wwPDB EM Validation Summary Report (i)

Jun 26, 2024 – 05:29 PM JST

PDB ID	:	7XR3
EMDB ID	:	EMD-33404
Title	:	3.4 Angstrom cryoEM D5 reconstruction of mud crab reovirus
Authors	:	Zhang, Q.F.; Gao, Y.Z.
Deposited on	:	2022-05-09
Resolution	:	3.70 Å(reported)

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

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

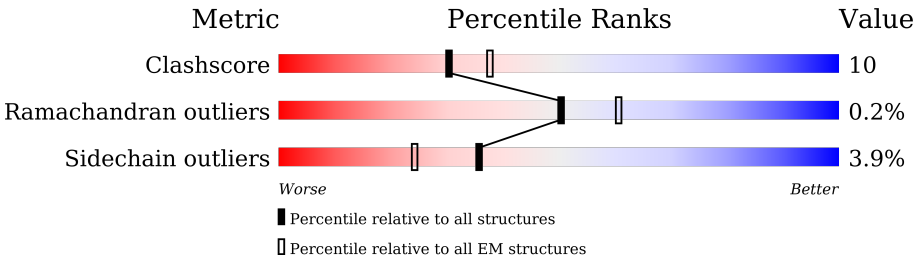
EMDB validation analysis	:	0.0.1.dev92
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance

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

The reported resolution of this entry is 3.70 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	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	A	854	26% 75% 19% • 5%
1	B	854	22% 75% 23% ••
1	C	854	22% 71% 21% • 7%
1	D	854	20% 78% 20% ••
1	E	854	29% 72% 19% • 7%
1	F	854	24% 71% 26% ••
1	G	854	33% 74% 18% 7%
1	H	854	30% 76% 21% ••

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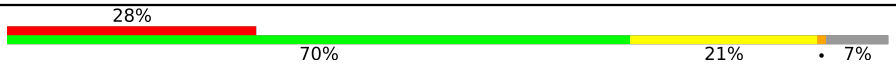
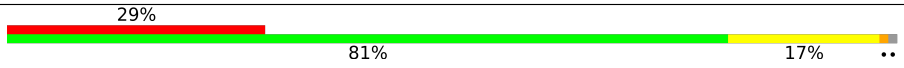
Mol	Chain	Length	Quality of chain
1	I	854	
1	J	854	
2	Z	1425	

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 76250 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 VP3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	815	Total	C	N	O	S	0	0
			6516	4128	1128	1232	28		
1	B	846	Total	C	N	O	S	0	0
			6746	4260	1175	1283	28		
1	C	794	Total	C	N	O	S	0	0
			6372	4043	1100	1201	28		
1	D	846	Total	C	N	O	S	0	0
			6746	4260	1175	1283	28		
1	E	794	Total	C	N	O	S	0	0
			6372	4043	1100	1201	28		
1	F	846	Total	C	N	O	S	0	0
			6746	4260	1175	1283	28		
1	G	794	Total	C	N	O	S	0	0
			6372	4043	1100	1201	28		
1	H	846	Total	C	N	O	S	0	0
			6746	4260	1175	1283	28		
1	I	794	Total	C	N	O	S	0	0
			6372	4043	1100	1201	28		
1	J	846	Total	C	N	O	S	0	0
			6746	4260	1175	1283	28		

- Molecule 2 is a protein called VP1.

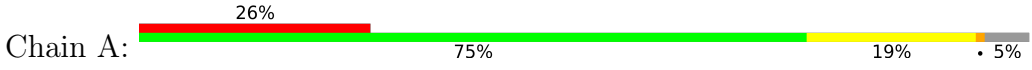
Mol	Chain	Residues	Atoms					AltConf	Trace
2	Z	1320	Total	C	N	O	S	0	0
			10516	6661	1799	2000	56		

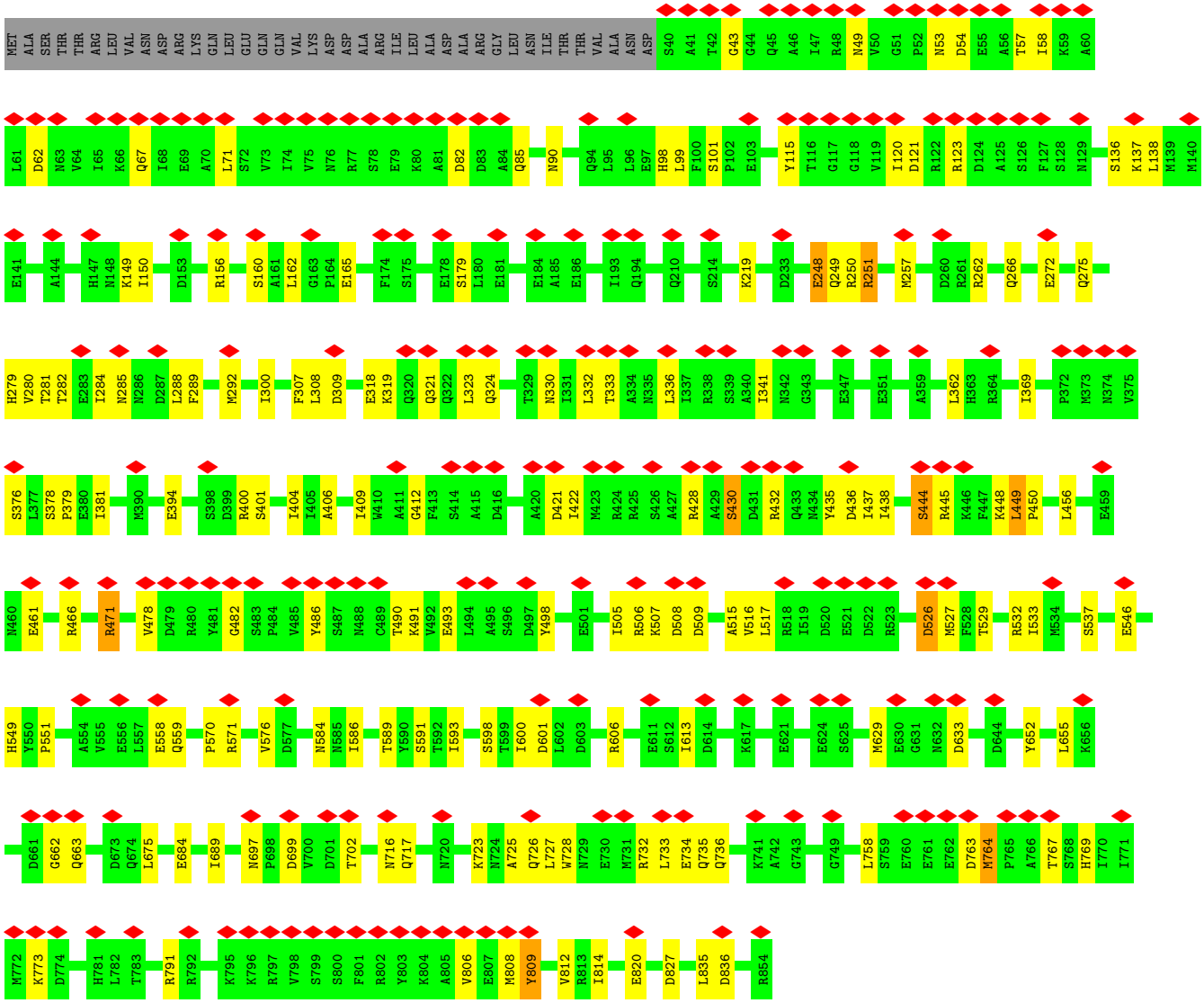
3 Residue-property plots (i)

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: VP3

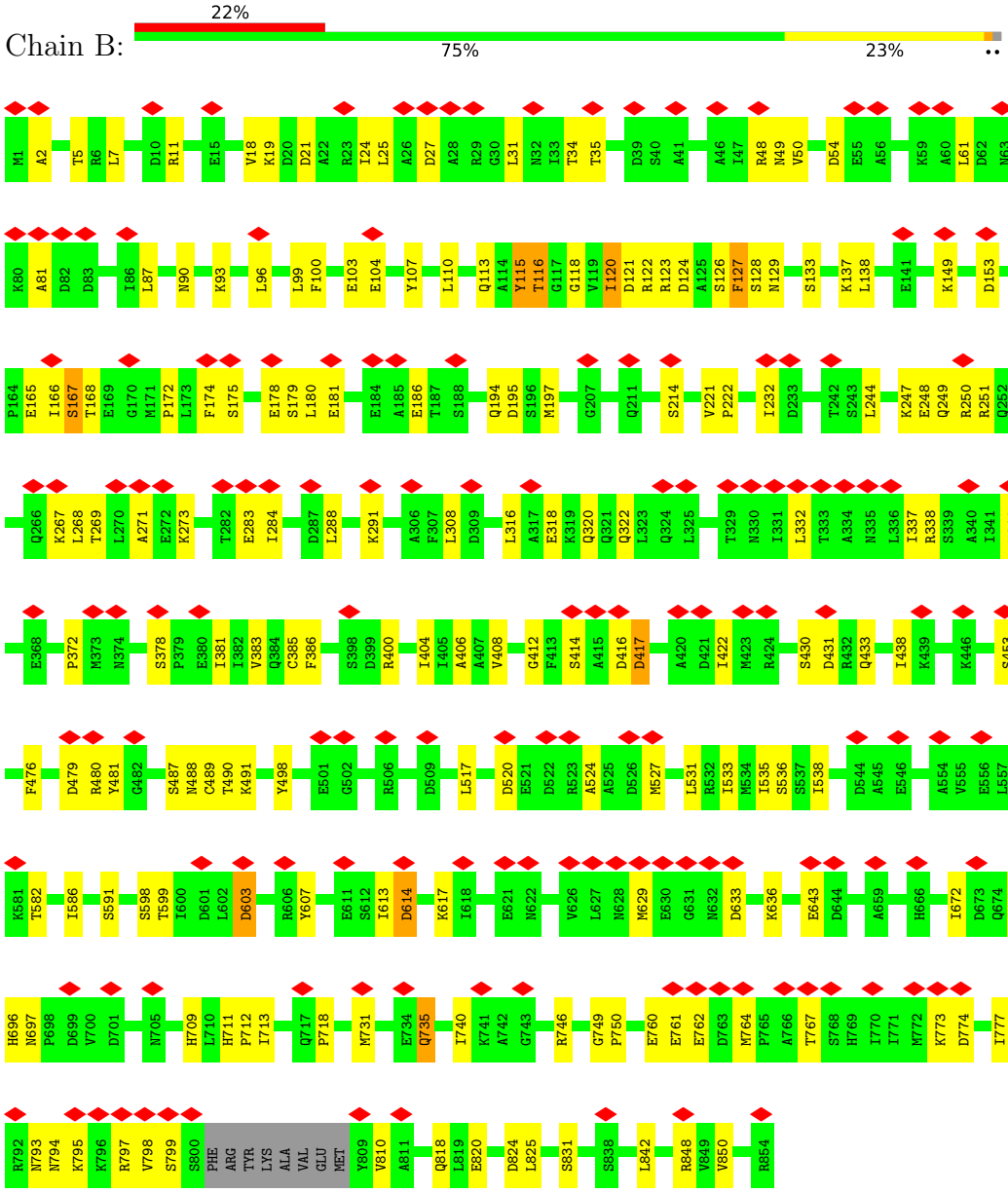
Chain A:





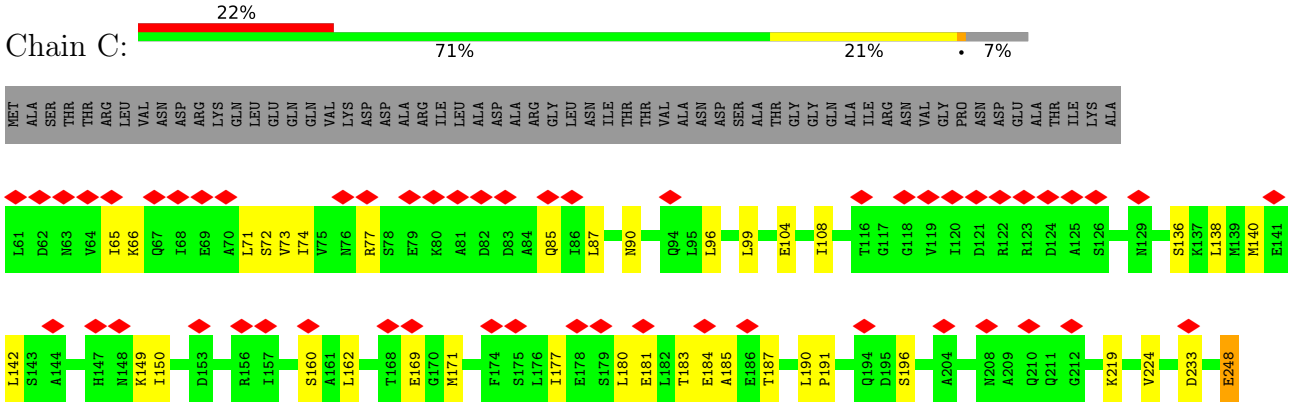
- Molecule 1: VP3

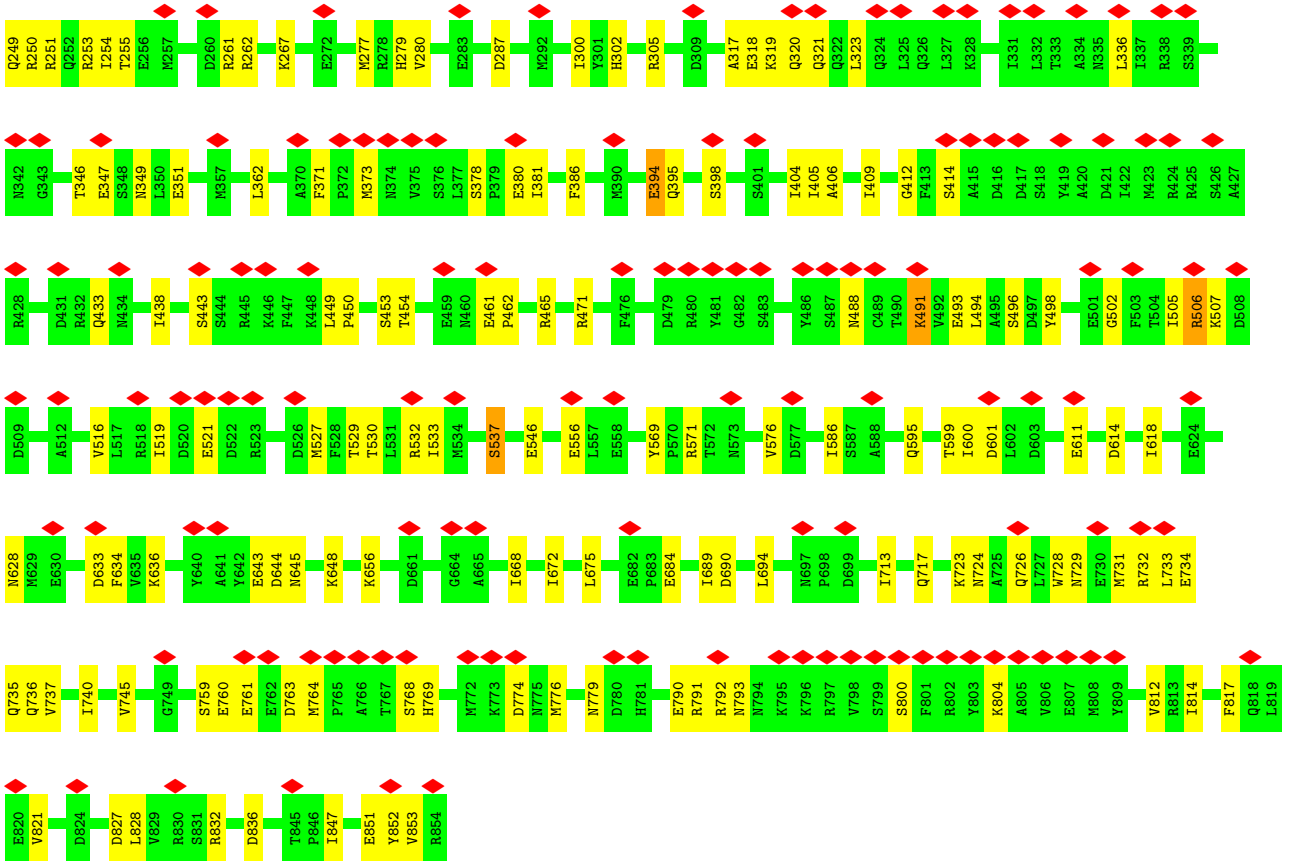
Chain B:



• Molecule 1: VP3

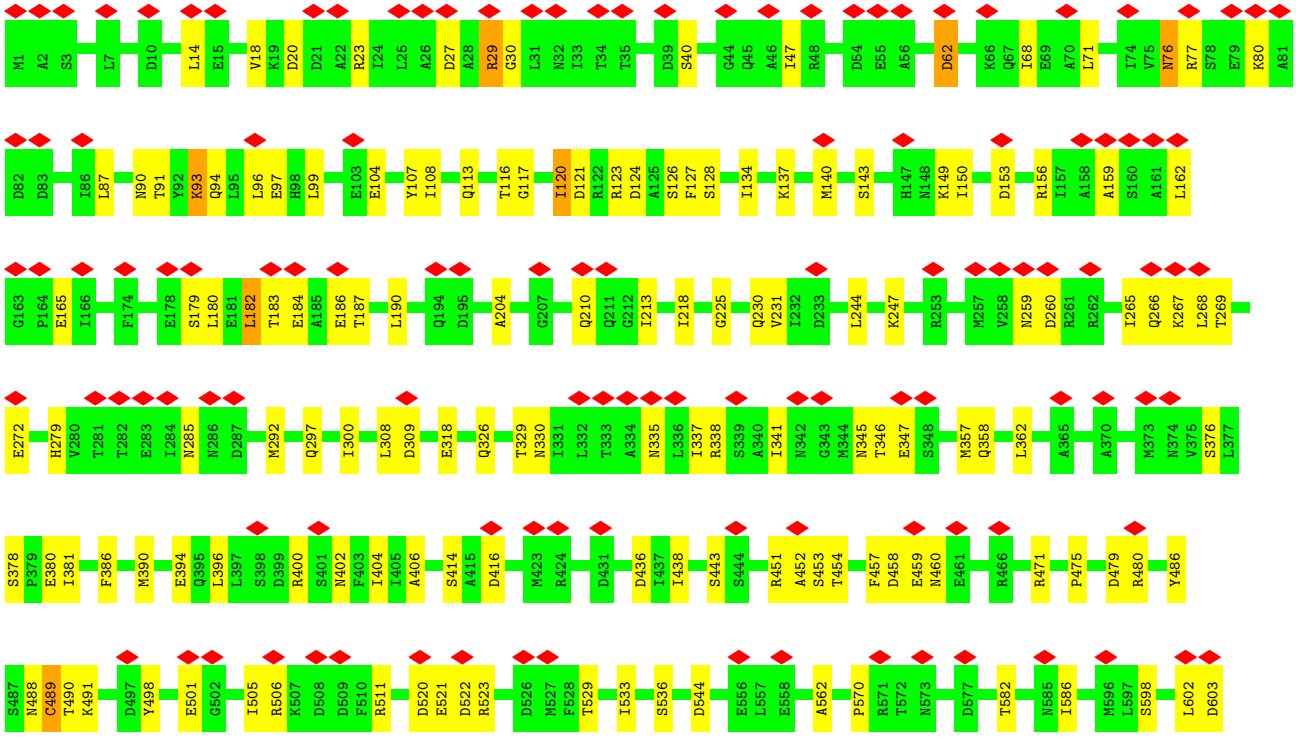
Chain C:

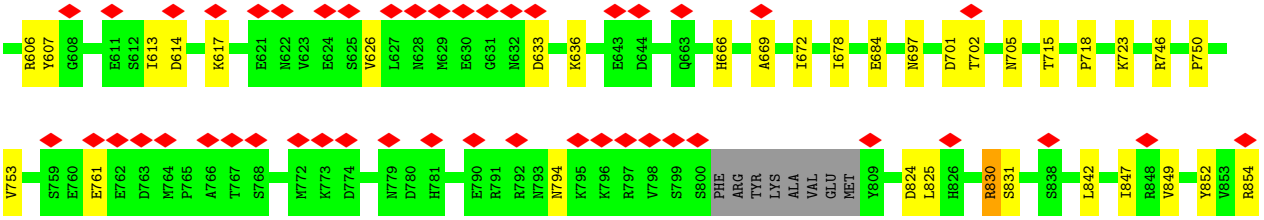




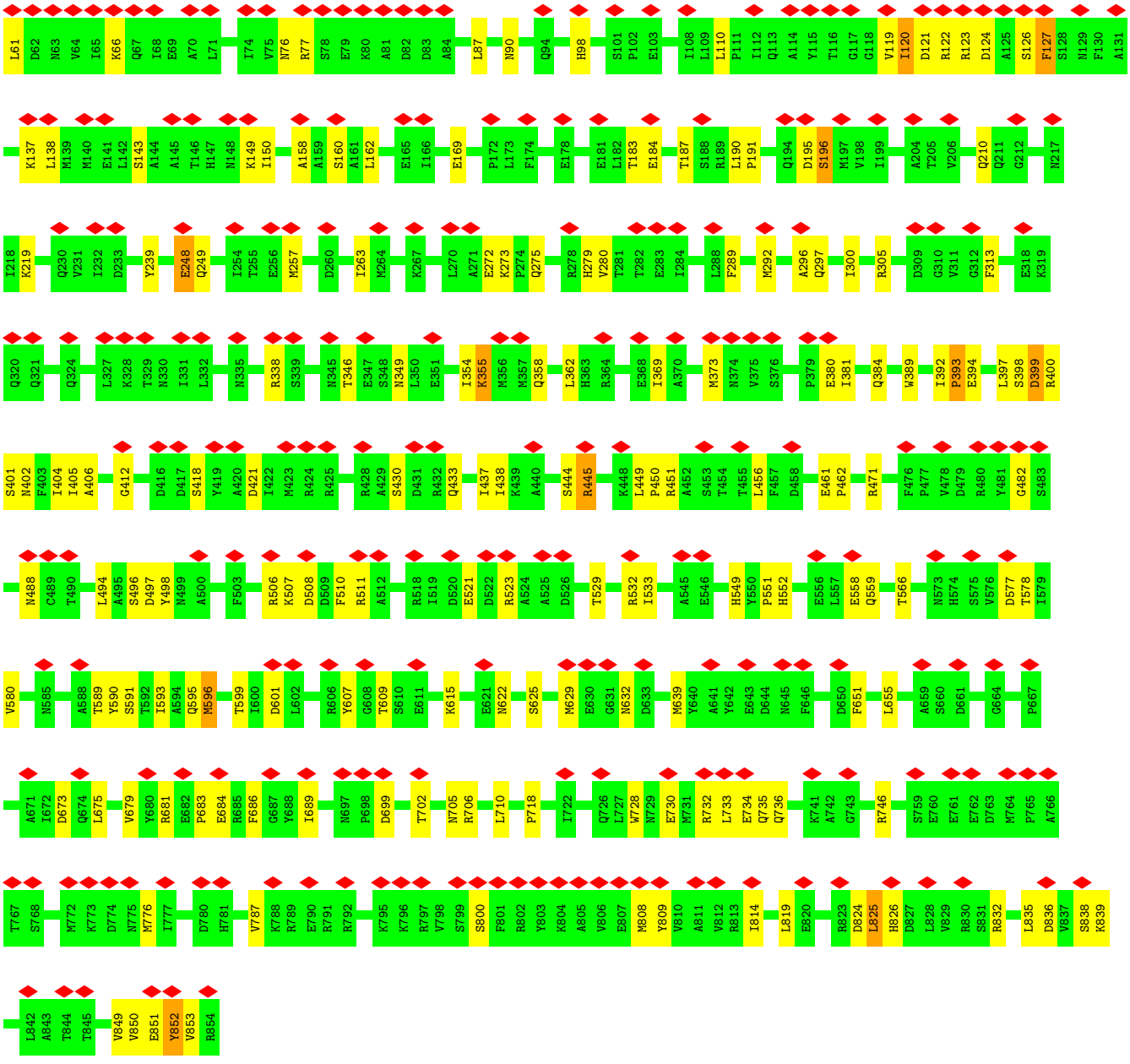
- Molecule 1: VP3

Chain D:



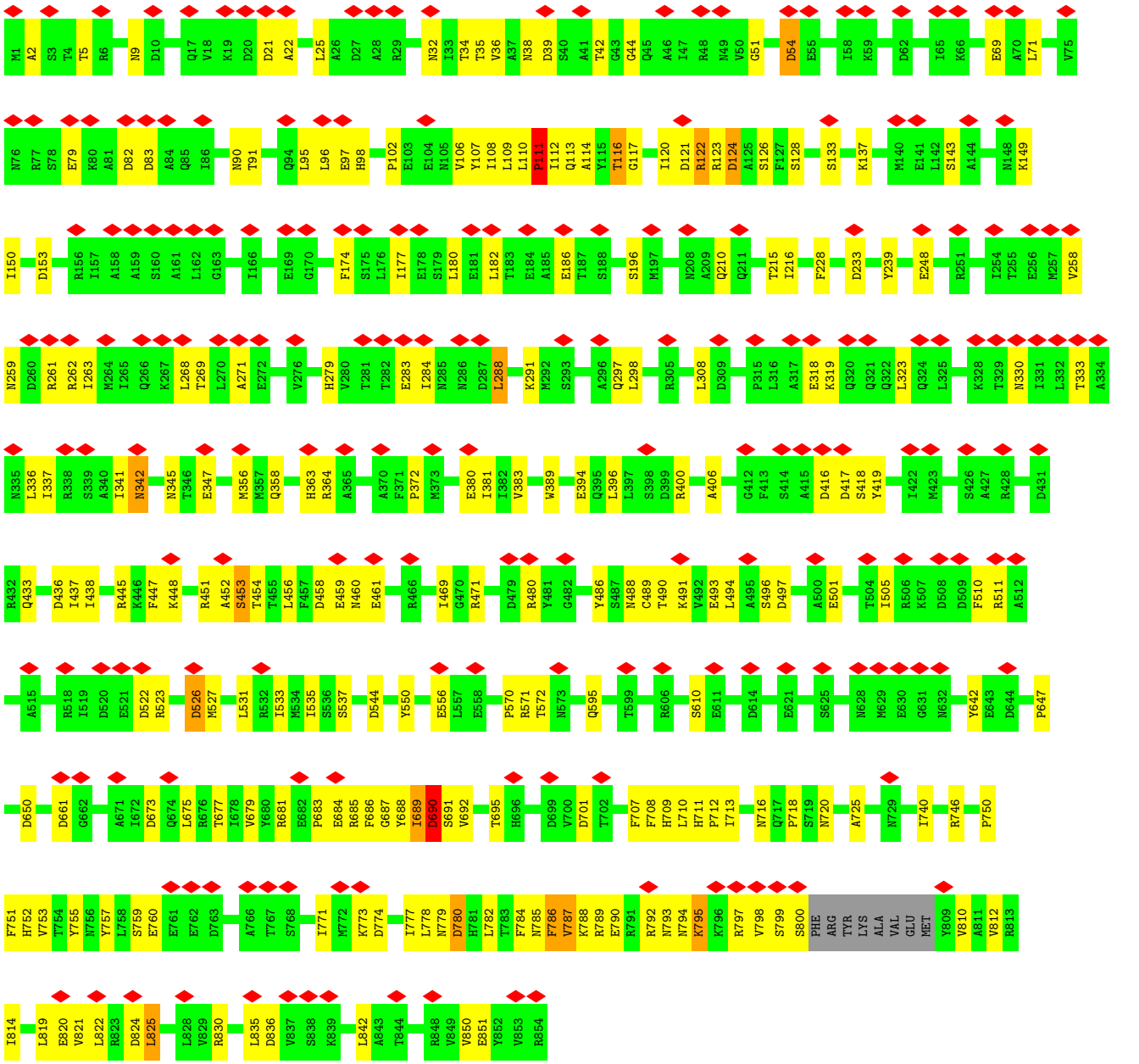


• Molecule 1: VP3



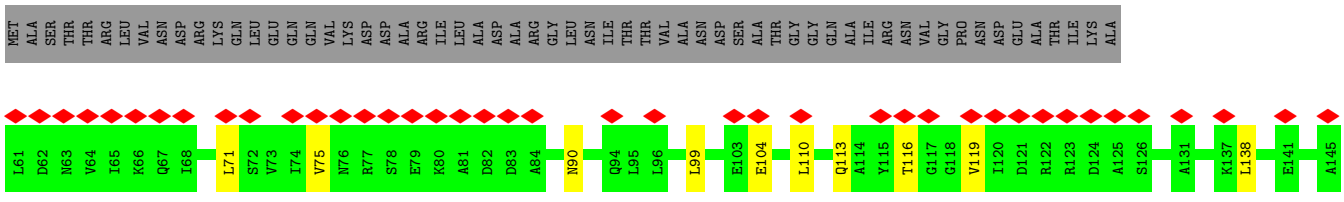
• Molecule 1: VP3

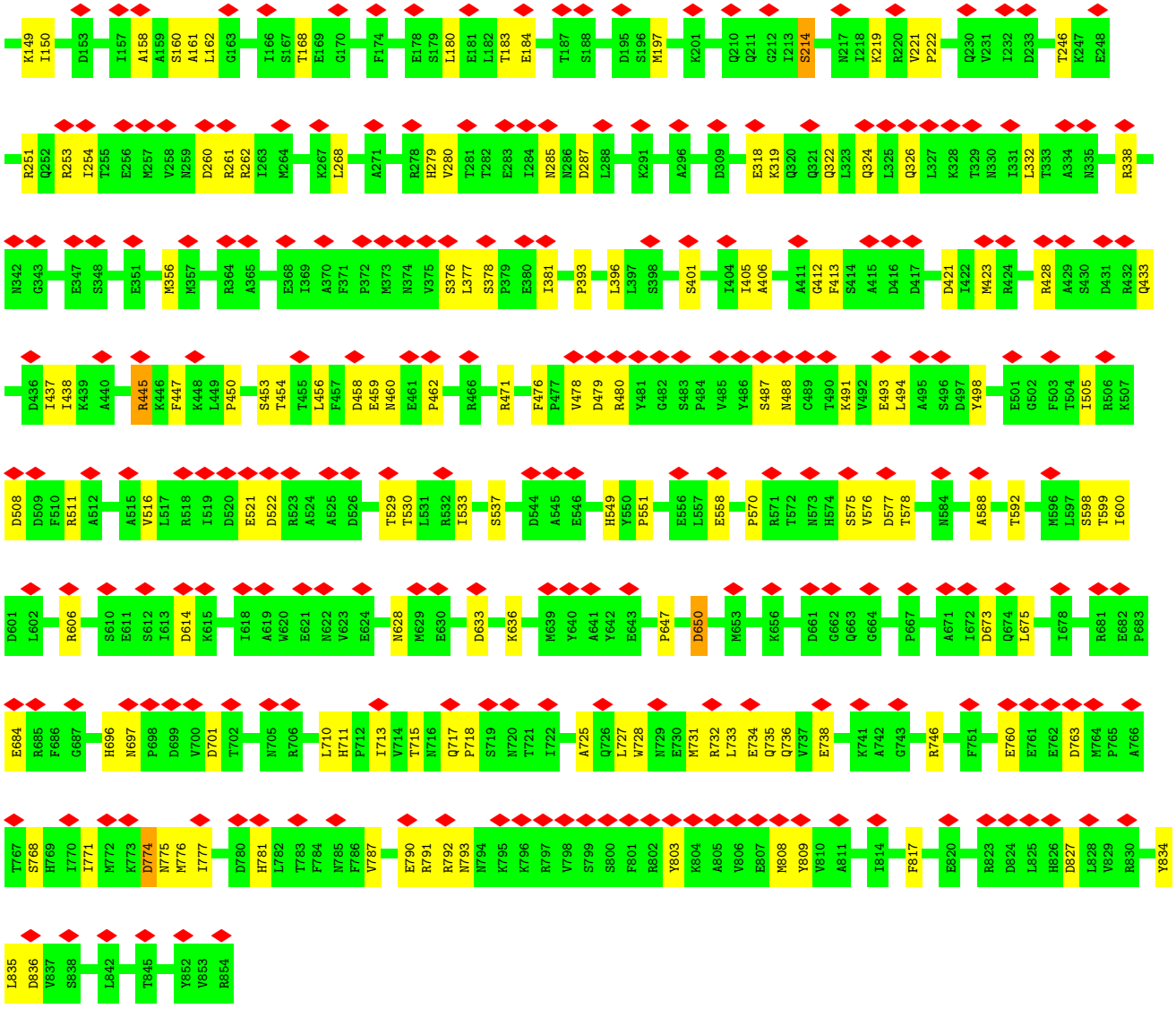
Chain F:



• Molecule 1: VP3

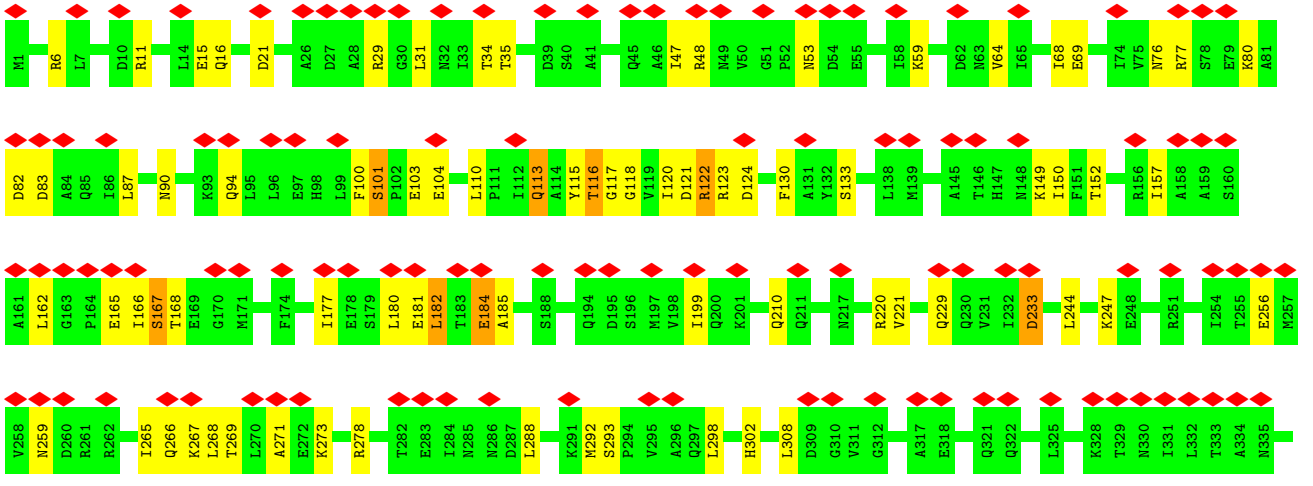
Chain G:

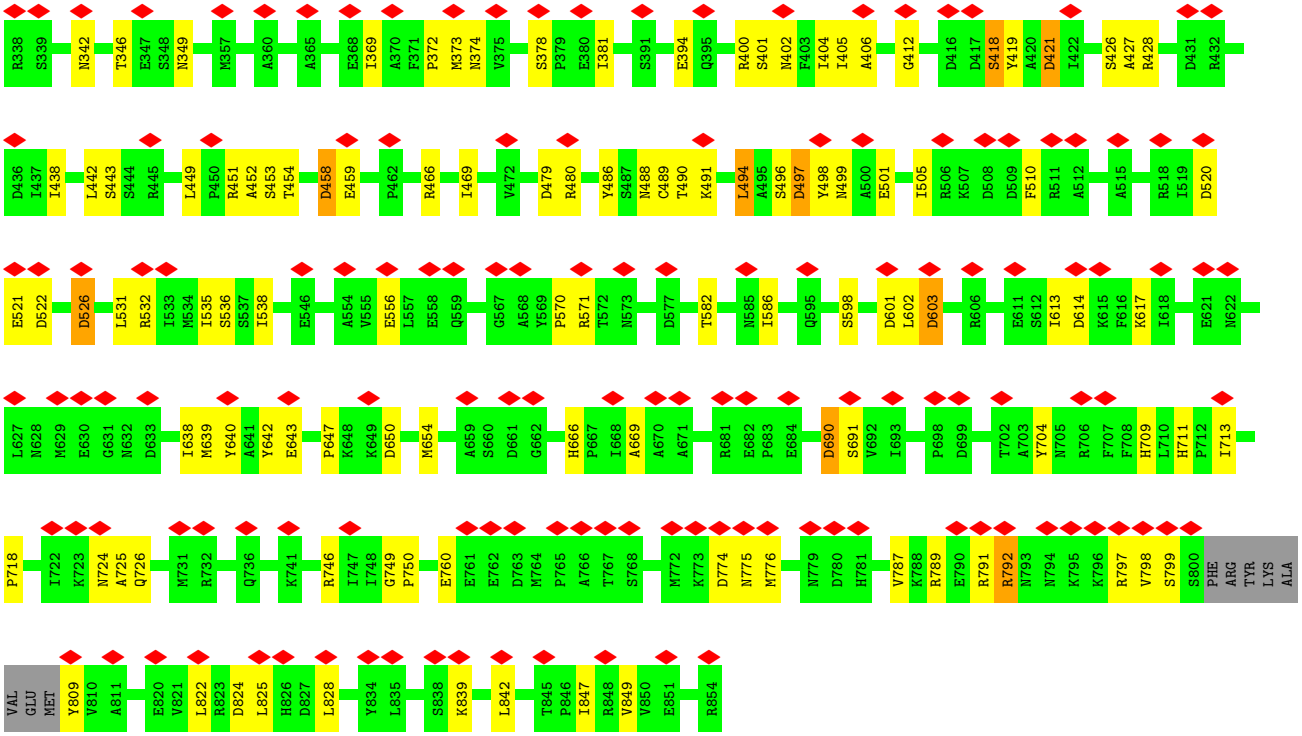




• Molecule 1: VP3

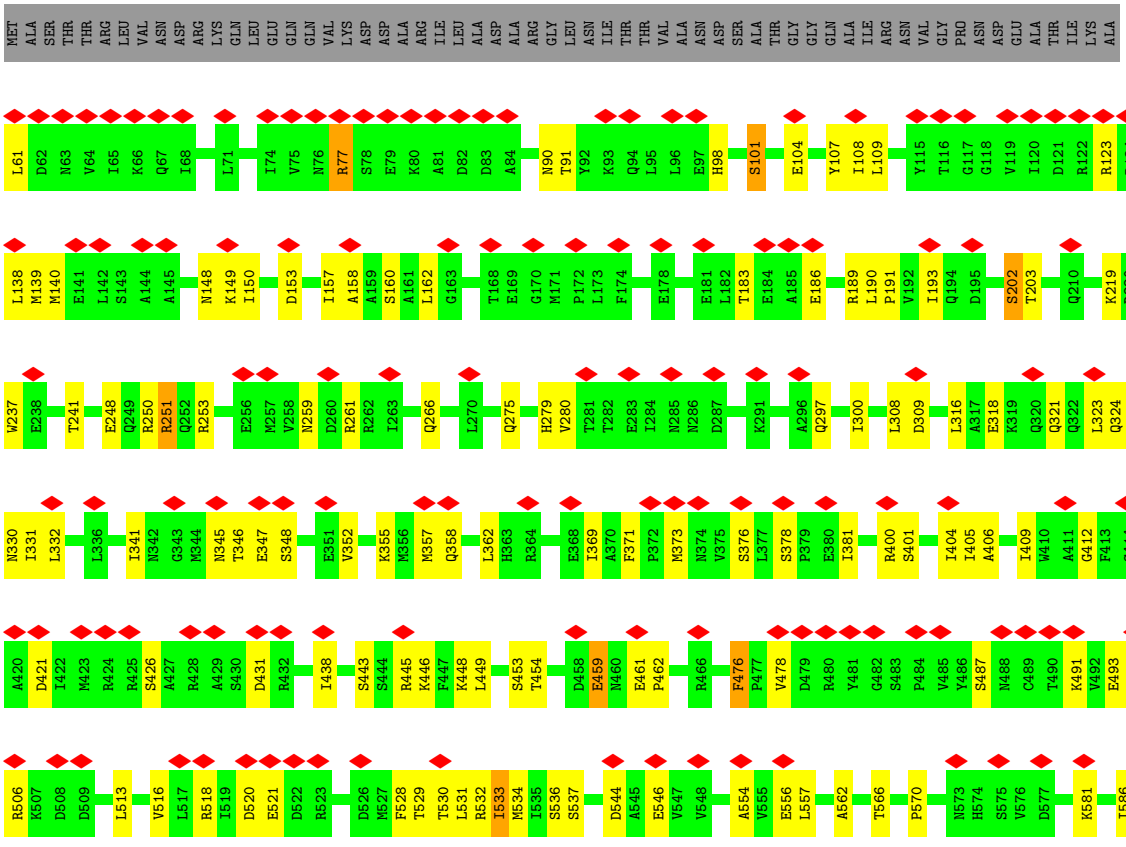
Chain H:

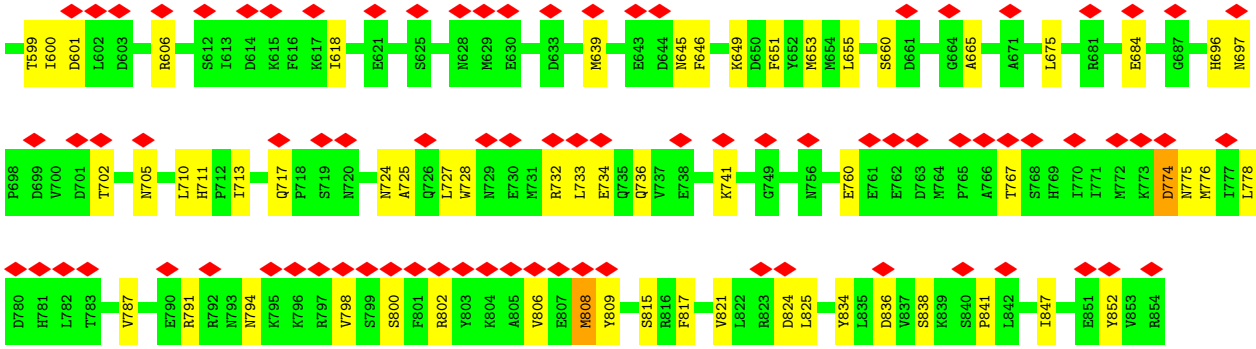




• Molecule 1: VP3

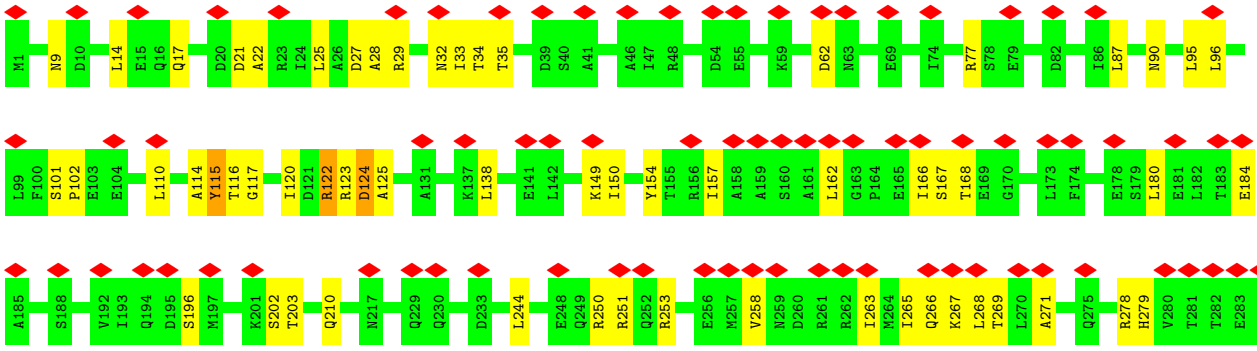
Chain I:





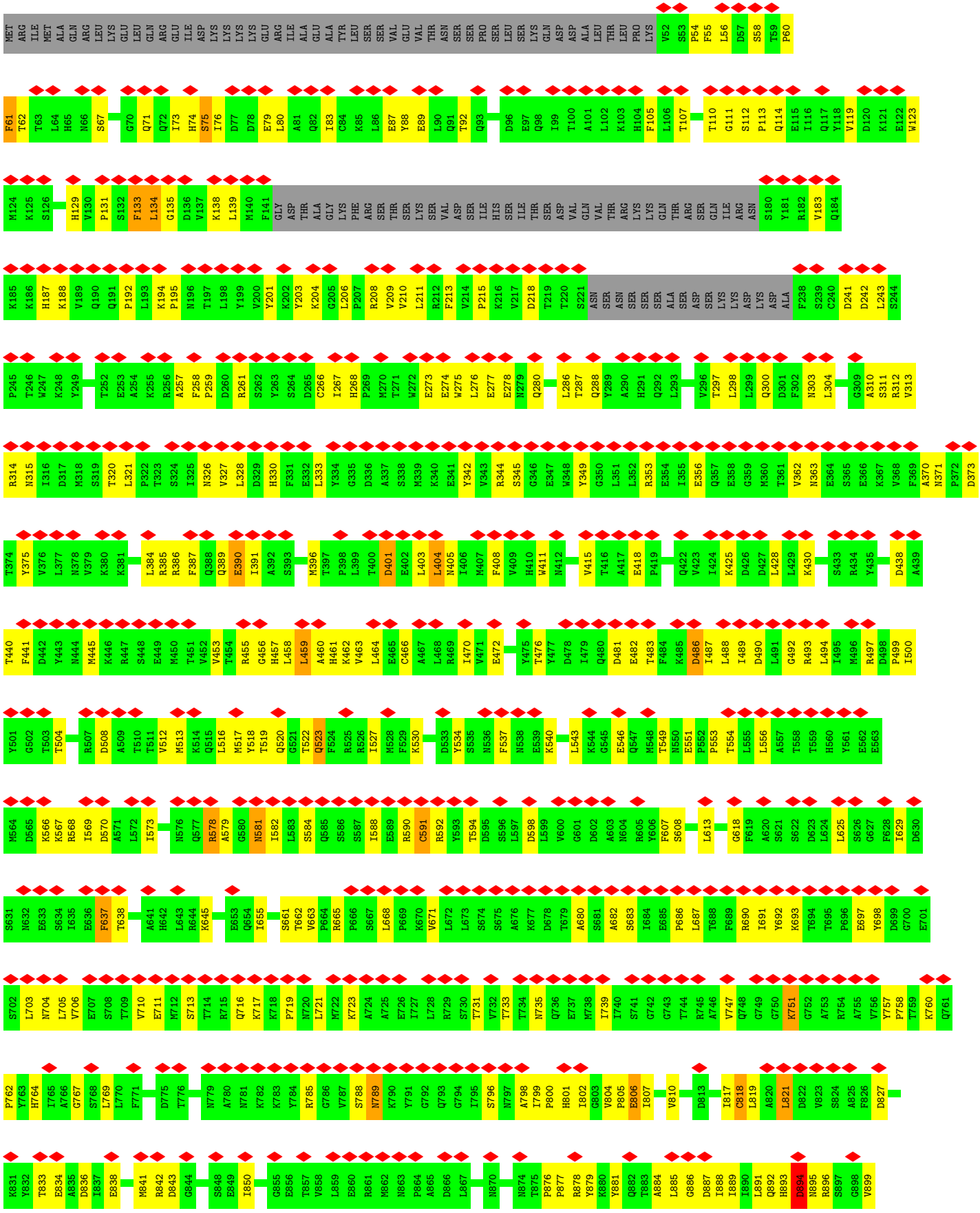
• Molecule 1: VP3

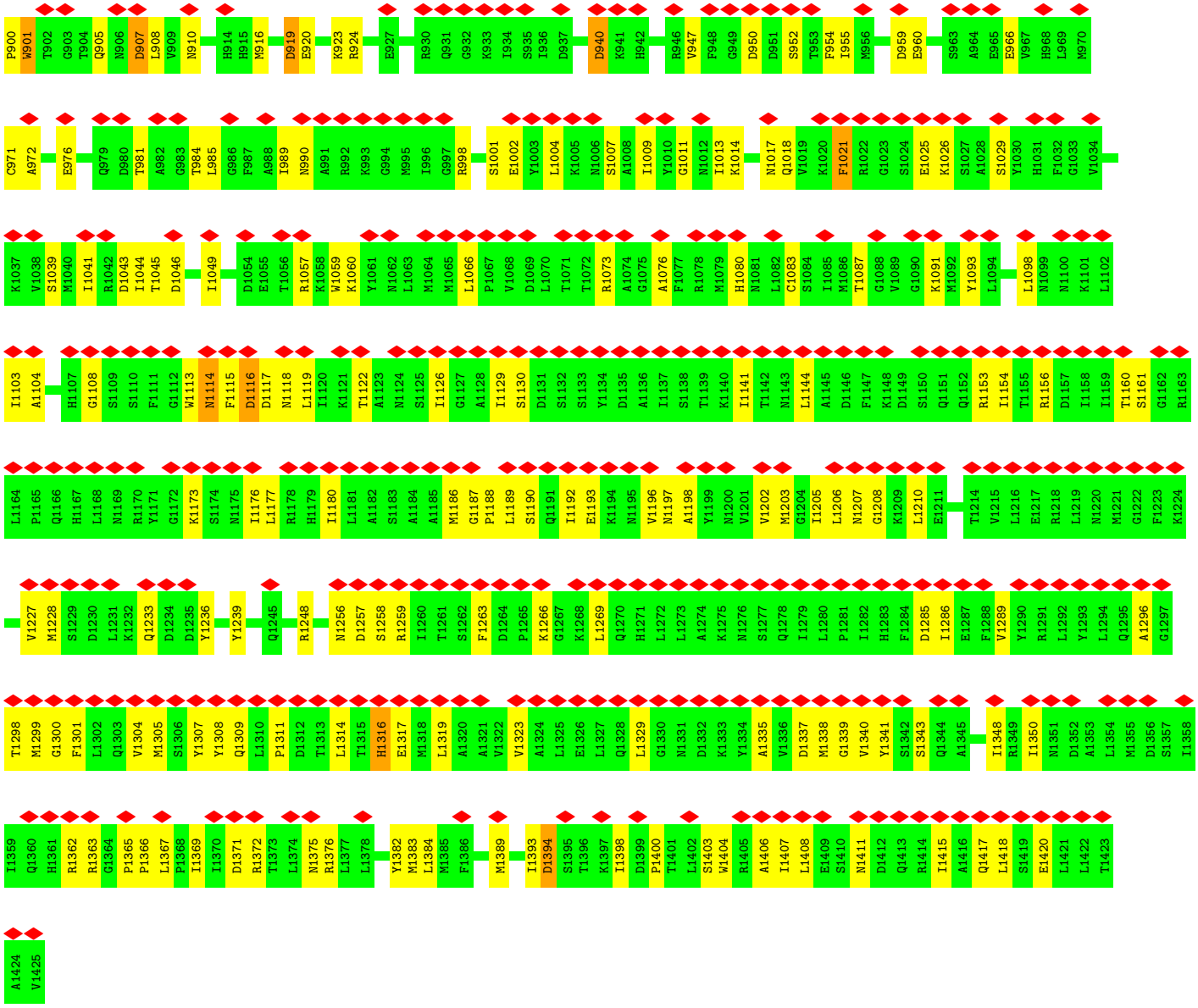
Chain J:



• Molecule 2: VP1

Chain Z:


MET ARG ILE MET ALA GLN ARG LEU LYS GLU LEU GLN ARG GLU ILE ASP LYS LYS LYS LYS GLU ARG ILE ALA GLU ALA TYR LEU SER SER VAL GLU VAL THR ASN SER SER PRO SER LEU SER LYS GLN ASP ALA LEU THR LEU PRO LYS V52 S53 P54 F55 L56 D57 S58 T59 P60
F61 T62 T63 L64 H65 N66 S67 G70 Q71 Q72 I73 H74 S75 I76 D77 D78 E79 L80 A81 Q82 I83 C84 K85 L86 E87 Y88 E89 L90 Q91 T92 Q93 D96 E97 Q98 I99 T100 A101 L102 K103 H104 F105 L106 T107 T110 G111 S112 P113 Q114 E115 I116 Q117 Y118 V119 D120 K121 E122 W123
M124 K125 S126 H129 V130 P131 S132 F133 L134 G135 D136 V137 K138 L139 M140 F141 GLY ASP THR ALA GLY LYS PHE ARG SER THR SER LYS SER VAL ASP SER ILE HIS SER ILE THR SER ASP VAL GLN VAL THR ARG LYS LYS GLN THR ARG SER GLN ILE ARG ASN S180 Y181 R182 V183 Q184
K185 K186 H187 K188 V189 Q190 Q191 P192 L193 K194 P195 N196 T197 L198 Y199 V200 Y201 K202 Y203 K204 G205 L206 P207 R208 V209 V210 L211 R212 F213 V214 P215 K216 V217 D218 T219 T220 S221 ASN SER ASN SER SER SER ALA SER ASP SER LYS LYS ASP LYS ASP ALA F238 S239 C240 D241 D242 L243 S244
P245 T246 W247 K248 Y249 T252 E253 A254 K255 R256 A257 F258 P259 D260 R261 S262 Y263 S264 D265 C266 I267 H268 P269 N270 T271 W272 E273 E274 W275 L276 E277 E278 N279 Q280 L286 T287 Q288 Y289 A290 H291 Q292 L293 V296 T297 L298 L299 Q300 D301 F302 N303 L304 G309 A310 S311 R312 V313
R314 N315 I316 D317 M318 S319 T320 L321 P322 T323 S324 I325 N326 V327 L328 D329 H330 F331 E332 L333 Y334 G335 D336 A337 S338 M339 K340 E341 Y342 V343 R344 S345 G346 E347 W348 Y349 G350 L351 L352 R353 E354 I355 E356 Q357 E358 G359 M360 T361 V362 N363 E364 S365 E366 K367 V368 F369 A370 N371 P372 D373
T374 Y375 V376 L377 N378 V379 K380 K381 L384 R385 R386 F387 Q388 Q389 E390 I391 A392 S393 M396 T397 P398 L399 T400 D401 E402 L403 L404 N405 I406 M407 F408 V409 H410 W411 N412 V415 T416 A417 E418 P419 Q422 V423 I424 K425 D426 D427 L428 L429 K430 S433 R434 Y435 D438 A439
T440 F441 D442 Y443 N444 M445 K446 R447 S448 E449 M450 T451 V452 V453 T454 R455 G456 H457 L458 L459 A460 H461 K462 V463 L464 E465 C466 A467 L468 R469 I470 V471 E472 Y475 T476 Y477 D478 I479 Q480 D481 E482 T483 F484 K485 D486 I487 L488 I489 D490 L491 G492 R493 L494 I495 M496 R497 D498 P499 I500
Y501 G502 T503 T504 R507 D508 A509 T510 T511 V512 M513 K514 Q515 L516 M517 Y518 T519 Q520 G521 T522 Q523 F524 R525 R526 I527 M528 F529 K530 D533 Y534 S535 N536 F537 N538 E539 K540 L543 K544 G545 E546 Q547 M548 T549 N550 E551 P552 P553 T554 L555 L556 A557 T558 T559 H560 Y561 E562 E563
M564 D565 K566 K567 R568 I569 D570 A571 L572 I573 N576 Q577 R578 A579 G580 N581 I582 L583 S584 Q585 S586 S587 I588 E589 R590 C591 R592 Y593 T594 D595 S596 L597 D598 L599 V600 G601 D602 A603 N604 R605 Y606 F607 S608 L613 G618 F619 A620 S621 S622 D623 L624 L625 S626 G627 F628 I629 D630
S631 N632 E633 S634 I635 E636 F637 T638 A641 H642 L643 R644 K645 E653 Q654 I655 S661 T662 V663 P664 R665 P666 S667 L668 P669 K670 V671 L672 L673 S674 S675 A676 K677 D678 T679 A680 S681 A682 S683 I684 E685 P686 L687 T688 F689 R690 I691 Y692 K693 T694 T695 P696 E697 Y698 D699 G700 E701
S702 L703 N704 L705 V706 E707 S708 T709 V710 E711 M712 S713 T714 R715 Q716 K717 K718 P719 N720 L721 M722 K723 A724 A725 E726 I727 L728 R729 S730 T731 V732 T733 T734 N735 Q736 E737 M738 I739 I740 S741 G742 G743 T744 R745 A746 V747 Q748 G749 G750 K751 G752 A753 R754 A755 V756 Y757 P758 T759 K760 Q761
P762 Y763 H764 I765 A766 G767 S768 L769 L770 F771 D775 T776 N779 A780 N781 K782 K783 Y784 R785 G786 V787 S788 N789 K790 Y791 G792 Q793 G794 I795 S796 N797 A798 I799 P800 H801 I802 G803 V804 P805 E806 I807 V810 D813 I817 C818 L819 A820 L821 D822 V823 S824 A825 F826 D827
K831 Y832 T833 E834 A835 D836 I837 E838 M841 R842 D843 G844 S848 E849 I850 G855 E856 T857 V858 L859 E860 R861 M862 N863 P864 A865 D866 L867 N870 N874 T875 P876 P877 R878 Y879 K880 Y881 Q882 T883 A884 L885 G886 D887 I888 I889 I890 L891 Q892 H893 D894 N895 R896 S897 G898 V899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C971 A972 E976 Q979 D980 T981 A982 G983 T984 L985 G986 F987 A988 I989 N990 A991 R992 K993 G994 M995 I996 G997 R998 S1001 E1002 Y1003 L1004 K1005 N1006 S1007 A1008 I1009 Y1010 G1011 N1012 I1013 K1014 N1017 Q1018 V1019 K1020 F1021 R1022 G1023 S1024 E1025 K1026 S1027 A1028 S1029 Y1030 H1031 F1032 G1033 V1034
K1037 V1038 S1039 M1040 I1041 R1042 D1043 I1044 T1045 D1046 I1049 D1054 E1055 T1056 R1057 K1058 W1059 K1060 Y1061 N1062 L1063 M1064 M1065 L1066 P1067 V1068 D1069 L1070 T1071 T1072 R1073 A1074 G1075 A1076 F1077 R1078 M1079 H1080 N1081 L1082 C1083 S1084 I1085 M1086 T1087 G1088 V1089 G1090 K1091 M1092 Y1093 L1094 L1098 N1099 N1100 K1101 L1102
I1103 A1104 H1107 G1108 S1109 S1110 F1111 G1112 W1113 N1114 F1115 D1116 D1117 N1118 L1119 I1120 K1121 T1122 A1123 N1124 S1125 I1126 G1127 A1128 I1129 S1130 D1131 S1132 S1133 Y1134 D1135 A1136 I1137 S1138 T1139 K1140 I1141 T1142 N1143 L1144 A1145 D1146 F1147 K1148 D1149 S1150 Q1151 Q1152 R1153 I1154 T1155 R1156 D1157 I1158 I1159 T1160 S1161 G1162 R1163
L1164 P1165 Q1166 H1167 L1168 N1169 R1170 Y1171 G1172 K1173 S1174 N1175 I1176 L1177 R1178 H1179 I1180 L1181 A1182 S1183 A1184 A1185 M1186 G1187 P1188 L1189 S1190 Q1191 I1192 E1193 K1194 N1195 V1196 N1197 A1198 Y1199 N1200 V1201 V1202 M1203 G1204 I1205 L1206 N1207 G1208 K1209 L1210 E1211 T1214 V1215 L1216 E1217 R1218 L1219 N1220 M1221 G1222 F1223 K1224
V1227 M1228 S1229 D1230 L1231 K1232 Q1233 D1234 D1235 Y1236 Y1239 Q1245 R1248 N1256 D1257 S1258 R1259 I1260 T1261 S1262 F1263 D1264 P1265 K1266 G1267 K1268 L1269 Q1270 H1271 L1272 L1273 A1274 K1275 N1276 S1277 Q1278 I1279 L1280 P1281 I1282 H1283 F1284 D1285 I1286 E1287 F1288 V1289 Y1290 R1291 L1292 Y1293 L1294 Q1295 A1296 G1297
T1298 M1299 G1300 F1301 L1302 Q1303 V1304 M1305 S1306 Y1307 Y1308 Q1309 L1310 P1311 D1312 T1313 L1314 T1315 H1316 E1317 M1318 L1319 A1320 A1321 V1322 V1323 A1324 L1325 E1326 L1327 Q1328 L1329 G1330 N1331 D1332 K1333 Y1334 A1335 V1336 D1337 M1338 G1339 V1340 Y1341 S1342 S1343 Q1344 A1345 I1348 R1349 I1350 N1351 D1352 A1353 L1354 M1355 D1356 S1357 I1358
I1359 Q1360 H1361 R1362 R1363 G1364 P1365 P1366 L1367 P1368 I1369 I1370 D1371 R1372 T1373 L1374 N1375 R1376 L1377 L1378 Y1382 M1383 L1384 M1385 F1386 M1389 I1393 D1394 S1395 T1396 K1397 I1398 D1399 P1400 T1401 L1402 S1403 W1404 R1405 A1406 I1407 L1408 E1409 S1410 N1411 D1412 Q1413 R1414 I1415 A1416 Q1417 L1418 S1419 E1420 L1421 L1422 T1423
A1424 V1425

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	58095	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	25	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	128440	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	33.537	Depositor
Minimum map value	-21.310	Depositor
Average map value	0.081	Depositor
Map value standard deviation	1.814	Depositor
Recommended contour level	6.0	Depositor
Map size (Å)	872.0, 872.0, 872.0	wwPDB
Map dimensions	800, 800, 800	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.09, 1.09, 1.09	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	A	0.32	0/6644	0.55	1/9015 (0.0%)
1	B	0.32	0/6871	0.56	1/9322 (0.0%)
1	C	0.31	0/6499	0.54	1/8818 (0.0%)
1	D	0.34	0/6871	0.55	0/9322
1	E	0.32	0/6499	0.56	2/8818 (0.0%)
1	F	0.34	0/6871	0.57	2/9322 (0.0%)
1	G	0.30	0/6499	0.53	1/8818 (0.0%)
1	H	0.32	0/6871	0.56	1/9322 (0.0%)
1	I	0.32	0/6499	0.55	1/8818 (0.0%)
1	J	0.32	0/6871	0.56	3/9322 (0.0%)
2	Z	0.40	0/10724	0.59	1/14518 (0.0%)
All	All	0.33	0/77719	0.56	14/105415 (0.0%)

There are no bond length outliers.

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	614	ASP	CB-CG-OD1	5.91	123.62	118.30
1	I	774	ASP	CB-CG-OD1	5.48	123.23	118.30
1	G	774	ASP	CB-CG-OD1	5.40	123.16	118.30
1	E	699	ASP	CB-CG-OD1	5.35	123.12	118.30
1	E	673	ASP	CB-CG-OD1	5.28	123.06	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6516	0	6517	104	0
1	B	6746	0	6755	144	0
1	C	6372	0	6375	117	0
1	D	6746	0	6755	118	0
1	E	6372	0	6375	124	0
1	F	6746	0	6755	180	0
1	G	6372	0	6375	115	0
1	H	6746	0	6755	138	0
1	I	6372	0	6375	130	0
1	J	6746	0	6755	107	0
2	Z	10516	0	10497	329	0
All	All	76250	0	76289	1515	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

The worst 5 of 1515 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Z:895:ASN:HB3	2:Z:905:GLN:OE1	1.66	0.96
1:F:98:HIS:HB2	1:F:112:ILE:HD11	1.44	0.96
2:Z:686:PRO:HG3	2:Z:717:LYS:HA	1.48	0.94
1:B:126:SER:HB3	1:B:129:ASN:OD1	1.68	0.93
1:E:119:VAL:HB	1:F:69:GLU:OE2	1.68	0.92

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	813/854 (95%)	741 (91%)	72 (9%)	0	100 100
1	B	842/854 (99%)	775 (92%)	65 (8%)	2 (0%)	47 78

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	792/854 (93%)	721 (91%)	71 (9%)	0	100	100
1	D	842/854 (99%)	785 (93%)	56 (7%)	1 (0%)	51	83
1	E	792/854 (93%)	719 (91%)	70 (9%)	3 (0%)	34	69
1	F	842/854 (99%)	761 (90%)	76 (9%)	5 (1%)	25	62
1	G	792/854 (93%)	726 (92%)	66 (8%)	0	100	100
1	H	842/854 (99%)	786 (93%)	55 (6%)	1 (0%)	51	83
1	I	792/854 (93%)	733 (93%)	58 (7%)	1 (0%)	51	83
1	J	842/854 (99%)	777 (92%)	64 (8%)	1 (0%)	51	83
2	Z	1314/1425 (92%)	1162 (88%)	144 (11%)	8 (1%)	25	62
All	All	9505/9965 (95%)	8686 (91%)	797 (8%)	22 (0%)	50	78

5 of 22 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	127	PHE
1	F	689	ILE
1	J	115	TYR
2	Z	894	ASP
2	Z	901	TRP

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	A	718/751 (96%)	688 (96%)	30 (4%)	30	59
1	B	744/751 (99%)	716 (96%)	28 (4%)	33	61
1	C	704/751 (94%)	679 (96%)	25 (4%)	35	63
1	D	744/751 (99%)	713 (96%)	31 (4%)	30	59
1	E	704/751 (94%)	681 (97%)	23 (3%)	38	64
1	F	744/751 (99%)	708 (95%)	36 (5%)	25	56
1	G	704/751 (94%)	689 (98%)	15 (2%)	53	74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	H	744/751 (99%)	705 (95%)	39 (5%)	23 55
1	I	704/751 (94%)	676 (96%)	28 (4%)	31 60
1	J	744/751 (99%)	722 (97%)	22 (3%)	41 66
2	Z	1167/1263 (92%)	1117 (96%)	50 (4%)	29 58
All	All	8421/8773 (96%)	8094 (96%)	327 (4%)	36 60

5 of 327 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	251	ARG
2	Z	384	LEU
1	I	487	SER
1	J	196	SER
2	Z	591	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 44 such sidechains are listed below:

Mol	Chain	Res	Type
1	J	736	GLN
2	Z	704	ASN
2	Z	268	HIS
2	Z	410	HIS
2	Z	748	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

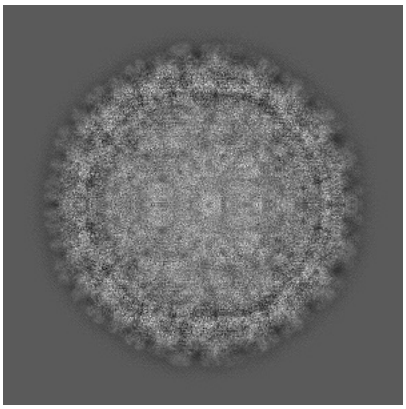
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-33404. These allow visual inspection of the internal detail of the map and identification of artifacts.

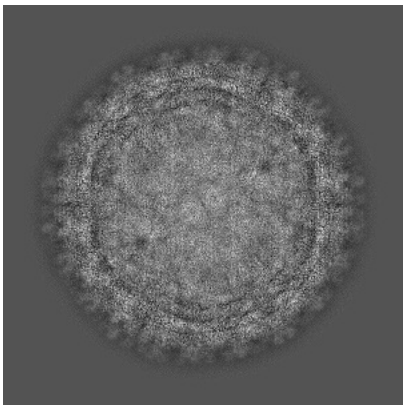
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

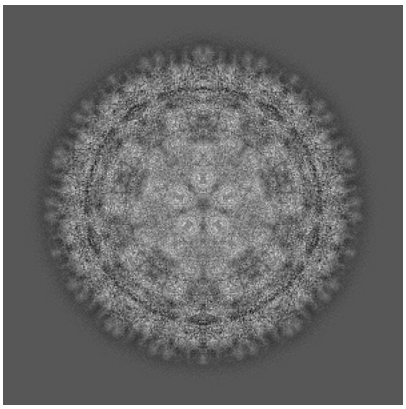
6.1.1 Primary map



X

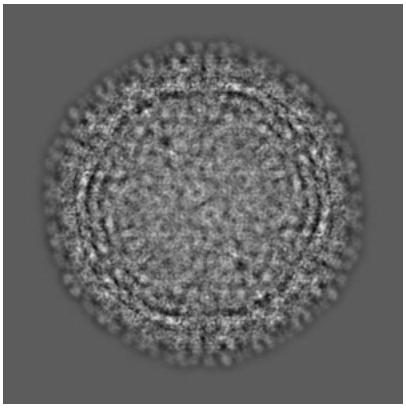


Y

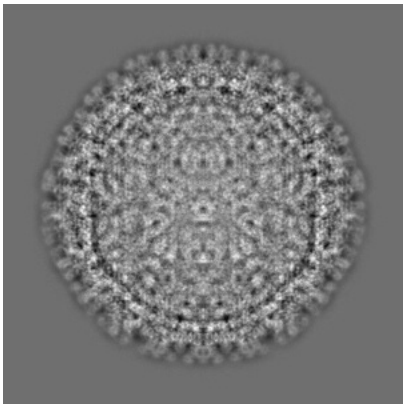


Z

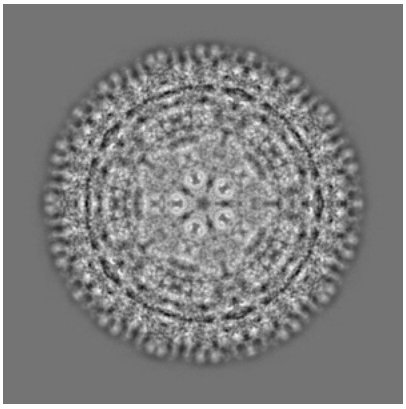
6.1.2 Raw map



X



Y

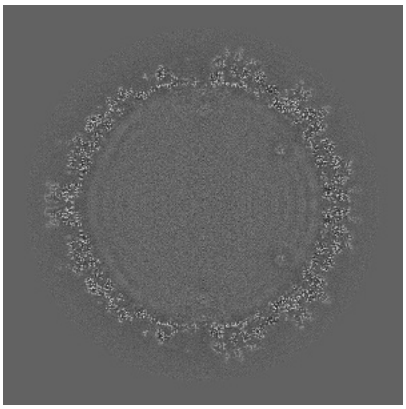


Z

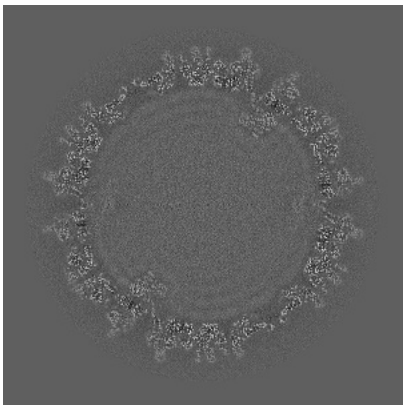
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

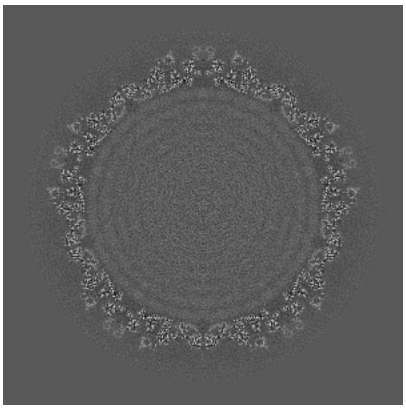
6.2.1 Primary map



X Index: 400

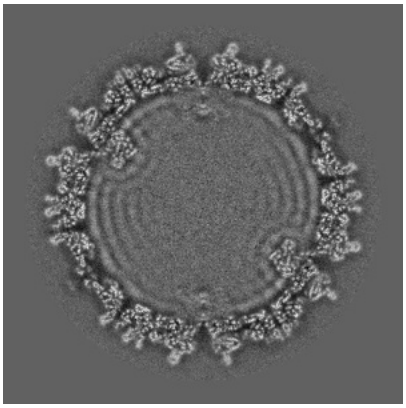


Y Index: 400

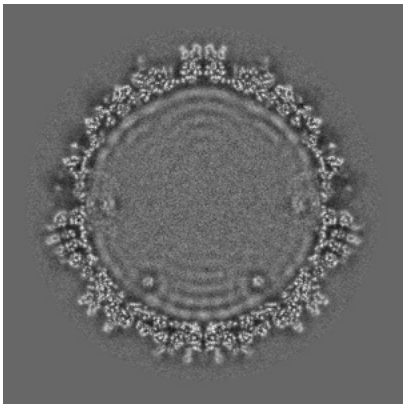


Z Index: 400

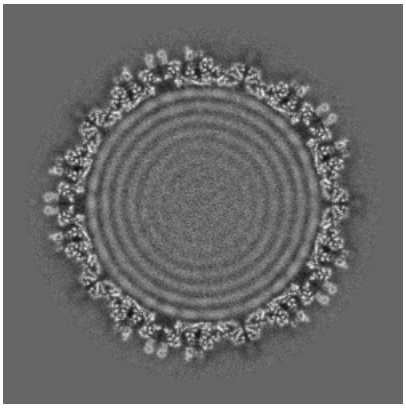
6.2.2 Raw map



X Index: 400



Y Index: 400

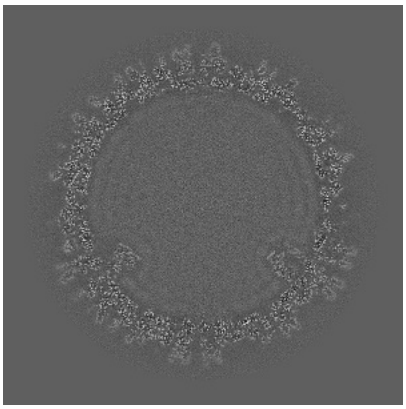


Z Index: 400

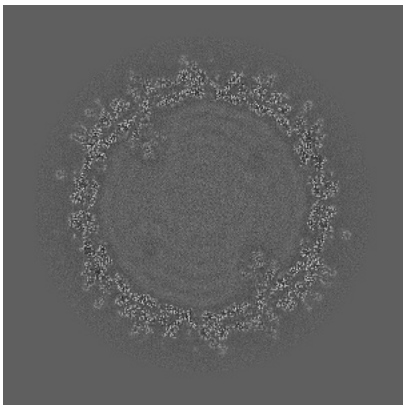
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

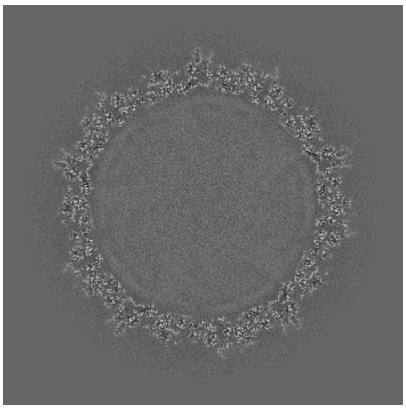
6.3.1 Primary map



X Index: 358

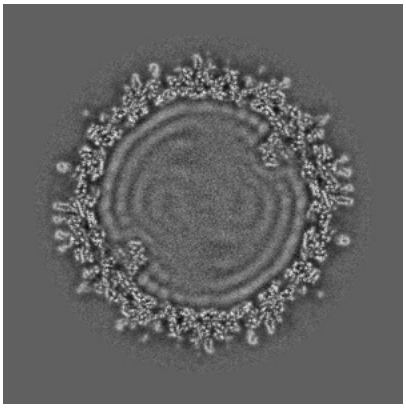


Y Index: 292

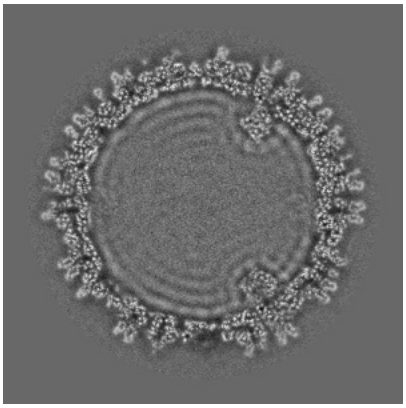


Z Index: 336

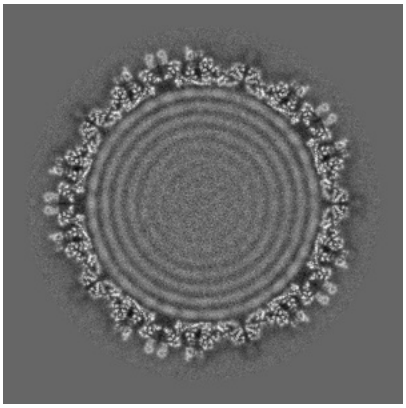
6.3.2 Raw map



X Index: 293



Y Index: 354

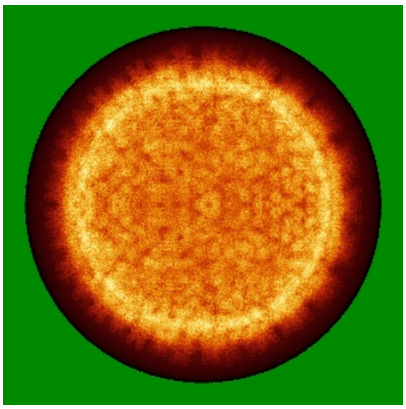


Z Index: 400

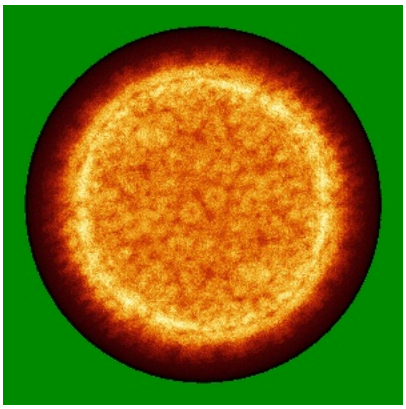
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

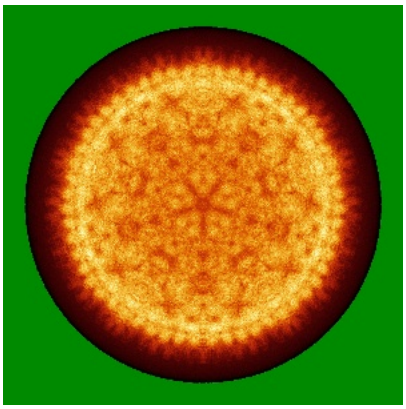
6.4.1 Primary map



X

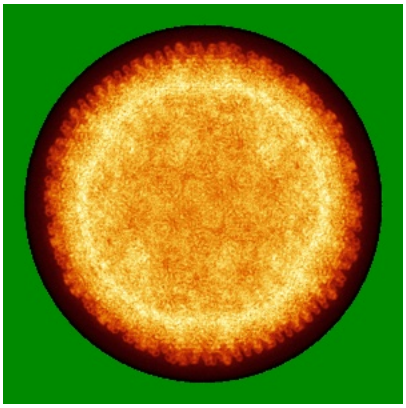


Y

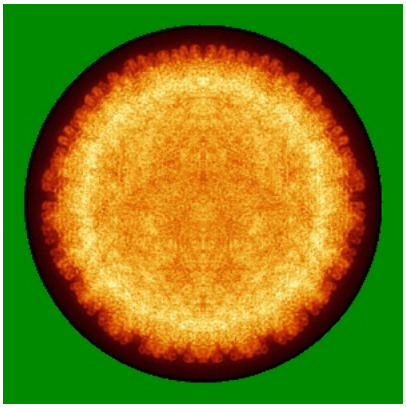


Z

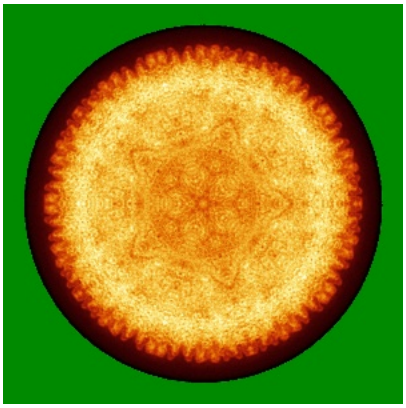
6.4.2 Raw map



X



Y

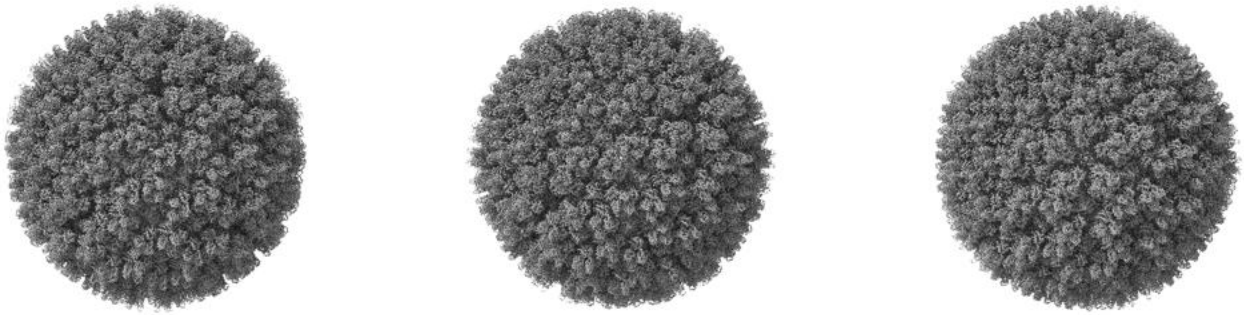


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 6.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

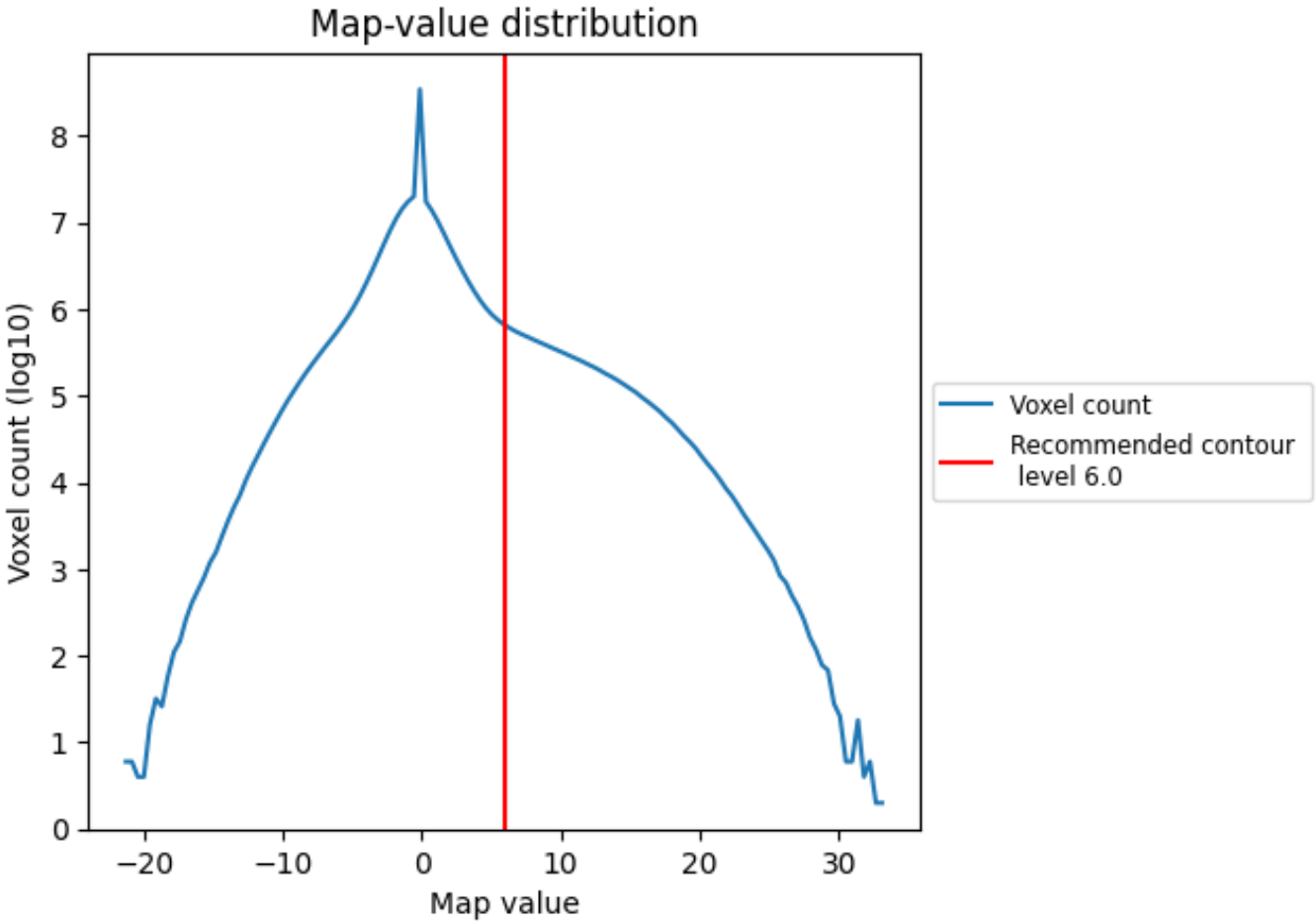
6.6 Mask visualisation (i)

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

7 Map analysis

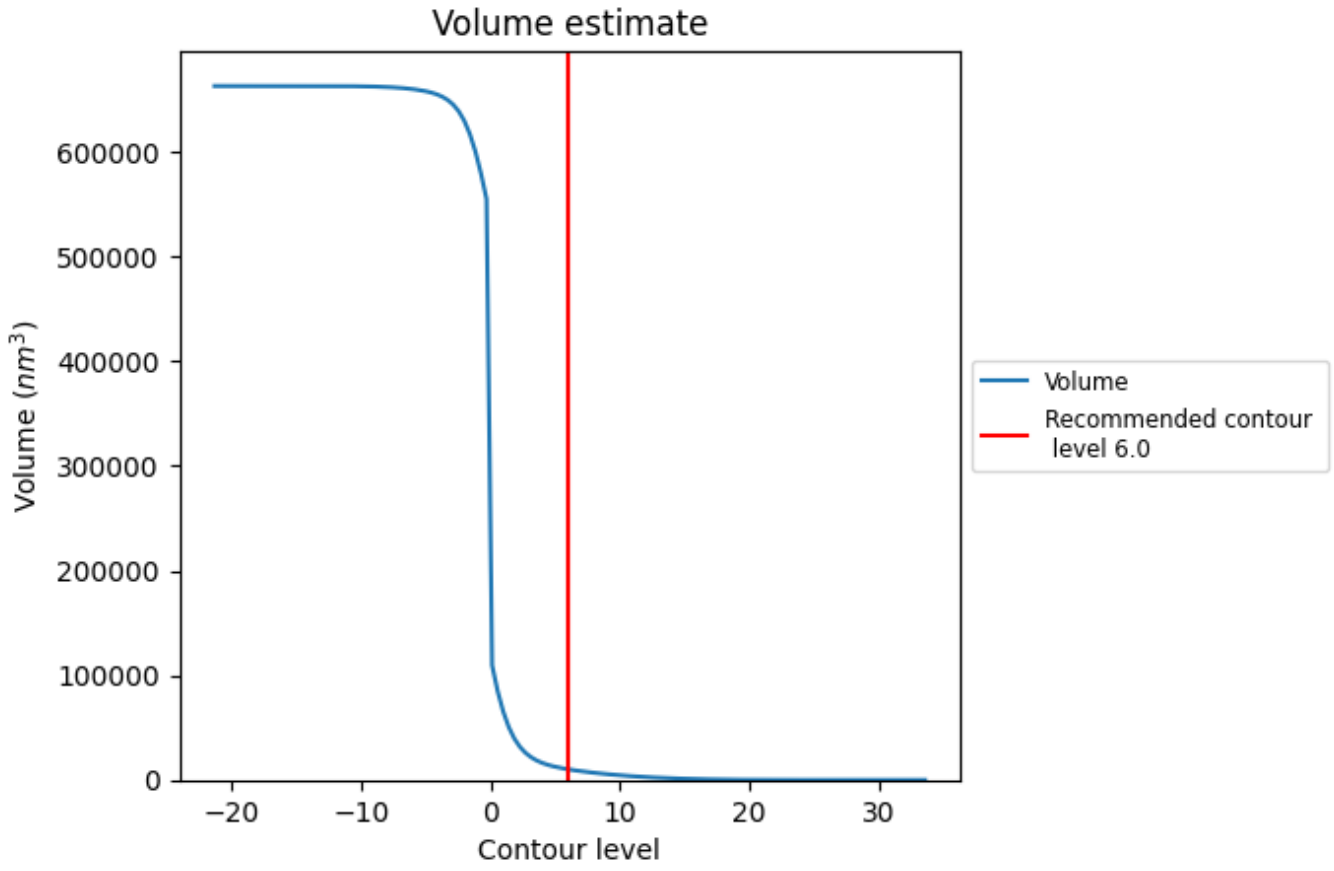
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

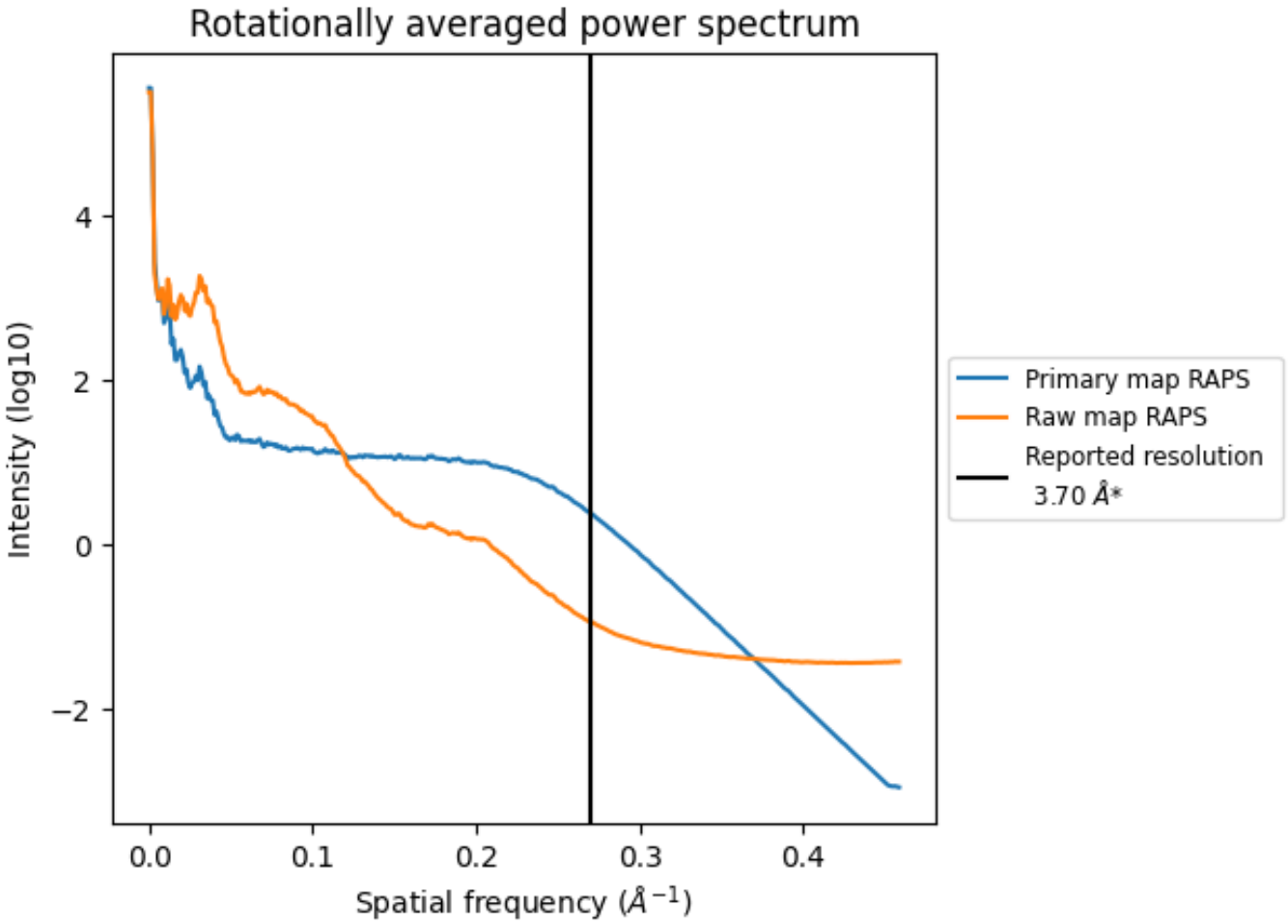
7.2 Volume estimate (i)



The volume at the recommended contour level is 10162 nm^3; this corresponds to an approximate mass of 9180 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

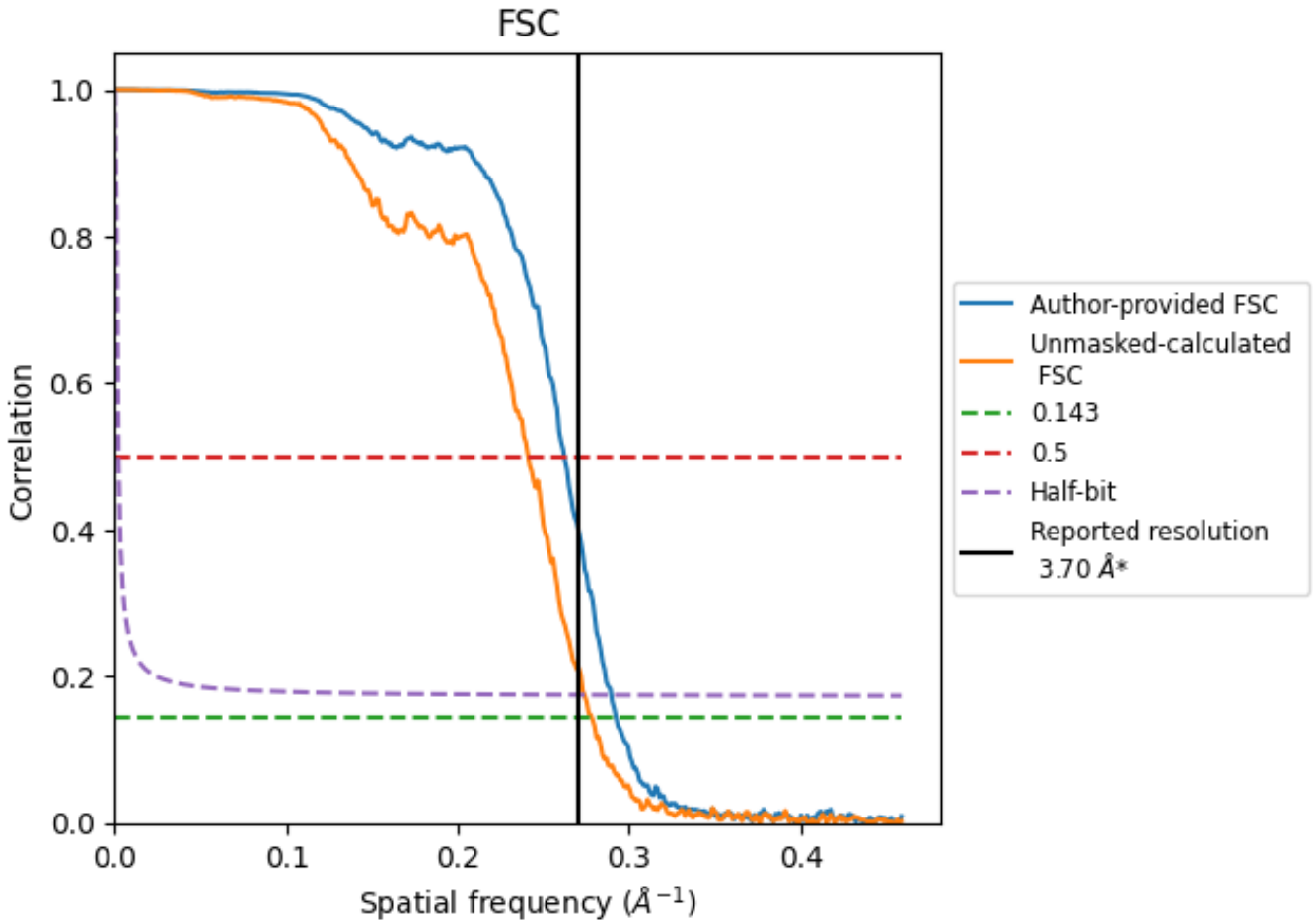


*Reported resolution corresponds to spatial frequency of 0.270 $Å^{-1}$

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.270 Å^{-1}

8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	3.42	3.82	3.45
Unmasked-calculated*	3.59	4.15	3.65

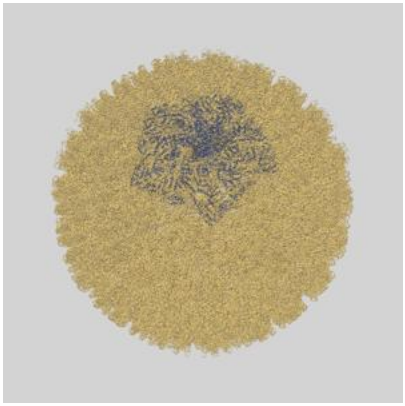
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-33404 and PDB model 7XR3. Per-residue inclusion information can be found in section 3 on page 5.

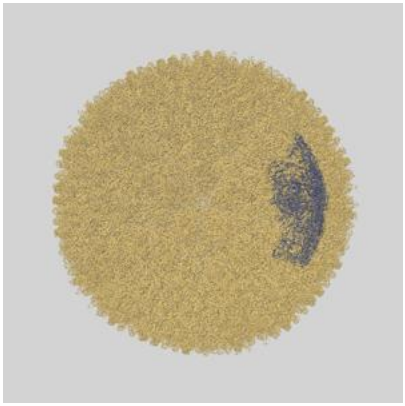
9.1 Map-model overlays

9.1.1 Map-model overlay



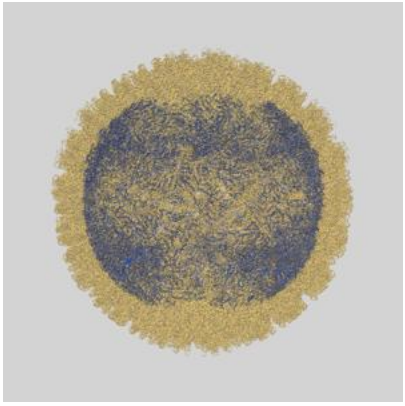
X

Y

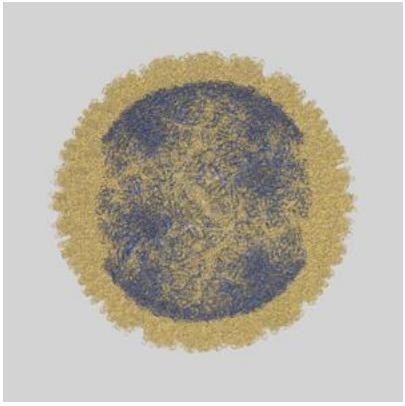


Z

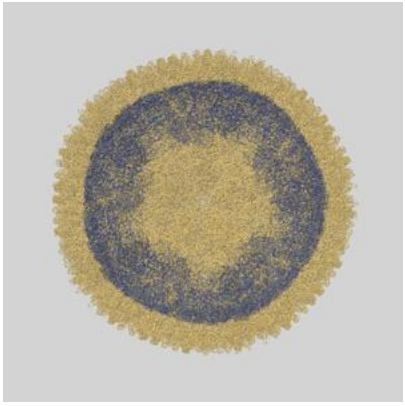
9.1.2 Map-model assembly overlay



X



Y



Z

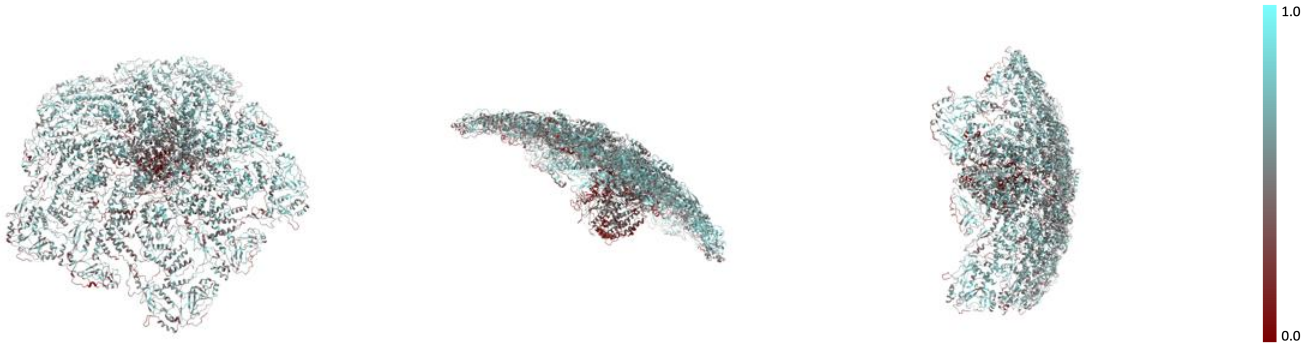
The images above show the 3D surface view of the map at the recommended contour level 6.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model

X Y Z

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.

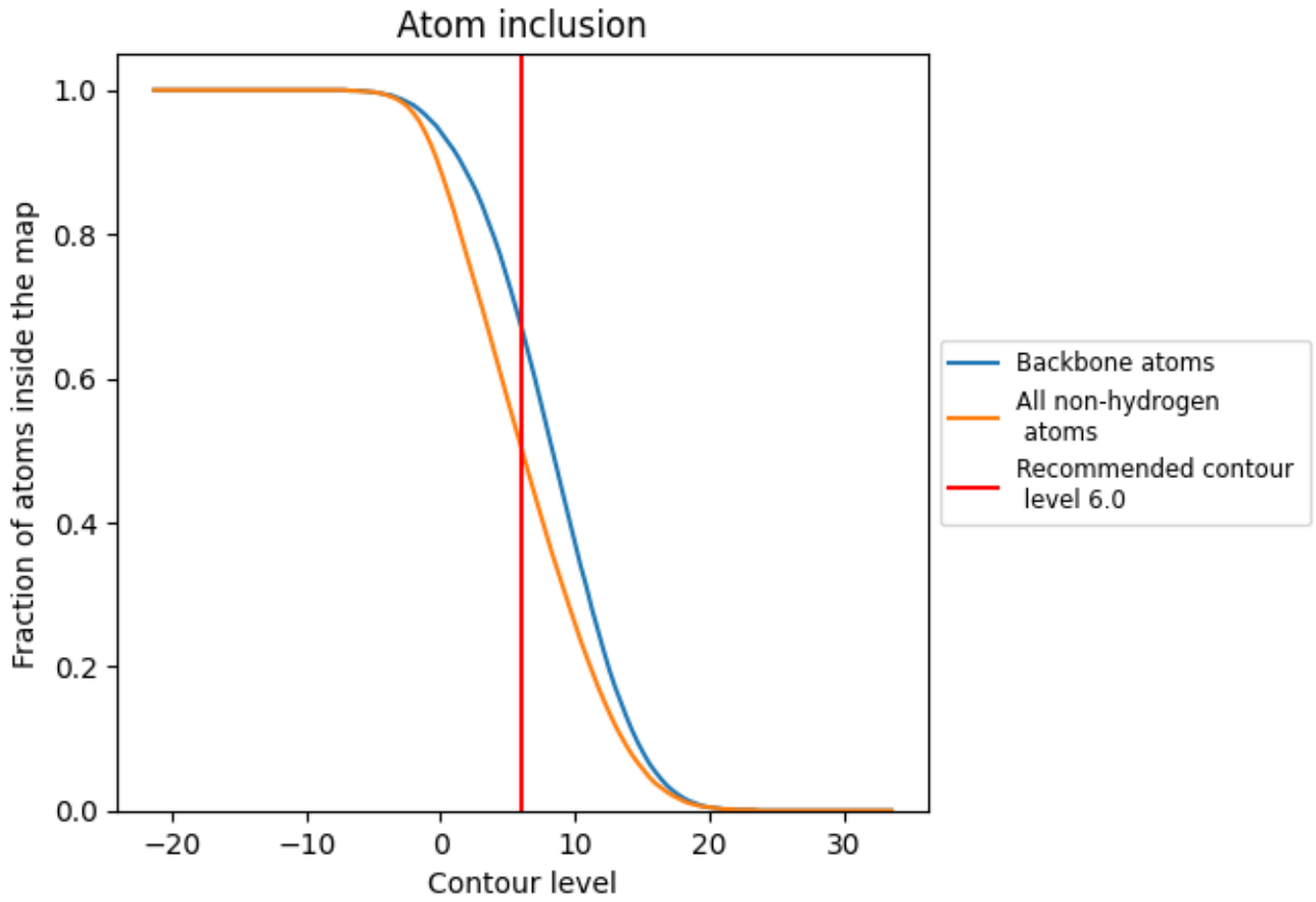
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (6.0).

9.4 Atom inclusion (i)



At the recommended contour level, 67% of all backbone atoms, 50% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (6.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5040	0.3580
A	0.5410	0.3990
B	0.5700	0.3920
C	0.5580	0.3950
D	0.5790	0.4090
E	0.5080	0.3430
F	0.5540	0.3670
G	0.4850	0.3300
H	0.5060	0.3160
I	0.5160	0.3590
J	0.5180	0.3340
Z	0.3130	0.3130