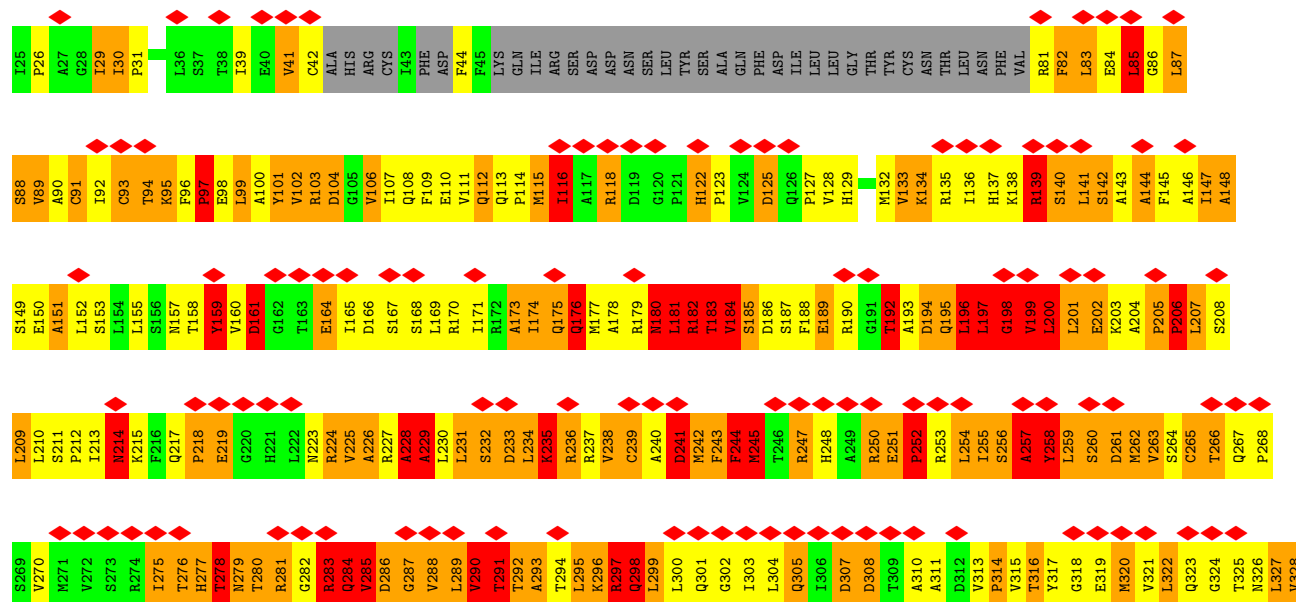
• Molecule 1: Major capsid protein

Chain I: 74% 23%

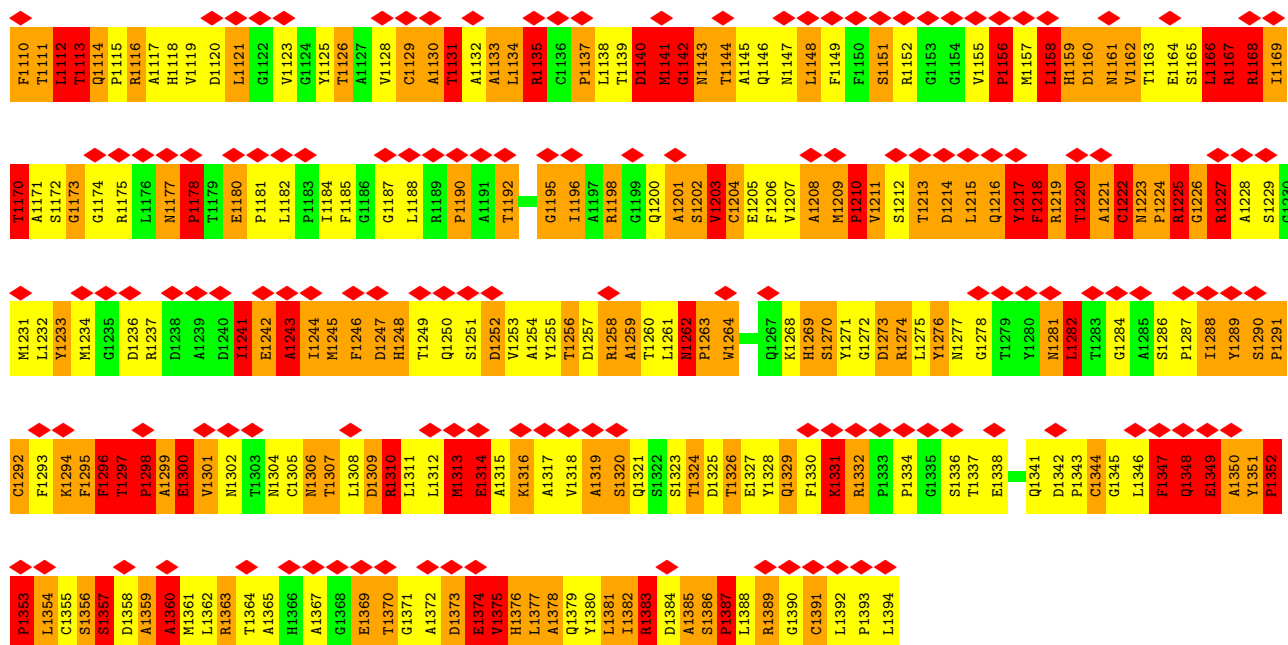




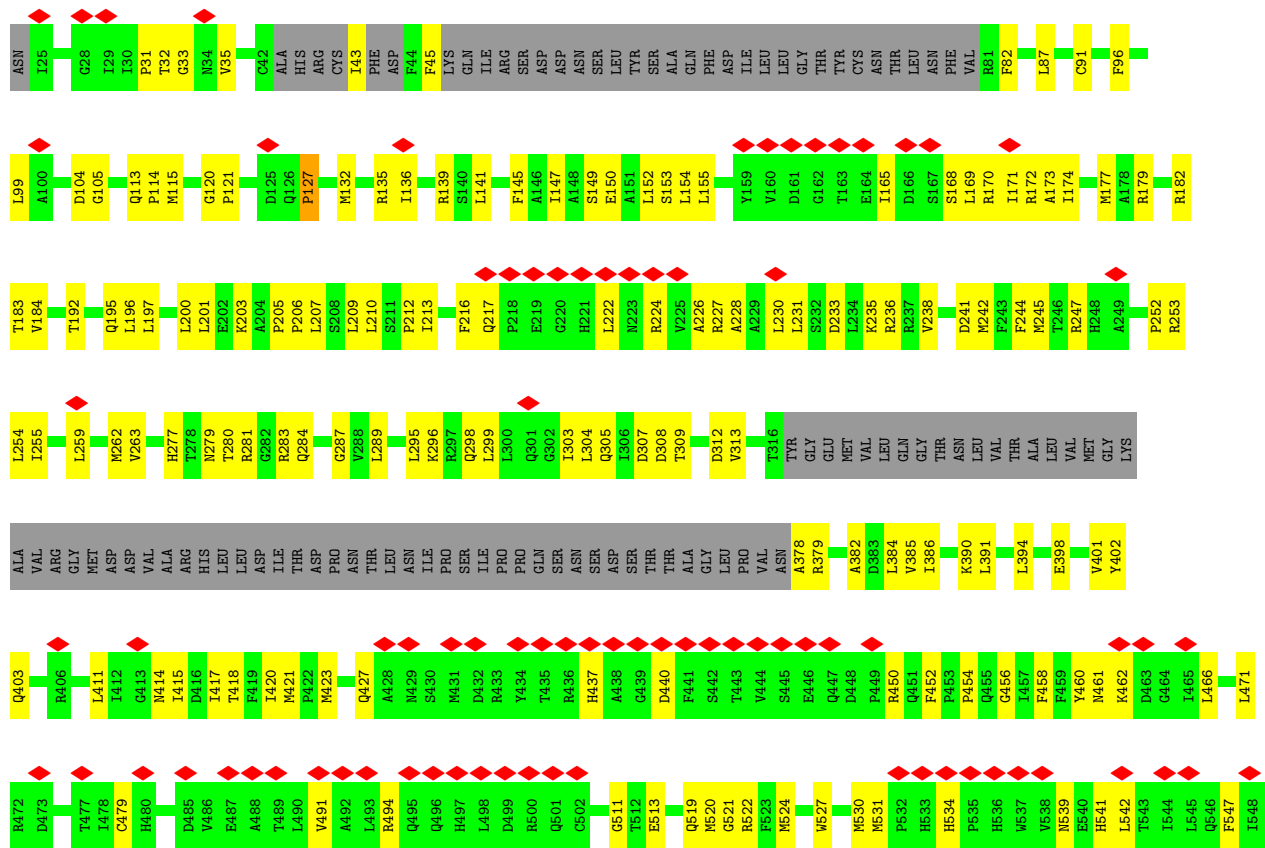
• Molecule 2: Major capsid protein



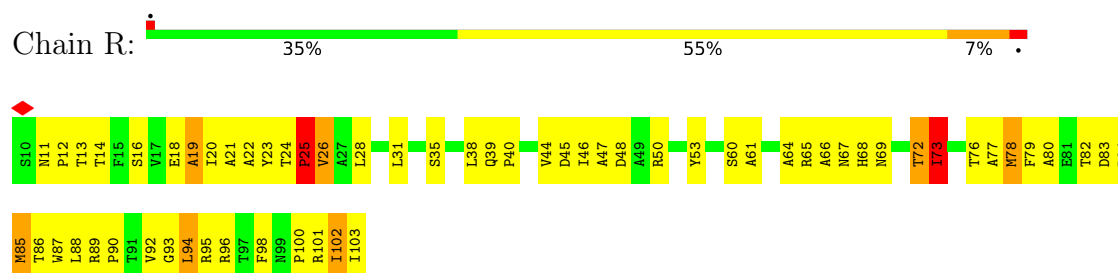
F1050	T1051	P1052	I1053	S1054	L1055	T1056	L1057	Q1058	R1059	R1060	T1061	G1062	F1063	H1064	P1065	G1066	I1067	A1068	V1069	F1069	T1070	I1071	T1072	R1073	Q1074	D1075	R1076	F1077	H1078	T1079	E1080	Q1081	L1082	L1083	Y1084	A1085	E1086	R1087	A1088	S1089	E1090	S1091	F1092	F1093	V1094	G1095	Q1096	I1097	G1098	V1099	H1100	H1101	H1102	D1103	A1104	L1105	G1106	G1107	V1108	N1109
A990	S991	L992	P993	D994	M995	T996	N997	A998	R999	R1000	V1001	L1002	A1003	K1004	H1005	V1006	P1007	P1008	I1009	P1010	F1011	F1012	L1013	G1014	A1015	N1016	H1017	L1018	A1019	T1020	I1021	L1022	Q1023	P1024	V1025	A1026	Y1027	H1028	V1029	T1030	H1031	S1032	K1033	S1034	D1035	F1036	N1037	T1038	L1039	T1040	Y1041	S1042	L1043	L1044	G1045	G1046	Y1047	F1048	K1049	
G809	D810	T811	G812	Q813	A814	L815	P816	L817	T818	P819	H820	H821	D822	R823	E824	W825	G826	L827	V828	S829	R830	Y831	Y832	Y833	Y834	L835	V836	L837	R838	A839	H840	S841	R842	G843	S844	C845	C846	T847	H848	G849	R850	R851	Y852	D853	R854	L855	Y856	P857	L858	Q859	A860	L861	R862	L863	R864	P865	F866	L867	P868	
E871	E872	A873	P874	T875	T876	P877	E878	D879	P880	R881	H882	P883	L884	H885	A886	H887	Q888	L889	V890	P891	N892	S893	L894	N895	V896	R897	F898	H899	A900	H901	H902	L903	T904	V905	D906	G907	D908	A909	L910	L911	T912	L913	Q914	E915	L916	R917	G918	D919	H920	A921	E922	R923	T924	T925	F926	L927	Y928			
S930	S931	A932	P933	D934	A935	G936	A937	A938	T939	A940	T941	T942	R943	H944	M945	R946	Y947	Y948	D949	G950	A951	L952	Y953	H954	G955	L956	T957	N958	A959	A960	Y961	Q962	A963	Y964	D965	E966	T967	L968	A969	T970	G971	T972	F973	F974	Y975	P976	Y977	P978	Y979	N980	P981	L982	F983	A984	C985	P986	E987	H988	L989	
E809	D810	T811	G812	Q813	A814	L815	P816	L817	T818	P819	H820	H821	D822	R823	E824	W825	G826	L827	V828	S829	R830	Y831	Y832	Y833	Y834	L835	V836	L837	R838	A839	H840	S841	R842	G843	S844	C845	C846	T847	H848	G849	R850	R851	Y852	D853	R854	L855	Y856	P857	L858	Q859	A860	L861	R862	L863	R864	P865	F866	L867	P868	
Y689	L690	T691	P692	G693	L694	G695	N696	G697	E698	L699	P700	E701	V702	C703	T704	N705	T706	Y707	R708	L709	L710	L711	Q712	H713	V714	R715	A716	L717	R718	Q719	T720	T721	D722	D723	T724	T725	T726	Q727	G728	E729	G730	H731	N732	G733	E734	T735	S736	E737	A738	L739	N740	N741	L742	L743	T744	D745	D746	T747	F748	
A629	V630	K631	D632	T633	F634	E635	D636	R637	A638	Y639	P640	T641	I642	F643	Y644	N645	L646	E647	A648	V649	I650	H651	G652	N653	E654	R655	V656	F657	C658	A659	L660	R661	R662	L663	L664	T665	C666	C667	L668	R669	G670	Y671	N672	E673	Q674	S675	H676	R677	V678	A679	F680	V681	N682	N683	F684	H685	L686	L687	M688	
P569	G570	D571	V572	D573	L574	P575	G576	P577	Q578	R579	P580	P581	E582	A583	M584	P585	T586	W587	N588	A589	D589	M590	L591	R592	I593	I594	N595	G596	L597	I598	P599	V600	L601	L602	C603	P604	L605	S606	F607	D608	A609	P610	L611	G612	T613	Q614	L615	G616	L617	R618	R619	H620	T621	M622	F623	D624	A625	T626	I627	K628
A509	E510	G511	T512	E513	D514	T515	L516	D517	V518	Q519	M520	G521	R522	F523	M524	E525	T526	W527	A528	D529	M530	M531	P532	H533	H534	P535	H536	W537	N538	E540	H541	L542	T543	I544	L545	Q546	F547	I548	A549	P550	S551	N552	P553	R554	L555	R556	F557	L559	N560	P561	A562	F563	D564	F565	G566	V567	A568			
P449	R450	Q451	F452	P453	P454	Q455	G456	I457	F458	E459	R460	N461	K462	D463	G464	I465	L466	T467	Q468	L469	T470	L471	R472	D473	A474	M475	G476	T477	I478	C479	H480	S481	S482	L483	L484	D485	V486	E487	A488	T489	L490	V491	A492	L493	R494	Q495	Q496	L497	L498	D499	R500	Q501	C502	Y503	F504	G505	V506	T507	V508	
D389	K390	L391	V392	F393	L394	E395	A396	L397	E398	R399	R400	V401	Y402	Q403	A404	H405	R406	Y407	A408	Y409	P410	L411	I412	G413	N414	I415	D416	I417	T418	F419	I420	M421	P422	M423	G424	V425	F426	Q427	L428	A428	N429	S430	M431	D432	R433	T434	R435	R436	H437	A438	C439	D440	F441	T442	V443	S444	E445	Q446	D447	D448
T329	A330	L331	V332	M333	G334	K335	A336	V337	R338	GLY	MET	ASP	ASP	VAL	ALA	ARG	HIS	LEU	LEU	ASP	ILE	THR	ASP	PRO	ASN	THR	LEU	ASN	ILE	PRO	GLN	SER	ASN	SER	ASP	THR	THR	ALA	GLY	LEU	PRO	VAL	N377	A378	R379	V380	P381	A382	D383	L384	V385	I386	V387	G388						



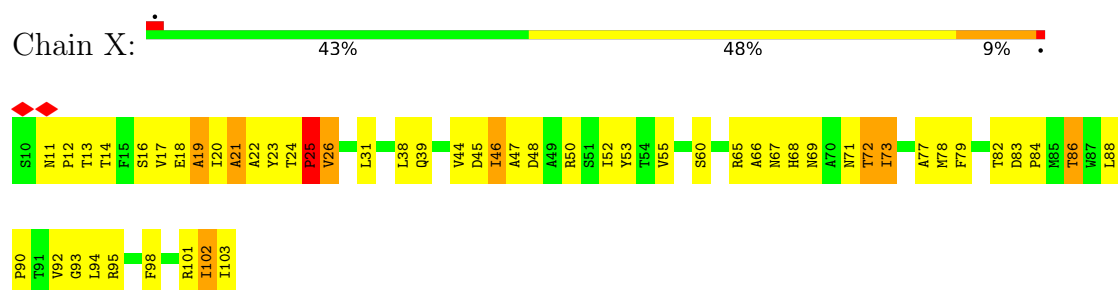
• Molecule 3: Major capsid protein



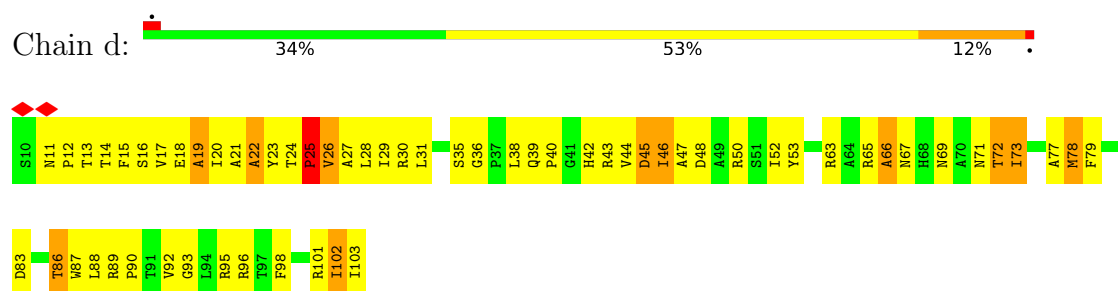
- Molecule 4: Small capsomere-interacting protein



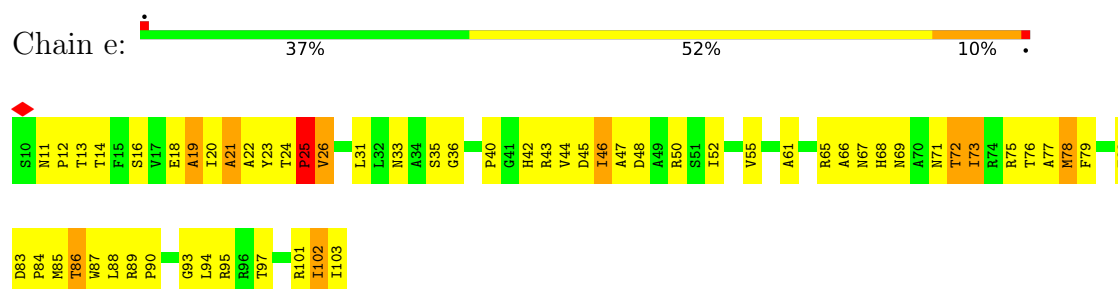
- Molecule 4: Small capsomere-interacting protein



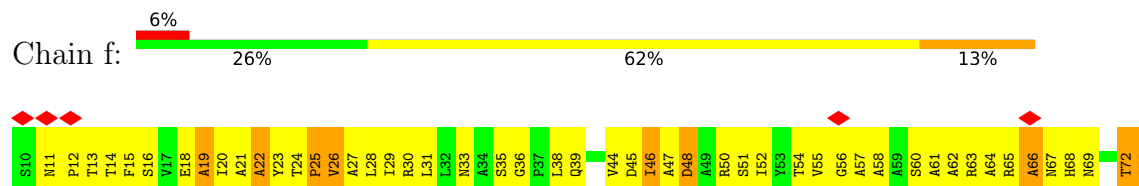
- Molecule 4: Small capsomere-interacting protein



- Molecule 4: Small capsomere-interacting protein

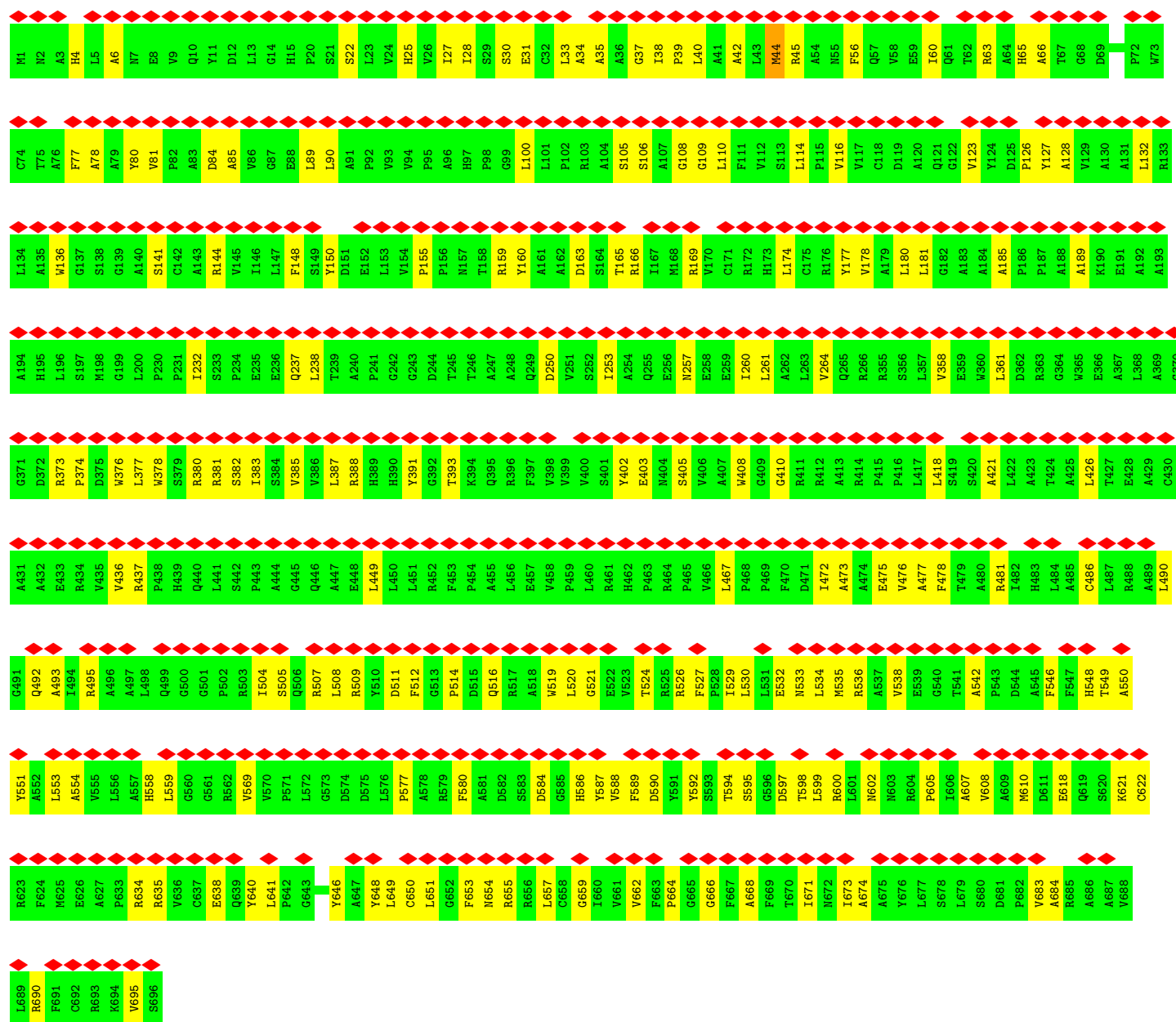
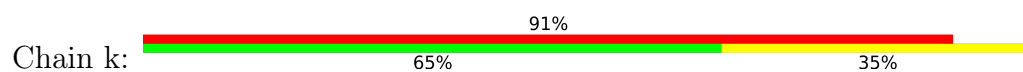


- Molecule 4: Small capsomere-interacting protein

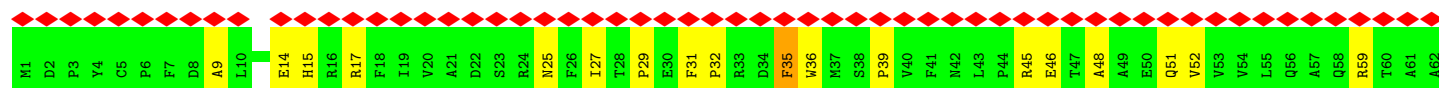
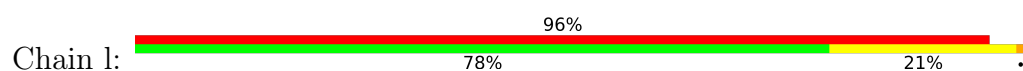


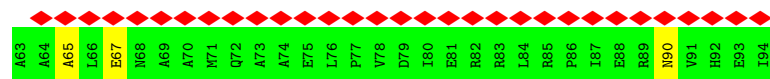


• Molecule 5: CVC1

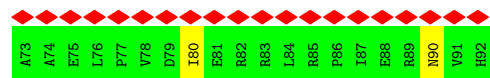
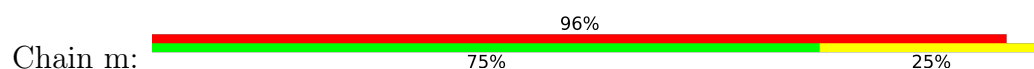


• Molecule 6: Capsid vertex component 2

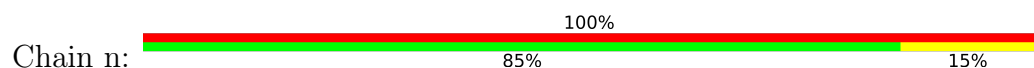




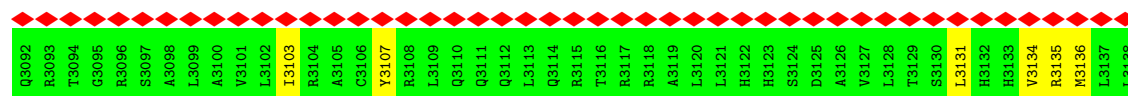
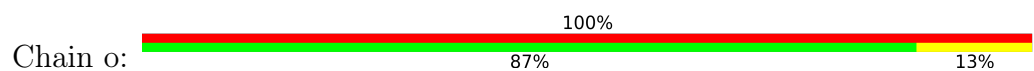
- Molecule 7: Capsid vertex component 2



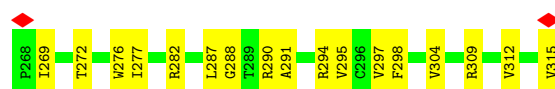
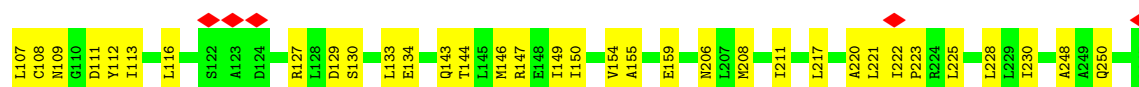
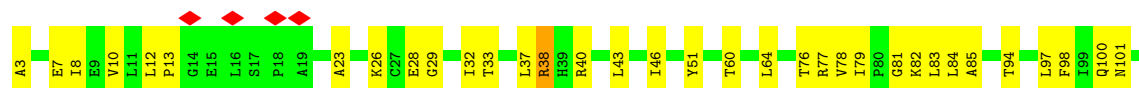
- Molecule 8: Large tegument protein deneddylase



- Molecule 8: Large tegument protein deneddylase

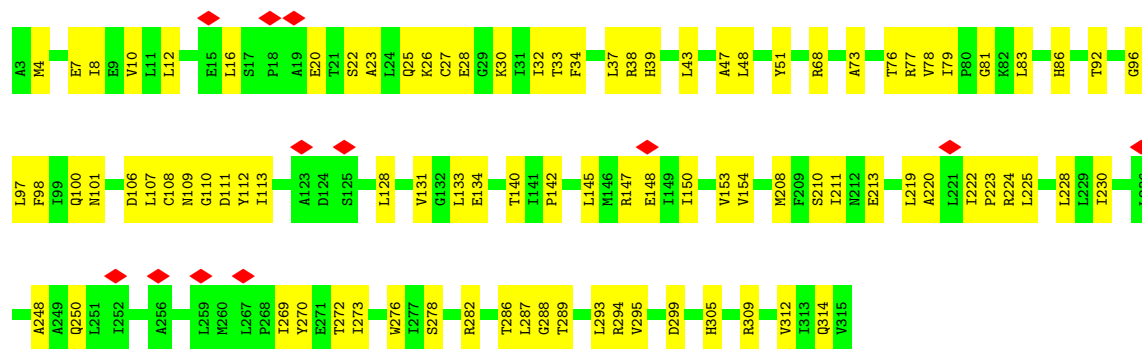


- Molecule 9: Tri2A



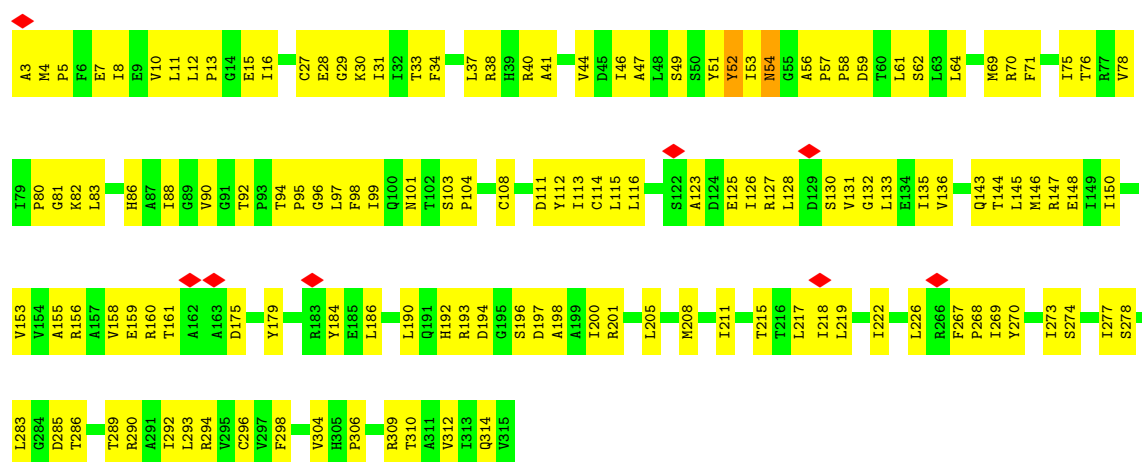
- Molecule 9: Tri2A





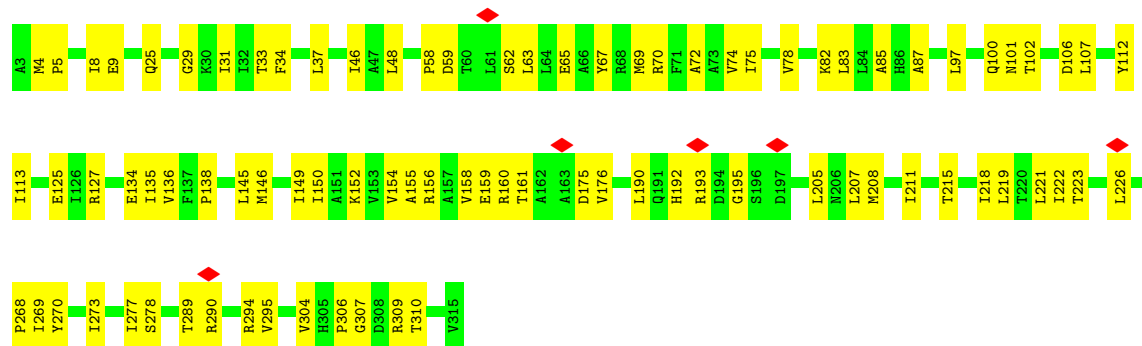
• Molecule 10: Tri2A

Chain V: 48% 52% .



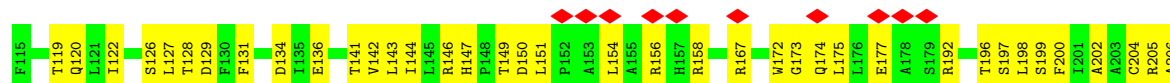
• Molecule 10: Tri2A

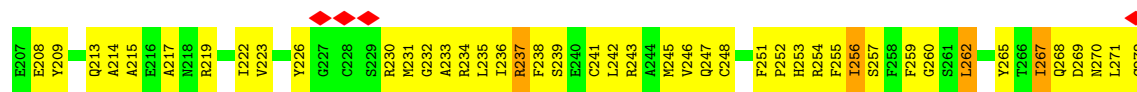
Chain b: 67% 33% .



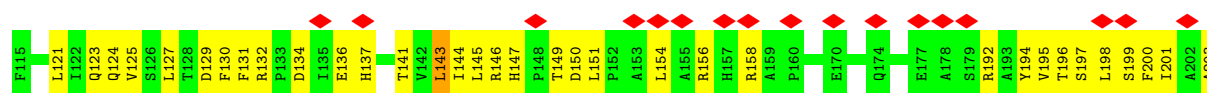
• Molecule 11: Tri1

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	2
1	F	1327/1369 (97%)	1209 (91%)	117 (9%)	1 (0%)	48	78
1	G	1327/1369 (97%)	1233 (93%)	93 (7%)	1 (0%)	48	78
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%)	43	73
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	47
9	a	248/256 (97%)	233 (94%)	14 (6%)	1 (0%)	30	61
10	V	257/263 (98%)	230 (90%)	26 (10%)	1 (0%)	30	61
10	b	257/263 (98%)	236 (92%)	20 (8%)	1 (0%)	30	61
11	c	280/286 (98%)	240 (86%)	35 (12%)	5 (2%)	6	28
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%)	86	87
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%)	81	85
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

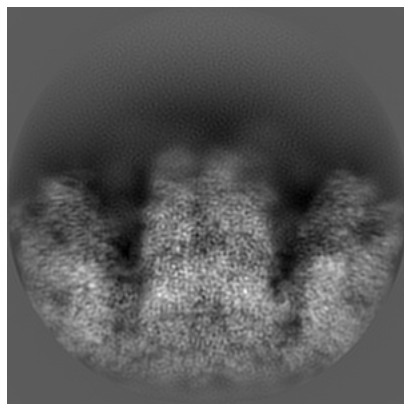
6 Map visualisation [i](#)

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.

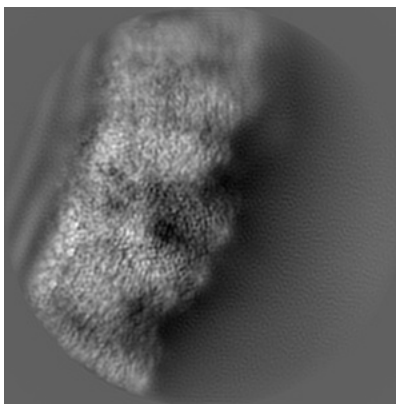
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

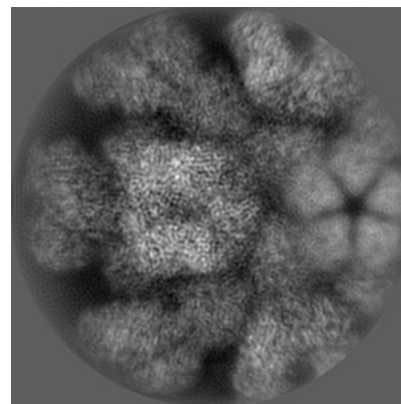
6.1.1 Primary map



X

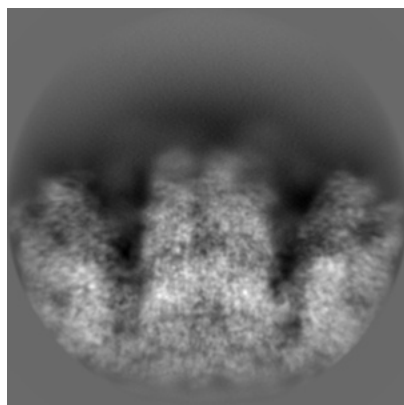


Y

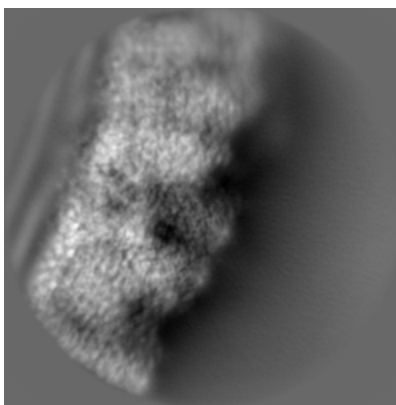


Z

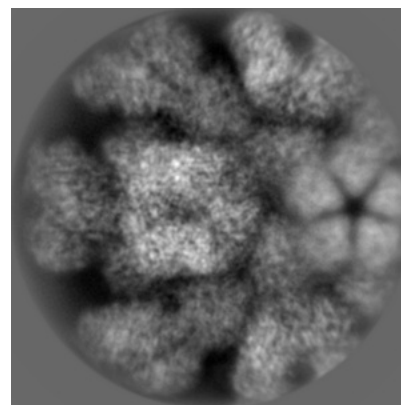
6.1.2 Raw map



X



Y

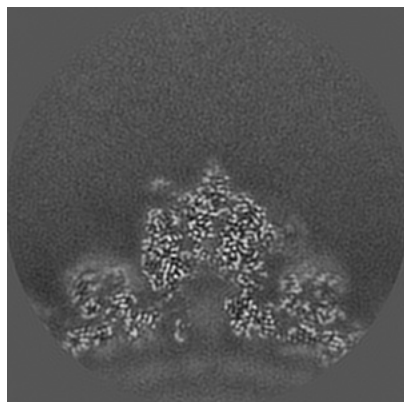


Z

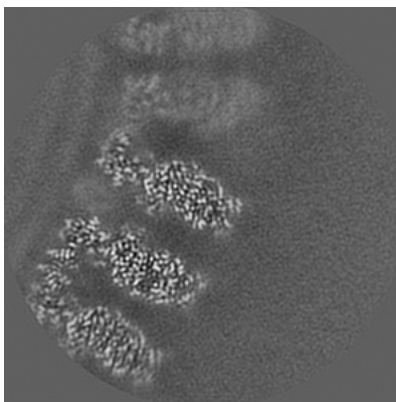
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

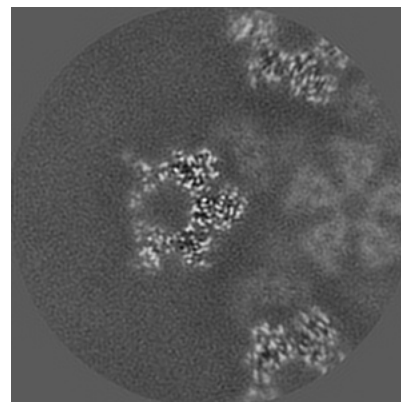
6.2.1 Primary map



X Index: 140

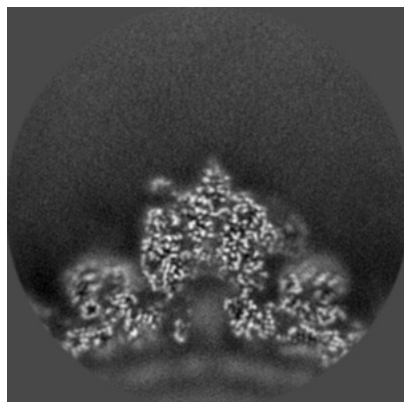


Y Index: 140

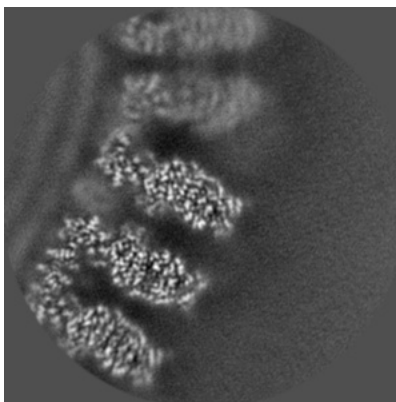


Z Index: 140

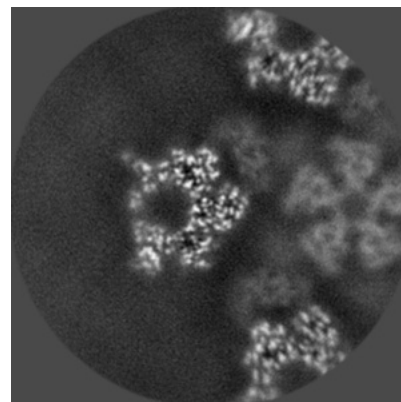
6.2.2 Raw map



X Index: 140



Y Index: 140

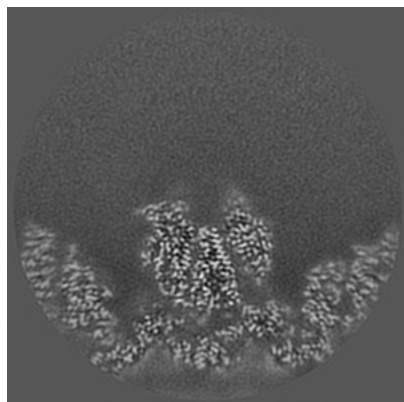


Z Index: 140

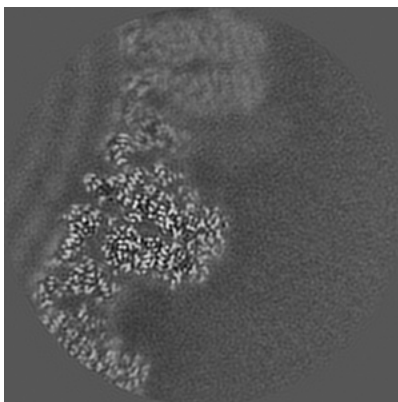
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

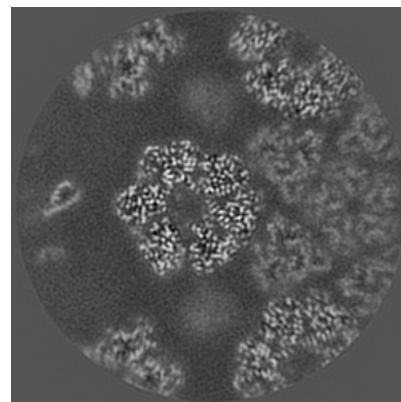
6.3.1 Primary map



X Index: 101

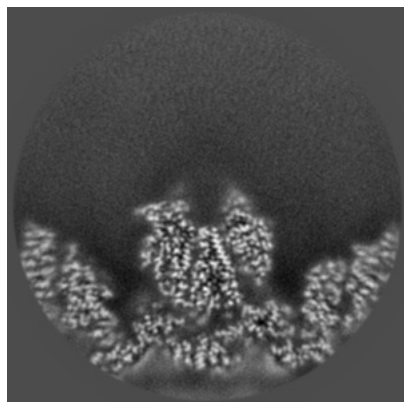


Y Index: 118

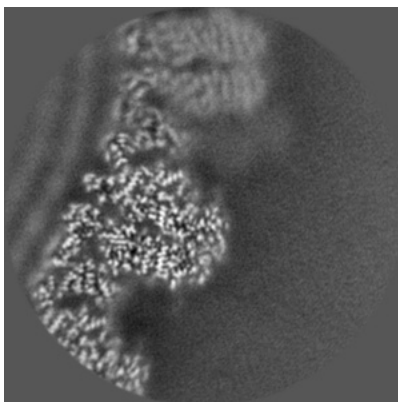


Z Index: 104

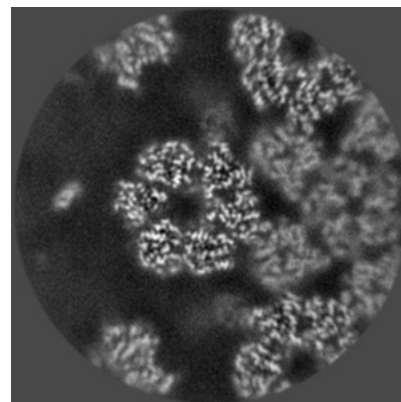
6.3.2 Raw map



X Index: 101



Y Index: 119

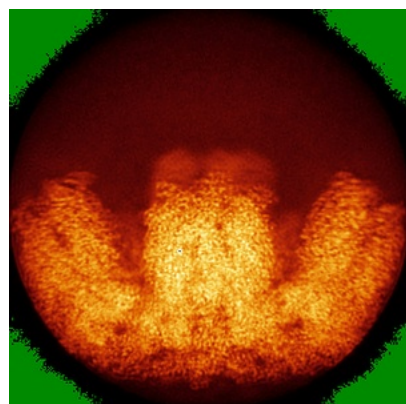


Z Index: 109

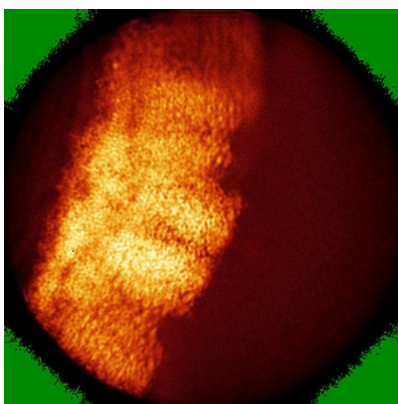
The images above show the largest variance slices of the map in three orthogonal directions.

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

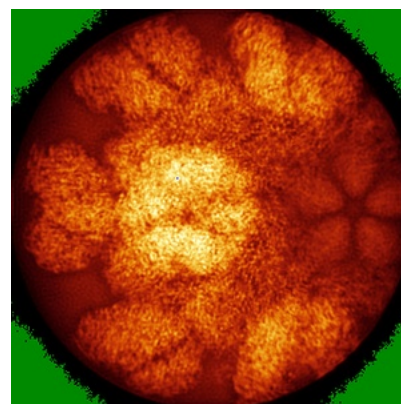
6.4.1 Primary map



X

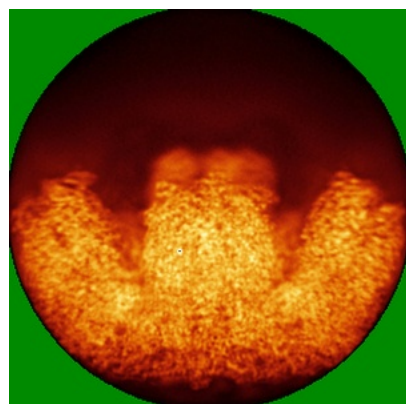


Y

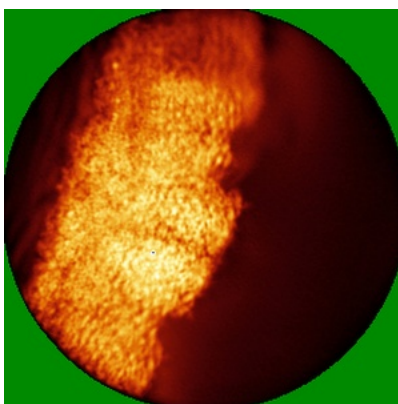


Z

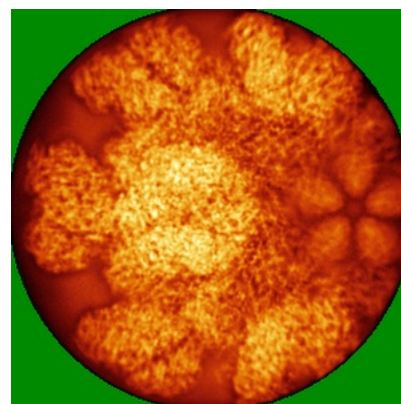
6.4.2 Raw map



X



Y

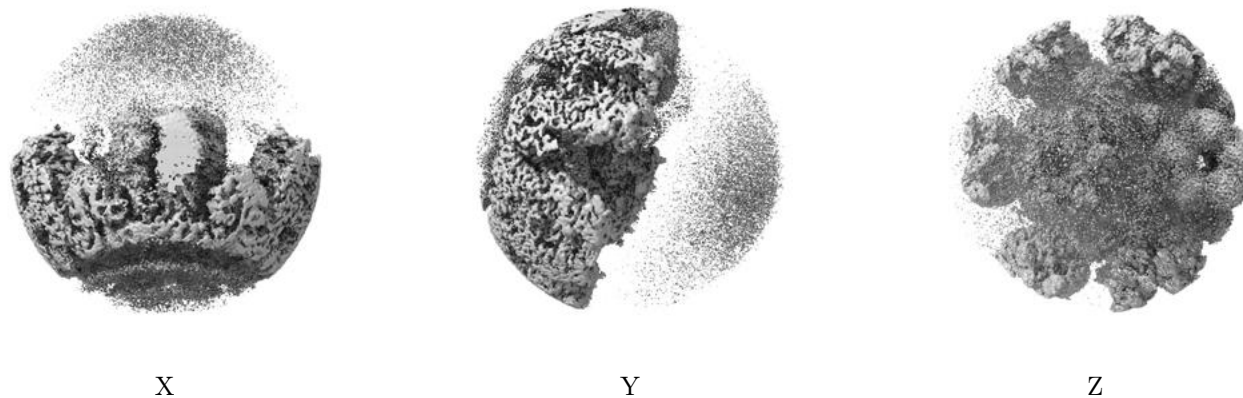


Z

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.

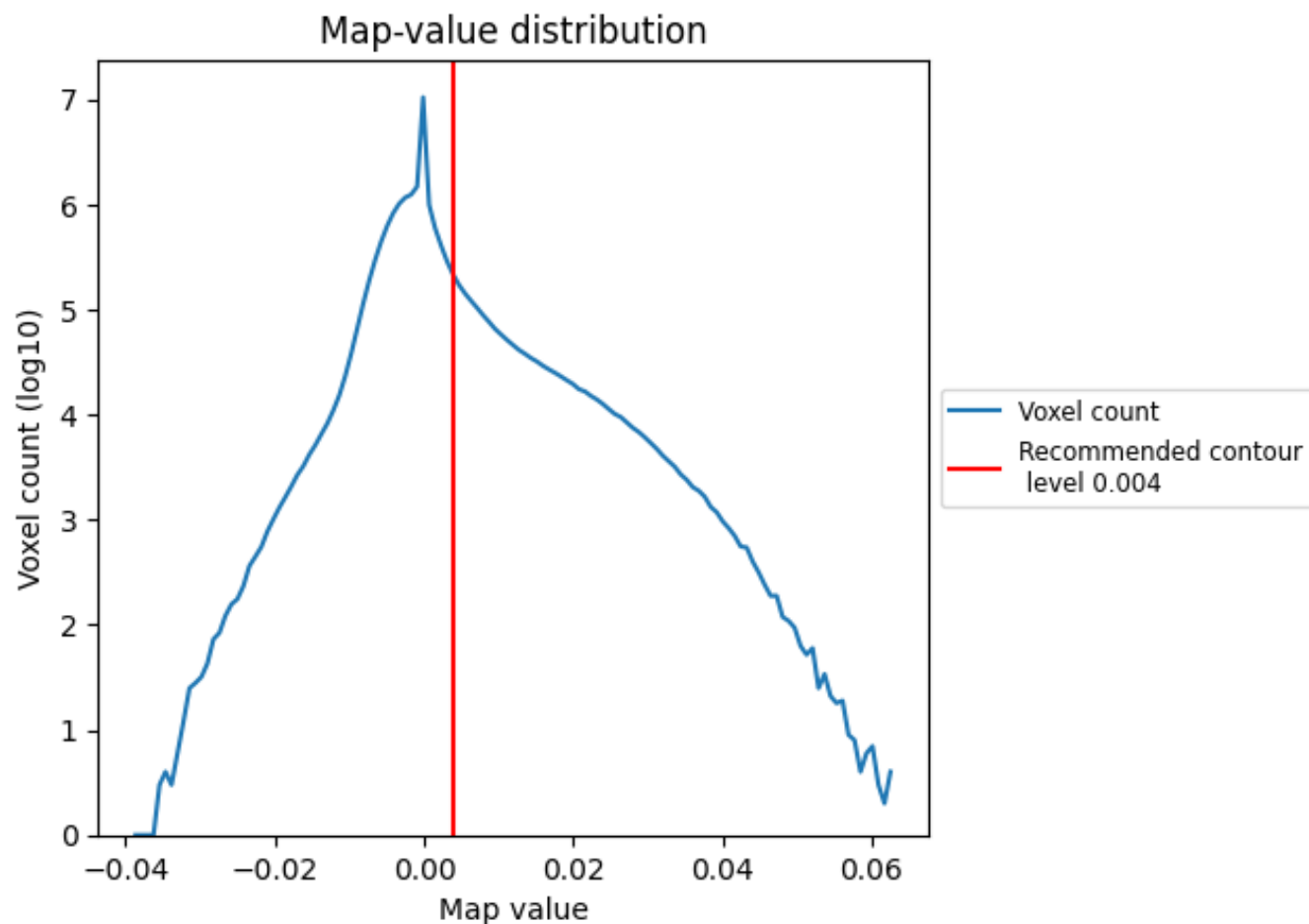
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

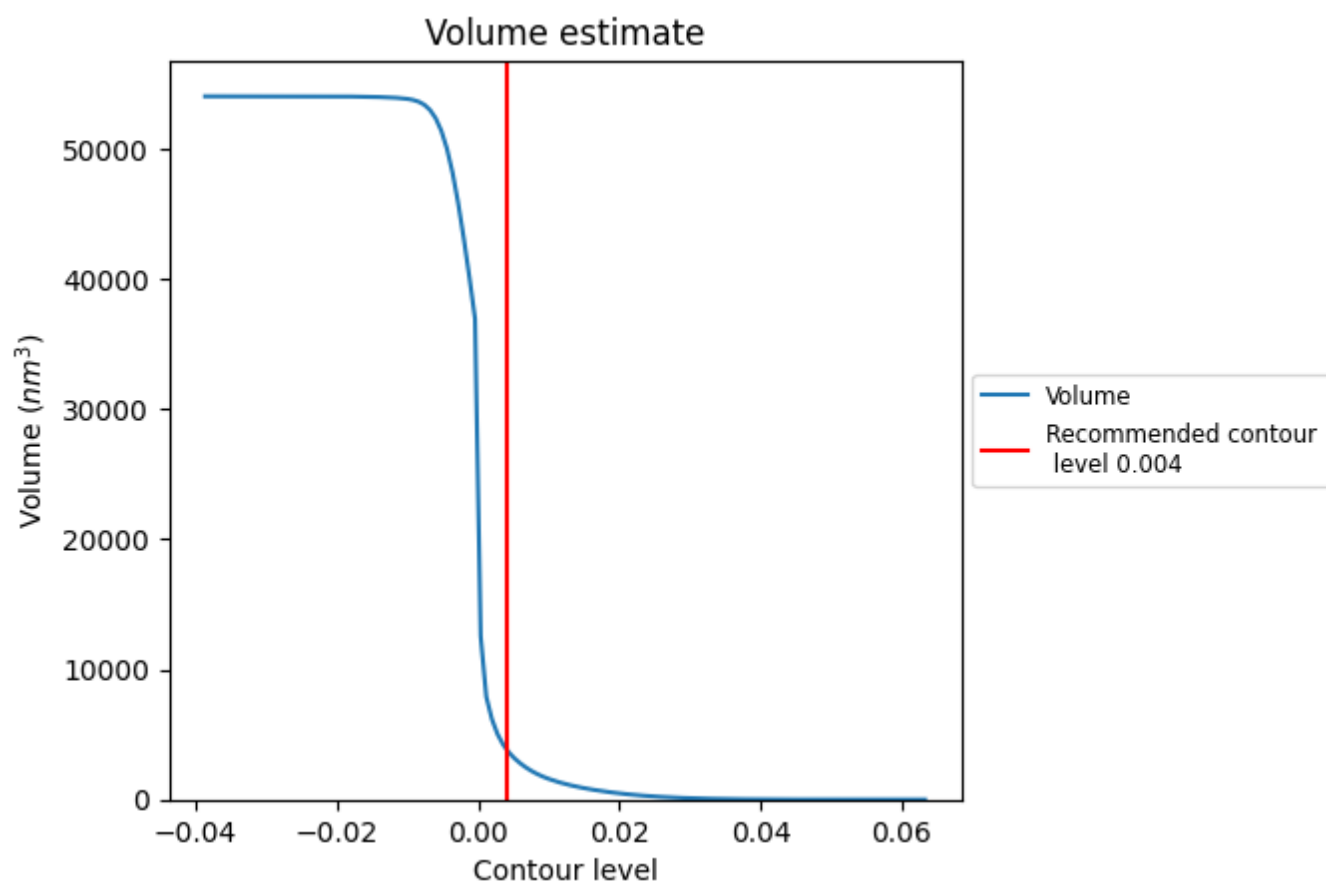
This section contains the results of statistical analysis of the map.

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.

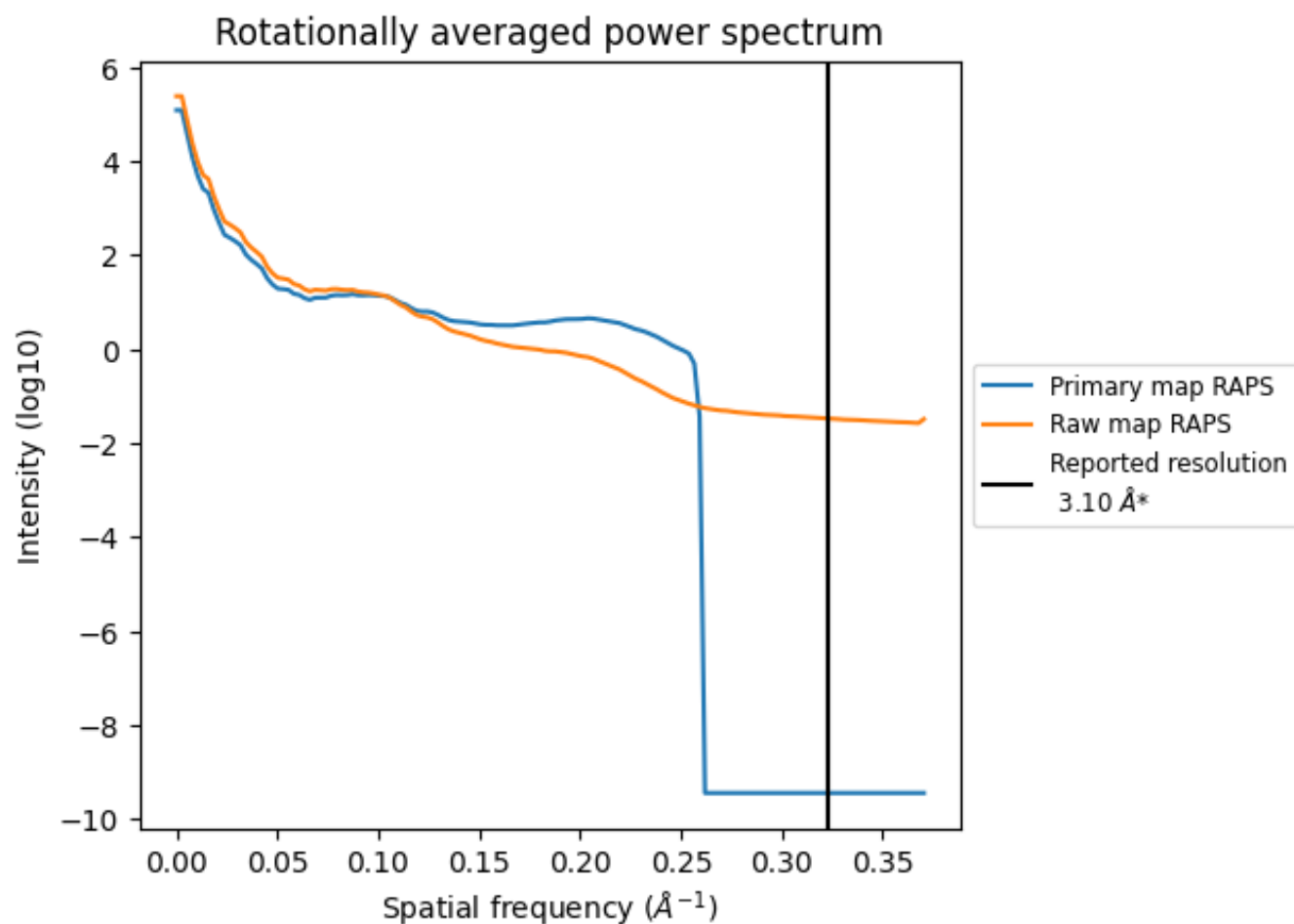
7.2 Volume estimate [i](#)



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 ⓘ

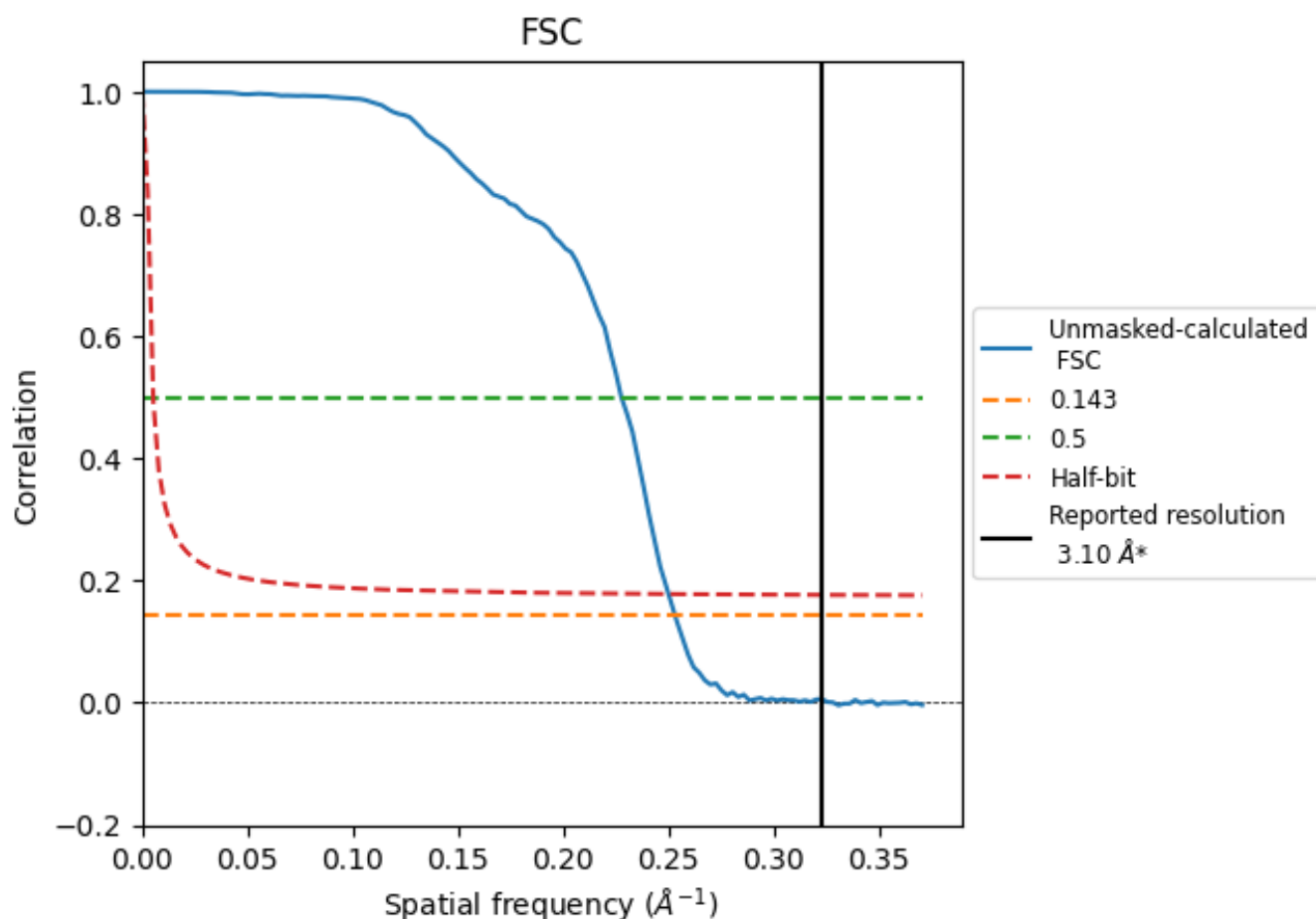


*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

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](#)

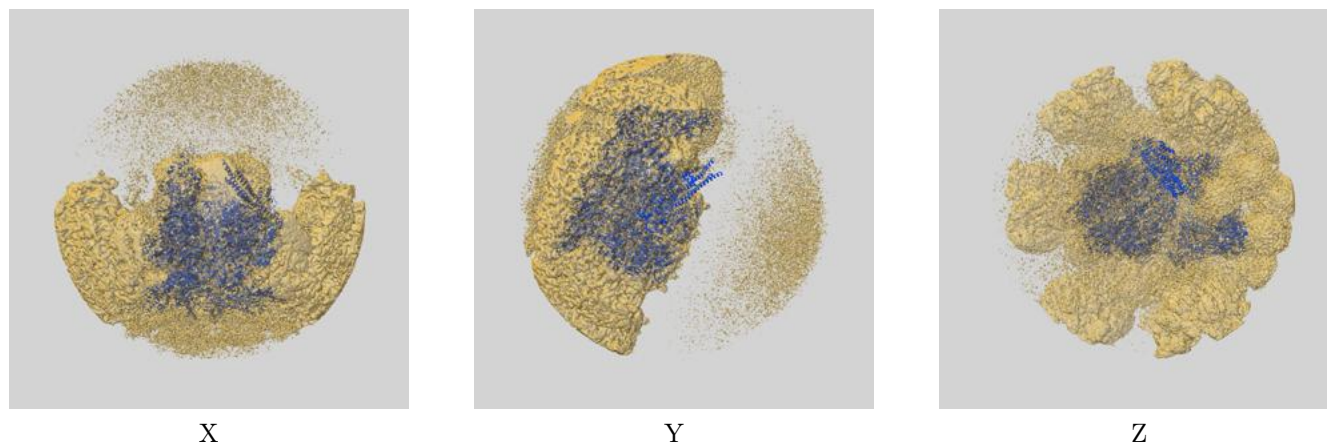
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.95	4.39	4.00

*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](#)

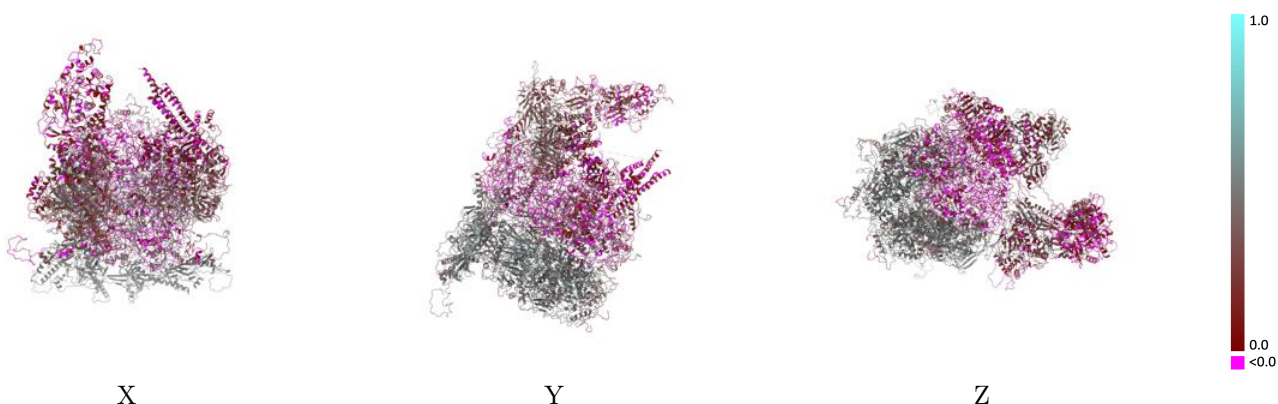
This section contains information regarding the fit between EMDB map EMD-38189 and PDB model 8X9Z. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



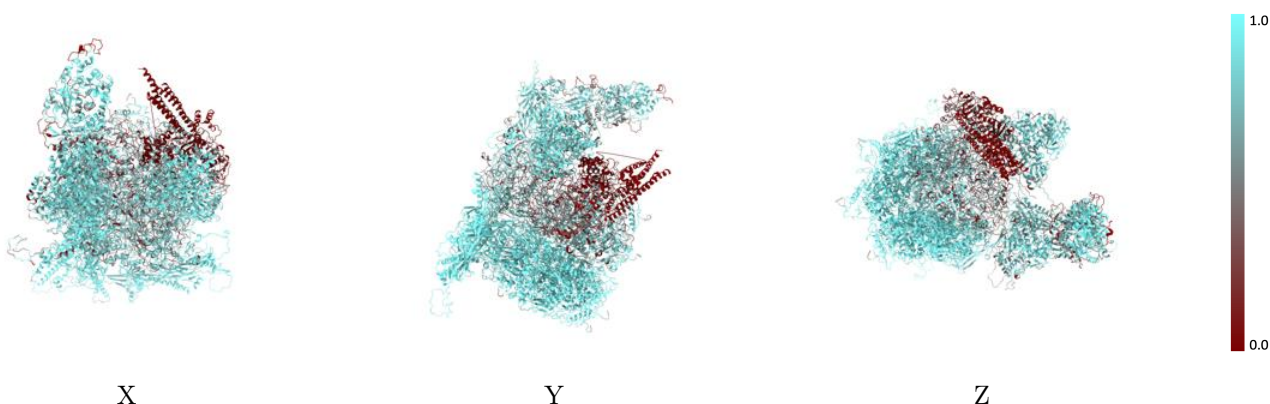
The images above show the 3D surface view of the map at the recommended contour level 0.004 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



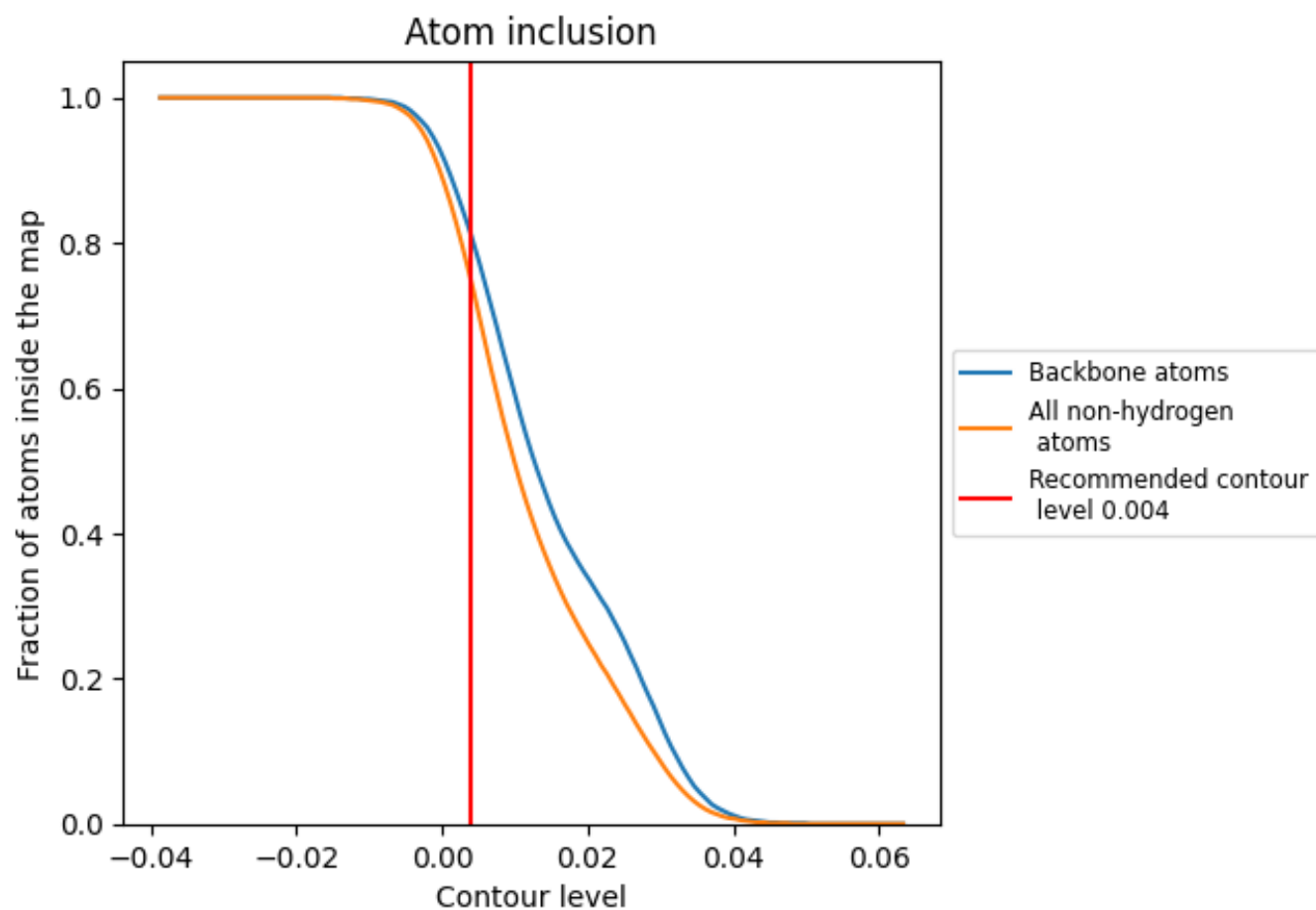
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

