



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 02:26 PM BST

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 EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>

MolProbity : 4.02b-467
Mogul : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : trunk27241

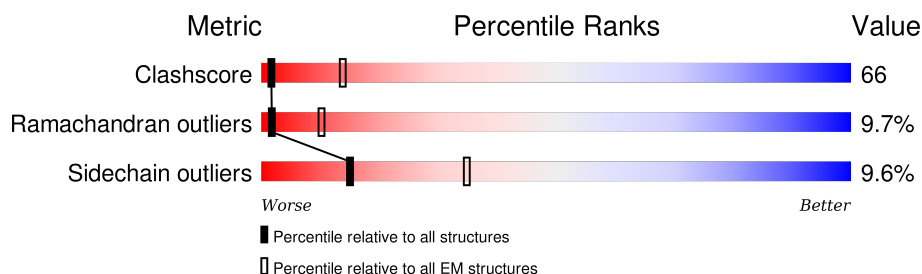
1 Overall quality at a glance

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	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

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 [i](#)

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 2085	C 1288	N 378	O 402	S 17	0	0
5	H	276	Total 2085	C 1288	N 378	O 402	S 17	0	0
5	L	276	Total 2085	C 1288	N 378	O 402	S 17	0	0
5	M	276	Total 2085	C 1288	N 378	O 402	S 17	0	0
5	N	276	Total 2085	C 1288	N 378	O 402	S 17	0	0
5	R	276	Total 2085	C 1288	N 378	O 402	S 17	0	0
5	S	276	Total 2085	C 1288	N 378	O 402	S 17	0	0
5	T	276	Total 2085	C 1288	N 378	O 402	S 17	0	0
5	Y	276	Total 2085	C 1288	N 378	O 402	S 17	0	0

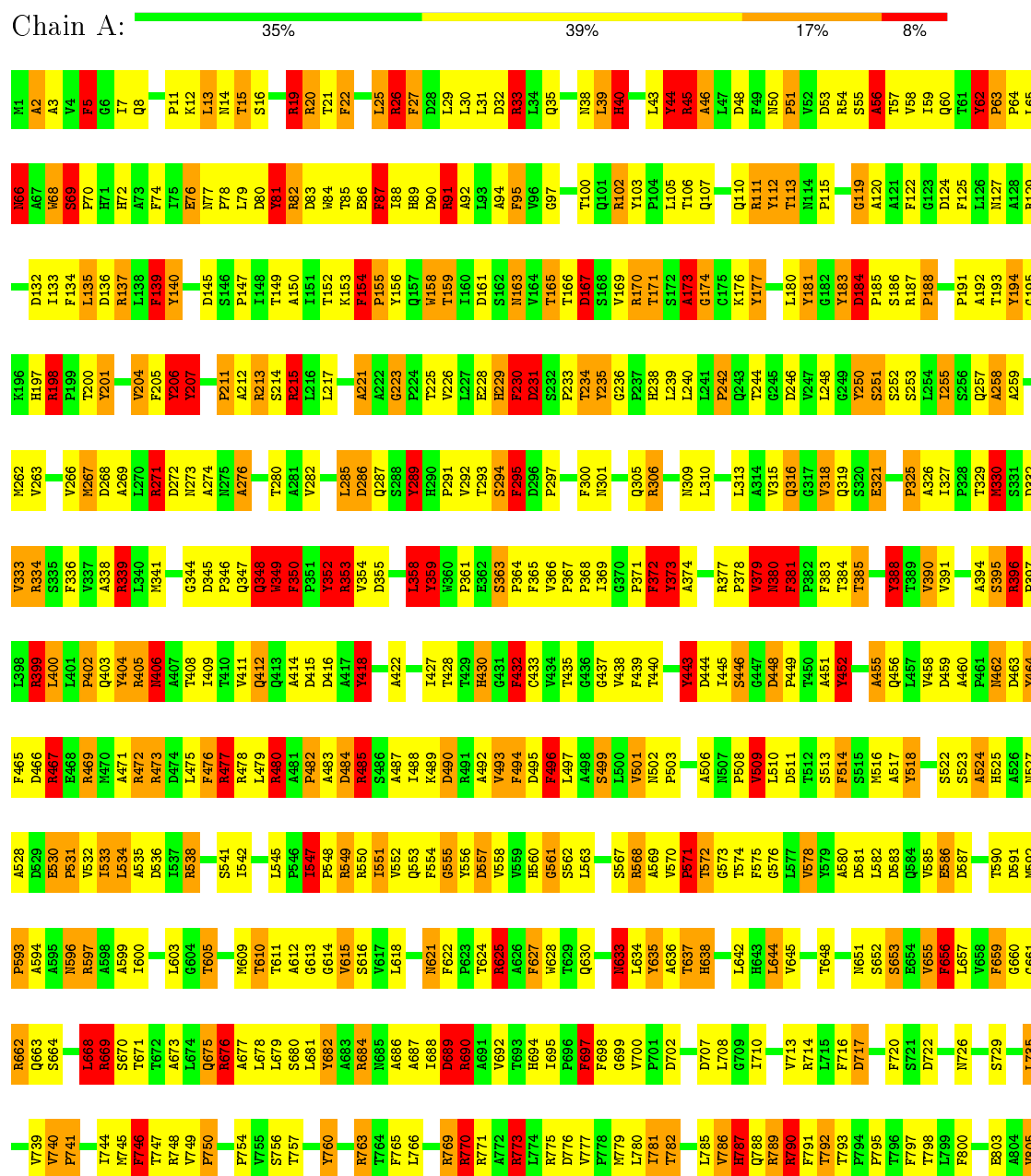
- Molecule 6 is a protein called Outer capsid VP5.

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

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 errors 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






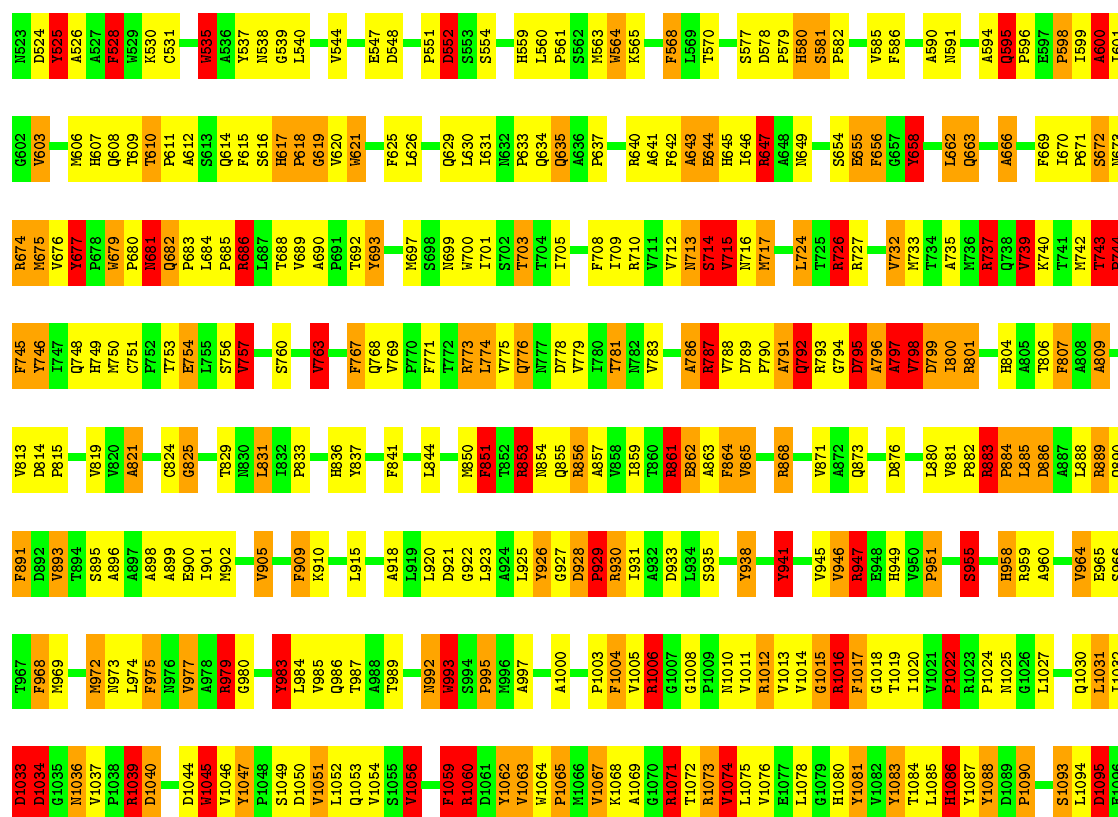
Frequency	Percentage
Daily	37%
Often	36%
Sometimes	20%
Not at all	6%



F445	G378	F304	E237	S175	D102	T19	D1174	E1101	L1031	S955	Q890	V820	H749	V677
F449	G379	T305	G238	S176	M106	N20	P1175	E1102	I1032	R956	F891	V821	H750	F678
F450	E380	L306	A239	K177	M107	V21	M1176	M1103	D1033	R957	D892	C824	C751	F679
F451	S382	S307	V240	K178	P110	V22	Y1177	L1104	D1034	R958	T894	G825	C752	G682
F452	A383	N312	N241	L179	P111	A24	R1178	I1107	V1037	A960	A897	G826	T753	G683
F453	N384	K313	R242	S180	N113	K25	G1180	L1108	P1038	L861	A898	T827	E754	P885
L463	S385	S314	T243	A181	P114	P28	M1182	A1110	R1039	Q862	A899	E828	L755	P886
Q464	C245	S315	C246	Y182	S115	N31	R1183	G1111	D1040	Q863	A900	T829	S756	L867
Q465	L183	L183	L183	L183	S116	N31	D1184	I1112	I1041	R830	E900	R830	V757	T688
Q466	T247	F317	T247	D184	Y117	S32	L1184	I1112	A1042	L831	E901	L832	V761	V689
Q467	N248	T318	N248	S185	V118	P33	P1185	V1115	G1043	M902	M902	H835	P765	V693
L468	N249	C119	A186	C119	C119	P34	R1187	F1117	D1044	A904	H903	H836	F766	D694
L469	A250	N120	V187	N120	N120	P39	R1188	C1118	W1046	V905	V905	T837	F767	M697
V460	D254	A188	A188	M189	C122	P39	T1189	I1119	Y1047	L974	N906	F841	P770	W700
V461	E255	G190	N123	G190	N123	A43	Y1191	S1048	P1048	F909	F909	A842	F771	W701
S463	G256	P191	R125	E192	R125	A44	N1192	D1050	I1051	K910	K910	P843	T772	L701
F471	G258	L193	F126	L193	F126	D45	S1193	A1057	V1052	A912	T911	L844	R773	S702
L472	L259	I194	S127	I194	S127	Q48	C1127	V1058	L1052	Y983	F913	L845	L774	T703
V473	E260	T195	T128	T195	T128	Q49	Y1195	Q1053	Q1053	L984	D914	L848	V775	T704
E474	V261	E196	M129	E196	M129	Q50	R1196	V1054	V1054	V985	L915	L849	W776	L705
R407	R262	D197	S130	D197	S130	P60	Y1197	S1055	S1055	Q886	D916	A849	D778	A706
H410	T198	A131	L132	T198	A131	A62	N1198	V1056	V1056	Q887	L916	K850	F779	F707
L479	G199	L132	L132	G199	L132	A67	F1199	A1057	A1057	T887	L919	F851	W788	F708
L480	L200	S133	E134	L200	S133	A67	T1200	V1058	V1058	A988	L920	T852	T782	L709
R481	C201	E134	E134	C201	E134	N73	Y1201	Q1059	Q1059	A1000	L921	R861	R710	R710
S482	T202	S134	S134	T202	S134	N73	P1202	R1061	R1061	P1002	G922	E862	L784	V711
T414	S203	R137	R137	S203	R137	N73	Y1207	Y1062	Y1062	P1003	G923	A863	W712	W712
Q415	F204	S138	S138	F204	S138	N73	M1208	V1063	V1063	P1004	L924	F864	G794	G794
V417	M205	R141	R141	M205	R141	N73	T1209	W1064	W1064	V1005	R930	C866	D795	D723
Q418	L207	D143	D143	L207	D143	N73	Y1210	V1067	V1067	R1006	I931	A867	L724	L724
T419	N209	A144	A144	N209	A144	N73	R1211	G1070	G1070	M1010	A932	R868	T725	T725
T420	T210	S145	S145	T210	S145	N73	A1213	V1074	V1074	N1011	D933	V871	R726	R726
E422	P211	S145	S145	P211	S145	N73	T1214	E1077	E1077	R1012	T934	A872	R727	R727
C423	S212	L148	L148	S212	L148	G76	M1207	Y1081	Y1081	S935	L934	A873	T728	T728
A424	A213	A149	A149	A213	A149	D77	M1208	V1082	V1082	A936	S936	Q873	R801	R801
M425	H214	T150	T150	H214	T150	D77	R1211	V1083	V1083	A937	A937	C874	A802	T730
N426	L215	P151	P151	L215	P151	T79	S1212	V1084	V1084	G1015	L939	Q875	T803	G731
T427	K216	M152	M152	K216	M152	R81	A1147	T1085	T1085	F1017	Q940	Q875	V831	V831
N285	K217	I153	I153	K217	I153	P82	S1148	L1086	L1086	T1019	Y941	A805	T743	T743
A286	E218	H154	H154	E218	H154	T83	S1149	H1086	H1086	T1019	Y941	A805	P815	P744
Q287	L219	A156	A156	L219	A156	D85	T1156	Y1088	Y1088	G1015	Y941	A805	A816	F745
R289	G221	I157	I157	G221	I157	S86	A1157	V1088	V1088	F1017	Q940	A805	A817	Y746
P290	F223	R158	R158	P290	F223	S86	E1160	T1088	T1088	G1015	Y941	A805	V813	W742
L291	T223	S159	S159	L291	T223	S86	A1163	Y1088	Y1088	G1015	Y941	A805	D814	T743
A292	W224	F160	F160	A292	W224	S86	V1164	Y1088	Y1088	G1015	Y941	A805	P815	P744
L293	F225	W164	W164	L293	F225	V90	S1165	D1089	D1089	T1021	N944	L880	A816	F745
R294	M226	D165	D165	R294	M226	K95	V1166	P1022	P1022	N944	N944	L880	A817	Y746
S295	Q227	N228	N228	S295	Q227	P96	S1166	P1023	P1023	V945	V945	L880	V813	W742
N296	M228	N228	N228	N296	M228	A97	S1166	P1024	P1024	V945	V945	L880	D814	T743
Y229	Y229	I167	I167	Y229	Y229	A98	R1168	M1025	M1025	R947	R947	L880	P815	P744
Q230	Q230	R168	R168	Q230	Q230	A98	W1169	N1025	N1025	P951	P951	L880	A816	F745
M231	M231	I169	I169	M231	M231	V99	P1170	E1028	E1028	P952	P952	L880	A817	Y746
P236	P236	L170	L170	P236	P236	V100	G1171	P1029	P1029	P953	P953	L880	V813	W742
Q303	Q303	S171	S171	Q303	Q303	S101	V1172	L1109	L1109	P954	P954	L880	D814	T743
							V1173	L1109	L1109	P954	P954	L880	P815	P744

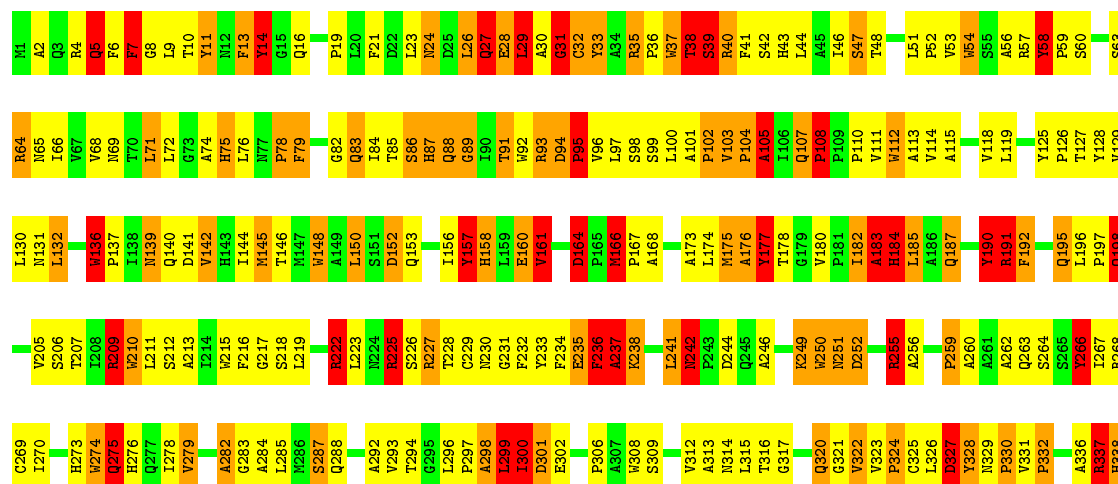
• Molecule 3: VP3B

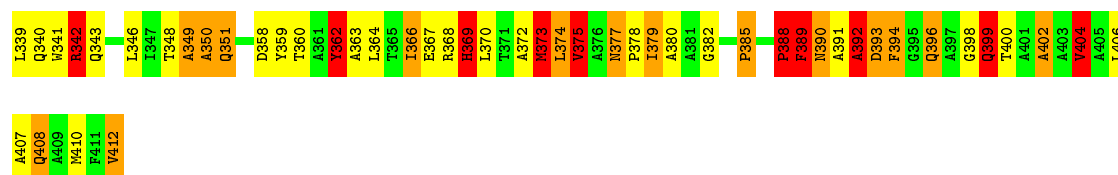
Chain C: 



• Molecule 4: Core protein VP6

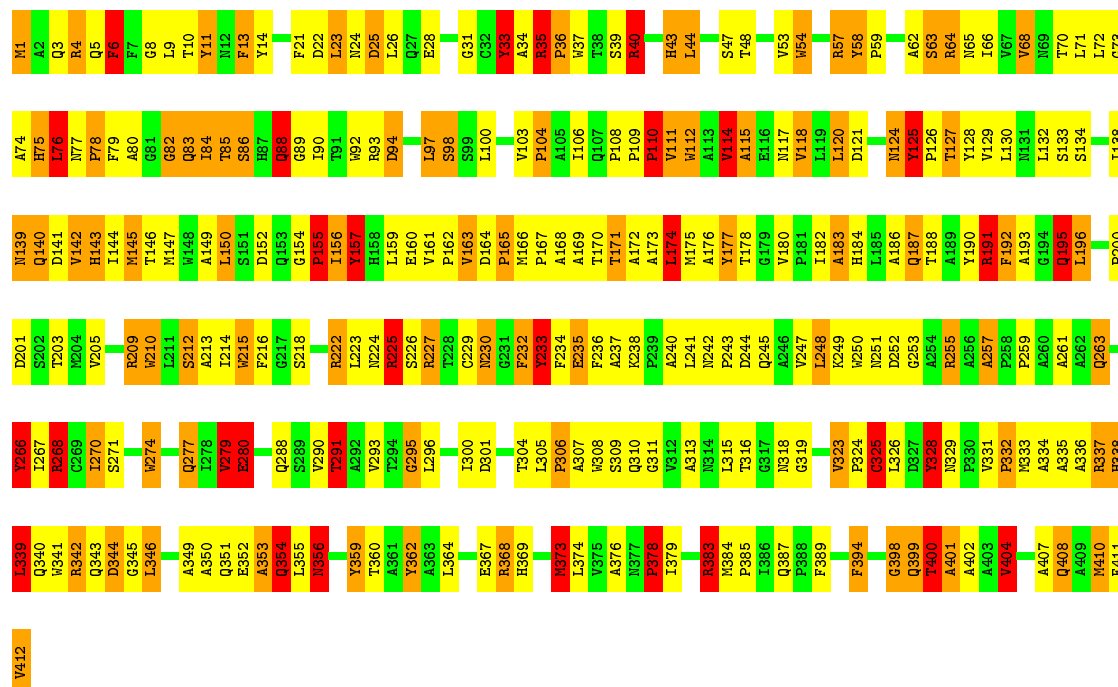
Chain D: 31% 38% 20% 11%





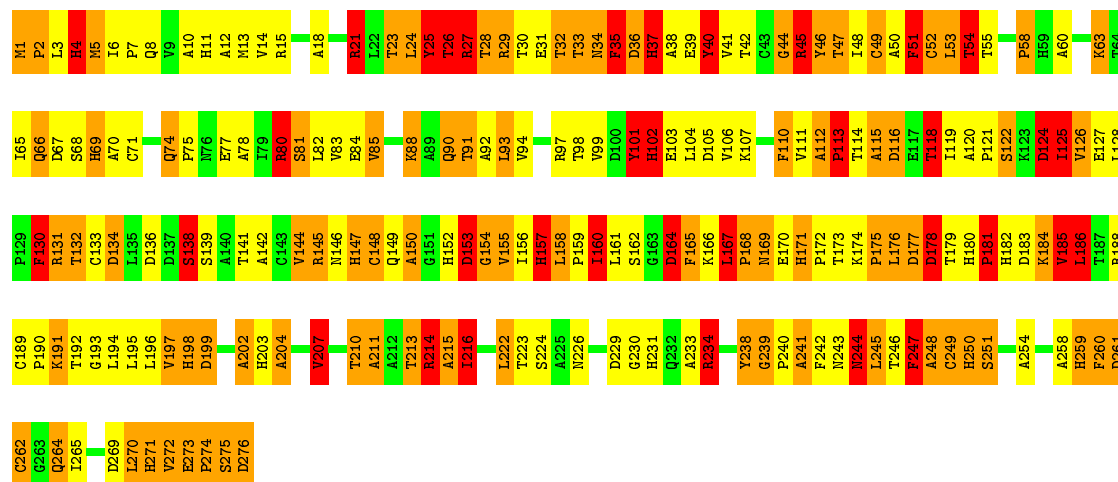
• Molecule 4: Core protein VP6

Chain E: 33% 39% 20% 8%

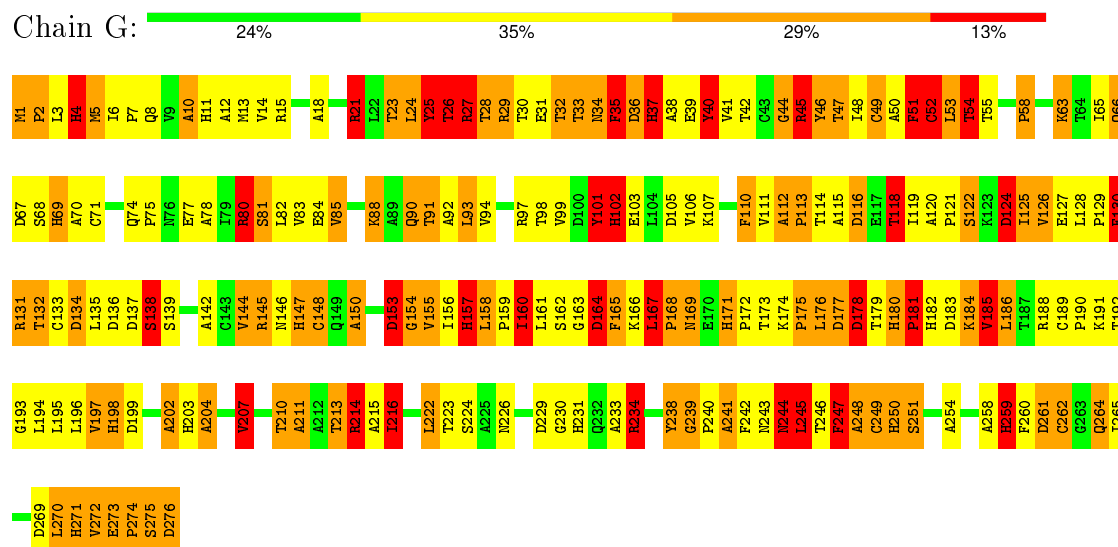


• Molecule 5: Outer capsid VP7

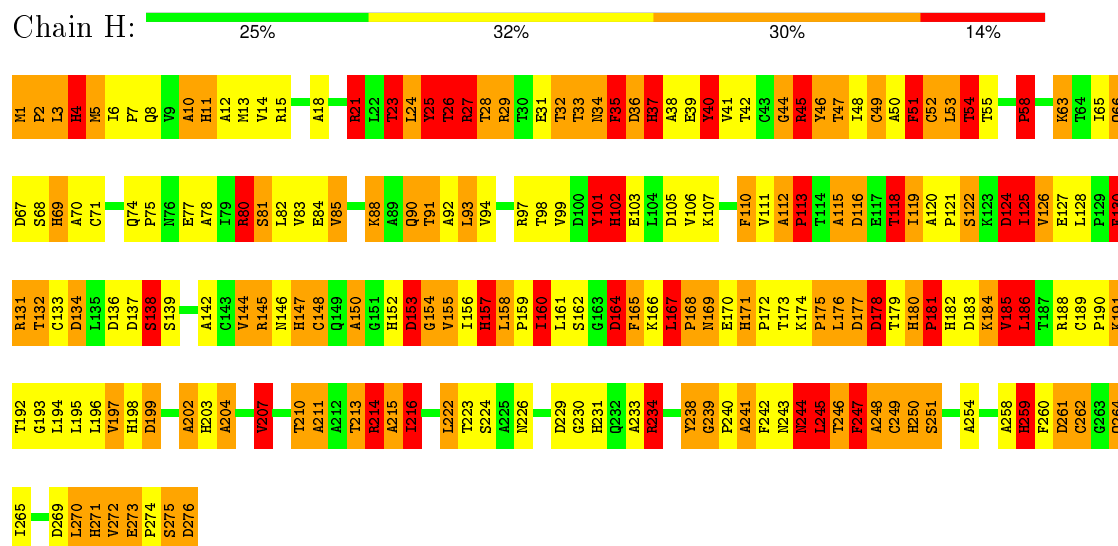
Chain F: 23% 34% 30% 13%



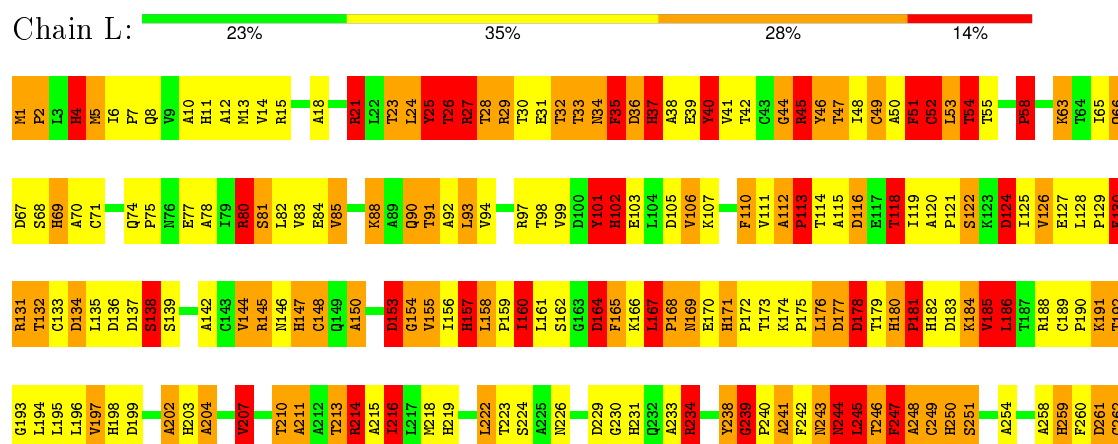
• Molecule 5: Outer capsid VP7

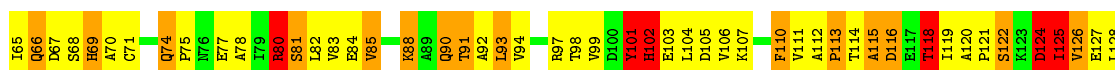


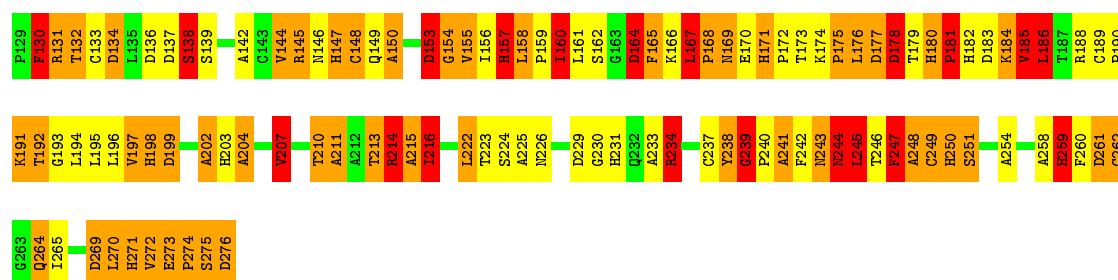
• Molecule 5: Outer capsid VP7



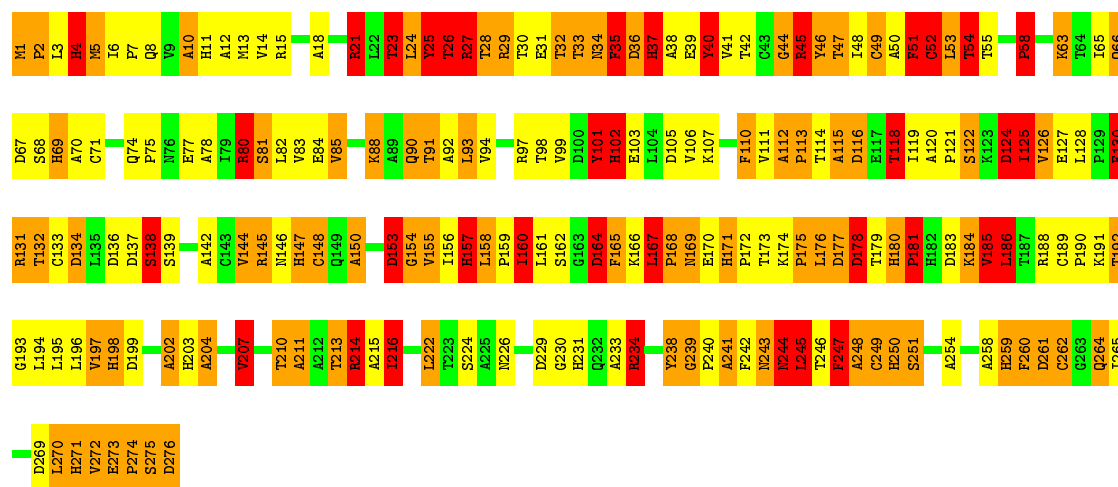
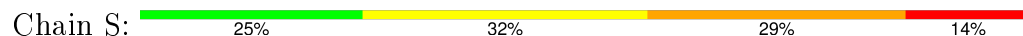
• Molecule 5: Outer capsid VP7



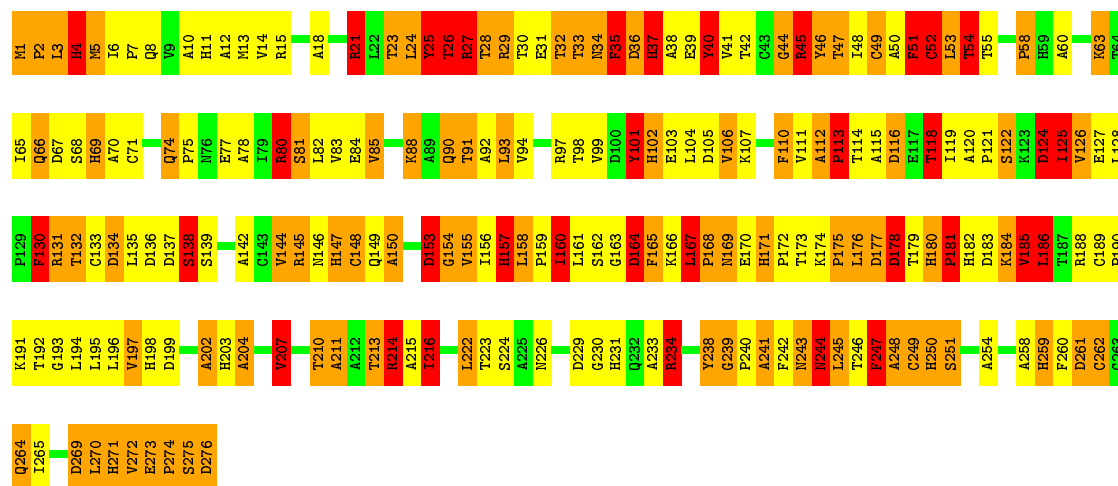
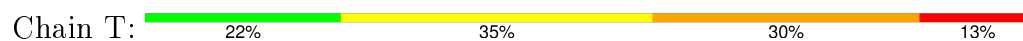




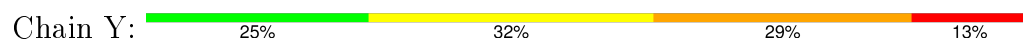
• Molecule 5: Outer capsid VP7



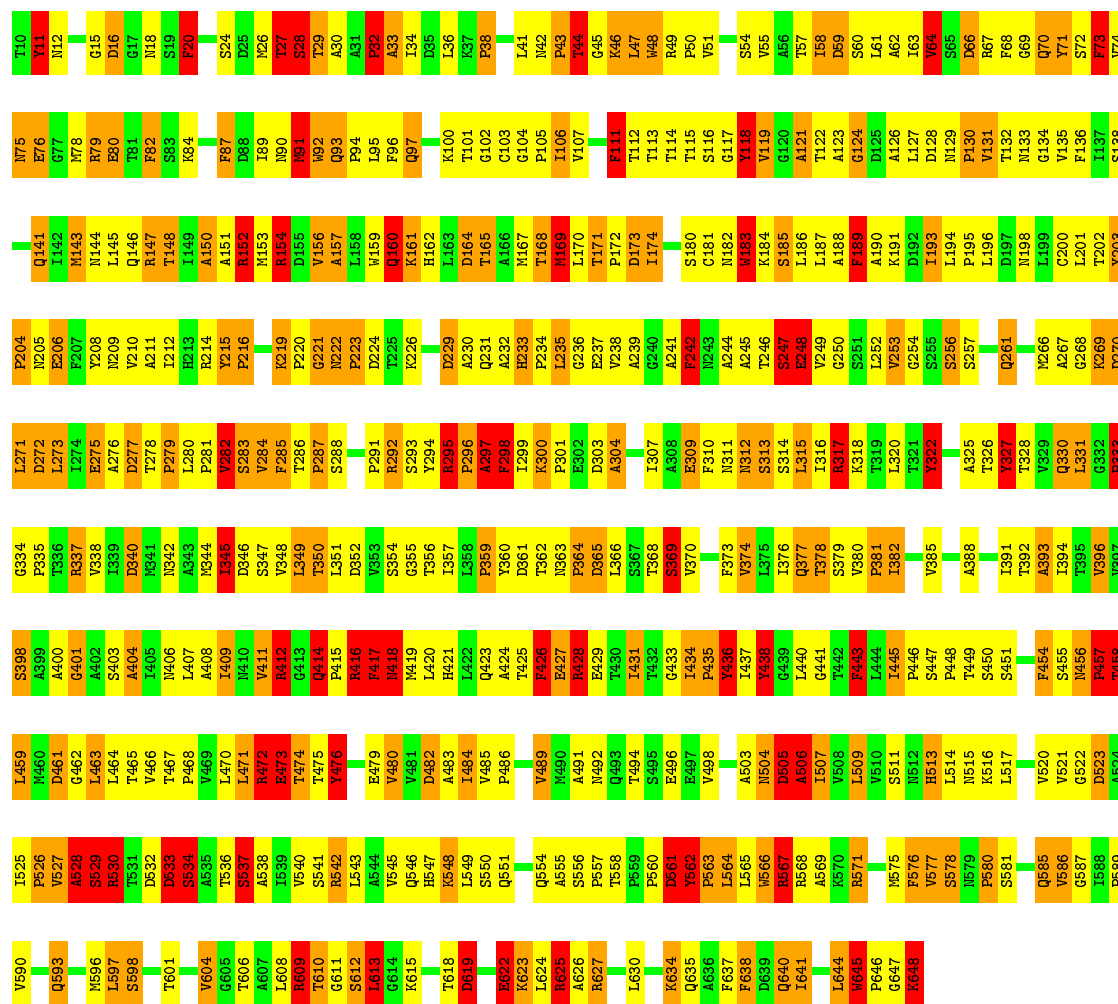
• Molecule 5: Outer capsid VP7



• Molecule 5: Outer capsid VP7

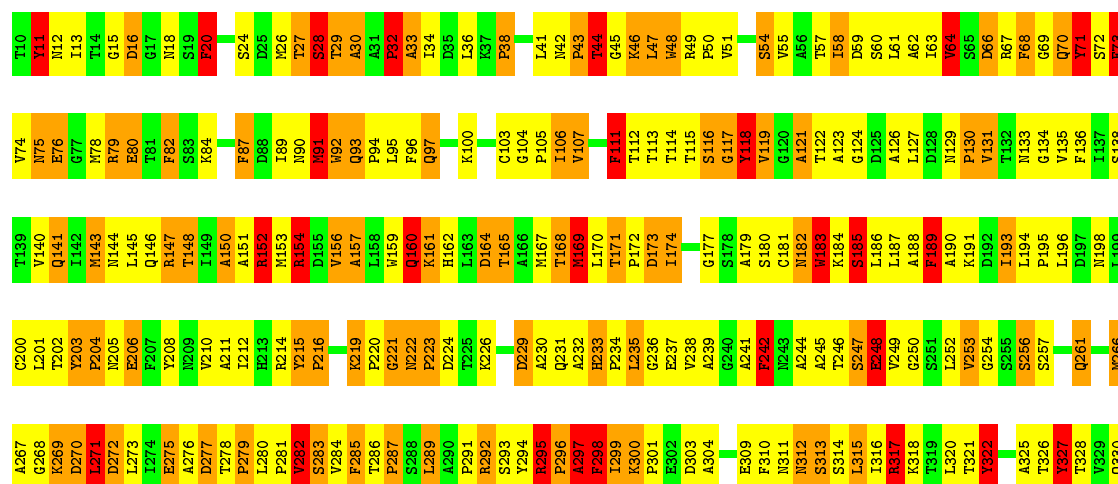


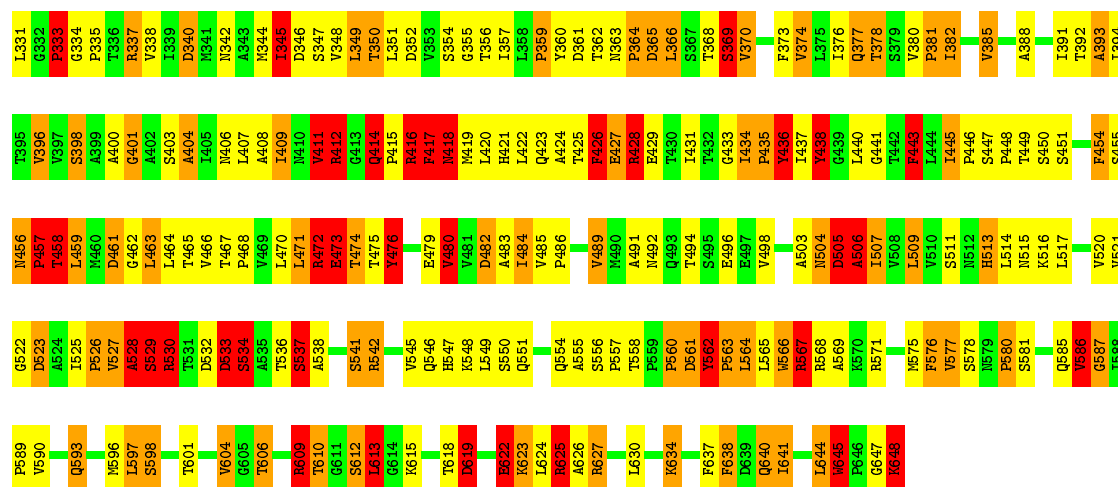
Chain J: 



• Molecule 6: Outer capsid VP5

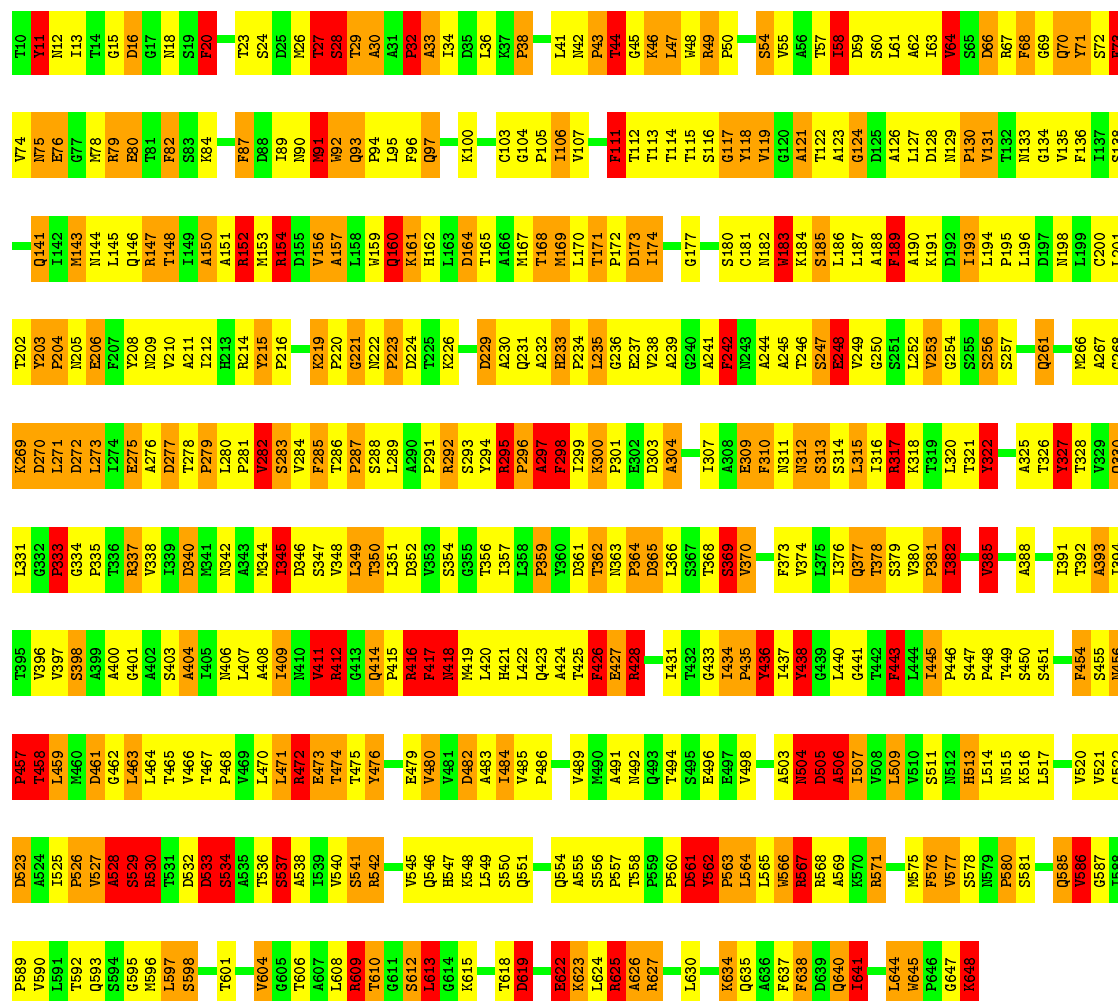
Chain K: 



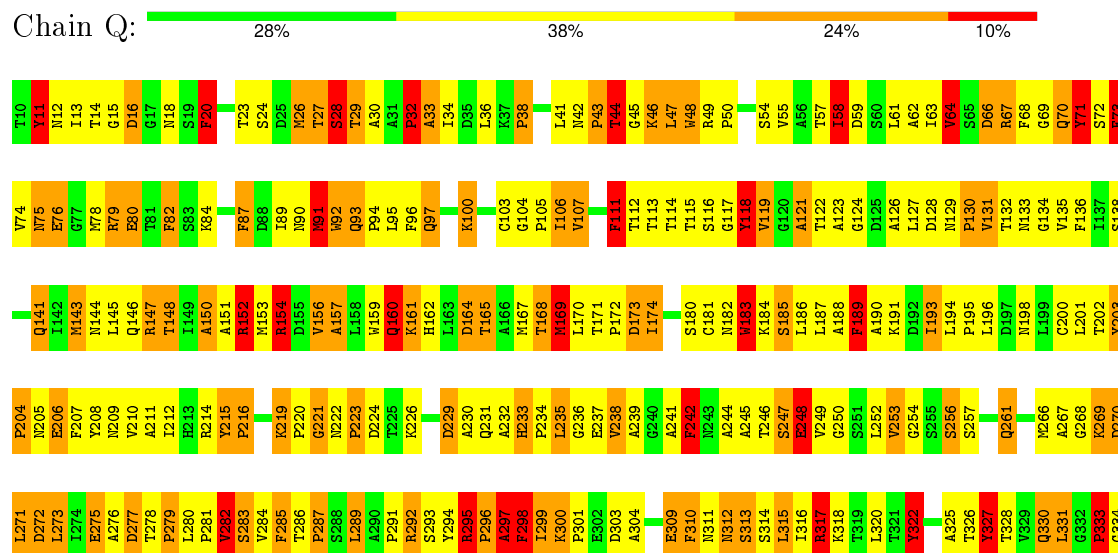
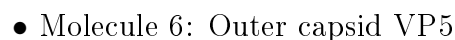


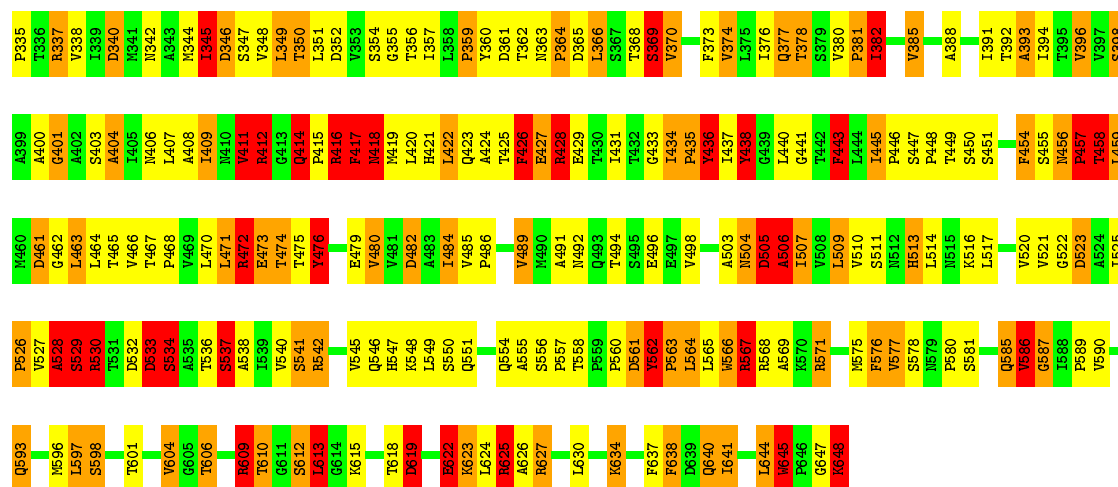
• Molecule 6: Outer capsid VP5

Chain O: 27% 41% 23% 10%



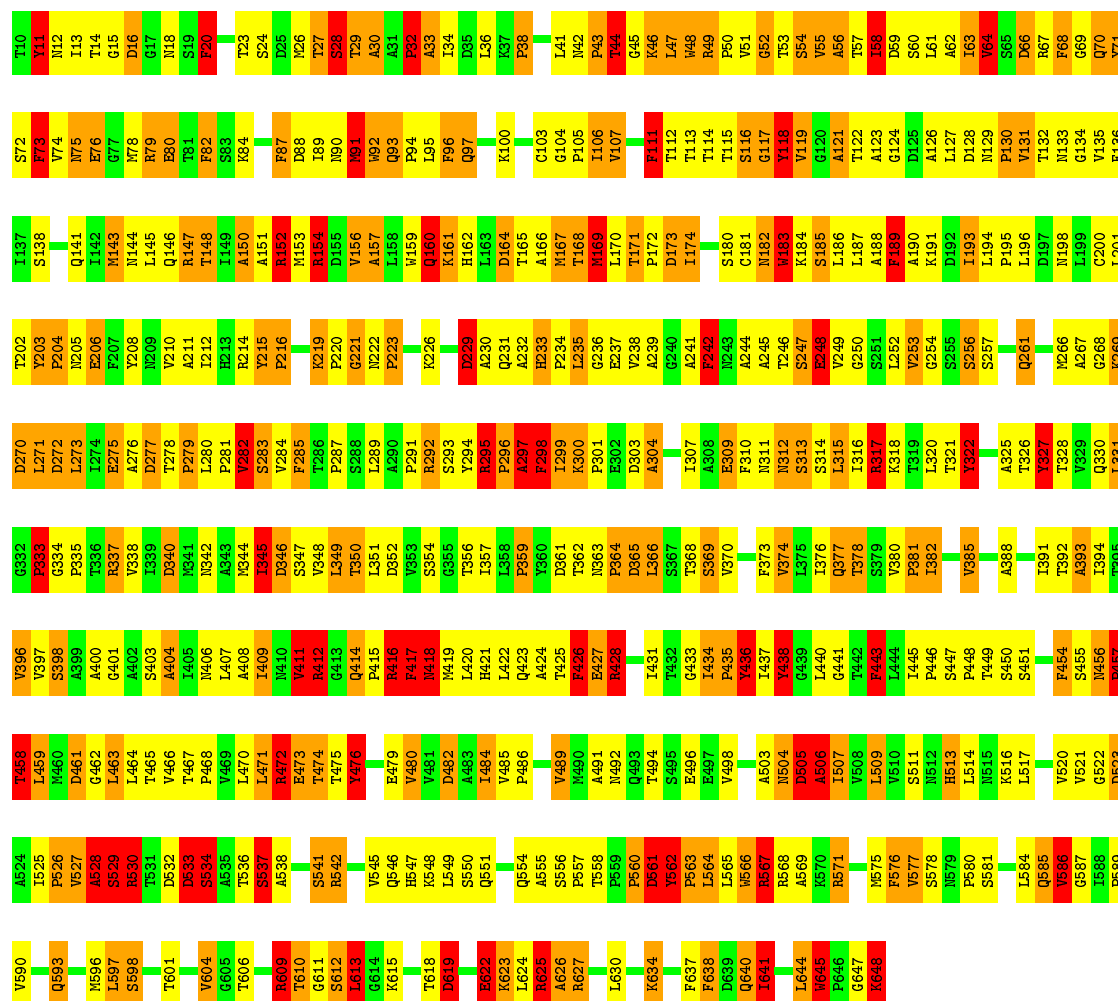
• Molecule 6: Outer capsid VP5



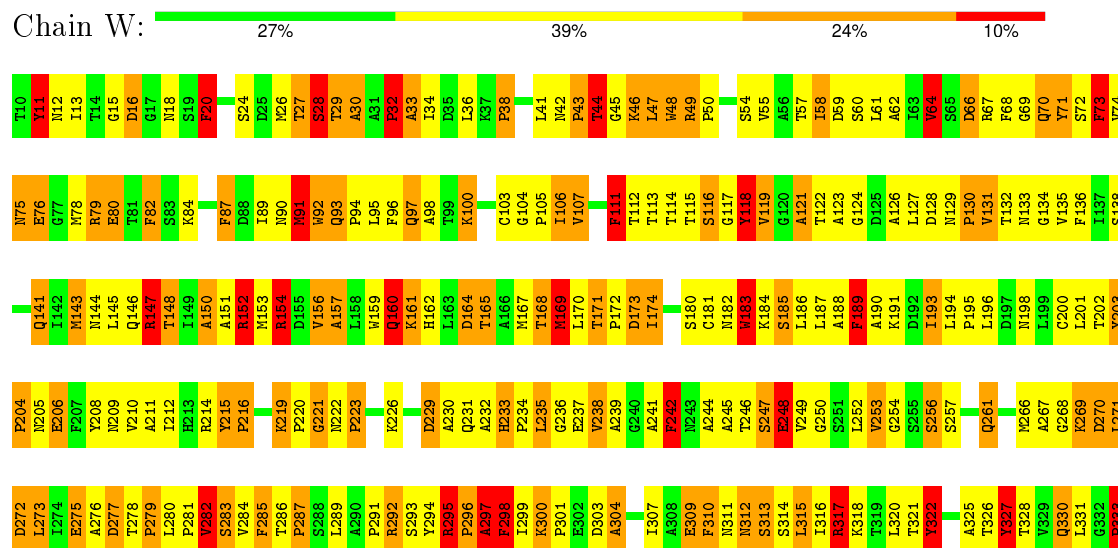
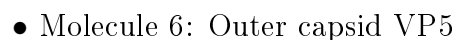


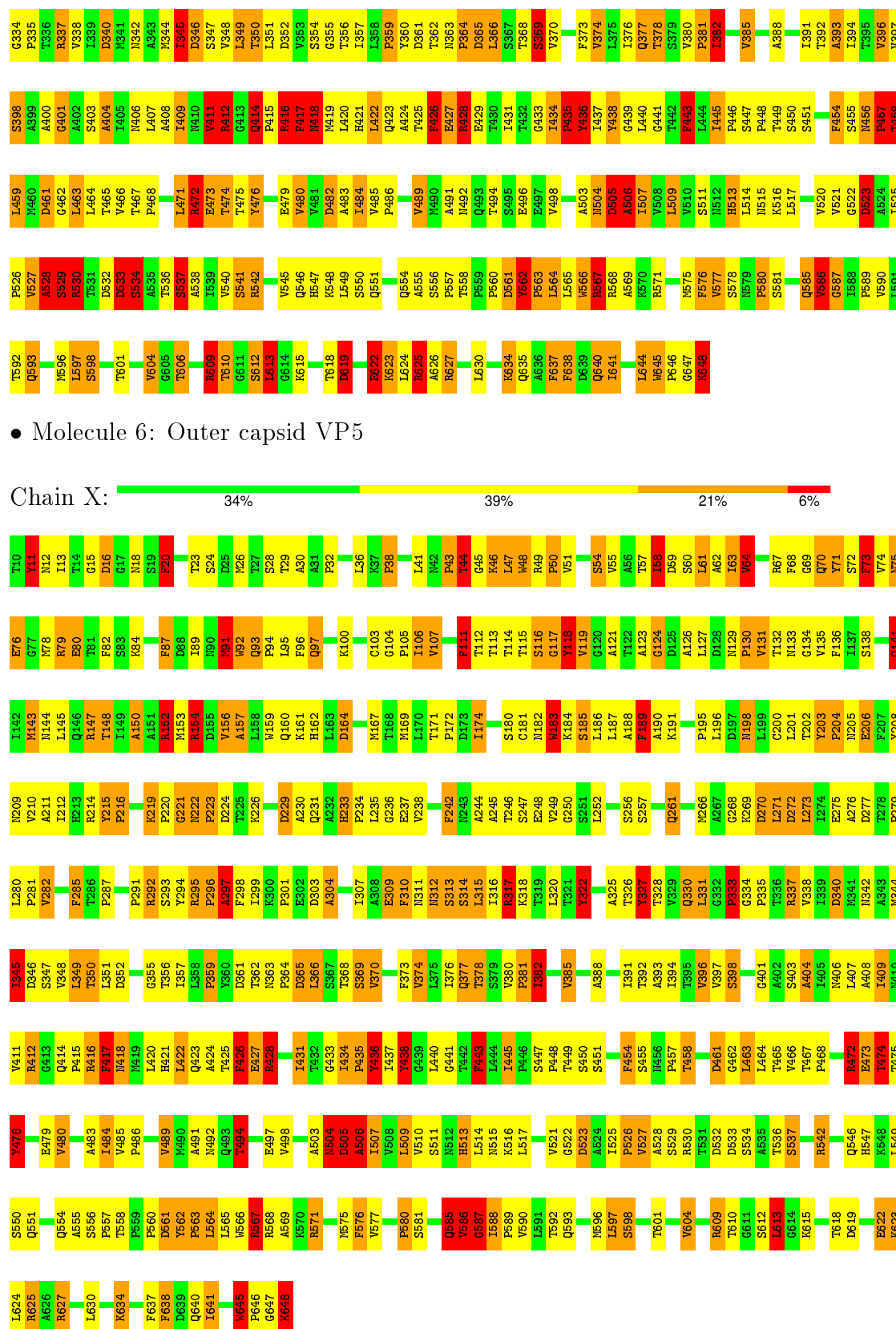
• Molecule 6: Outer capsid VP5

Chain U: 27% 38% 24% 10%



• Molecule 6: Outer capsid VP5





• Molecule 6: Outer capsid VP5

4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of images	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 [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	1297/1299 (100%)	974 (75%)	214 (16%)	109 (8%)	1 17
2	B	1025/1027 (100%)	842 (82%)	136 (13%)	47 (5%)	3 33

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	1194/1196 (100%)	904 (76%)	201 (17%)	89 (8%)	1	21
4	D	410/412 (100%)	317 (77%)	54 (13%)	39 (10%)	1	15
4	E	410/412 (100%)	307 (75%)	75 (18%)	28 (7%)	1	24
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	5
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	5
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	5
5	S	274/276 (99%)	170 (62%)	61 (22%)	43 (16%)	0	5
5	T	274/276 (99%)	169 (62%)	62 (23%)	43 (16%)	0	5
5	Y	274/276 (99%)	169 (62%)	62 (23%)	43 (16%)	0	5
6	I	637/639 (100%)	477 (75%)	105 (16%)	55 (9%)	1	17
6	J	637/639 (100%)	476 (75%)	106 (17%)	55 (9%)	1	17
6	K	637/639 (100%)	479 (75%)	102 (16%)	56 (9%)	1	17
6	O	637/639 (100%)	478 (75%)	102 (16%)	57 (9%)	1	17
6	P	637/639 (100%)	476 (75%)	103 (16%)	58 (9%)	1	16
6	Q	637/639 (100%)	481 (76%)	102 (16%)	54 (8%)	1	17
6	U	637/639 (100%)	477 (75%)	105 (16%)	55 (9%)	1	17
6	V	637/639 (100%)	479 (75%)	100 (16%)	58 (9%)	1	16
6	W	637/639 (100%)	482 (76%)	99 (16%)	56 (9%)	1	17
6	X	637/639 (100%)	482 (76%)	99 (16%)	56 (9%)	1	17
All	All	13446/13496 (100%)	9824 (73%)	2324 (17%)	1298 (10%)	2	14

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	43
2	B	875/875 (100%)	788 (90%)	87 (10%)	10	42
3	C	1017/1017 (100%)	926 (91%)	91 (9%)	12	47
4	D	326/326 (100%)	283 (87%)	43 (13%)	5	30
4	E	326/326 (100%)	286 (88%)	40 (12%)	6	32
5	F	228/228 (100%)	199 (87%)	29 (13%)	5	31
5	G	228/228 (100%)	200 (88%)	28 (12%)	6	32
5	H	228/228 (100%)	199 (87%)	29 (13%)	5	31
5	L	228/228 (100%)	200 (88%)	28 (12%)	6	32
5	M	228/228 (100%)	200 (88%)	28 (12%)	6	32
5	N	228/228 (100%)	200 (88%)	28 (12%)	6	32
5	R	228/228 (100%)	199 (87%)	29 (13%)	5	31
5	S	228/228 (100%)	200 (88%)	28 (12%)	6	32
5	T	228/228 (100%)	199 (87%)	29 (13%)	5	31
5	Y	228/228 (100%)	200 (88%)	28 (12%)	6	32
6	I	528/528 (100%)	483 (92%)	45 (8%)	13	50
6	J	528/528 (100%)	486 (92%)	42 (8%)	15	53
6	K	528/528 (100%)	486 (92%)	42 (8%)	15	53
6	O	528/528 (100%)	485 (92%)	43 (8%)	15	52
6	P	528/528 (100%)	488 (92%)	40 (8%)	16	55
6	Q	528/528 (100%)	485 (92%)	43 (8%)	15	52
6	U	528/528 (100%)	485 (92%)	43 (8%)	15	52
6	V	528/528 (100%)	487 (92%)	41 (8%)	16	54
6	W	528/528 (100%)	485 (92%)	43 (8%)	15	52
6	X	528/528 (100%)	484 (92%)	44 (8%)	14	51
All	All	11196/11196 (100%)	10120 (90%)	1076 (10%)	15	43

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.