wwPDB EM Validation Summary Report

Dec 17, 2022 – 04:51 pm GMT

PDB ID	:	6ZTZ
EMDB ID	:	EMD-22166
Title	:	Assembly intermediates of orthoreovirus captured in the cell
Authors	:	Sutton, G.C.; Stuart, D.I.
Deposited on	:	2020-07-20
Resolution	:	Not provided

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

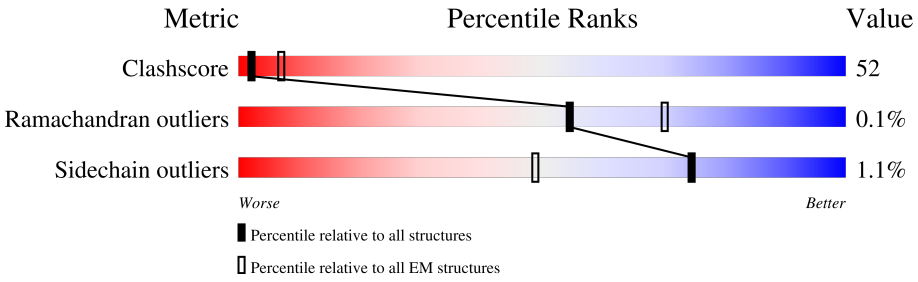
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is unknown.

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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	B	1035	100% 30% 69% .
2	C	1008	95% 26% 73% .
3	D	417	96% 27% 71% .
3	P	417	84% 25% 73% .
4	K	641	89% 28% 71% .
4	L	641	91% 32% 68% .
4	M	641	92% 32% 67% .
5	O	1284	91% 26% 73% .

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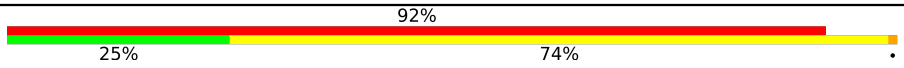
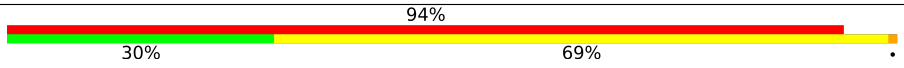
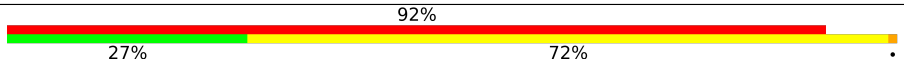
Mol	Chain	Length	Quality of chain
6	X	365	
6	Y	365	
6	Z	365	

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 56150 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

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

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

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

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

There are 8 discrepancies between the modelled and reference sequences:

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

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

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

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

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

There are 81 discrepancies between the modelled and reference sequences:

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

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

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

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

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

There are 4 discrepancies between the modelled and reference sequences:

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

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

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

There are 6 discrepancies between the modelled and reference sequences:

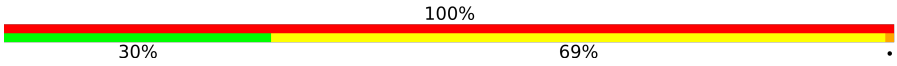
Chain	Residue	Modelled	Actual	Comment	Reference
X	104	CYS	ALA	conflict	UNP P07939
X	325	ASN	ASP	conflict	UNP P07939
Y	104	CYS	ALA	conflict	UNP P07939
Y	325	ASN	ASP	conflict	UNP P07939
Z	104	CYS	ALA	conflict	UNP P07939
Z	325	ASN	ASP	conflict	UNP P07939

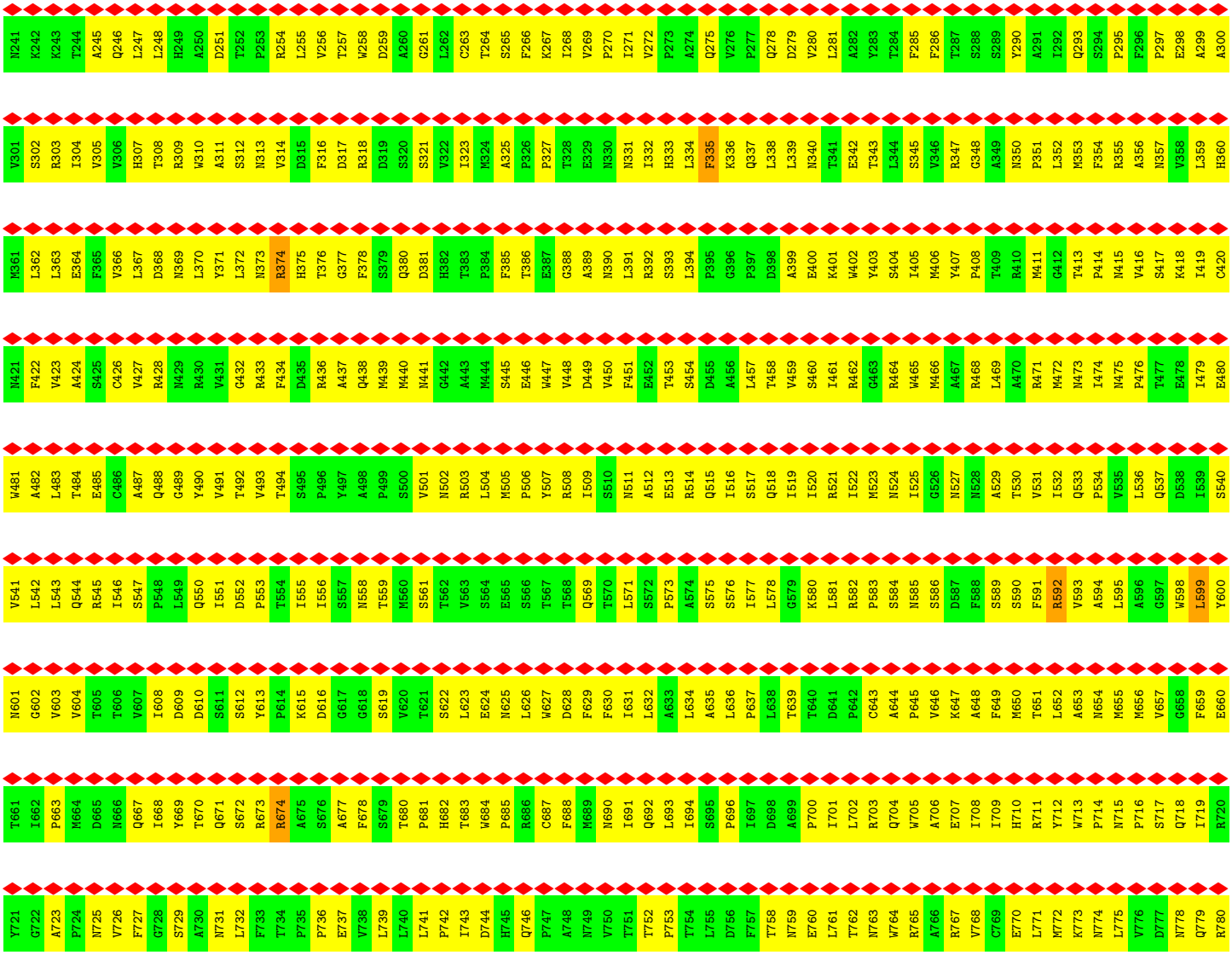
3 Residue-property plots (i)

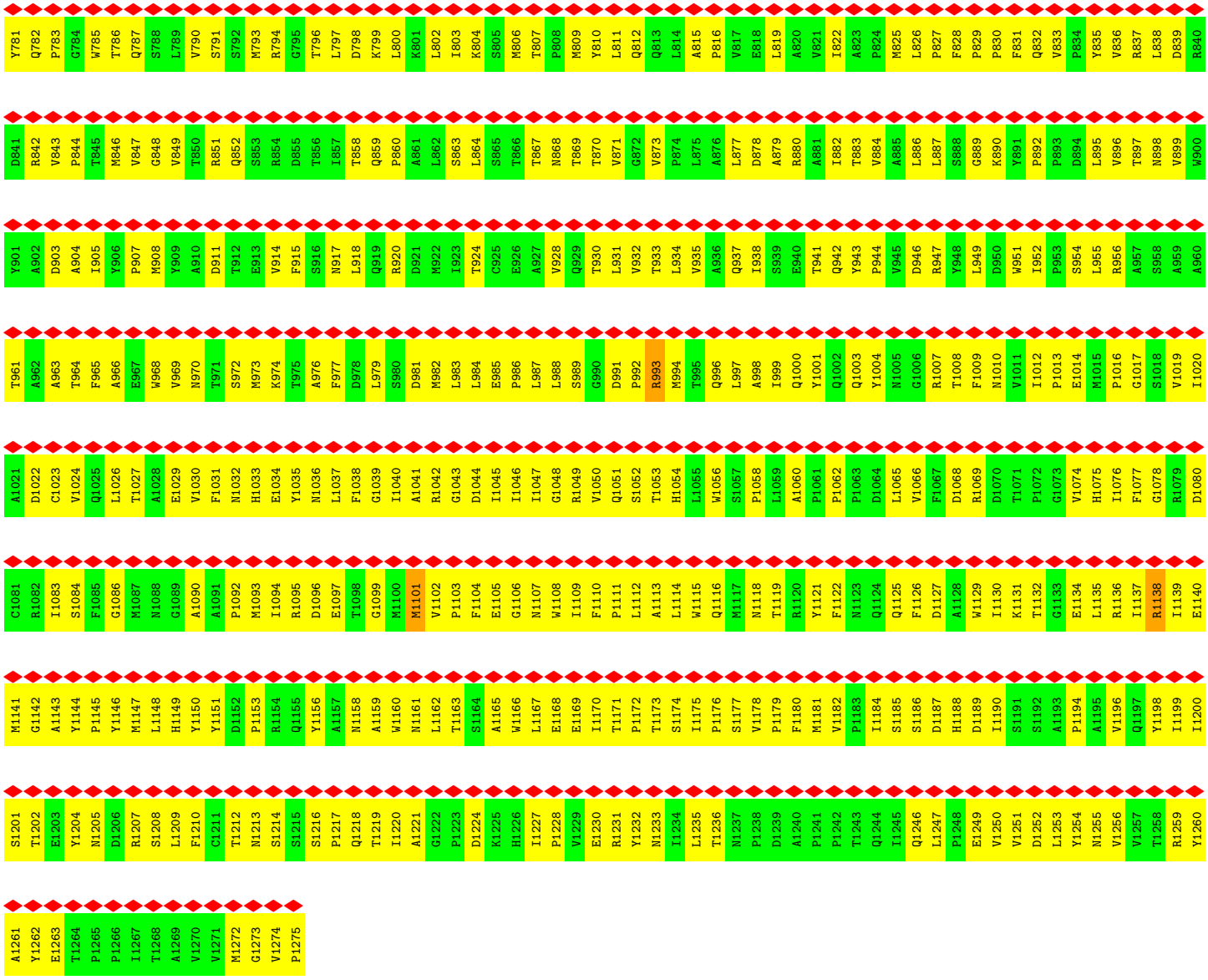
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: Inner capsid protein lambda-1

Chain B:

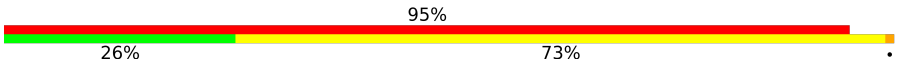


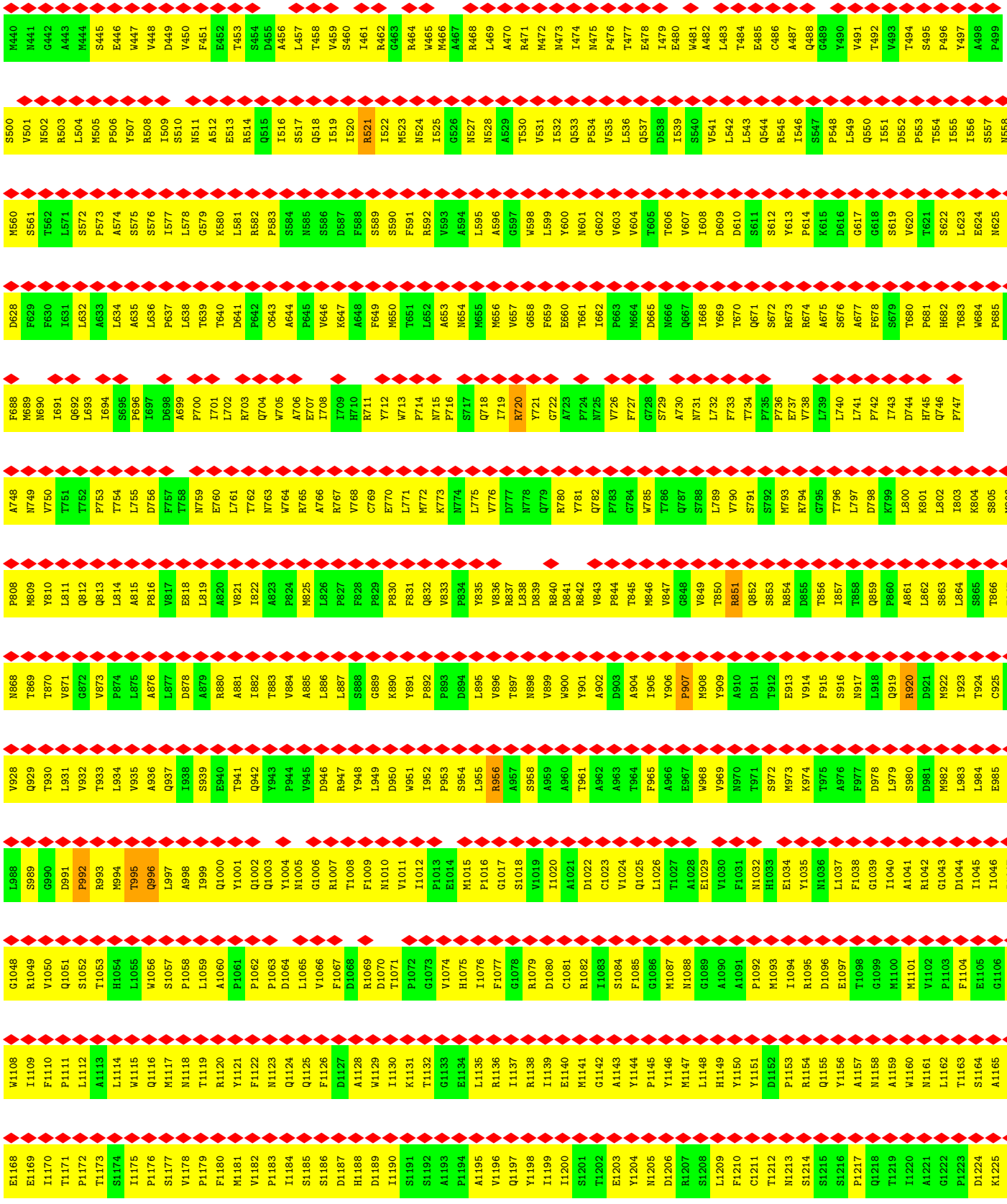


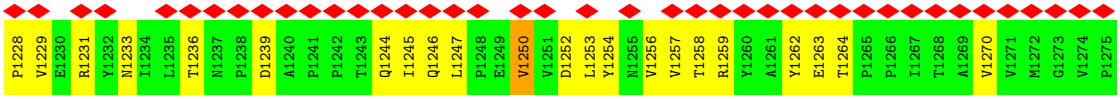


• Molecule 2: Inner capsid protein lambda-1

Chain C:

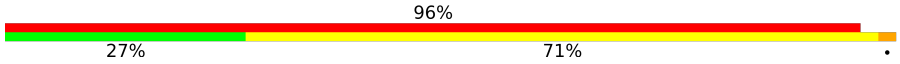


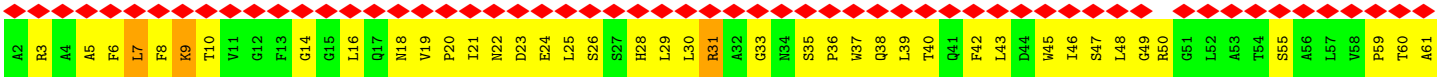

M440 N441 G442 A443 M444 S445 E446 W447 V448 D449 V450 F451 E452 T453 S454 D455 A456 L457 T458 V459 S460 I461 R462 G463 R464 W465 M466 A467 R468 L469 A470 R471 M472 N473 I474 N475 P476 T477 E478 I479 E480 W481 A482 L483 T484 E485 C486 A487 Q488 G489 Y490 V491 T492 V493 T494 S495 P496 Y497 A498 P499
S500 V501 N502 R503 L504 M505 P506 Y507 R508 I509 S510 N511 A512 E513 R514 Q515 I516 S517 Q518 I519 I520 R521 I522 M523 N524 I525 G526 N527 N528 A529 T530 V531 I532 Q533 P534 V535 L536 Q537 D538 I539 S540 V541 L542 L543 Q544 R545 I546 S547 P548 L549 Q550 I551 D552 P553 T554 I555 I556 S557 N558 T559
M560 S561 T562 L571 S572 P573 A574 S575 S576 I577 L578 G579 K580 L581 R582 P583 S584 N585 S586 D587 F588 S589 S590 F591 R592 V593 A594 L595 A596 G597 W598 L599 Y600 N601 G602 V603 V604 T605 T606 V607 I608 D609 D610 S611 S612 Y613 P614 K615 D616 G617 G618 S619 V620 T621 S622 L623 E624 N625 L626 W627
D628 F629 F630 I631 L632 A633 L634 A635 L636 P637 L638 T639 T640 D641 P642 C643 A644 P645 V646 K647 A648 F649 M650 T651 L652 A653 N654 M655 M656 V657 G658 F659 E660 T661 I662 P663 M664 D665 N666 Q667 I668 Y669 T670 Q671 S672 R673 R674 A675 S676 A677 F678 S679 T680 P681 H682 T683 W684 P685 R686 C687
F688 M689 M690 I691 Q692 L693 I694 S695 P696 I697 D698 A699 P700 I701 L702 R703 Q704 W705 A706 E707 I708 I709 H710 R711 Y712 W713 P714 N715 P716 S717 Q718 I719 R720 Y721 G722 A723 P724 N725 V726 F727 G728 S729 A730 N731 L732 F733 T734 P735 P736 E737 V738 L739 L740 L741 P742 I743 D744 H745 Q746 P747
A748 N749 V750 T751 T752 P753 T754 L755 D756 F757 T758 N759 E760 L761 T762 N763 W764 R765 A766 R767 V768 C769 E770 L771 W772 K773 N774 L775 V776 D777 N778 Q779 R780 Y781 Q782 P783 G784 W785 T786 Q787 S788 L789 V790 S791 S792 W793 R794 G795 T796 L797 D798 K799 L800 K801 L802 I803 K804 S805 M806 T807
P808 M809 Y810 L811 Q812 Q813 L814 A815 P816 V817 E818 L819 A820 V821 I822 A823 P824 M825 L826 P827 F828 P829 P830 F831 Q832 V833 P834 Y835 V836 R837 L838 D839 R840 D841 R842 V843 P844 T845 M846 V847 G848 V849 T850 R851 Q852 S853 R854 D855 T856 I857 T858 Q859 P860 A861 L862 S863 L864 S865 T866 T867
N868 T869 T870 V871 G872 V873 P874 L875 A876 L877 D878 A879 R880 A881 I882 T883 V884 A885 L886 L887 S888 G889 K890 Y891 P892 P893 D894 L895 V896 T897 N898 V899 W900 Y901 A902 D903 A904 I905 Y906 P907 M908 Y909 A910 D911 T912 E913 V914 F915 S916 N917 L918 Q919 R920 D921 M922 I923 T924 C925 E926 A927
V928 Q929 T930 L931 V932 T933 L934 V935 A936 Q937 I938 S939 E940 T941 Q942 Y943 P944 V945 D946 R947 Y948 L949 D950 W951 I952 P953 S954 L955 R956 A957 S958 A959 A960 T961 A962 A963 T964 F965 A966 E967 W968 V969 N970 T971 S972 M973 K974 T975 A976 F977 D978 L979 S980 D981 M982 L983 L984 E985 P986 L987
L988 S989 G990 D991 P992 R993 M994 T995 Q996 L997 A998 I999 Q1000 Y1001 Q1002 Q1003 Y1004 N1005 G1006 R1007 T1008 F1009 N1010 V1011 I1012 P1013 E1014 M1015 P1016 G1017 S1018 V1019 I1020 A1021 D1022 C1023 V1024 Q1025 L1026 T1027 A1028 E1029 V1030 F1031 N1032 H1033 E1034 Y1035 N1036 L1037 F1038 G1039 I1040 A1041 R1042 G1043 D1044 I1045 I1046 I1047
G1048 R1049 V1050 Q1051 S1052 T1053 H1054 L1055 W1056 S1057 P1058 L1059 A1060 P1061 P1062 P1063 D1064 L1065 V1066 F1067 D1068 R1069 D1070 T1071 P1072 G1073 V1074 H1075 I1076 F1077 G1078 R1079 D1080 C1081 R1082 I1083 S1084 F1085 G1086 N1087 N1088 G1089 A1090 A1091 P1092 M1093 I1094 R1095 D1096 E1097 T1098 G1099 M1100 M1101 V1102 P1103 F1104 E1105 G1106 N1107
W1108 I1109 F1110 P1111 L1112 A1113 L1114 W1115 Q1116 M1117 N1118 T1119 R1120 Y1121 F1122 N1123 Q1124 Q1125 F1126 D1127 A1128 W1129 I1130 K1131 T1132 G1133 E1134 L1135 R1136 I1137 R1138 I1139 E1140 M1141 G1142 A1143 Y1144 P1145 Y1146 M1147 L1148 H1149 Y1150 Y1151 D1152 P1153 R1154 Q1155 Y1156 A1157 N1158 A1159 W1160 N1161 L1162 T1163 S1164 A1165 W1166 L1167
E1168 E1169 I1170 T1171 P1172 T1173 S1174 I1175 P1176 S1177 V1178 P1179 F1180 M1181 V1182 P1183 I1184 S1185 S1186 D1187 H1188 D1189 I1190 S1191 S1192 A1193 P1194 A1195 V1196 Q1197 Y1198 I1199 I1200 S1201 T1202 E1203 Y1204 N1205 D1206 R1207 S1208 L1209 F1210 C1211 T1212 N1213 S1214 S1215 S1216 P1217 Q1218 T1219 I1220 A1221 G1222 P1223 D1224 K1225 H1226 I1227

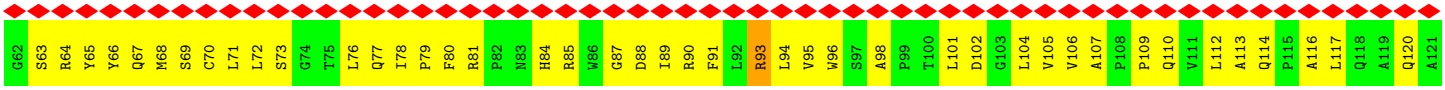


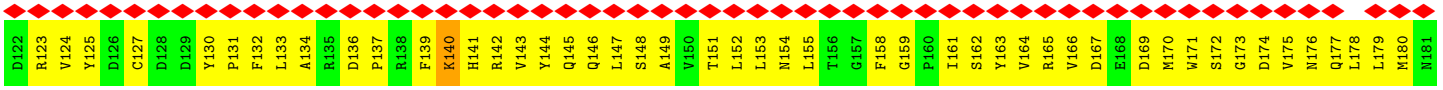
• Molecule 3: Inner capsid protein sigma-2

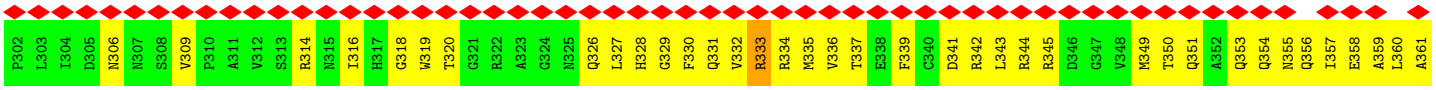
Chain D:

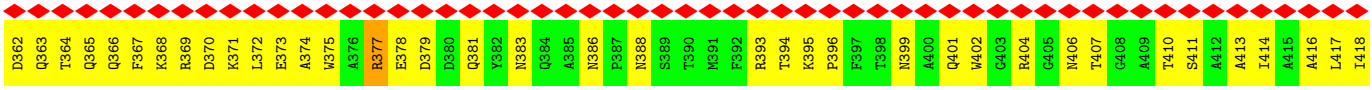






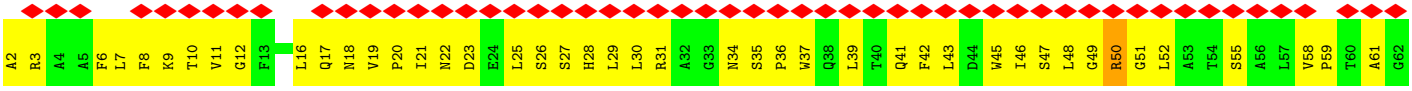


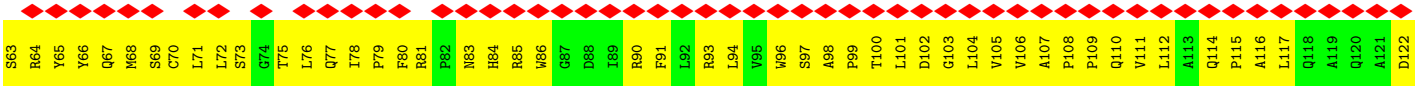


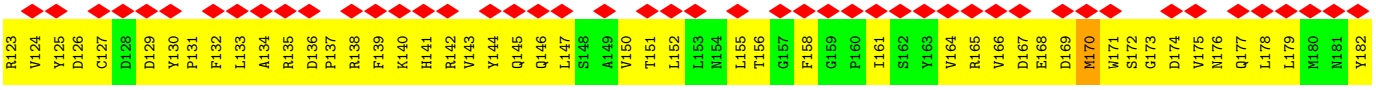


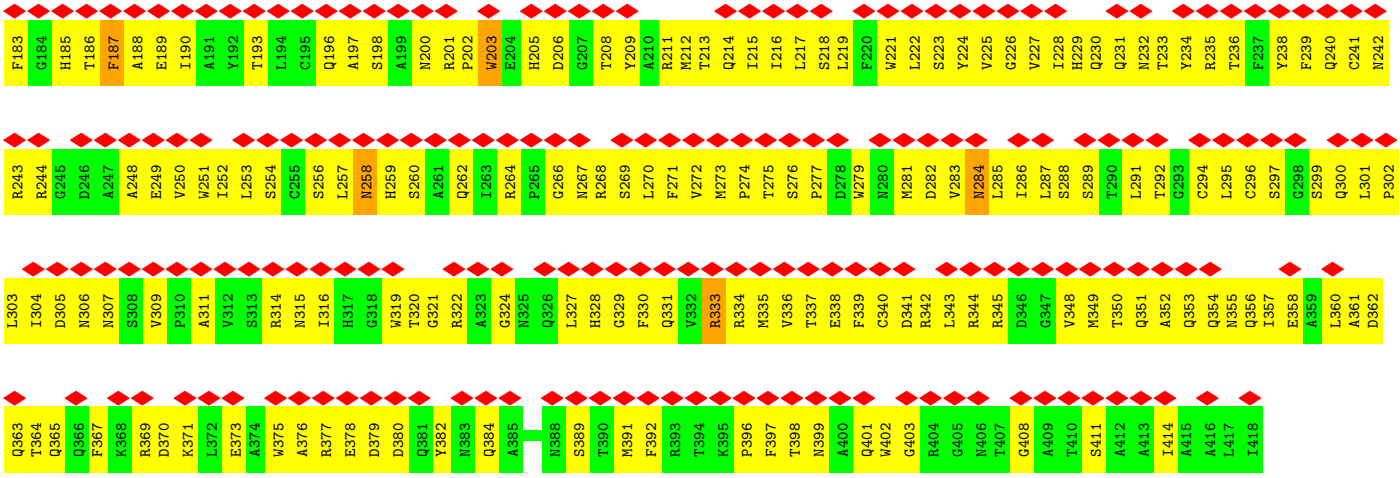
• Molecule 3: Inner capsid protein sigma-2

Chain P:



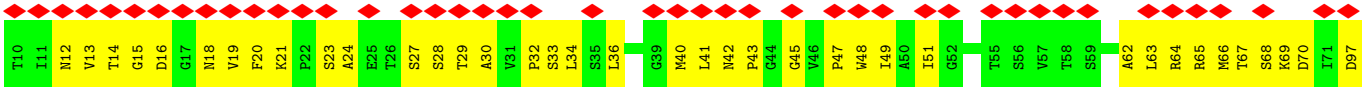


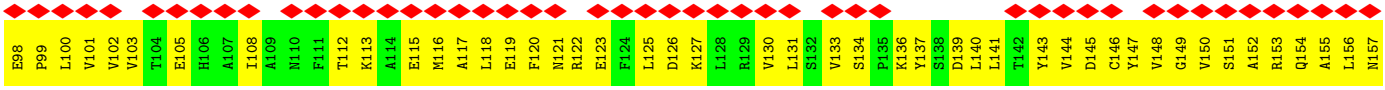


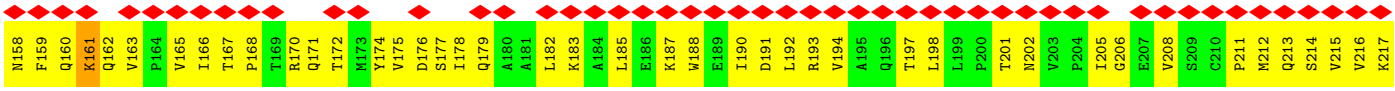


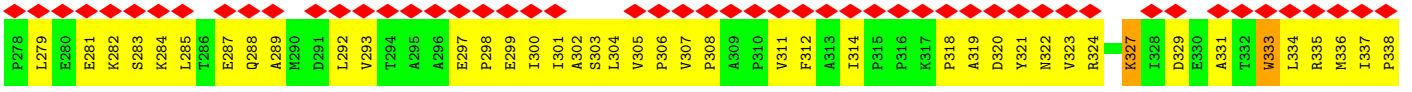
- Molecule 4: Outer capsid protein mu-1

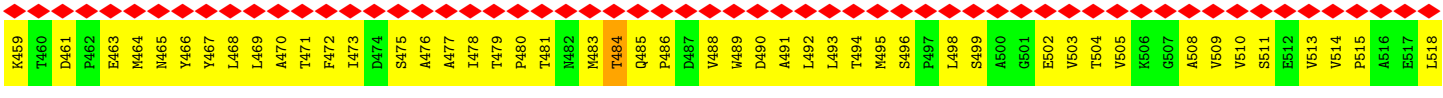
Chain K:

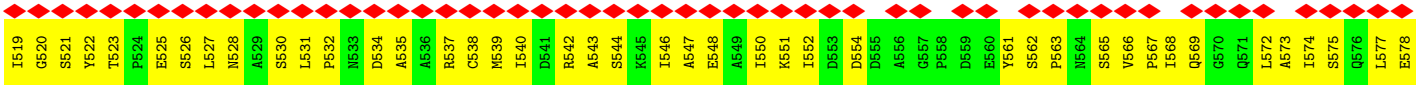


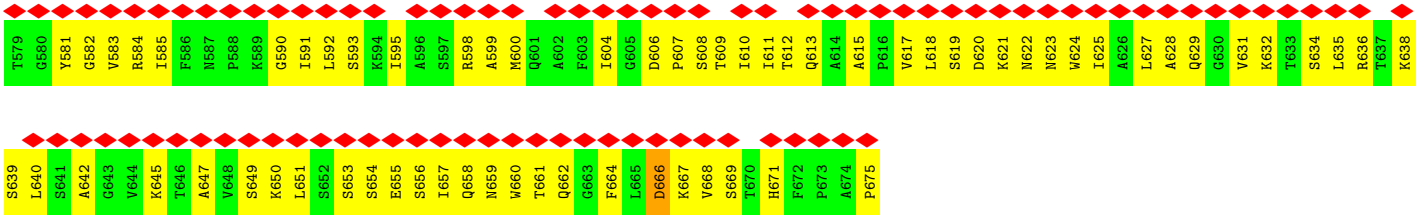






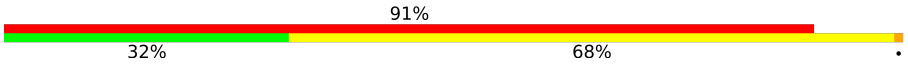


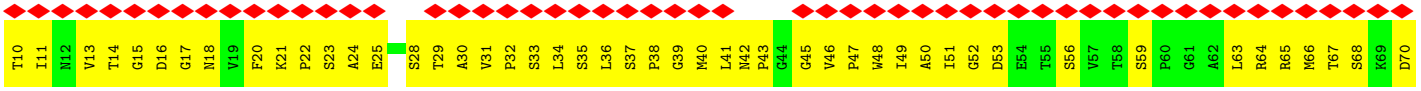


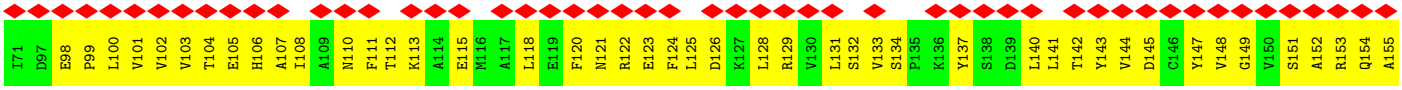


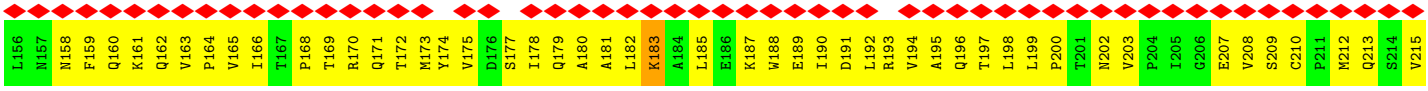
• Molecule 4: Outer capsid protein mu-1

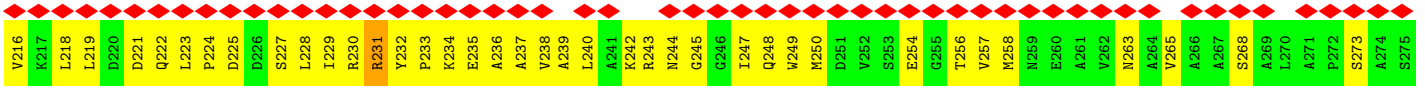
Chain L:

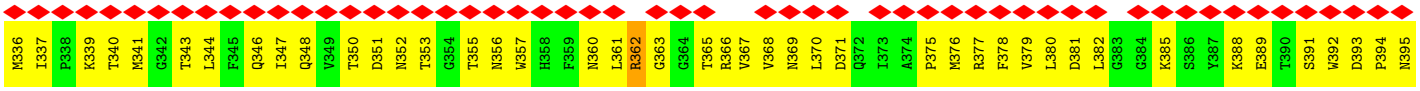


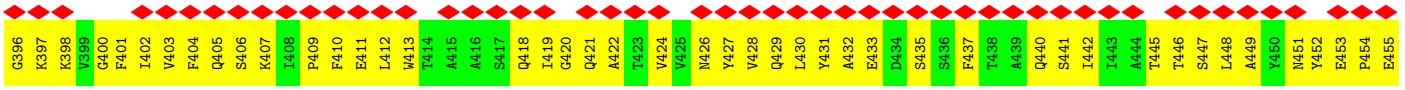


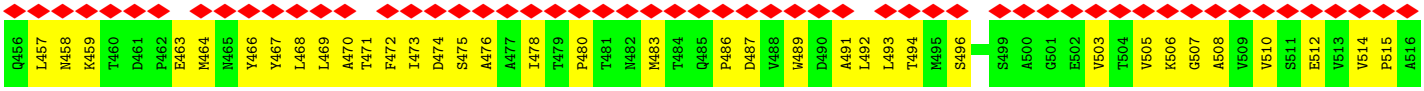


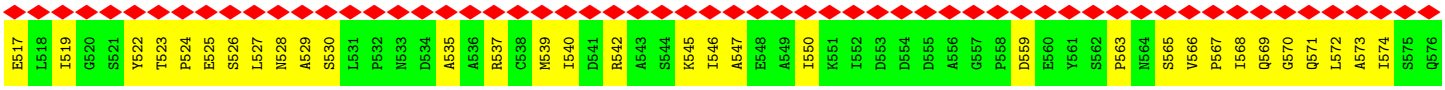


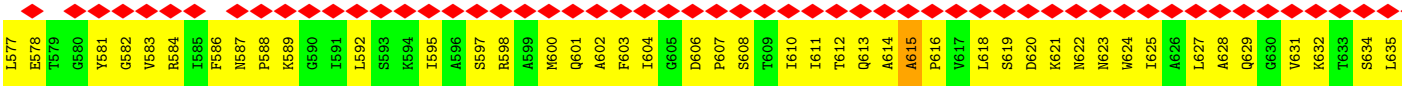


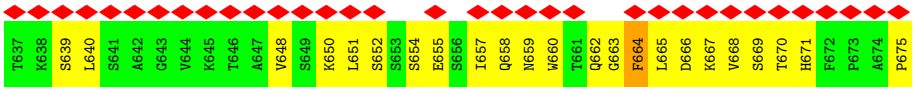






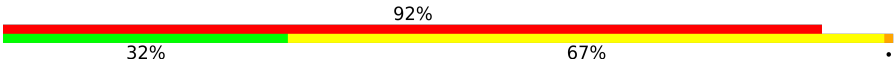


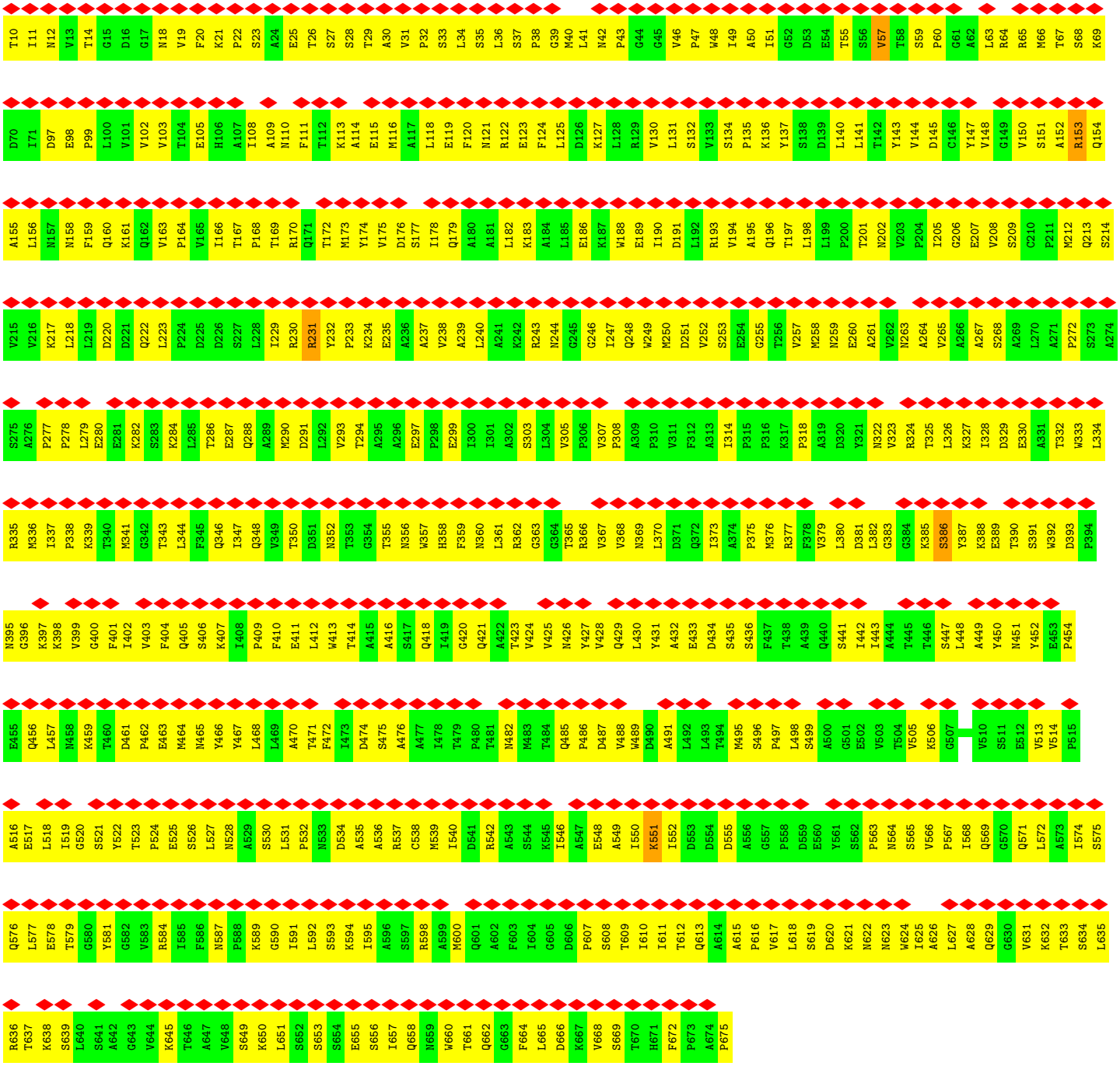




• Molecule 4: Outer capsid protein mu-1

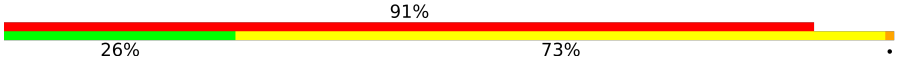
Chain M:

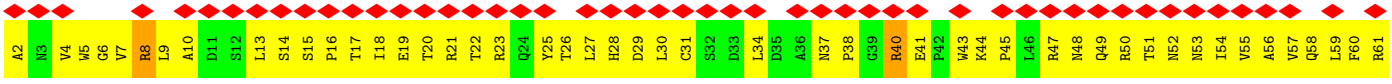


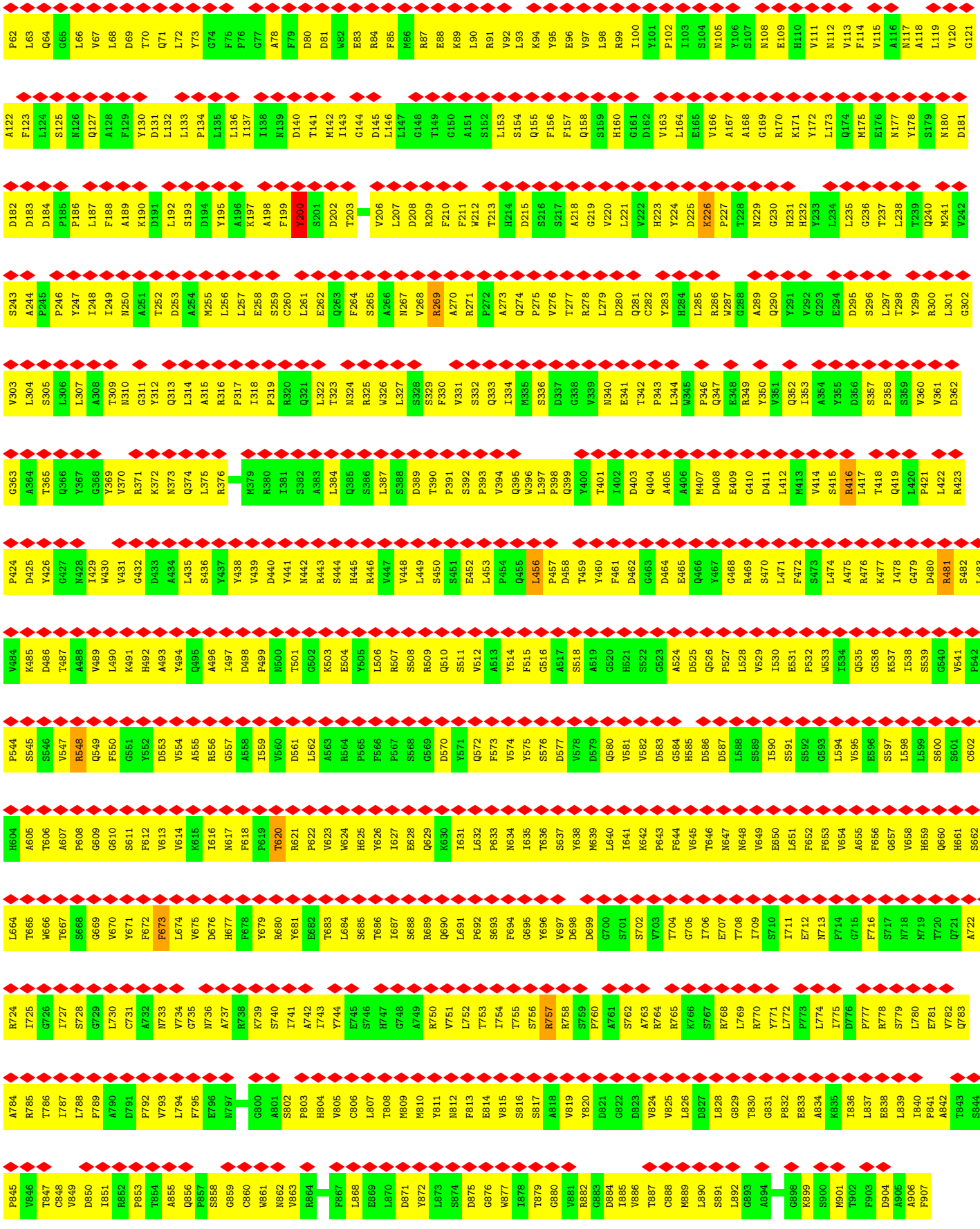


• Molecule 5: Outer capsid protein lambda-2

Chain O:



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A122 F123 L124 S125 N126 Q127 A128 F129 Y130 D131 L132 L133 P134 L135 L136 I137 I138 N139 D140 T141 M142 I143 G144 D145 L146 L147 G148 T149 G150 A151 S152 L153 S154 Q155 F156 F157 Q158 S159 H160 G161 D162 V163 L164 E165 V166 A167 A168 G169 R170 K171 Y172 L173 Q174 M175 E176 N177 Y178 S179 N180 D181
D182 D183 D184 P185 P186 L187 F188 A189 K190 D191 L192 S193 D194 Y195 A196 K197 A198 F199 Y200 S201 D202 T203 V206 L207 D208 R209 F210 F211 W212 T213 H214 D215 S216 S217 A218 G219 V220 L221 V222 H223 Y224 D225 K226 P227 T228 N229 G230 H231 H232 Y233 L234 L235 G236 T237 L238 T239 Q240 M241 V242
S243 A244 P245 P246 Y247 I248 I249 N250 A251 T252 D253 A254 M255 L256 L257 E258 S259 C260 L261 E262 Q263 F264 S265 A266 N267 V268 R269 A270 R271 P272 A273 Q274 P275 V276 T277 R278 L279 D280 Q281 C282 Y283 H284 L285 R286 W287 G288 A289 Q290 Y291 V292 G293 E294 D295 S296 L297 T298 Y299 R300 L301 G302
V303 L304 S305 L306 L307 A308 T309 N310 G311 Y312 Q313 L314 A315 R316 P317 I318 P319 R320 Q321 L322 T323 N324 R325 W326 L327 S328 S329 F330 V331 S332 Q333 I334 M335 S336 D337 G338 V339 N340 E341 T342 P343 L344 W345 P346 Q347 E348 R349 Y350 V351 Q352 I353 A354 Y355 D356 S357 P358 S359 V360 V361 D362
G363 A364 T365 Q366 Y367 G368 Y369 V370 R371 K372 N373 Q374 L375 R376 M379 R380 I381 S382 A383 L384 Q385 S386 L387 S388 D389 T390 P391 S392 P393 V394 Q395 W396 L397 P398 Q399 Y400 T401 I402 D403 Q404 A405 A406 M407 D408 E409 G410 D411 L412 M413 V414 S415 R416 L417 T418 Q419 L420 P421 L422 R423
P424 D425 Y426 G427 N428 I429 W430 V431 G432 D433 A434 L435 S436 Y437 Y438 V439 D440 Y441 N442 R443 S444 H445 R446 V447 V448 L449 S450 S451 E452 L453 P454 Q455 L456 P457 D458 T459 Y460 F461 D462 G463 D464 E465 Q466 Y467 G468 R469 S470 L471 F472 S473 L474 A475 R476 K477 I478 G479 D480 R481 S482 L483
V484 K485 D486 T487 A488 V489 L490 K491 H492 A493 Y494 Q495 A496 I497 D498 P499 N500 T501 Q502 K503 E504 Y505 L506 R507 S508 R509 Q510 S511 V512 A513 Y514 F515 G516 A517 S518 A519 G520 H521 S522 G523 A524 D525 Q526 P527 L528 V529 I530 E531 P532 W533 I534 Q535 G536 K537 I538 S539 G540 V541 P542 P543
P544 S545 S546 V547 R548 Q549 F550 G551 Y552 D553 V554 A555 R556 G557 A558 I559 V560 D561 L562 A563 R564 P565 F566 P567 S568 G569 D570 Y571 Q572 F573 V574 Y575 S576 D577 V578 D579 Q580 V581 V582 D583 G584 H585 D586 D587 L588 S589 I590 S591 S592 G593 L594 V595 E596 S597 L598 L599 S600 S601 C602 M603
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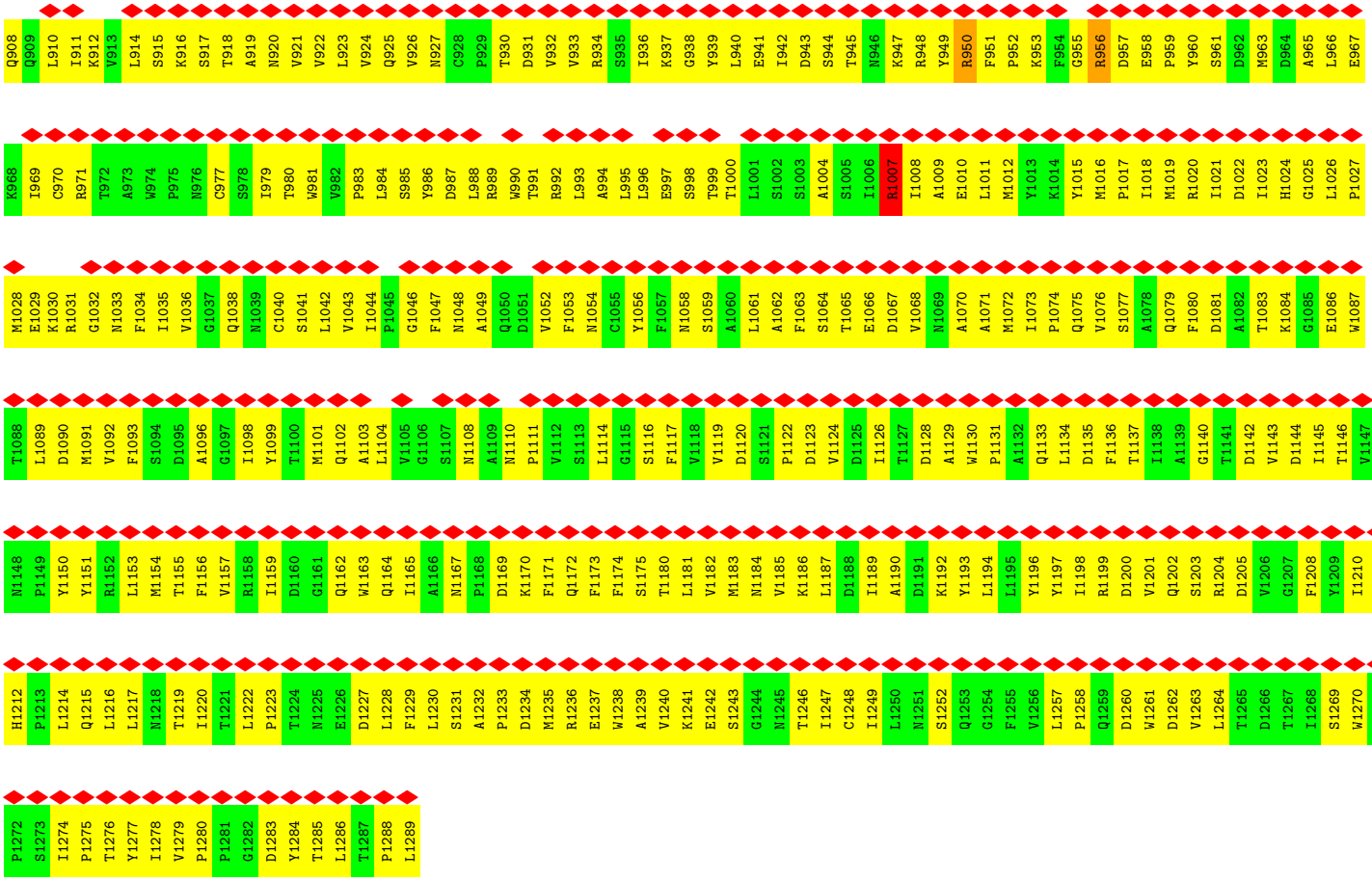
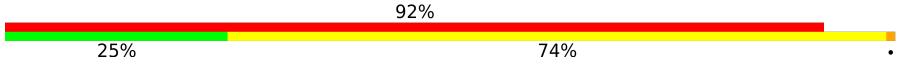
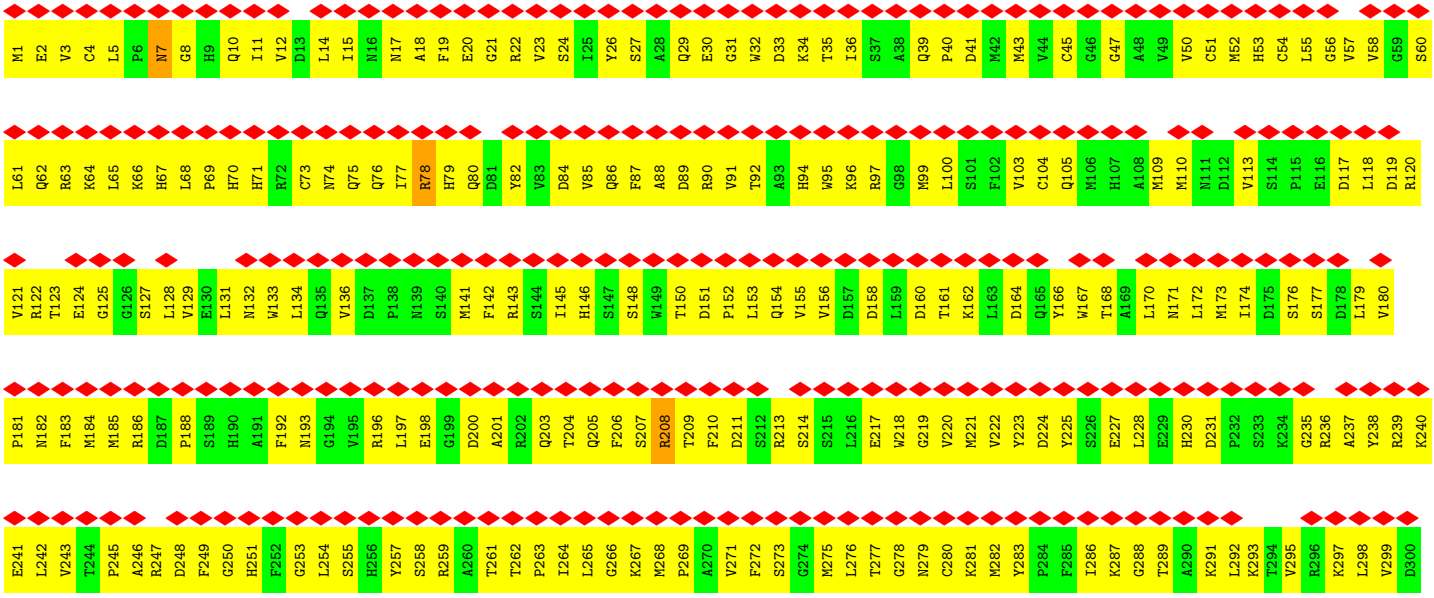
L664 T665 W666 T667 S668 G669 V670 Y671 F672 F673 L674 V675 D676 H677 F678 Y679 R680 Y681 E682 T683 L684 S685 T686 I687 S688 R689 Q690 L691 P692 S693 F694 G695 Y696 V697 D698 D699 G700 S701 S702 V703 T704 G705 I706 E707 T708 I709 S710 I711 E712 N713 P714 G715 F716 S717 N718 M719 T720 Q721 A722 A723
R724 I725 G726 I727 S728 G729 L730 C731 A732 N733 V734 G735 N736 A737 R738 K739 S740 I741 A742 I743 Y744 E745 S746 H747 G748 A749 R750 V751 L752 T753 I754 T755 S756 R757 R758 S759 P760 A761 S762 A763 R764 R765 K766 S767 R768 L769 R770 Y771 L772 P773 L774 I775 D776 P777 R778 S779 L780 E781 V782 Q783
A784 R785 T786 I787 L788 P789 A790 D791 P792 V793 L794 F795 E796 N797 G800 A801 S802 P803 H804 V805 C806 L807 T808 M809 M810 Y811 N812 F813 E814 V815 S816 S817 A818 V819 Y820 D821 G822 D823 V824 V825 L826 D827 L828 G829 T830 G831 P832 E833 A834 K835 I836 L837 E838 L839 I840 P841 A842 T843 S844
P845 V846 T847 C848 V849 D850 I851 R852 P853 T854 A855 Q856 P857 S858 G859 C860 W861 N862 V863 R864 F867 L868 E869 L870 D871 Y872 L873 S874 D875 G876 W877 I878 T879 G880 V881 R882 G883 D884 I885 V886 T887 C888 M889 L890 S891 L892 G893 A894 G898 K899 S900 M901 T902 F903 D904 A905 A906 F907

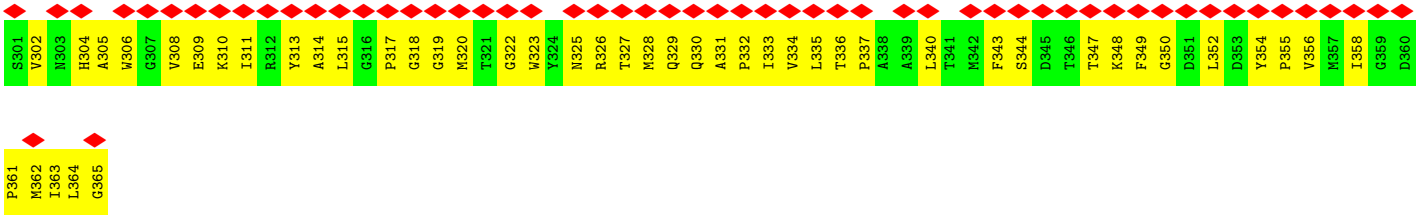


• Molecule 6: Outer capsid protein sigma-3

Chain X:

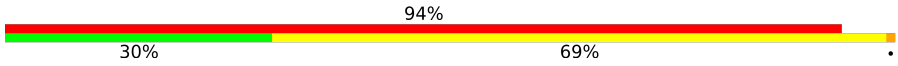


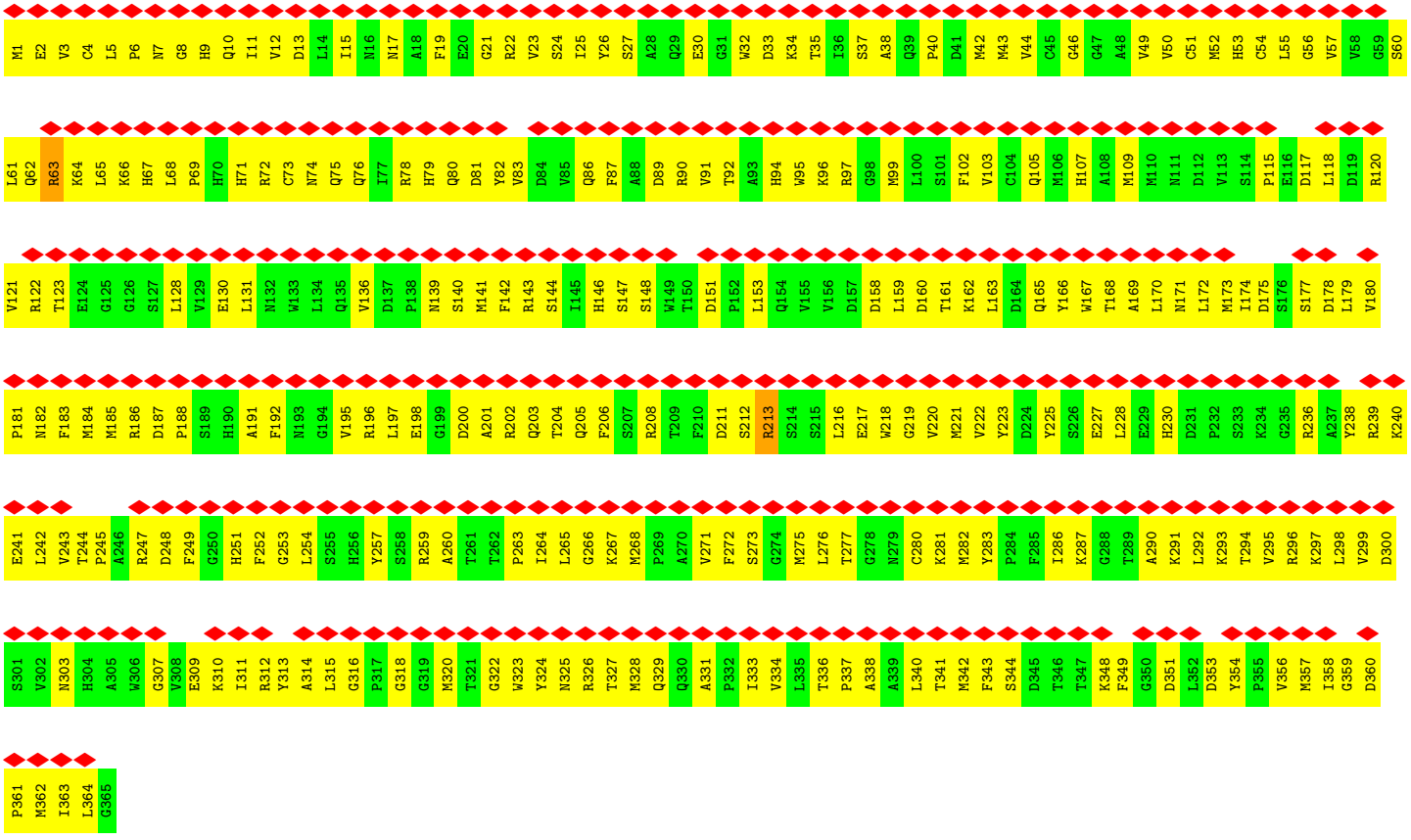




• Molecule 6: Outer capsid protein sigma-3

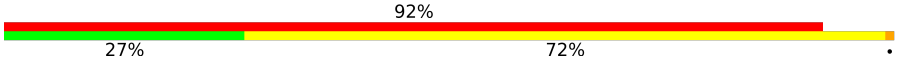
Chain Y:

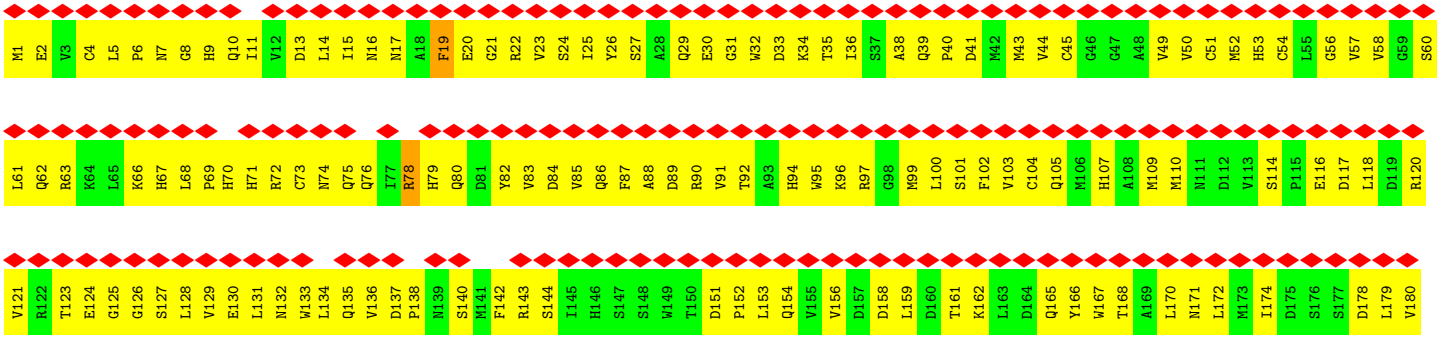




• Molecule 6: Outer capsid protein sigma-3

Chain Z:



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E241 L242 V243 T244 P245 A246 R247 D248 F249 G250 H251 F252 G253 L254 S255 H256 Y257 S258 R259 A260 T261 T262 P263 I264 L265 G266 K267 M268 P269 A270 V271 F272 S273 G274 M275 L276 T277 G278 N279 C280 K281 M282 Y283 P284 F285 I286 K287 G288 T289 A290 K291 L292 K293 T294 V295 R296 K297 L298 V299 D300
S301 V302 N303 H304 A305 W306 G307 V308 E309 K310 I311 R312 Y313 A314 L315 G316 P317 G318 G319 M320 T321 G322 W323 Y324 N325 R326 T327 M328 Q329 Q330 A331 P332 I333 V334 L335 T336 P337 A338 A339 L340 T341 M342 F343 S344 D345 T346 T347 K348 F349 G350 D351 L352 D353 Y354 P355 V356 M357 I358 G359 D360
P361 M362 I363 L364 G365

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	TOMOGRAPHY	Depositor
Imposed symmetry	POINT, Not provided	
Number of tilted images used	41	Depositor
Resolution determination method	Not provided	
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	2	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum voxel value	8.955	Depositor
Minimum voxel value	-5.801	Depositor
Average voxel value	0.054	Depositor
Voxel value standard deviation	0.430	Depositor
Recommended contour level	2.7	Depositor
Tomogram size (Å)	648.0, 648.0, 648.0	wwPDB
Tomogram dimensions	360, 360, 360	wwPDB
Tomogram angles (°)	90.0, 90.0, 90.0	wwPDB
Grid spacing (Å)	1.8, 1.8, 1.8	Depositor

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	B	0.38	0/8391	0.56	1/11492 (0.0%)
2	C	0.40	0/8174	0.56	0/11194
3	D	0.39	0/3398	0.56	2/4626 (0.0%)
3	P	0.40	0/3398	0.56	1/4626 (0.0%)
4	K	0.36	0/4971	0.54	1/6787 (0.0%)
4	L	0.36	0/4971	0.56	0/6787
4	M	0.35	0/4971	0.54	0/6787
5	O	0.40	0/10385	0.56	1/14172 (0.0%)
6	X	0.39	0/2957	0.53	0/4005
6	Y	0.36	0/2957	0.53	0/4005
6	Z	0.37	0/2957	0.53	0/4005
All	All	0.38	0/57530	0.55	6/78486 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
2	C	0	1
4	L	0	1
4	M	0	2
5	O	0	1
6	X	0	1
All	All	0	7

There are no bond length outliers.

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

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

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

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	977	PHE	Peptide
2	C	383	THR	Peptide
4	L	615	ALA	Peptide
4	M	386	SER	Peptide
4	M	57	VAL	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	8171	0	8083	851	0
2	C	7958	0	7871	867	0
3	D	3313	0	3215	361	0
3	P	3313	0	3215	415	0
4	K	4871	0	4900	587	0
4	L	4871	0	4900	541	0
4	M	4871	0	4900	524	0
5	O	10127	0	9910	1080	0
6	X	2885	0	2816	282	0
6	Y	2885	0	2816	296	0
6	Z	2885	0	2816	298	0
All	All	56150	0	55442	5837	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 52.

The worst 5 of 5837 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:O:1230:LEU:O	5:O:1276:THR:HA	1.45	1.14
1:B:760:GLU:O	1:B:764:TRP:HB2	1.46	1.14
5:O:704:THR:HA	5:O:758:ARG:O	1.47	1.12
4:K:68:SER:HG	4:K:97:ASP:N	1.47	1.11
4:L:142:THR:O	4:L:164:PRO:HA	1.50	1.10

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	1031/1035 (100%)	841 (82%)	190 (18%)	0	100	100
2	C	1004/1008 (100%)	820 (82%)	179 (18%)	5 (0%)	29	29
3	D	415/417 (100%)	343 (83%)	71 (17%)	1 (0%)	47	47
3	P	415/417 (100%)	352 (85%)	62 (15%)	1 (0%)	47	47
4	K	637/641 (99%)	548 (86%)	88 (14%)	1 (0%)	47	47
4	L	637/641 (99%)	536 (84%)	100 (16%)	1 (0%)	47	47
4	M	637/641 (99%)	550 (86%)	86 (14%)	1 (0%)	47	47
5	O	1280/1284 (100%)	1069 (84%)	211 (16%)	0	100	100
6	X	363/365 (100%)	309 (85%)	54 (15%)	0	100	100
6	Y	363/365 (100%)	317 (87%)	46 (13%)	0	100	100
6	Z	363/365 (100%)	296 (82%)	67 (18%)	0	100	100
All	All	7145/7179 (100%)	5981 (84%)	1154 (16%)	10 (0%)	54	51

5 of 10 Ramachandran outliers are listed below:

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

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

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	915/915 (100%)	908 (99%)	7 (1%)	81	81
2	C	890/890 (100%)	882 (99%)	8 (1%)	78	78
3	D	352/352 (100%)	346 (98%)	6 (2%)	60	60
3	P	352/352 (100%)	346 (98%)	6 (2%)	60	60
4	K	541/541 (100%)	534 (99%)	7 (1%)	69	69
4	L	541/541 (100%)	537 (99%)	4 (1%)	84	84
4	M	541/541 (100%)	538 (99%)	3 (1%)	86	86
5	O	1118/1118 (100%)	1101 (98%)	17 (2%)	65	65
6	X	317/317 (100%)	312 (98%)	5 (2%)	62	62
6	Y	317/317 (100%)	315 (99%)	2 (1%)	86	86
6	Z	317/317 (100%)	314 (99%)	3 (1%)	78	78
All	All	6201/6201 (100%)	6133 (99%)	68 (1%)	74	73

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

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

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

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

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	C	1
4	L	1
4	M	1
4	K	1
1	B	1
5	O	1

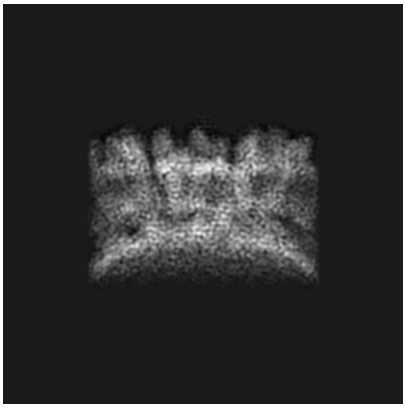
The worst 5 of 6 chain breaks are listed below:

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

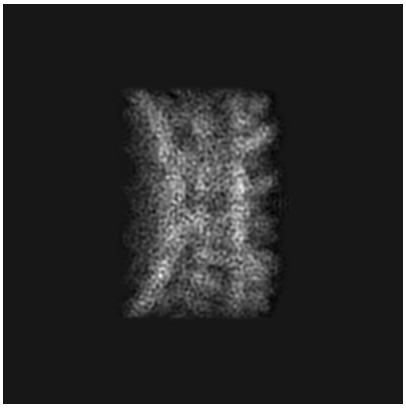
6 Tomogram visualisation

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

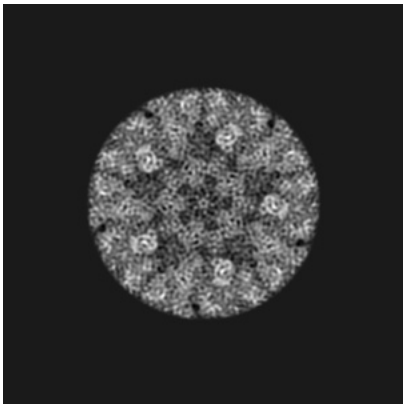
6.1 Orthogonal projections



X



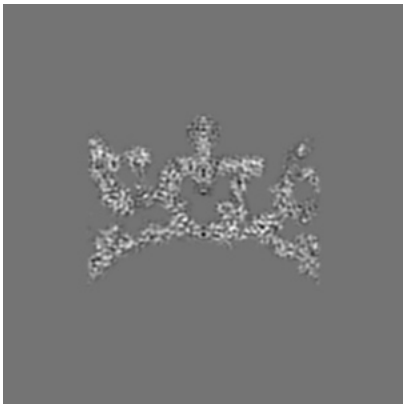
Y



Z

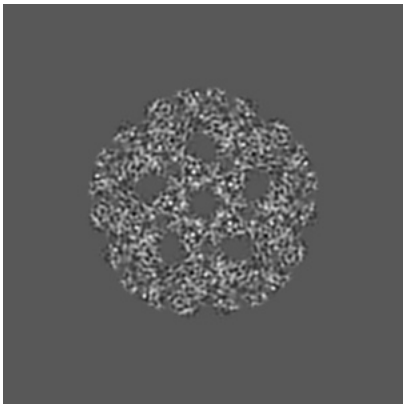
The images above show the tomogram projected in three orthogonal directions.

6.2 Central slices



X Index: 180

Y Index: 180

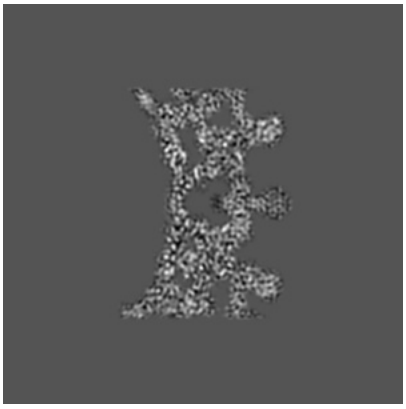


Z Index: 180

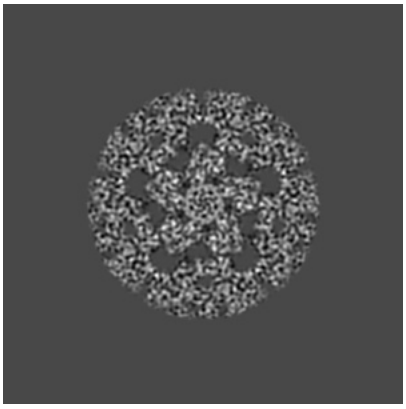
The images above show central slices of the tomogram in three orthogonal directions.

6.3 Largest variance slices (i)

X Index: 195



Y Index: 176



Z Index: 213

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

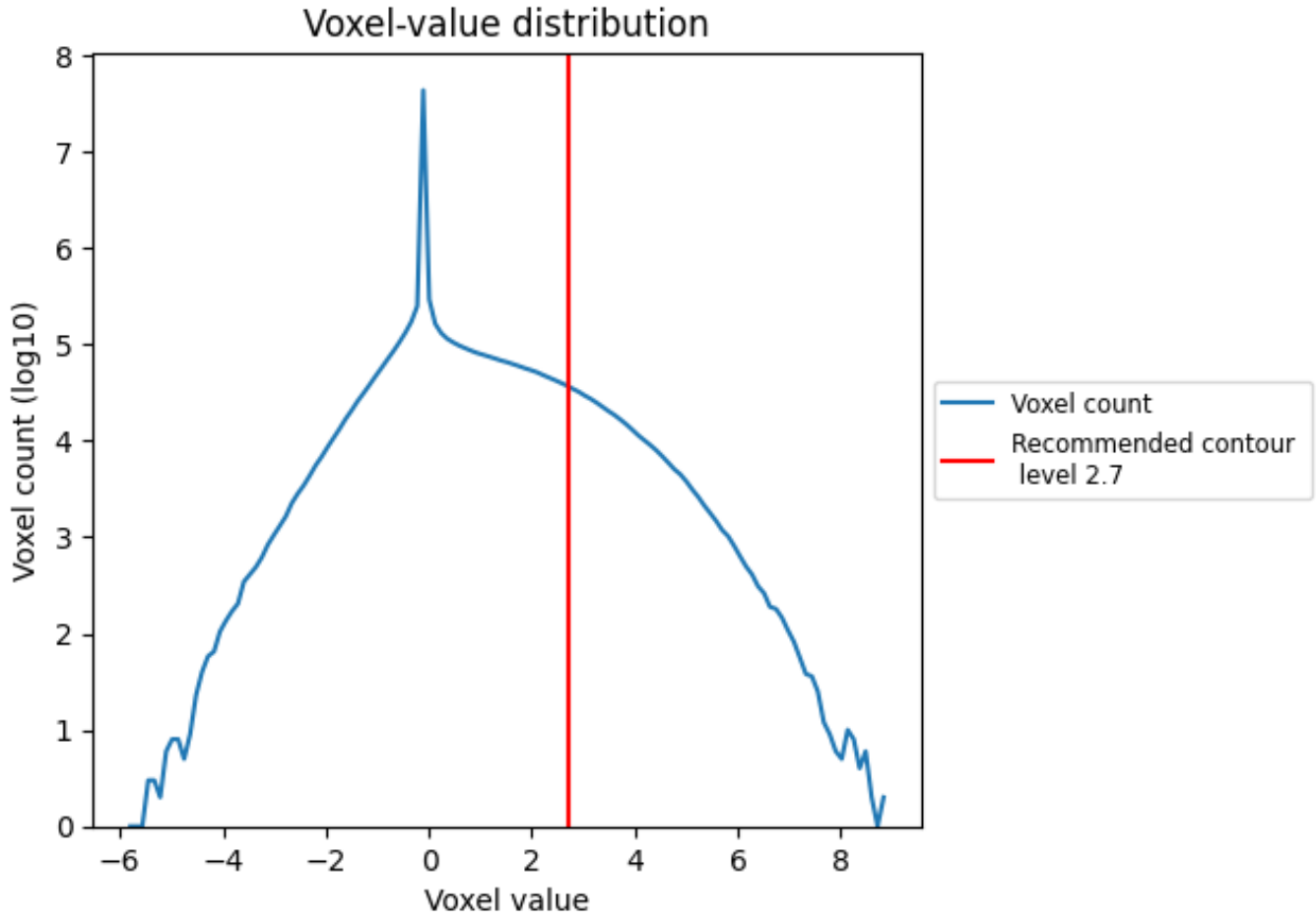
6.4 Mask visualisation (i)

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

7 Tomogram analysis (i)

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

7.1 Voxel-value distribution (i)



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

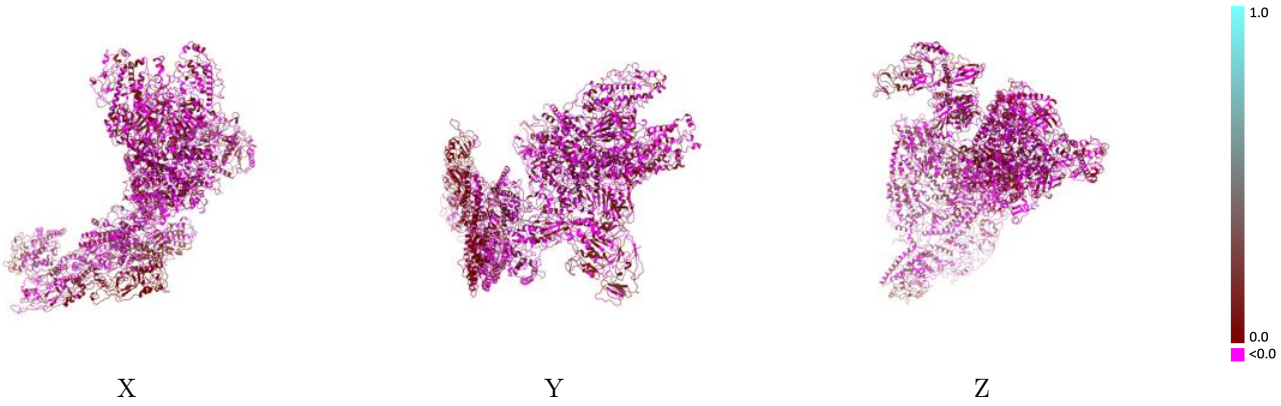
8 Map-model fit

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

8.1 Map-model overlay

This section was not generated.

8.2 Q-score mapped to coordinate model

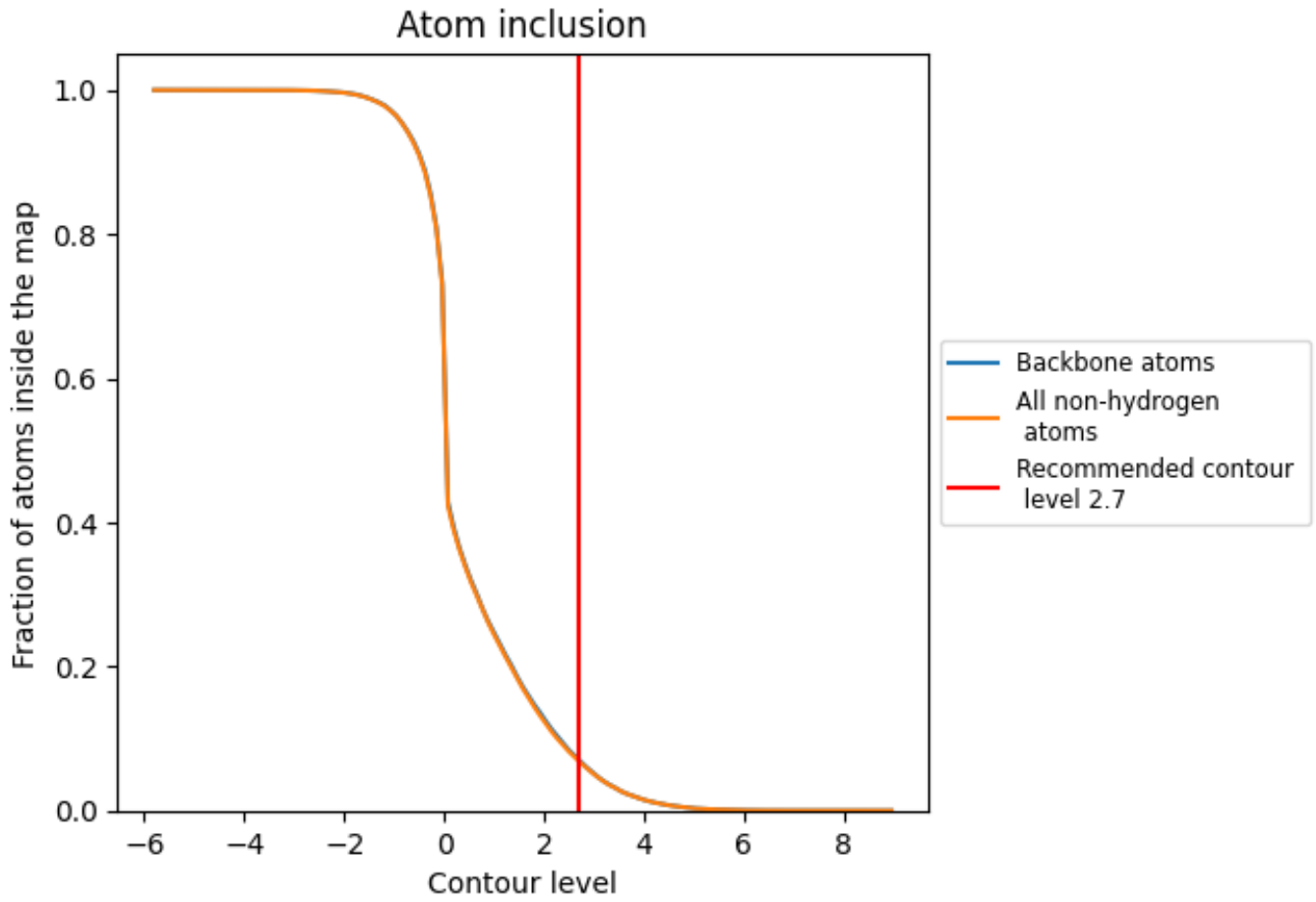


The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

8.3 Atom inclusion mapped to coordinate model

This section was not generated.

8.4 Atom inclusion (i)



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

8.5 Map-model fit summary

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

Chain	Atom inclusion	Q-score
All	0.0687	0.0100
B	0.0011	0.0230
C	0.0532	0.0150
D	0.0446	0.0040
K	0.0868	-0.0040
L	0.0866	0.0090
M	0.0828	0.0020
O	0.0912	0.0230
P	0.1510	-0.0060
X	0.0719	-0.0060
Y	0.0559	-0.0050
Z	0.0825	0.0030