



wwPDB EM Validation Summary Report ⓘ

Mar 27, 2025 – 12:26 pm GMT

PDB ID : 6ZTZ
EMDB ID : EMD-22166
Title : Assembly intermediates of orthoreovirus captured in the cell
Authors : Sutton, G.C.; Stuart, D.I.
Deposited on : 2020-07-20
Resolution : 6.50 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.dev117
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) : 2.41.5

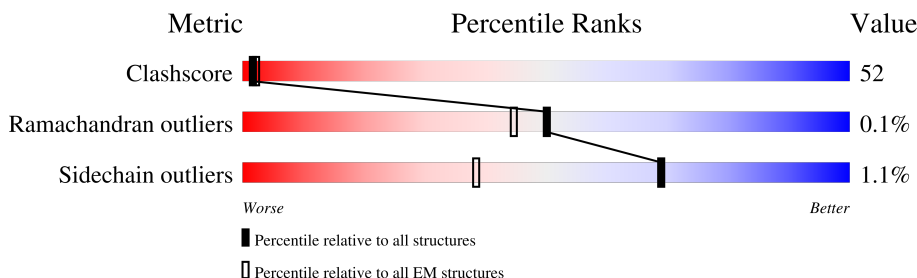
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 6.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
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 ≥ 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	B	1035	<div> <div>100%</div> <div> <div>30%</div> <div>69%</div> <div>.</div> </div> </div>
2	C	1008	<div> <div>95%</div> <div> <div>26%</div> <div>73%</div> <div>.</div> </div> </div>
3	D	417	<div> <div>96%</div> <div> <div>27%</div> <div>71%</div> <div>.</div> </div> </div>
3	P	417	<div> <div>84%</div> <div> <div>25%</div> <div>73%</div> <div>.</div> </div> </div>
4	K	641	<div> <div>89%</div> <div> <div>28%</div> <div>71%</div> <div>.</div> </div> </div>
4	L	641	<div> <div>91%</div> <div> <div>32%</div> <div>68%</div> <div>.</div> </div> </div>
4	M	641	<div> <div>92%</div> <div> <div>32%</div> <div>67%</div> <div>.</div> </div> </div>
5	O	1284	<div> <div>91%</div> <div> <div>26%</div> <div>73%</div> <div>.</div> </div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
6	X	365	<div><div></div><div>92%</div><div>25%</div><div>74%</div><div></div></div>
6	Y	365	<div><div></div><div>94%</div><div>30%</div><div>69%</div><div></div></div>
6	Z	365	<div><div></div><div>92%</div><div>27%</div><div>72%</div><div></div></div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 56150 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 Inner capsid protein lambda-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	1035	Total	C	N	O	S	0	0
			8171	5222	1380	1519	50		

- Molecule 2 is a protein called Inner capsid protein lambda-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	1008	Total	C	N	O	S	0	0
			7958	5091	1342	1475	50		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	VAL	deletion	UNP Q9WAB2
C	?	-	SER	deletion	UNP Q9WAB2
C	?	-	GLU	deletion	UNP Q9WAB2
C	?	-	SER	deletion	UNP Q9WAB2
C	?	-	THR	deletion	UNP Q9WAB2
C	?	-	THR	deletion	UNP Q9WAB2
C	?	-	GLN	deletion	UNP Q9WAB2
C	?	-	THR	deletion	UNP Q9WAB2

- Molecule 3 is a protein called Inner capsid protein sigma-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	417	Total	C	N	O	S	0	0
			3313	2092	600	604	17		
3	P	417	Total	C	N	O	S	0	0
			3313	2092	600	604	17		

- Molecule 4 is a protein called Outer capsid protein mu-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	K	641	Total 4871	C 3091	N 807	O 954	S 19	0	0
4	L	641	Total 4871	C 3091	N 807	O 954	S 19	0	0
4	M	641	Total 4871	C 3091	N 807	O 954	S 19	0	0

There are 81 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	?	-	PRO	deletion	UNP P11077
K	?	-	GLU	deletion	UNP P11077
K	?	-	THR	deletion	UNP P11077
K	?	-	ALA	deletion	UNP P11077
K	?	-	ILE	deletion	UNP P11077
K	?	-	ILE	deletion	UNP P11077
K	?	-	ASN	deletion	UNP P11077
K	?	-	THR	deletion	UNP P11077
K	?	-	ASP	deletion	UNP P11077
K	?	-	ASN	deletion	UNP P11077
K	?	-	SER	deletion	UNP P11077
K	?	-	SER	deletion	UNP P11077
K	?	-	GLY	deletion	UNP P11077
K	?	-	ALA	deletion	UNP P11077
K	?	-	VAL	deletion	UNP P11077
K	?	-	PRO	deletion	UNP P11077
K	?	-	SER	deletion	UNP P11077
K	?	-	GLU	deletion	UNP P11077
K	?	-	SER	deletion	UNP P11077
K	?	-	ALA	deletion	UNP P11077
K	?	-	LEU	deletion	UNP P11077
K	?	-	VAL	deletion	UNP P11077
K	?	-	PRO	deletion	UNP P11077
K	?	-	TYR	deletion	UNP P11077
K	?	-	ASN	deletion	UNP P11077
K	344	LEU	PRO	conflict	UNP P11077
K	359	PHE	LEU	conflict	UNP P11077
L	?	-	PRO	deletion	UNP P11077
L	?	-	GLU	deletion	UNP P11077
L	?	-	THR	deletion	UNP P11077
L	?	-	ALA	deletion	UNP P11077
L	?	-	ILE	deletion	UNP P11077
L	?	-	ILE	deletion	UNP P11077

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
L	?	-	ASN	deletion	UNP P11077
L	?	-	THR	deletion	UNP P11077
L	?	-	ASP	deletion	UNP P11077
L	?	-	ASN	deletion	UNP P11077
L	?	-	SER	deletion	UNP P11077
L	?	-	SER	deletion	UNP P11077
L	?	-	GLY	deletion	UNP P11077
L	?	-	ALA	deletion	UNP P11077
L	?	-	VAL	deletion	UNP P11077
L	?	-	PRO	deletion	UNP P11077
L	?	-	SER	deletion	UNP P11077
L	?	-	GLU	deletion	UNP P11077
L	?	-	SER	deletion	UNP P11077
L	?	-	ALA	deletion	UNP P11077
L	?	-	LEU	deletion	UNP P11077
L	?	-	VAL	deletion	UNP P11077
L	?	-	PRO	deletion	UNP P11077
L	?	-	TYR	deletion	UNP P11077
L	?	-	ASN	deletion	UNP P11077
L	344	LEU	PRO	conflict	UNP P11077
L	359	PHE	LEU	conflict	UNP P11077
M	?	-	PRO	deletion	UNP P11077
M	?	-	GLU	deletion	UNP P11077
M	?	-	THR	deletion	UNP P11077
M	?	-	ALA	deletion	UNP P11077
M	?	-	ILE	deletion	UNP P11077
M	?	-	ILE	deletion	UNP P11077
M	?	-	ASN	deletion	UNP P11077
M	?	-	THR	deletion	UNP P11077
M	?	-	ASP	deletion	UNP P11077
M	?	-	ASN	deletion	UNP P11077
M	?	-	SER	deletion	UNP P11077
M	?	-	SER	deletion	UNP P11077
M	?	-	GLY	deletion	UNP P11077
M	?	-	ALA	deletion	UNP P11077
M	?	-	VAL	deletion	UNP P11077
M	?	-	PRO	deletion	UNP P11077
M	?	-	SER	deletion	UNP P11077
M	?	-	GLU	deletion	UNP P11077
M	?	-	SER	deletion	UNP P11077
M	?	-	ALA	deletion	UNP P11077
M	?	-	LEU	deletion	UNP P11077

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
M	?	-	VAL	deletion	UNP P11077
M	?	-	PRO	deletion	UNP P11077
M	?	-	TYR	deletion	UNP P11077
M	?	-	ASN	deletion	UNP P11077
M	344	LEU	PRO	conflict	UNP P11077
M	359	PHE	LEU	conflict	UNP P11077

- Molecule 5 is a protein called Outer capsid protein lambda-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	O	1284	Total	C	N	O	S	0	0
			10127	6468	1700	1917	42		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	?	-	SER	deletion	UNP P11079
O	?	-	ALA	deletion	UNP P11079
O	?	-	SER	deletion	UNP P11079
O	?	-	GLY	deletion	UNP P11079

- Molecule 6 is a protein called Outer capsid protein sigma-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	X	365	Total	C	N	O	S	0	0
			2885	1818	508	531	28		
6	Y	365	Total	C	N	O	S	0	0
			2885	1818	508	531	28		
6	Z	365	Total	C	N	O	S	0	0
			2885	1818	508	531	28		

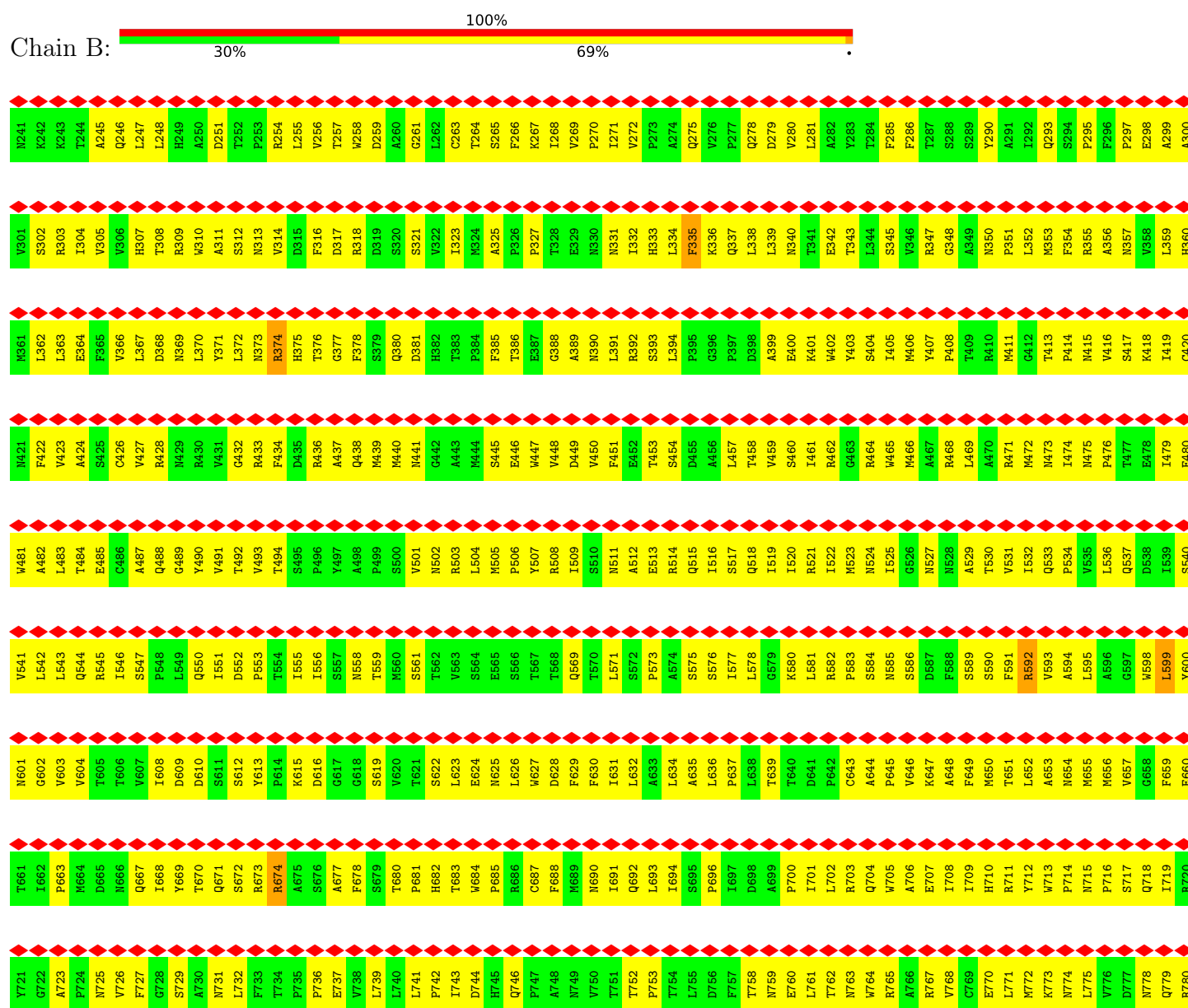
There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	104	CYS	ALA	conflict	UNP P07939
X	325	ASN	ASP	conflict	UNP P07939
Y	104	CYS	ALA	conflict	UNP P07939
Y	325	ASN	ASP	conflict	UNP P07939
Z	104	CYS	ALA	conflict	UNP P07939
Z	325	ASN	ASP	conflict	UNP P07939

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: Inner capsid protein lambda-1



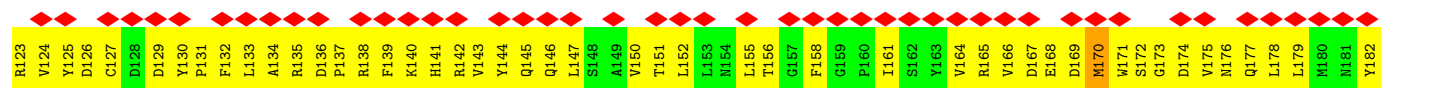
Y781	D841	Y901	T961	A1021	G1081	M1141	S1201	A1261	Y781
Q782	R842	A902	A962	D1022	I1082	G1142	T1202	Y1262	Q782
P783	V843	D903	A963	C1023	I1083	A1143	E1203	E1263	P783
G784	P844	A904	T964	V1024	S1084	Y1144	Y1204	T1264	G784
W785	T845	I905	F965	Q1025	F1085	P1145	N1205	P1265	W785
T786	M846	Y906	A966	L1026	G1086	Y1146	D1206	P1266	T786
Q787	V847	P907	E967	T1027	M1087	M1147	R1207	I1267	Q787
S788	G848	M908	W968	A1028	N1088	L1148	S1208	T1268	S788
L789	V849	Y909	W969	E1029	N1089	H1149	L1209	A1269	L789
W790	T850	A910	N970	Y1030	A1090	Y1150	F1210	V1270	W790
S791	R851	D911	T971	F1031	A1091	Y1151	C1211	V1271	S791
S792	Q852	T912	S972	M1032	P1092	D1152	T1212	G1272	S792
M793	S853	E913	M973	H1033	M1093	P1153	N1213	M1273	M793
R794	R854	V914	K974	E1034	I1094	R1154	S1214	V1274	R794
G795	D855	F915	T975	Y1035	R1095	Q1155	S1215	P1275	G795
T796	T856	S916	A976	M1036	D1096	Y1156	S1216	A1276	T796
L797	I857	N917	F977	L1037	E1097	A1157	P1217	V1277	L797
D798	T858	L918	L978	F1038	T1098	M1158	Q1218	T1278	D798
K799	Q859	Q919	L979	G1039	G1099	A1159	T1219	A1279	K799
L800	P860	R920	S980	I1040	M1100	W1160	I1220	V1280	L800
K801	A861	D921	D981	A1041	M1101	L1161	A1221	A1281	K801
L802	L862	M922	M982	R1042	Y1102	L1162	G1222	A282	L802
I803	S863	I923	L983	G1043	P1103	T1163	P1223	Y283	I803
K804	L864	T924	L984	D1044	F1104	S1164	D1224	Z284	K804
S805	S865	C925	E985	I1045	E1105	A1165	K1225	T285	S805
M806	T866	E926	P986	I1046	G1106	L1166	H1226	F286	M806
T807	T867	A927	L987	I1047	M1107	L1167	I1227	T287	T807
P808	N868	V928	L988	G1048	W1108	E1168	P1228	P1288	P808
M809	T869	Q929	S989	I1049	I1109	E1169	V1229	S288	M809
Y810	T870	T930	G990	V1050	F1110	I1170	R1230	S289	Y810
L811	B871	L931	D991	Q1051	P1111	T1171	R1231	Y290	L811
Q812	G872	V932	P992	S1052	L1112	P1172	Y1232	A291	Q812
Q813	B873	T933	R993	T1053	A1113	S1173	N1233	L292	Q813
L814	P874	L934	M994	H1054	L1114	I1174	I1234	S294	L814
A815	L875	V935	T995	L1055	W1115	I1175	L1235	P295	A815
P816	A876	A936	Q996	V1056	Q1116	P1176	T1236	G296	P816
V817	L877	Q937	L997	S1057	M1117	S1177	M1237	F297	V817
E818	D878	I938	A998	P1058	N1118	Y1178	P1238	P298	E818
L819	A879	S939	I999	L1059	T1119	P1179	D1239	E298	L819
A820	R880	E940	Q1000	A1060	R1120	F1180	A1240	A299	A820
V821	A881	T941	Y1001	P1061	M1121	M1181	P1241	A300	V821
I822	I882	Q942	Q1002	P1062	F1122	Y1182	P1242	V301	I822
A823	T883	Y943	Q1003	P1063	M1123	P1183	T1243	S302	A823
P824	V884	P944	Y1004	D1064	Q1124	L1184	Q1244	R303	P824
M825	A885	V945	M1005	L1065	Q1125	S1185	I1245	T304	M825
L826	L886	D946	G1006	V1066	Q1126	S1186	Q1246	V305	L826
P827	L887	R947	A1007	F1067	D1127	D1187	L1247	V306	P827
F828	S888	Y948	T1008	D1068	A1128	H1188	P1248	H307	F828
P829	G889	L949	F1009	R1069	W1129	L1189	E1249	T308	P829
P830	K890	D950	M1010	D1070	I1130	D1190	V1250	N309	P830
F831	Y891	W951	Y1011	T1071	K1131	S1191	V1251	W310	F831
Q832	P892	I952	T1012	P1072	T1132	S1192	D1252	A311	Q832
V833	P893	P953	P1013	G1073	G1133	A1193	L1253	S312	V833
P834	D894	S954	E1014	L1074	E1134	P1194	Y1254	N313	P834
Y835	L895	L955	M1015	H1075	L1135	A1195	N1255	V314	Y835
V836	V896	R956	P1016	T1076	R1136	V1196	V1256	D315	V836
R837	T897	A957	G1017	F1077	I1137	Q1197	T1257	F316	R837
L838	N898	S958	S1018	G1078	R1138	Y1198	T1258	D317	L838
D839	W899	A959	V1019	R1079	I1139	T1199	R1259	R318	D839
R840	W900	A960	I1020	D1080	E1140	T1200	Y1260	D319	R840

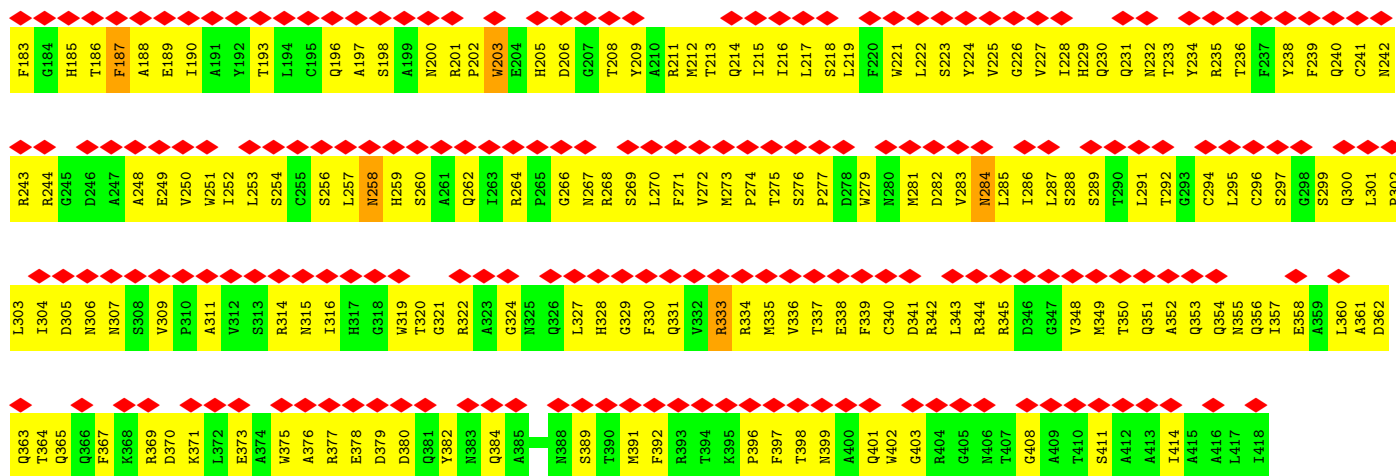
• Molecule 2: Inner capsid protein lambda-1



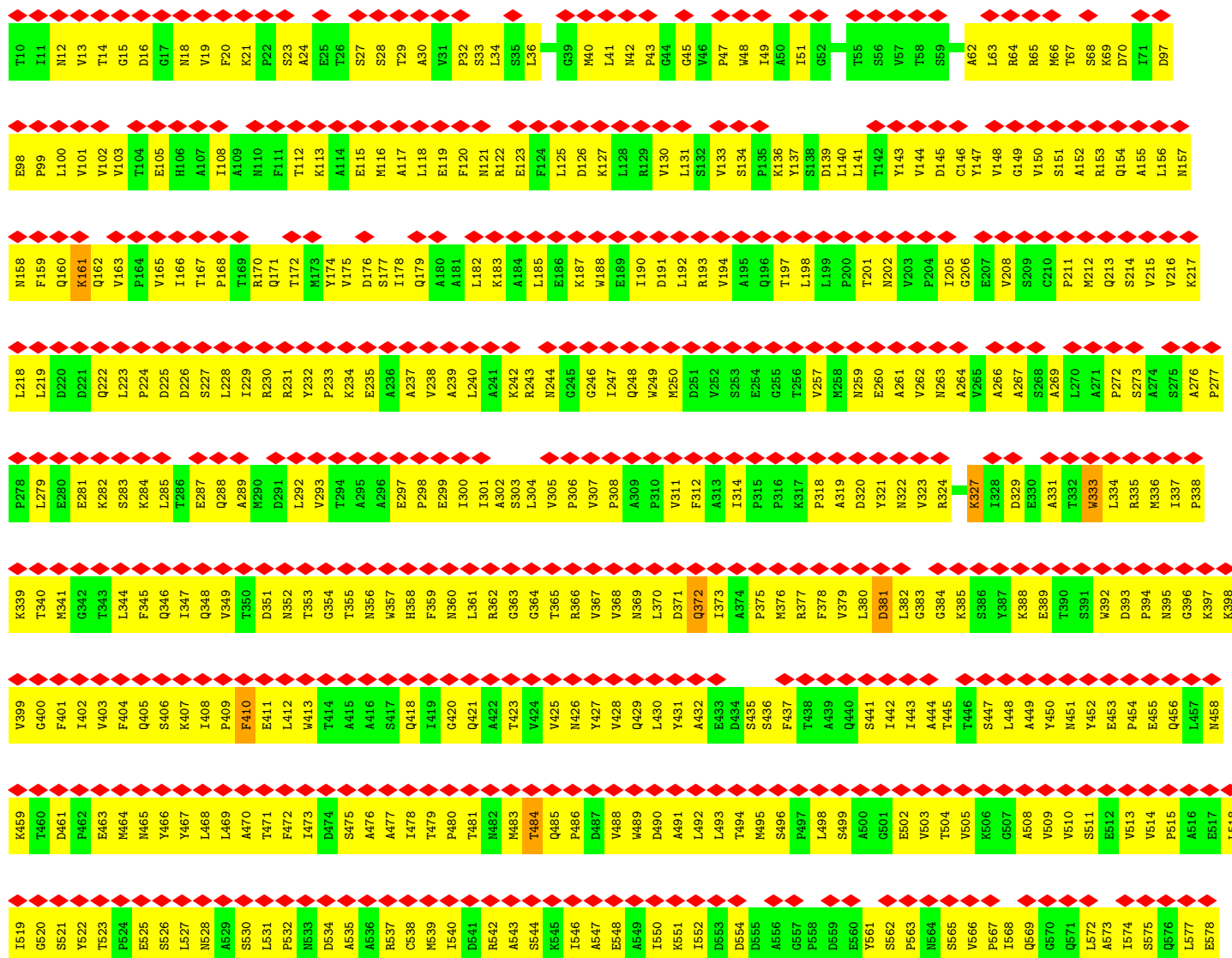
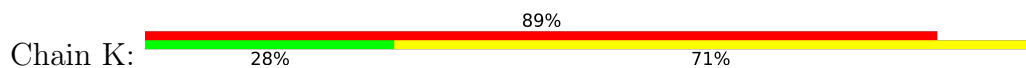
A260	S320	Q380
G261	S321	D381
L262	V322	H382
C263	I323	T383
T264	K324	F384
S265	A325	F385
F266	P326	T386
K267	P327	E387
L268	T328	G388
V269	E329	A389
P270	N330	N390
L271	N331	L391
V272	I332	R392
P273	K333	S393
A274	L334	L394
Q275	F335	P395
V276	K336	G396
T277	Q337	P397
Q278	L338	D398
D279	L339	A399
V280	N340	E400
L281	T341	K401
A282	E342	W402
Y283	T343	Y403
T284	L344	S404
F285	S345	I405
F286	V346	M406
T287	R347	Y407
S288	G348	P408
S289	A349	T409
Y290	N350	R410
A291	P351	M411
L292	L352	G412
Q293	K353	T413
S294	F354	P414
P295	R355	M415
F296	A356	V416
P297	N357	S417
E298	V358	K418
A299	L359	I419
A300	H360	C420
V301	K361	N421
S302	L362	F422
R303	L363	V423
T304	E364	A424
V305	F365	S425
V306	V366	C426
H307	L367	V427
T308	D368	R428
R309	N369	N429
W310	L370	R430
A311	Y371	V431
S312	L372	G432
N313	K373	R433
V314	R374	F434
D315	H375	D435
F316	T376	R436
D317	G377	A437
R318	F378	Q438
D319	S379	M439

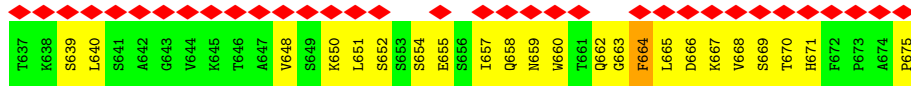
E1168	G1048	L988	V928	N868	P808	A748	F888	D828	M560	S500	M440
E1169	R1049	S989	Q929	T869	M809	N749	M889	F829	S561	V501	N441
I1170	V1050	G990	T930	T870	Y810	V750	N690	F830	T562	N502	G442
T1171	Q1051	D991	L931	V871	L811	T751	I691	I831	L571	R503	A443
P1172	S1052	D992	V932	G872	Q812	T752	Q892	L632	S572	L504	M444
T1173	T1053	R993	T933	V873	Q813	P753	L693	A833	S573	M505	S445
S1174	H1054	M994	L934	P874	L814	T754	S895	L634	A574	P506	E446
I1175	L1055	T995	V935	L875	A815	L755	P896	A635	S575	Y507	E447
P1176	W1056	Q996	A936	A876	P816	D756	I897	L636	S576	L508	V448
S1177	S1057	L997	Q937	L877	V817	T757	D898	P637	I577	I509	D449
V1178	P1058	A998	T938	D878	B818	T758	A699	L638	L578	S510	V450
P1179	L1059	I999	S939	A879	L819	N759	P700	T639	G579	N511	F451
F1180	A1060	Q1000	E940	R880	A820	E760	I701	T640	K580	A512	E452
M1181	P1061	Y1001	T941	A881	V821	L761	L702	D641	L581	E513	T453
V1182	P1062	Q1002	Q942	T882	T822	T762	Q704	P642	R582	R514	S454
P1183	P1063	Q1003	Y943	T883	A823	N763	W705	C643	P583	Q515	D455
I1184	D1064	Y1004	P944	V884	P824	A764	A706	A644	S584	I516	A456
S1185	L1065	M1005	V945	A885	M825	R765	E707	P645	N585	S517	L457
L1186	V1066	L886	D946	L886	L826	A766	I708	V646	S586	Q518	T458
D1187	F1067	R947	R947	L887	P827	R767	I709	K647	D587	I519	V459
H1188	D1068	Y948	Y948	S888	F828	V768	I710	A648	F588	I520	S460
A1189	R1069	F1009	L949	G889	P829	C769	R711	F649	S589	R521	I461
I1190	D1070	N1010	D950	K890	P830	E770	Y712	M650	I522	I522	R462
I1191	T1071	V1011	D951	Y891	P831	L771	W713	M650	S590	I523	G463
S1192	P1072	I1012	P952	P892	Q832	M772	P714	L951	F591	N524	R464
A1193	G1073	P953	P953	P893	V833	K773	W715	A653	R592	I525	W465
P1194	V1074	S954	S954	D894	P834	N774	P716	N654	A594	G526	M466
I1195	H1075	M1015	L955	L895	Y835	L775	Q718	M655	L595	N527	R468
V1196	I1076	P1016	R956	V896	V836	V776	I719	M656	A596	N528	L469
Q1197	F1077	G1017	A957	T897	R837	D777	R720	V657	G597	A529	A470
Y1198	G1078	S1018	S958	N898	L838	N778	Y721	G658	W598	T530	R471
I1199	R1079	V1019	A959	V899	D839	Q779	Y721	F659	L599	V531	M472
I1200	D1080	I1020	A960	W900	R840	R780	G722	E660	Y600	I532	N473
C1201	C1081	A1021	T961	Y901	R842	Y781	A723	T661	N601	Q533	I474
T1202	I1082	D1022	A962	A902	V843	Q782	W725	I662	G602	P534	N475
E1203	S1084	C1023	A963	D903	P844	P783	V726	P663	V603	V535	P476
Y1204	F1085	V1024	T964	A904	T845	G784	F727	M664	L536	L536	T477
M1205	G1086	Q1025	F965	I905	M846	W785	G728	D665	T605	Q537	E478
D1206	M1087	L1026	A966	Y906	V847	T786	S729	M666	T606	D538	I479
R1207	N1088	T1027	E967	P907	G848	Q787	A730	Q667	V607	I539	E480
S1208	G1089	A1028	W968	N908	V849	Q788	N731	I668	I608	S540	W481
L1209	A1090	E1029	V969	Y909	T850	L789	L732	Y669	D609	V541	A482
F1210	A1091	V1030	A970	A910	R851	V790	F733	T670	D610	L542	L483
C1211	P1092	F1031	T971	D911	Q852	S791	T734	Q671	S611	L543	T484
T1212	M1093	H1033	S972	T912	S853	S792	P735	S672	S612	Q544	E485
N1213	I1094	E1034	N973	E913	R854	W793	E737	S673	S613	R545	C486
R1214	R1095	Y1035	K974	V914	D855	R794	V738	R674	P614	I546	A487
S1215	D1096	N1036	T975	F915	T856	G795	L739	A675	K615	S547	Q488
T1216	E1097	F1037	A976	S916	T857	L796	L740	S676	D616	P548	G489
P1217	T1098	L1038	F977	N917	T858	L797	L741	A677	L549	Y491	Y490
Q1218	G1099	G1039	D978	L918	Q859	D798	P742	G618	Q550	T492	T492
T1219	M1100	I1040	L979	Q919	P860	K799	I743	S679	S619	V493	V493
I1220	M1101	A1041	S980	R920	A861	L800	D744	T880	V620	D552	T494
A1221	V1102	R1042	D981	D921	L862	K801	H745	P681	T621	P553	S495
G1222	P1103	G1043	N982	N922	S863	L802	Q746	H882	S622	T554	P496
P1223	F1104	D1044	L983	I923	L864	I803	P747	T883	L623	I555	I555
D1224	E1105	I1045	L984	T924	S865	K804		W884	E624	I556	A498
K1225	G1106	I1046	E985	C925	T866	N806		P885	N625	S557	P499
H1226	N1107	I1047	P986	E926	T867	T807		N886	L626	N558	
I1227			L987	A927				C887	W627	S559	



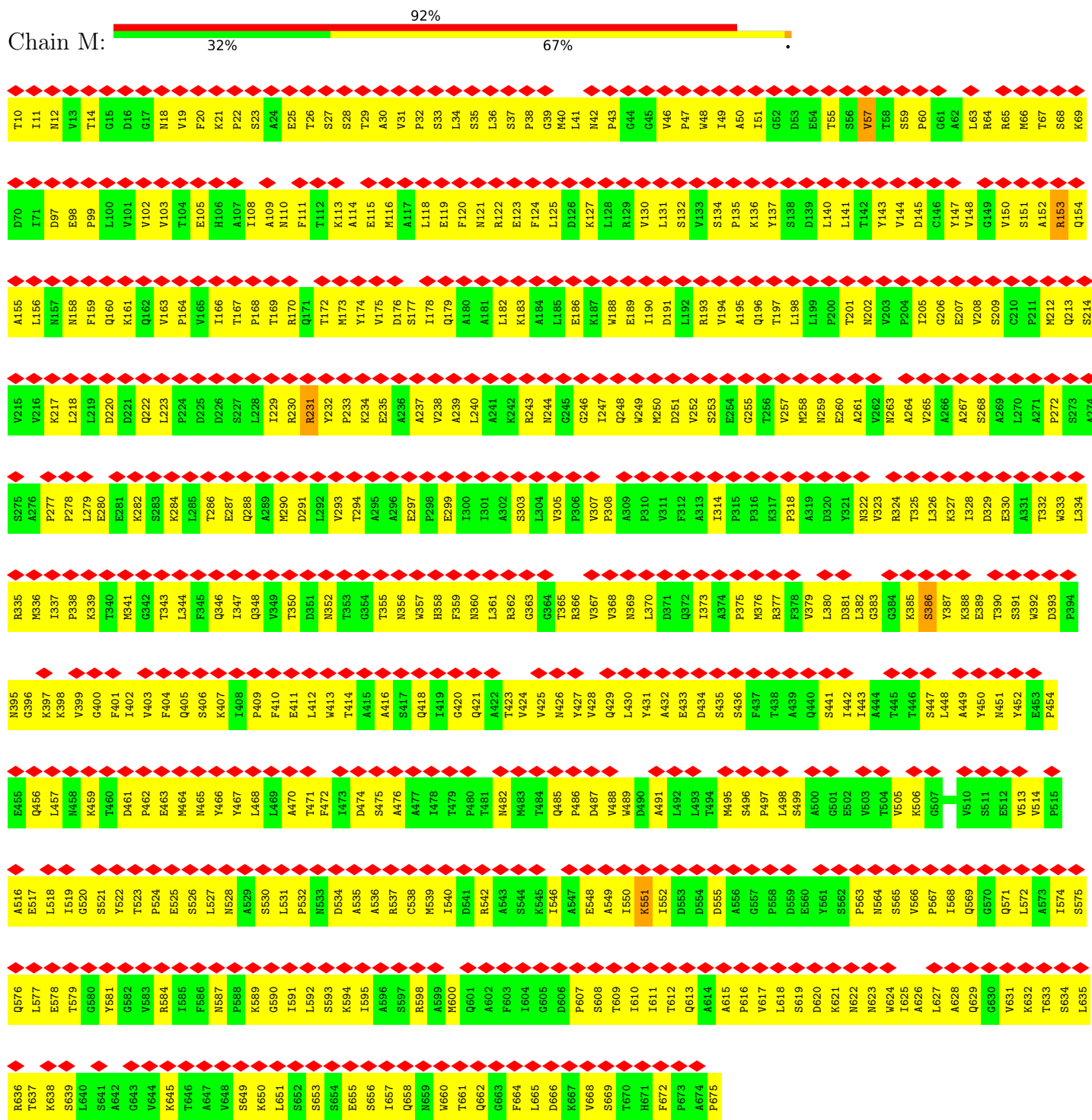


• Molecule 4: Outer capsid protein mu-1

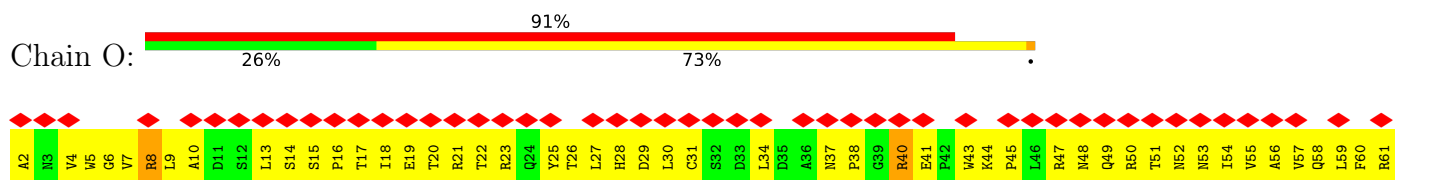




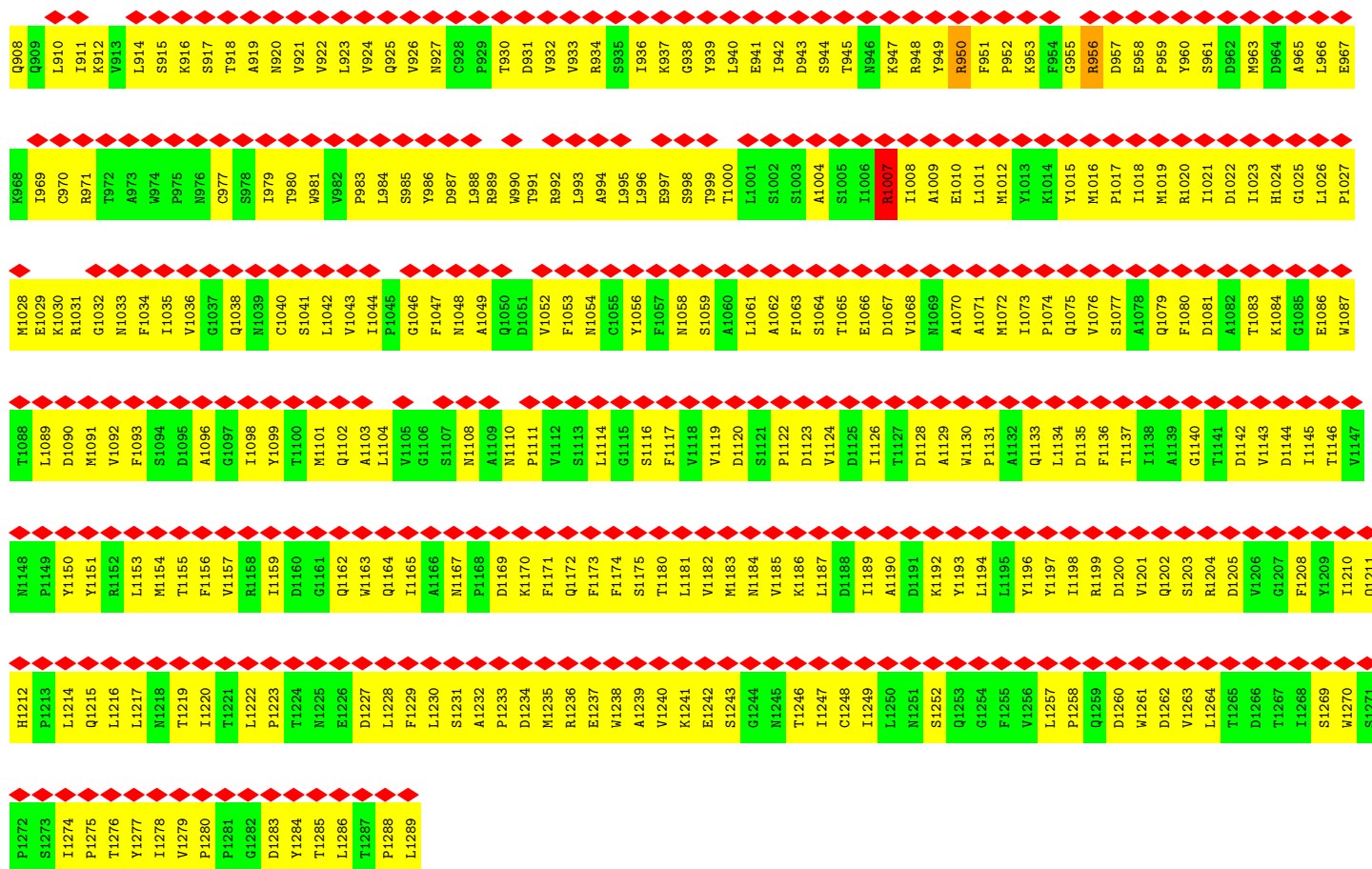
• Molecule 4: Outer capsid protein mu-1



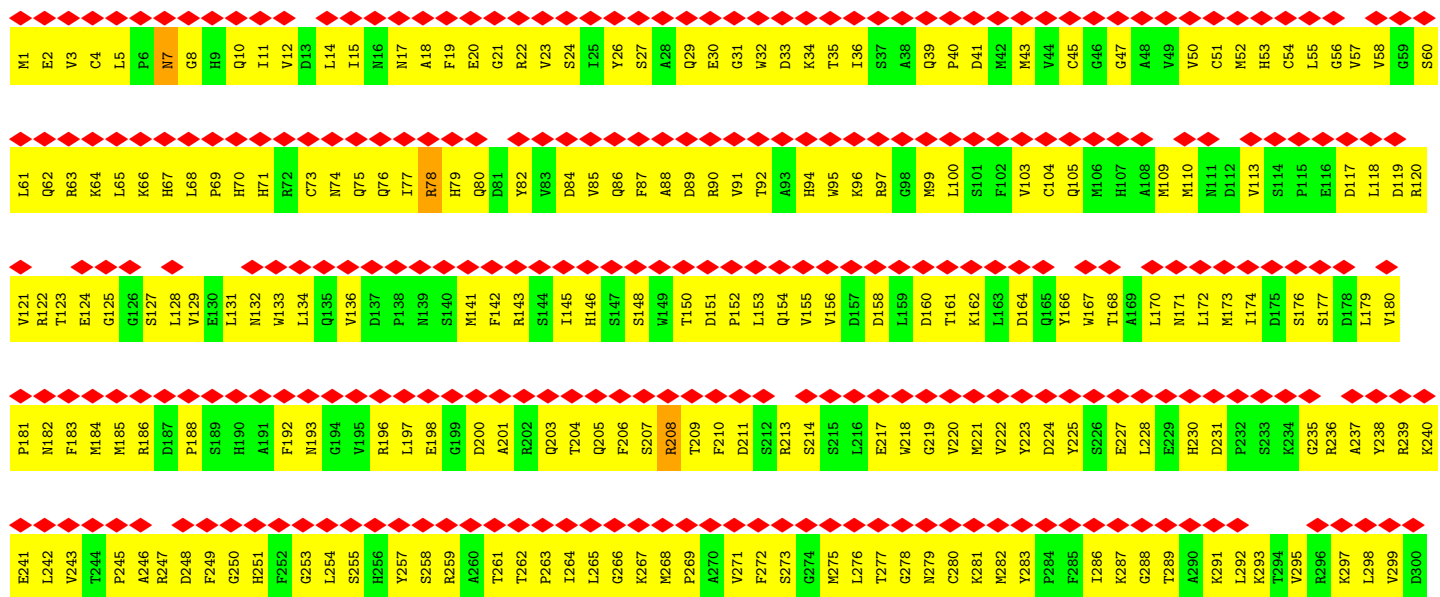
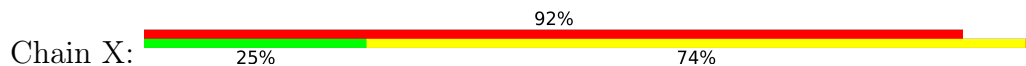
• Molecule 5: Outer capsid protein lambda-2

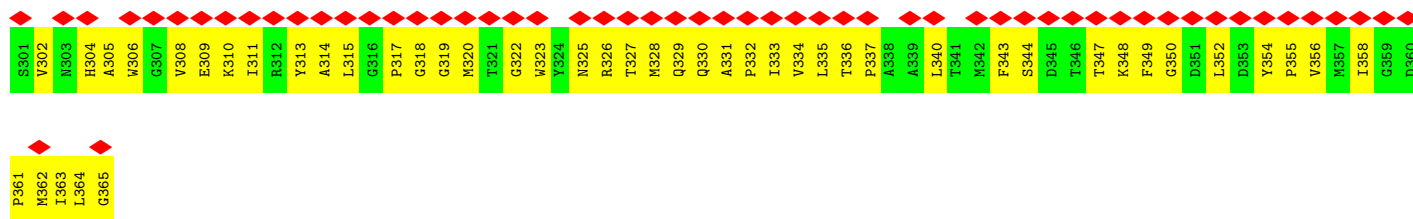




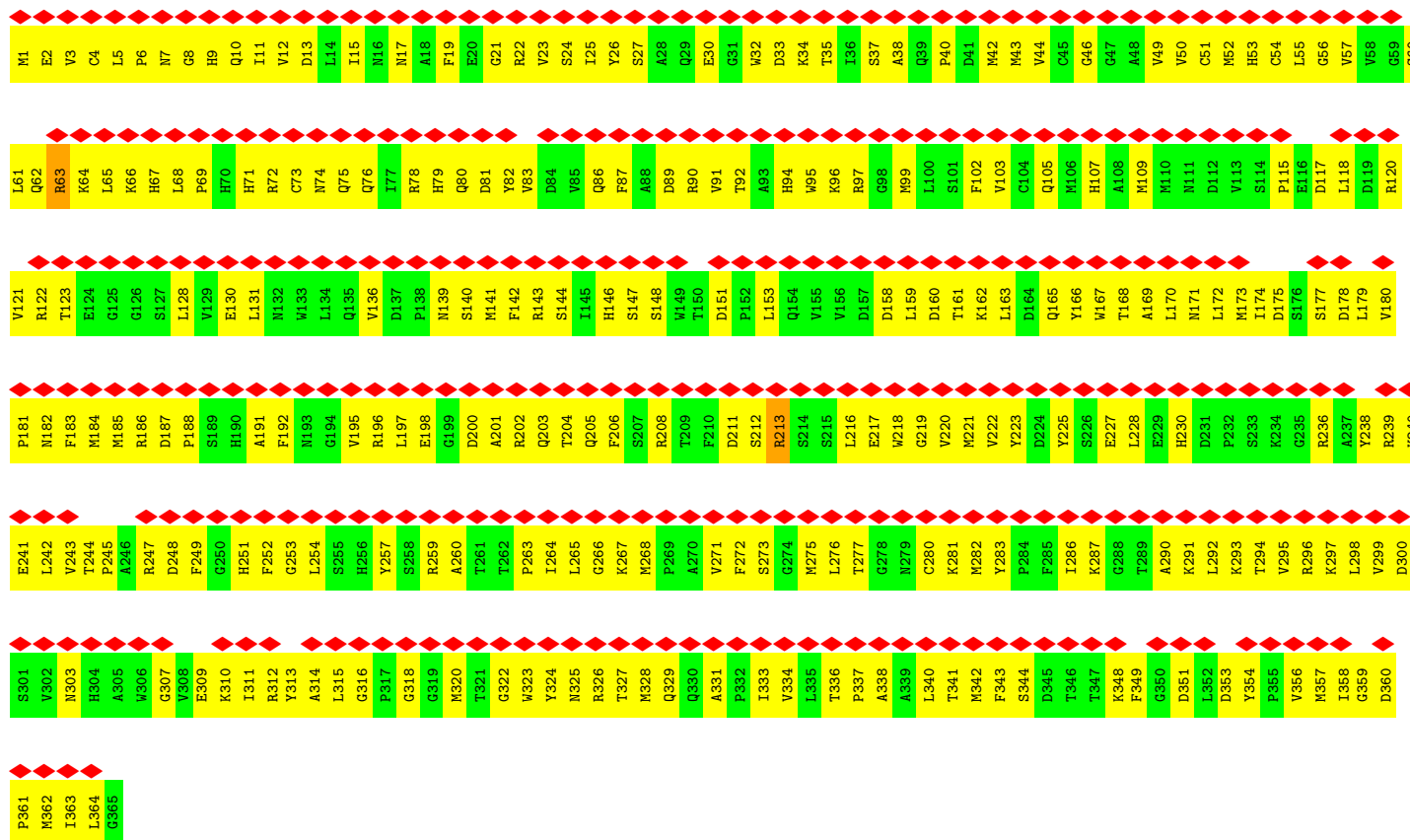


● Molecule 6: Outer capsid protein sigma-3

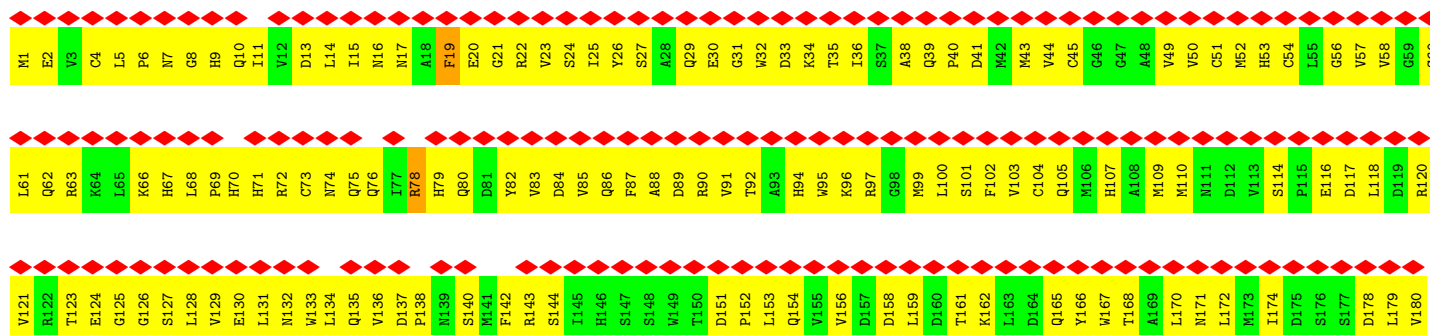
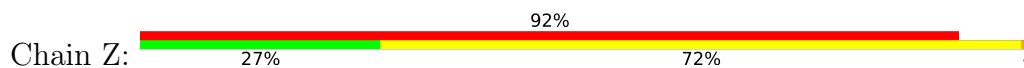




• Molecule 6: Outer capsid protein sigma-3



• Molecule 6: Outer capsid protein sigma-3





4 Experimental information

Property	Value	Source
EM reconstruction method	TOMOGRAPHY	Depositor
Imposed symmetry	POINT, Not provided	
Number of tilted images used	Not provided	
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 ($e^-/\text{\AA}^2$)	2	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum voxel value	8.955	Depositor
Minimum voxel value	-5.801	Depositor
Average voxel value	0.054	Depositor
Voxel value standard deviation	0.430	Depositor
Recommended contour level	2.7	Depositor
Tomogram size (Å)	648.0, 648.0, 648.0	wwPDB
Tomogram dimensions	360, 360, 360	wwPDB
Tomogram angles (°)	90.0, 90.0, 90.0	wwPDB
Grid spacing (Å)	1.8, 1.8, 1.8	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	B	0.38	0/8391	0.56	1/11492 (0.0%)
2	C	0.40	0/8174	0.56	0/11194
3	D	0.39	0/3398	0.56	2/4626 (0.0%)
3	P	0.40	0/3398	0.56	1/4626 (0.0%)
4	K	0.36	0/4971	0.54	1/6787 (0.0%)
4	L	0.36	0/4971	0.56	0/6787
4	M	0.35	0/4971	0.54	0/6787
5	O	0.40	0/10385	0.56	1/14172 (0.0%)
6	X	0.39	0/2957	0.53	0/4005
6	Y	0.36	0/2957	0.53	0/4005
6	Z	0.37	0/2957	0.53	0/4005
All	All	0.38	0/57530	0.55	6/78486 (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
1	B	0	1
2	C	0	1
4	L	0	1
4	M	0	2
5	O	0	1
6	X	0	1
All	All	0	7

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	O	1007	ARG	NE-CZ-NH1	-5.83	117.39	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	K	484	THR	C-N-CA	-5.68	107.50	121.70
3	D	7	LEU	CA-CB-CG	5.38	127.68	115.30
3	D	217	LEU	CA-CB-CG	-5.16	103.42	115.30
1	B	599	LEU	CA-CB-CG	-5.05	103.69	115.30

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	977	PHE	Peptide
2	C	383	THR	Peptide
4	L	615	ALA	Peptide
4	M	386	SER	Peptide
4	M	57	VAL	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	B	8171	0	8083	851	0
2	C	7958	0	7871	867	0
3	D	3313	0	3215	361	0
3	P	3313	0	3215	415	0
4	K	4871	0	4900	587	0
4	L	4871	0	4900	541	0
4	M	4871	0	4900	524	0
5	O	10127	0	9910	1080	0
6	X	2885	0	2816	282	0
6	Y	2885	0	2816	296	0
6	Z	2885	0	2816	298	0
All	All	56150	0	55442	5837	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 52.

The worst 5 of 5837 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)
5:O:1230:LEU:O	5:O:1276:THR:HA	1.45	1.14
1:B:760:GLU:O	1:B:764:TRP:HB2	1.46	1.14
5:O:704:THR:HA	5:O:758:ARG:O	1.47	1.12
4:K:68:SER:HG	4:K:97:ASP:N	1.47	1.11
4:L:142:THR:O	4:L:164:PRO:HA	1.50	1.10

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	B	1031/1035 (100%)	841 (82%)	190 (18%)	0	100	100
2	C	1004/1008 (100%)	820 (82%)	179 (18%)	5 (0%)	25	64
3	D	415/417 (100%)	343 (83%)	71 (17%)	1 (0%)	44	78
3	P	415/417 (100%)	352 (85%)	62 (15%)	1 (0%)	44	78
4	K	637/641 (99%)	548 (86%)	88 (14%)	1 (0%)	44	78
4	L	637/641 (99%)	536 (84%)	100 (16%)	1 (0%)	44	78
4	M	637/641 (99%)	550 (86%)	86 (14%)	1 (0%)	44	78
5	O	1280/1284 (100%)	1069 (84%)	211 (16%)	0	100	100
6	X	363/365 (100%)	309 (85%)	54 (15%)	0	100	100
6	Y	363/365 (100%)	317 (87%)	46 (13%)	0	100	100
6	Z	363/365 (100%)	296 (82%)	67 (18%)	0	100	100
All	All	7145/7179 (100%)	5981 (84%)	1154 (16%)	10 (0%)	50	83

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	1088	ASN
3	D	49	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	M	387	TYR
4	K	372	GLN
3	P	170	MET

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	B	915/915 (100%)	908 (99%)	7 (1%)	79	85
2	C	890/890 (100%)	882 (99%)	8 (1%)	75	83
3	D	352/352 (100%)	346 (98%)	6 (2%)	56	72
3	P	352/352 (100%)	346 (98%)	6 (2%)	56	72
4	K	541/541 (100%)	534 (99%)	7 (1%)	65	77
4	L	541/541 (100%)	537 (99%)	4 (1%)	81	87
4	M	541/541 (100%)	538 (99%)	3 (1%)	84	88
5	O	1118/1118 (100%)	1101 (98%)	17 (2%)	60	75
6	X	317/317 (100%)	312 (98%)	5 (2%)	58	74
6	Y	317/317 (100%)	315 (99%)	2 (1%)	84	88
6	Z	317/317 (100%)	314 (99%)	3 (1%)	75	83
All	All	6201/6201 (100%)	6133 (99%)	68 (1%)	69	80

5 of 68 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	P	333	ARG
6	X	78	ARG
6	Z	19	PHE
4	K	333	TRP
4	K	327	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 189 such sidechains are listed below:

Mol	Chain	Res	Type
4	M	613	GLN
3	P	84	HIS
5	O	180	ASN
5	O	804	HIS
3	P	242	ASN

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
2	C	1
4	L	1
4	M	1
4	K	1
1	B	1
5	O	1

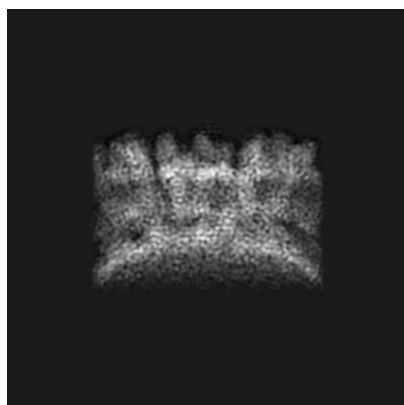
The worst 5 of 6 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	562:THR	C	571:LEU	N	14.85
1	L	71:ILE	C	97:ASP	N	12.37
1	M	71:ILE	C	97:ASP	N	11.46
1	K	71:ILE	C	97:ASP	N	9.27
1	B	583:PRO	C	584:SER	N	8.38

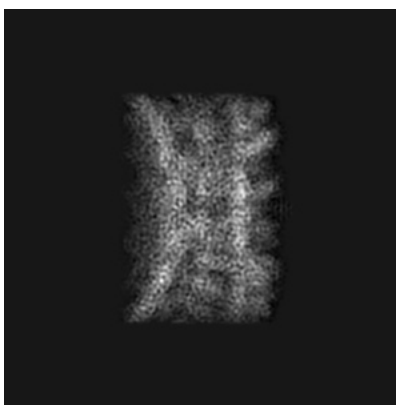
6 Tomogram visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-22166. These allow visual inspection of the internal detail of the tomogram and identification of artifacts.

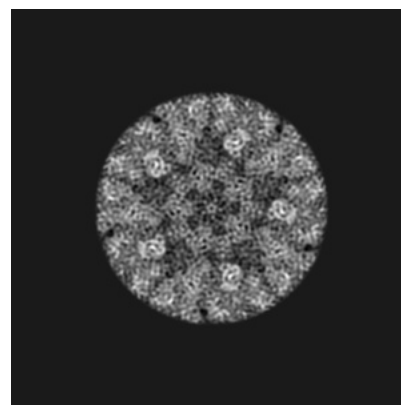
6.1 Orthogonal projections [i](#)



X



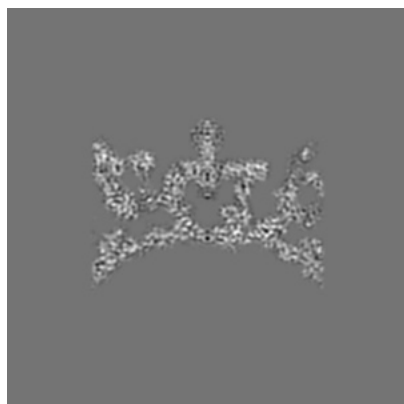
Y



Z

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

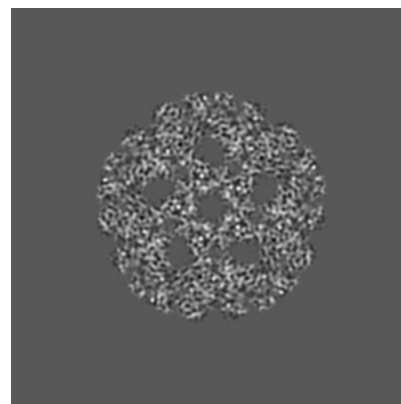
6.2 Central slices [i](#)



X Index: 180



Y Index: 180



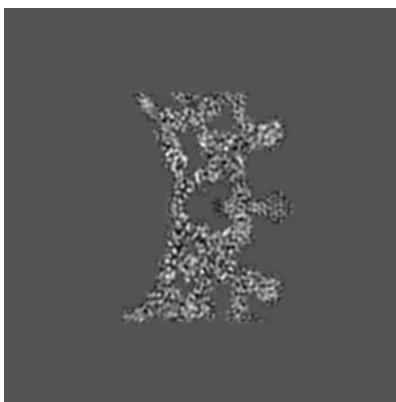
Z Index: 180

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

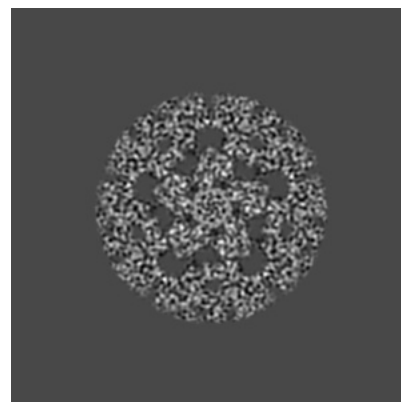
6.3 Largest variance slices [i](#)



X Index: 195



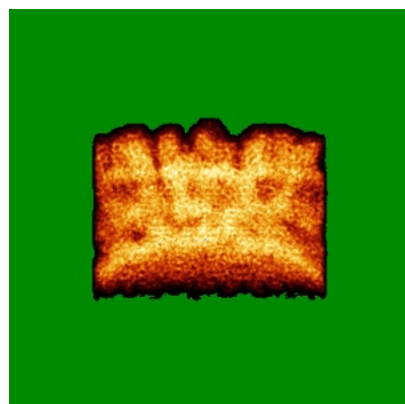
Y Index: 176



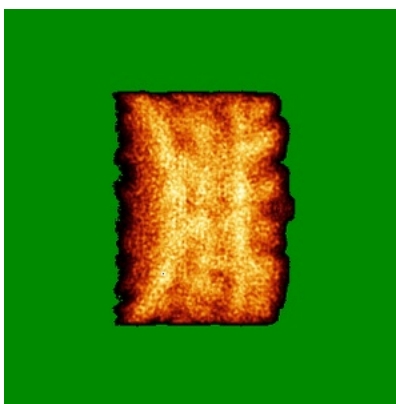
Z Index: 213

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

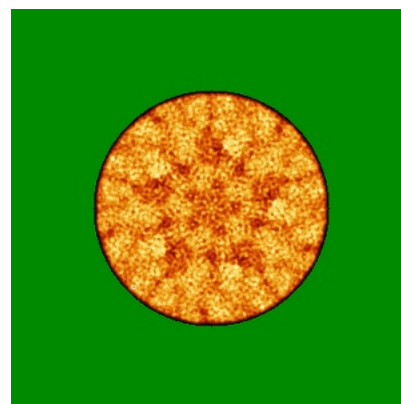
6.4 Orthogonal standard-deviation projections (False-color) [i](#)



X



Y



Z

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

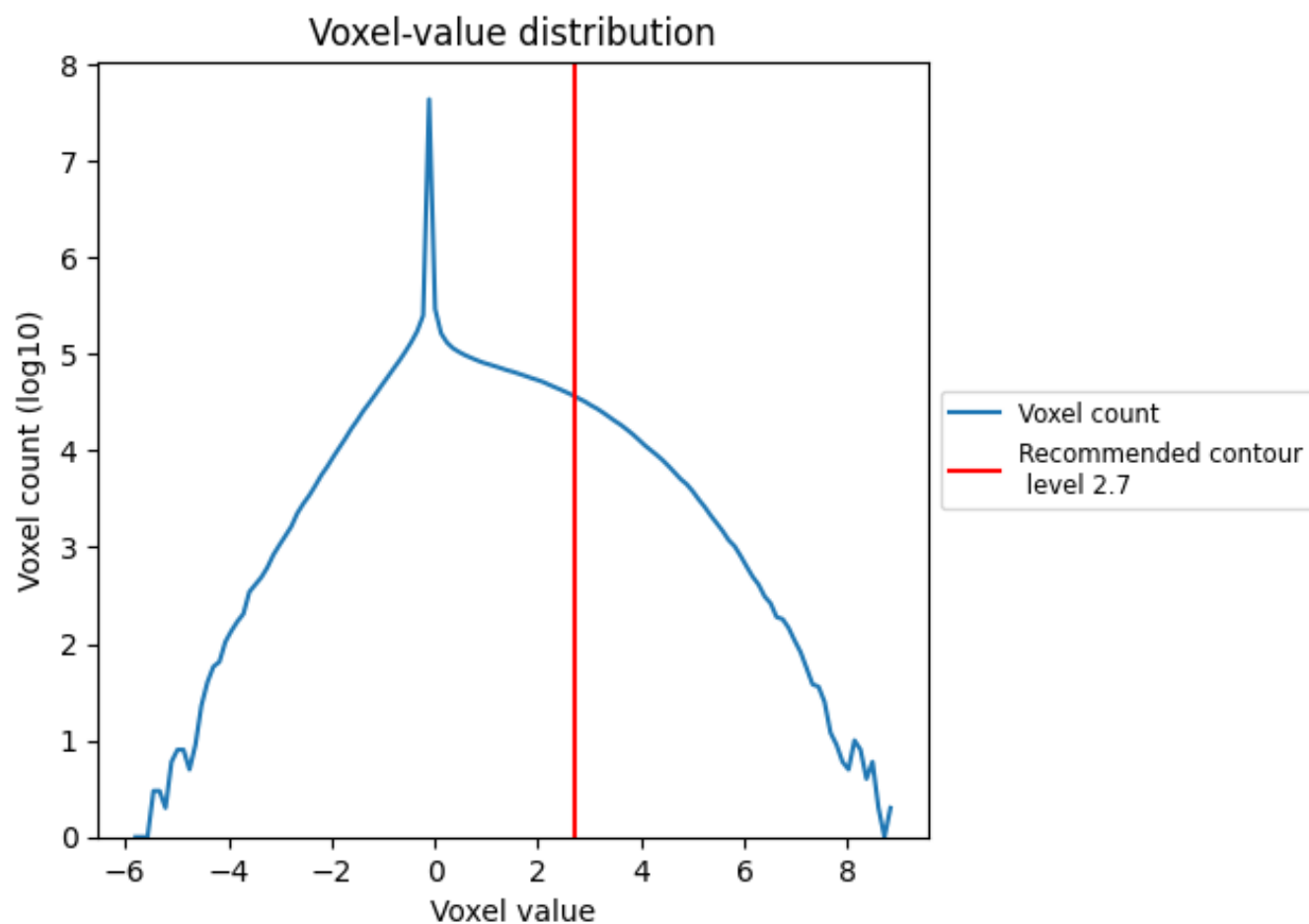
6.5 Mask visualisation [i](#)

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

7 Tomogram analysis [i](#)

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

7.1 Voxel-value distribution [i](#)



The voxel-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic.

8 Map-model fit [i](#)

This section contains information regarding the fit between EMD map EMD-22166 and PDB model 6ZTZ. Per-residue inclusion information can be found in section 3 on page 8.

8.1 Map-model overlay [i](#)

This section was not generated.

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

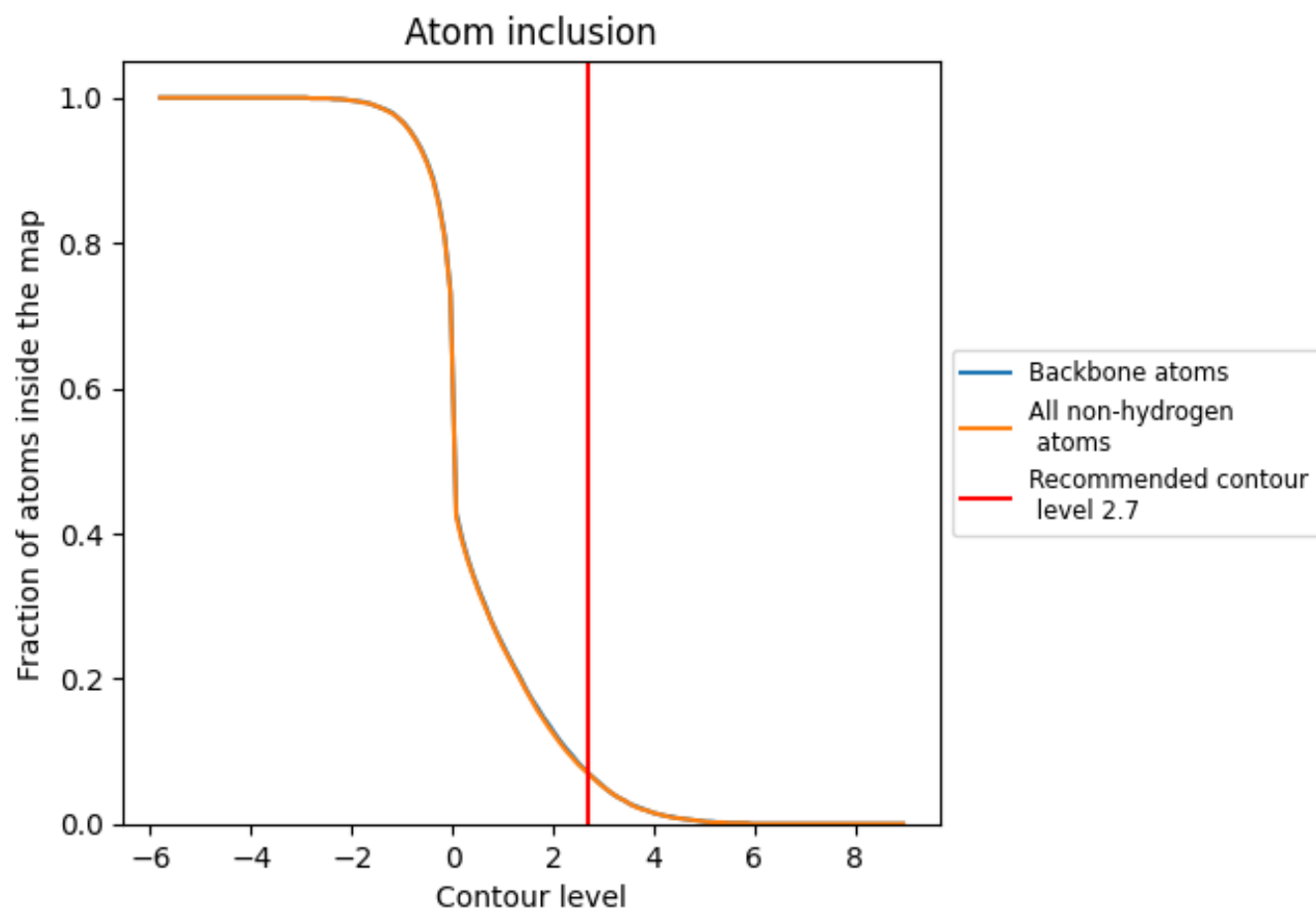


The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

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

This section was not generated.

8.4 Atom inclusion [i](#)



At the recommended contour level, 7% of all backbone atoms, 7% of all non-hydrogen atoms, are inside the map.

8.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (2.7) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.0690	<div></div> 0.0100
B	<div></div> 0.0010	<div></div> 0.0230
C	<div></div> 0.0530	<div></div> 0.0150
D	<div></div> 0.0450	<div></div> 0.0040
K	<div></div> 0.0870	<div></div> -0.0040
L	<div></div> 0.0870	<div></div> 0.0090
M	<div></div> 0.0830	<div></div> 0.0020
O	<div></div> 0.0910	<div></div> 0.0230
P	<div></div> 0.1510	<div></div> -0.0060
X	<div></div> 0.0720	<div></div> -0.0060
Y	<div></div> 0.0560	<div></div> -0.0050
Z	<div></div> 0.0830	<div></div> 0.0030

1.0

0.0

<0.0