



## wwPDB EM Validation Summary Report ⓘ

Oct 1, 2024 – 11:19 AM JST

PDB ID : 7BR8  
EMDB ID : EMD-30159  
Title : Epstein-Barr virus, C5 penton vertex, CATC absent.  
Authors : Li, Z.; Yu, X.  
Deposited on : 2020-03-26  
Resolution : 3.80 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](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

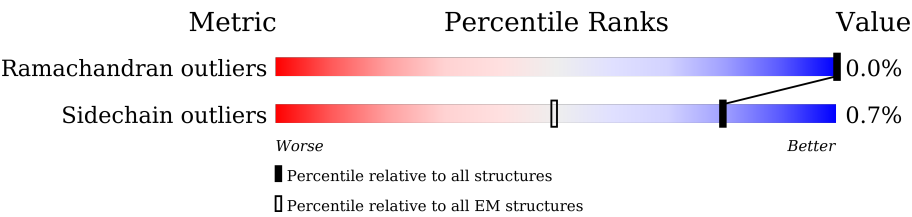
EMDB validation analysis : 0.0.1.dev113  
MolProbity : 4.02b-467  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

# 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 3.80 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)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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  $\geq 3$ , 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	2	176	<div><div>39%</div><div>41%</div><div>58%</div></div>
1	Y	176	<div><div>35%</div><div>41%</div><div>58%</div></div>
1	Z	176	<div><div>37%</div><div>42%</div><div>58%</div></div>
1	m	176	<div><div>38%</div><div>40%</div><div>60%</div></div>
1	y	176	<div><div>36%</div><div>42%</div><div>58%</div></div>
2	S	1381	<div><div>54%</div><div>96%</div><div>9%</div></div>
2	T	1381	<div><div>49%</div><div>95%</div><div>9%</div></div>
2	W	1381	<div><div>43%</div><div>95%</div><div>9%</div></div>
2	l	1381	<div><div>57%</div><div>90%</div><div>9%</div></div>

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Mol	Chain	Length	Quality of chain
2	x	1381	<p>49% 96% .</p>
3	5	364	<p>54% 84% . 15%</p>
3	e	364	<p>35% 87% . 12%</p>
4	6	301	<p>73% 94% . .</p>
4	7	301	<p>77% 92% . 7%</p>
4	f	301	<p>41% 96% .</p>
4	g	301	<p>41% 92% . 7%</p>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 68602 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 Small capsomere-interacting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	m	71	Total	C	N	O	S	0	0
			600	381	111	107	1		
1	Y	74	Total	C	N	O	S	0	0
			621	394	114	112	1		
1	Z	74	Total	C	N	O	S	0	0
			621	394	114	112	1		
1	2	74	Total	C	N	O	S	0	0
			621	394	114	112	1		
1	y	74	Total	C	N	O	S	0	0
			621	394	114	112	1		

- Molecule 2 is a protein called Major capsid protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	S	1333	Total	C	N	O	S	0	0
			10491	6665	1820	1946	60		
2	T	1323	Total	C	N	O	S	0	0
			10398	6600	1808	1929	61		
2	W	1331	Total	C	N	O	S	0	0
			10463	6650	1810	1944	59		
2	x	1325	Total	C	N	O	S	0	0
			10404	6607	1803	1935	59		
2	l	1251	Total	C	N	O	S	0	0
			9883	6283	1717	1824	59		

- Molecule 3 is a protein called Triplex capsid protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	e	319	Total	C	N	O	S	0	0
			2505	1608	444	446	7		
3	5	311	Total	C	N	O	S	0	0
			2446	1568	435	436	7		

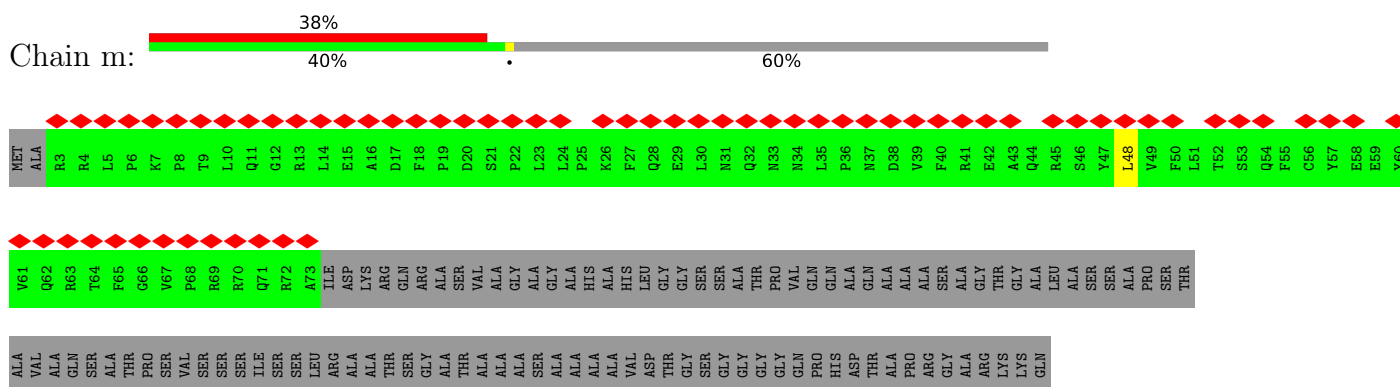
- Molecule 4 is a protein called Triplex capsid protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	f	290	Total	C	N	O	S	0	0
			2279	1466	378	419	16		
4	g	281	Total	C	N	O	S	0	0
			2190	1413	358	401	18		
4	6	289	Total	C	N	O	S	0	0
			2272	1461	377	418	16		
4	7	279	Total	C	N	O	S	0	0
			2187	1406	358	405	18		

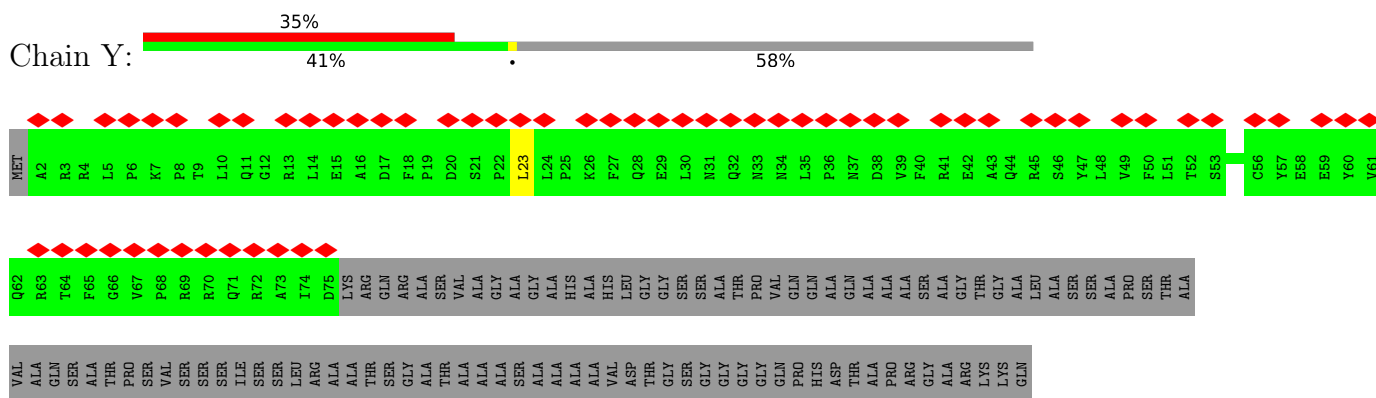
### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

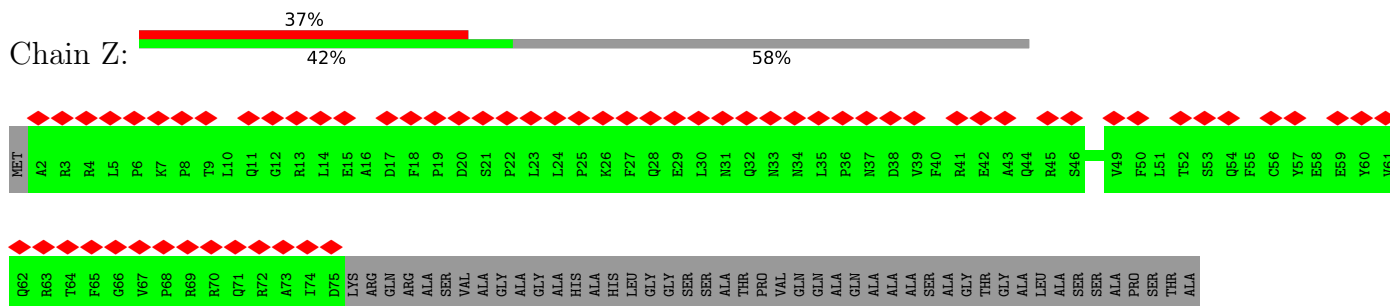
- Molecule 1: Small capsomere-interacting protein



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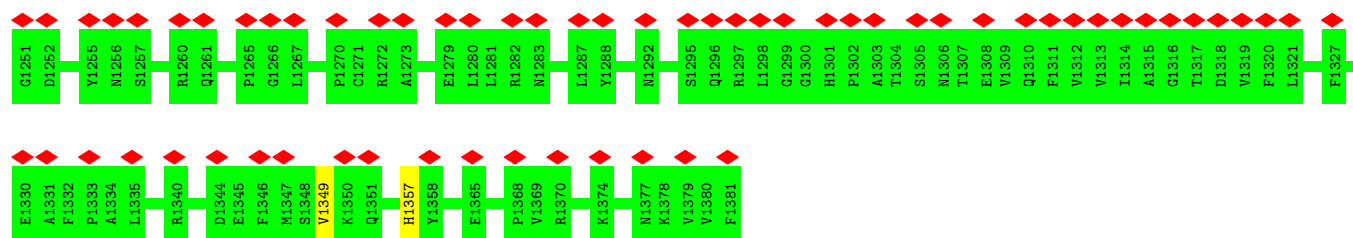
- Molecule 1: Small capsomere-interacting protein



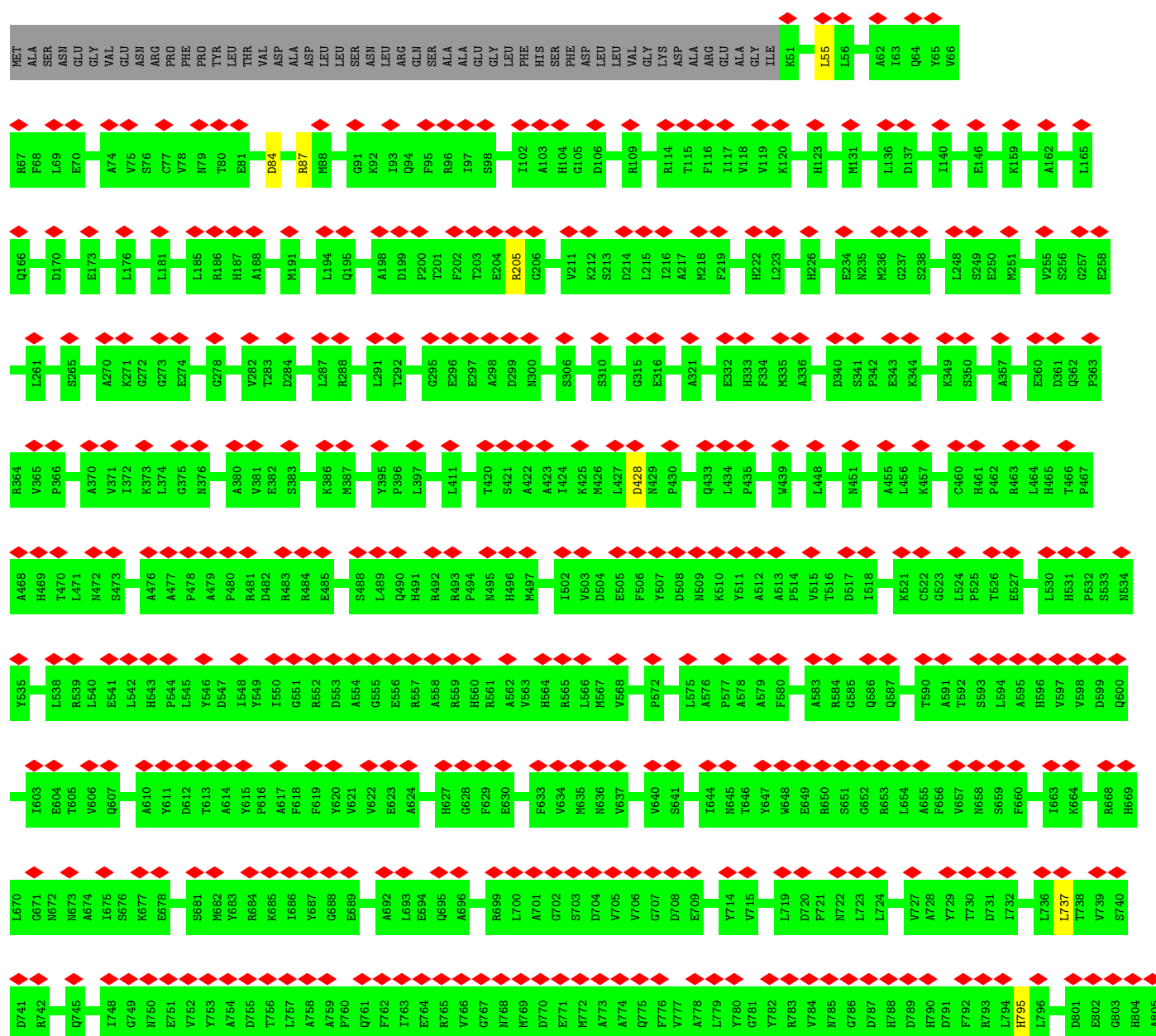


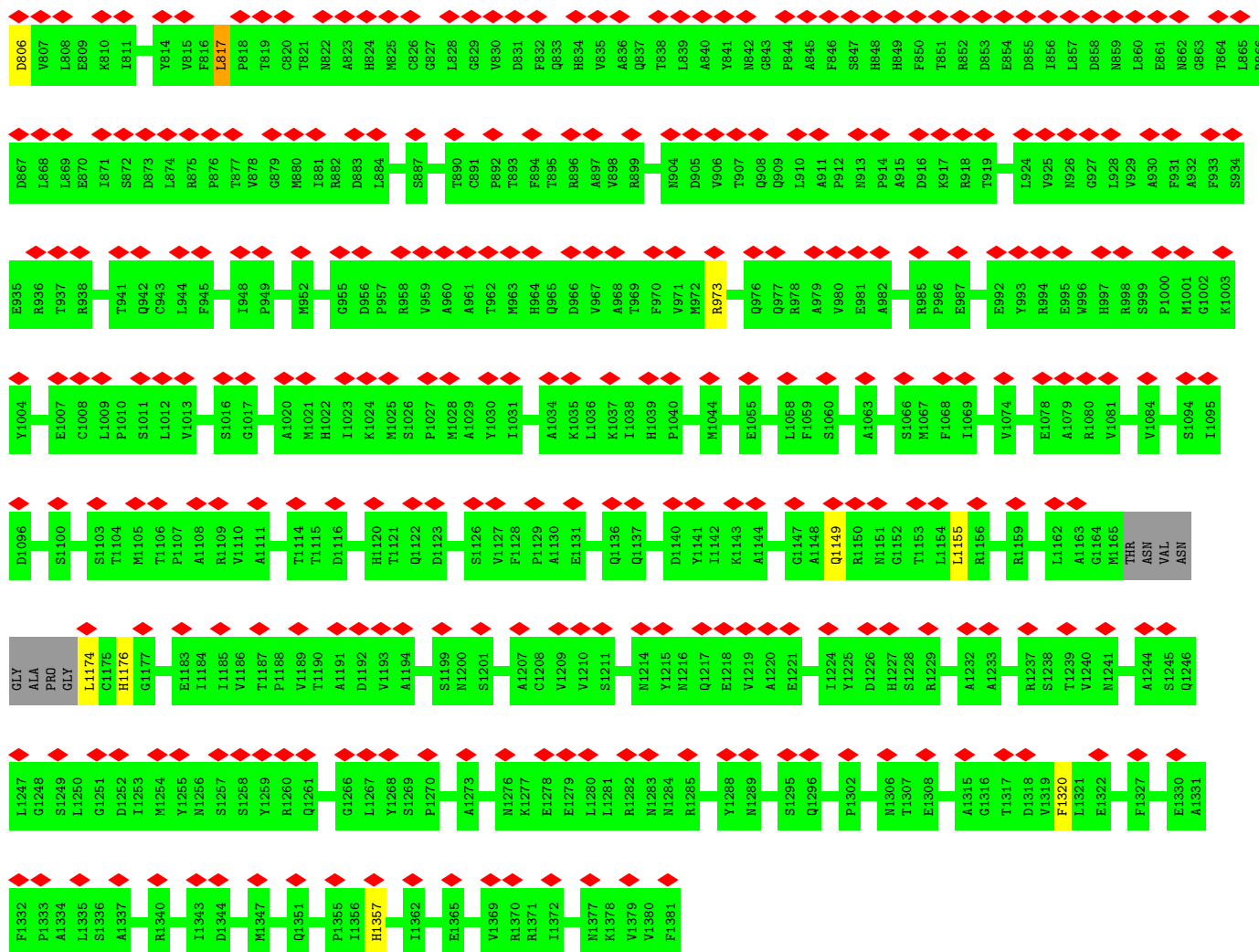
ASP	LEU	PRO	ALA	VAL	ALA	ALA	GLY	GLU	ASP	GLN	PRO	R364	V365	P366	I367	S368	A369	A370	V371	A378	V379	A380	V381	E382	S383	K386	N389	D390	S393	L397	N398	R399	R400	N401	F407	L411	P414	N415	P416	T420	S421	A422	A423	I424	K425	D428	N429	P430										
												L448	M454	A455	L456	K457	V458	L459	C460	H461	P462	R463	L464	H465	T466	H469	T470	L471	M472	S473	A476	A477	P478	A479	P480	R481	D482	R483	R484	T486	Y487	S488	L489	Q490	H491	R492	R493	H496	M497	M498	V499	L500	V501	I502	V503			
D504	E505	F506	Y507	D508	N509	K510	Y511	A512	A513	P514	V515	T516	D517	I518	K521	C522	G523	L524	P525	T526	E527	D528	F529	L530	H531	N534	Y535	L538	R539	L540	E541	L542	H543	Y546	D547	I548	Y549	G551	R552	D553	A554	G555	E556	R557	A558	R559	H560	R561	A562	V563	H564	R565	V568					
L571	P572	T573	P574	L575	A579	F580	Q581	E582	A583	R584	Q585	Q586	Q587	T590	A591	C592	S593	L594	A595	H596	V597	V598	D599	Q600	I603	E604	T605	V606	Q607	D608	T609	A610	Y611	D612	T613	A614	Y615	P616	F618	F619	Y620	V621	V622	E623	A624	M625	I626	H627	G628	F629	E630	E631	K632	F633				
V634	M635	N636	V637	P638	L639	V640	S641	L642	C643	I644	N645	T646	Y647	W648	E649	R650	S651	G652	R653	L654	A655	F656	V657	N658	S659	F660	I663	K664	F665	I666	C667	L668	H669	L670	G671	N672	N673	A674	I675	S676	K677	E678	A679	Y680	S681	M682	Y683	R684	K685	I686	E689	A692	L693	E694	Q695	A696		
L697	M698	R699	L700	A701	G702	S703	D704	V705	G706	G707	D708	E709	G712	Q713	Y714	V715	C716	A717	L718	L719	D720	P721	N722	L723	L724	P725	P726	V727	A728	Y729	T730	D731	I732	F733	T734	H735	L736	L737	T738	V739	S740	D741	R742	A743	P744	G745	I746	I747	I748	G749	N750	E751	V752	Y753	A754	D755	T756	L757
A758	A759	P760	Q761	F762	I763	E764	R765	V766	G767	N768	M769	D770	E771	M772	A773	A774	Q775	F776	V777	A778	L779	Y780	G781	Y782	W784	N785	G786	D787	Y788	D789	H790	D791	F792	R793	L794	H795	L796	G797	P798	Y799	D800	E802	G803	H804	A805	D806	N807	L808	E809	K810	T811	W815	R816	L817	P818	T819		
C820	T821	N822	A823	H824	H825	L828	G829	V830	D831	F832	Q833	H834	V835	A836	Q837	T838	L839	A840	Y841	N842	C843	P844	F846	S847	H848	H849	F850	T851	R852	D853	E854	D855	L856	L857	D858	N859	L860	E861	C863	T864	L865	R866	D867	L868	L869	E870	T871	S872	D873	L874	R875	P876	N880	T881	R882			
D883	L884	S885	A886	S887	F888	M889	T890	C891	P892	R896	A897	V898	R899	V900	S901	V902	D903	N904	D905	V906	T907	L910	A911	P912	N913	D916	K917	R918	T919	E920	Q921	T922	V923	L924	V925	N926	Q927	L928	V929	F931	A932	F933	S934	E935	R936	T937	R938	A939	V940	T941	L942	Q942	F945	H946	A947			
I948	P949	F950	H951	N952	F953	Y954	G955	D956	P957	R958	V959	A960	A961	T962	M963	H964	Q965	D966	V967	A968	V971	M972	R973	N974	P975	Q976	Q977	R978	A979	V980	E981	A982	R985	P986	E987	E992	Y993	R994	E995	W996	H997	R998	S999	P1000	M1001	G1002	K1003	Y1004	E1007	C1008	L1009	P1010	S1011	L1012	V1013			
S1016	G1017	A1020	M1021	I1023	K1024	M1025	S1026	P1027	Y1030	I1031	A1032	Q1033	A1034	K1035	L1036	K1037	I1038	H1039	M1044	T1045	V1046	E1055	M1056	I1057	L1058	F1059	S1060	S1061	R1062	A1063	S1066	M1067	F1068	E1078	A1079	R1080	V1081	V1084	I1095	D1096	T1097	S1100	Y1101	S1102	S1103	T1104	M1105	T1106										
P1107	A1108	R1109	V1110	A1111	D1116	M1117	H1120	T1121	Q1122	D1123	S1126	V1127	A1130	E1131	M1135	Q1136	V1138	M1139	D1140	Y1141	I1142	K1143	G1147	A1148	GLN	ASN	GLY	LEU	LEU	ARG	ASP	PRO	ARG	THR	THR	TVR	LEU	GLY	MET	THR	ASN	VAL	ASN	GLY	ALA	PRO	GLY	L1174	C1175	H1176								
G1177	Q1178	Q1179	A1180	E1183	I1184	I1185	V1186	P1187	P1188	V1189	D1192	V1193	A1194	K1198	S1199	R1203	A1206	V1210	S1211	C1212	E1213	N1214	Y1215	N1216	Q1217	E1218	V1219	A1220	L1223	I1224	Y1225	D1226	S1228	R1229	A1232	A1233	R1237	T1238	V1239	V1240	N1241	A1244	S1245	Q1246	L1247	G1248	S1249	L1250										



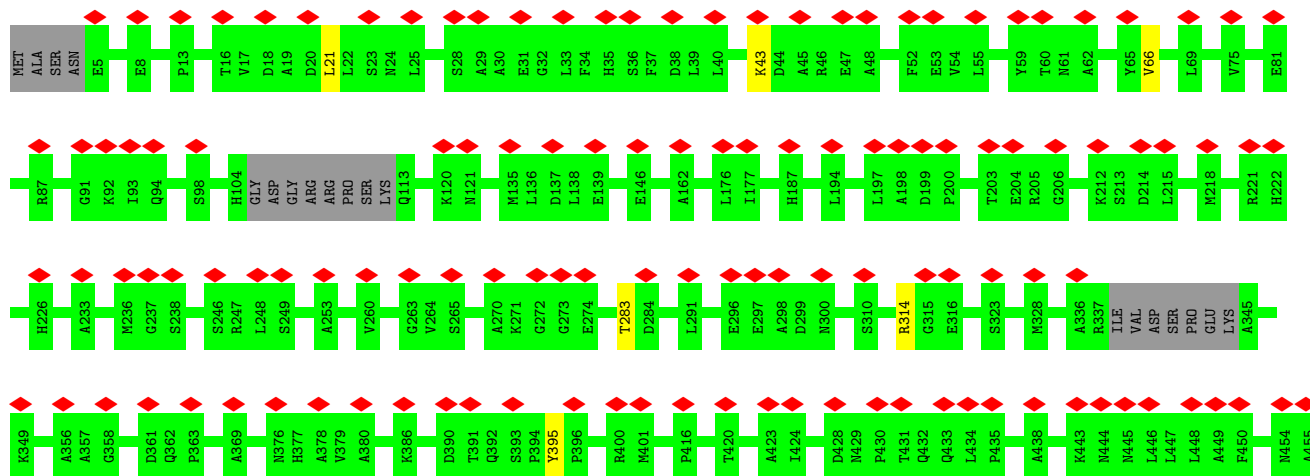
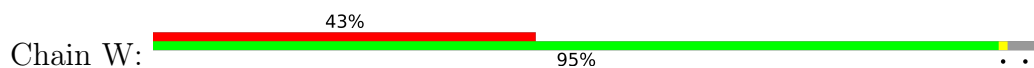


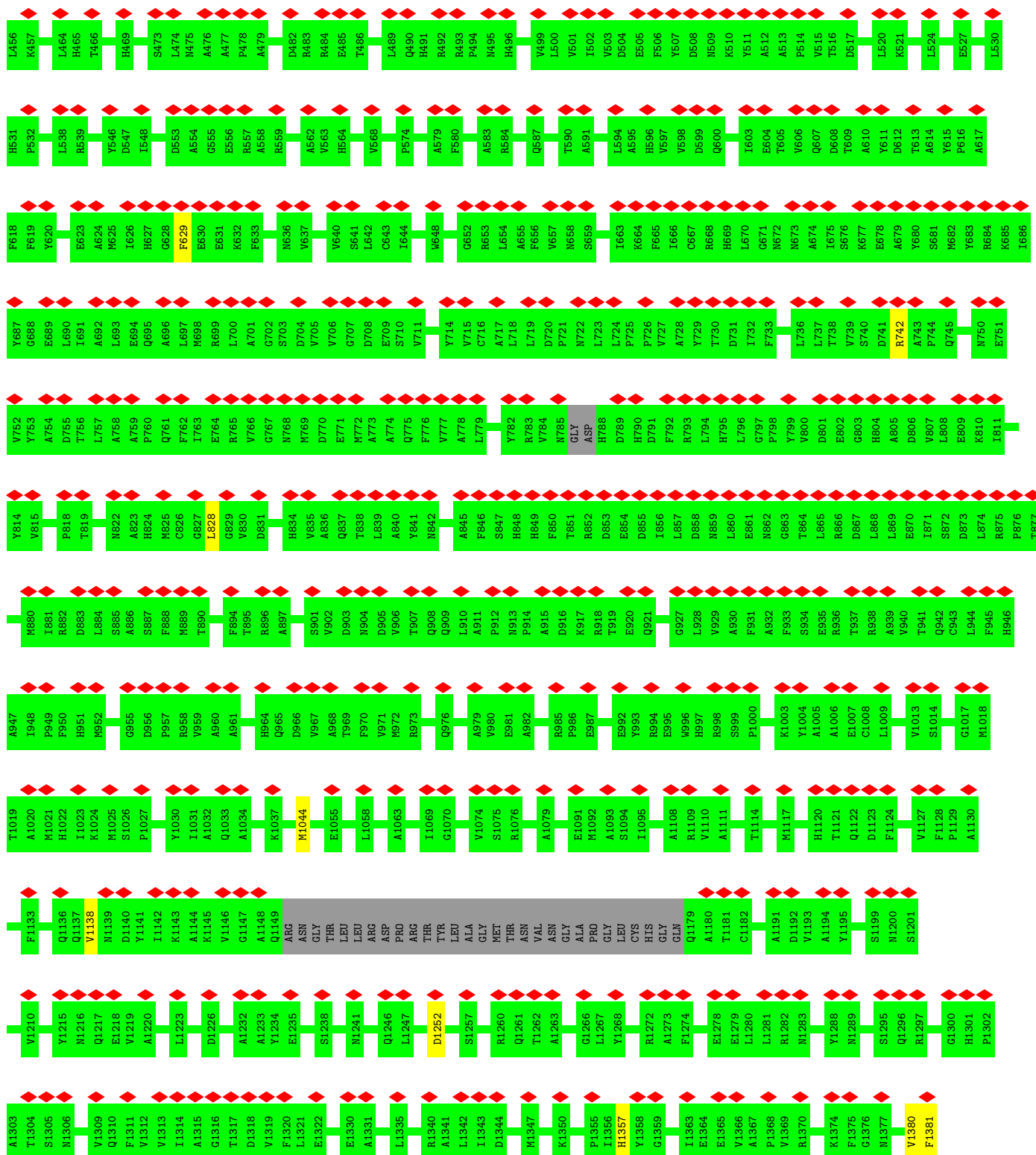
• Molecule 2: Major capsid protein





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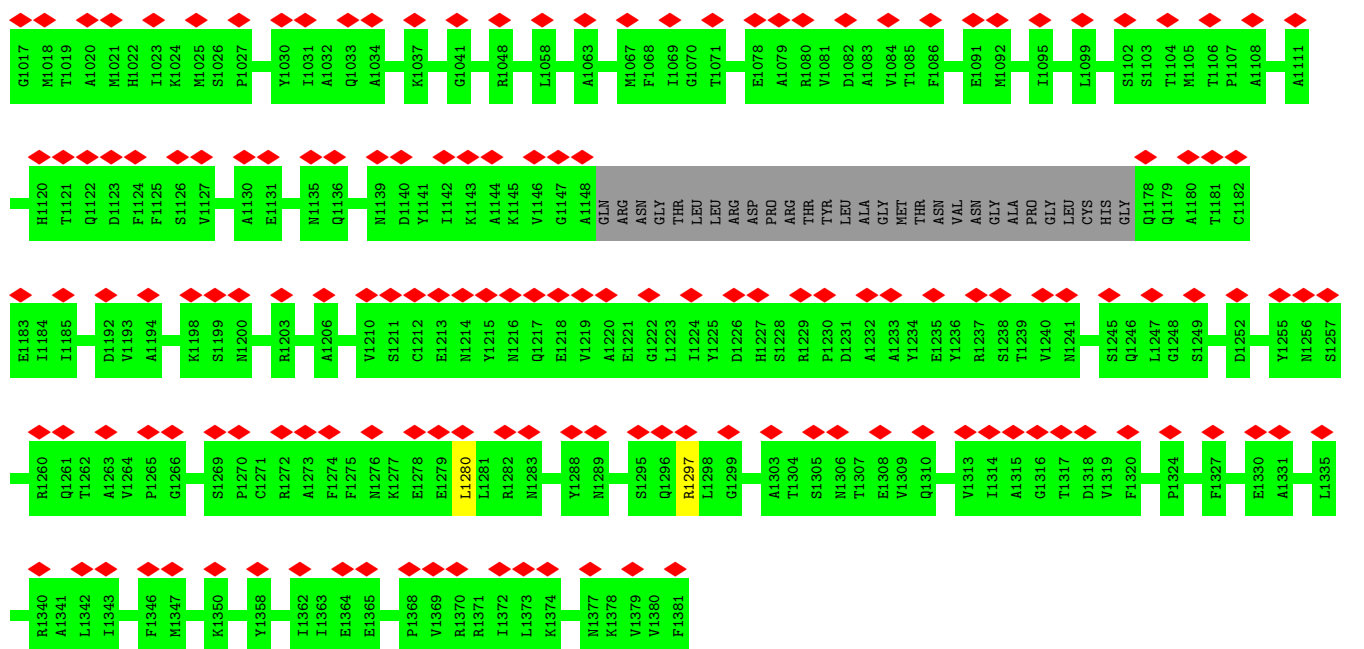




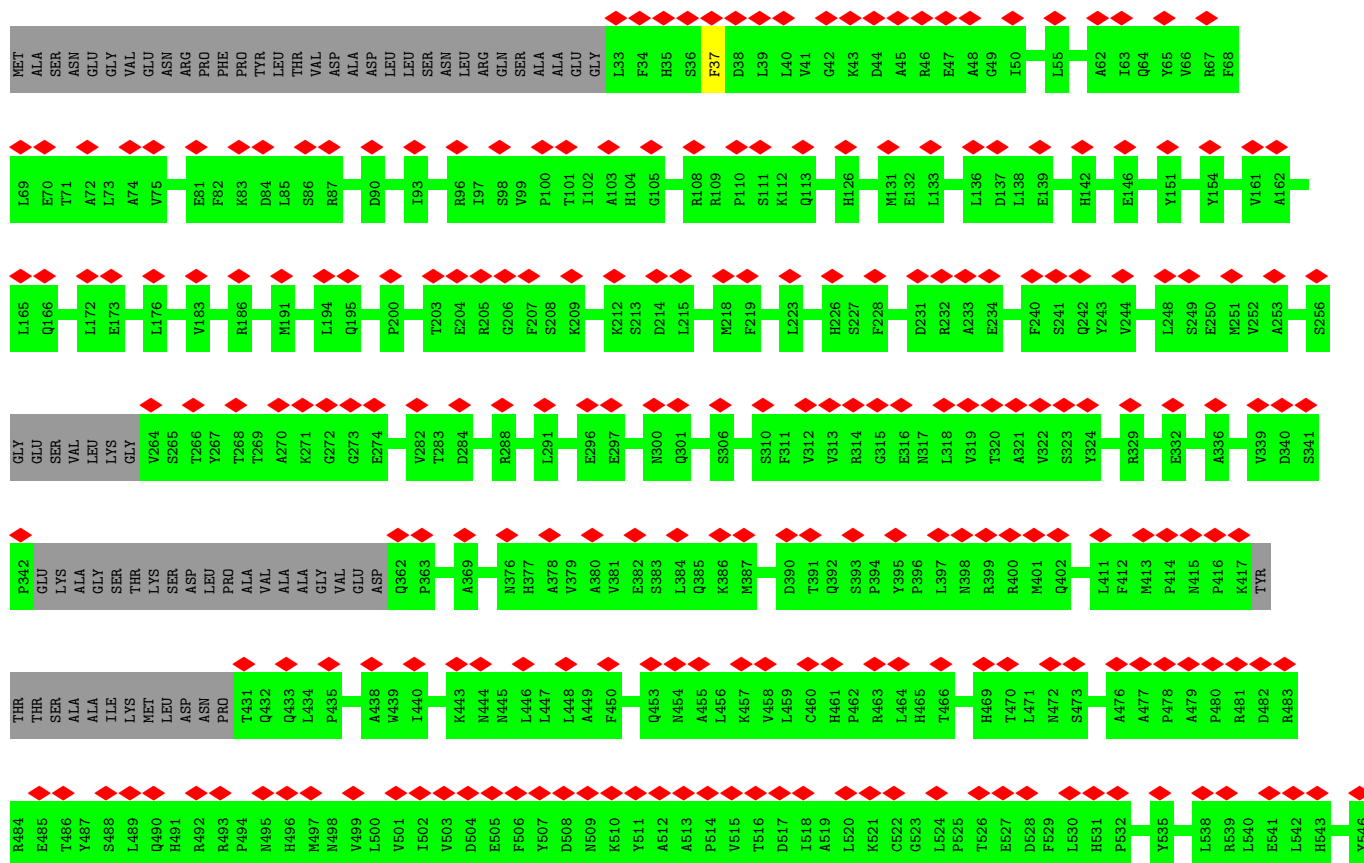
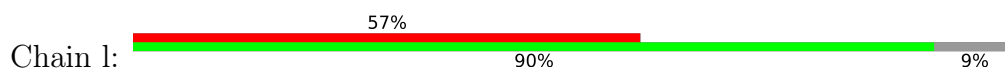
• Molecule 2: Major capsid protein



MET	ALA	SER	ASN	GLU	GLY	VAL	GLU	ASN	ARG	PRO	PHE	PRO	LEU	THR	VAL	ASP	ALA	ASP	LEU	SER	ASN	LEU	ARG	GLN	S28	A29	A30	E31	G32	L33	F34	H35	S36	F37	L40	V41	G42	K43	D44	A45	R46	E47	A48	G49	H61	Y65	L69	A72	V78	N79	T80							
E81		R67		K92	I93	Q94	R95	R96	I97	S98			I102	A103	H104	G105		P110	S111	K112	Q113		I117	K124	I127	S134	D137	L138	H142	P145	E146	T147	P148	Y151	A152	K159	L165	L172	I177	V183	H187	A188	P189	L194	Q195													
A198	S310	F311	V312	V313	R314	M328	E332	H333	A336	R337	D340	E343	K344	A345	G346	S347	T348	K349	S350	A356	A357	G358	V359	E360	D361	Q362	P363	R364	A369	N376	A380	L384	Q385	K386	D390	S393	L397	N398	R399	Y406	L411	F412	P416															
K417	Y418	T419	T420	S421	A422	A423	M426	L427	D428	N429	P430	T431	Q432	Q433	L434	P435	A438	V441	N442	K443	N444	N445	L448	A449	F450	M454	A455	L456	K457	H461	P462	R463	L464	H465	T466	H469	T470	S473	L474	N475	A476	A477	P478	A479	D482	R483	R484	E485	T486	Y487								
S488	L489	R492	R493	P494	M495	H496	V499	L500	V501	I502	V503	E505	F506	D508	N509	K510	V511	A512	A513	P514	V515	T516	D517	I518	A519	L520	K521	L524	E527	D528	F529	L530	Y535	L538	R539	L540	E541	L542	Y546	D547	I548	V549	I550	G551	R552	D553	A554	G555	E556	R557								
A558	R559	A562	V563	H564	V568	G569	P572	I573	P574	L575	A579	F580	A583	R584	G585	Q586	Q587	F588	E589	T590	A591	T592	S593	L594	A595	H596	V597	D599	Q600	L603	E604	Q607	D608	T609	A610	T613	A614	V615	P616	A617	F618	F619	E623	A624	N625	L626	H627	G628	F629									
E630	E631	R632	F633	M636	V637	P638	L639	V640	S641	L642	C643	I644	N645	M648	E649	R650	G651	R652	L654	A655	F656	V657	N658	S659	I663	K664	F665	L666	C667	R668	H669	L670	G671	N672	N673	A674	L675	K677	E678	A679	V680	S681	H682	V683	R684	K685	L686	E689	L690	I691	A692	L693						
A696	L697	M698	R699	L700	G702	S703	D704	V705	V706	G707	D708	E709	S710	V711	G712	Q713	V714	V715	C716	A717	L718	L719	D720	P721	N722	R723	L724	P725	F726	G727	F728	H729	T730	D731	I732	F733	T734	H735	L736	L737	T738	V739	S740	D741	R742	A743	P744	Q745	L746	I747	L748	G749	N750	E751	V752	Y753	A754	D755
T756	L757	A758	A759	P760	Q761	F762	I763	E764	R765	V766	G767	N768	M769	D770	E771	M772	Q775	F776	V777	A778	L779	Y780	G781	P782	R783	V784	N785	G786	D787	H788	D789	H790	D791	F792	R793	L794	H795	L796	G797	V800	D801	E802	C803	H804	A805	D806	V807	L808	E809	K810	I811	R812	Y813	Y814	V815	F816	L817	
P818	T819	C820	T821	N822	A823	H824	C826	G827	L828	G829	V830	D831	H834	V835	A836	Q837	T838	L839	D840	Y841	N842	G843	P844	A845	F846	S847	H848	H849	F850	T851	R852	D853	E854	D855	L856	L857	N858	H859	L860	E861	N862	G863	T864	L865	R866	D867	L868	L869	E870	I871	S872	D873	L874	R875	P876	T877		
M880	T881	R882	D883	L884	S885	A886	S887	F888	F894	T895	R896	A897	S901	V902	D903	N904	D905	V906	T907	Q908	Q909	L910	A911	P912	Q913	P914	A915	D916	K917	R918	T919	E920	D921	T922	V923	L924	G927	A930	F931	A932	F933	S934	E935	R936	T937	Y938	T941	Q942	C943	L944	F945	H946	A947	I948				
P949	F950	H951	M952	F953	Y954	G955	D956	P957	R958	A961	T962	M963	H964	Q965	D966	V967	A968	T969	F970	V971	N972	R973	N974	P975	Q976	Q977	R978	A979	E981	A982	R985	P986	E987	E992	E995	H996	H997	R998	S999	P1000	K1003	Y1004	E1007	C1008	L1009	P1010	S1011	L1012	V1013	S1014	I1015	S1016						




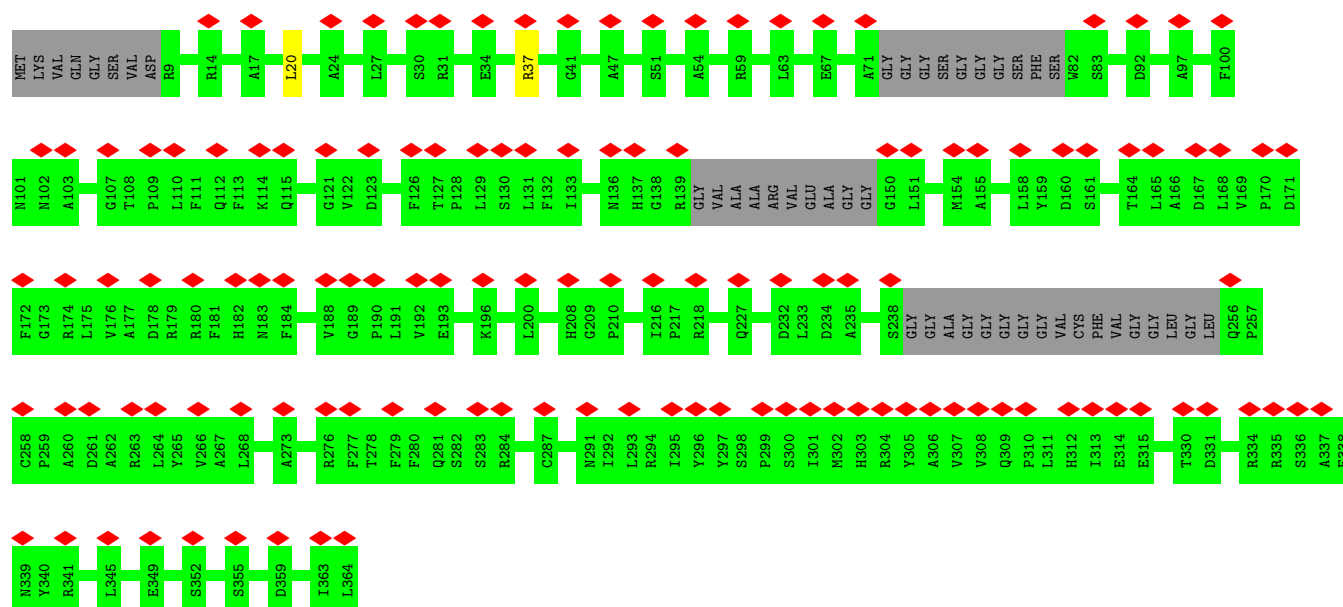
• Molecule 2: Major capsid protein




P1324	S1257	I1185	D1123	D1050	V980	E920	D858	L796	L736	I675	Y615	D547
F1327	S1258	T1187	S1126	E1051	E981	Q921	N859	G797	L737	S676	P616	I548
E1330	S1259	P1188	V1127	I1052	A982	T922	L860	P798	T738	K677	F618	I550
A1331	R1260	F1128	F1128	S1054	R985	L924	E861	V799	V739	E878	F619	G551
A1334	Q1261	P1129	P1129	E1055	P986	V925	G863	D801	S740	A679	Y620	R552
L1335	A1263	D1192	A1130	L1056	E987	N926	T864	E802	R742	Y680	V621	D553
	V1264	V1193	E1131	I1057	Q988	G927	L865	G803	R743	S681	V622	A554
	P1265	A1194	A1132	L1058	L989	L928	R866	H804	F744	M682	E923	G555
	G1266	Y1195	F1133	A1063	F990	V929	D867	A805	Q745	Y683	A624	E556
S1339	L1267	G1134	A991	A1063	A991	A930	L868	D806	I746	K685	M625	R557
R1340	Y1268	N1135	E992	S1066	E992	F931	L869	V807	I747	I686	I626	A558
A1341	S1269	Q1136	Y993	M1067	R994	A932	E870	L808	I748	Y687	G628	R559
L1342	P1270	V1137	R993	F1068	E995	F933	I871	E809	G749	G688	G629	H560
I1343	C1271	V1138	E995	I1069	W996	S934	S872	K810	N750	E689	E630	R561
D1344	R1272	R1203	N1139	I1069	H997	E935	D873	I811	E751	L690	E562	A562
E1345	A1273		D1140			R936	D873			V563	E631	R563
F1346		V1210	Y1141	V1074	R998	T937	R875	Y814	V752	I691	K632	H564
M1347	E1278	S1211	I1142	R1075	S999	R938	R875	W815	A754	A692	F633	R565
S1348	E1279	C1212	K1143	R1077	P1000	A939	P876		D755	L693	V634	L566
VAL		E1213	A1144	E1078	M1001	V940	T877	P818	T756	E694	M635	M567
LYS	R1282	M1214	A1144	A1079	G1002	T941	V878	T819	L757	A696	N636	V568
GLN	N1283	Y1215	K1145		K1003	Q942	G879	C820			V637	
THR		M1216				Q942	M880	T821	A758	L697	P638	F574
HIS	Q1217	M1216			Y1004	C943	L881	N822	F760	L697	L639	L575
ALA	E1218	V1219			A1005	L944	R882	A823	Q761	L700	V640	A579
PRO	V1219	A1220			A1006	F945	D883	H824	F762	A701	L642	F580
ILE	A1220				E1007	H946	L884	M825	I763	G702	C643	
					C1008	A947	L884	M825	I763	S703	I644	A583
H1357					L1009	I948	S885	C826	E764	D704	N645	R584
	E1293	L1223			P1010	I948	S887	G827	R765	L828	G585	H584
H1360	Y1294	I1224			S1011	P949	S887	L828	V766	V705	T646	Q586
Y1361	S1295	Y1225			V1011	F950	F888	G829	G767	V706	Y647	Q587
I1362	Q1296	D1226			L1012	H951	M889	V830	N768	G707	W648	
	R1297				V1013	M952	T890	D831	M769	D708	E649	T590
E1365	L1298				S1014	F953	T890	F832	E710	E709	R650	A591
	GLY	R1229			I1015	Y954	C891	Q833	D770	S710	S651	T592
P1368	GLY	P1230			S1016	G1017	P892	Q833	E771	S710	G652	S593
V1369	HIS	D1231			D1096	G1017	T893	H834	M772	V711	R653	L594
R1370	R1370	A1232			T1097	M1018	D956	V835	A773		L654	A595
R1371	ALA	A1233			G1098	T1019	P957	A836			A655	H596
I1372	THR	Y1234			L1099	A1020	R958	Q837	Q775	C716	F656	V597
L1373	THR	E1235				M1021	R958	T838	F776	A717	N657	V597
K1374	ASN					H1022	A960	L839	V777	L718	M658	D599
F1375	THR	S1238				I1023	A960	A840	A778	L719	S659	Q600
GLY	THR	T1239				I1023	A961	Y841	L779	L719	F660	A601
ASN	GLU	V1240				M1025	N963	N842	Y780	D720	F660	V602
VAL	VAL	M1241				S1026	H964	G843	G781	P721	S661	I603
VAL	PHE					P1027	D903	P844	T782	N722	M662	I603
VAL	ILE	A1244					N904	F846	R783	L723	I663	E604
PHE	ALA	S1245					D905	S847	V784	P725	F665	T605
	GLY	Q1246					V906	H848	N785	L724	F665	V606
LYS	THR	L1247					T907	H849	G786	F726	I666	Q607
VAL	THR	G1248					Q908	F850	D787	V727	C667	D608
VAL	ASP	S1249					Q909	T851	H788	A728	R668	T609
VAL	VAL	L1250					L910	R852	D789	Y729	H669	A610
	VAL	A1180					A911	D853	H790	T730	Y611	D612
	VAL	T1181					P912	R913	D791	I732	T613	A614
	VAL	G1251					N913	P914	F792	F733	N672	
	VAL	D1252					P912	R914	D791	F733	N672	
	VAL	I1253					N913	R914	D791	F733	N672	
	VAL	M1254					P912	R914	D791	F733	N672	
	VAL	Y1255					N913	R914	D791	F733	N672	
	VAL	M1256					N913	R914	D791	F733	N672	
	VAL						N913	R914	D791	F733	N672	
	VAL						N913	R914	D791	F733	N672	
	VAL						N913	R914	D791	F733	N672	
	VAL						N913	R914	D791	F733	N672	
	VAL						N913	R914	D791	F733	N672	
	VAL						N913	R914	D791	F733	N672	
	VAL						N913	R914	D791	F733	N672	
	VAL						N913	R914	D791	F733	N672	
	VAL						N913	R914	D791	F733	N672	
	VAL						N913	R914	D791	F733	N672	
	VAL						N913	R914	D791	F733	N672	
	VAL						N913	R914	D791	F733	N672	
	VAL						N913	R914	D791	F733	N672	
	VAL						N913	R914	D791	F733	N672	
	VAL						N913	R914	D791	F733	N672	
	VAL						N913	R914	D791	F733	N672	
	VAL						N913	R914	D791	F733	N672	
	VAL						N913	R914	D791	F733	N672	
	VAL						N913	R914	D791	F733	N672	
	VAL						N913	R914	D791	F733	N672	
	VAL						N913	R914	D791	F733	N672	
	VAL						N913	R914	D791	F733	N672	
	VAL						N913	R914	D791	F733	N672	
	VAL						N913	R914	D791	F733	N672	
	VAL						N913	R914	D791	F733	N672	
	VAL						N913	R914	D791	F733	N672	
	VAL						N913	R914	D791	F733	N672	
	VAL						N913	R914	D791	F733	N672	
	VAL						N913	R914	D791	F733	N672	
	VAL						N913	R914	D791	F733	N672	
	VAL						N913	R914	D791	F733	N672	
	VAL						N913	R914	D791	F733	N672	
	VAL						N913	R914	D791	F733	N672	
	VAL						N913	R914	D791	F733	N672	
	VAL						N913	R914	D791	F733	N672	
	VAL						N913	R914	D791	F733	N672	
	VAL						N913	R914	D791	F733	N672	
	VAL						N913	R914	D791	F733	N672	
	VAL						N913					

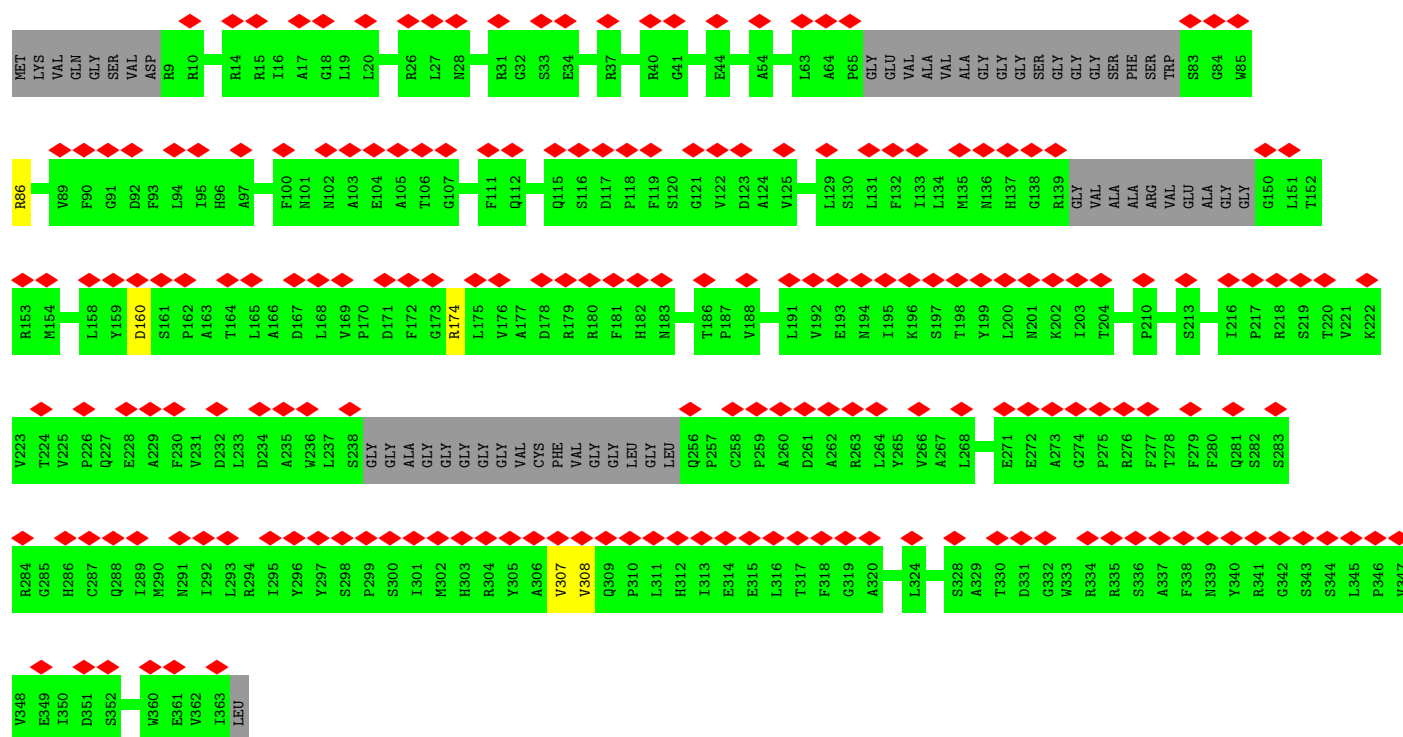
- Molecule 3: Triplex capsid protein 1

Chain e: 

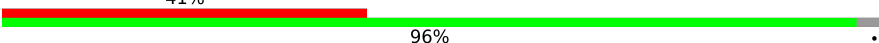


• Molecule 3: Triplex capsid protein 1

Chain 5: 

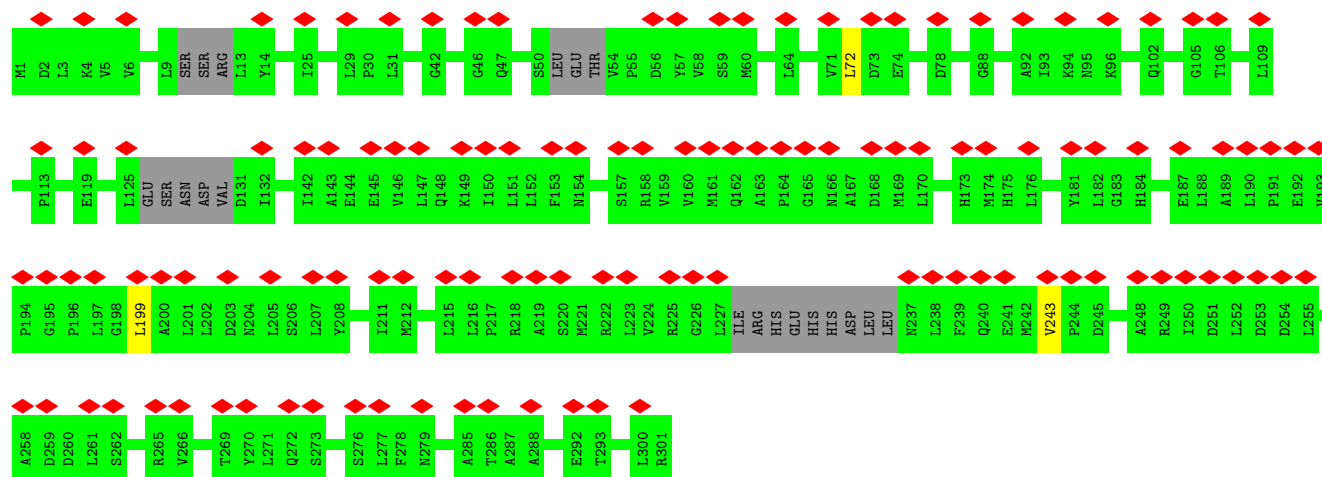
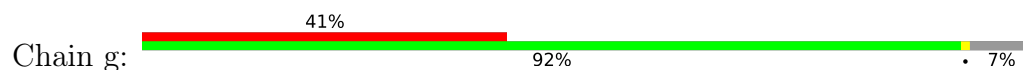


• Molecule 4: Triplex capsid protein 2

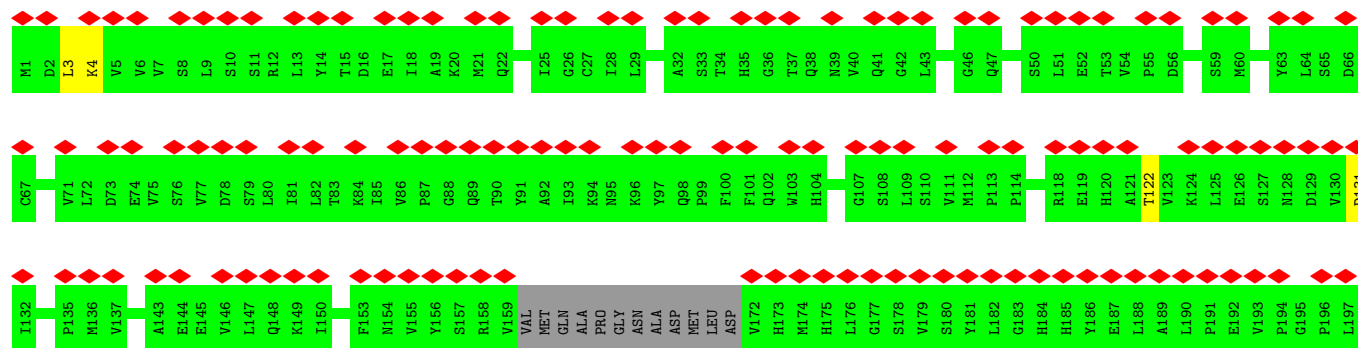
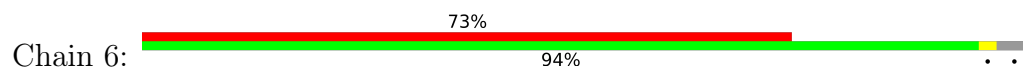
Chain f: 



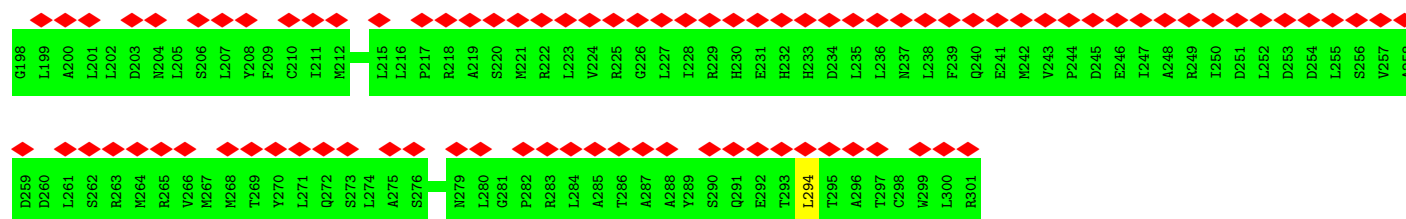
• Molecule 4: Triplex capsid protein 2



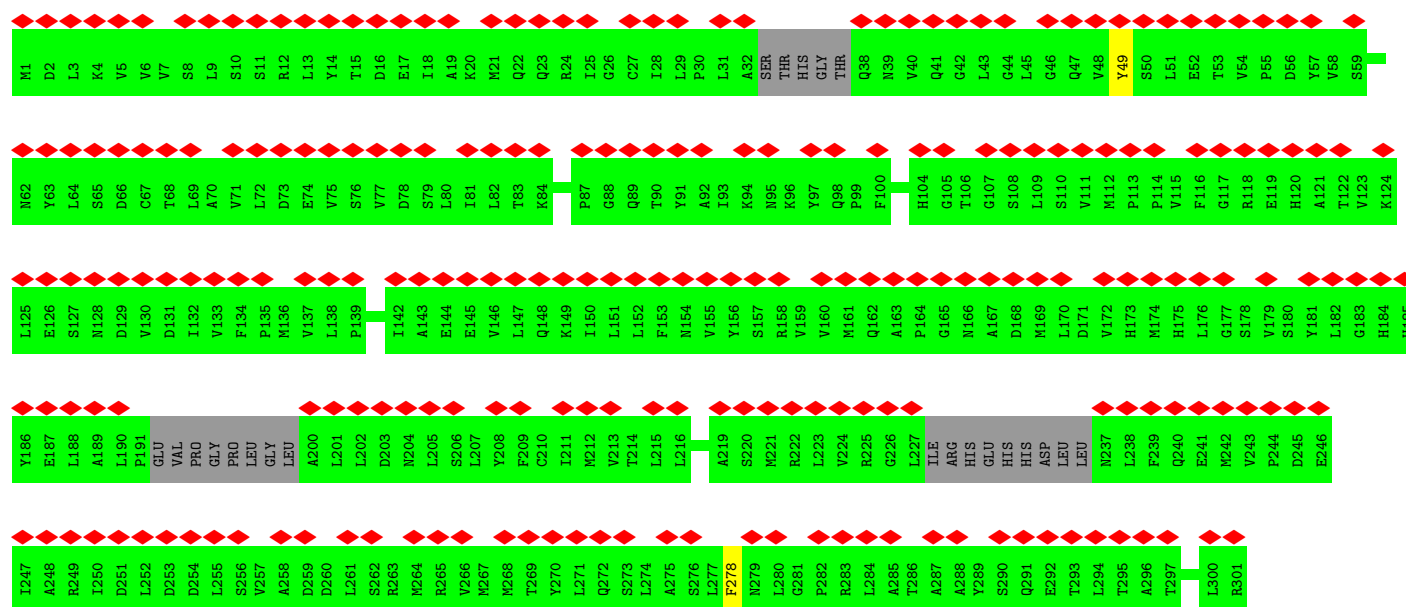
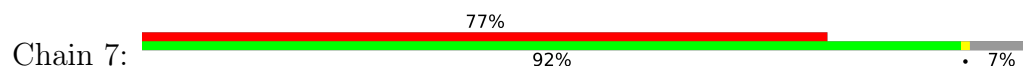
• Molecule 4: Triplex capsid protein 2







• Molecule 4: Triplex capsid protein 2



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C5	Depositor
Number of particles used	137356	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	48	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.064	Depositor
Minimum map value	-0.033	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.011	Depositor
Map size (Å)	392.99997, 392.99997, 392.99997	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.31, 1.31, 1.31	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	2	0.30	0/636	0.61	0/861
1	Y	0.28	0/636	0.52	1/861 (0.1%)
1	Z	0.29	0/636	0.49	0/861
1	m	0.31	0/615	0.57	1/832 (0.1%)
1	y	0.31	0/636	0.54	0/861
2	S	0.37	0/10737	0.53	0/14589
2	T	0.37	0/10642	0.56	4/14463 (0.0%)
2	W	0.34	0/10706	0.54	2/14549 (0.0%)
2	l	0.32	0/10114	0.52	0/13734
2	x	0.36	0/10648	0.54	1/14471 (0.0%)
3	5	0.29	0/2511	0.52	0/3418
3	e	0.33	0/2572	0.54	1/3503 (0.0%)
4	6	0.30	0/2320	0.59	2/3159 (0.1%)
4	7	0.29	0/2228	0.57	0/3029
4	f	0.31	0/2327	0.56	1/3169 (0.0%)
4	g	0.31	0/2233	0.59	2/3037 (0.1%)
All	All	0.34	0/70197	0.54	15/95397 (0.0%)

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
2	S	0	1
2	T	0	2
2	W	0	1
3	5	0	1
4	6	0	1
4	7	0	1
All	All	0	7

There are no bond length outliers.

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	T	817	LEU	CA-CB-CG	8.76	135.45	115.30
4	6	3	LEU	CA-CB-CG	6.49	130.22	115.30
4	g	72	LEU	CA-CB-CG	6.07	129.26	115.30
4	f	129	ASP	CB-CG-OD1	5.98	123.69	118.30
4	g	199	LEU	CA-CB-CG	5.86	128.78	115.30

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	5	307	VAL	Peptide
2	S	1357	HIS	Peptide
2	T	1357	HIS	Peptide
2	T	817	LEU	Peptide
2	W	1357	HIS	Peptide

## 5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

## 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	2	72/176 (41%)	64 (89%)	8 (11%)	0	100	100
1	Y	72/176 (41%)	65 (90%)	7 (10%)	0	100	100
1	Z	72/176 (41%)	67 (93%)	5 (7%)	0	100	100
1	m	69/176 (39%)	64 (93%)	5 (7%)	0	100	100
1	y	72/176 (41%)	65 (90%)	7 (10%)	0	100	100
2	S	1327/1381 (96%)	1246 (94%)	80 (6%)	1 (0%)	48	79

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	T	1319/1381 (96%)	1222 (93%)	97 (7%)	0	100	100
2	W	1321/1381 (96%)	1243 (94%)	78 (6%)	0	100	100
2	l	1237/1381 (90%)	1164 (94%)	73 (6%)	0	100	100
2	x	1321/1381 (96%)	1243 (94%)	78 (6%)	0	100	100
3	5	303/364 (83%)	285 (94%)	17 (6%)	1 (0%)	37	69
3	e	311/364 (85%)	300 (96%)	11 (4%)	0	100	100
4	6	285/301 (95%)	269 (94%)	16 (6%)	0	100	100
4	7	271/301 (90%)	255 (94%)	16 (6%)	0	100	100
4	f	286/301 (95%)	276 (96%)	10 (4%)	0	100	100
4	g	271/301 (90%)	261 (96%)	10 (4%)	0	100	100
All	All	8609/9717 (89%)	8089 (94%)	518 (6%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	S	1176	HIS
3	5	308	VAL

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	2	68/128 (53%)	66 (97%)	2 (3%)	37	58
1	Y	68/128 (53%)	68 (100%)	0	100	100
1	Z	68/128 (53%)	68 (100%)	0	100	100
1	m	66/128 (52%)	66 (100%)	0	100	100
1	y	68/128 (53%)	68 (100%)	0	100	100
2	S	1136/1171 (97%)	1125 (99%)	11 (1%)	73	80
2	T	1126/1171 (96%)	1115 (99%)	11 (1%)	73	80
2	W	1132/1171 (97%)	1120 (99%)	12 (1%)	70	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	l	1070/1171 (91%)	1068 (100%)	2 (0%)	92	94
2	x	1125/1171 (96%)	1120 (100%)	5 (0%)	89	91
3	5	263/289 (91%)	260 (99%)	3 (1%)	70	79
3	e	268/289 (93%)	267 (100%)	1 (0%)	89	91
4	6	258/267 (97%)	256 (99%)	2 (1%)	79	84
4	7	248/267 (93%)	247 (100%)	1 (0%)	89	91
4	f	259/267 (97%)	258 (100%)	1 (0%)	89	91
4	g	247/267 (92%)	246 (100%)	1 (0%)	89	91
All	All	7470/8141 (92%)	7418 (99%)	52 (1%)	80	86

5 of 52 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	W	395	TYR
2	W	1381	PHE
4	6	4	LYS
2	W	629	PHE
2	W	1138	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 116 such sidechains are listed below:

Mol	Chain	Res	Type
2	W	1310	GLN
4	6	98	GLN
2	x	984	ASN
3	5	312	HIS
2	l	586	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

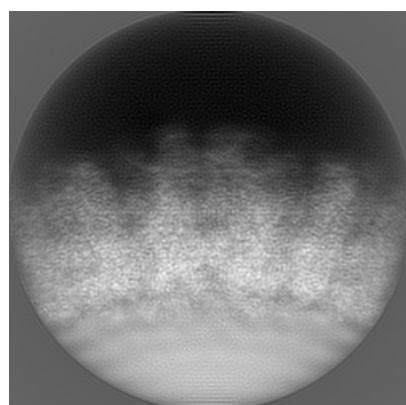
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30159. These allow visual inspection of the internal detail of the map and identification of artifacts.

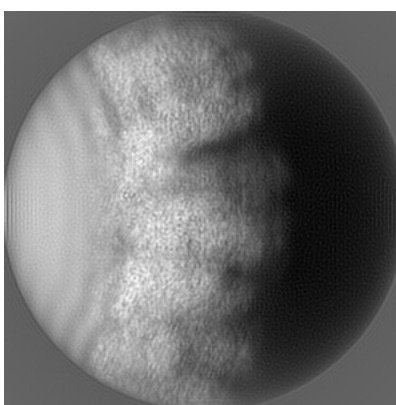
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

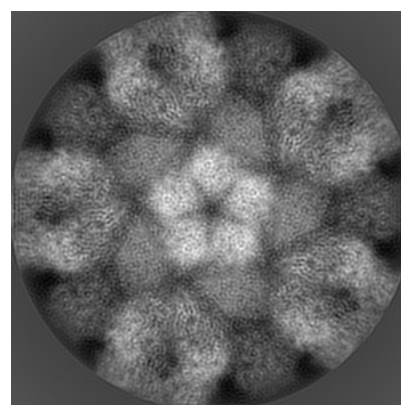
#### 6.1.1 Primary map



X



Y

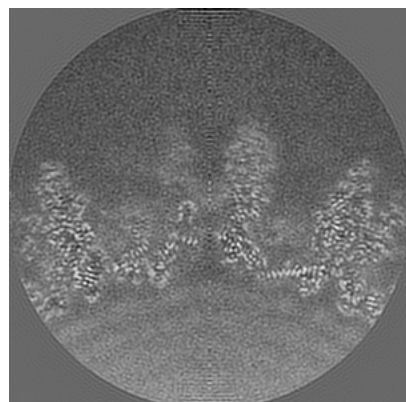


Z

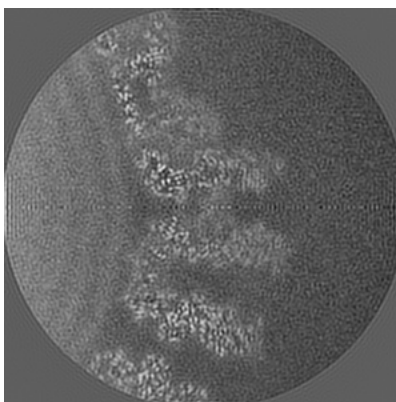
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

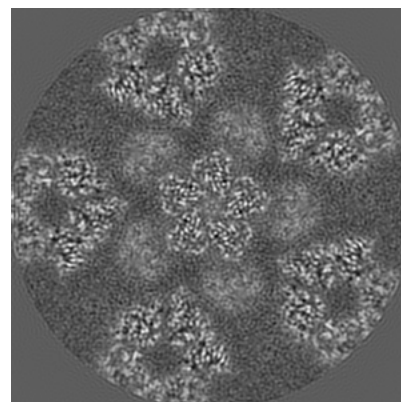
#### 6.2.1 Primary map



X Index: 150



Y Index: 150



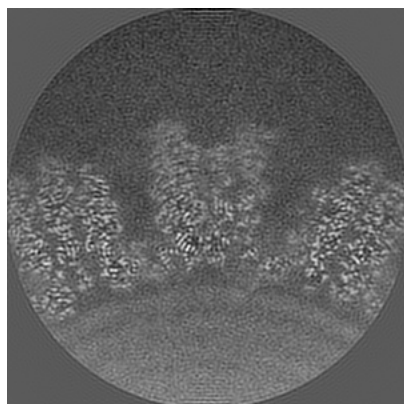
Z Index: 150



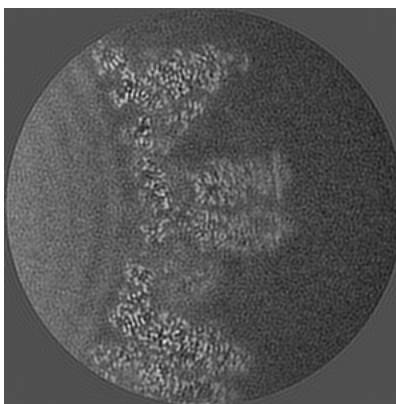
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

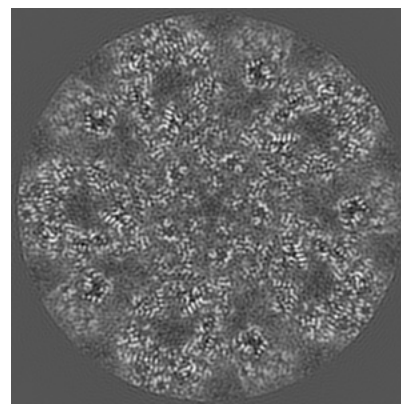
### 6.3.1 Primary map



X Index: 137



Y Index: 122

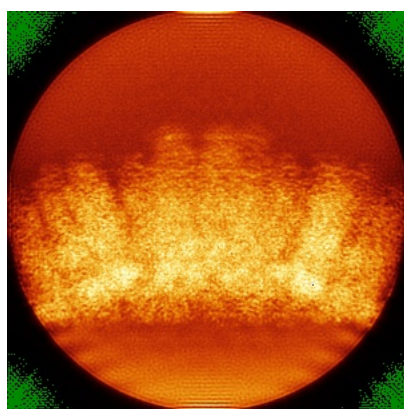


Z Index: 108

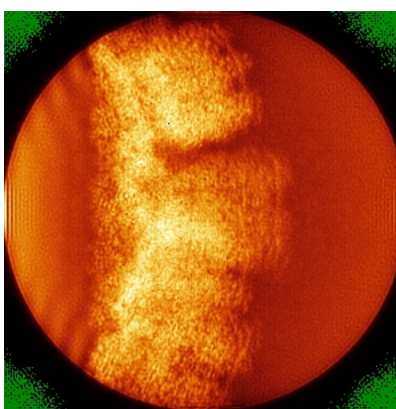
The images above show the largest variance slices of the map in three orthogonal directions.

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

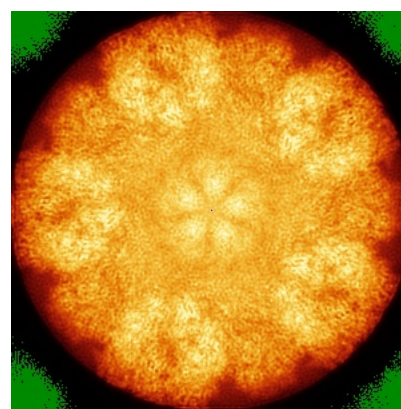
### 6.4.1 Primary map



X



Y

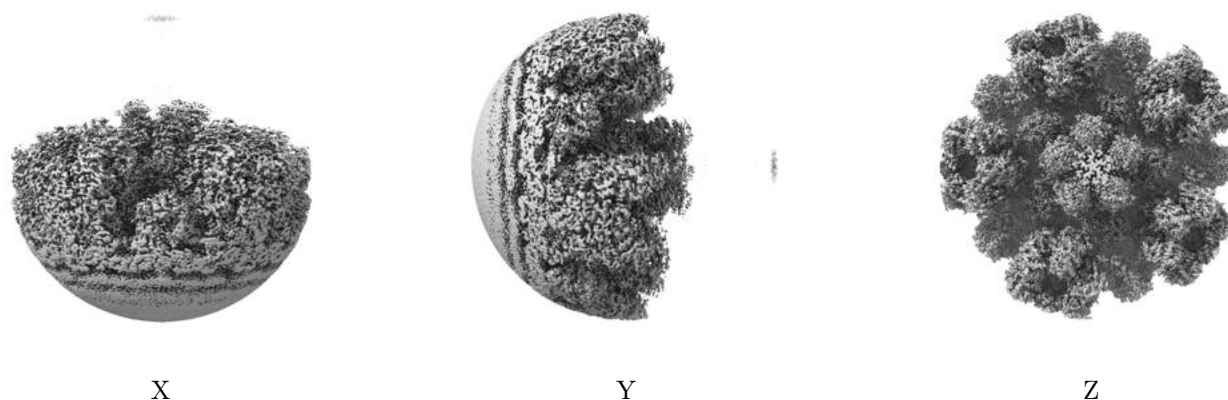


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.011. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

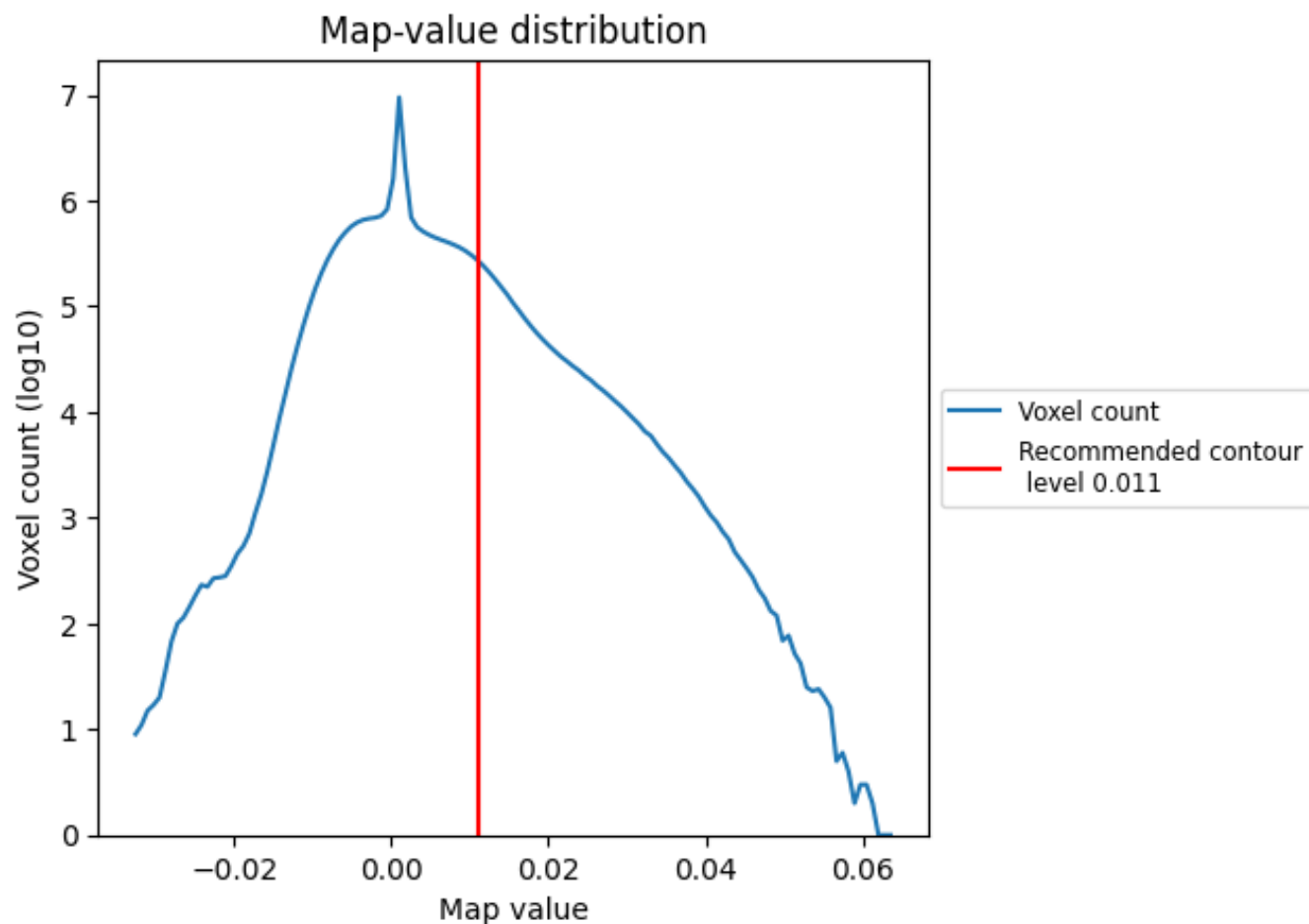
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

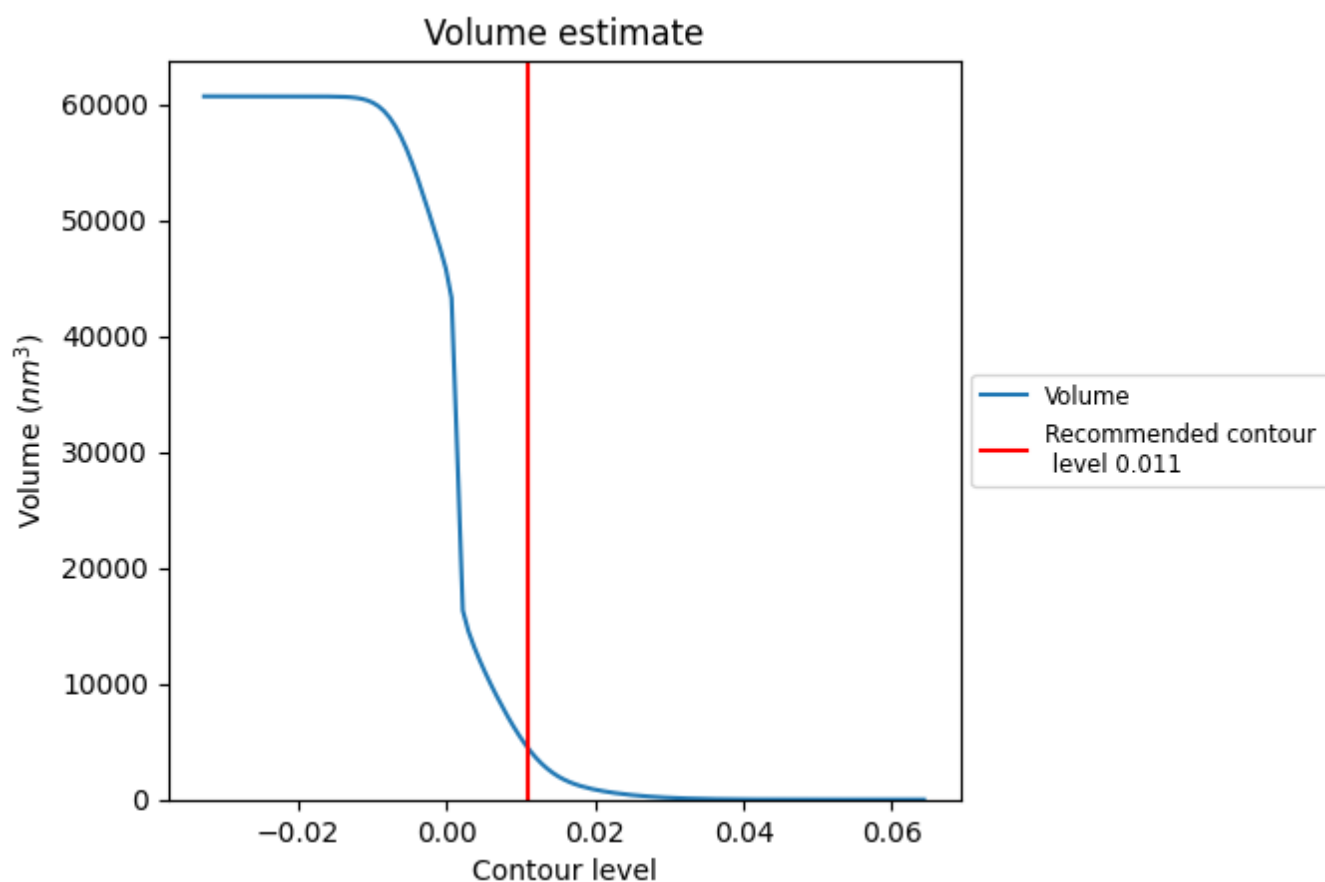
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

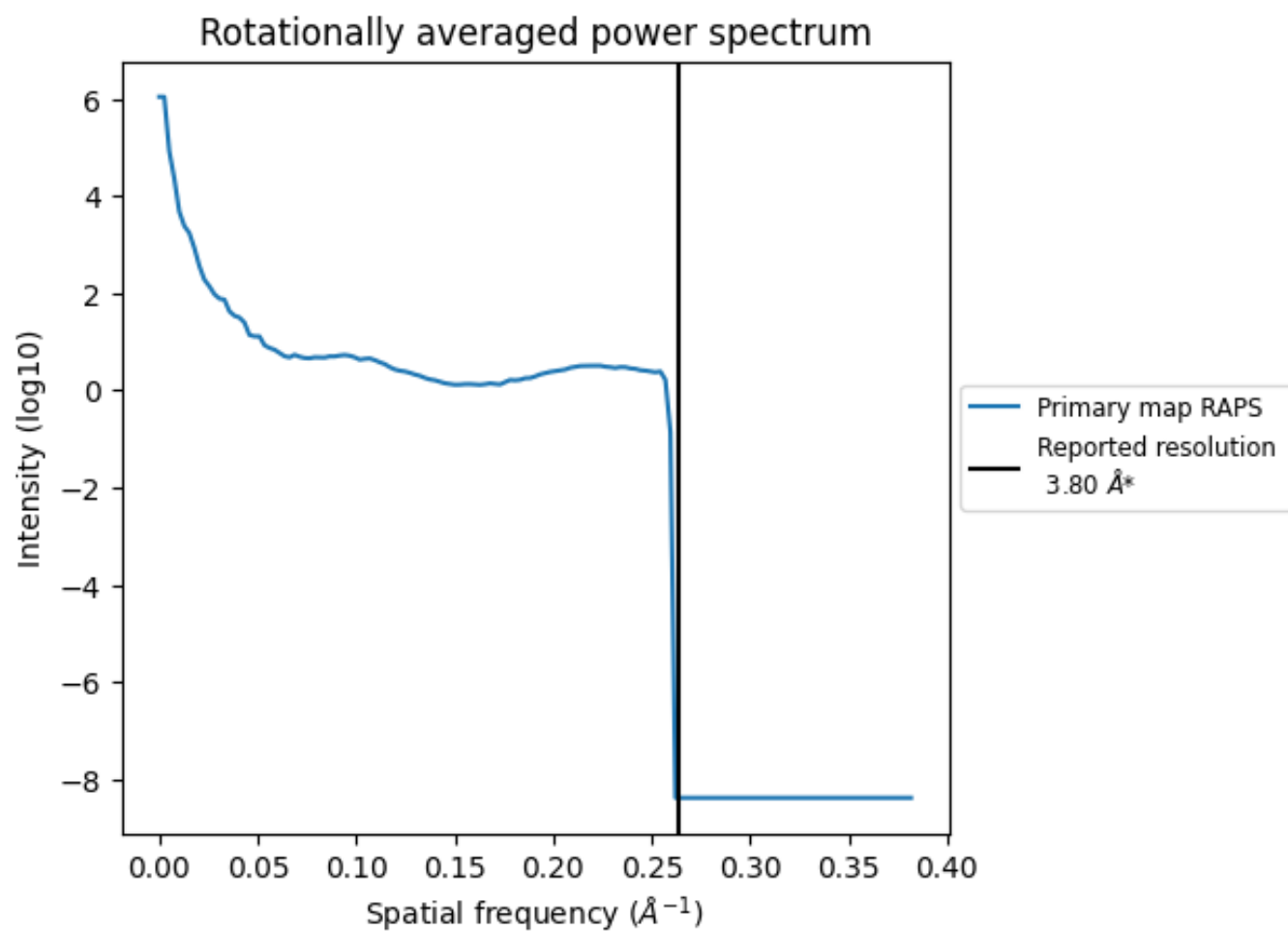
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 4476 nm<sup>3</sup>; this corresponds to an approximate mass of 4043 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 0.263 Å<sup>-1</sup>

## 8 Fourier-Shell correlation

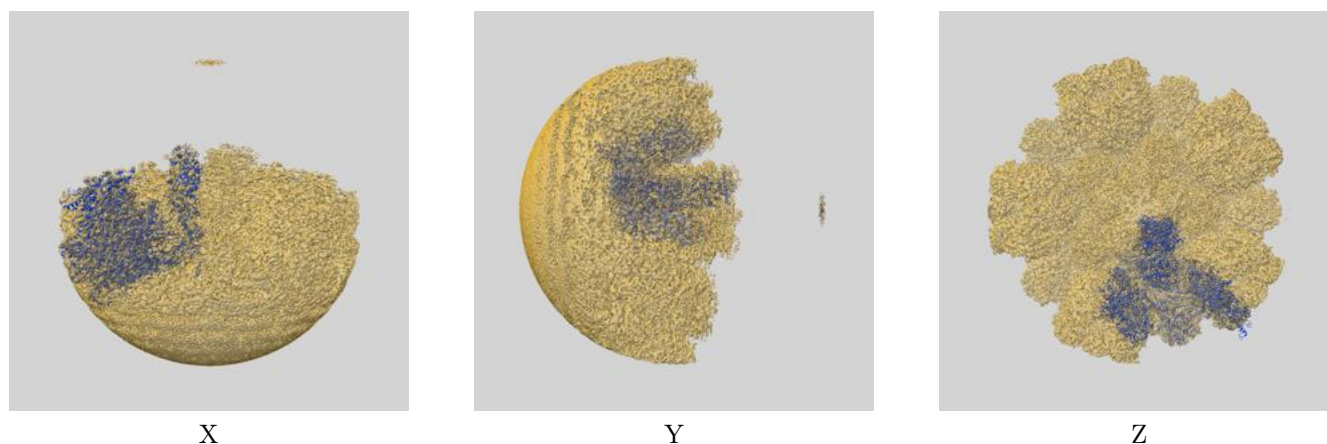
This section was not generated. No FSC curve or half-maps provided.

## 9 Map-model fit [i](#)

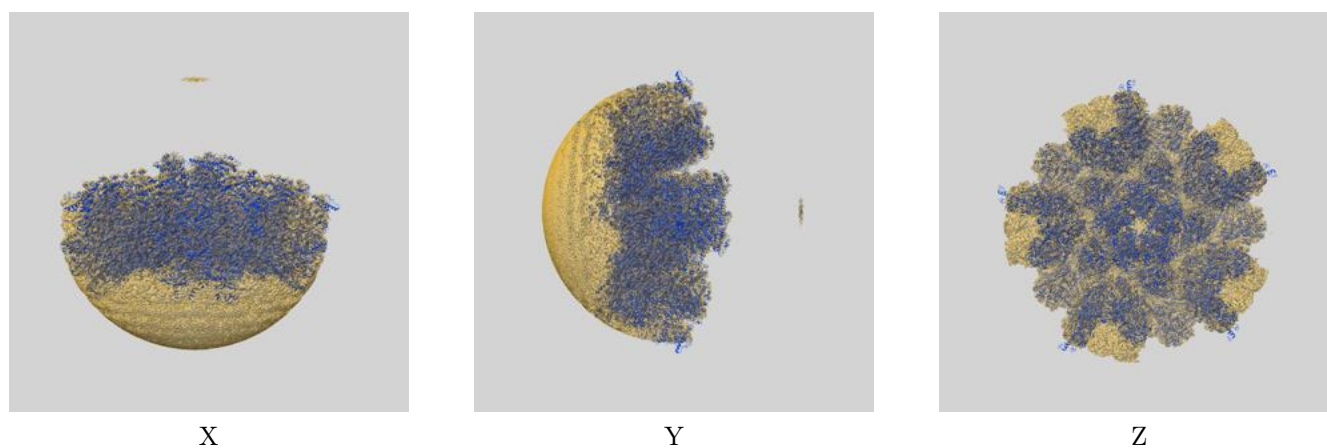
This section contains information regarding the fit between EMDB map EMD-30159 and PDB model 7BR8. Per-residue inclusion information can be found in section 3 on page 6.

### 9.1 Map-model overlays

#### 9.1.1 Map-model overlay [i](#)



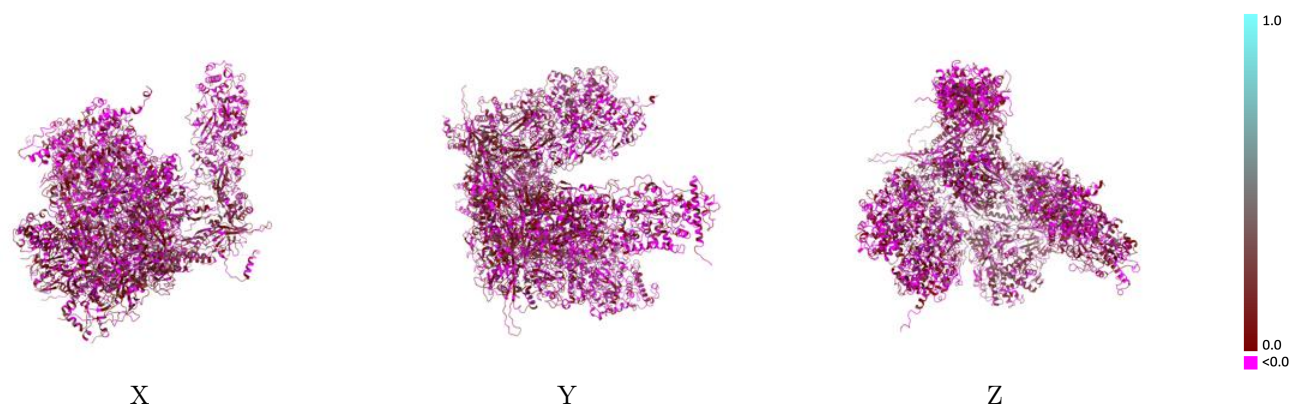
#### 9.1.2 Map-model assembly overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.011 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.

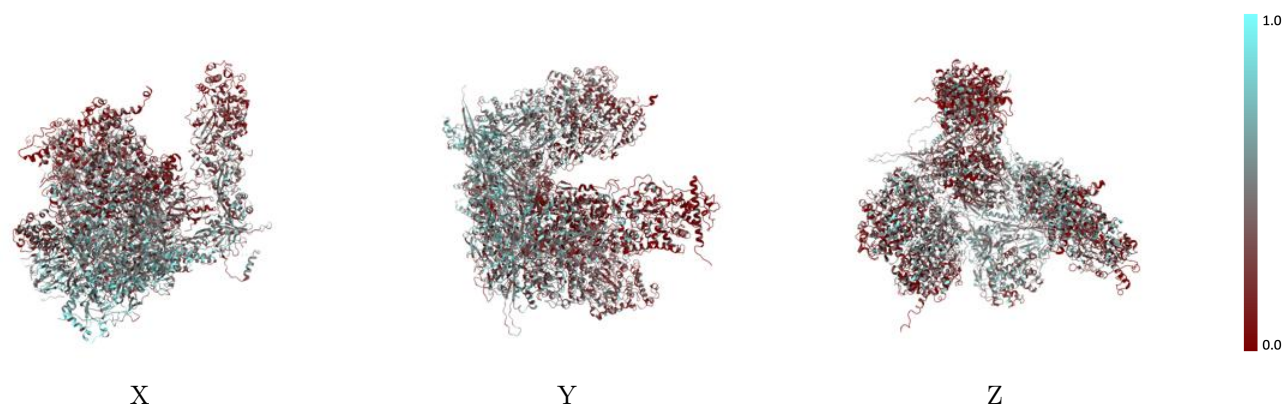


## 9.2 Q-score mapped to coordinate model [i](#)



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.

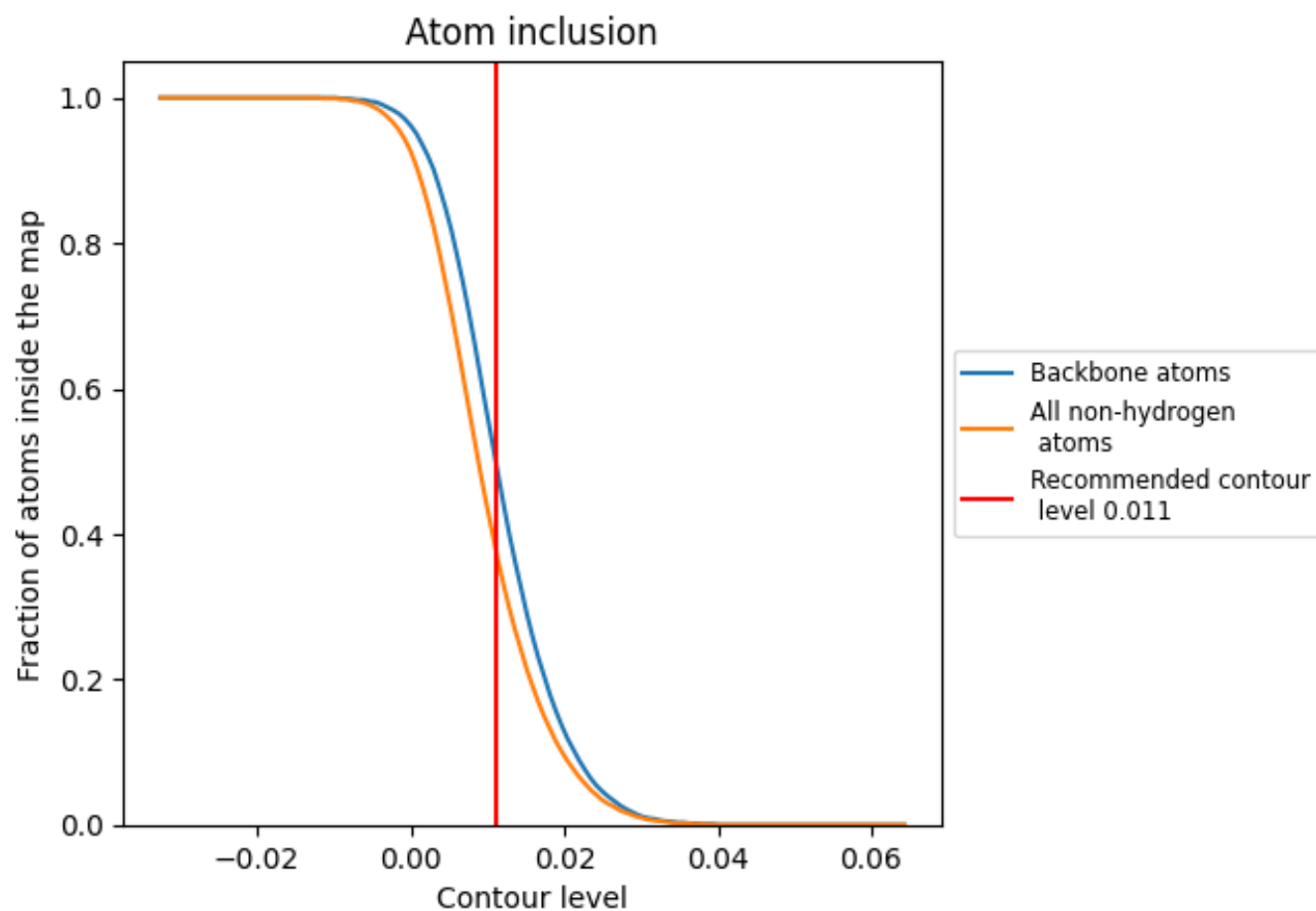
## 9.3 Atom inclusion mapped to coordinate model [i](#)



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 (0.011).





































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 50% of all backbone atoms, 38% 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 (0.011) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.3840	 0.0390
2	 0.0900	 0.0040
5	 0.3400	 0.0580
6	 0.2570	 0.0380
7	 0.2150	 0.0200
S	 0.3920	 0.0270
T	 0.4150	 0.0250
W	 0.4590	 0.0620
Y	 0.1880	 -0.0060
Z	 0.1430	 -0.0060
e	 0.4820	 0.0630
f	 0.4460	 0.0640
g	 0.4600	 0.0620
l	 0.3240	 0.0360
m	 0.0830	 -0.0260
x	 0.4190	 0.0370
y	 0.1570	 0.0320

