



## wwPDB/EMDatabank EM Map/Model Validation Summary Report ⓘ

Sep 3, 2017 – 11:34 PM EDT

PDB ID : 5VKU  
EMDB ID: : EMD-8703  
Title : An atomic structure of the human cytomegalovirus (HCMV) capsid with its  
securing layer of pp150 tegument protein  
Authors : Yu, X.; Jih, J.; Jiang, J.; Zhou, H.  
Deposited on : unknown  
Resolution : 3.90 Å(reported)

This is a wwPDB/EMDatabank EM Map/Model Validation Summary Report  
for a publicly released PDB/EMDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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MolProbity : 4.02b-467  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20029824

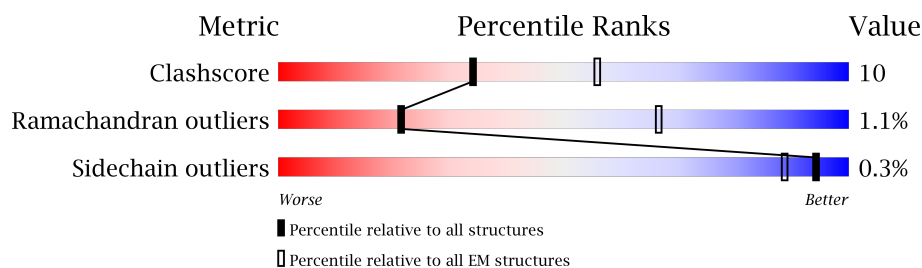
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.90 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.




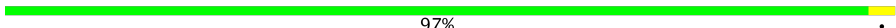
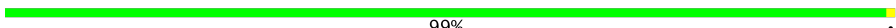
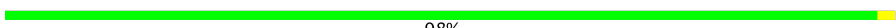
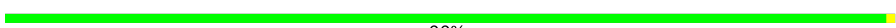








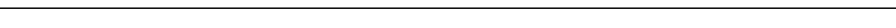











Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	0	285	
1	1	285	
1	2	285	
1	3	285	
1	4	285	
1	5	285	
1	6	285	
1	7	285	
1	8	285	
















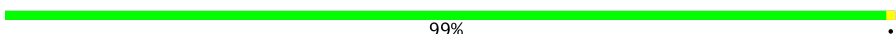
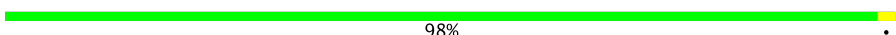
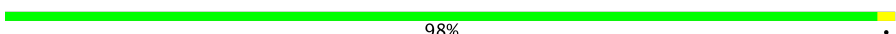


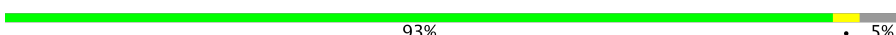
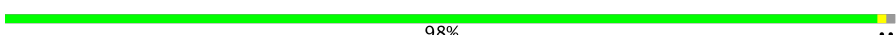
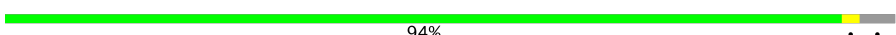
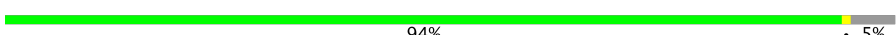
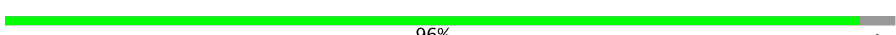
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Mol	Chain	Length	Quality of chain
1	9	285	
1	v	285	
1	w	285	
1	x	285	
1	y	285	
1	z	285	
2	A	1370	
2	B	1370	
2	C	1370	
2	D	1370	
2	E	1370	
2	F	1370	
2	G	1370	
2	H	1370	
2	I	1370	
2	J	1370	
2	K	1370	
2	L	1370	
2	M	1370	
2	N	1370	
2	O	1370	
2	P	1370	
3	Q	75	
3	R	75	
3	S	75	

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Mol	Chain	Length	Quality of chain
3	T	75	
3	U	75	
3	V	75	
3	W	75	
3	X	75	
3	Y	75	
3	Z	75	
3	a	75	
3	b	75	
3	c	75	
3	d	75	
3	e	75	
3	f	75	
4	g	290	
4	j	290	
4	m	290	
4	p	290	
4	s	290	
5	h	306	
5	i	306	
5	k	306	
5	l	306	
5	n	306	
5	o	306	
5	q	306	

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Mol	Chain	Length	Quality of chain
5	r	306	<div><div></div><div>97%</div><div></div></div> <div>..</div>
5	t	306	<div><div></div><div>95%</div><div></div></div> <div>. .</div>
5	u	306	<div><div></div><div>98%</div><div></div></div> <div>..</div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 248627 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 Tegument protein pp150.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	285	Total	C	N	O	S	0	0
			2328	1468	426	421	13		
1	1	285	Total	C	N	O	S	0	0
			2328	1468	426	421	13		
1	2	285	Total	C	N	O	S	0	0
			2328	1468	426	421	13		
1	3	285	Total	C	N	O	S	0	0
			2328	1468	426	421	13		
1	4	285	Total	C	N	O	S	0	0
			2328	1468	426	421	13		
1	5	285	Total	C	N	O	S	0	0
			2328	1468	426	421	13		
1	6	285	Total	C	N	O	S	0	0
			2328	1468	426	421	13		
1	7	285	Total	C	N	O	S	0	0
			2328	1468	426	421	13		
1	8	285	Total	C	N	O	S	0	0
			2328	1468	426	421	13		
1	9	285	Total	C	N	O	S	0	0
			2328	1468	426	421	13		
1	v	285	Total	C	N	O	S	0	0
			2328	1468	426	421	13		
1	w	285	Total	C	N	O	S	0	0
			2328	1468	426	421	13		
1	x	285	Total	C	N	O	S	0	0
			2328	1468	426	421	13		
1	y	285	Total	C	N	O	S	0	0
			2328	1468	426	421	13		
1	z	285	Total	C	N	O	S	0	0
			2328	1468	426	421	13		

- Molecule 2 is a protein called Major capsid protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	1329	Total	C	N	O	S	0	0
			10527	6711	1822	1933	61		
2	B	1335	Total	C	N	O	S	0	0
			10574	6733	1830	1950	61		
2	C	1349	Total	C	N	O	S	0	0
			10686	6805	1852	1968	61		
2	D	1346	Total	C	N	O	S	0	0
			10670	6796	1849	1964	61		
2	E	1347	Total	C	N	O	S	0	0
			10676	6799	1850	1966	61		
2	F	1350	Total	C	N	O	S	0	0
			10693	6809	1853	1970	61		
2	G	1351	Total	C	N	O	S	0	0
			10705	6816	1854	1974	61		
2	H	1352	Total	C	N	O	S	0	0
			10710	6819	1855	1975	61		
2	I	1347	Total	C	N	O	S	0	0
			10676	6799	1850	1966	61		
2	J	1335	Total	C	N	O	S	0	0
			10581	6739	1837	1945	60		
2	K	1348	Total	C	N	O	S	0	0
			10681	6802	1851	1967	61		
2	L	1353	Total	C	N	O	S	0	0
			10717	6823	1856	1977	61		
2	M	1353	Total	C	N	O	S	0	0
			10717	6823	1856	1977	61		
2	N	1350	Total	C	N	O	S	0	0
			10693	6809	1853	1970	61		
2	O	1348	Total	C	N	O	S	0	0
			10681	6802	1851	1967	61		
2	P	1348	Total	C	N	O	S	0	0
			10681	6802	1851	1967	61		

- Molecule 3 is a protein called Small capsomere-interacting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	Q	63	Total	C	N	O	S	0	0
			513	321	97	91	4		
3	R	63	Total	C	N	O	S	0	0
			513	321	97	91	4		
3	S	63	Total	C	N	O	S	0	0
			513	321	97	91	4		
3	T	63	Total	C	N	O	S	0	0
			513	321	97	91	4		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	U	63	Total	C	N	O	S	0	0
			513	321	97	91	4		
3	V	63	Total	C	N	O	S	0	0
			513	321	97	91	4		
3	W	63	Total	C	N	O	S	0	0
			513	321	97	91	4		
3	X	63	Total	C	N	O	S	0	0
			513	321	97	91	4		
3	Y	63	Total	C	N	O	S	0	0
			513	321	97	91	4		
3	Z	63	Total	C	N	O	S	0	0
			513	321	97	91	4		
3	a	63	Total	C	N	O	S	0	0
			513	321	97	91	4		
3	b	63	Total	C	N	O	S	0	0
			513	321	97	91	4		
3	c	63	Total	C	N	O	S	0	0
			513	321	97	91	4		
3	d	63	Total	C	N	O	S	0	0
			513	321	97	91	4		
3	e	63	Total	C	N	O	S	0	0
			513	321	97	91	4		
3	f	63	Total	C	N	O	S	0	0
			513	321	97	91	4		

- Molecule 4 is a protein called Triplex capsid protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	g	260	Total	C	N	O	S	0	0
			2091	1344	365	371	11		
4	j	290	Total	C	N	O	S	0	0
			2325	1485	411	417	12		
4	m	290	Total	C	N	O	S	0	0
			2325	1485	411	417	12		
4	p	290	Total	C	N	O	S	0	0
			2325	1485	411	417	12		
4	s	290	Total	C	N	O	S	0	0
			2325	1485	411	417	12		

- Molecule 5 is a protein called Triplex capsid protein 2.

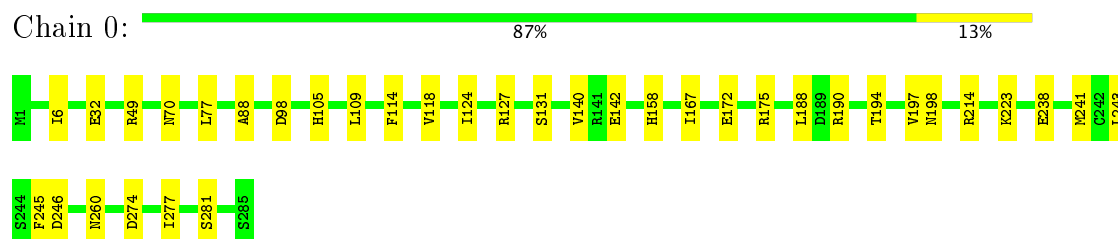


Mol	Chain	Residues	Atoms					AltConf	Trace
5	h	292	Total	C	N	O	S	0	0
			2316	1490	399	409	18		
5	i	285	Total	C	N	O	S	0	0
			2258	1454	386	401	17		
5	k	292	Total	C	N	O	S	0	0
			2317	1491	399	408	19		
5	l	303	Total	C	N	O	S	0	0
			2406	1541	419	428	18		
5	n	295	Total	C	N	O	S	0	0
			2334	1501	402	412	19		
5	o	291	Total	C	N	O	S	0	0
			2311	1484	398	411	18		
5	q	295	Total	C	N	O	S	0	0
			2334	1501	402	412	19		
5	r	304	Total	C	N	O	S	0	0
			2411	1544	420	429	18		
5	t	296	Total	C	N	O	S	0	0
			2342	1505	403	415	19		
5	u	304	Total	C	N	O	S	0	0
			2411	1544	420	429	18		

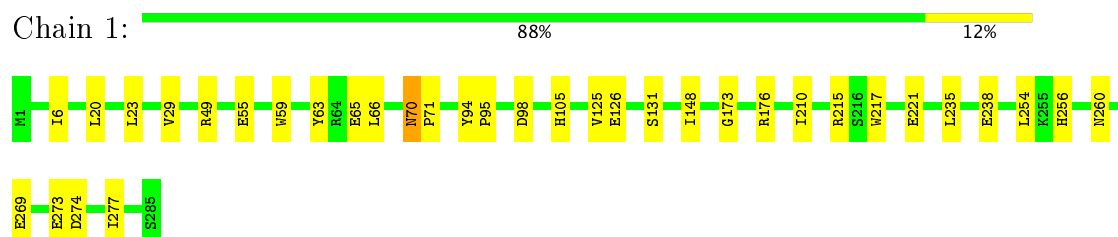
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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. 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. 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.

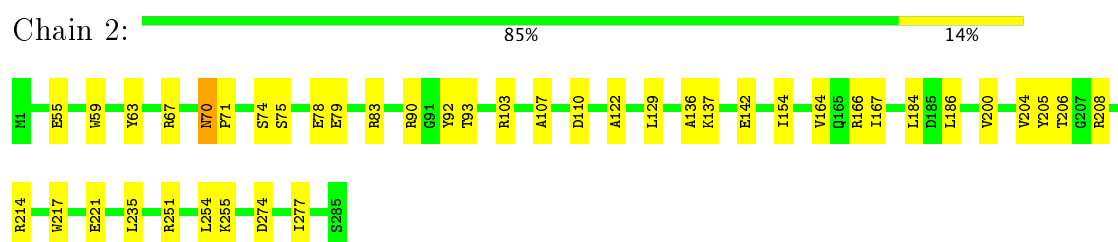
- Molecule 1: Tegument protein pp150



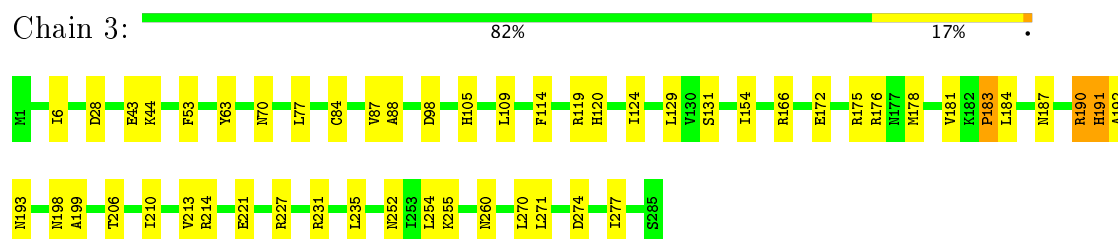
- Molecule 1: Tegument protein pp150




- Molecule 1: Tegument protein pp150

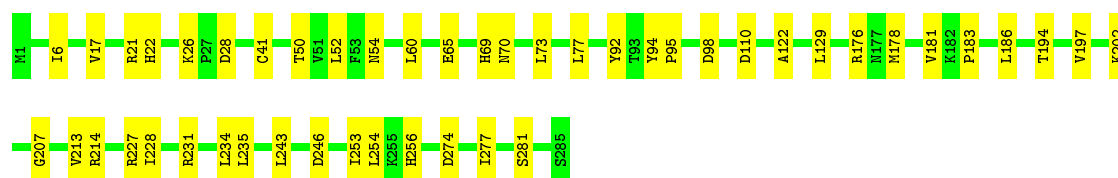


- Molecule 1: Tegument protein pp150




- Molecule 1: Tegument protein pp150

Chain 4:  84% 16%




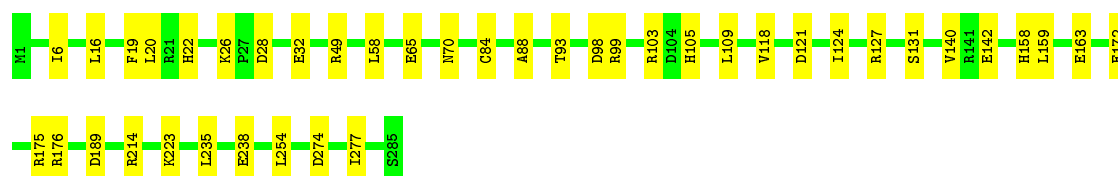
- Molecule 1: Tegument protein pp150

Chain 5:  84% 16%




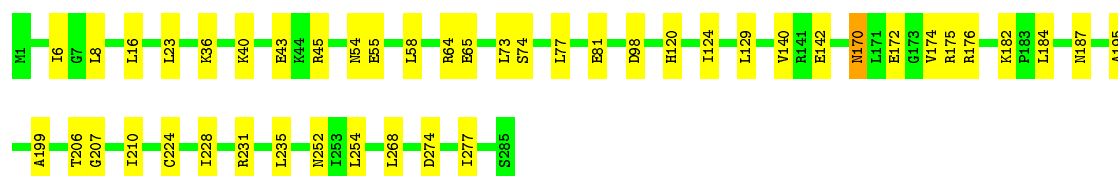
- Molecule 1: Tegument protein pp150

Chain 6:  86% 14%




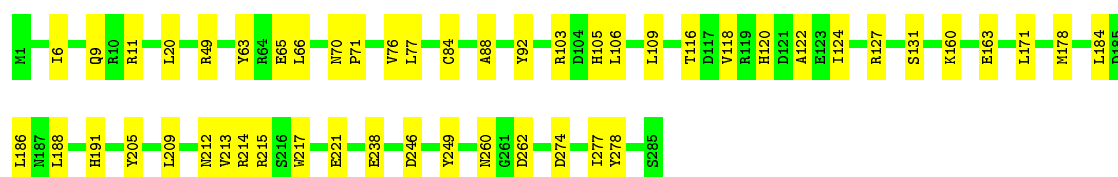
- Molecule 1: Tegument protein pp150

Chain 7:  84% 15%




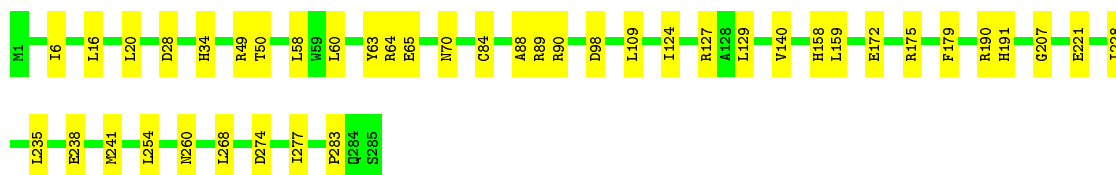
- Molecule 1: Tegument protein pp150

Chain 8:  82% 18%



- Molecule 1: Tegument protein pp150

Chain 9:  85% 15%



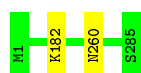
- Molecule 1: Tegument protein pp150

Chain v: 97%



- Molecule 1: Tegument protein pp150

Chain w: 99%



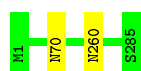
- Molecule 1: Tegument protein pp150

Chain x: 98%



- Molecule 1: Tegument protein pp150

Chain y: 99%



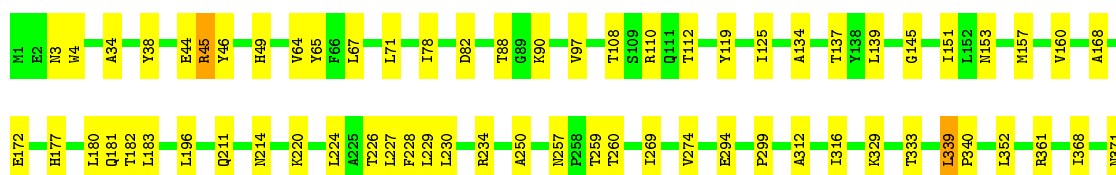
- Molecule 1: Tegument protein pp150

Chain z: 99%

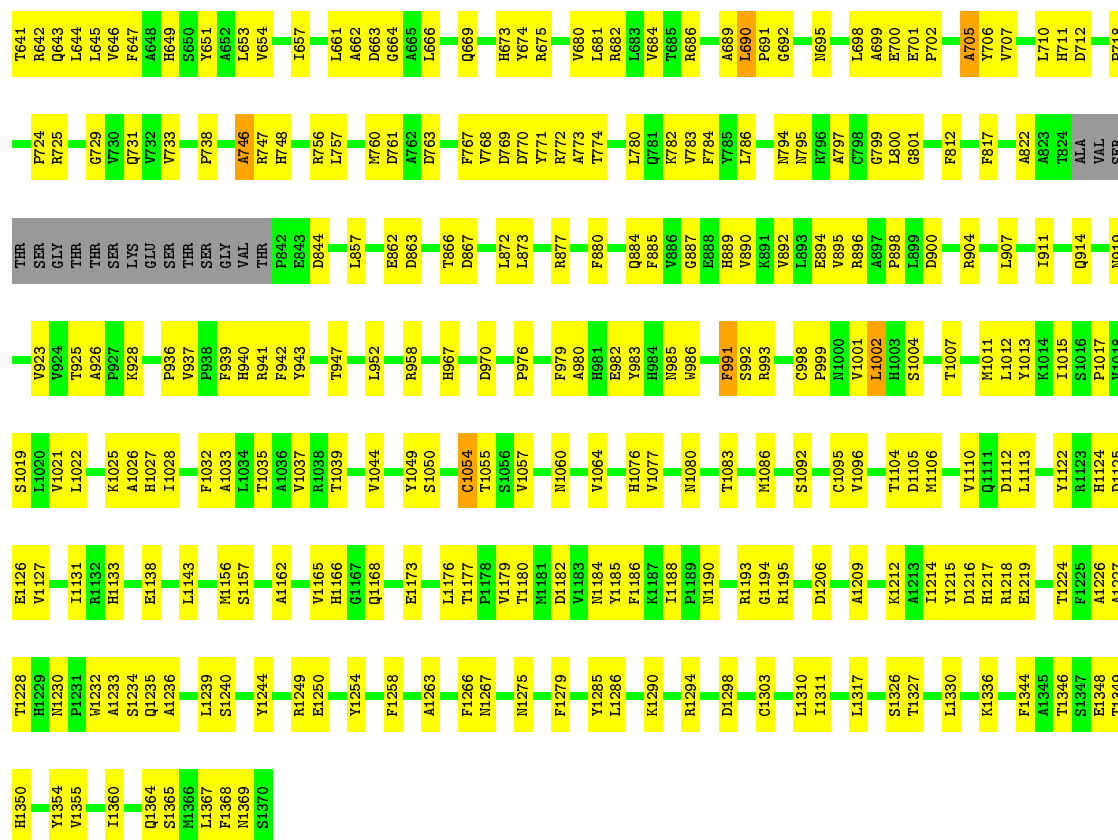


- Molecule 2: Major capsid protein

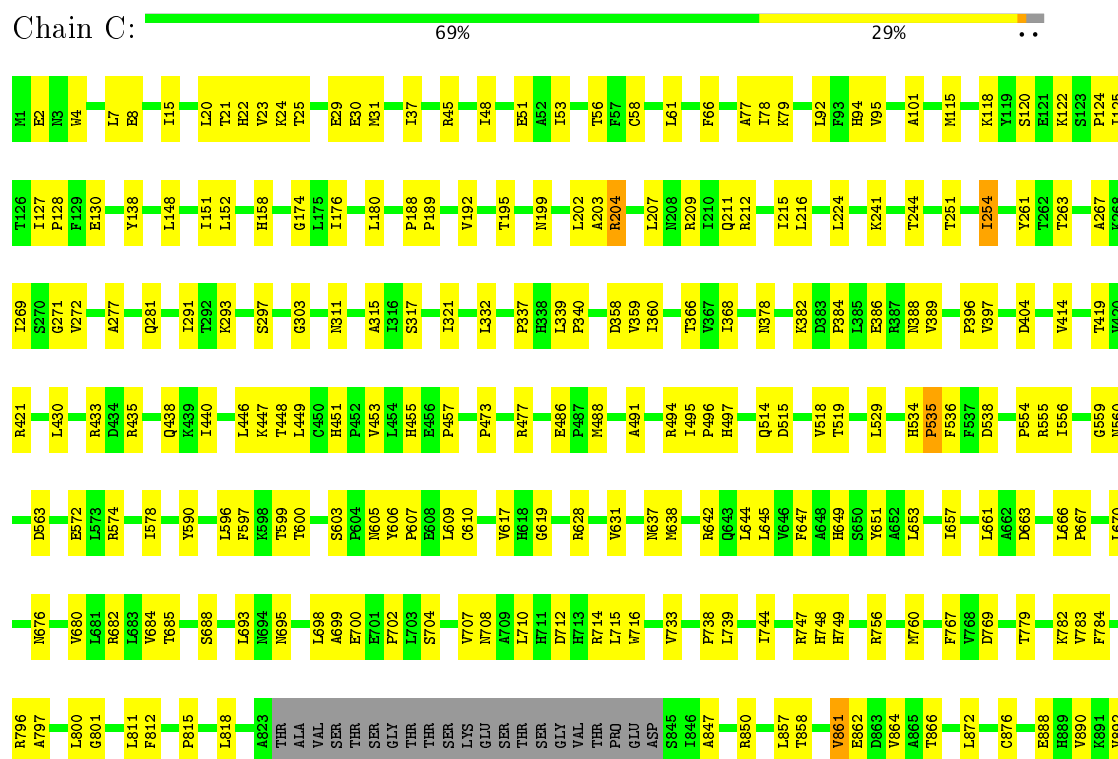
Chain A: 68%

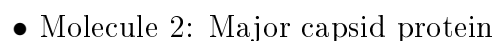


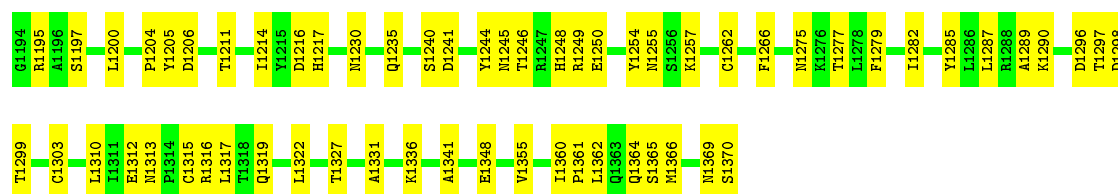
L372	A373	R374	V375	L385	P386	R387	P388	V389	L391	P395	P396	P397	Y400	P403	ASP	ARG	GLY	THR	THR	THR	VAL	GLU	SER	LYS	VAL	LYS	LEU	ASN	T419	L424	P425	T426	T427	L430	L431	R432	D434	R435	Q438	D441	F442	G564	L565	A566	P567	G568	H571																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																			
P457	A458	P459	C460	P469	P470	M475	Q476	R477	L478	L479	E480	C481	Q484	M488	I495	P496	R502	Q514	V517	V518	F521	Y522	K523	N524	N526	I527	Y530	H534	P535	F536	F537	Q543	R555	N560	L561	D562	G564	L565	A566	P567	G568	H571																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																								
E572	L573	L578	P587	T600	P607	G610	V611	H618	A623	S627	P630	R633	R638	L645	L653	L657	L661	P667	L670	L683	L687	S688	R694	R695	L703	S704	A705	Y706	L710	H711	D712	L715	H716	P717	P718	L772	R725	R726	R727	R728	R729	R730	R731	R732	R733	R734	R735	R736	R737	R738	R739	R740	R741	R742	R743	R744	R745	R746	R747	R748	R749	R750	R751	R752	R753	R754	R755	R756	R757	R758	R759	R760	R761	R762	R763	R764	R765	R766	R767	R768	R769	R770	R771	R772	R773	R774	R775	R776	R777	R778	R779	R780	R781	R782	R783	R784	R785	R786	R787	R788	R789	R790	R791	R792	R793	R794	R795	R796	R797	R798	R799	R800	R801	R802	R803	R804	R805	R806	R807	R808	R809	R810	R811	R812	R813	R814	R815	R816	R817	R818	R819	R820	R821	R822	R823	R824	R825	R826	R827	R828	R829	R830	R831	R832	R833	R834	R835	R836	R837	R838	R839	R840	R841	R842	R843	R844	R845	R846	R847	R848	R849	R850	R851	R852	R853	R854	R855	R856	R857	R858	R859	R860	R861	R862	R863	R864	R865	R866	R867	R868	R869	R870	R871	R872	R873	R874	R875	R876	R877	R878	R879	R880	R881	R882	R883	R884	R885	R886	R887	R888	R889	R890	R891	R892	R893	R894	R895	R896	R897	R898	R899	R900	R901	R902	R903	R904	R905	R906	R907	R908	R909	R910	R911	R912	R913	R914	R915	R916	R917	R918	R919	R920	R921	R922	R923	R924	R925	R926	R927	R928	R929	R930	R931	R932	R933	R934	R935	R936	R937	R938	R939	R940	R941	R942	R943	R944	R945	R946	R947	R948	R949	R950	R951	R952	R953	R954	R955	R956	R957	R958	R959	R960	R961	R962	R963	R964	R965	R966	R967	R968	R969	R970	R971	R972	R973	R974	R975	R976	R977	R978	R979	R980	R981	R982	R983	R984	R985	R986	R987	R988	R989	R990	R991	R992	R993	R994	R995	R996	R997	R998	R999	A1000	A1001	A1002	A1003	A1004	A1005	A1006	A1007	A1008	A1009	A1010	A1011	A1012	A1013	A1014	A1015	A1016	A1017	A1018	A1019	A1020	A1021	A1022	A1023	A1024	A1025	A1026	A1027	A1028	A1029	A1030	A1031	A1032	A1033	A1034	A1035	A1036	A1037	A1038	A1039	A1040	A1041	A1042	A1043	A1044	A1045	A1046	A1047	A1048	A1049	A1050	A1051	A1052	A1053	A1054	A1055	A1056	A1057	A1058	A1059	A1060	A1061	A1062	A1063	A1064	A1065	A1066	A1067	A1068	A1069	A1070	A1071	A1072	A1073	A1074	A1075	A1076	A1077	A1078	A1079	A1080	A1081	A1082	A1083	A1084	A1085	A1086	A1087	A1088	A1089	A1090	A1091	A1092	A1093	A1094	A1095	A1096	A1097	A1098	A1099	A1100	A1101	A1102	A1103	A1104	A1105	A1106	A1107	A1108	A1109	A1110	A1111	A1112	A1113	A1114	A1115	A1116	A1117	A1118	A1119	A1120	A1121	A1122	A1123	A1124	A1125	A1126	A1127	A1128	A1129	A1130	A1131	A1132	A1133	A1134	A1135	A1136	A1137	A1138	A1139	A1140	A1141	A1142	A1143	A1144	A1145	A1146	A1147	A1148	A1149	A1150	A1151	A1152	A1153	A1154	A1155	A1156	A1157	A1158	A1159	A1160	A1161	A1162	A1163	A1164	A1165	A1166	A1167	A1168	A1169	A1170	A1171	A1172	A1173	A1174	A1175	A1176	A1177	A1178	A1179	A1180	A1181	A1182	A1183	A1184	A1185	A1186	A1187	A1188	A1189	A1190	A1191	A1192	A1193	A1194	A1195	A1196	A1197	A1198	A1199	A1200	A1201	A1202	A1203	A1204	A1205	A1206	A1207	A1208	A1209	A1210	A1211	A1212	A1213	A1214	A1215	A1216	A1217	A1218	A1219	A1220	A1221	A1222	A1223	A1224	A1225	A1226	A1227	A1228	A1229	A1230	A1231	A1232	A1233	A1234	A1235	A1236	A1237	A1238	A1239	A1240	A1241	A1242	A1243	A1244	A1245	A1246	A1247	A1248	A1249	A1250	A1251	A1252	A1253	A1254	A1255	A1256	A1257	A1258	A1259	A1260	A1261	A1262	A1263	A1264	A1265	A1266	A1267	A1268	A1269	A1270	A1271	A1272	A1273	A1274	A1275	A1276	A1277	A1278	A1279	A1280	A1281	A1282	A1283	A1284	A1285	A1286	A1287	A1288	A1289	A1290	A1291	A1292	A1293	A1294	A1295	A1296	A1297	A1298	A1299	A1300	A1301	A1302	A1303	A1304	A1305	A1306	A1307	A1308	A1309	A1310	A1311	A1312	A1313	A1314	A1315	A1316	A1317	A1318	A1319	A1320	A1321	A1322	A1323	A1324	A1325	A1326	A1327	A1328	A1329	A1330	A1331	A1332	A1333	A1334	A1335	A1336	A1337	A1338	A1339	A1340	A1341	A1342	A1343	A1344	A1345	A1346	A1347	A1348	A1349	A1350	A1351	A1352	A1353	A1354	A1355	A1356	A1357	A1358	A1359	A1360	A1361	A1362	A1363	A1364	A1365	A1366	A1367	A1368	A1369	A1370	A1371	A1372	A1373	A1374	A1375	A1376	A1377	A1378	A1379	A1380	A1381	A1382	A1383	A1384	A1385	A1386	A1387	A1388	A1389	A1390	A1391	A1392	A1393	A1394	A1395	A1396	A1397	A1398	A1399	A1400	A1401	A1402	A1403	A1404	A1405	A1406	A1407	A1408	A1409	A1410	A1411	A1412	A1413	A1414	A1415	A1416	A1417	A1418	A1419	A1420	A1421	A1422	A1423	A1424	A1425	A1426	A1427	A1428	A1429	A1430	A1431	A1432	A1433	A1434	A1435	A1436	A1437	A1438	A1439	A1440	A1441	A1442	A1443	A1444	A1445	A1446	A1447	A1448	A1449	A1450	A1451	A1452	A1453	A1454	A1455	A1456	A1457	A1458	A1459	A1460	A1461	A1462	A1463	A1464	A1465	A1466	A1467	A1468	A1469	A1470	A1471	A1472	A1473	A1474	A1475	A1476	A1477	A1478	A1479	A1480	A1481	A1482	A1483	A1484	A1485	A1486	A1487	A1488	A1489	A1490	A1491	A1492	A1493	A1494	A1495	A1496	A1497	A1498	A1499	A1500	A1501	A1502	A1503	A1504	A1505	A1506	A1507	A1508	A1509	A1510	A1511	A1512	A1513	A1514	A1515	A1516	A1517	A1518	A1519	A1520	A1521	A1522	A1523	A1524	A1525	A1526	A1527	A1528	A1529	A1530	A1531	A1532	A1533	A1534	A1535	A1536	A1537	A1538	A1539	A1540	A1541	A1542	A1543	A1544	A1545	A1546	A1547	A1548	A1549	A1550	A1551	A1552	A1553	A1554	A1555	A1556	A1557	A1558	A1559	A1560	A1561	A1562	A1563	A1564	A1565	A1566	A1567	A1568	A1569	A1570	A1571	A1572	A1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- Molecule 2: Major capsid protein

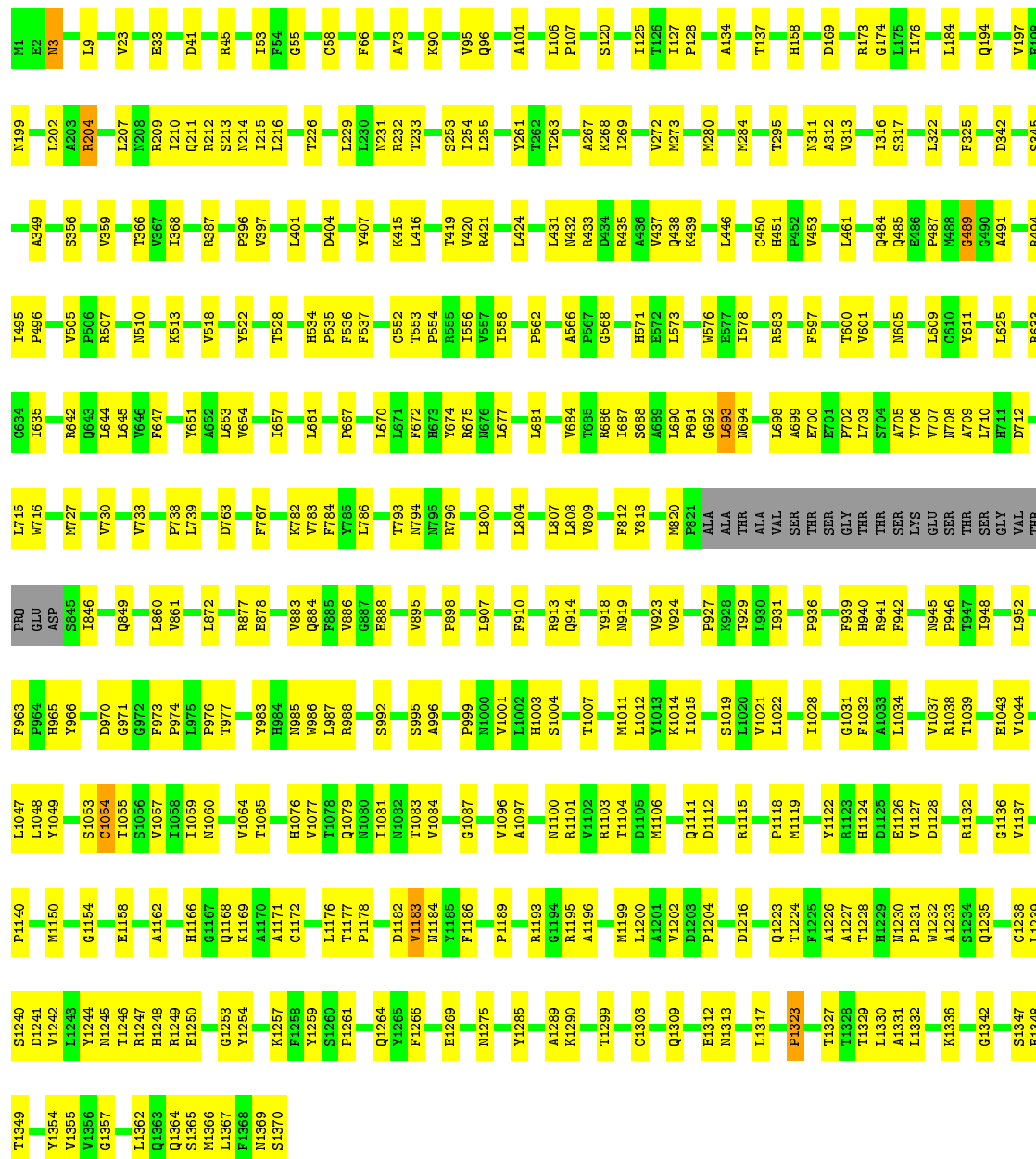






• Molecule 2: Major capsid protein

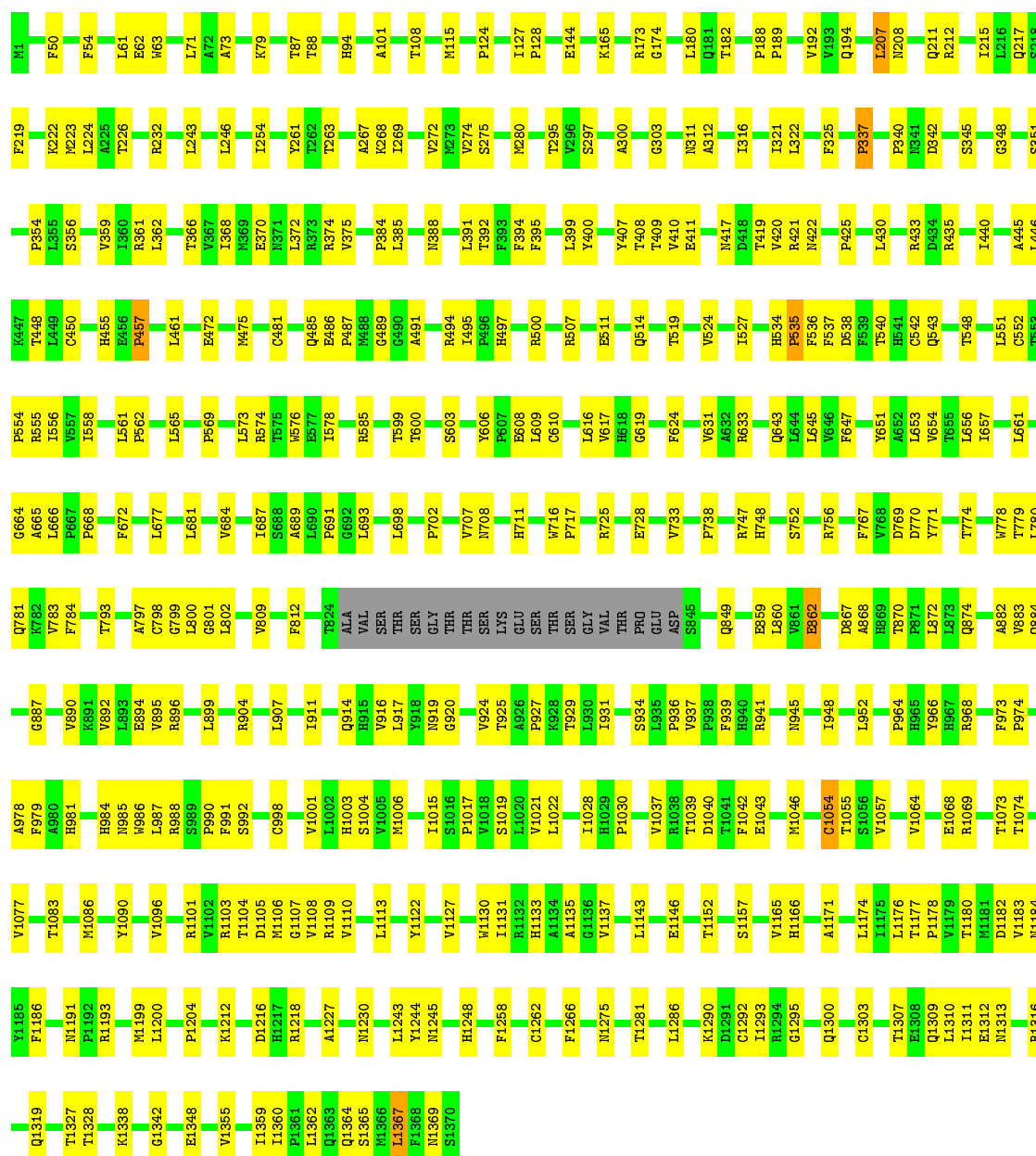
Chain E: 69% 28% ..



• Molecule 2: Major capsid protein

Chain F: 70% 28% ..

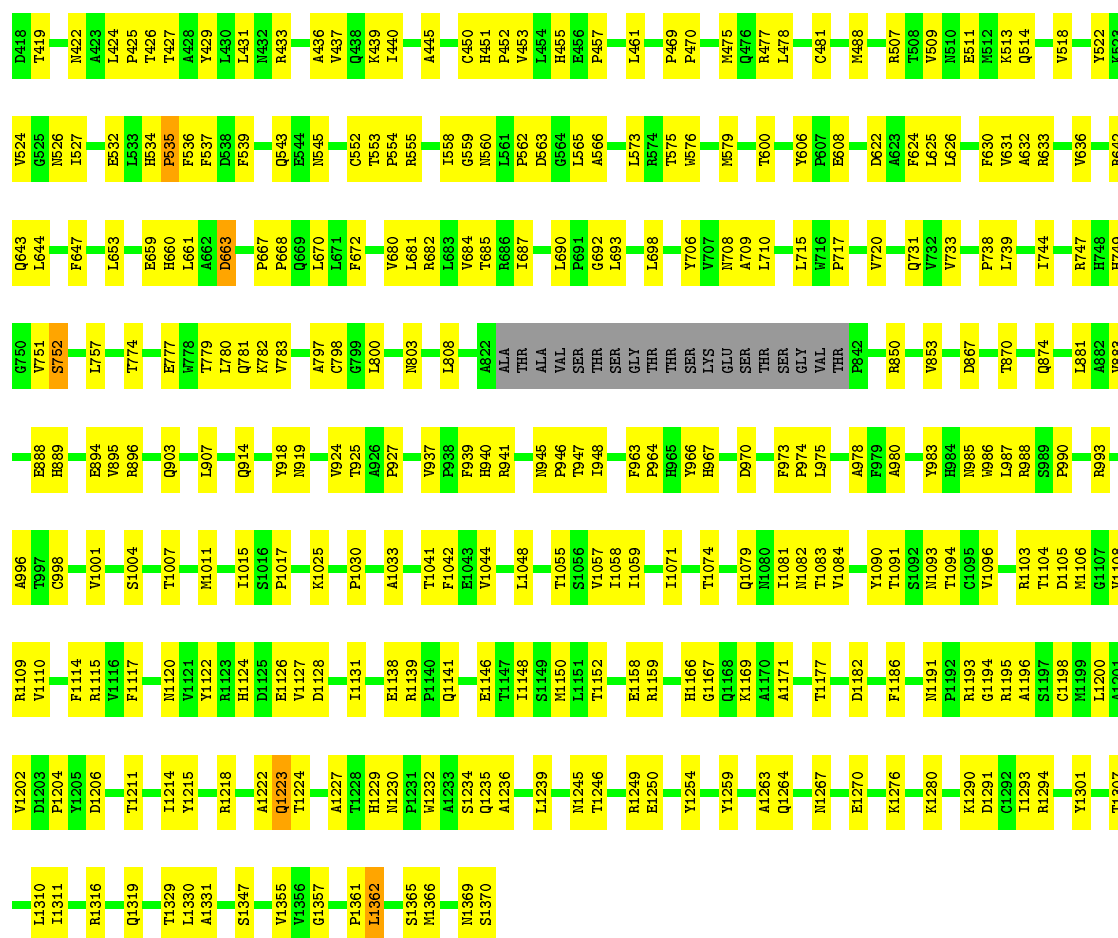




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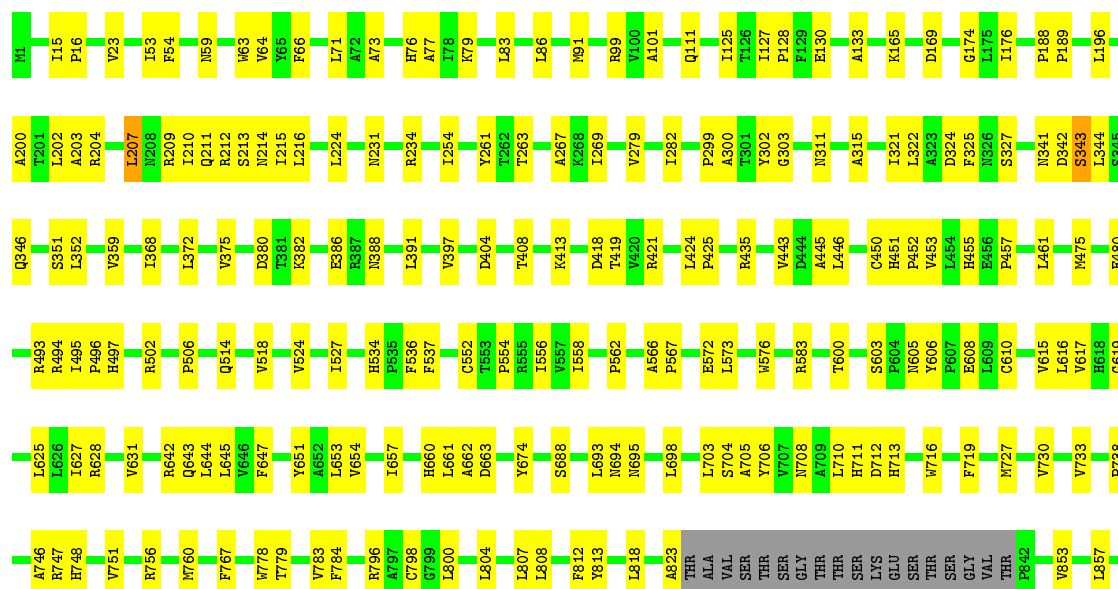
Chain G: 70% 28% .





- Molecule 2: Major capsid protein

Chain H:  73% 26%

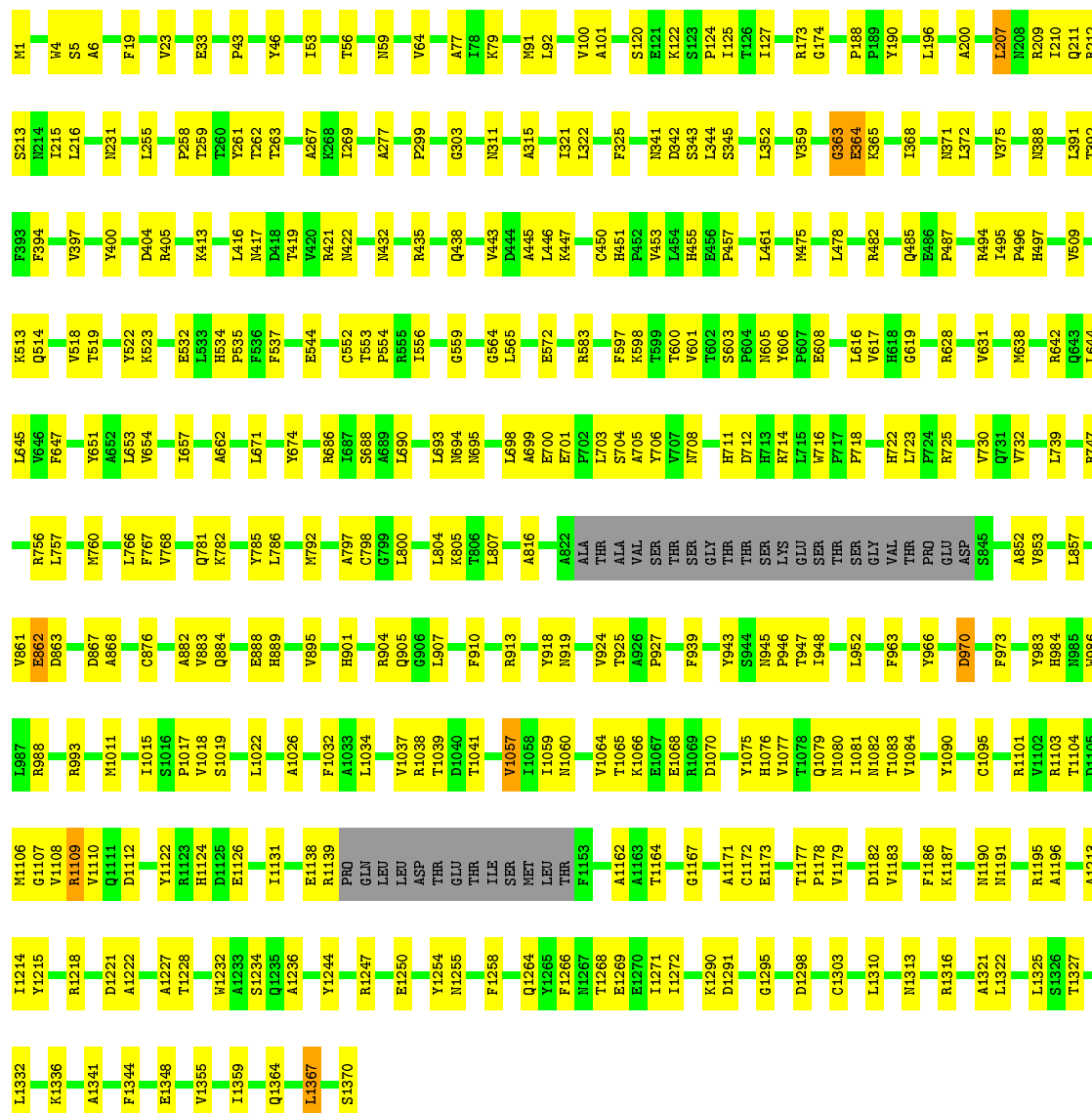






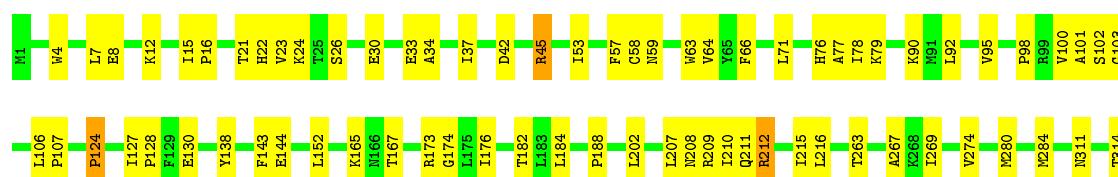
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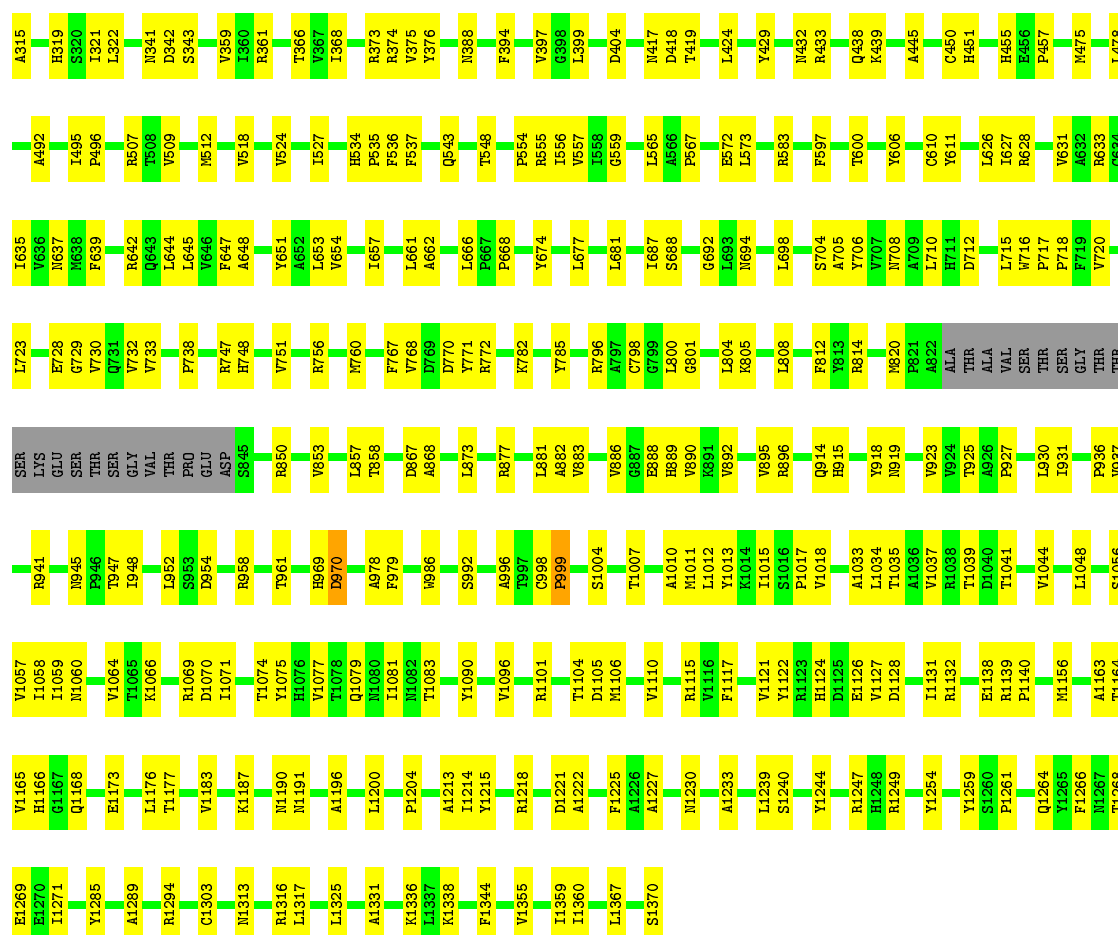
Chain J: 72% 25%



• Molecule 2: Major capsid protein

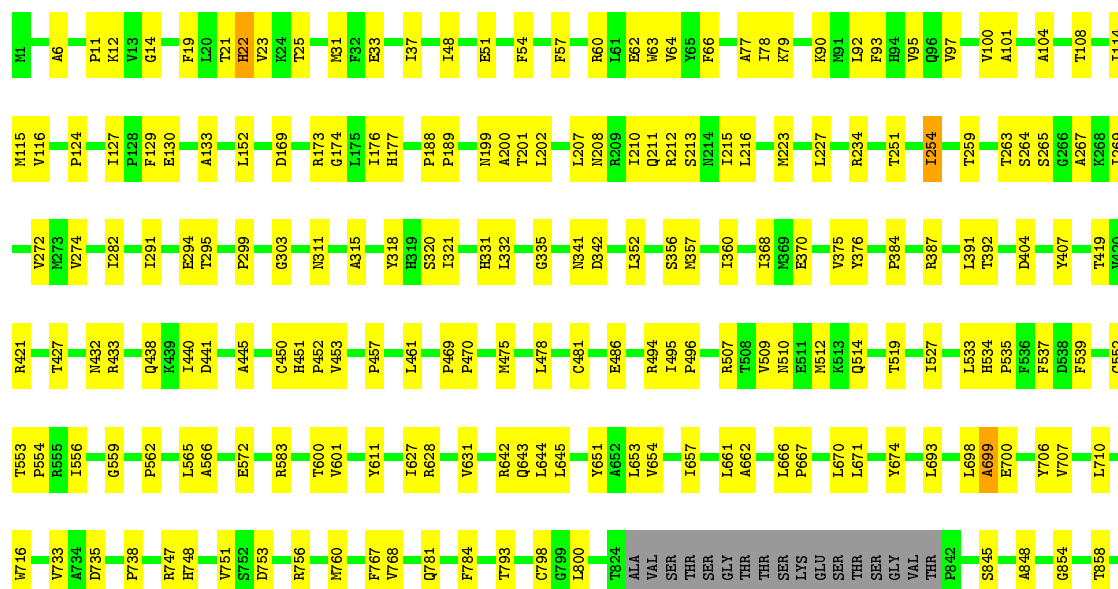
Chain K: 72% 26%

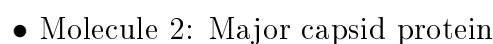




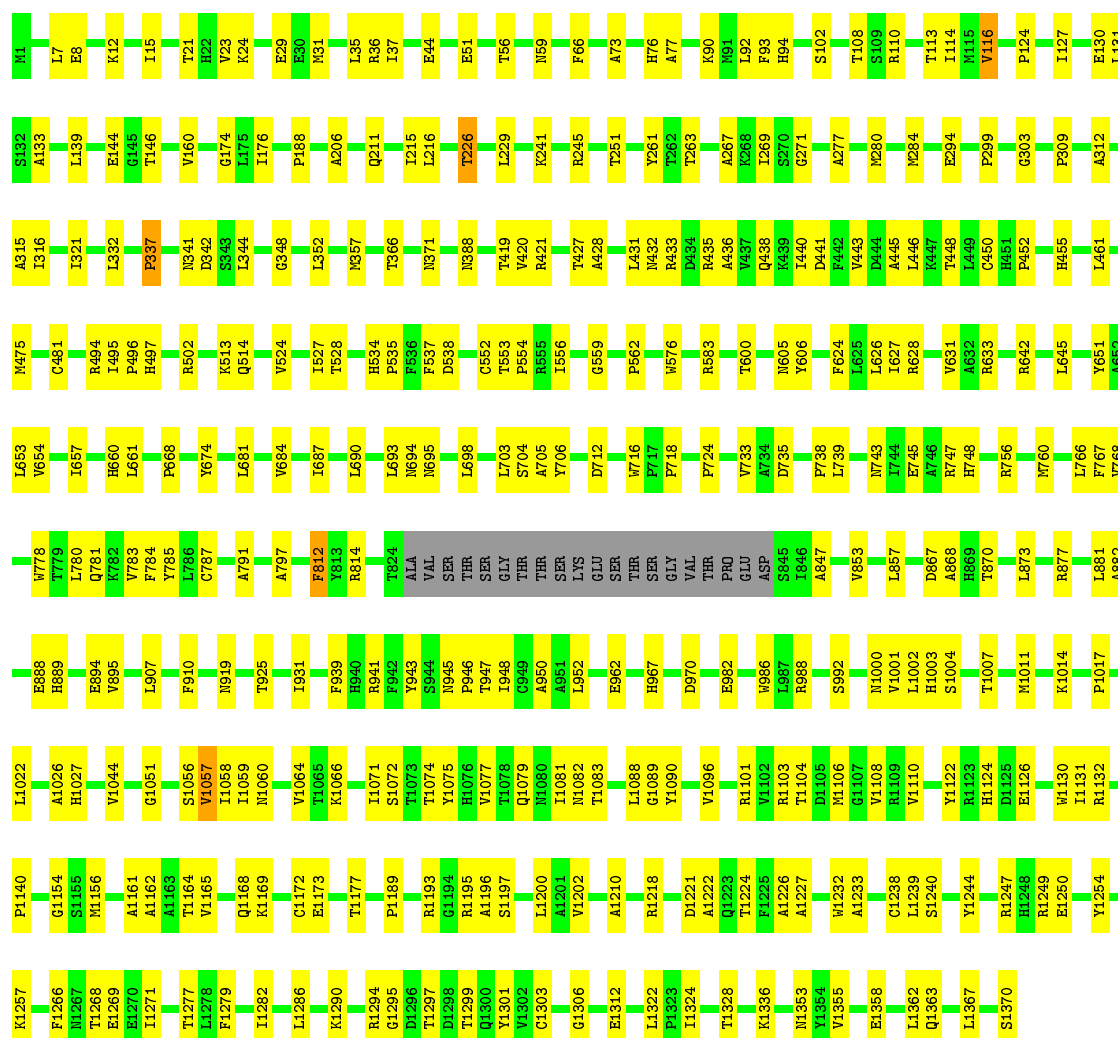
- Molecule 2: Major capsid protein

Chain L:  74% 24% ..



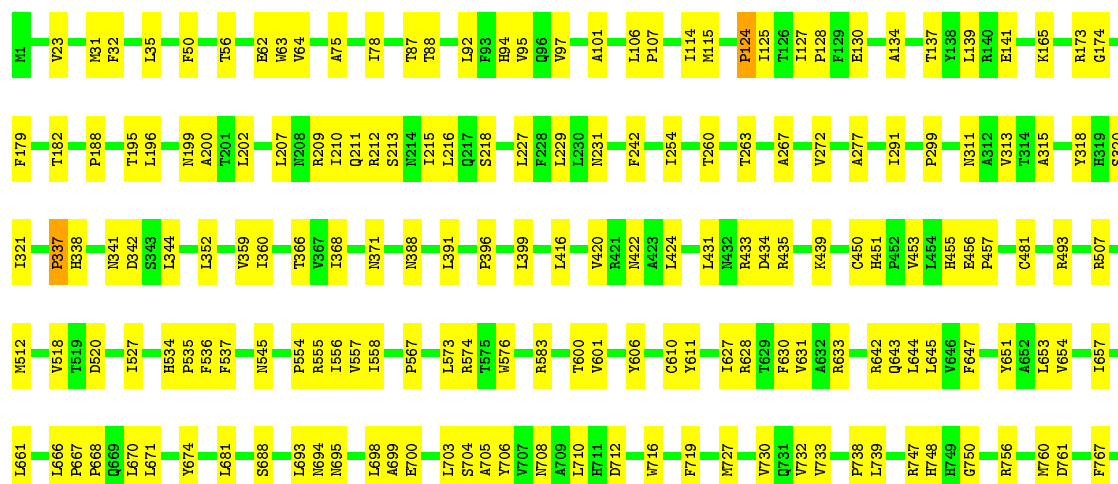


Chain N:  75% 24%



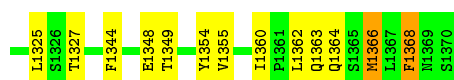
- Molecule 2: Major capsid protein

Chain 0:  73% 25%

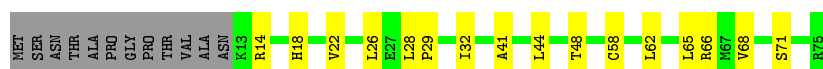


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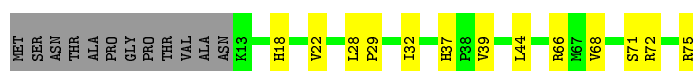




- Molecule 3: Small capsomere-interacting protein



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- Molecule 3: Small capsomere-interacting protein



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- Molecule 3: Small capsomere-interacting protein



- Molecule 3: Small capsomere-interacting protein

Chain X:  64% 20% 16%



- Molecule 3: Small capsomere-interacting protein

Chain Y:  71% 13% 16%




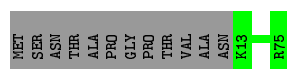
- Molecule 3: Small capsomere-interacting protein

Chain Z:  73% 11% 16%




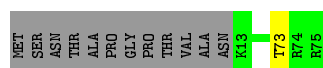
- Molecule 3: Small capsomere-interacting protein

Chain a:  84% 16%




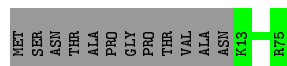
- Molecule 3: Small capsomere-interacting protein

Chain b:  83% 16%




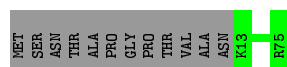
- Molecule 3: Small capsomere-interacting protein

Chain c:  84% 16%




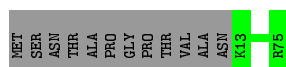
- Molecule 3: Small capsomere-interacting protein

Chain d:  84% 16%



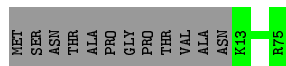
- Molecule 3: Small capsomere-interacting protein

Chain e:  84% 16%



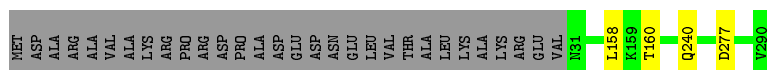
- Molecule 3: Small capsomere-interacting protein

Chain f: 84% 16%



- Molecule 4: Triplex capsid protein 1

Chain g: 88% 10%



- Molecule 4: Triplex capsid protein 1

Chain j: 98%



- Molecule 4: Triplex capsid protein 1

Chain m: 99%



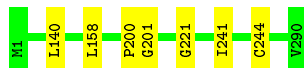
- Molecule 4: Triplex capsid protein 1

Chain p: 98%



- Molecule 4: Triplex capsid protein 1

Chain s: 98%



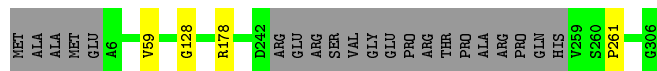
- Molecule 5: Triplex capsid protein 2

Chain h: 92% 5%



- Molecule 5: Triplex capsid protein 2

Chain i:  92% • 7%



- Molecule 5: Triplex capsid protein 2

Chain k:  93% • 5%



- Molecule 5: Triplex capsid protein 2

Chain l:  98% ••



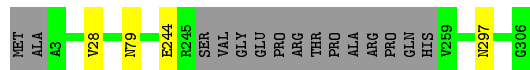
- Molecule 5: Triplex capsid protein 2

Chain n:  94% ••



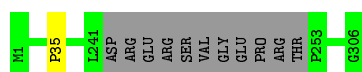
- Molecule 5: Triplex capsid protein 2

Chain o:  94% • 5%



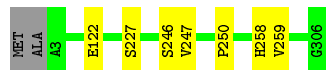
- Molecule 5: Triplex capsid protein 2

Chain q:  96% •



- Molecule 5: Triplex capsid protein 2

Chain r:  97% ••



- Molecule 5: Triplex capsid protein 2

Chain t: 

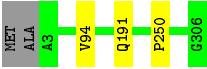
95%



• Molecule 5: Triplex capsid protein 2

Chain u: 

98%



## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, 1	Depositor
Number of particles used	39600	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 ( $e^-/\text{\AA}^2$ )	2.7	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	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	$\# Z  > 2$	RMSZ	$\# Z  > 2$
1	0	0.23	0/2366	0.37	0/3192
1	1	0.23	0/2366	0.38	0/3192
1	2	0.23	0/2366	0.38	0/3192
1	3	0.23	0/2366	0.37	0/3192
1	4	0.23	0/2366	0.38	0/3192
1	5	0.23	0/2366	0.37	0/3192
1	6	0.23	0/2366	0.37	0/3192
1	7	0.23	0/2366	0.38	0/3192
1	8	0.23	0/2366	0.37	0/3192
1	9	0.23	0/2366	0.38	0/3192
1	v	0.23	0/2366	0.38	0/3192
1	w	0.23	0/2366	0.38	0/3192
1	x	0.23	0/2366	0.38	0/3192
1	y	0.23	0/2366	0.37	0/3192
1	z	0.23	0/2366	0.37	0/3192
2	A	0.25	0/10780	0.44	0/14685
2	B	0.25	0/10824	0.44	0/14743
2	C	0.25	0/10942	0.44	1/14906 (0.0%)
2	D	0.25	0/10926	0.44	0/14884
2	E	0.25	0/10932	0.44	0/14892
2	F	0.25	0/10949	0.43	0/14916
2	G	0.25	0/10962	0.43	0/14933
2	H	0.25	0/10967	0.43	0/14940
2	I	0.25	0/10932	0.43	1/14892 (0.0%)
2	J	0.25	0/10835	0.43	1/14757 (0.0%)
2	K	0.25	0/10937	0.44	0/14899
2	L	0.25	0/10974	0.43	0/14950
2	M	0.25	0/10974	0.43	0/14950
2	N	0.25	0/10949	0.43	0/14916
2	O	0.25	0/10937	0.43	0/14899
2	P	0.25	0/10937	0.43	0/14899
3	Q	0.22	0/520	0.38	0/697
3	R	0.23	0/520	0.38	0/697
3	S	0.24	0/520	0.38	0/697

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >2	RMSZ	# Z  >2
3	T	0.24	0/520	0.38	0/697
3	U	0.23	0/520	0.38	0/697
3	V	0.23	0/520	0.37	0/697
3	W	0.23	0/520	0.37	0/697
3	X	0.23	0/520	0.38	0/697
3	Y	0.23	0/520	0.37	0/697
3	Z	0.23	0/520	0.38	0/697
3	a	0.23	0/520	0.37	0/697
3	b	0.23	0/520	0.37	0/697
3	c	0.23	0/520	0.38	0/697
3	d	0.23	0/520	0.37	0/697
3	e	0.23	0/520	0.37	0/697
3	f	0.23	0/520	0.37	0/697
4	g	0.24	0/2138	0.44	0/2903
4	j	0.25	0/2374	0.43	0/3221
4	m	0.24	0/2374	0.43	0/3221
4	p	0.25	0/2374	0.43	0/3221
4	s	0.25	0/2374	0.43	0/3221
5	h	0.25	0/2361	0.44	0/3206
5	i	0.25	0/2300	0.46	0/3124
5	k	0.25	0/2361	0.43	0/3207
5	l	0.24	0/2453	0.43	0/3332
5	n	0.24	0/2379	0.45	1/3230 (0.0%)
5	o	0.24	0/2353	0.42	0/3193
5	q	0.24	0/2379	0.43	0/3230
5	r	0.24	0/2458	0.43	0/3339
5	t	0.25	0/2387	0.45	0/3241
5	u	0.24	0/2458	0.43	0/3339
All	All	0.25	0/254090	0.42	4/345321 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1367	LEU	CB-CG-CD2	-6.90	99.26	111.00
2	J	1367	LEU	CB-CG-CD1	-6.42	100.09	111.00
2	I	1367	LEU	CB-CG-CD2	-5.55	101.56	111.00
5	n	124	LEU	CA-CB-CG	5.21	127.28	115.30

There are no chirality outliers.

There are no planarity outliers.



## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	2328	0	2363	20	0
1	1	2328	0	2363	19	0
1	2	2328	0	2363	21	0
1	3	2328	0	2363	29	0
1	4	2328	0	2363	25	0
1	5	2328	0	2363	23	0
1	6	2328	0	2363	23	0
1	7	2328	0	2363	24	0
1	8	2328	0	2363	29	0
1	9	2328	0	2363	23	0
1	v	2328	0	2363	0	0
1	w	2328	0	2363	0	0
1	x	2328	0	2363	0	0
1	y	2328	0	2363	0	0
1	z	2328	0	2363	0	0
2	A	10527	0	10474	280	0
2	B	10574	0	10522	296	0
2	C	10686	0	10628	298	0
2	D	10670	0	10613	311	0
2	E	10676	0	10618	281	0
2	F	10693	0	10635	259	0
2	G	10705	0	10641	270	0
2	H	10710	0	10646	258	0
2	I	10676	0	10618	238	0
2	J	10581	0	10518	248	0
2	K	10681	0	10623	267	0
2	L	10717	0	10653	254	0
2	M	10717	0	10653	250	0
2	N	10693	0	10635	225	0
2	O	10681	0	10623	248	0
2	P	10681	0	10623	224	0
3	Q	513	0	539	14	0
3	R	513	0	539	9	0
3	S	513	0	539	7	0
3	T	513	0	539	10	0
3	U	513	0	539	11	0
3	V	513	0	539	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	W	513	0	539	5	0
3	X	513	0	539	11	0
3	Y	513	0	539	7	0
3	Z	513	0	539	7	0
3	a	513	0	539	0	0
3	b	513	0	539	0	0
3	c	513	0	539	0	0
3	d	513	0	539	0	0
3	e	513	0	539	0	0
3	f	513	0	539	0	0
4	g	2091	0	2120	0	0
4	j	2325	0	2363	0	0
4	m	2325	0	2363	0	0
4	p	2325	0	2363	0	0
4	s	2325	0	2363	0	0
5	h	2316	0	2409	0	0
5	i	2258	0	2350	0	0
5	k	2317	0	2415	0	0
5	l	2406	0	2495	0	0
5	n	2334	0	2431	0	0
5	o	2311	0	2402	0	0
5	q	2334	0	2431	0	0
5	r	2411	0	2500	0	0
5	t	2342	0	2435	0	0
5	u	2411	0	2500	0	0
All	All	248627	0	249732	4113	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 10.

The worst 5 of 4113 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)
2:L:512:MET:CE	2:L:527:ILE:HD11	1.81	1.10
2:L:512:MET:HE2	2:L:527:ILE:HD11	1.33	1.08
2:A:475:MET:O	2:A:478:LEU:HG	1.64	0.95
2:A:1361:PRO:HB2	2:A:1364:GLN:HB3	1.49	0.92
2:D:478:LEU:HD13	2:D:512:MET:SD	2.12	0.90

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	0	283/285 (99%)	274 (97%)	6 (2%)	3 (1%)	17	60
1	1	283/285 (99%)	267 (94%)	13 (5%)	3 (1%)	17	60
1	2	283/285 (99%)	267 (94%)	14 (5%)	2 (1%)	25	67
1	3	283/285 (99%)	266 (94%)	11 (4%)	6 (2%)	8	48
1	4	283/285 (99%)	271 (96%)	10 (4%)	2 (1%)	25	67
1	5	283/285 (99%)	272 (96%)	7 (2%)	4 (1%)	13	55
1	6	283/285 (99%)	271 (96%)	10 (4%)	2 (1%)	25	67
1	7	283/285 (99%)	267 (94%)	13 (5%)	3 (1%)	17	60
1	8	283/285 (99%)	275 (97%)	5 (2%)	3 (1%)	17	60
1	9	283/285 (99%)	271 (96%)	8 (3%)	4 (1%)	13	55
1	v	283/285 (99%)	262 (93%)	13 (5%)	8 (3%)	6	43
1	w	283/285 (99%)	269 (95%)	12 (4%)	2 (1%)	25	67
1	x	283/285 (99%)	264 (93%)	14 (5%)	5 (2%)	10	51
1	y	283/285 (99%)	270 (95%)	11 (4%)	2 (1%)	25	67
1	z	283/285 (99%)	272 (96%)	7 (2%)	4 (1%)	13	55
2	A	1321/1370 (96%)	1230 (93%)	78 (6%)	13 (1%)	18	61
2	B	1329/1370 (97%)	1226 (92%)	80 (6%)	23 (2%)	11	52
2	C	1345/1370 (98%)	1259 (94%)	71 (5%)	15 (1%)	17	60
2	D	1342/1370 (98%)	1233 (92%)	94 (7%)	15 (1%)	17	60
2	E	1343/1370 (98%)	1233 (92%)	90 (7%)	20 (2%)	12	54
2	F	1346/1370 (98%)	1242 (92%)	87 (6%)	17 (1%)	14	57
2	G	1347/1370 (98%)	1250 (93%)	82 (6%)	15 (1%)	17	60
2	H	1348/1370 (98%)	1253 (93%)	86 (6%)	9 (1%)	25	67
2	I	1343/1370 (98%)	1243 (93%)	88 (7%)	12 (1%)	20	63
2	J	1329/1370 (97%)	1239 (93%)	76 (6%)	14 (1%)	17	60

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	K	1344/1370 (98%)	1249 (93%)	87 (6%)	8 (1%)	28	70
2	L	1349/1370 (98%)	1259 (93%)	77 (6%)	13 (1%)	18	61
2	M	1349/1370 (98%)	1250 (93%)	89 (7%)	10 (1%)	25	67
2	N	1346/1370 (98%)	1256 (93%)	81 (6%)	9 (1%)	25	67
2	O	1344/1370 (98%)	1243 (92%)	84 (6%)	17 (1%)	14	57
2	P	1344/1370 (98%)	1249 (93%)	81 (6%)	14 (1%)	18	61
3	Q	61/75 (81%)	58 (95%)	3 (5%)	0	100	100
3	R	61/75 (81%)	57 (93%)	4 (7%)	0	100	100
3	S	61/75 (81%)	58 (95%)	3 (5%)	0	100	100
3	T	61/75 (81%)	58 (95%)	3 (5%)	0	100	100
3	U	61/75 (81%)	56 (92%)	5 (8%)	0	100	100
3	V	61/75 (81%)	56 (92%)	4 (7%)	1 (2%)	11	53
3	W	61/75 (81%)	58 (95%)	3 (5%)	0	100	100
3	X	61/75 (81%)	59 (97%)	2 (3%)	0	100	100
3	Y	61/75 (81%)	57 (93%)	4 (7%)	0	100	100
3	Z	61/75 (81%)	58 (95%)	3 (5%)	0	100	100
3	a	61/75 (81%)	59 (97%)	2 (3%)	0	100	100
3	b	61/75 (81%)	58 (95%)	3 (5%)	0	100	100
3	c	61/75 (81%)	60 (98%)	1 (2%)	0	100	100
3	d	61/75 (81%)	58 (95%)	3 (5%)	0	100	100
3	e	61/75 (81%)	57 (93%)	4 (7%)	0	100	100
3	f	61/75 (81%)	58 (95%)	3 (5%)	0	100	100
4	g	258/290 (89%)	234 (91%)	21 (8%)	3 (1%)	15	58
4	j	288/290 (99%)	267 (93%)	17 (6%)	4 (1%)	13	55
4	m	288/290 (99%)	272 (94%)	14 (5%)	2 (1%)	25	67
4	p	288/290 (99%)	269 (93%)	16 (6%)	3 (1%)	18	61
4	s	288/290 (99%)	266 (92%)	17 (6%)	5 (2%)	11	52
5	h	288/306 (94%)	260 (90%)	21 (7%)	7 (2%)	7	45
5	i	281/306 (92%)	257 (92%)	20 (7%)	4 (1%)	13	55
5	k	288/306 (94%)	268 (93%)	14 (5%)	6 (2%)	8	48
5	l	301/306 (98%)	274 (91%)	24 (8%)	3 (1%)	18	61

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	n	291/306 (95%)	271 (93%)	15 (5%)	5 (2%)	11	52
5	o	287/306 (94%)	266 (93%)	18 (6%)	3 (1%)	18	61
5	q	291/306 (95%)	279 (96%)	11 (4%)	1 (0%)	44	80
5	r	302/306 (99%)	275 (91%)	21 (7%)	6 (2%)	9	49
5	t	292/306 (95%)	269 (92%)	19 (6%)	4 (1%)	13	55
5	u	302/306 (99%)	275 (91%)	24 (8%)	3 (1%)	18	61
All	All	31023/31905 (97%)	28879 (93%)	1807 (6%)	337 (1%)	21	60

5 of 337 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	3	183	PRO
2	A	694	ASN
2	A	805	LYS
2	B	203	ALA
2	B	844	ASP

### 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	0	256/257 (100%)	256 (100%)	0	100	100
1	1	256/257 (100%)	256 (100%)	0	100	100
1	2	256/257 (100%)	256 (100%)	0	100	100
1	3	256/257 (100%)	256 (100%)	0	100	100
1	4	256/257 (100%)	256 (100%)	0	100	100
1	5	256/257 (100%)	256 (100%)	0	100	100
1	6	256/257 (100%)	256 (100%)	0	100	100
1	7	256/257 (100%)	255 (100%)	1 (0%)	93	96
1	8	256/257 (100%)	256 (100%)	0	100	100
1	9	256/257 (100%)	256 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	v	256/257 (100%)	256 (100%)	0	100	100
1	w	256/257 (100%)	256 (100%)	0	100	100
1	x	256/257 (100%)	256 (100%)	0	100	100
1	y	256/257 (100%)	256 (100%)	0	100	100
1	z	256/257 (100%)	256 (100%)	0	100	100
2	A	1156/1192 (97%)	1153 (100%)	3 (0%)	94	97
2	B	1162/1192 (98%)	1158 (100%)	4 (0%)	94	97
2	C	1174/1192 (98%)	1171 (100%)	3 (0%)	94	97
2	D	1173/1192 (98%)	1167 (100%)	6 (0%)	91	96
2	E	1174/1192 (98%)	1166 (99%)	8 (1%)	87	94
2	F	1175/1192 (99%)	1170 (100%)	5 (0%)	93	96
2	G	1177/1192 (99%)	1175 (100%)	2 (0%)	94	97
2	H	1177/1192 (99%)	1173 (100%)	4 (0%)	94	97
2	I	1174/1192 (98%)	1171 (100%)	3 (0%)	94	97
2	J	1161/1192 (97%)	1156 (100%)	5 (0%)	93	96
2	K	1174/1192 (98%)	1170 (100%)	4 (0%)	94	97
2	L	1178/1192 (99%)	1176 (100%)	2 (0%)	94	97
2	M	1178/1192 (99%)	1176 (100%)	2 (0%)	94	97
2	N	1175/1192 (99%)	1170 (100%)	5 (0%)	93	96
2	O	1174/1192 (98%)	1170 (100%)	4 (0%)	94	97
2	P	1174/1192 (98%)	1170 (100%)	4 (0%)	94	97
3	Q	59/68 (87%)	59 (100%)	0	100	100
3	R	59/68 (87%)	59 (100%)	0	100	100
3	S	59/68 (87%)	59 (100%)	0	100	100
3	T	59/68 (87%)	59 (100%)	0	100	100
3	U	59/68 (87%)	59 (100%)	0	100	100
3	V	59/68 (87%)	59 (100%)	0	100	100
3	W	59/68 (87%)	59 (100%)	0	100	100
3	X	59/68 (87%)	59 (100%)	0	100	100
3	Y	59/68 (87%)	58 (98%)	1 (2%)	66	86
3	Z	59/68 (87%)	59 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	a	59/68 (87%)	59 (100%)	0	100	100
3	b	59/68 (87%)	58 (98%)	1 (2%)	66	86
3	c	59/68 (87%)	59 (100%)	0	100	100
3	d	59/68 (87%)	59 (100%)	0	100	100
3	e	59/68 (87%)	59 (100%)	0	100	100
3	f	59/68 (87%)	59 (100%)	0	100	100
4	g	228/252 (90%)	227 (100%)	1 (0%)	93	96
4	j	252/252 (100%)	251 (100%)	1 (0%)	93	96
4	m	252/252 (100%)	250 (99%)	2 (1%)	85	93
4	p	252/252 (100%)	250 (99%)	2 (1%)	85	93
4	s	252/252 (100%)	250 (99%)	2 (1%)	85	93
5	h	262/273 (96%)	260 (99%)	2 (1%)	85	93
5	i	256/273 (94%)	256 (100%)	0	100	100
5	k	262/273 (96%)	260 (99%)	2 (1%)	85	93
5	l	272/273 (100%)	272 (100%)	0	100	100
5	n	263/273 (96%)	262 (100%)	1 (0%)	93	96
5	o	261/273 (96%)	260 (100%)	1 (0%)	93	96
5	q	263/273 (96%)	263 (100%)	0	100	100
5	r	272/273 (100%)	271 (100%)	1 (0%)	93	96
5	t	264/273 (97%)	263 (100%)	1 (0%)	93	96
5	u	272/273 (100%)	272 (100%)	0	100	100
All	All	27423/28005 (98%)	27340 (100%)	83 (0%)	94	97

5 of 83 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	I	1303	CYS
2	K	1303	CYS
5	o	297	ASN
2	I	1370	SER
2	J	1303	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 102 such sidechains are listed below:

Mol	Chain	Res	Type
2	I	901	HIS
2	K	749	HIS
4	p	211	HIS
2	I	985	ASN
2	J	901	HIS

### 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 carbohydrates 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.