



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Mar 2, 2017 – 11:55 am GMT

PDB ID : 3K1Q
EMDB ID: : EMD-1653
Title : Backbone model of an aquareovirus virion by cryo-electron microscopy and bioinformatics
Authors : Cheng, L.P.; Zhu, J.; Hiu, W.H.; Zhang, X.K.; Honig, B.; Fang, Q.; Zhou, Z.H.
Deposited on : 2009-09-28
Resolution : 4.50 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
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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) : recalc29047

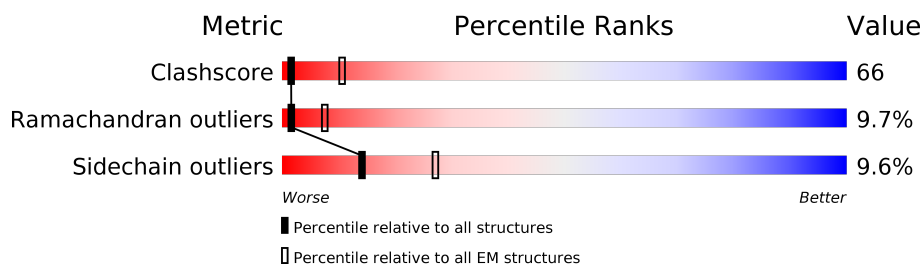
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.50 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.



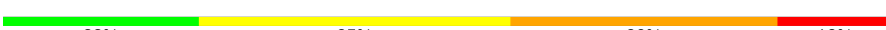
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

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 ≥ 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	A	1299	35% 39% 17% 8%
2	B	1027	37% 36% 20% 6%
3	C	1196	39% 37% 17% 8%
4	D	412	31% 38% 20% 11%
4	E	412	33% 39% 20% 8%
5	F	276	23% 34% 30% 13%
5	G	276	24% 35% 29% 13%
5	H	276	25% 32% 30% 14%
5	L	276	23% 35% 28% 14%

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Mol	Chain	Length	Quality of chain
5	M	276	
5	N	276	
5	R	276	
5	S	276	
5	T	276	
5	Y	276	
6	I	639	
6	J	639	
6	K	639	
6	O	639	
6	P	639	
6	Q	639	
6	U	639	
6	V	639	
6	W	639	
6	X	639	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 101798 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 VP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1299	Total	C	N	O	S	0	0
			9989	6395	1700	1866	28		

- Molecule 2 is a protein called VP3A.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1027	Total	C	N	O	S	0	0
			7935	5067	1359	1462	47		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	455	GLU	GLN	CONFLICT	UNP Q9E3V8

- Molecule 3 is a protein called VP3B.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	1196	Total	C	N	O	S	0	0
			9154	5805	1575	1722	52		

- Molecule 4 is a protein called Core protein VP6.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	412	Total	C	N	O	S	0	0
			3145	2013	545	571	16		
4	E	412	Total	C	N	O	S	0	0
			3145	2013	545	571	16		

- Molecule 5 is a protein called Outer capsid VP7.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	276	Total	C	N	O	S	0	0
			2085	1288	378	402	17		

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Mol	Chain	Residues	Atoms					AltConf	Trace
5	G	276	Total	C	N	O	S	0	0
			2085	1288	378	402	17		
5	H	276	Total	C	N	O	S	0	0
			2085	1288	378	402	17		
5	L	276	Total	C	N	O	S	0	0
			2085	1288	378	402	17		
5	M	276	Total	C	N	O	S	0	0
			2085	1288	378	402	17		
5	N	276	Total	C	N	O	S	0	0
			2085	1288	378	402	17		
5	R	276	Total	C	N	O	S	0	0
			2085	1288	378	402	17		
5	S	276	Total	C	N	O	S	0	0
			2085	1288	378	402	17		
5	T	276	Total	C	N	O	S	0	0
			2085	1288	378	402	17		
5	Y	276	Total	C	N	O	S	0	0
			2085	1288	378	402	17		

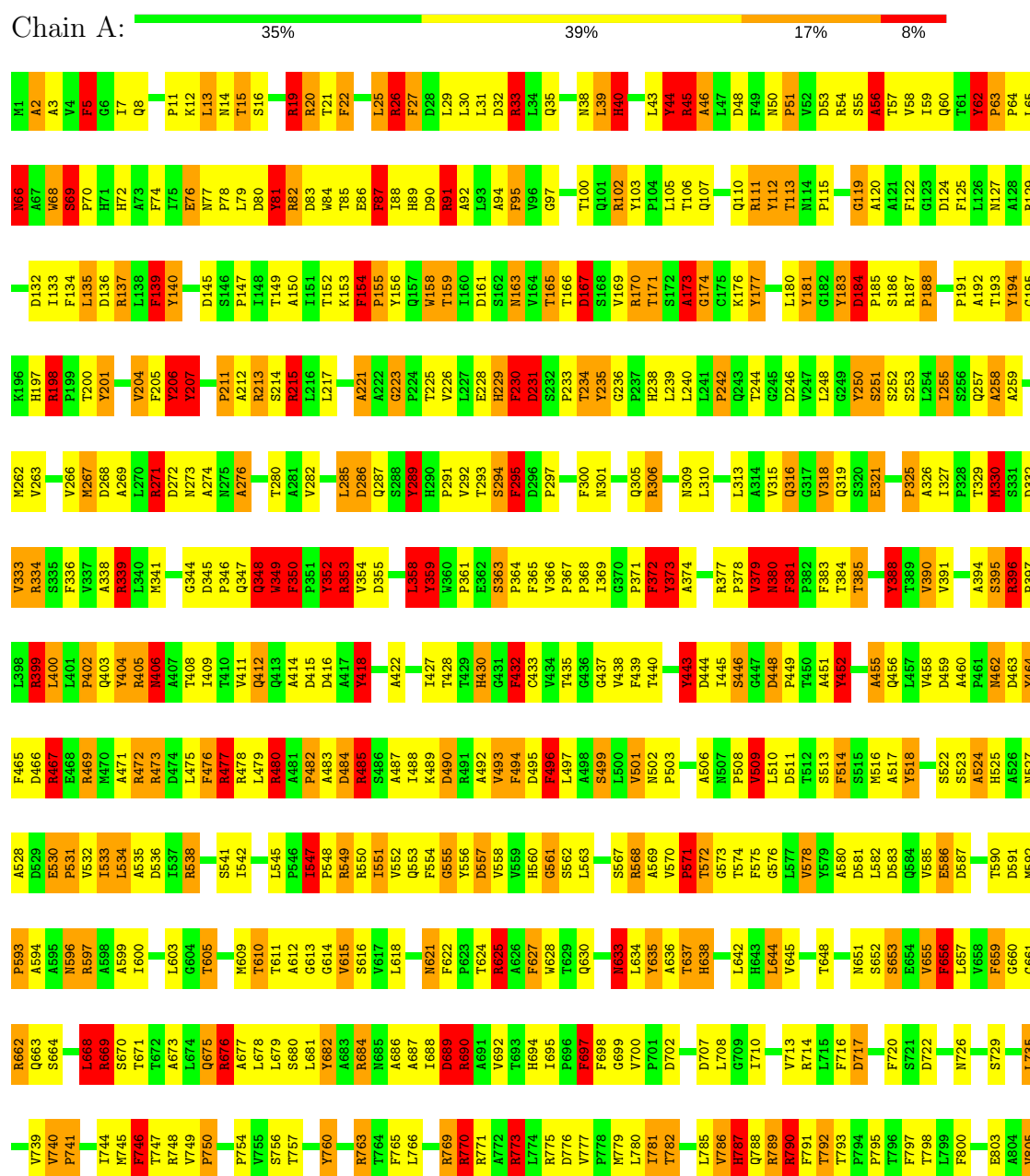
- Molecule 6 is a protein called Outer capsid VP5.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	I	639	Total	C	N	O	S	0	0
			4758	3012	801	927	18		
6	J	639	Total	C	N	O	S	0	0
			4758	3012	801	927	18		
6	K	639	Total	C	N	O	S	0	0
			4758	3012	801	927	18		
6	O	639	Total	C	N	O	S	0	0
			4758	3012	801	927	18		
6	P	639	Total	C	N	O	S	0	0
			4758	3012	801	927	18		
6	Q	639	Total	C	N	O	S	0	0
			4758	3012	801	927	18		
6	U	639	Total	C	N	O	S	0	0
			4758	3012	801	927	18		
6	V	639	Total	C	N	O	S	0	0
			4758	3012	801	927	18		
6	W	639	Total	C	N	O	S	0	0
			4758	3012	801	927	18		
6	X	639	Total	C	N	O	S	0	0
			4758	3012	801	927	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: VP1

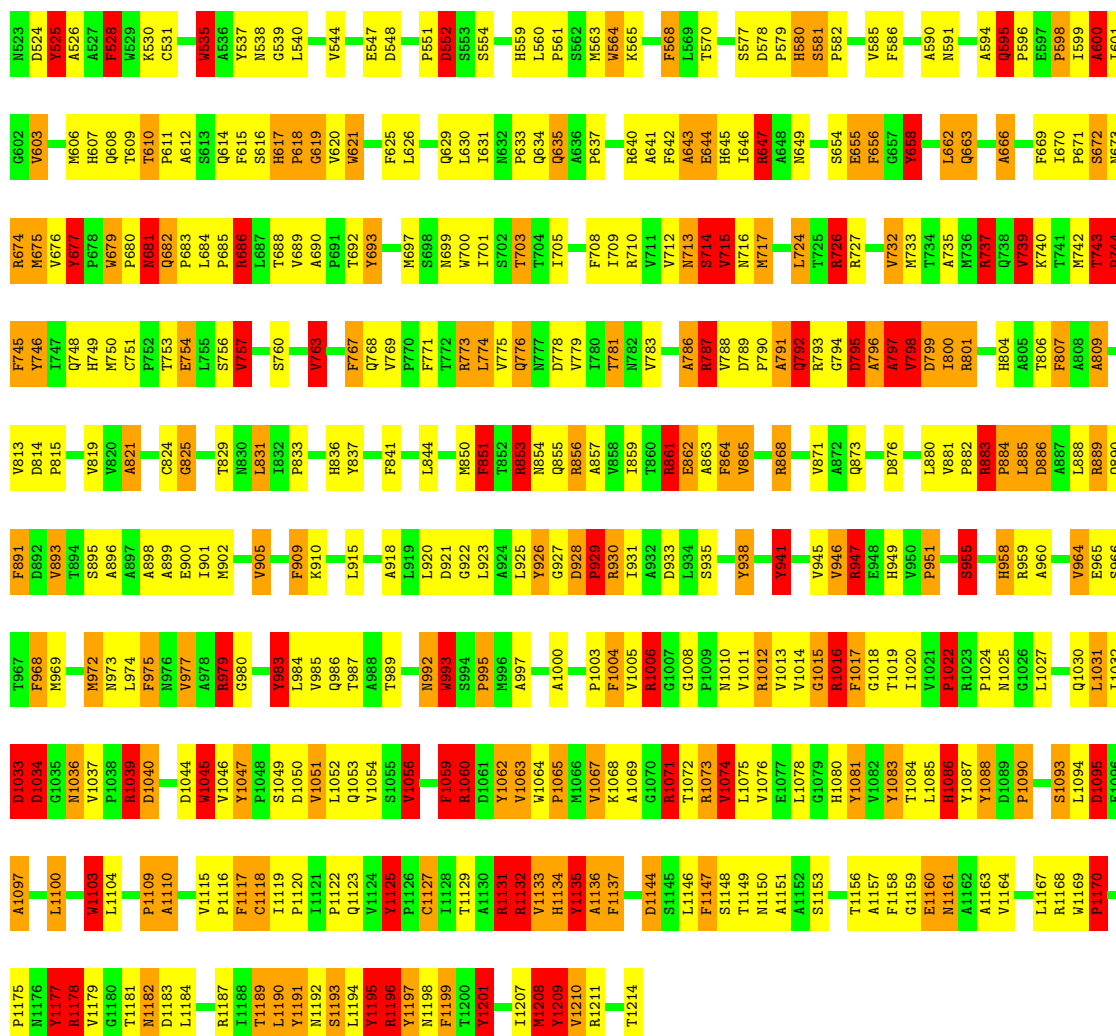




Frequency	Percentage
Daily	37%
Often	36%
Sometimes	20%
Not at all	6%

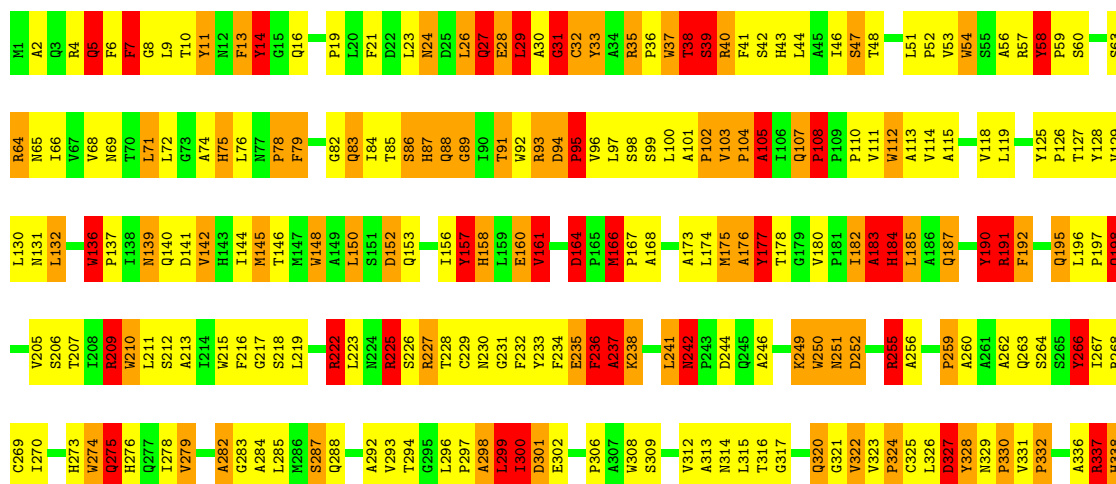


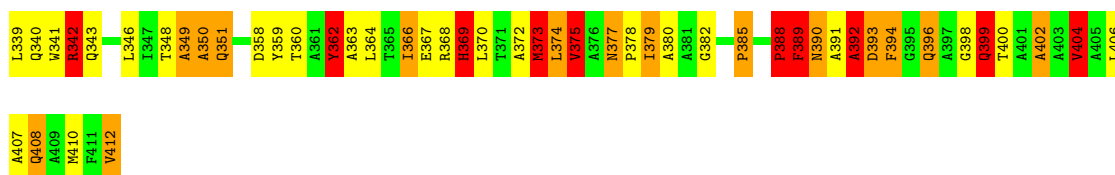
Y677	H749	V820	Q890	S955	L1031	E1101	D1174	L1032	E1102	D1175	E1103	D1176	L1033	E1104	D1177	E1105	D1178	L1034	E1106	D1179	E1107	D1180	L1035	E1108	D1181	E1109	D1182	L1036	E1110	D1183	E1111	D1184	L1037	E1112	D1185	E1113	D1186	L1038	E1114	D1187	E1115	D1188	L1039	E1116	D1189	E1117	D1190	L1040	E1118	D1191	E1119	D1192	L1041	E1120	D1193	E1121	D1194	L1042	E1122	D1195	E1123	D1196	L1043	E1124	D1197	E1125	D1198	L1044	E1126	D1199	E1127	D1200	L1045	E1128	D1201	E1129	D1202	L1046	E1130	D1203	E1131	D1204	L1047	E1132	D1205	E1133	D1206	L1048	E1134	D1207	E1135	D1208	L1049	E1136	D1209	E1137	D1210	L1050	E1138	D1211	E1139	D1212	L1051	E1140	D1213	E1141	D1214	L1052	E1142	D1215	E1143	D1216	L1053	E1144	D1217	E1145	D1218	L1054	E1146	D1219	E1147	D1220	L1055	E1148	D1221	E1149	D1222	L1056	E1150	D1223	E1151	D1224	L1057	E1152	D1225	E1153	D1226	L1058	E1154	D1227	E1155	D1228	L1059	E1156	D1229	E1157	D1230	L1060	E1158	D1231	E1159	D1232	L1061	E1160	D1233	E1161	D1234	L1062	E1162	D1235	E1163	D1236	L1063	E1164	D1237	E1165	D1238	L1064	E1166	D1239	E1167	D1240	L1065	E1168	D1241	E1169	D1242	L1066	E1170	D1243	E1171	D1244	L1067	E1172	D1245	E1173	D1246	L1068	E1174	D1247	E1175	D1248	L1069	E1176	D1249	E1177	D1250	L1070	E1178	D1251	E1179	D1252	L1071	E1180	D1253	E1181	D1254	L1072	E1182	D1255	E1183	D1256	L1073	E1184	D1257	E1185	D1258	L1074	E1186	D1259	E1187	D1260	L1075	E1188	D1261	E1189	D1262	L1076	E1190	D1263	E1191	D1264	L1077	E1192	D1265	E1193	D1266	L1078	E1194	D1267	E1195	D1268	L1079	E1196	D1269	E1197	D1270	L1080	E1198	D1271	E1199	D1272	L1081	E1200	D1273	E1201	D1274	L1082	E1202	D1275	E1203	D1276	L1083	E1204	D1277	E1205	D1278	L1084	E1206	D1279	E1207	D1280	L1085	E1208	D1281	E1209	D1282	L1086	E1210	D1283	E1211	D1284	L1087	E1212	D1285	E1213	D1286	L1088	E1214	D1287	E1215	D1288	L1089	E1216	D1289	E1217	D1290	L1090	E1218	D1291	E1219	D1292	L1091	E1220	D1293	E1221	D1294	L1092	E1222	D1295	E1223	D1296	L1093	E1224	D1297	E1225	D1298	L1094	E1226	D1299	E1227	D1300	L1095	E1228	D1301	E1229	D1302	L1096	E1230	D1303	E1231	D1304	L1097	E1232	D1305	E1233	D1306	L1098	E1234	D1307	E1235	D1308	L1099	E1236	D1309	E1237	D1310	L1100	E1238	D1311	E1239	D1312	L1101	E1240	D1313	E1241	D1314	L1102	E1242	D1315	E1243	D1316	L1103	E1244	D1317	E1245	D1318	L1104	E1246	D1319	E1247	D1320	L1105	E1248	D1321	E1249	D1322	L1106	E1250	D1323	E1251	D1324	L1107	E1252	D1325	E1253	D1326	L1108	E1254	D1327	E1255	D1328	L1109	E1256	D1329	E1257	D1330	L1110	E1258	D1331	E1259	D1332	L1111	E1260	D1333	E1261	D1334	L1112	E1262	D1335	E1263	D1336	L1113	E1264	D1337	E1265	D1338	L1114	E1266	D1339	E1267	D1340	L1115	E1268	D1341	E1269	D1342	L1116	E1270	D1343	E1271	D1344	L1117	E1272	D1345	E1273	D1346	L1118	E1274	D1347	E1275	D1348	L1119	E1276	D1349	E1277	D1350	L1120	E1278	D1351	E1279	D1352	L1121	E1280	D1353	E1281	D1354	L1122	E1282	D1355	E1283	D1356	L1123	E1284	D1357	E1285	D1358	L1124	E1286	D1359	E1287	D1360	L1125	E1288	D1361	E1289	D1362	L1126	E1290	D1363	E1291	D1364	L1127	E1292	D1365	E1293	D1366	L1128	E1294	D1367	E1295	D1368	L1129	E1296	D1369	E1297	D1370	L1130	E1298	D1371	E1299	D1372	L1131	E1300	D1373	E1301	D1374	L1132	E1302	D1375	E1303	D1376	L1133	E1304	D1377	E1305	D1378	L1134	E1306	D1379	E1307	D1380	L1135	E1308	D1381	E1309	D1382	L1136	E1310	D1383	E1311	D1384	L1137	E1312	D1385	E1313	D1386	L1138	E1314	D1387	E1315	D1388	L1139	E1316	D1389	E1317	D1390	L1140	E1318	D1391	E1319	D1392	L1141	E1320	D1393	E1321	D1394	L1142	E1322	D1395	E1323	D1396	L1143	E1324	D1397	E1325	D1398	L1144	E1326	D1399	E1327	D1400	L1145	E1328	D1401	E1329	D1402	L1146	E1330	D1403	E1331	D1404	L1147	E1332	D1405	E1333	D1406	L1148	E1334	D1407	E1335	D1408	L1149	E1336	D1409	E1337	D1410	L1150	E1338	D1411	E1339	D1412	L1151	E1340	D1413	E1341	D1414	L1152	E1342	D1415	E1343	D1416	L1153	E1344	D1417	E1345	D1418	L1154	E1346	D1419	E1347	D1420	L1155	E1348	D1421	E1349	D1422	L1156	E1350	D1423	E1351	D1424	L1157	E1352	D1425	E1353	D1426	L1158	E1354	D1427	E1355	D1428	L1159	E1356	D1429	E1357	D1430	L1160	E1358	D1431	E1359	D1432	L1161	E1360	D1433	E1361	D1434	L1162	E1362	D1435	E1363	D1436	L1163	E1364	D1437	E1365	D1438	L1164	E1366	D1439	E1367	D1440	L1165	E1368	D1441	E1369	D1442	L1166	E1370	D1443	E1371	D1444	L1167	E1372	D1445	E1373	D1446	L1168	E1374	E1375	D1447	E1376	D1448	L1169	E1377	D1449	E1378	D1450	L1170	E1379	D1451	E1380	D1452	L1171	E1381	D1453	E1382	D1454	L1172	E1383	D1455	E1384	D1456	L1173	E1385	D1457	E1386	D1458	L1174	E1387	D1459	E1388	D1460	L1175	E1389	D1461	E1390	D1462	L1176	E1391	D1463	E1392	D1464	L1177	E1393	D1465	E1394	D1466	L1178	E1395	D1467	E1396	D1468	L1179	E1397	D1469	E1398	D1470	L1180	E1399	D1471	E1400	D1472	L1181	E1401	D1473	E1402	D1474	L1182	E1403	D1475	E1404	D1476	L1183	E1405	D1477	E1406	D1478	L1184	E1407	D1479	E1408	D1480	L1185	E1409	D1481	E1410	D1482	L1186	E1411	D1483	E1412	D1484	L1187	E1413	D1485	E1414	D1486	L1188	E1415	D1487	E1416	D1488	L1189	E1417	D1489	E1418	D1490	L1190	E1419	D1491	E1420	D1492	L1191	E1421	D1493	E1422	D1494	L1192	E1423	D1495	E1424	D1496	L1193	E1425	D1497	E1426	D1498	L1194	E1427	D1499	E1430	D1500	L1195	E1431	D1501	E1432	D1502	L1196	E1433	D1503	E1434	D1504	L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• Molecule 4: Core protein VP6

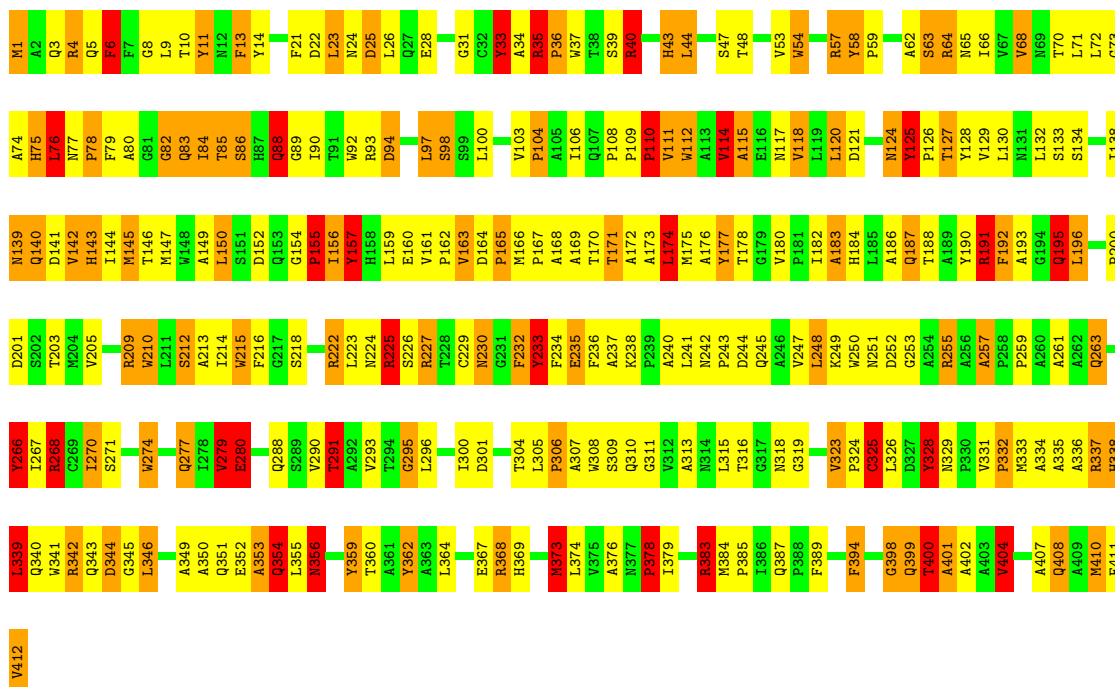
Chain D: 31% 38% 20% 11%





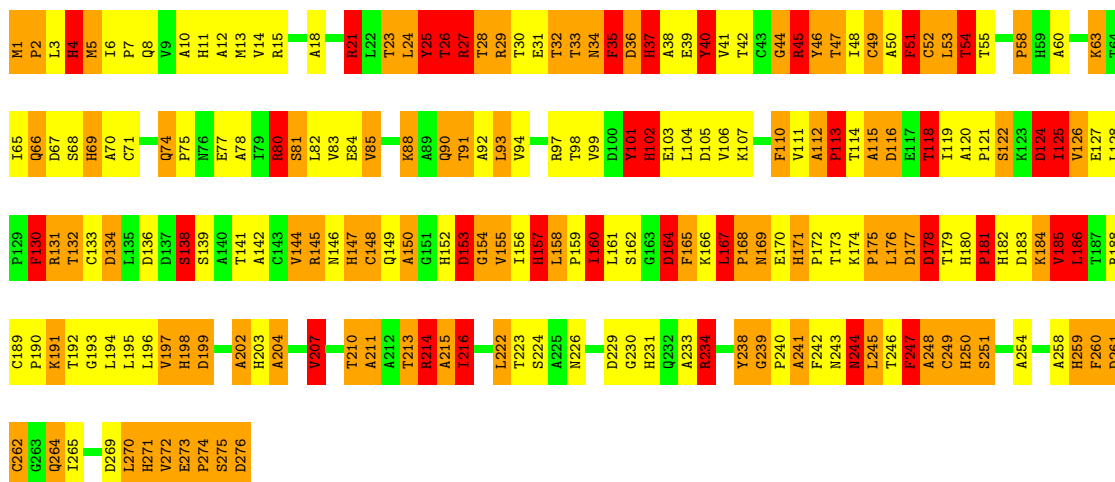
• Molecule 4: Core protein VP6

Chain E: 33% 39% 20% 8%



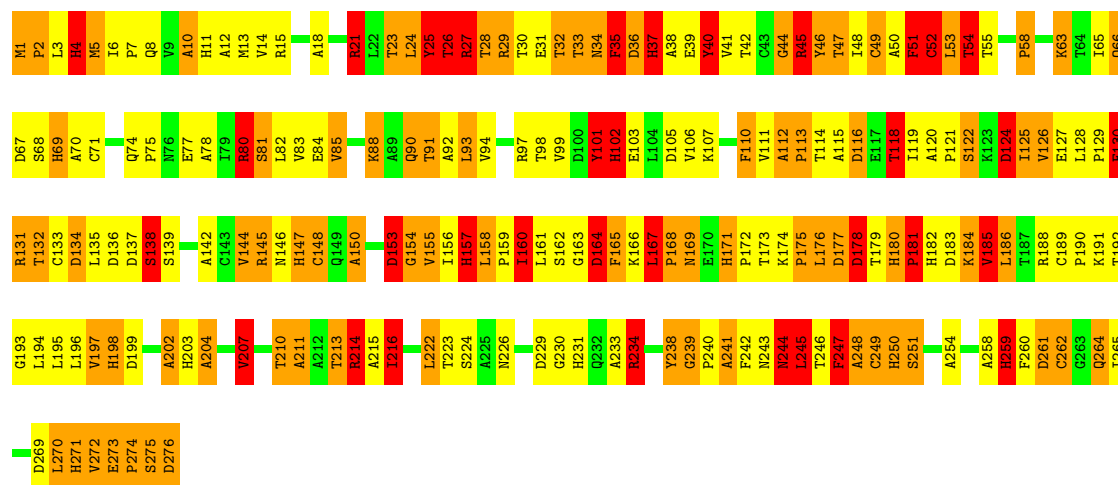
• Molecule 5: Outer capsid VP7

Chain F: 23% 34% 30% 13%



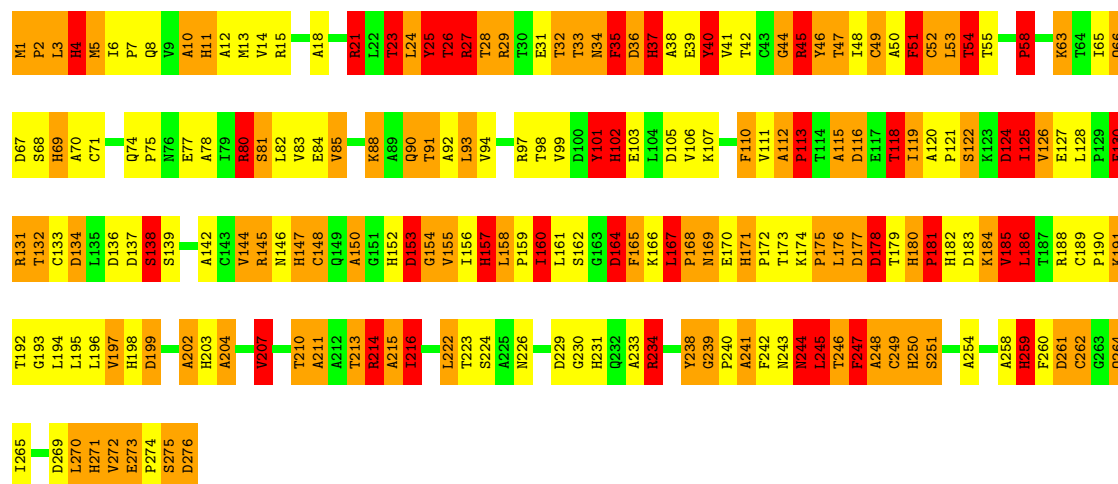
• Molecule 5: Outer capsid VP7

Chain G: 24% 35% 29% 13%



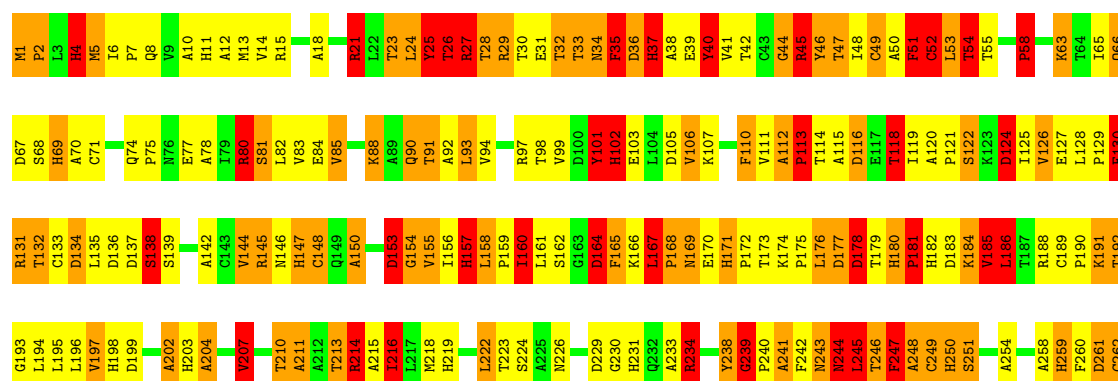
• Molecule 5: Outer capsid VP7

Chain H: 25% 32% 30% 14%



• Molecule 5: Outer capsid VP7

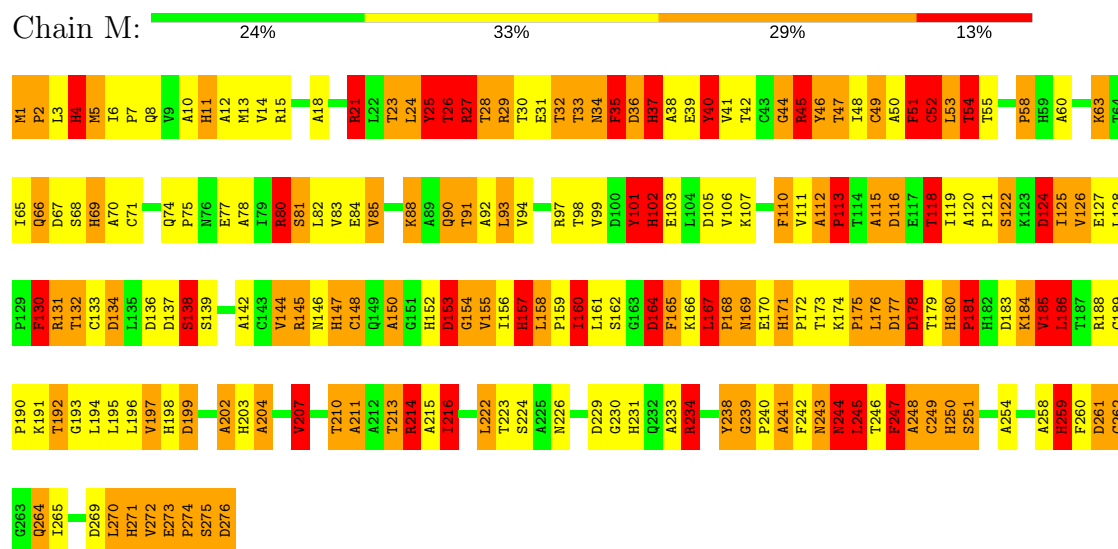
Chain L: 23% 35% 28% 14%





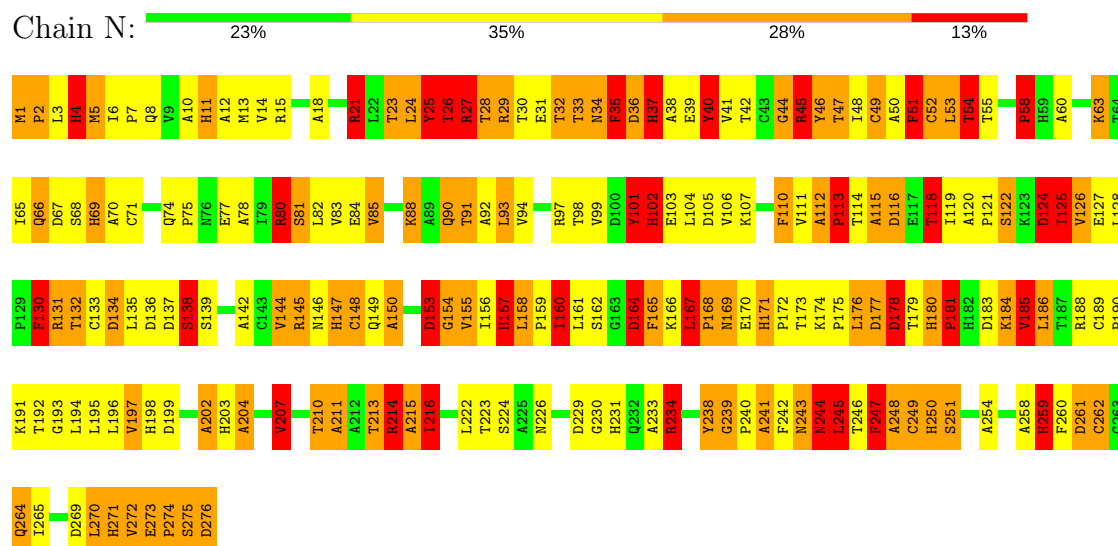
• Molecule 5: Outer capsid VP7

Chain M:



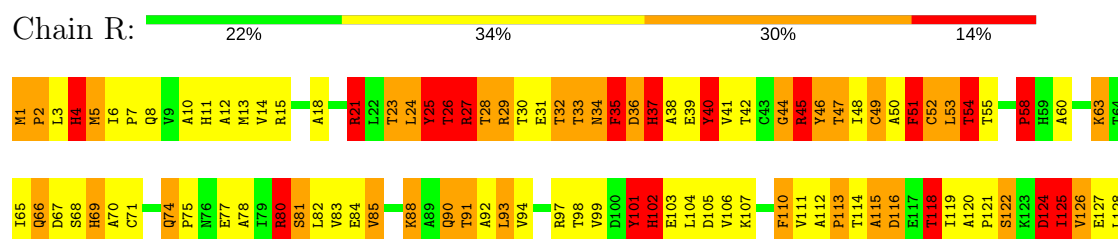
• Molecule 5: Outer capsid VP7

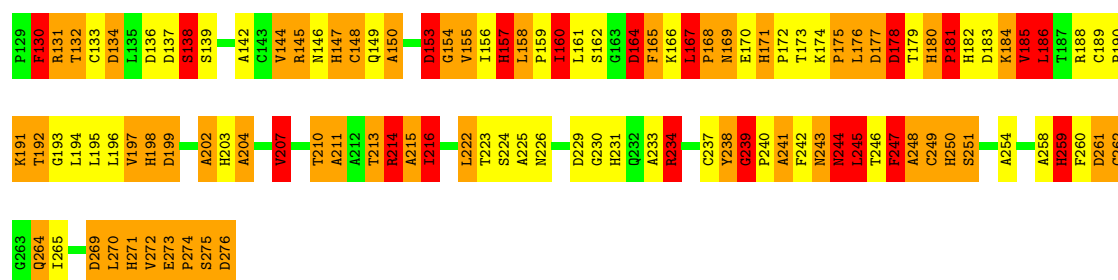
Chain N:



• Molecule 5: Outer capsid VP7

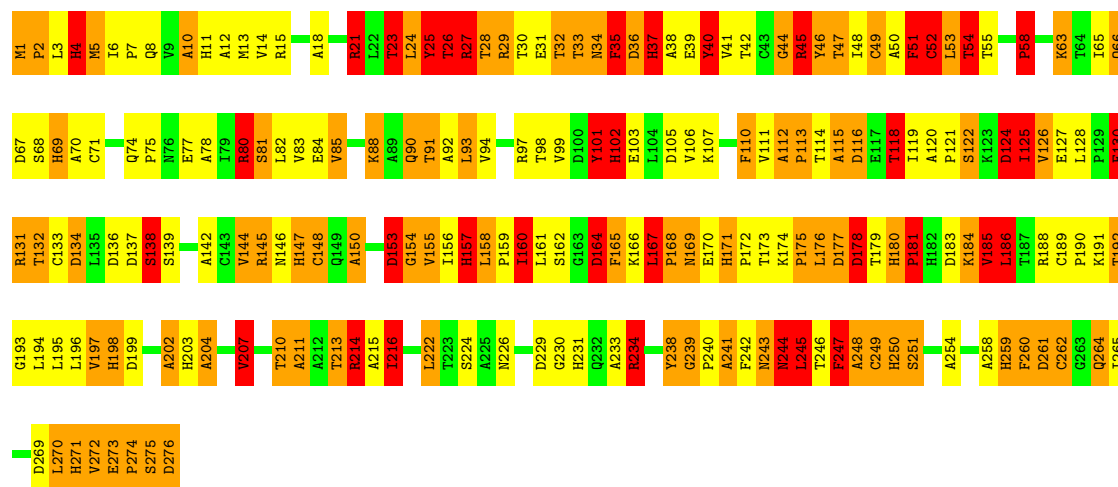
Chain R:





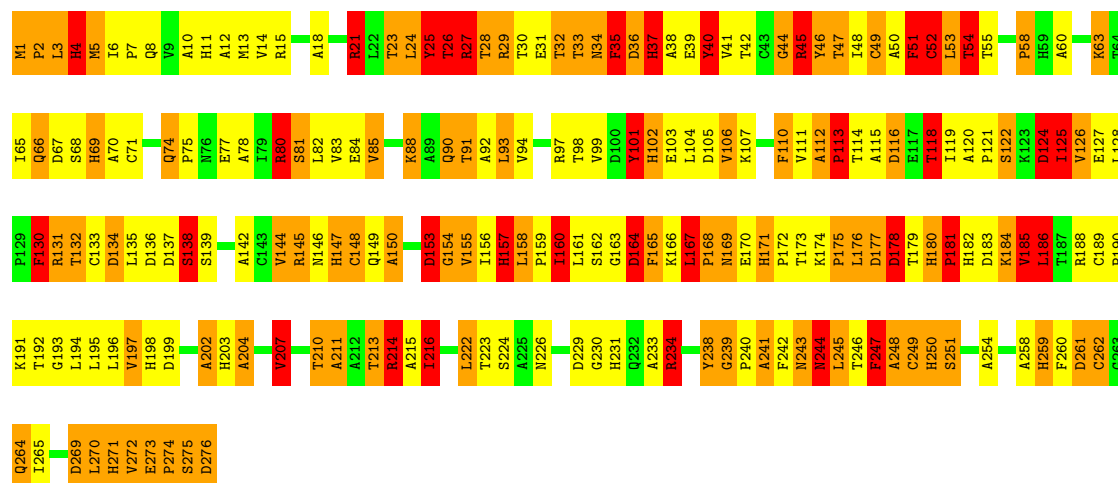
• Molecule 5: Outer capsid VP7

Chain S: 25% 32% 29% 14%



• Molecule 5: Outer capsid VP7

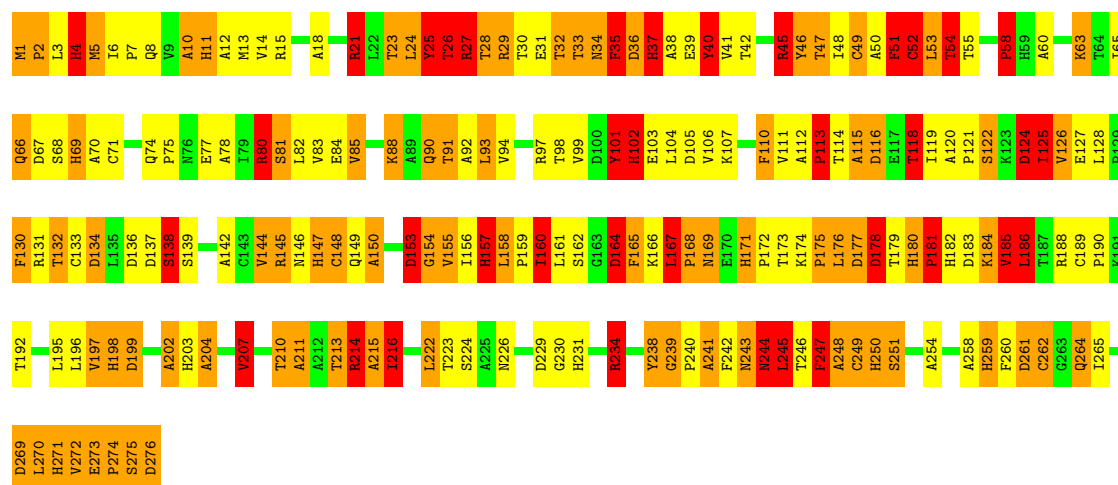
Chain T: 22% 35% 30% 13%



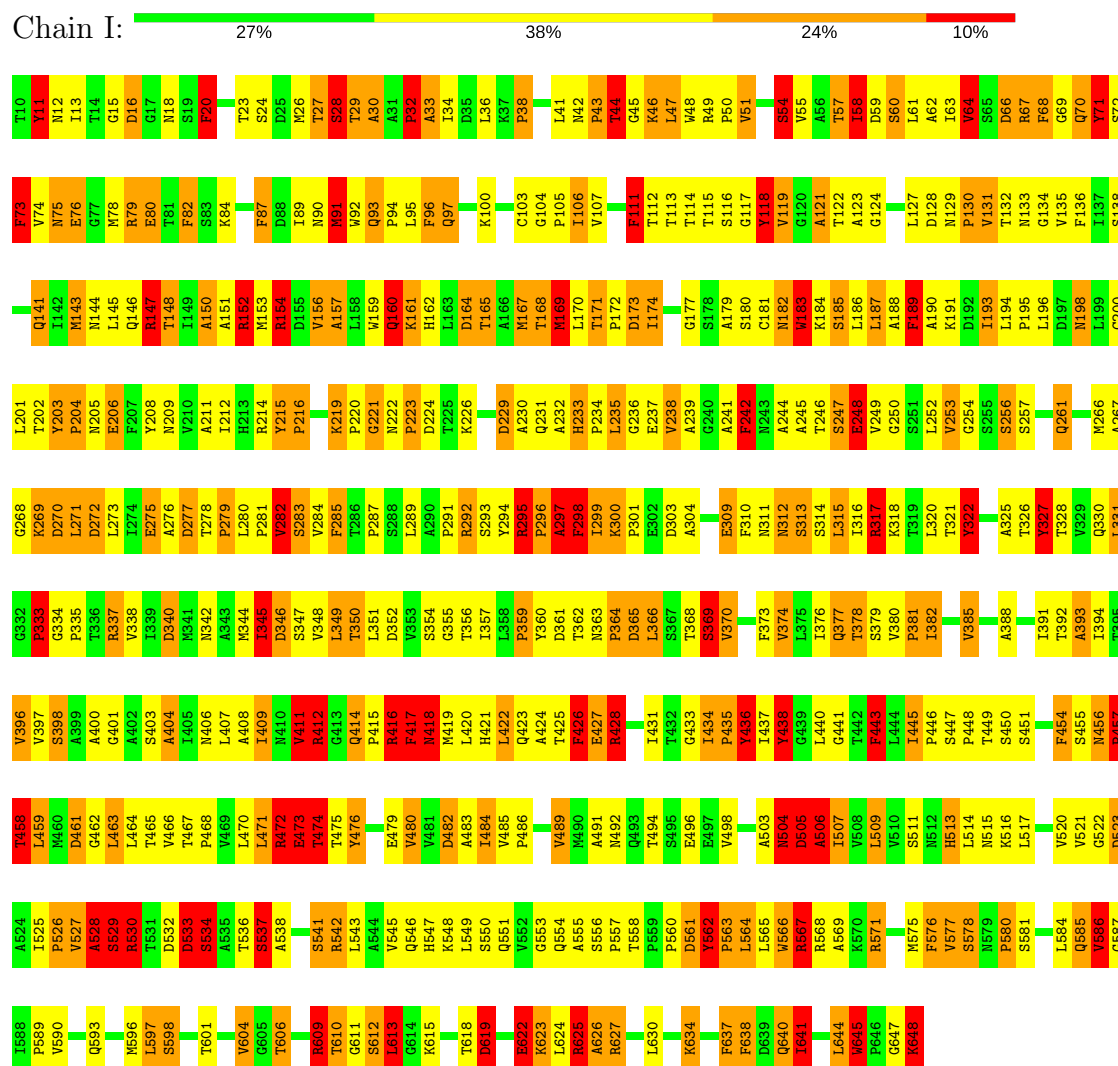
• Molecule 5: Outer capsid VP7

Chain Y: 25% 32% 29% 13%

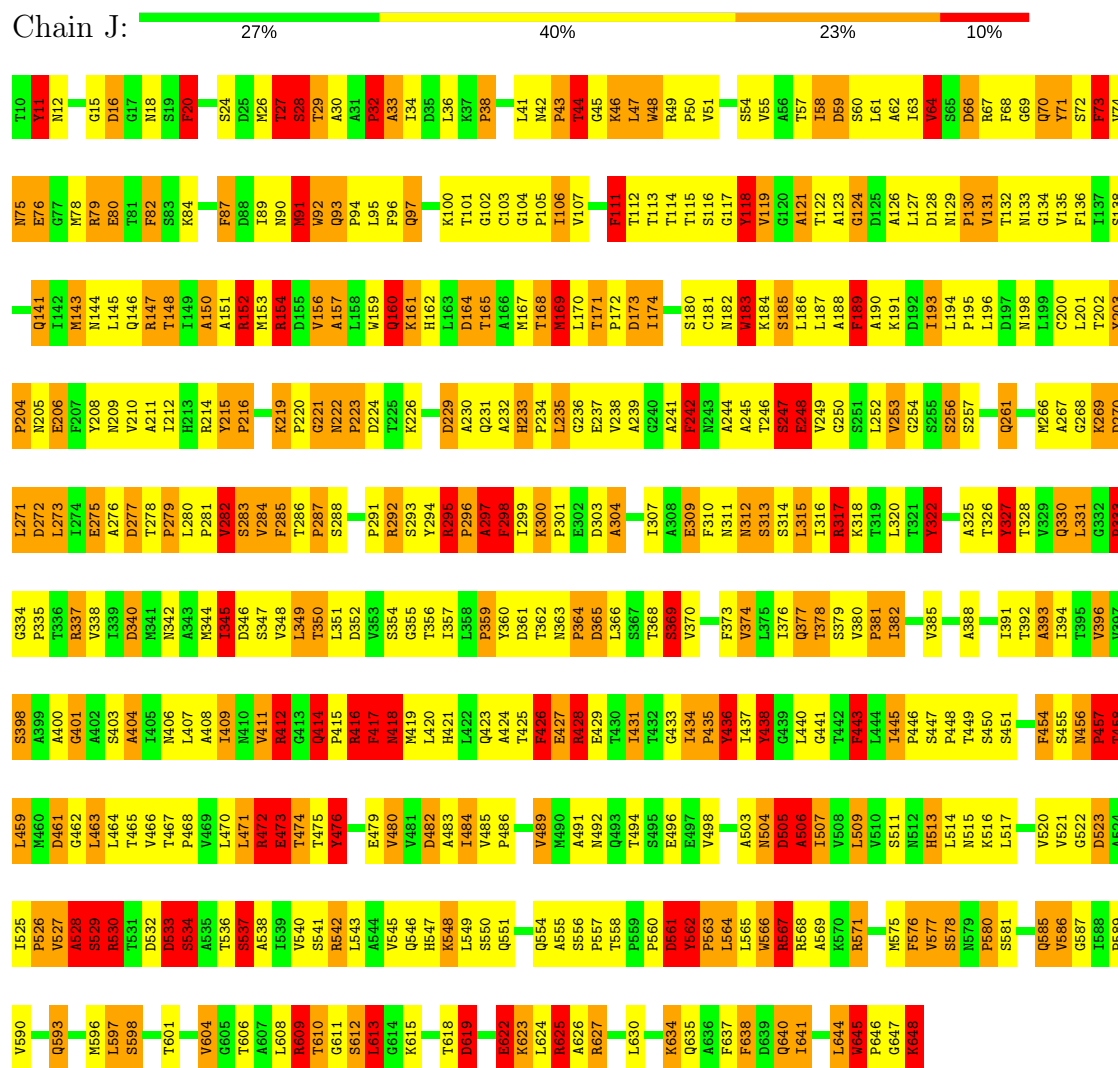




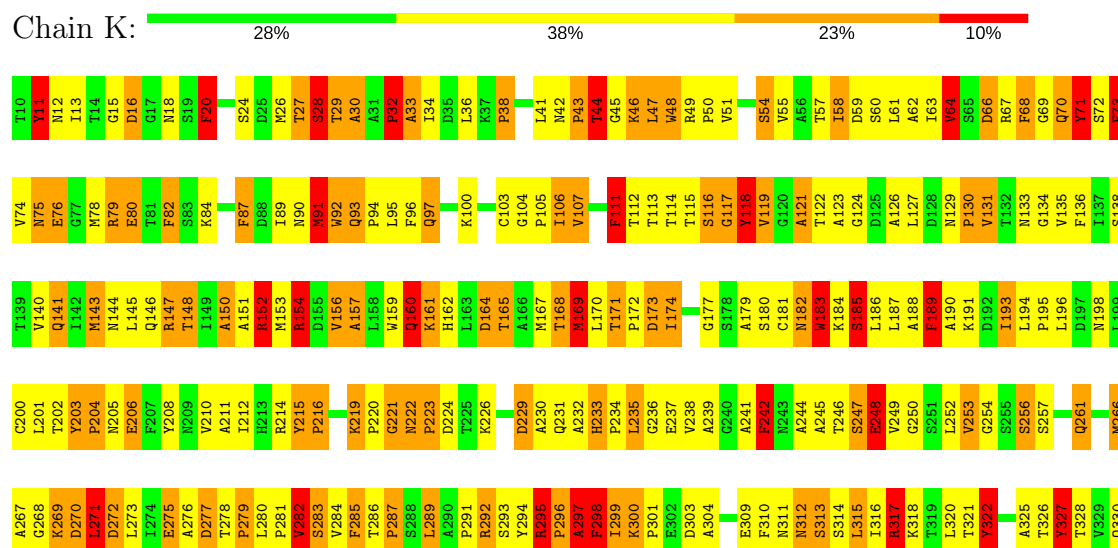
• Molecule 6: Outer capsid VP5

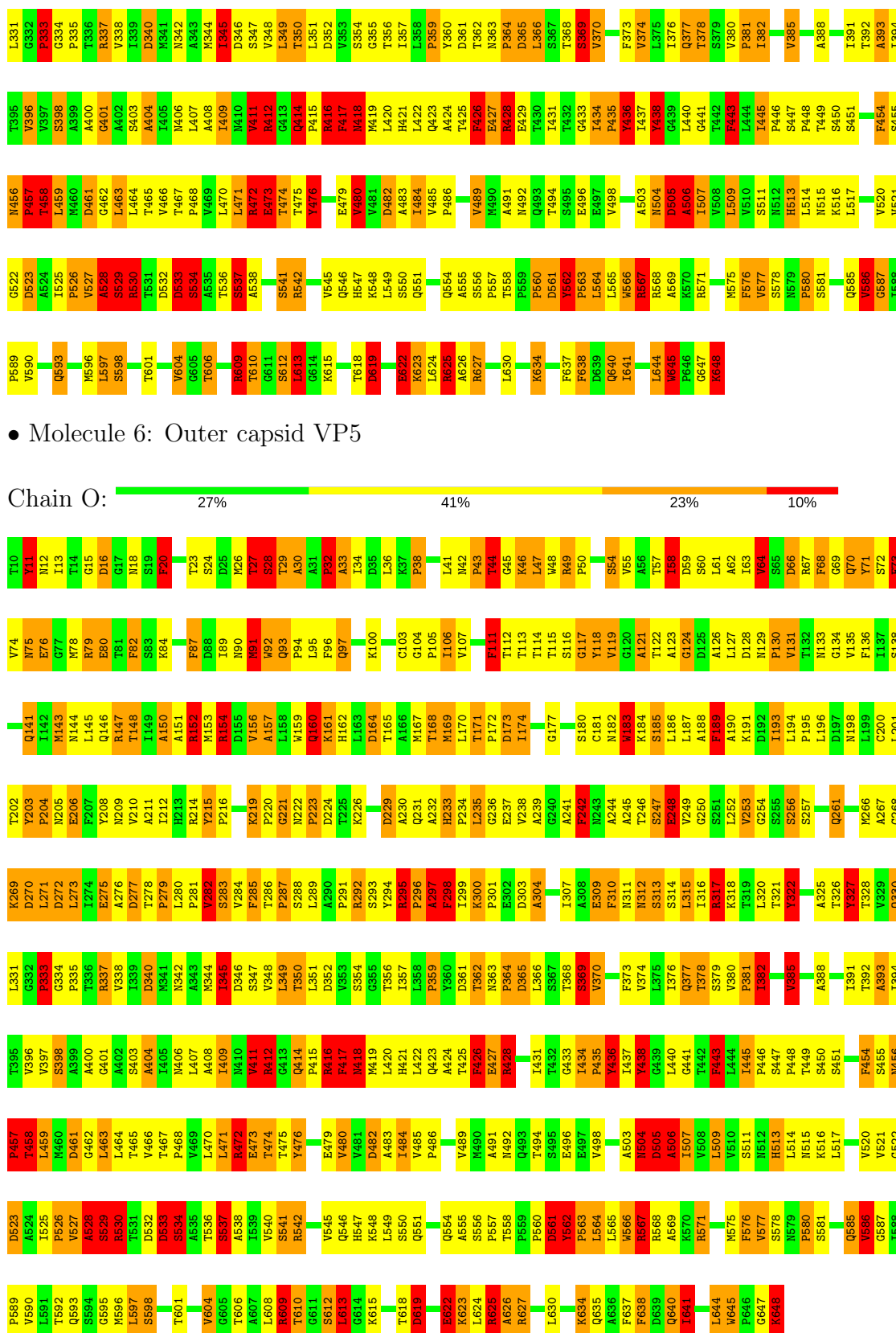


• Molecule 6: Outer capsid VP5



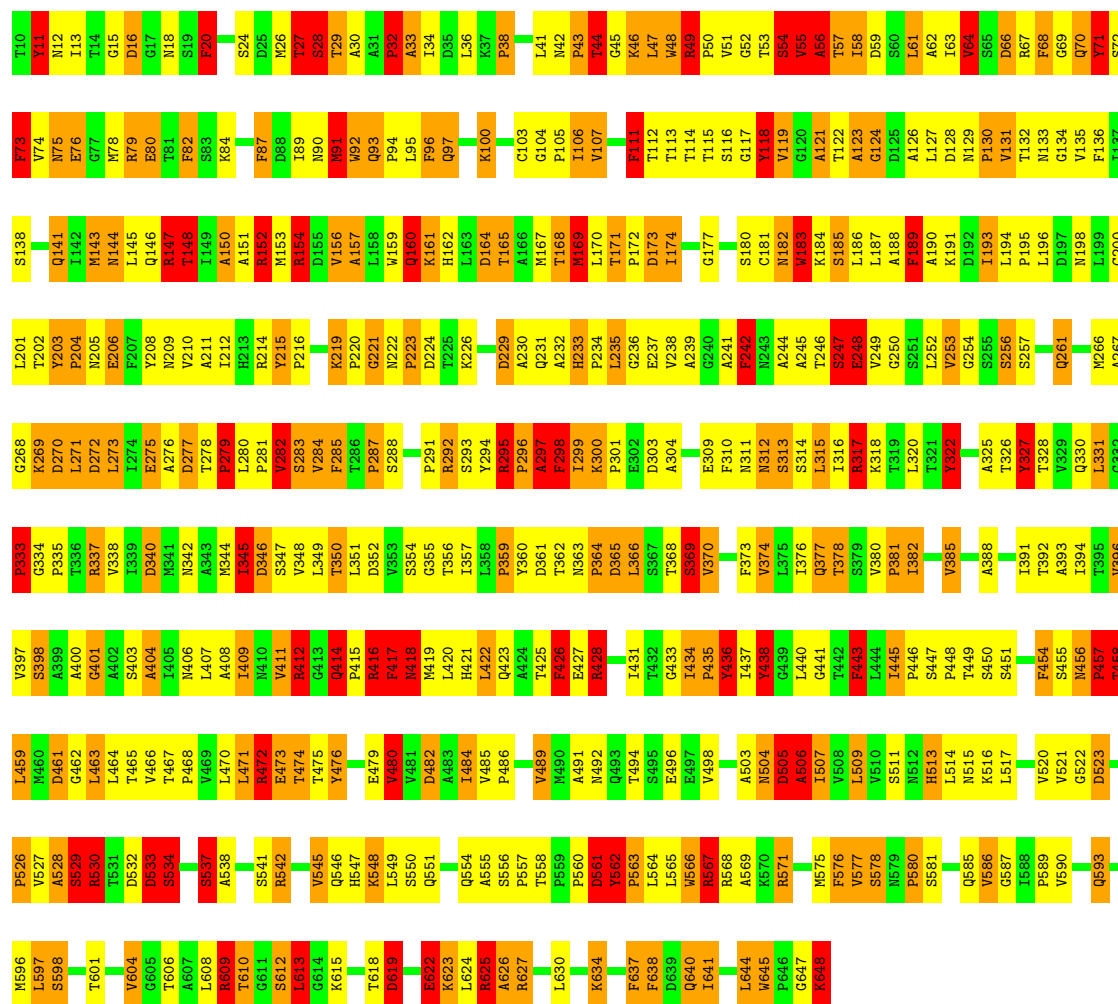
- Molecule 6: Outer capsid VP5



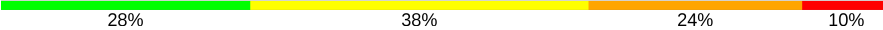


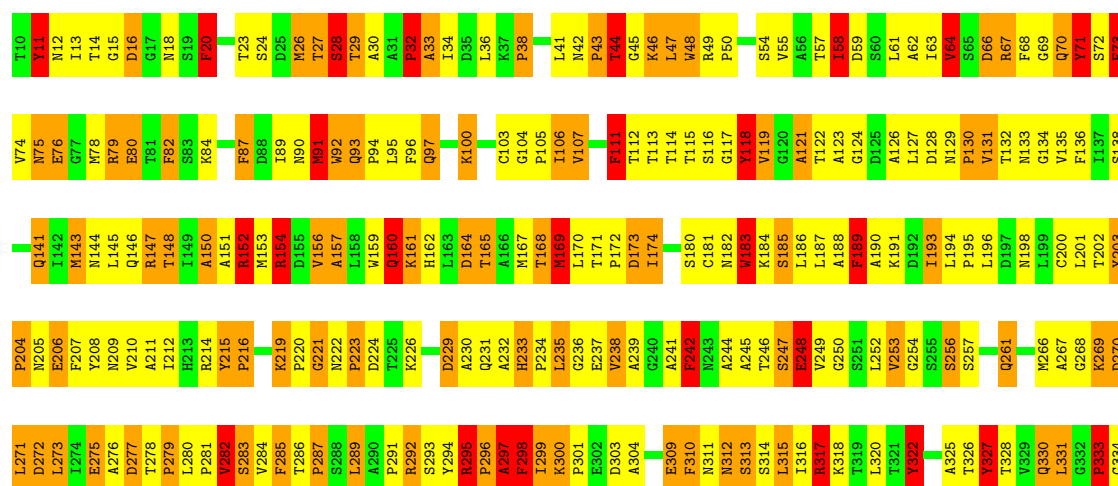
Molecule 6: Outer capsid VP5

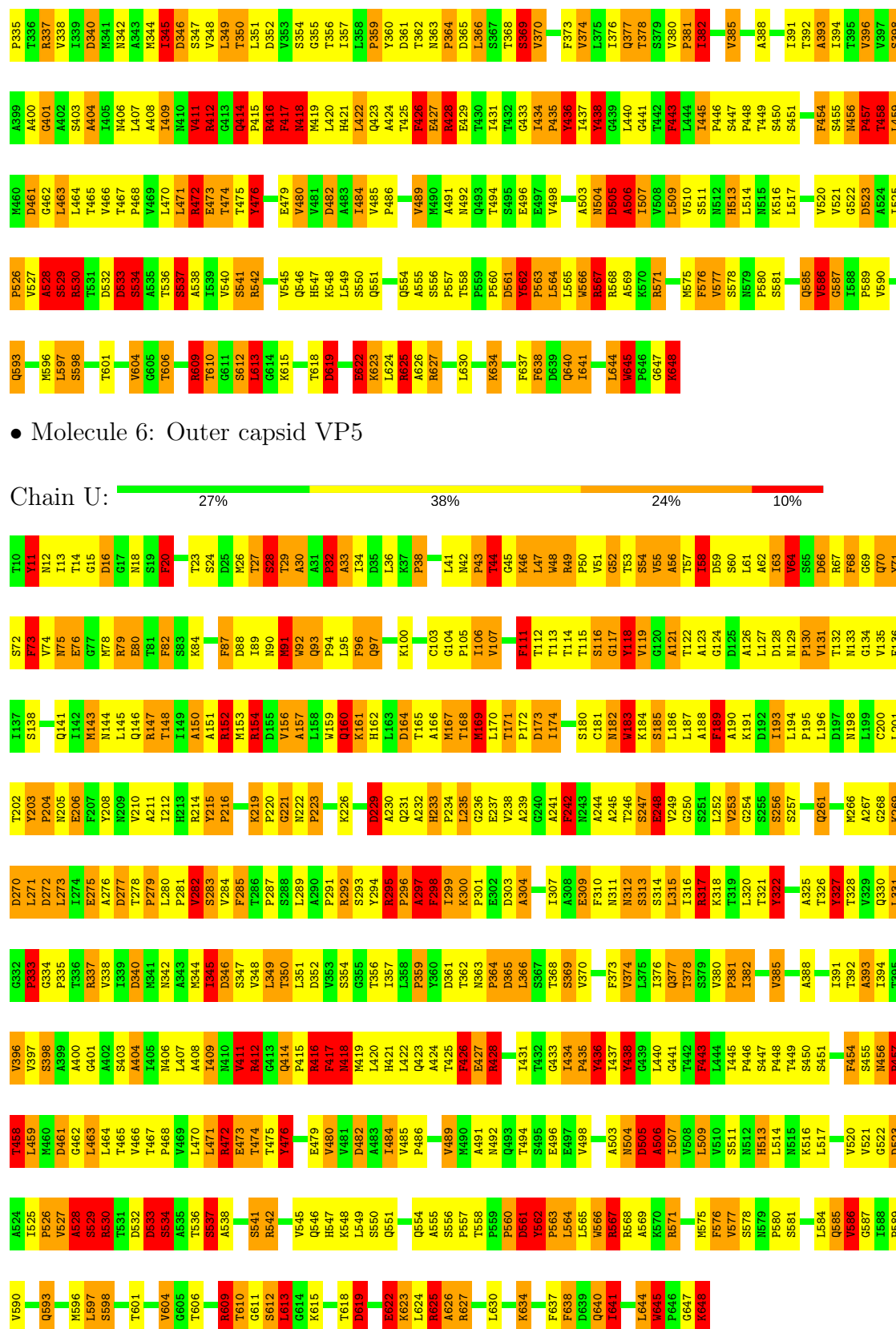
Chain P: 



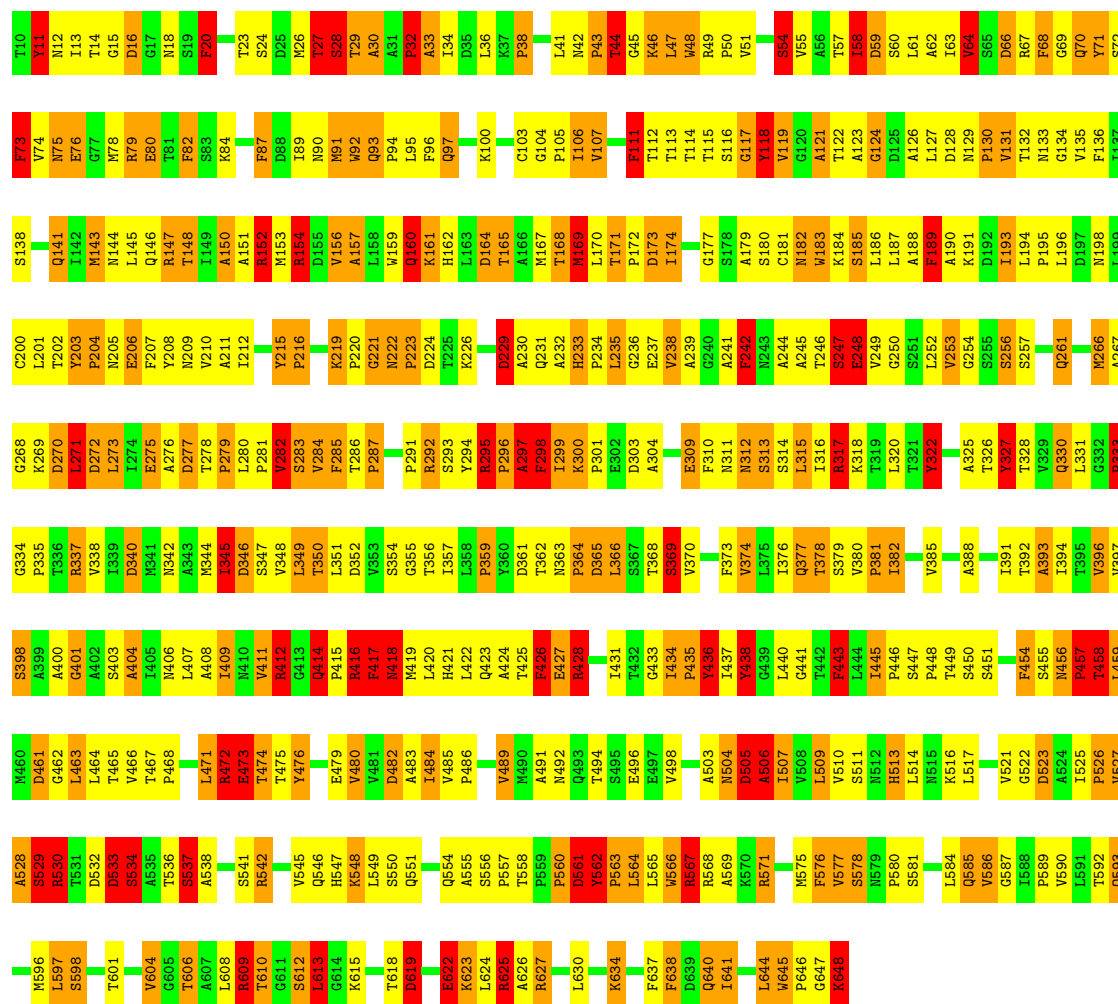
• Molecule 6: Outer capsid VP5

Chain Q: 

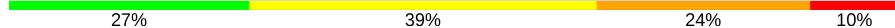


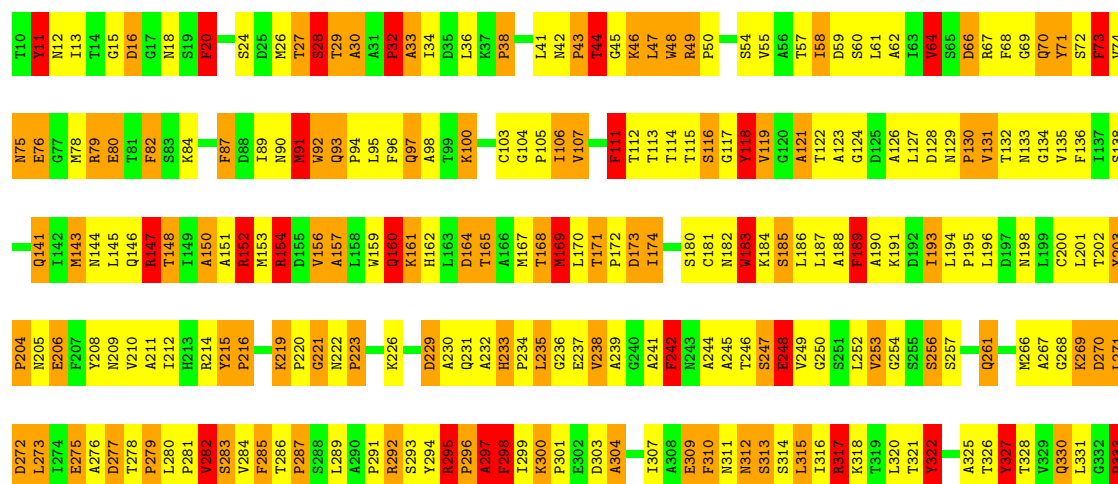


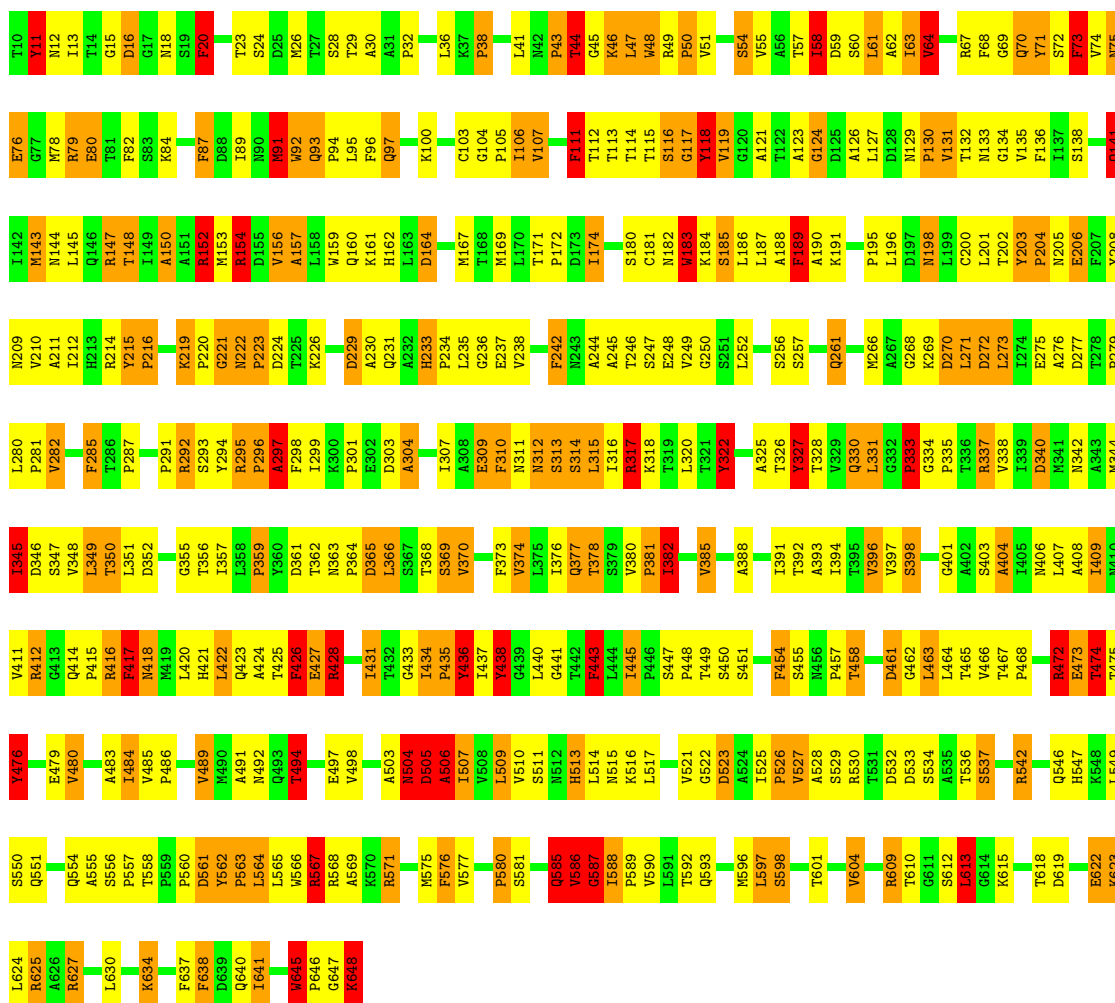
Chain V: 



• Molecule 6: Outer capsid VP5

Chain W: 





4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	Fully corrected. See Zhou et al., 1999, J. Virol. 73, 3210-3218	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	2000	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2300	Depositor
Magnification	154380	Depositor
Image detector	Not provided	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	A	0.56	0/10259	2.41	538/14091 (3.8%)
2	B	0.55	0/8142	2.55	420/11160 (3.8%)
3	C	0.55	0/9383	2.56	471/12866 (3.7%)
4	D	0.55	0/3240	2.54	172/4453 (3.9%)
4	E	0.56	0/3240	2.44	181/4453 (4.1%)
5	F	0.50	0/2132	2.40	115/2912 (3.9%)
5	G	0.50	0/2132	2.41	113/2912 (3.9%)
5	H	0.50	0/2132	2.40	116/2912 (4.0%)
5	L	0.50	0/2132	2.40	116/2912 (4.0%)
5	M	0.51	0/2132	2.39	114/2912 (3.9%)
5	N	0.51	0/2132	2.39	111/2912 (3.8%)
5	R	0.51	0/2132	2.41	121/2912 (4.2%)
5	S	0.51	0/2132	2.40	116/2912 (4.0%)
5	T	0.51	0/2132	2.40	116/2912 (4.0%)
5	Y	0.50	0/2132	2.43	114/2912 (3.9%)
6	I	0.53	0/4856	3.09	312/6646 (4.7%)
6	J	0.53	0/4856	3.03	308/6646 (4.6%)
6	K	0.52	0/4856	3.02	312/6646 (4.7%)
6	O	0.53	0/4856	3.03	302/6646 (4.5%)
6	P	0.70	3/4856 (0.1%)	3.26	317/6646 (4.8%)
6	Q	0.53	0/4856	3.12	316/6646 (4.8%)
6	U	0.53	0/4856	3.04	312/6646 (4.7%)
6	V	0.53	0/4856	3.03	315/6646 (4.7%)
6	W	0.52	0/4856	3.08	313/6646 (4.7%)
6	X	0.53	0/4856	2.38	226/6646 (3.4%)
All	All	0.54	3/104144 (0.0%)	2.74	5967/142603 (4.2%)

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.

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Mol	Chain	#Chirality outliers	#Planarity outliers
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Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	285
2	B	0	206
3	C	1	274
4	D	0	87
4	E	0	98
5	F	0	68
5	G	0	67
5	H	0	68
5	L	0	66
5	M	0	69
5	N	0	67
5	R	0	68
5	S	0	67
5	T	0	67
5	Y	0	68
6	I	0	155
6	J	0	142
6	K	0	149
6	O	0	145
6	P	0	147
6	Q	0	146
6	U	0	145
6	V	0	141
6	W	0	146
6	X	0	135
All	All	1	3076

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	P	56	ALA	CA-CB	25.04	2.05	1.52
6	P	56	ALA	N-CA	-14.68	1.17	1.46
6	P	56	ALA	CA-C	-11.44	1.23	1.52

The worst 5 of 5967 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	W	248	GLU	OE1-CD-OE2	-80.62	26.56	123.30
6	Q	248	GLU	OE1-CD-OE2	-80.09	27.19	123.30
6	K	248	GLU	OE1-CD-OE2	-77.76	29.99	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	O	248	GLU	OE1-CD-OE2	-76.08	32.01	123.30
6	U	248	GLU	OE1-CD-OE2	-75.94	32.18	123.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	C	315	SER	CA

5 of 3076 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	11	PRO	Mainchain
1	A	13	LEU	Mainchain
1	A	19	ARG	Sidechain
1	A	20	ARG	Sidechain
1	A	5	PHE	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	9989	0	9916	381	0
2	B	7935	0	7904	765	0
3	C	9154	0	9092	604	0
4	D	3145	0	3071	587	0
4	E	3145	0	3071	274	0
5	F	2085	0	2019	225	0
5	G	2085	0	2019	232	0
5	H	2085	0	2019	238	0
5	L	2085	0	2019	221	0
5	M	2085	0	2019	226	0
5	N	2085	0	2019	241	0
5	R	2085	0	2019	221	0
5	S	2085	0	2019	235	0
5	T	2085	0	2019	244	0
5	Y	2085	0	2019	168	0
6	I	4758	0	4791	1941	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	J	4758	0	4792	1863	0
6	K	4758	0	4793	1854	0
6	O	4758	0	4792	1888	0
6	P	4758	0	4791	2017	0
6	Q	4758	0	4792	1844	0
6	U	4758	0	4792	2037	0
6	V	4758	0	4793	1877	0
6	W	4758	0	4790	1906	0
6	X	4758	0	4797	224	0
All	All	101798	0	101167	13378	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 66.

The worst 5 of 13378 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:N:4:HIS:CG	6:O:586:VAL:HG22	1.19	1.72
6:U:66:ASP:HB2	6:V:232:ALA:CB	1.22	1.68
6:V:193:ILE:HG22	6:W:562:TYR:CE1	1.24	1.68
6:U:193:ILE:HG22	6:V:562:TYR:CE1	1.27	1.67
6:U:459:LEU:CB	6:V:414:GLN:HE22	1.05	1.67

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	A	1297/1299 (100%)	974 (75%)	214 (16%)	109 (8%)	1 16
2	B	1025/1027 (100%)	842 (82%)	136 (13%)	47 (5%)	3 30

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	1194/1196 (100%)	904 (76%)	201 (17%)	89 (8%)	1	19
4	D	410/412 (100%)	317 (77%)	54 (13%)	39 (10%)	1	14
4	E	410/412 (100%)	307 (75%)	75 (18%)	28 (7%)	1	21
5	F	274/276 (99%)	167 (61%)	66 (24%)	41 (15%)	0	5
5	G	274/276 (99%)	170 (62%)	61 (22%)	43 (16%)	0	4
5	H	274/276 (99%)	170 (62%)	62 (23%)	42 (15%)	0	5
5	L	274/276 (99%)	168 (61%)	62 (23%)	44 (16%)	0	4
5	M	274/276 (99%)	170 (62%)	62 (23%)	42 (15%)	0	5
5	N	274/276 (99%)	170 (62%)	62 (23%)	42 (15%)	0	5
5	R	274/276 (99%)	170 (62%)	61 (22%)	43 (16%)	0	4
5	S	274/276 (99%)	170 (62%)	61 (22%)	43 (16%)	0	4
5	T	274/276 (99%)	169 (62%)	62 (23%)	43 (16%)	0	4
5	Y	274/276 (99%)	169 (62%)	62 (23%)	43 (16%)	0	4
6	I	637/639 (100%)	477 (75%)	105 (16%)	55 (9%)	1	16
6	J	637/639 (100%)	476 (75%)	106 (17%)	55 (9%)	1	16
6	K	637/639 (100%)	479 (75%)	102 (16%)	56 (9%)	1	16
6	O	637/639 (100%)	478 (75%)	102 (16%)	57 (9%)	1	15
6	P	637/639 (100%)	476 (75%)	103 (16%)	58 (9%)	1	15
6	Q	637/639 (100%)	481 (76%)	102 (16%)	54 (8%)	1	16
6	U	637/639 (100%)	477 (75%)	105 (16%)	55 (9%)	1	16
6	V	637/639 (100%)	479 (75%)	100 (16%)	58 (9%)	1	15
6	W	637/639 (100%)	482 (76%)	99 (16%)	56 (9%)	1	16
6	X	637/639 (100%)	482 (76%)	99 (16%)	56 (9%)	1	16
All	All	13446/13496 (100%)	9824 (73%)	2324 (17%)	1298 (10%)	1	13

5 of 1298 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	39	LEU
1	A	40	HIS
1	A	69	SER
1	A	76	GLU
1	A	153	LYS

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1092/1092 (100%)	987 (90%)	105 (10%)	10	38
2	B	875/875 (100%)	788 (90%)	87 (10%)	9	36
3	C	1017/1017 (100%)	926 (91%)	91 (9%)	11	42
4	D	326/326 (100%)	283 (87%)	43 (13%)	5	26
4	E	326/326 (100%)	286 (88%)	40 (12%)	5	28
5	F	228/228 (100%)	199 (87%)	29 (13%)	5	27
5	G	228/228 (100%)	200 (88%)	28 (12%)	5	28
5	H	228/228 (100%)	199 (87%)	29 (13%)	5	27
5	L	228/228 (100%)	200 (88%)	28 (12%)	5	28
5	M	228/228 (100%)	200 (88%)	28 (12%)	5	28
5	N	228/228 (100%)	200 (88%)	28 (12%)	5	28
5	R	228/228 (100%)	199 (87%)	29 (13%)	5	27
5	S	228/228 (100%)	200 (88%)	28 (12%)	5	28
5	T	228/228 (100%)	199 (87%)	29 (13%)	5	27
5	Y	228/228 (100%)	200 (88%)	28 (12%)	5	28
6	I	528/528 (100%)	483 (92%)	45 (8%)	12	45
6	J	528/528 (100%)	486 (92%)	42 (8%)	14	47
6	K	528/528 (100%)	486 (92%)	42 (8%)	14	47
6	O	528/528 (100%)	485 (92%)	43 (8%)	14	47
6	P	528/528 (100%)	488 (92%)	40 (8%)	15	49
6	Q	528/528 (100%)	485 (92%)	43 (8%)	14	47
6	U	528/528 (100%)	485 (92%)	43 (8%)	14	47
6	V	528/528 (100%)	487 (92%)	41 (8%)	15	48
6	W	528/528 (100%)	485 (92%)	43 (8%)	14	47
6	X	528/528 (100%)	484 (92%)	44 (8%)	13	46
All	All	11196/11196 (100%)	10120 (90%)	1076 (10%)	14	38

5 of 1076 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	I	537	SER
5	L	210	THR
6	W	554	GLN
6	J	113	THR
6	K	148	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 252 such sidechains are listed below:

Mol	Chain	Res	Type
6	K	209	ASN
5	N	90	GLN
6	W	593	GLN
6	K	546	GLN
5	L	231	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 ⓘ

There are no chain breaks in this entry.