Full wwPDB EM Validation Report (i)

Mar 11, 2024 – 01:47 PM EDT

PDB ID	:	6Q1F
EMDB ID	:	EMD-20557
Title	:	Atomic structure of the Human Herpesvirus 6B Capsid and Capsid-Associated Tegument Complexes
Authors	:	Zhang, Y.B.; Liu, W.; Li, Z.H.; Kumar, V.; Alvarez-Cabrera, A.L.; Leibovitch, E.; Cui, Y.X.; Mei, Y.; Bi, G.Q.; Jacobson, S.; Zhou, Z.H.
Deposited on	:	2019-08-03
Resolution	:	9.00 Å(reported)

This is a Full wwPDB EM Validation 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:

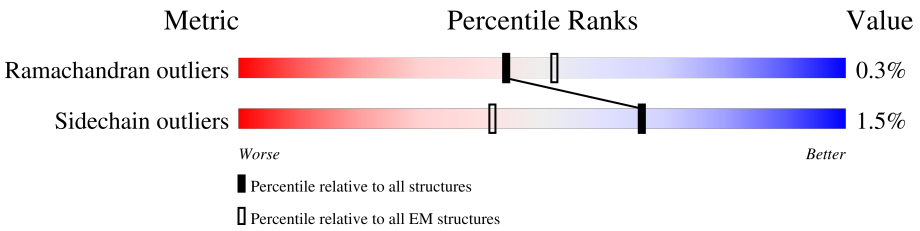
EMDB validation analysis	:	0.0.1.dev70
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 9.00 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)
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	1345	39% 99%
1	B	1345	41% 98%
1	C	1345	42% 97%
1	D	1345	38% 98%
1	E	1345	37% 98%
1	F	1345	43% 98%
1	G	1345	42% 98%
1	H	1345	34% 98%
1	I	1345	40% 99%

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Mol	Chain	Length	Quality of chain
1	q	1345	54% / 95%
1	r	1345	49% / 99%
1	s	1345	47% / 99%
1	t	1345	45% / 99%
1	u	1345	49% / 99%
1	v	1345	51% / 96%
1	w	1345	77% / 92% / 7%
2	e	858	27% / 31% / 69%
2	f	858	28% / 31% / 69%
2	g	858	25% / 30% / 69%
2	h	858	29% / 31% / 69%
2	i	858	26% / 30% / 69%
2	j	858	29% / 30% / 69%
2	k	858	25% / 30% / 69%
2	l	858	30% / 30% / 69%
2	m	858	24% / 31% / 69%
2	n	858	22% / 30% / 69%
2	o	858	21% / 30% / 69%
2	p	858	25% / 31% / 69%
3	1	89	45% / 67% / 31%
3	2	89	53% / 67% / 31%
3	3	89	61% / 67% / 31%
3	4	89	65% / 64% / 35%
3	J	89	48% / 65% / 31%
3	K	89	47% / 67% / 31%

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Mol	Chain	Length	Quality of chain
3	L	89	53% 66% 31%
3	M	89	49% 67% 31%
3	N	89	47% 67% 31%
3	O	89	58% 67% 31%
3	P	89	45% 67% 31%
3	Q	89	54% 67% 31%
3	R	89	49% 67% 31%
3	x	89	64% 67% 31%
3	y	89	61% 67% 31%
3	z	89	57% 67% 31%
4	5	299	56% 83% 16%
4	S	299	45% 98%
4	T	299	57% 99%
4	U	299	48% 97%
4	V	299	47% 97%
5	6	296	69% 95% 5%
5	7	296	71% 98%
5	W	296	48% 98%
5	X	296	58% 99%
5	Y	296	50% 98%
5	Z	296	46% 96%
5	a	296	48% 98%
5	b	296	54% 97%
5	c	296	46% 98%
5	d	296	47% 97%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 238552 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 Major capsid protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1343	10682	6792	1813	2017	60	0	0
1	B	1343	10682	6792	1813	2017	60	0	0
1	C	1325	10552	6709	1792	1991	60	0	0
1	D	1343	10682	6792	1813	2017	60	0	0
1	E	1343	10682	6792	1813	2017	60	0	0
1	F	1343	10682	6792	1813	2017	60	0	0
1	G	1343	10682	6792	1813	2017	60	0	0
1	H	1343	10682	6792	1813	2017	60	0	0
1	I	1343	10682	6792	1813	2017	60	0	0
1	q	1296	10313	6561	1751	1942	59	0	0
1	r	1343	10682	6792	1813	2017	60	0	0
1	s	1343	10682	6792	1813	2017	60	0	0
1	t	1343	10682	6792	1813	2017	60	0	0
1	u	1344	10690	6797	1814	2018	61	0	0
1	v	1301	10331	6564	1759	1948	60	0	0
1	w	1248	9933	6324	1691	1860	58	0	0

- Molecule 2 is a protein called Large structural phosphoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	e	269	2224	1417	376	426	5	0	0
2	f	269	2224	1417	376	426	5	0	0
2	g	269	2224	1417	376	426	5	0	0
2	h	269	2224	1417	376	426	5	0	0
2	i	269	2224	1417	376	426	5	0	0
2	j	269	2224	1417	376	426	5	0	0
2	k	269	2224	1417	376	426	5	0	0
2	l	269	2224	1417	376	426	5	0	0
2	m	269	2224	1417	376	426	5	0	0
2	n	269	2224	1417	376	426	5	0	0
2	o	269	2224	1417	376	426	5	0	0
2	p	269	2224	1417	376	426	5	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	J	61	483	308	89	83	3	0	0
3	K	61	483	308	89	83	3	0	0
3	L	61	483	308	89	83	3	0	0
3	M	61	483	308	89	83	3	0	0
3	N	61	483	308	89	83	3	0	0
3	O	61	483	308	89	83	3	0	0
3	P	61	483	308	89	83	3	0	0
3	Q	61	483	308	89	83	3	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	R	61	483	308	89	83	3	0	0
3	x	61	483	308	89	83	3	0	0
3	y	61	483	308	89	83	3	0	0
3	z	61	483	308	89	83	3	0	0
3	1	61	483	308	89	83	3	0	0
3	2	61	483	308	89	83	3	0	0
3	3	61	483	308	89	83	3	0	0
3	4	58	456	292	85	76	3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	5	251	2023	1306	327	376	14	0	0
4	S	299	2398	1542	395	446	15	0	0
4	T	299	2398	1542	395	446	15	0	0
4	U	299	2398	1542	395	446	15	0	0
4	V	299	2398	1542	395	446	15	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	6	282	2226	1422	370	415	19	0	0
5	W	296	2337	1486	393	437	21	0	0
5	X	296	2337	1486	393	437	21	0	0
5	Y	296	2337	1486	393	437	21	0	0

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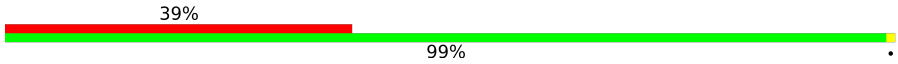
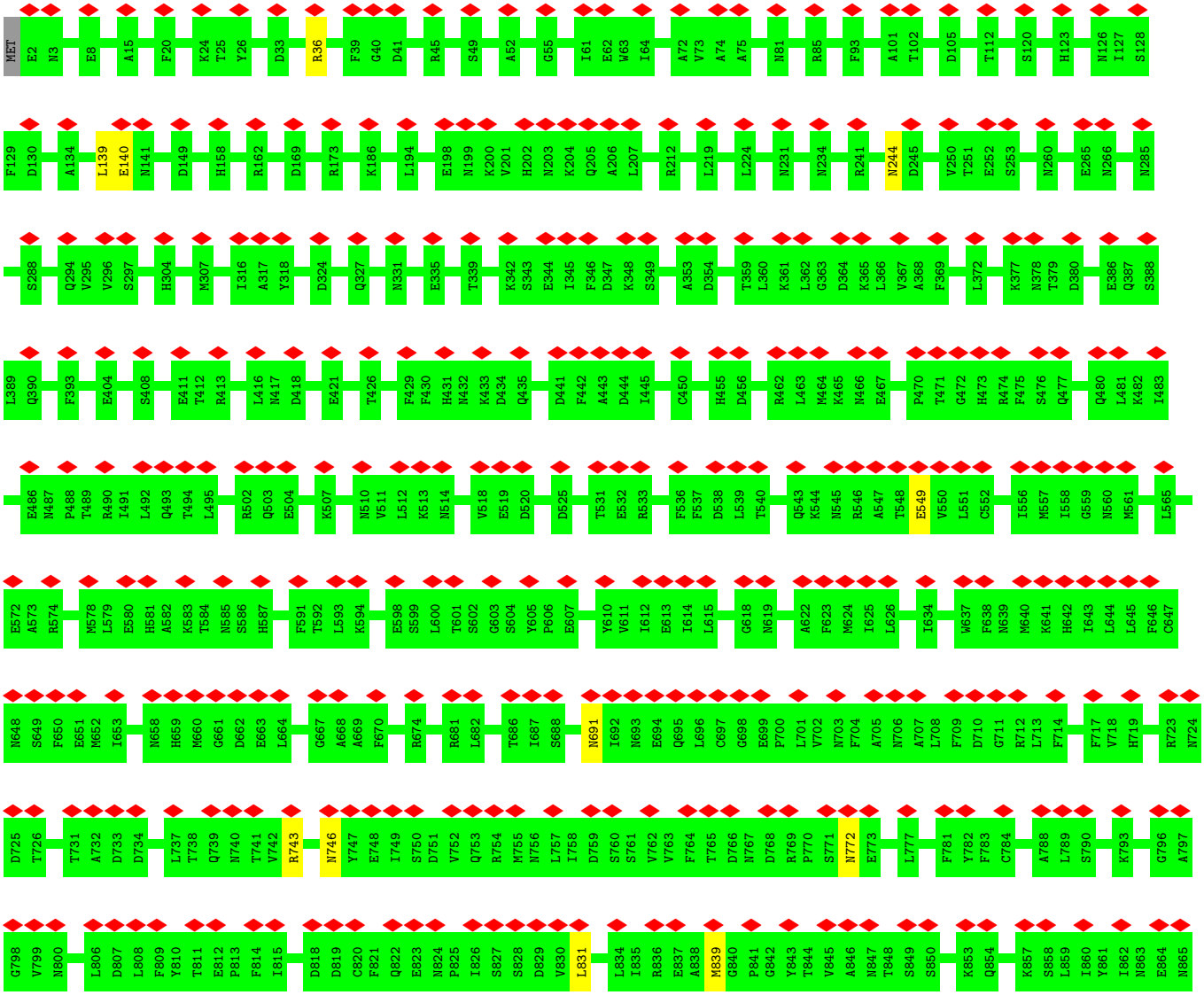
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	Z	296	2337	1486	393	437	21	0	0
			Total	C	N	O	S		
5	7	296	2337	1486	393	437	21	0	0
			Total	C	N	O	S		
5	a	295	2329	1481	392	436	20	0	0
			Total	C	N	O	S		
5	b	295	2329	1481	392	436	20	0	0
			Total	C	N	O	S		
5	c	295	2329	1481	392	436	20	0	0
			Total	C	N	O	S		
5	d	295	2329	1481	392	436	20	0	0

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: Major capsid protein

Chain A: 



T866 K867 I868 L869 E872 D876 P877 A878 Q879 R880 H881 G882 H886 F887 Q888 S889 L890 Q891 H892 I893 L894 Y895 N896 G897 L898 C899 L900 I901 T905 T906 L907 R908 R909 F916 F920 S921 D922 P923 G924 G927 T928 M929 I933 N938 Y943 Q944 R945 N946 D947 G948

G949 F950 P951 L952 P955 L956 A957 L958 E959 F960 Y961 N962 W963 Q964 R965 F968 A973 S978 A986 A987 M988 H989 S990 K991 I997 Q1000 S1001 K1002 S1003 K1004 I1005 H1006 P1007 G1008 F1009 R1015 T1016 D1017 D1020 V1021 E1022 C1023 R1029 A1030 A1031 T1032 D1037 D1038

A1045 K1046 D1047 L1065 G1066 T1073 A1074 N1075 R1078 K1086 I1087 Q1088 N1089 F1094 H1097 A1098 F1099 D1103 R1109 H1110 H1111 V1112 G1113 I1114 E1115 P1119 S1120 E1121 G1122 E1123 N1126 I1127 G1131 G1132 I1133 N1134 K1135 I1140 H1143 G1144 C1149 I1152 I1160 N1161

F1162 F1163 K1164 R1170 G1171 R1172 E1173 M1176 M1177 D1180 P1181 H1182 N1183 E1184 R1188 H1194 T1195 D1198 S1199 D1200 T1201 F1202 A1203 A1204 A1210 S1211 L1212 P1213 G1214 S1215 I1219 N1222 R1226 E1227 Q1228 L1229 C1230 F1242 D1247 I1248 L1249 K1250 T1251 N1252 K1257 E1261

Y1262 C1263 M1264 N1267 S1268 C1269 L1270 N1271 E1275 I1276 Q1277 Y1278 E1282 G1283 T1284 D1285 S1286 F1287 V1288 S1289 R1290 P1291 C1292 A1298 L1301 H1302 C1303 S1304 R1313 S1314 K1315 T1316 G1317 N1318 T1319 G1332 E1333 L1339 E1342 S1343 S1344 ILE

- Molecule 1: Major capsid protein

Chain B: 41% 98%

MET E2 E8 E14 N18 I19 F20 N21 D22 I23 K24 A28 L31 F32 D33 Y38 F39 G40 D41 D42 N47 I48 S49 F50 E51 A52 L53 L54 G55 K60 I61 E62 A74 A75 R79 F80 N81 R85 M86 G89 F94 L97 P98 R99 N104

D105 V106 T107 A108 E111 T112 K118 H119 S120 E121 K122 I125 S128 F129 D130 H138 L139 E140 N141 T142 F143 K144 N145 D149 N153 H158 R162 D169 R173 F179 L184 R185 E198 N199 K200 V201 H202 N203 K204 Q205 A206 R209 R212 S213

F216 L219 L227 N231 R232 N233 N234 R241 N244 T258 S263 K264 E265 N266 D270 N285 Y290 I291 S292 T293 S297 H304 F305 I306 M307 A315 I316 A317 Y318 D324 Q327 N331 A332 G333 T334 E335 T339 I345 K348 S349

R350 A351 D354 K361 L362 G363 D364 K365 D370 H371 L372 H373 Y376 K377 D380 D383 E386 Q390 F393 F394 L397 G398 E404 M410 M420 E421 N422 N423 F429 K433 D434 Q435 R439 F442 A443 D444 C450 I453 V454 H455 D456

R462 L463 M464 K465 N466 E467 P468 L469 P470 T471 G472 H473 R474 L478 C479 Q480 L481 K482 I483 T484 R485 R490 I491 L492 Q493 T494 N497 L498 Y499 R502 Q503 E504 K507 L512 K513 N514 E515 L516 N517 V518 E519 D520 K523 F527 T531 E532 R533 F536 F537

D538 L539 T540 Q543 K544 N545 R546 A547 T548 E549 V550 L551 C552 R555 I556 M557 I558 M561 L565 H571 E572 E580 K583 T584 N585 S586 H587 D590 F591 K594 E598 S599 L600 G603 S604 Y605 P606 E607 L608 A609 I612 E613 I614 L615 G618 N619 K620

M624 I625 L626 K627 Q628 S631 S635 Y636 W637 F638 N639 H642 I643 L644 L645 F646 C647 N648 E651 M652 I653 M654 L655 I656 S657 N658 H659 M660 G661 D662 E663 L664 G667 A668 A669 S678 I687 S688 I689 S690 N691 I692 N693 E694 C697 L701 V702 N703 F704

A707 L708 F709 D710 G711 R712 L713 F714 C715 P716 F717 V718 H719 T720 M721 P722 R723 N724 D725 T726 N727 A728 K729 I730 T731 A732 D733 D734 T735 P736 L737 T738 Q739 N740 T741 V742 R743 V744 R745 N746 Y747 E748 I749 S750 R754 M755 N756 L757 I758 D759 S760 F764 T765 D766 N767 D768 R769

N772 E773 N774 T775 I776 L777 S778 K779 I780 F781 Y782 F783 L786 P787 A788 N792 A797 G798 V799 N800 E803 L804 D807 L808 F809 Y810 T811 E812 P813 F814 I815 D818 D819 G820 F821 Q822 E823 N824 P825 I826 S827 S828 D829 V830 S833 L834 I835 R836 E837 A838 M839 G840 P841

G842 Y843 T844 V845 A846 N847 T848 S849 S850 I851 A852 K853 Q854 L855 F856 K857 S858 L859 E864 N865 I868 E872 Q879 R880 H881 G882 V885 H886 F887 Q888 H892 I893 L894 Y895 N896 G897 L898 C899 L900 I904 T905 R908 R909 Y910 Y911 F916 F920 S921 D922

G927 T928 M929 N930 Q934 V935 F936 T939 F940 Y943 Q944 R945 N946 D947 G948 G949 F950 P951 L952 P955 L956 A957 Y961 N962 W963 Q964 R965 F968 S969 A973 F974 N977 S978 M988 H989 S990 K991 L992 S993 A996 I999 Q1000 S1001 K1002 S1003 G1008 D1020

C1023 R1029 D1037 T1042 A1043 E1044 A1045 K1046 D1047 T1050 L1058 D1062 L1065 T1073 A1074 N1075 L1076 K1077 R1078 S1085 K1086 I1087 Q1088 N1089 H1097 A1098 F1099 D1103 R1109 H1110 H1111 V1112 G1113 I1114 E1115 K1116 P1117 N1118 P1119 S1120 E1121 G1122 E1123 A1124 L1125 N1126 I1127

I1128 T1129 F1130 G1131 G1132 I1133 N1134 K1135 I1140 H1143 G1144 Q1145 Q1146 A1147 I1148 C1149 P1155 I1160 N1161 F1162 R1170 G1171 R1172 E1173 S1174 C1175 M1176 M1177 G1178 T1179 D1180 P1181 H1182 N1183 E1184 E1185 A1186 A1187 R1188 L1191 Y1192 D1198 S1199 D1200 T1201 F1202 A1203 A1204 T1205 A1210 G1214

S1215 L1216 G1217 D1218 I1219 N1222 T1223 A1224 H1225 R1226 E1227 Q1228 L1229 K1234 A1240 Q1241 F1242 S1246 D1247 I1248 L1249 K1250 T1251 N1252 K1253 K1257 M1264 K1265 S1266 N1267 S1268 C1269 L1270 N1271 S1272 D1273 Q1277 Y1278 S1279 C1280 S1281 E1282 G1283 T1284 D1285 S1286 F1287 A1298 L1301 Q1307

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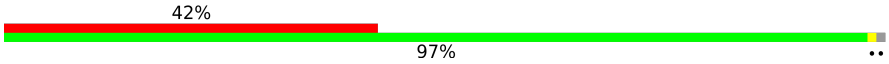
- Molecule 1: Major capsid protein

Chain C:



MET E2 E8 I9 L10 A15 N18 I19 P20 D33 N34 L35 R36 I37 G40 D41 R45 S49 F50 E51 A52 L53 L54 G55 N59 K60 I61 E62 W63 I64 A74 A75 R79 F80 R85 M86 T87 L88 L97 P98 R99 D105 E111 A117

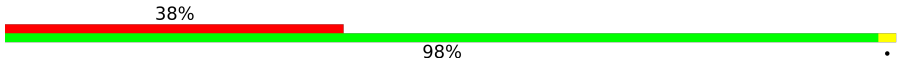
E121 K122 D130 L131 S132 H138 L139 E140 N141 T142 F143 K144 N145 D149 H158 R162 S167 R173 G174 A178 F179 M180 L184 R185 K186 M196 N197 E198 N199 K200 V201 H202 N203 K204 Q205 A206 R212 S213 L219 R222 L223 L227 N231 S237

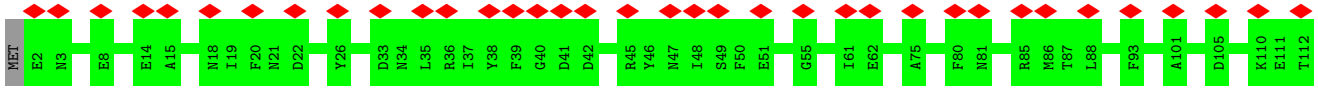
R241 N244 D245 E248 S253 I254 D257 T258 K264 E265 D270 G271 L274 L283 T284 N285 S292 S297 S301 K309 I316 A317 Y318 R319 A320 A323 D324 N331 A332 G333 T334 E335 D338 T339 K342 I345 R350 A351 Y352 A353

D354 L355 K356 K361 L362 G363 D364 K365 L366 V367 D370 H371 L372 H373 K377 D380 E386 Q387 S388 L389 Q390 F393 F394 G398 I399 E404 S408 T409 M410 E411 T412 R413 D418 T419 M420 E421 N422 N423 L424 F429 F430 H431 N432 K433 D434 Q435 F442 A443

- Molecule 1: Major capsid protein

Chain D:





T113 A117 K118 H119 S120 S128 F129 D130 L131 S132 A133 A134 E140 N141 T142 F143 D149 N153 H158 R162 S163 L164 R173 I192 E198 N199 K200 V201 H202 N203 K204 Q205 R212 F216 N221 L227 N231 R232 N233 N234 N244 E248 S249

E252 L255 N256 D257 T258 E265 N266 G271 N285 Y290 V296 S297 A298 Y302 M307 I316 A317 Y318 M322 Q327 N331 A332 G333 T334 E335 D338 T339 K342 S343 E344 I345 K348 S349 R350 A351 D354 T359 L360 G363 D364 K365

A368 F369 D370 H373 K374 K377 N378 T379 D380 F393 L397 E404 M410 E411 K415 D418 T419 M420 E421 M422 P425 F429 F430 H431 N432 K433 D434 Q435 R439 I440 D441 F442 A443 D444 I445 C450 D456 M464 K465 N466 T471 G472 H473 R474

Q477 L478 C479 Q480 L481 T484 R485 R490 Q493 T494 N497 L498 Y499 R502 Q503 E504 V505 P506 K507 N514 E515 V518 E519 D520 F521 D525 T531 E532 R533 F536 F537 D538 L539 T540 Q543 K544 N545 R546 A547 T548 E549 V550 L551 I558 G559 N560 M561

L565 E572 A573 R574 T575 N576 E580 H581 A582 K583 S586 H587 N588 Y589 D590 F591 E598 S599 L600 G603 S604 Y605 P606 E607 V611 I612 E613 I614 L615 V616 H617 G618 N619 A622 F623 M624 I625 L626 K627 H642 I643 L644 L645 N648 I653 M654 N658 H659

M660 G661 D662 E663 L664 H672 Y673 R681 R685 T686 I687 S688 I689 S690 N691 I692 N693 E694 Q695 L701 V702 N703 F704 A705 N706 A707 L708 F709 D710 G711 R712 L713 P716 F717 V718 H719 R723 N724 D725 T726 N727 A728 K729 T730 T731 A732 D733 D734 L737 T738 Q739 N740

R743 V744 R745 N746 Y747 D751 V752 Q753 R754 M755 N756 L757 I758 D759 V763 F764 T765 D766 N767 D768 R769 N772 E773 L777 S778 K779 I780 F781 Y782 A788 L789 K793 A794 C795 G796 A797 G798 V799 N800 E803 L804 V805 L806 D807 L808 F809 Y810 T811 F814 I815 C816 P817

D818 D819 C820 F821 Q822 E823 N824 P825 I826 S827 S828 D829 V830 L831 M832 S833 L834 M839 G840 V845 A846 N847 I851 A852 K853 Q854 L855 F856 K857 S858 L859 I860 Y861 I862 N863 E864 E870 V871 E872 A878 Q879 R880 H881 S884 V885 H886 F887 Q888 S889 L890 N896 G897 L898

C899 L900 I901 S902 P903 R908 R909 Y910 Y911 P915 F916 S921 D922 C926 G927 T928 M929 N938 T939 F940 Y943 Q944 R945 N946 D947 G948 G949 F950 P951 L952 P955 L956 A957 L958 E959 F960 Y961 N962 W963 Q964 R965 F968 F974 N977 S978 S981 I982 M983

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- Molecule 1: Major capsid protein

Chain E: 37% 98%

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R241 N244 D245 E248 D257 E265 G271 L274 N285 S288 Q289 Y290 T293 Q294 S297 A298 H304 I316 D324 N331 A332 G333 T334 E335 D338 T339 I345 F346 D347 K348 S349 R350 A351 Y352 A353 T359 K365 D370 Y376

K377 D380 E386 F393 I399 E404 T405 R413 D418 T426 F429 K433 D434 Q435 R439 F442 A443 D444 C450 H455 D456 S457 T458 I459 R462 L463 M464 K465 N466 E467 G472 H473 R474 Q477 L478 C479 Q480 L481 R485 R490 I491

L492 Q493 T494 L495 L498 Y499 R502 Q503 E504 K507 N514 E515 L516 N517 V518 E519 D520 D525 L529 P530 T531 E532 R533 F536 F537 D538 L539 T540 Q543 R546 E549 V550 L551 C552 R555 I556 H557 L565 A566 F567 I568 H571 E572 A573 R574 M578

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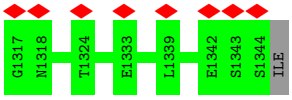
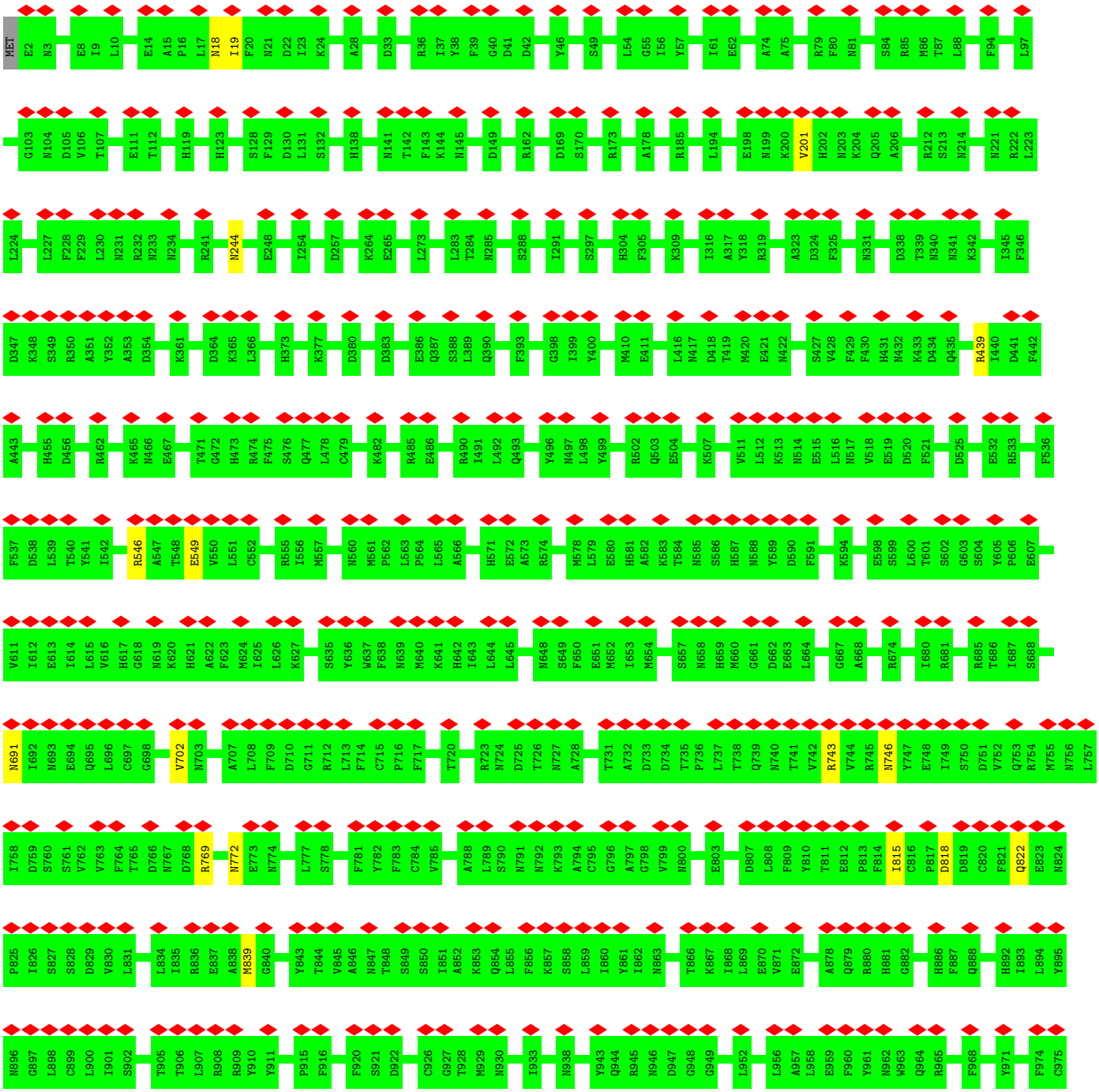
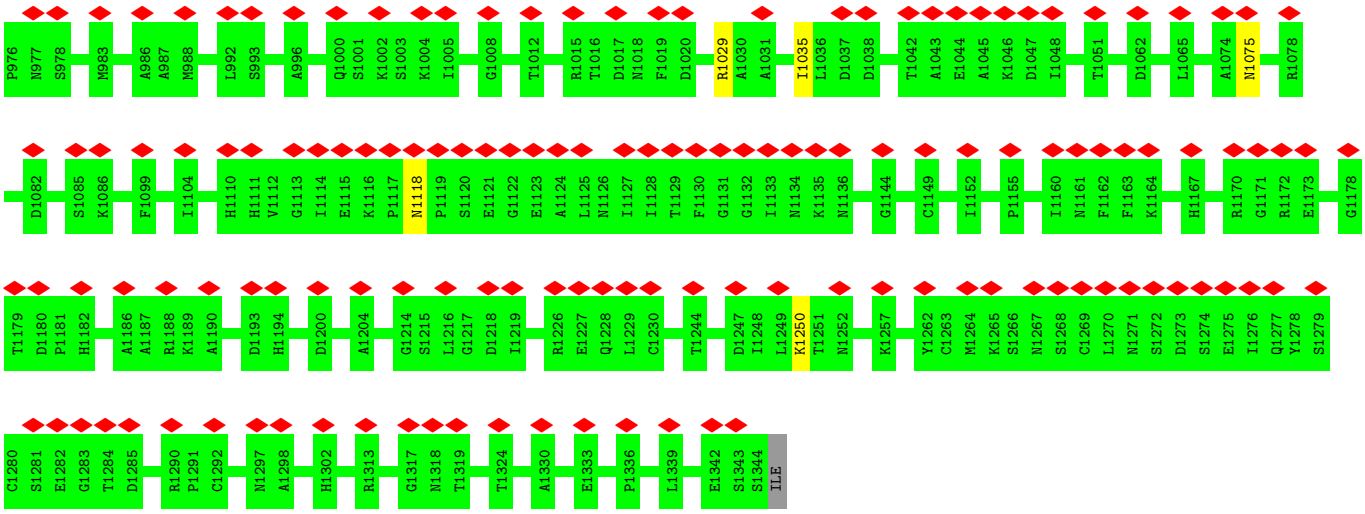


- Molecule 1: Major capsid protein

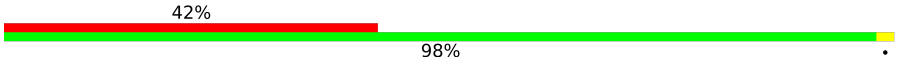
Chain F: 43% 98%

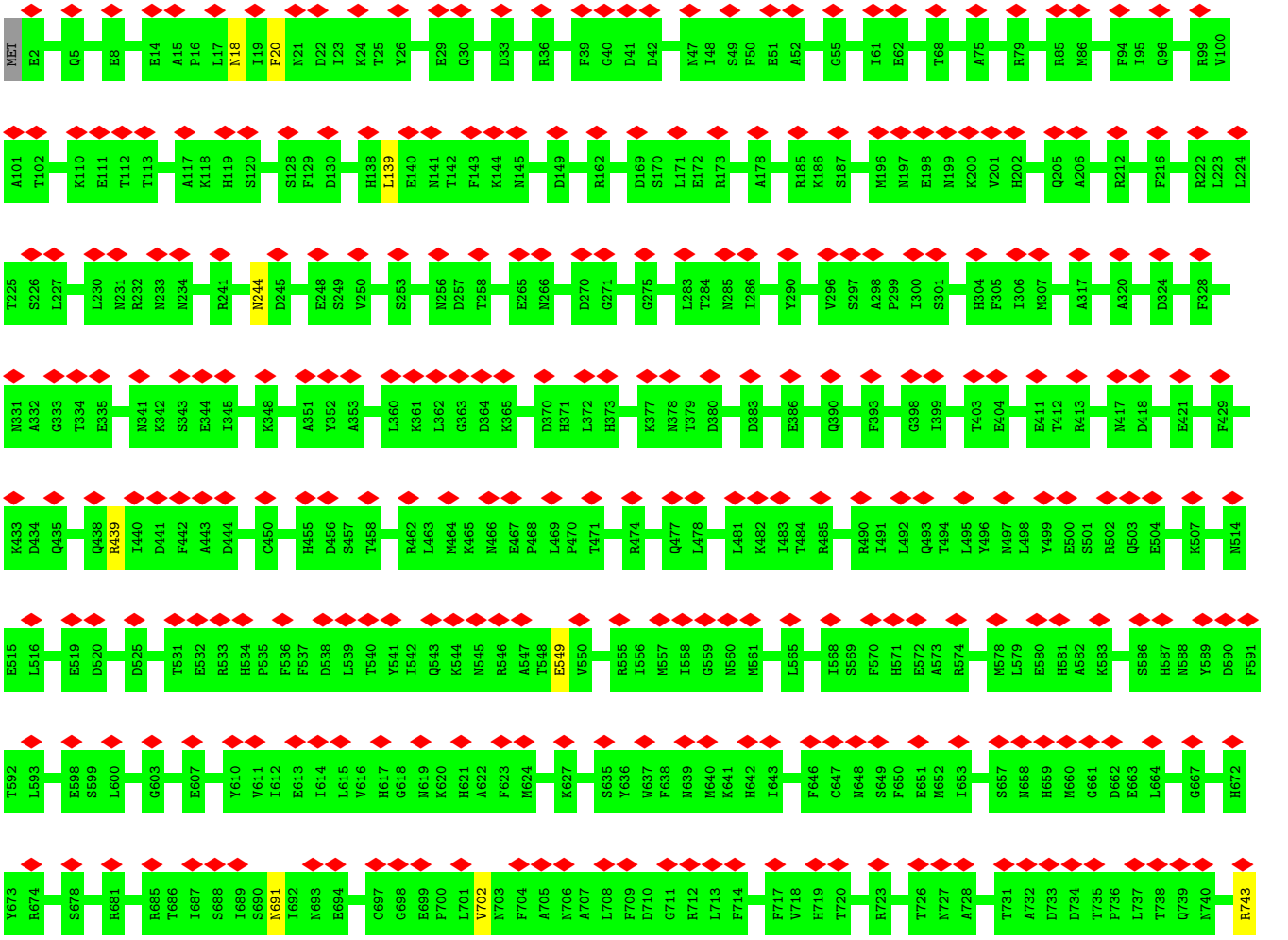




- Molecule 1: Major capsid protein

Chain G:





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F887 Q888 H892 I893 L894 Y895 N896 G897 L898 C899 L900 I901 S902 P903 I904 T905 T906 L907 R908 R909 Y910 Y911 I914 F920 S921 D922 P923 G924 G927 T928 M929 N938 Y943 Q944 D947 G948 G949 F950 P951 L956 A957 L958 E959 N962 W963 Q964 F968 F974 C975

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- Molecule 1: Major capsid protein

Chain H: 34% 98%

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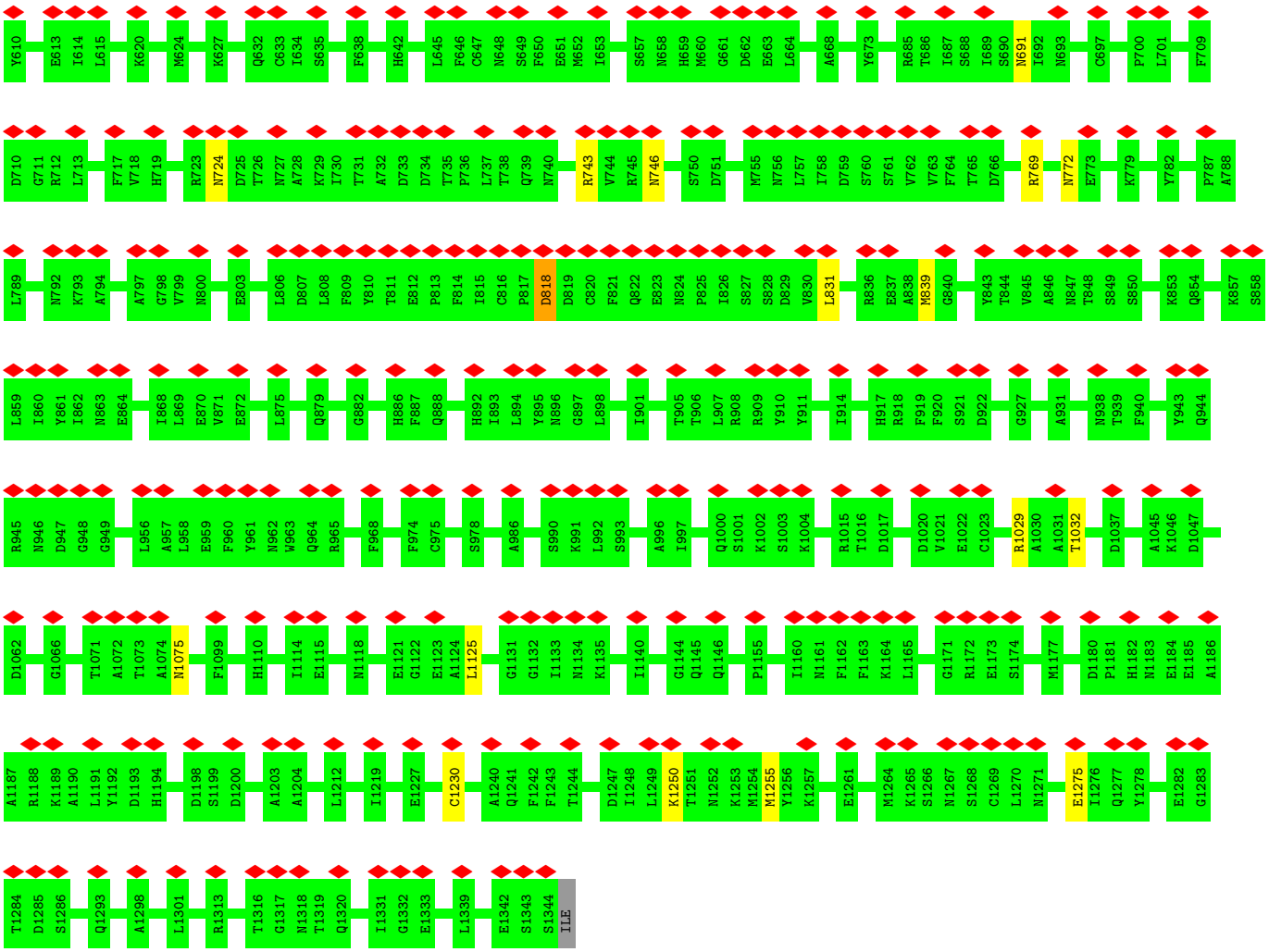
N126 I127 S128 F129 D130 L131 E140 N141 T142 F143 D149 R162 D169 S170 R173 M180 E198 N199 K200 V201 H202 N203 K204 Q205 A206 R209 R212 Q217 S218 L219 R222 L223 L224 L230 N231 N234 S237 R241 N244 D245 E248 E252

S253 T254 D257 E265 N266 D270 G271 G275 G278 N285 Y290 I291 Q294 V295 V296 S297 M307 A315 T316 R319 N331 A332 G333 T334 E335 D338 T339 K342 S343 E344 K348 A351 G363 D364 K365 D370 H371 L372 H373 N378 T379

D380 E386 Q390 F393 F394 F395 G398 I399 Y400 T403 E404 M410 E411 D418 E421 N422 N423 F429 K433 D434 Q435 R439 I440 D441 F442 C450 D456 R462 L463 M464 K465 L469 P470 T471 G472 H473 R474 L478 L481 K482 R485

R490 I491 L492 Q493 T494 R502 Q503 E504 L512 K513 N514 E515 L516 N517 V518 E519 D520 R533 F536 F537 D538 Q543 K544 N545 R546 A547 T548 E549 V550 L551 N560 M561 L565 E572 A573 R574 E580 K583 T584 N585 S586 H587 N588 Y589 T601 S602 E607



- Molecule 1: Major capsid protein

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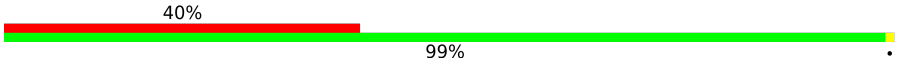

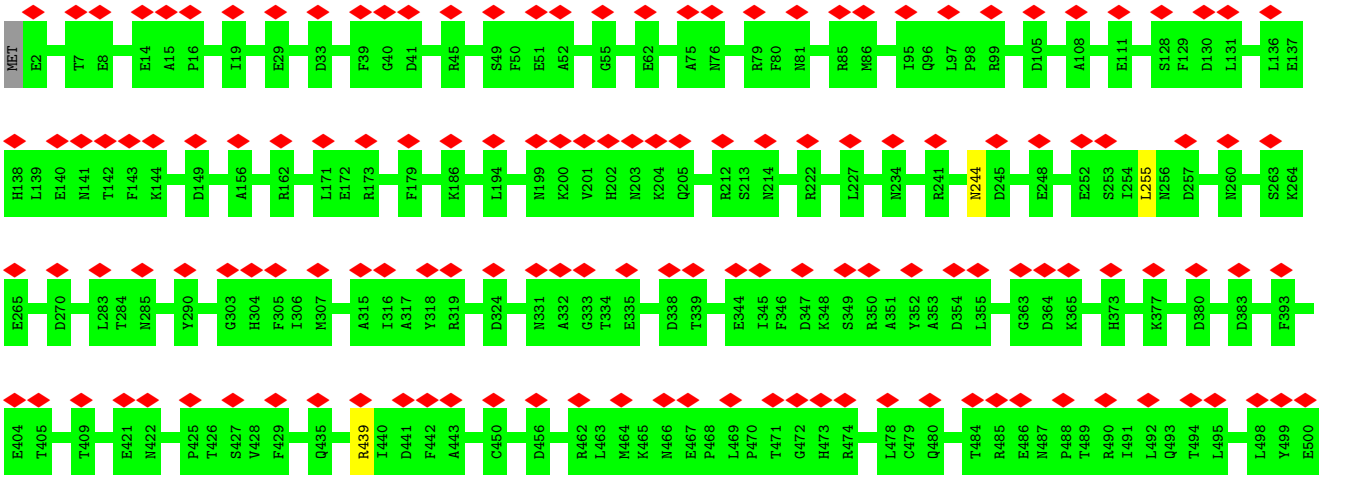

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N585 S586 H587 D590 F591 K594 E598 T601 S602 G603 S604 Y605 P606 E607 L608 A609 Y610 V611 I612 E613 I614 L615 V616 H617 G618 N619 A622 F623 M624 K627 S631 F638 N639 M640 K641 H642 I643 L644 L645 F646 C647 N648 S649 F650 E651 M652 I653 M654 S657 N658

G661 L664 G667 H672 S678 R681 R685 T686 I687 S688 I689 S690 N691 I692 N693 E694 Q695 L696 L701 V702 N703 A707 L708 F709 D710 G711 R712 L713 F717 V718 H719 T720 R723 N724 D725 T726 N727 A728 A732 D733 D734 T735 P736 L737 T738 Q739 N740 R743

V744 R745 N746 Y747 E748 I749 S750 D751 V752 Q753 R754 L757 I758 D759 V762 V763 F764 T765 D766 N767 D768 R769 P770 S771 N772 E773 Y782 F783 A788 L789 N792 K793 A794 C795 G796 A797 G798 V799 N800 E803 L804 V805 L806 D807 L808 F809 Y810 T811 E812 P813 F814 I815 C816 P817

D818 D819 C820 F821 Q822 E823 N824 P825 I826 S827 S828 D829 V830 L831 L834 I835 R836 E837 A838 G842 Y843 T844 V845 A846 N847 T848 S849 S850 K853 Q854 L855 F856 K857 S858 L859 I860 Y861 I862 N863 E864 N865 T866 A878 Q879 R880 H881 G882 N883 H886 F887 Q888 S889 L890 Q891 H892

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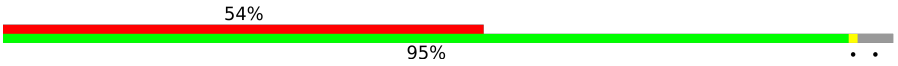
- Molecule 1: Major capsid protein

Chain q:



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R241
N244
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S253
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L274 G275
N285
S288
T293
V296 S297
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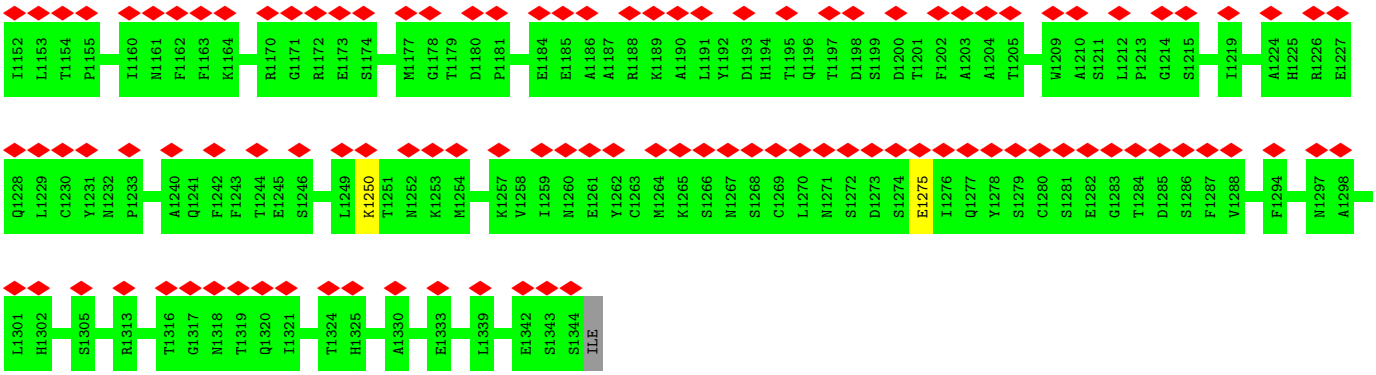

- Molecule 1: Major capsid protein

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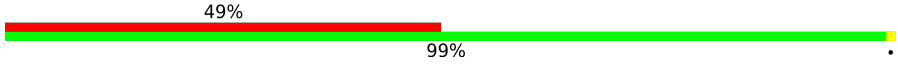

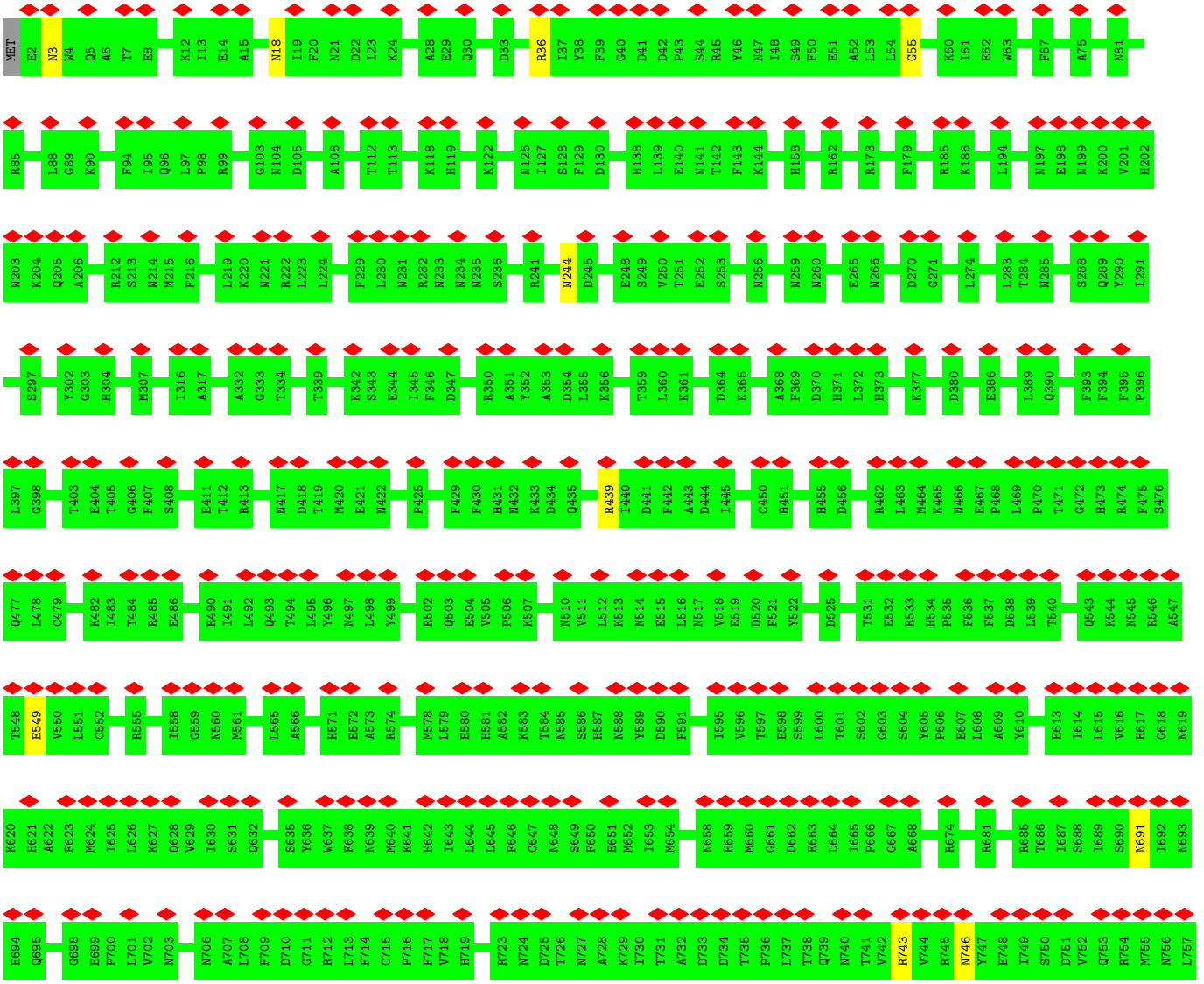

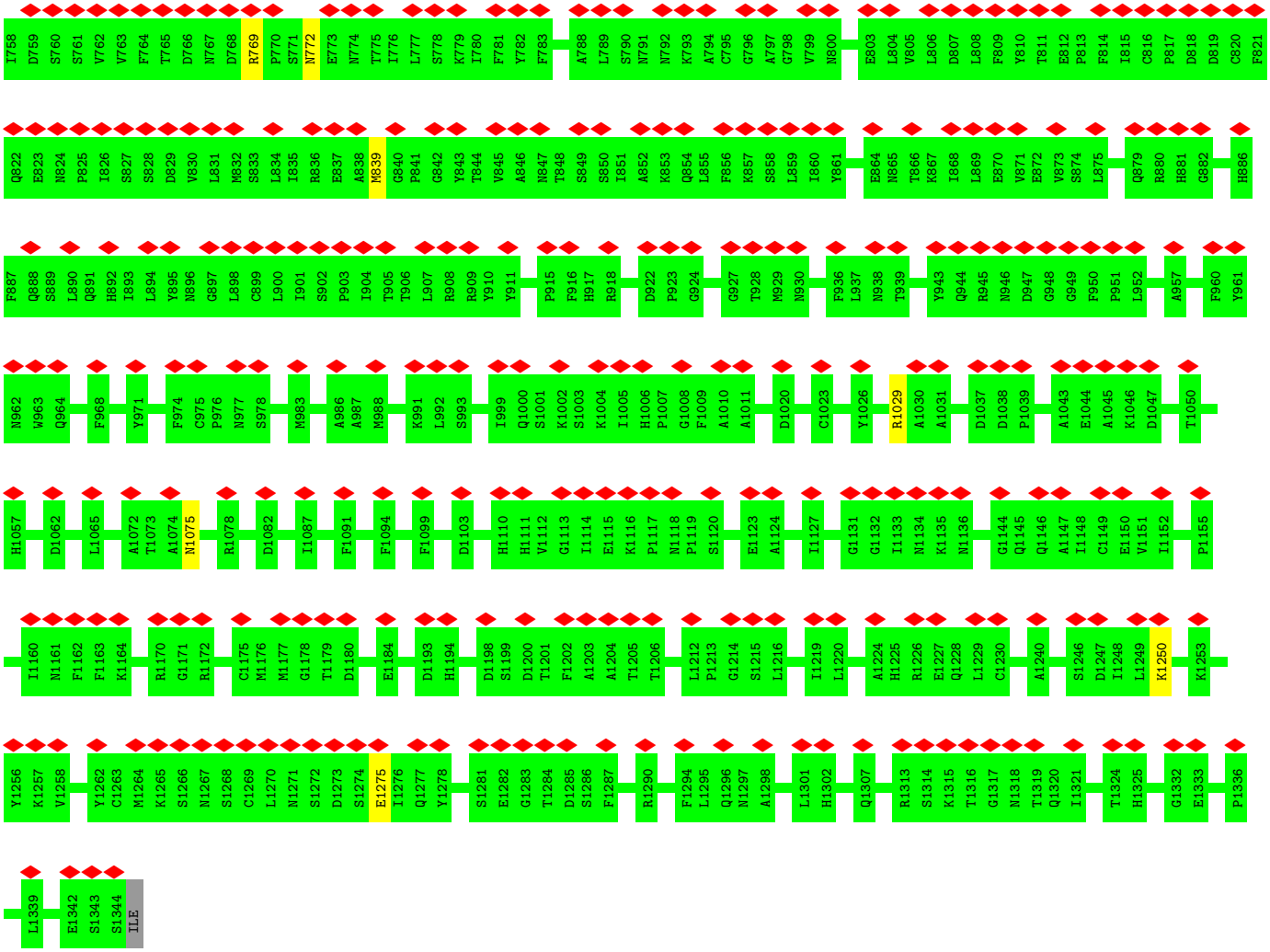

- Molecule 1: Major capsid protein

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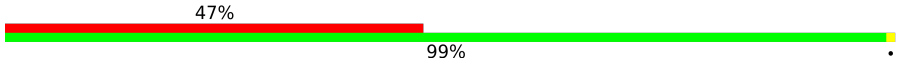

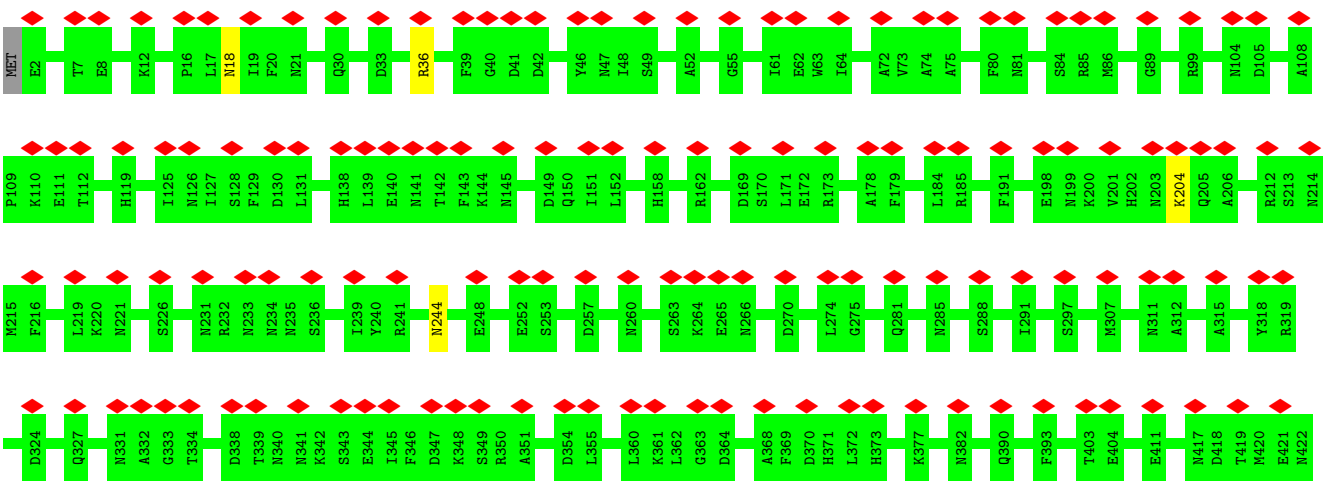

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- Molecule 1: Major capsid protein

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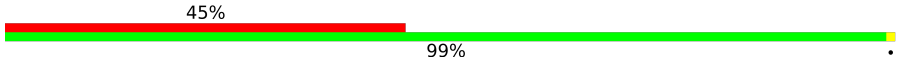

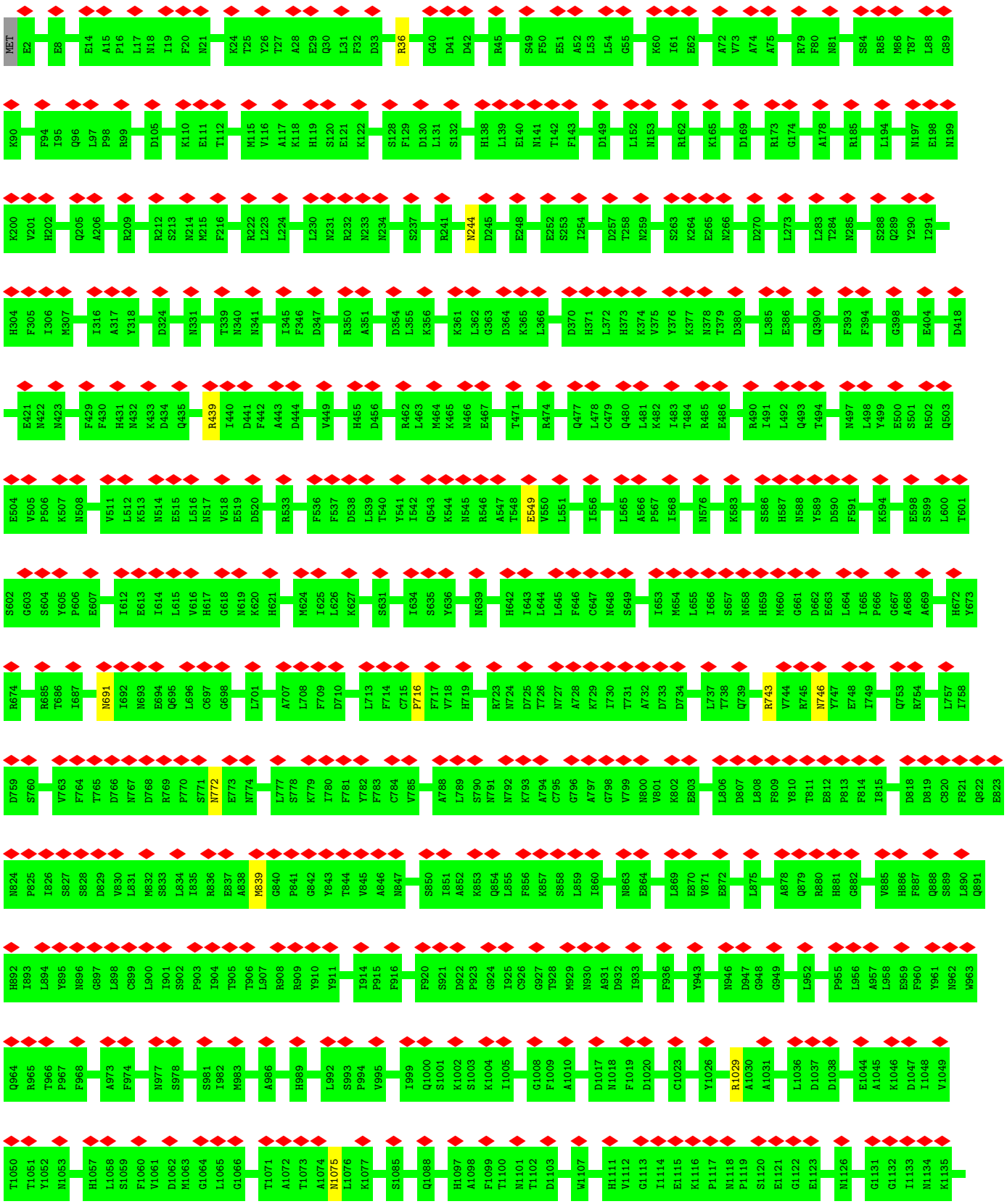
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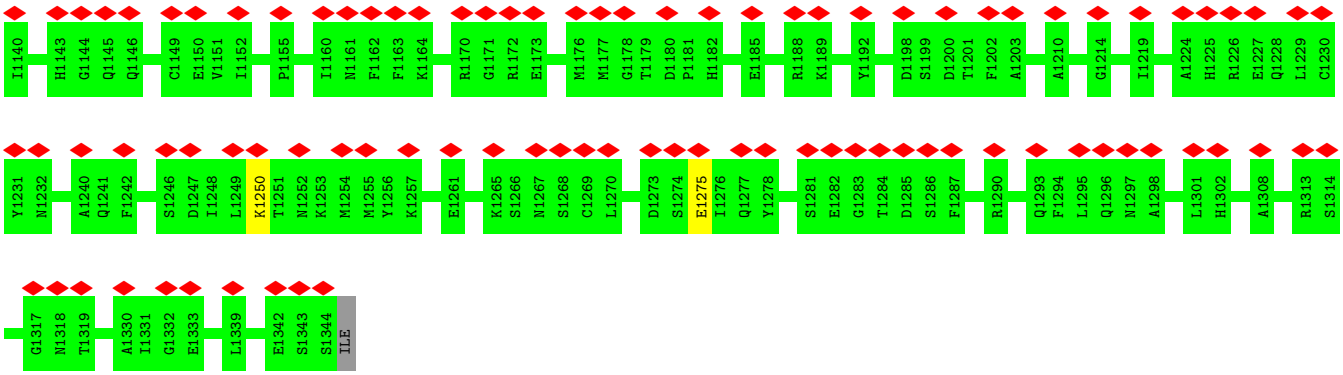

- Molecule 1: Major capsid protein

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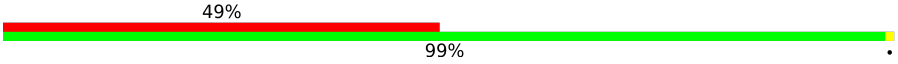

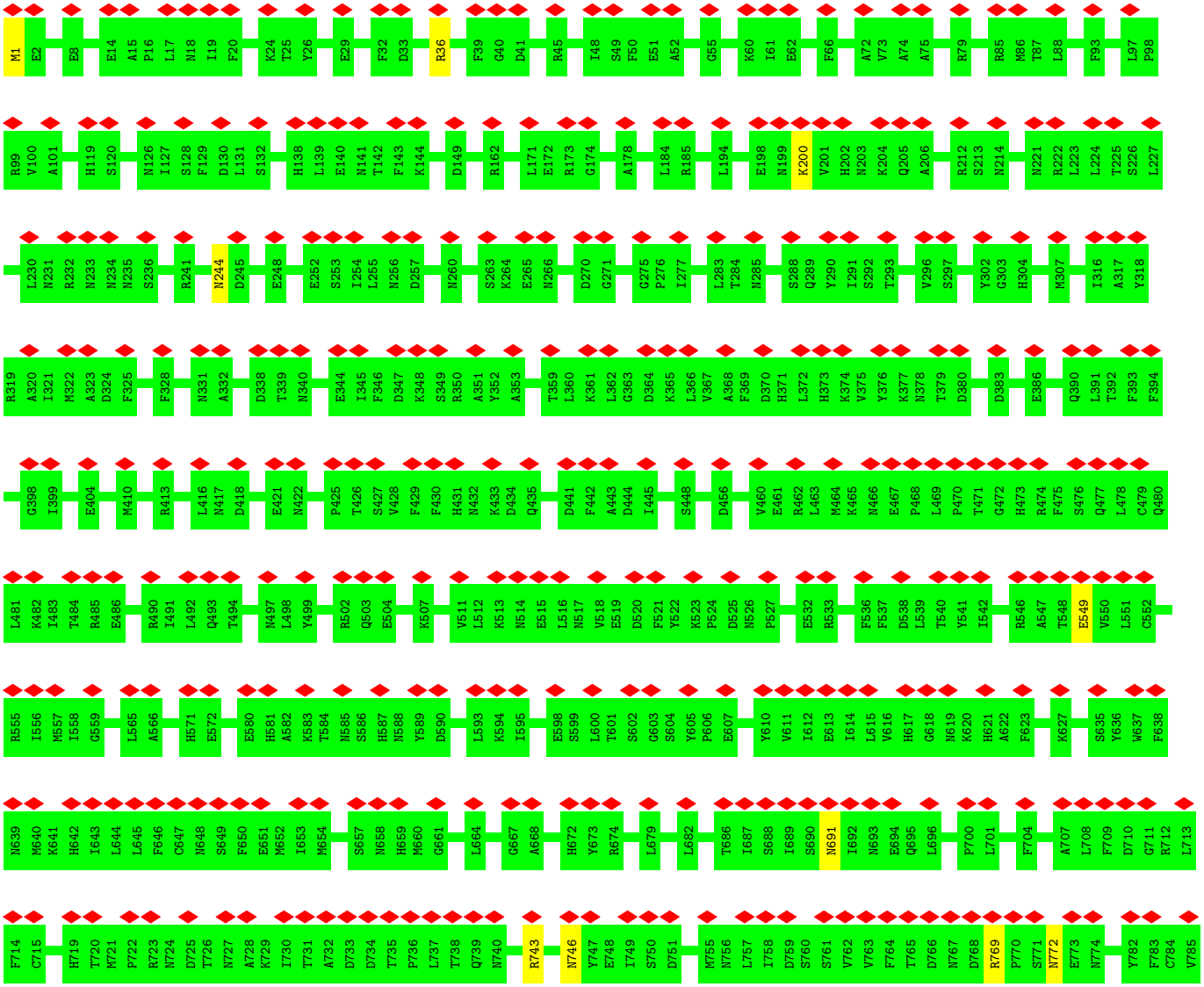

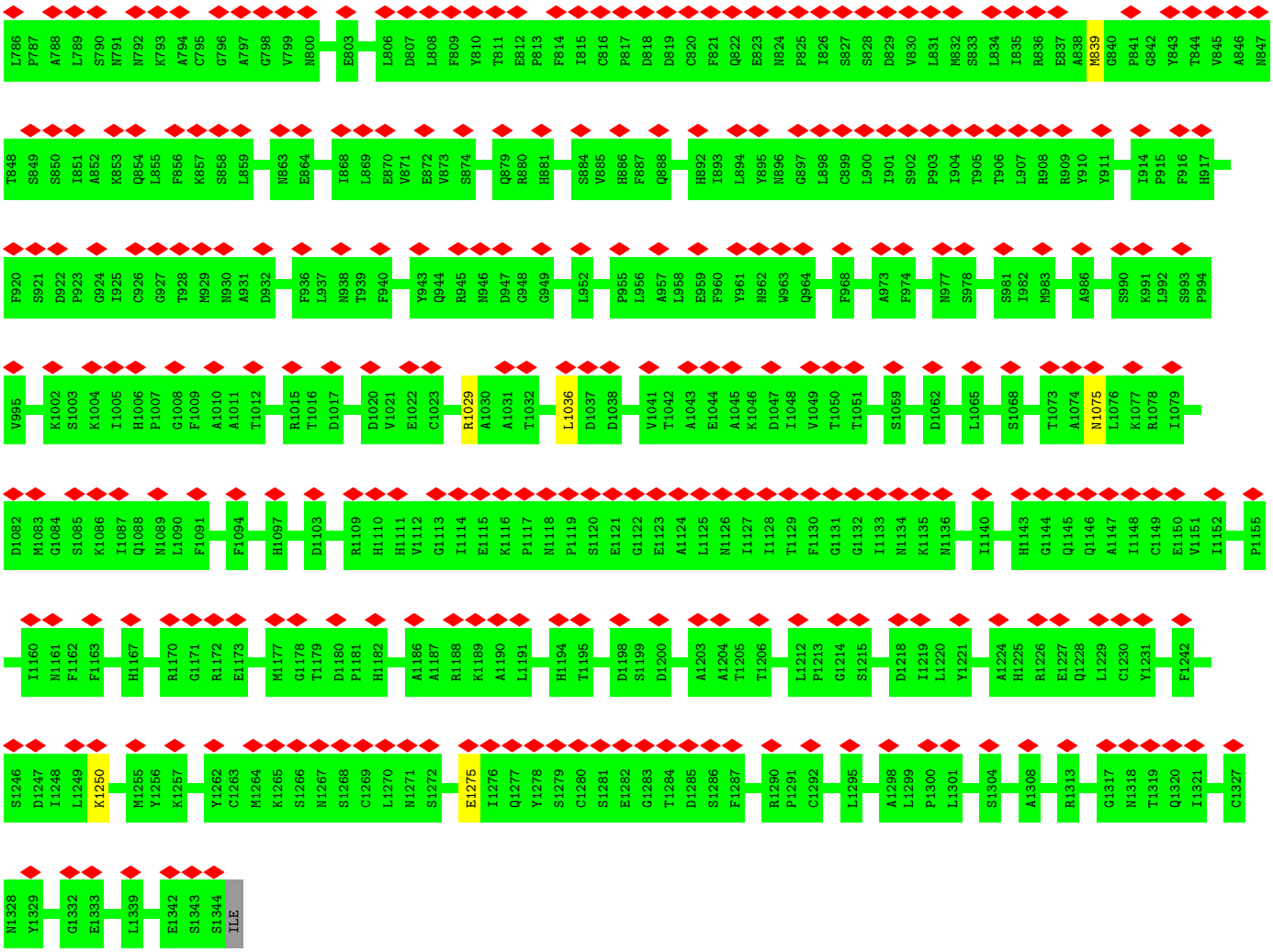

- Molecule 1: Major capsid protein

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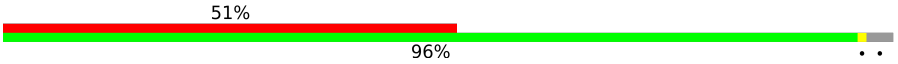

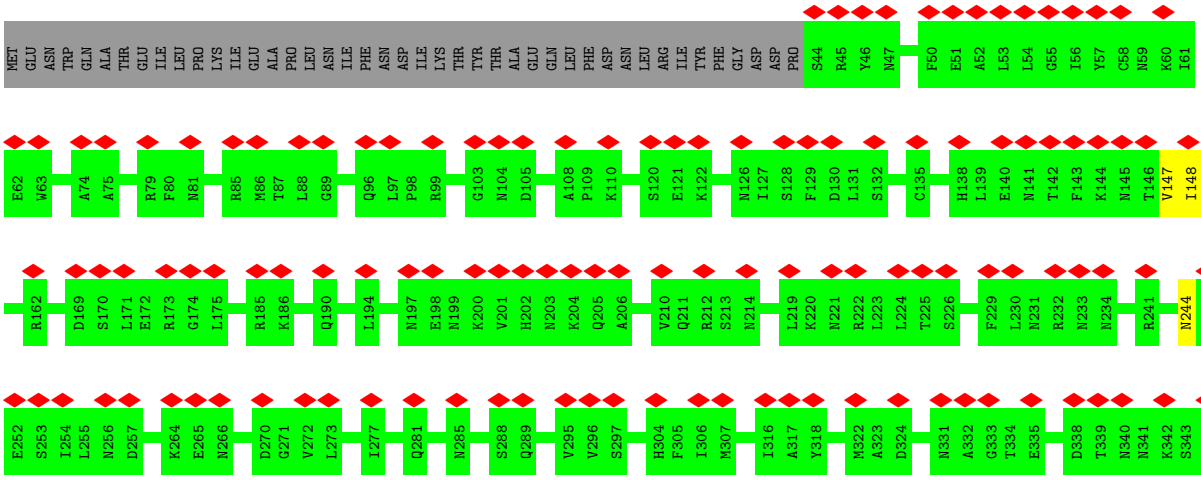

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ILE

- Molecule 1: Major capsid protein

Chain w: 77% 92% • 7%

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V596 T597 E598 S599 L600 T601 S602 G603 S604 Y605 P606 E607 L608 A609 Y610 V611 I612 E613 I614 L615 V616 H617 G618 N619 K620 H621 A622 F623 M624 I625 L626 K627 Q628 V629 I630 S631 Q632 C633 I634 S635 Y636 W637 F638 N639 M640 K641 H642 I643 L644 L645 F646 C647 N648 S649 F650 E651 M652 I653 M654 L655

I656 S657 N658 H659 M660 G661 D662 E663 L664 I665 P666 G667 A668 A669 F670 A671 H672 Y673 R674 N675 L676 V677 S678 L679 I680 R681 L682 V683 K684 R685 T686 I687 S688 I689 S690 N691 I692 N693 E694 Q695 L696 C697 G698 E699 P700 L701 V702 N703 F704 A705 N706 A707 L708 F709 D710 G711 R712 L713 F714 C715

P716 F717 V718 H719 T720 M721 P722 R723 N724 D725 T726 N727 A728 K729 I730 T731 A732 D733 D734 T735 P736 L737 T738 Q739 N740 T741 V742 R743 V744 R745 N746 Y747 E748 I749 S750 D751 V752 Q753 R754 M755 N756 L757 I758 D759 S760 S761 V762 V763 F764 T765 D766 N767 D768 R769 P770 S771 N772 E773 N774 T775

I776 L777 S778 K779 I780 F781 Y782 F783 C784 V785 L786 P787 A788 L789 S790 N791 N792 K793 A794 C795 G796 A797 G798 V799 N800 V801 K802 E803 L804 V805 L806 D807 L808 F809 Y810 T811 E812 P813 F814 I815 C816 P817 D818 D819 C820 F821 Q822 E823 N824 P825 I826 S827 S828 D829 V830 L831 M832 S833 L834 I835

R836 E837 A838 M839 G840 P841 G842 Y843 T844 V845 A846 N847 T848 S849 S850 I851 A852 K853 Q854 L855 F856 K857 S858 L859 I860 Y861 I862 N863 E864 N865 T866 K867 I868 L869 E870 V871 E872 V873 S874 L875 D876 P877 A878 Q879 R880 H881 G882 N883 S884 V885 H886 F887 Q888 S889 L890 Q891 H892 I893 L894 Y895

N896 G897 L898 C899 L900 I901 S902 P903 I904 T905 T906 L907 R908 R909 Y910 Y911 Q912 P913 I914 P915 F916 H917 R918 F919 F920 S921 D922 P923 G924 I925 C926 G927 T928 N929 N930 A931 D932 I933 Q934 V935 F936 L937 N938 T939 F940 P941 H942 Y943 Q944 R945 N946 D947 G948 G949 F950 P951 L952 P953 P954 P955

L956 A957 L958 E959 F960 Y961 N962 W963 Q964 R965 T966 P967 F968 S969 V970 Y971 S972 A973 F974 C975 P976 N977 S978 L979 L980 S981 T984 L985 A986 A987 M988 H989 S990 K991 L992 V995 A996 I997 A998 I999 Q1000 S1001 K1002 S1003 K1004 I1005 H1006 P1007 G1008 F1009 A1010 A1011 T1012 L1013 V1014 R1015 T1016 D1017

N1018 F1019 D1020 V1021 E1022 C1023 Y1026 R1029 A1030 A1031 T1032 S1033 L1036 D1037 D1038 P1039 T1040 V1041 T1042 A1043 E1044 A1045 K1046 D1047 I1048 V1049 T1050 T1051 Y1052 T1055 Q1056 H1057 L1058 S1059 F1060 V1061 D1062 M1063 G1064 L1065 G1066 F1067 T1073 A1074 N1075 L1076 K1077 R1078 I1079 K1080 S1081 D1082 M1083 G1084 S1085

K1086 I1087 Q1088 N1089 L1090 F1091 S1092 A1093 F1094 P1095 I1096 H1097 A1098 F1099 T1100 N1101 T1102 D1103 I1104 N1105 T1106 R1109 H1110 H1111 V1112 G1113 I1114 GLU LYS PRO ASN PRO SER GLU GLY GLY GLU ALA LEU ASN ILE ILE ILE THR PHE GLY GLY ILE ASN LYS ASN PRO PRO SER ILE LEU LEU HIS G1144 Q1145 Q1146

A1147 I1148 C1149 I1152 L1153 T1154 P1155 V1156 T1157 T1158 N1159 I1160 N1161 F1162 F1163 K1164 L1165 R1170 G1171 R1172 E1173 S1174 C1175 M1176 M1177 G1178 T1179 D1180 P1181 H1182 N1183 E1184 E1185 A1186 A1187 R1188 K1189 A1190 L1191 Y1192 D1193 H1194 T1195 Q1196 T1197 D1198 S1199 D1200 T1201 F1202 A1203 A1204 T1205 T1206 N1207 P1208 W1209 A1210

S1211 L1212 P1213 G1214 S1215 L1216 G1217 D1218 I1219 L1220 Y1221 N1222 T1223 A1224 H1225 R1226 E1227 Q1228 L1229 C1230 K1234 T1235 Y1236 S1237 P1238 N1239 A1240 Q1241 F1242 F1243 T1244 E1245 S1246 D1247 K1250 T1251 N1252 K1253 Y1256 K1257 N1260 E1261 Y1262 C1263 M1264 K1265 S1266 N1267 S1268 C1269 L1270 N1271 S1272 D1273 S1274 E1275

I1276 Q1277 Y1278 S1279 C1280 S1281 E1282 G1283 T1284 D1285 S1286 F1287 V1288 S1289 R1290 P1291 C1292 Q1293 F1294 L1295 Q1296 N1297 A1298 L1299 P1300 L1301 H1302 C1303 S1304 S1305 N1306 Q1307 A1308 E1311 S1312 R1313 S1314 K1315 T1316 G1317 N1318 T1319 Q1320 I1321 S1322 E1323 T1324 H1325 Y1326 C1327 N1328 Y1329 A1330 I1331 G1332 E1333 T1334 I1335 P1336

L1337 Q1338 L1339 I1340 I1341 E1342 S1343 S1344 ILE

- Molecule 2: Large structural phosphoprotein

Chain e: 27% 31% 69%

MET ASP LEU LYS ALA GLN S7 I8 P9 F10 A11 W12 L13 D14 R15 D16 K17 V18 Q19 R20 L21 T22 N23 F24 L25 S26 N27 L28 E29 N30 L31 E32 N33 V34 D35 L36 R37 E38 H39 P40 Y41 V42 T43 N44 S45 C46 V47 Y48 R49 E50 G51 E52 D53 V54 D55 E56 L57 K58 T59 L60

Y61 N62 T63 F64 I65 L66 W67 L68 M69 Y70 H71 Y72 V73 L74 S75 K76 R77 K78 P79 D80 Y81 N82 A83 I84 W85 Q86 D87 K90 L91 Q92 N93 V94 V95 N96 E97 Y98 L99 K100 S101 K102 G103 L104 N105 K106 G107 N108 F109 E110 N111 M112 F113 T114 N115 K116 E117 K118 F119 E120 S121

Q122 F123 S124 D125 I126 H127 R128 A129 L130 L131 R132 L133 S136 I137 R138 W139 V143 P144 I145 D146 T147 P148 Y149 V150 N151 A154 E155 D156 S157 S158 E161 N162 N163 L164 Q165 D166 A167 E168 K169 N170 M171 L172 W173 Y174 T175 V176 Y177 N178 I179 N180 D181 P182 W183 D184 E185 N186

G187 Y188 S192 I193 N194 K195 L196 V197 Y198 L199 L202 F203 N207 Q208 S209 W210 S211 K212 L213 E214 K215 V216 A217 M218 S219 Q220 I221 V222 T223 T224 Q225 N226 H227 L228 S229 G230 H231 L232 R233 K234 N235 E236 N237 F238 N239 A240 V241 Y242 S243 Q244 R245 V246 L247 Q248 T249 P250 L251

T252 G253 Q254 R255 V256 E257 S258 F259 L260 K261 T262 I263 T264 S265 D266 Y267 E268 T269 I270 K271 S272 S273 L274 E275 SER TYR SER ALA SER LYS ALA PHE SER VAL PRO GLU ASN GLY PRO HIS SER LEU MET ASP PHE ALA SER LEU ASP GLY ARG MET PRO SER ASP LEU SER LEU PRO SER

ILE SER ILE ASP THR LYS ARG PRO SER ALA ASP LEU ALA ARG LEU LYS ILE SER GLN PRO LYS SER LEU ASP ALA PRO LEU LYS THR GLN ARG ARG HIS LYS PHE PRO GLU SER ASP SER VAL ASP ASN ALA GLY GLY LYS ILE LEU ILE LYS LYS GLU THR LEU GLY GLY VAL

ARG ALA THR THR PRO VAL SER SER VAL SER LEU MET SER GLY VAL GLU PRO LEU SER SER SER LEU THR SER THR ASN LEU ASP LEU ARG ASP LYS SER HIS GLY ASN TYR ARG ILE GLY PRO SER GLY ILE LEU ASP PHE GLY VAL LYS LEU PRO ALA GLU ALA GLN SER ASN THR GLY ASP

VAL ASP LEU LEU GLN ASP LYS THR SER ILE ARG SER PRO SER SER GLY ILE THR ASP VAL VAL ASN GLY LEU ALA ASN LEU ASN LEU ARG GLN ASN LYS SER ASP VAL SER ARG PRO TRP SER LYS ASN THR ALA ALA ASN ALA ASP VAL PHE ASP PRO VAL HIS ARG LEU VAL SER GLU

GLN THR GLY THR PRO PHE VAL LEU ASN ASN SER ASP VAL ALA GLY SER GLU ALA LYS LEU THR THR HIS SER THR GLU THR GLY VAL SER PRO HIS ASN VAL SER LEU LEU ILE LYS ASP LEU ARG ASP LYS ASP PHE ARG LYS GLN LYS LYS LEU ASP LEU LEU GLY SER TRP THR LYS

GLU LYS ASN ASP LYS ALA ILE VAL HIS SER ARG GLU VAL THR GLY ASP SER GLY ASP ALA THR GLU THR VAL THR ALA ARG ASP SER PRO VAL LEU ARG LYS THR LYS HIS ALA ASN ASP ILE PHE ALA GLY LEU ASN LYS LYS TYR ALA ARG ASP VAL SER ARG GLY GLY GLY LYS ASN

SER ARG ASP LEU TYR SER GLY GLY ASN ALA GLU LYS LYS GLU THR SER GLY LYS PHE ASN VAL ASP LYS GLU MET THR GLN ASN GLU GLN GLU PRO LEU PRO ASN LEU MET GLU ALA ALA ARG ASN ALA GLY GLU GLU GLN TYR VAL GLN ALA GLY LEU GLY GLN ARG VAL ASN LYS ILE

LEU ALA GLU PHE THR ASN LEU ILE SER LEU GLY GLU LYS GLY ILE GLN ASP ILE LEU HIS ASN GLN SER GLY THR GLU LEU LYS LEU PRO THR GLU ASN LYS LEU GLY ARG GLU SER GLU GLU ALA ASN VAL GLU ARG ILE LEU GLU VAL SER ASP PRO GLN ASN LEU PHE LYS ASN PHE

LYS LEU GLN ASN ASP LEU ASP SER VAL GLN SER PRO PHE ARG LEU PRO ASN ALA ASP LEU ASP SER VAL SER PHE LYS ASP ALA LEU ASP VAL LYS LEU PRO GLY ASN GLY GLU ARG GLU ILE ASP LEU ALA LEU GLU GLN LYS VAL LYS ALA GLY GLU ARG GLU THR SER

ASP PHE LYS VAL GLY GLN ASP GLU THR LEU ILE PRO THR GLN LEU MET LYS VAL GLU THR PRO GLU GLU LYS ASP ASP VAL ILE GLU LYS MET VAL LEU ARG ILE ARG GLN ASP GLY GLU THR ASP GLU GLU THR VAL PRO GLY PRO GLY VAL ALA GLU SER LEU GLY ILE ALA ALA LYS

ASP LYS SER VAL ILE ALA SER

- Molecule 2: Large structural phosphoprotein

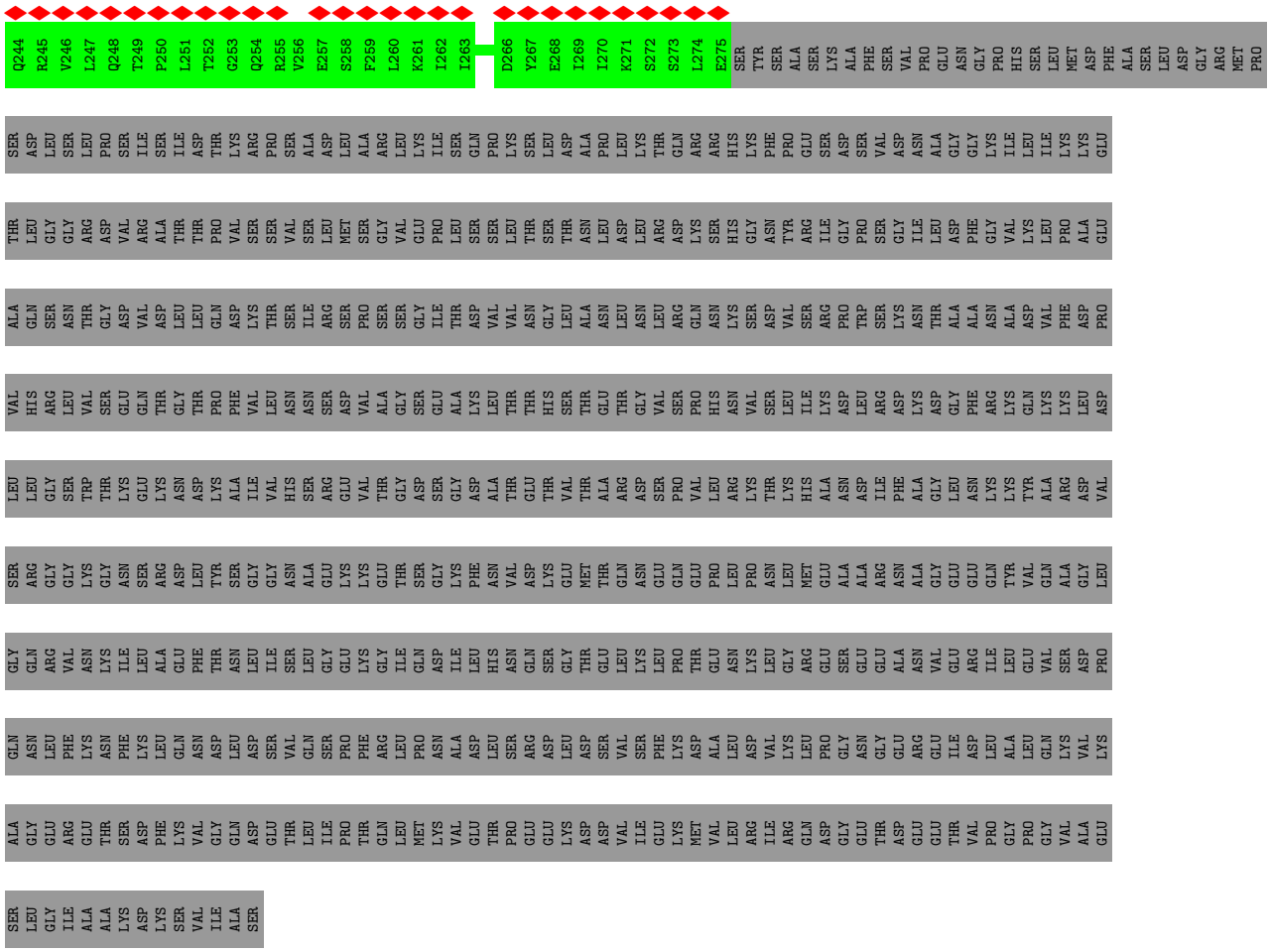
Chain f: 28% 31% 69%

MET ASP LEU LYS ALA GLN S7 I8 P9 F10 A11 W12 L13 D14 R15 D16 Q19 R20 L21 T22 N23 F24 L25 S26 N27 L28 E29 N30 L31 E32 N33 V34 D35 L36 R37 E38 H39 P40 Y41 V42 T43 N44 S45 C46 V47 V48 R49 E50 G51 E52 D53 V54 D55 E56 L57 L60 Y61 N62

T63 F64 I65 L66 W67 L68 M69 Y70 H71 Y72 S75 K76 R77 K78 P79 D80 Y81 N82 A83 I84 W85 Q86 D87 I88 T89 K90 L91 Q92 N93 V94 V95 N96 E97 Y98 L99 K100 S101 K102 G103 L104 N105 K106 G107 N108 F109 E110 N111 M112 F113 T114 N115 K116 E117 K118 F119 E120 S121 Q122 F123

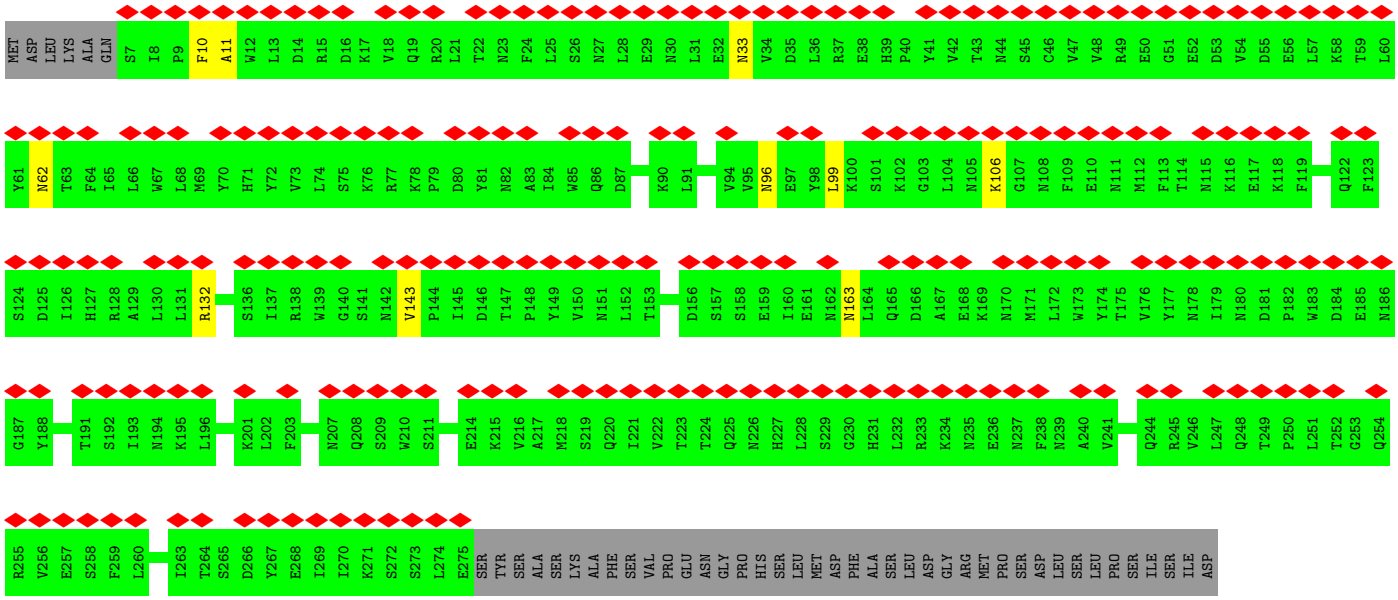
S124 D125 I126 H127 R128 A129 L130 L131 R132 L133 G134 N135 S136 I137 R138 W139 G140 S141 N142 V143 P144 I145 D146 T147 P148 Y149 V150 N151 L152 T153 A154 E155 D156 S157 S158 E159 I160 E161 N162 N163 L164 Q165 D166 A167 E168 K169 N170 M171 L172 W173 Y174 T175 V176 Y177 N178 I179 N180 D181 P182 W183

D184 E185 N186 G187 Y188 L189 V190 T191 S192 I193 N194 K195 L196 V197 Y198 L199 G200 K201 L202 F203 V204 T205 L206 N207 Q208 S209 W210 S211 K212 L213 E214 K215 V216 A217 M218 S219 Q220 I221 V222 T223 T224 Q225 N226 H227 L228 S229 G230 H231 L232 R233 K234 N235 E236 N237 F238 N239 A240 V241 Y242 S243



- Molecule 2: Large structural phosphoprotein

Chain g:



THR LYS ARG PRO SER ALA ASP LEU LEU ALA ARG LEU LYS ILE SER GLN PRO LYS SER LEU ASP ALA PRO LEU LYS THR GLN ARG ARG HIS LYS PHE PRO GLU SER ASP SER VAL ASP ASN ALA GLY GLY LYS ILE LEU ILE LYS LYS GLU THR LEU GLY GLY ARG ASP VAL ARG ALA THR THR

PRO VAL SER SER VAL SER LEU MET SER GLY VAL GLU PRO LEU SER SER LEU THR SER THR ASN LEU ASP LEU ARG ASP LYS SER HIS GLY ASN TYR ARG ILE SER GLY ILE LEU ASP PHE GLY VAL LYS LEU PRO ALA GLU ALA GLN SER ASN THR GLY ASP VAL LEU LEU

GLN ASP LYS THR SER ILE ARG SER PRO SER SER GLY ILE THR ASP VAL VAL ASN GLY LEU ALA ASN LEU ASN LEU ARG GLN ASN LYS SER ASP VAL SER ARG PRO TRP SER LYS ASN THR ALA ALA ASN ALA ASP VAL PHE ASP PRO VAL HIS ARG LEU VAL SER GLU GLN THR GLY THR

PRO PHE VAL LEU ASN ASN SER ASP VAL ALA GLY SER GLU ALA LYS LEU THR THR HIS SER THR GLU THR GLY VAL SER PRO HIS ASN VAL SER LEU ILE LYS ASP LEU ARG ASP LYS ASP GLY PHE ARG LYS GLN LYS LYS LEU ASP LEU LEU GLY SER SER TRP THR LYS GLU LYS ASN ASP

LYS ALA ILE VAL HIS SER ARG GLU VAL THR GLY ASP SER GLY ASP ALA THR GLU THR ALA ARG ASP SER PRO VAL LEU ARG LYS THR LYS HIS ALA ASN ASP ILE PHE ALA GLY LEU ASN LYS LYS TYR ALA ARG ASP VAL SER ARG GLY GLY GLY VAL LYS GLY ASN SER ARG ASP LEU

TYR SER GLY GLY ASN ALA GLU LYS LYS GLU THR GLU GLU MET THR GLN ASN GLU GLN GLU PRO LEU PRO ASN LEU MET GLU ALA ALA ARG ASN ALA GLY GLU GLU GLN TYR TYR VAL GLN ALA GLY LEU GLY GLN ARG VAL ASN LYS ILE LEU ALA GLU PHE

THR ASN LEU ILE SER LEU GLY GLU LYS GLY ILE GLN ASP ILE LEU HIS ASN GLN SER GLY THR GLU LEU LYS LEU PRO THR GLU ASN LYS LEU GLY ARG GLU SER GLU GLU ALA ASN VAL GLU ARG ILE LEU GLU VAL SER ASP PRO GLN ASN LEU PHE LYS ASN PHE LYS LEU GLN ASN

ASP LEU ASP SER VAL GLN SER PRO PHE ARG LEU PRO ASN ALA ASP LEU SER ARG ASP LEU ASP SER VAL SER PHE LYS ASP ALA LEU ASP VAL LYS LEU PRO GLY ASN GLY GLU ARG GLU ILE ASP LEU ALA LEU GLN LYS VAL LYS ALA GLY GLU ARG GLU THR SER ASP PHE LYS VAL

GLY GLN ASP GLU THR LEU ILE PRO THR GLN LEU MET LYS VAL GLU THR PRO GLU GLU LYS ASP ASP VAL ILE GLU LYS MET VAL LEU ARG ILE ARG GLN ASP GLY GLU THR ASP GLU GLU THR VAL PRO GLY PRO GLY VAL ALA GLU SER LEU GLY ILE ALA ALA LYS ASP LYS SER VAL

ILE ALA SER

- Molecule 2: Large structural phosphoprotein

Chain h: 29% 31% 69%

MET ASP LEU LYS ALA GLN S7 I8 P9 F10 A11 W12 L13 D14 R15 D16 K17 V18 Q19 R20 L21 T22 N23 F24 L25 S26 N27 L28 E29 N30 L31 E32 N33 V34 D35 L36 R37 E38 H39 P40 Y41 V42 T43 N44 S45 C46 V47 V48 R49 E50 G51 E52 D53 V54 D55 E56 L57 K58 T59 L60

Y61 N62 T63 F64 I65 L66 W67 L68 M69 Y70 H71 Y72 V73 L74 S75 K76 R77 K78 P79 D80 Y81 N82 A83 I84 W85 Q86 D87 I88 T89 K90 L91 Q92 N93 V94 V95 N96 E97 Y98 L99 K100 S101 K102 G103 L104 N105 K106 G107 N108 F109 E110 N111 M112 F113 T114 N115 K116 E117 K118 F119 E120

S121 Q122 F123 S124 D125 I126 H127 R128 A129 L130 L131 R132 L133 G134 N135 S136 I137 R138 W139 G140 S141 N142 V143 P144 I145 D146 T147 P148 Y149 V150 N151 L152 T153 A154 E155 D156 S157 S158 E159 I160 E161 N162 N163 L164 Q165 D166 A167 E168 K169 N170 M171 L172 W173 Y174 T175 V176 Y177 N178 I179 N180

W183 D184 E185 N186 G187 Y188 S192 I193 N194 K195 L196 V197 Y198 L199 G200 K201 L202 F203 V204 T205 L206 N207 Q208 S209 W210 S211 K212 L213 E214 K215 V216 A217 M218 S219 Q220 I221 V222 T223 T224 Q225 N226 H227 L228 S229 G230 H231 L232 R233 K234 N235 E236 N237 F238 N239 A240 V241 Y242 S243

Q244 R245 V246 L247 Q248 T249 P250 L251 T252 G253 Q254 R255 V256 E257 S258 F259 L260 K261 I262 I263 I264 S265 D266 Y267 E268 I269 I270 K271 S272 S273 L274 E275 SER TYR SER ALA SER LYS ALA PHE SER VAL PRO GLU ASN GLY PRO HIS SER LEU MET ASP PHE ALA SER LEU ASP GLY ARG MET

PRO SER ASP LEU SER LEU PRO SER ILE SER ILE ASP THR LYS ARG PRO SER ALA ASP LEU ALA ARG LEU LYS ILE SER GLN PRO LYS SER LEU ASP ALA PRO LEU LYS THR GLN ARG ARG HIS LYS PHE PRO GLU SER ASP SER VAL ASP ASN ALA ALA GLY GLY LYS ILE LEU ILE LYS LYS

GLU THR LEU GLY ARG ASP VAL ARG ALA THR THR PRO VAL SER SER VAL SER LEU MET SER GLY VAL GLU PRO LEU SER SER LEU THR SER THR ASN LEU ASP LEU ARG ASP LYS SER HIS GLY ASN TYR ARG ILE GLY PRO SER GLY ILE LEU ASP PHE GLY VAL LYS LEU PRO ALA

GLU ALA GLN SER ASN THR GLY ASP VAL ASP LEU LEU GLN ASP LYS THR SER ILE ARG SER PRO SER SER GLY ILE THR ASP VAL THR ASN GLY LEU ALA ASN LEU ASN LEU ARG GLN ASN LYS SER ASP VAL SER ARG PRO TRP SER LYS ASN THR ALA ALA ASN ALA ASP VAL PHE ASP

PRO VAL HIS ARG LEU VAL SER GLU GLN THR GLY THR PRO PHE VAL LEU ASN ASN SER ASP VAL ALA GLY SER GLU ALA LYS LEU THR THR HIS SER THR GLU THR GLY VAL SER PRO HIS ASN VAL SER LEU ILE LYS ASP LEU ARG LYS ASP GLY PHE ARG LYS GLN LYS LEU

ASP LEU LEU GLY SER TRP THR LYS GLU LYS ASN ASP LYS ALA ILE VAL HIS SER ARG GLU VAL THR GLY ASP SER GLY ASP ALA THR GLU THR VAL THR ALA ARG ASP SER PRO VAL LEU ARG LYS THR LYS HIS ALA ASN ASP ILE PHE ALA GLY LEU ASN LYS LYS TYR ALA ARG ASP

VAL SER ARG GLY GLY LYS GLY ASN SER ARG ASP LEU TYR SER GLY GLY ASN ALA GLU LYS LYS GLU THR SER GLY LYS PHE ASN VAL ASP LYS GLU MET THR GLN ASN GLU GLN GLU PRO LEU PRO ASN LEU MET GLU ALA ALA ARG ASN ALA GLY GLU GLU GLN TYR VAL GLN ALA GLY

LEU GLY GLN ARG VAL ASN LYS ILE LEU ALA GLU PHE THR ASN LEU ILE SER LEU GLY LYS LYS GLY ILE GLN ASP LYS GLU GLN ASN LYS LEU GLU GLU ASN GLN SER GLY THR GLU LEU LYS LEU PRO THR GLU ASN LYS LEU GLY ARG GLU SER GLU GLU ALA ASN VAL GLU ARG ILE LEU GLU VAL SER ASP

PRO GLN ASN LEU PHE LYS ASN PHE LYS LEU GLN ASN ASP LEU ASP SER VAL GLN SER PRO PHE ARG LEU PRO ASN ALA ASP LEU SER ARG ASP LEU ASP SER VAL SER PHE LYS ASP ALA LEU ASP VAL LYS LEU PRO GLY ASN GLY GLU ARG GLU ILE ASP LEU ALA LEU GLN LYS VAL

LYS ALA GLY GLU ARG GLU THR SER ASP PHE LYS VAL GLY GLN ASP GLU THR LEU ILE PRO THR GLN LEU MET LYS VAL GLU THR PRO GLU GLU LYS ASP ASP VAL ILE GLU LYS MET VAL LEU ARG ILE ARG GLN ASP GLY GLU THR ASP GLU GLU THR VAL PRO GLY PRO GLY VAL VAL ALA

GLU SER LEU GLY ILE ALA ALA LYS ASP LYS SER VAL ILE ALA SER

- Molecule 2: Large structural phosphoprotein

Chain i:

MET ASP LEU LYS ALA GLN S7 I8 P9 F10 A11 W12 L13 D14 R15 D16 K17 V18 Q19 R20 L21 T22 N23 F24 L25 S26 N27 L28 E29 N30 L31 E32 N33 V34 D35 L36 R37 E38 H39 P40 Y41 V42 T43 N44 S45 C46 V47 V48 R49 E50 G51 E52 D53 V54 D55 E56 L57 K58 T59 L60

Y61 N62 T63 F64 I65 L66 W67 L68 M69 Y70 H71 Y72 V73 L74 S75 K76 R77 K78 P79 D80 Y81 N82 A83 I84 W85 Q86 D87 I88 T89 Q92 N93 V94 V95 N96 E97 Y98 L99 K102 G103 L104 N105 K106 G107 N108 F109 E110 N111 M112 F113 T114 N115 K116 E117 K118 F119 E120 S121 Q122

F123 S124 D125 I126 H127 R128 A129 L130 L131 R132 L133 S136 I137 R138 W139 N142 V143 P144 I145 D146 T147 P148 Y149 V150 A154 E155 D156 S157 S158 E161 N162 N163 L164 Q165 D166 A167 E168 K169 N170 M171 L172 W173 Y174 T175 V176 Y177 N178 I179 N180 D181 P182 W183 D184 E185 N186 G187

Y188 T191 S192 I193 N194 K195 L196 V197 Y198 L199 G200 K201 L202 F203 L206 N207 Q208 S209 W210 S211 K212 L213 E214 K215 V216 A217 M218 S219 Q220 I221 V222 Q225 N226 H227 L228 S229 G230 H231 L232 R233 K234 N235 E236 N237 F238 N239 A240 V241 Y242 S243 Q244 R245 V246 L247 Q248 T249 P250

L251 T252 G253 Q254 R255 V256 E257 S258 F259 L260 K261 I262 I263 T264 S265 D266 Y267 E268 I269 I270 K271 S272 S273 L274 E275 SER TYR SER ALA SER LYS ALA PHE SER VAL PRO GLU ASN GLY PRO HIS SER LEU MET ASP PHE ALA SER LEU ASP GLY ARG MET PRO SER ASP LEU SER LEU PRO

SER ILE SER ILE ASP THR LYS ARG PRO SER ALA ASP LEU ALA ARG LEU LYS ILE SER GLN PRO LYS SER LEU ASP ALA PRO LEU LYS THR GLN ARG ARG HIS LYS PHE PRO GLU SER ASP SER VAL ASP ASN ALA GLY GLY LYS ILE LEU ILE LYS GLU THR LEU GLY GLY ARG ASP

VAL ARG ALA THR THR PRO VAL SER SER VAL SER LEU MET SER GLY VAL GLU PRO LEU SER LEU THR SER THR ASN LEU ASP LEU ARG ASP LYS SER HIS GLY ASN TYR ARG ILE GLY PRO SER GLY ILE LEU ASP PHE GLY VAL LYS LEU PRO ALA GLU ALA GLN SER ASN THR GLY

ASP VAL ASP LEU LEU GLN ASP LYS THR SER ILE ARG SER PRO SER SER GLY ILE THR ASP VAL VAL ASN GLY LEU ALA ASN LEU ASN LEU ARG GLN ASN LYS SER ASP VAL SER ARG PRO TRP SER LYS ASN THR ALA ALA ASN ALA ASP VAL PHE ASP PRO VAL HIS ARG LEU VAL SER

GLU GLN THR GLY THR PRO PHE VAL LEU ASN ASN SER ASP VAL ALA GLY SER GLU ALA LYS LEU THR THR HIS SER THR GLU THR GLY VAL SER PRO HIS ASN VAL SER LEU ILE LYS ASP LEU ARG ASP LYS ASP GLY PHE ARG LYS GLN LYS LYS LEU ASP LEU LEU GLY SER TRP THR

LYS GLU LYS ASN ASP LYS ALA ILE VAL HIS SER ARG GLU VAL THR GLY ASP SER GLY ASP ALA THR GLU THR VAL THR ALA ARG ASP SER PRO VAL LEU ARG LYS THR LYS HIS ALA ASN ASP ILE PHE ALA GLY LEU ASN LYS LYS TYR ALA ARG ASP VAL SER ARG GLY GLY LYS GLY

ASN SER ARG ASP LEU TYR SER GLY GLY ASN ALA GLU LYS LYS GLU THR SER GLY LYS PHE ASN VAL ASP LYS GLU MET THR GLN ASN GLU GLN GLU PRO LEU PRO ASN LEU MET GLU ALA ALA ARG ASN ALA GLY GLU GLU GLN TYR VAL GLN ALA GLY LEU GLY GLN ARG VAL ASN LYS

ILE LEU ALA GLU PHE THR ASN LEU ILE SER LEU GLY GLU LYS GLY ILE GLN ASP ILE LEU HIS ASN GLU SER GLY THR GLU LEU LYS LEU PRO THR GLU ASN LYS LEU GLY ARG GLU SER GLU GLU ALA ASN VAL GLU ARG ILE LEU GLU VAL SER ASP PRO GLN ASN LEU PHE LYS ASN

PHE LYS LEU GLN ASN ASP LEU ASP SER VAL GLN SER PRO PHE ARG LEU PRO ASN ALA ASP LEU SER ARG ASP LEU ASP SER VAL SER PHE LYS ASP ALA LEU ASP VAL LYS LEU PRO GLY ASN GLY GLU ARG GLU ILE ASP LEU ALA LEU GLN LYS VAL LYS ALA GLY GLU ARG GLU THR

SER ASP PHE LYS VAL GLY GLN ASP GLU THR LEU ILE PRO THR GLN LEU MET LYS VAL GLU THR PRO GLU GLU GLU LYS ASP ASP VAL ILE GLU LYS MET VAL LEU ARG ILE ARG GLN ASP GLY GLU THR ASP GLU GLU THR VAL PRO GLY PRO GLY VAL ALA GLU SER LEU GLY ILE ALA ALA

LYS ASP LYS SER VAL ILE ALA SER

- Molecule 2: Large structural phosphoprotein

Chain j: 29% 30% 69%

MET ASP LEU LYS ALA GLN S7 I8 P9 F10 A11 W12 L13 D14 R15 D16 K17 V18 Q19 R20 L21 T22 N23 F24 L25 S26 N27 L28 E29 N30 L31 E32 N33 V34 D35 L36 R37 E38 H39 P40 Y41 V42 T43 N44 S45 C46 V47 V48 R49 E50 G51 E52 D53 V54 D55 E56 L57 K58 T59 L60

Y61 N62 T63 F64 I65 L66 W67 L68 M69 Y70 H71 Y72 V73 L74 S75 K76 R77 K78 P79 D80 Y81 N82 A83 I84 W85 Q86 D87 I88 Q92 N93 V94 V95 N96 E97 Y98 L99 K100 S101 K102 G103 L104 N105 K106 G107 N108 F109 E110 N111 M112 F113 T114 N115 K116 E117 K118 F119 E120 S121 Q122

F123 S124 D125 I126 H127 R128 A129 L130 L131 R132 L133 G134 N135 S136 I137 R138 W139 G140 S141 N142 V143 P144 I145 D146 T147 P148 Y149 V150 N151 L152 T153 A154 E155 D156 S157 S158 E159 I160 E161 N162 N163 L164 Q165 D166 A167 E168 K169 N170 M171 L172 W173 Y174 T175 V176 Y177 N178 I179 N180 D181 P182

W183 D184 E185 N186 G187 Y188 L189 V190 T191 S192 I193 N194 K195 L196 V197 Y198 L199 G200 K201 L202 F203 V204 T205 L206 N207 Q208 S209 W210 S211 K212 L213 E214 K215 V216 A217 M218 S219 Q220 I221 V222 T223 T224 Q225 N226 H227 L228 S229 G230 H231 L232 R233 K234 N235 E236 N237 F238 N239 A240 V241 Y242

S243 Q244 R245 V246 L247 Q248 T249 P250 L251 T252 G253 Q254 R255 V256 E257 S258 F259 L260 K261 I262 I263 T264 S265 D266 Y267 E268 I269 I270 K271 S272 S273 L274 E275 SER TYR SER ALA SER LYS ALA PHE SER VAL PRO GLU ASN GLY PRO HIS SER LEU MET ASP PHE ALA SER LEU ASP GLY ARG

MET PRO SER ASP LEU SER L247 LEU PRO SER ILE SER ILE ASP THR LYS ARG PRO SER ALA ASP LEU ALA ARG LEU LYS ILE SER GLN PRO LYS SER LEU ASP ALA PRO LEU LYS THR GLN ARG ARG HIS LYS PHE PRO GLU SER ASP SER VAL ASP ASN ALA GLY GLY LYS ILE LEU ILE LYS

LYS GLU THR LEU GLY GLY ARG ASP VAL ARG ALA THR THR PRO VAL SER SER VAL SER LEU MET SER GLY VAL GLU PRO LEU SER SER LEU THR SER THR ASN LEU ASP LEU ARG ASP LYS SER HIS GLY ASN TYR ARG ILE GLY PRO SER GLY ILE LEU ASP PHE GLY VAL LYS LEU PRO

ALA GLU ALA GLN SER ASN THR GLY ASP VAL ASP LEU LEU GLN ASP LYS THR SER ILE ARG SER PRO SER SER GLY ILE THR ASP VAL VAL ASN GLY LEU ALA ASN LEU ASN LEU ARG GLN ASN LYS SER ASP VAL SER ARG PRO TRP SER LYS ASN THR ALA ALA ASN ALA ASP VAL PHE

ASP PRO VAL HIS ARG LEU VAL SER GLU GLN THR GLY THR PRO PHE VAL LEU ASN ASN SER ASP VAL ALA GLY SER GLU ALA LYS LEU THR THR HIS SER THR GLU THR GLY VAL SER PRO HIS ASN VAL SER LEU ILE LYS ASP LEU ARG ASP LYS ASP GLY PHE ARG LYS GLN LYS LYS

LEU ASP LEU LEU GLY SER TRP THR LYS GLU LYS ASN ASP LYS ALA ILE VAL HIS SER ARG GLU VAL THR GLY ASP SER GLY ASP ALA THR GLU THR VAL THR ALA ARG ASP SER PRO VAL LEU ARG LYS THR LYS HIS ALA ASN ASP ILE PHE ALA GLY LEU ASN LYS LYS TYR ALA ARG

ASP VAL SER ARG GLY GLY LYS LYS GLY ASN SER ARG ASP LEU TYR SER GLY GLY ASN ALA GLU LYS LYS GLU THR SER GLY LYS PHE ASN VAL ASP LYS GLU MET THR GLN ASN GLU GLN GLU PRO LEU PRO ASN LEU MET GLU ALA ALA ARG ASN ALA GLY GLU GLU GLN TYR VAL GLN ALA

GLY LEU GLY GLN ARG VAL ASN LYS ILE LEU LEU ALA GLU PHE THR ASN LEU ILE SER LEU GLY GLU LYS LYS GLU ILE GLN ASP ILE LEU HIS ASN GLN SER GLY THR GLU LEU LYS LEU GLY ARG GLU SER GLU GLU ALA ASN VAL GLU ARG ILE LEU GLU VAL SER

ASP PRO GLN ASN LEU PHE LYS ASN PHE LYS LEU GLN ASN ASP LEU ASP SER VAL GLN SER PRO PHE ARG LEU PRO ASN ALA ASP LEU SER ARG ASP LEU ASP SER VAL SER PHE LYS ASP ALA LEU ASP VAL LYS LEU PRO GLY ASN GLY GLU ARG GLU ILE ASP LEU ALA LEU GLN LYS

VAL LYS ALA GLY GLU ARG GLU THR SER ASP PHE LYS VAL GLY GLN ASP GLU THR LEU ILE PRO THR GLN LEU MET LYS VAL GLU THR PRO GLU GLU LYS ASP ASP VAL ILE GLU LYS MET VAL LEU ARG ILE ARG GLN ASP GLY GLU THR ASP GLU GLU THR VAL PRO GLY PRO GLY VAL

ALA GLU SER LEU GLY ILE ALA ALA LYS ASP LYS SER VAL ILE ALA SER

- Molecule 2: Large structural phosphoprotein

Chain k: 25% 30% • 69%

MET ASP LEU LYS ALA GLN S7 I8 P9 F10 A11 W12 L13 D14 R15 D16 K17 V18 Q19 R20 N23 F24 L25 S26 N27 L28 E29 N30 L31 E32 N33 V34 D35 L36 R37 E38 H39 P40 Y41 V42 T43 N44 S45 C46 V47 V48 R49 E50 G51 E52 D53 V54 D55 E56 L57 K58 T59 L60 Y61

N62 T63 F64 I65 L66 W67 L68 M69 Y70 H71 Y72 V73 L74 S75 K76 R77 A83 I84 W85 Q86 D87 I88 T89 K90 L91 Q92 N93 V94 V95 N96 E97 Y98 L99 K100 S101 K102 G103 L104 N105 K106 G107 N108 F109 E110 N111 M112 F113 T114 N115 K116 E117 K118 F119 E120 S121 Q122 F123 S124 D125

I126 H127 R128 L131 R132 N135 S136 I137 R138 W139 G140 S141 N142 V143 P144 I145 D146 T147 P148 Y149 V150 N151 L152 T153 A154 E155 D156 S157 S158 E159 I160 E161 M162 N163 L164 Q165 D166 A167 E168 K169 N170 M171 L172 W173 Y174 T175 V176 Y177 N178 I179 N180 D181 P182 W183 D184 E185 N186 G187

Y188 T191 S192 I193 N194 K195 L199 G200 K201 L202 F203 L206 N207 Q208 S209 W210 S211 K212 L213 E214 K215 V216 A217 M218 I221 V222 T223 T224 Q225 N226 H227 L228 S229 G230 H231 L232 R233 K234 N235 E236 N237 F238 N239 A240 V241 Y242 S243 Q244 R245 V246 L247 Q248 P249 P250 L251

Q254 R255 V256 E257 S258 F259 L260 K261 I262 S265 D266 Y267 E268 I269 I270 K271 S272 S273 L274 E275 SER TYR SER ALA SER LYS ALA PHE SER VAL PRO GLU ASN GLY PRO HIS SER LEU MET ASP PHE ALA SER LEU ASP GLY ARG MET PRO SER ASP LEU SER LEU PRO SER ILE SER ILE

ASP THR LYS ARG PRO SER ALA ASP LEU ALA ARG LEU LYS ILE SER GLN PRO LYS SER LEU ASP ALA PRO LEU LYS THR GLN ARG ARG HIS LYS PHE PRO GLU SER ASP SER VAL ASP ASN ALA GLY GLY LYS ILE LEU ILE LYS LYS GLU THR LEU GLY GLY ARG ASP VAL ARG ALA THR

THR PRO VAL SER SER VAL SER LEU MET SER GLY VAL GLU PRO LEU SER SER LEU THR SER THR ASN LEU ASP LEU ARG ASP LYS SER HIS GLY ASN TYR ARG ILE GLY PRO SER GLY ILE LEU ASP PHE GLY VAL LYS LEU PRO ALA GLU ALA GLN SER ASN THR GLY ASP VAL ASP LEU

LEU GLN ASP LYS THR SER ILE ARG SER PRO SER SER GLY ILE THR ASP VAL VAL ASN GLY LEU ALA ASN LEU ASN LEU ARG GLN ASN LYS SER ASP VAL SER ARG PRO TRP SER LYS ASN THR ALA ALA ASN ALA ASP VAL PHE ASP PRO VAL HIS ARG LEU VAL SER GLU GLN THR GLY

THR PRO PHE VAL LEU ASN ASN SER ASP VAL ALA GLY SER GLU ALA LYS LEU THR THR HIS SER THR GLU THR GLY VAL SER PRO HIS ASN VAL SER LEU ILE LYS ASP LEU ARG ASP LYS ASP GLY PHE ARG LYS GLN LYS LYS LEU ASP LEU LEU GLY SER TRP THR LYS GLU LYS ASN

ASP LYS ALA ILE VAL HIS SER ARG GLU VAL THR GLY ASP SER GLY ASP ALA THR GLU THR VAL THR ALA ARG ASP SER PRO VAL LEU ARG LYS THR LYS HIS ALA ASN ASP ILE PHE ALA GLY LEU ASN LYS LYS TYR ALA ARG ASP VAL SER ARG GLY GLY LYS GLY ASN SER ARG ASP

LEU TYR SER GLY GLY ASN ALA GLU LYS LYS THR SER GLY LYS PHE ASN VAL ASP LYS GLU MET THR GLN ASN GLU GLN GLU PRO LEU PRO ASN LEU MET GLU ALA ALA ARG ASN ALA GLY GLU GLU GLN TYR VAL GLN ALA GLY LEU LEU GLY GLN ARG VAL ASN LYS ILE LEU ALA GLU

PHE THR ASN LEU ILE SER LEU GLY GLU LYS GLY ILE GLN ASP ILE LEU HIS ASN GLN SER GLY THR GLU LEU LYS LEU PRO THR GLU ASN LYS LEU GLY ARG GLU SER GLU GLU ALA ASN VAL GLU ARG ILE LEU GLU VAL SER ASP PRO GLN ASN LEU PHE LYS ASN LEU

ASN ASP LEU ASP SER VAL GLN SER PRO PHE ARG LEU PRO ASN ALA ASP LEU SER ARG ASP LEU ASP SER VAL SER PHE LYS ASP ALA LEU ASP VAL ILE ASP LEU ALA LEU GLN LYS VAL LYS ALA GLY GLU ARG GLU THR SER ASP PHE LYS

VAL GLY GLN ASP GLU THR LEU ILE PRO THR GLN LEU MET LYS VAL GLU THR PRO GLU GLU LYS ASP ASP VAL ILE GLU LYS MET VAL LEU ARG ILE ARG GLN ASP GLY GLU THR ASP GLU GLU THR VAL PRO GLY PRO GLY VAL ALA GLU SER LEU GLY ILE ALA ALA LYS ASP LYS SER

VAL ILE ALA SER

- Molecule 2: Large structural phosphoprotein

Chain l: 30% 30% 69%

MET ASP LEU LYS ALA GLN S7 I8 P9 F10 A11 W12 L13 D14 R15 D16 K17 V18 Q19 R20 L21 T22 N23 F24 L25 S26 N27 L28 E29 N30 L31 E32 N33 V34 D35 L36 R37 E38 H39 P40 Y41 V42 T43 N44 S45 C46 V47 V48 R49 E50 G51 E52 D53 V54 D55 E56 L57 K58 T59 L60

Y61 N62 T63 F64 I65 L66 W67 L68 M69 Y70 H71 Y72 V73 L74 S75 K76 R77 K78 P79 D80 Y81 N82 A83 I84 W85 Q86 D87 I88 T89 K90 N93 V94 V95 N96 E97 Y98 L99 K100 S101 K102 G103 L104 N105 K106 G107 N108 F109 E110 N111 M112 F113 T114 N115 K116 E117 K118 F119 E120 S121

Q122 F123 S124 D125 I126 H127 R128 A129 L130 L131 R132 L133 G134 N135 S136 I137 R138 W139 G140 S141 N142 V143 P144 I145 D146 T147 P148 Y149 V150 N151 L152 T153 A154 E155 D156 S157 S158 E159 I160 E161 N162 N163 L164 Q165 D166 A167 E168 K169 N170 M171 L172 W173 Y174 T175 V176 Y177 N178 I179 N180 D181

P182 W183 D184 E185 N186 G187 Y188 L189 V190 T191 S192 I193 N194 K195 L196 V197 Y198 L199 G200 K201 L202 F203 L206 N207 Q208 S209 W210 S211 K212 L213 E214 K215 V216 A217 M218 S219 Q220 I221 V222 T223 T224 Q225 N226 H227 L228 S229 G230 H231 L232 R233 K234 N235 E236 N237 F238 N239 A240 V241 Y242

S243 Q244 R245 V246 L247 Q248 T249 P250 L251 T252 G253 Q254 R255 V256 E257 S258 F259 L260 K261 I262 I263 T264 S265 D266 Y267 E268 I269 I270 K271 S272 S273 L274 E275 SER TYR SER ALA SER LYS ALA PHE SER VAL PRO GLU ASN GLY PRO HIS SER LEU MET ASP PHE ALA SER LEU ASP GLY ARG

MET PRO SER ASP LEU SER LEU PRO SER ILE SER ILE ASP THR LYS ARG PRO SER ALA ASP LEU ALA ARG LEU LYS ILE SER GLN PRO LYS SER LEU ASP ALA PRO LEU LYS THR GLN ARG ARG HIS LYS PHE PRO GLU SER ASP SER VAL ASP ASN ALA GLY GLY LYS ILE LEU LEU LYS

LYS GLU THR LEU GLY GLY ARG ASP VAL ARG ALA THR THR PRO VAL SER SER VAL SER LEU MET SER GLY VAL GLU PRO LEU SER SER LEU THR SER THR ASN LEU ASP LEU ARG ASP LYS SER HIS GLY ASN TYR ARG ILE GLY PRO VAL SER GLY ILE LEU ASP PHE GLY VAL LYS LEU PRO

ALA GLU ALA GLN SER ASN THR GLY ASP VAL ASP LEU LEU GLN ASP LYS THR SER ILE ARG SER PRO SER SER GLY ILE THR ASP VAL VAL ASN GLY LEU ALA ASN LEU ASN LEU ARG GLN ASN LYS SER ASP VAL SER ARG PRO TRP SER LYS ASN THR ALA ALA ASN ALA ASP VAL PHE

ASP PRO VAL HIS ARG LEU VAL SER GLU GLN THR GLY THR PRO PHE VAL LEU ASN ASN SER ASP VAL ALA GLY SER GLU ALA LYS LEU THR THR HIS SER THR GLU THR GLY VAL SER PRO HIS ASN VAL SER LEU ILE LYS ASP LEU ARG LYS THR LYS ASP ASP LYS ASP GLY PHE ARG LYS GLN LYS LYS

LEU ASP LEU LEU GLY SER TRP THR LYS GLU LYS ASN ASP LYS ALA ILE VAL HIS SER ARG GLU VAL THR GLY ASP SER GLY ASP ALA THR GLU THR VAL THR ALA ALA ARG ASP SER PRO VAL LEU ARG LYS THR LYS HIS ALA ASN ASP ILE PHE ALA GLY LEU ASN LYS LYS TYR ALA ARG

ASP VAL SER ARG GLY GLY ASN SER ARG GLY ASP LYS ALA GLU LYS LYS GLU THR SER GLY LYS PHE ASN VAL ASP LYS GLU MET THR GLN ASN GLU GLN GLU PRO LEU PRO ASN LEU MET GLU ALA ALA ARG ASN ALA ALA GLY GLU GLU GLN TYR VAL GLN ALA

GLY LEU GLY GLN ARG VAL ASN LYS ILE LEU GLU PHE THR ASN LEU ILE SER LEU GLY LYS GLY ILE GLN ASP ILE LEU HIS ASN GLN SER GLY THR GLU LEU LYS LEU PRO THR GLU ASN LYS LEU GLY ARG GLU SER GLU GLU ALA ASN LEU VAL GLU ARG ILE LEU GLU VAL SER

ASP PRO GLN ASN LEU PHE LYS LEU GLN ASN ASP LEU ASP SER VAL GLN SER PHE LYS ASP ALA LEU ASP VAL SER PHE LYS ASP LEU ARG ASP LEU ASP SER VAL SER ARG GLY LEU PRO ASN ALA ASP LEU HIS ASN GLN SER GLY THR GLU LEU LYS LEU PRO THR GLU GLN GLN GLU ALA ALA GLY GLU GLU GLN ARG ILE LEU GLU VAL SER

• Molecule 2: Large structural phosphoprotein

Chain n: 22% 30% • 69%

MET ASP LEU LYS ALA GLN S7 I8 P9 F10 A11 W12 L13 D14 R15 D16 K17 R20 L25 S26 N27 L28 E29 N30 L31 E32 N33 V34 D35 L36 R37 E38 H39 P40 Y41 V42 T43 N44 S45 C46 V47 V48 R49 E50 G51 E52 D53 V54 D55 E56 L57 K58 T59 L60 Y61 N62 T63 F64

I65 L66 W67 L68 M69 Y70 H71 Y72 K76 R77 T89 Q92 N93 V94 V95 N96 E97 Y98 L99 K100 S101 K102 G103 L104 N105 K106 G107 N108 F109 E110 N111 M112 F113 T114 N115 K116 E117 K118 F119 E120 S121 Q122 F123 S124 D125 I126 H127 R128 A129 L130 L131 R132 L133 G134 N135 S136 I137

R138 W139 G140 S141 N142 V143 P144 I145 D146 T147 P148 Y149 V150 N151 L152 T153 A154 E155 D156 S157 S158 E159 I160 E161 N162 N163 L164 Q165 D166 A167 E168 K169 N170 M171 L172 W173 Y174 T175 V176 Y177 N178 I179 N180 D181 P182 W183 D184 E185 N186 G187 Y188 L189 S192 I193 N194 K195 L196 V197 Y198

L199 G200 K201 L202 F203 Q208 S211 K212 K215 S219 V222 N226 H227 L228 S229 G230 H231 L232 R233 K234 N235 E236 N237 F238 Y242 R245 V246 L247 Q248 T249 P250 L251 T252 G253 Q254 R255 V256 E257 S258 F259 D266 Y267 E268 I269 I270 K271 S272 S273 L274 E275 SER

TYR SER ALA SER LYS ALA PHE SER VAL PRO GLU ASN GLY PRO HIS SER LEU MET ASP PHE ALA SER LEU ASP GLY ARG MET PRO SER ASP LEU SER LEU PRO SER ILE SER ILE ASP THR LYS ARG PRO SER ALA ASP LEU ALA ARG LEU LYS ILE SER GLN PRO LYS SER LEU ASP ALA

PRO LEU LYS THR GLN ARG ARG HIS LYS PHE PRO GLU SER ASP SER VAL ASP ASN ALA ALA GLY GLY LYS ILE LEU ILE LYS LYS GLU THR LEU GLY GLY ARG ASP VAL ARG ALA THR THR PRO VAL SER SER VAL SER LEU MET SER GLY VAL GLU PRO LEU SER SER LEU THR SER THR ASN

LEU ASP LEU ARG ASP LYS SER HIS GLY ASN TYR ARG ILE GLY PRO SER GLY ILE LEU ASP PHE GLY VAL LYS LEU PRO ALA GLU ALA GLN SER ASN THR GLY ASP VAL ASP LEU LEU GLN ASP LYS THR SER ILE ARG SER PRO SER SER GLY ILE THR ASP VAL VAL ASN GLY ALA

ASN LEU ASN LEU ARG GLN ASN LYS SER ASP VAL SER ARG PRO TRP SER LYS ASN THR ALA ALA ASN ASN ALA ASP VAL PHE ASP PRO ALA VAL HIS ARG LEU VAL SER GLU GLN THR GLY GLY ASP PHE VAL LEU ASN ASN SER ASP VAL ALA GLY SER GLU ALA LYS LEU THR THR HIS SER THR

GLU THR GLY VAL SER PRO HIS ASN VAL SER LEU ILE LYS ASP LEU ARG ASP LYS ASP GLY PHE ARG LYS GLN LYS LYS LEU ASP LEU LEU GLY SER TRP THR LYS GLU LYS ASN ASP LYS ALA ILE VAL HIS SER ARG GLU VAL THR GLY ASP SER GLY ASP ALA THR GLU THR VAL THR

ALA ARG ASP SER PRO VAL LEU ARG LYS THR LYS HIS ALA ASN ASP ILE PHE ALA GLY LEU ASN LYS LYS TYR ALA ARG ASP VAL SER ARG GLY GLY LYS GLY ASN SER ARG ASP LEU TYR SER GLY GLY ASN ALA GLU LYS LYS GLU THR SER GLY LYS PHE ASN VAL ASP LYS GLU MET

THR GLN ASN GLU GLN GLU PRO LEU PRO ASN LEU MET GLU ALA ALA ARG ASN ALA GLY GLU GLU GLN TYR VAL GLN ALA GLY LEU GLY GLN ARG VAL ASN LYS ILE LEU ALA GLU PHE THR ASN LEU ILE SER LEU GLY GLU LYS GLY ILE GLN ASP ILE LEU HIS ASN GLN SER GLY THR

GLU LEU LYS LEU PRO THR GLU ASN LYS LEU GLY ARG GLU SER GLU GLU ALA ASN VAL GLU ARG ILE LEU GLU VAL SER ASP PRO GLN ASN LEU PHE LYS ASN PHE LYS LEU GLN ASN ASP LEU ASP SER VAL GLN SER PRO PHE ARG LEU PRO ASN ALA ASP LEU SER ASP LEU

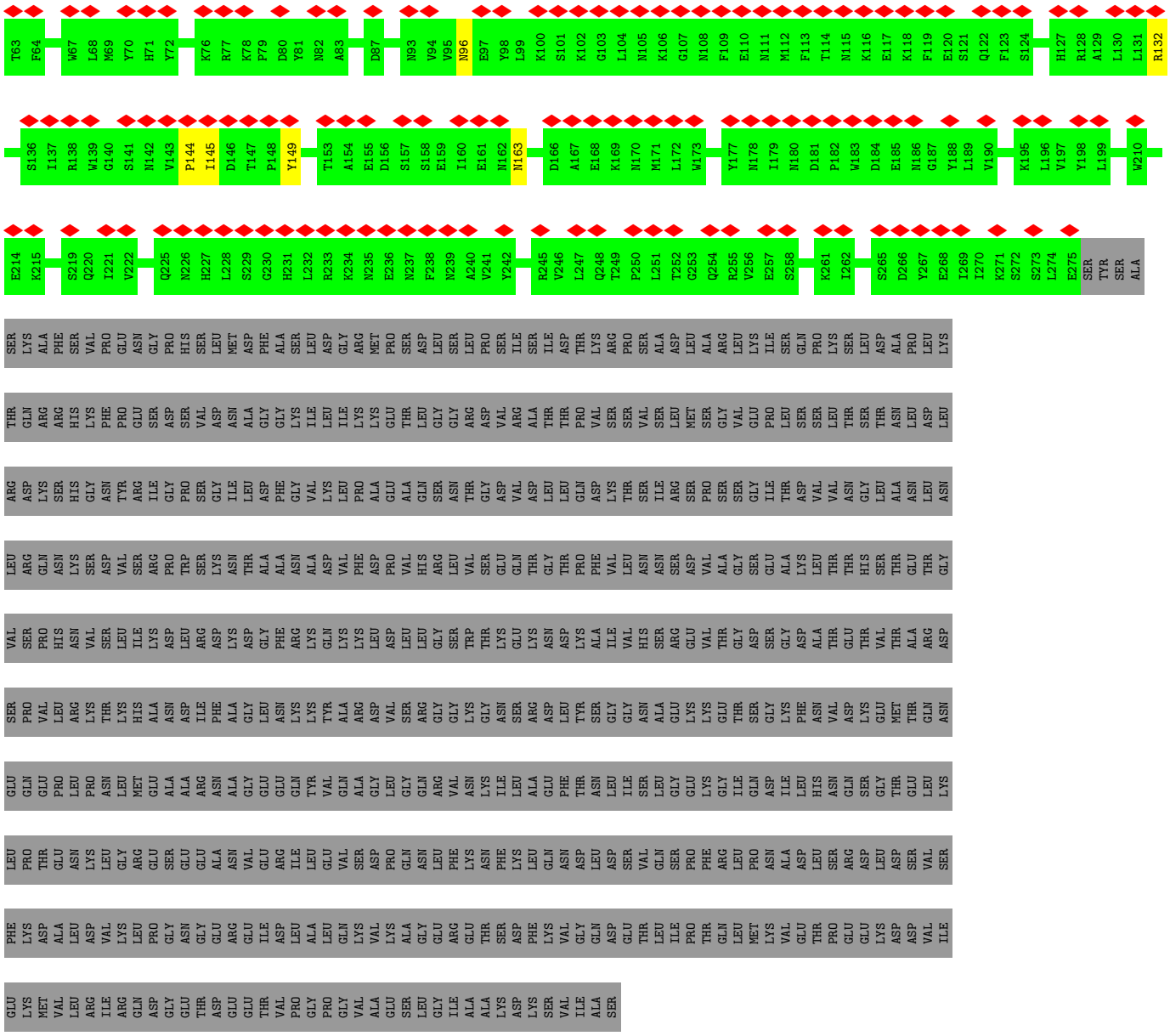
SER VAL SER PHE PHE LYS ASP ALA LEU ASP VAL LYS LEU PRO GLY ASN GLY GLU GLU ILE ASP LEU ALA LEU GLN LYS VAL LYS ALA GLY GLU ARG GLU THR SER ASP PHE LYS VAL GLY GLN ASP GLU THR LEU ILE PRO THR GLN LEU MET LYS VAL GLU THR PRO GLU GLU LYS ASP

ASP VAL ILE GLU LYS MET VAL LEU ARG ILE ARG GLN ASP GLY GLU THR ASP GLU GLU THR VAL PRO GLY PRO GLY VAL ALA GLU SER LEU GLY ILE ALA ALA LYS ASP LYS SER VAL ILE ALA SER

• Molecule 2: Large structural phosphoprotein

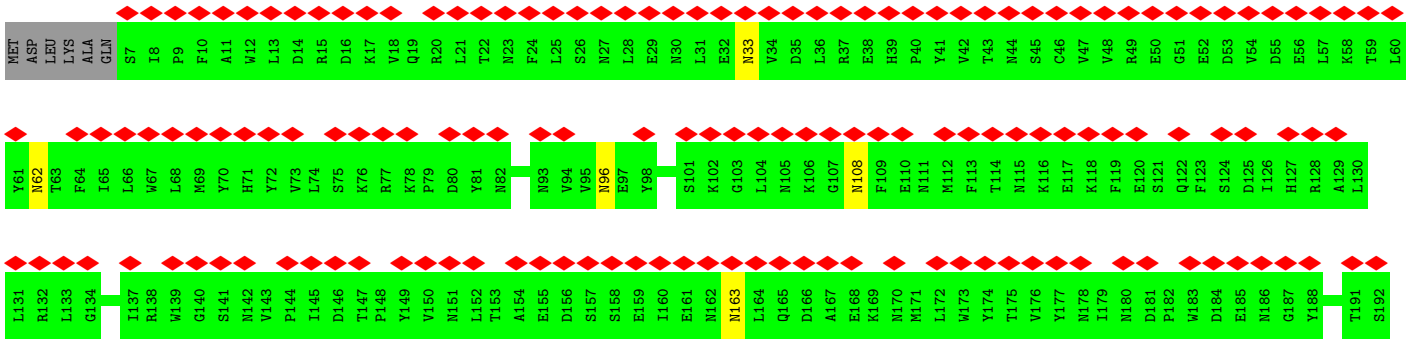
Chain o: 21% 30% • 69%

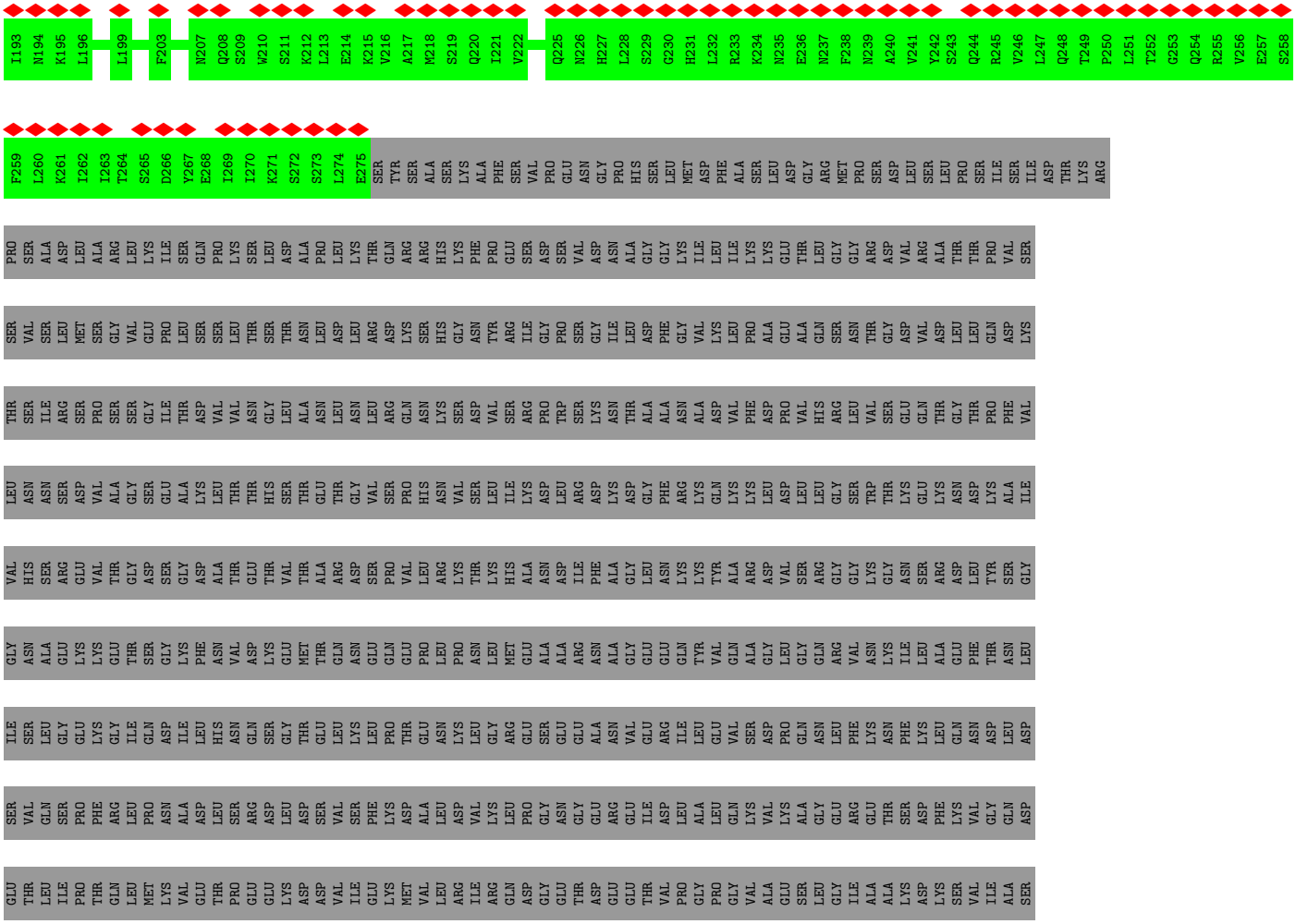
MET ASP LEU LYS ALA GLN S7 I8 P9 F10 A11 W12 L13 D14 R15 D16 Q19 R20 L21 T22 N23 F24 L25 S26 N27 L28 E29 N30 L31 E32 N33 V34 D35 L36 R37 E38 H39 P40 Y41 V42 T43 N44 S45 C46 V47 V48 R49 E50 G51 E52 D53 V54 D55 E56 T59 L60 Y61 N62



• Molecule 2: Large structural phosphoprotein

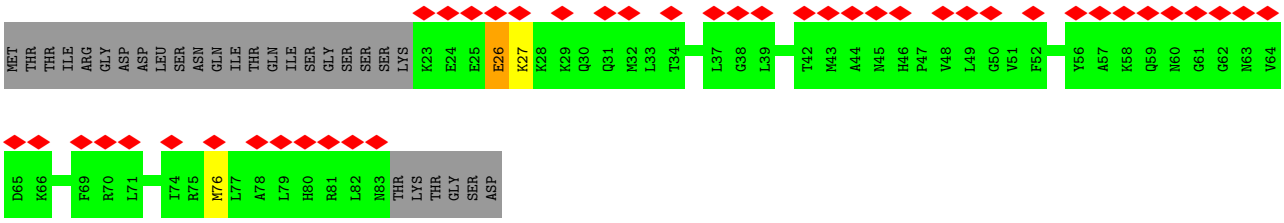
Chain p:





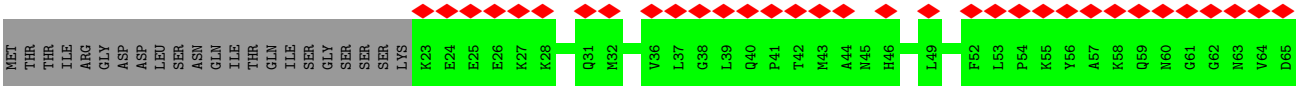
• Molecule 3: Small capsomere-interacting protein

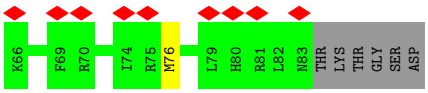
Chain J:



• Molecule 3: Small capsomere-interacting protein

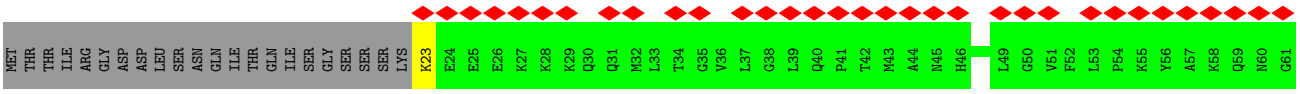
Chain K:

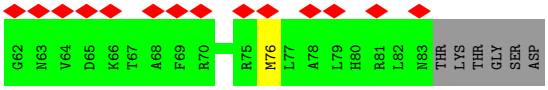




• Molecule 3: Small capsomere-interacting protein

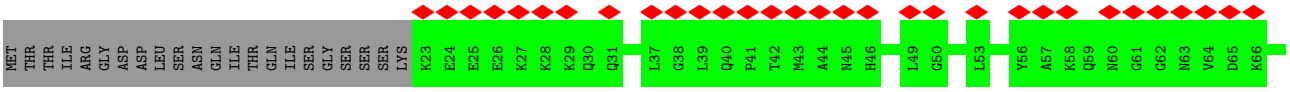
Chain L:

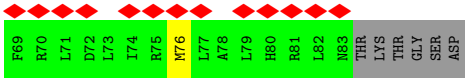




• Molecule 3: Small capsomere-interacting protein

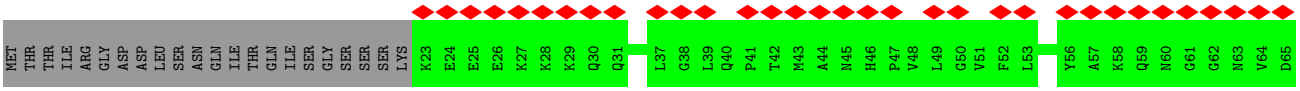
Chain M:

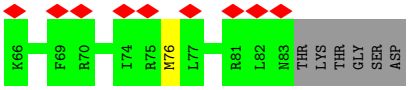




• Molecule 3: Small capsomere-interacting protein

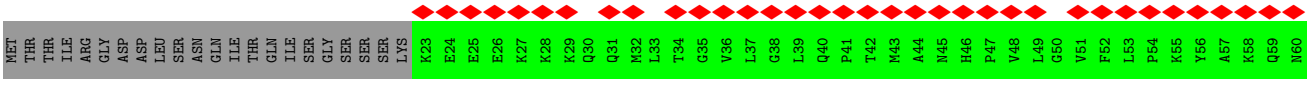
Chain N:

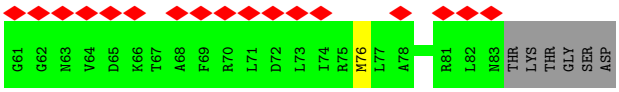




• Molecule 3: Small capsomere-interacting protein

Chain O:



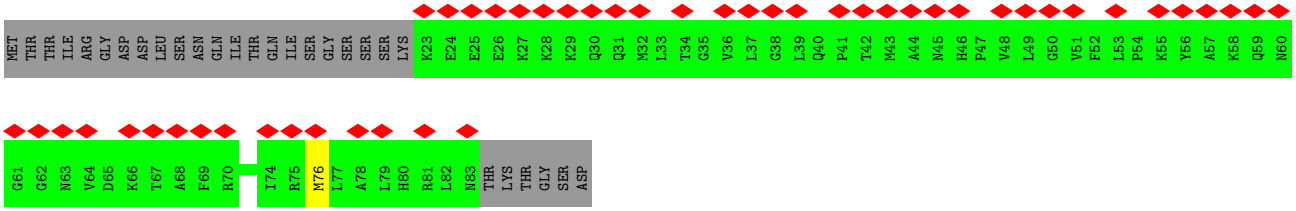


• Molecule 3: Small capsomere-interacting protein

Chain P:

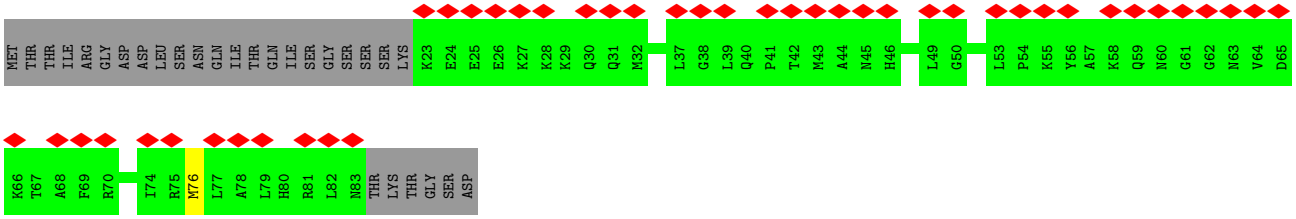
- Molecule 3: Small capsomere-interacting protein

Chain Q:



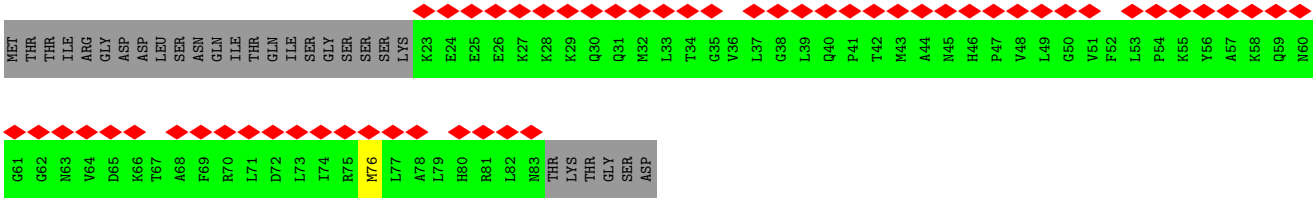
- Molecule 3: Small capsomere-interacting protein

Chain R:



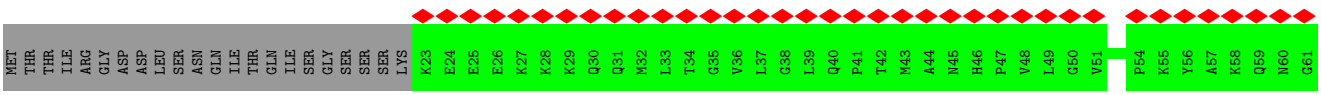
- Molecule 3: Small capsomere-interacting protein

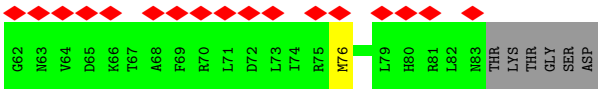
Chain x:



- Molecule 3: Small capsomere-interacting protein

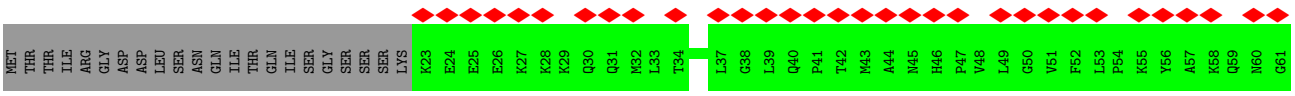
Chain y:

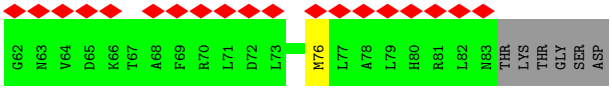




- Molecule 3: Small capsomere-interacting protein

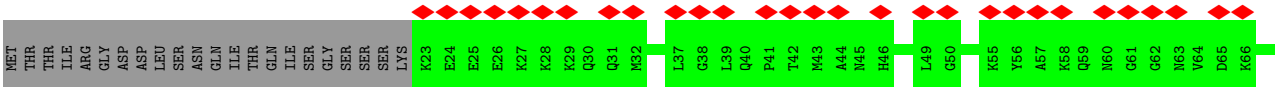
Chain z:

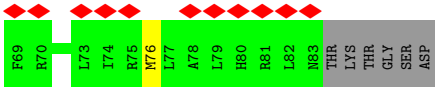




- Molecule 3: Small capsomere-interacting protein

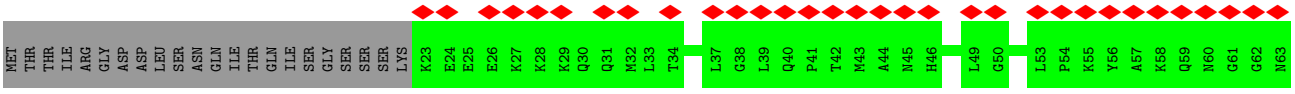
Chain 1:

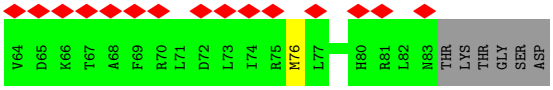




- Molecule 3: Small capsomere-interacting protein

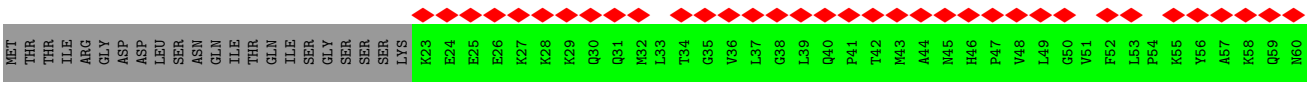
Chain 2:

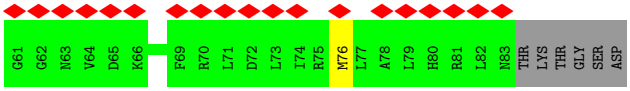




- Molecule 3: Small capsomere-interacting protein

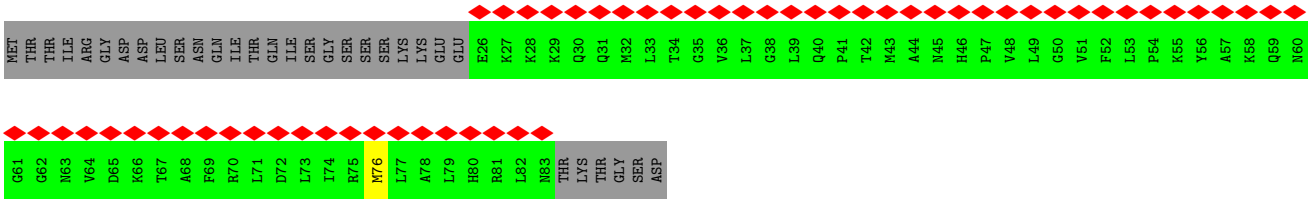
Chain 3:





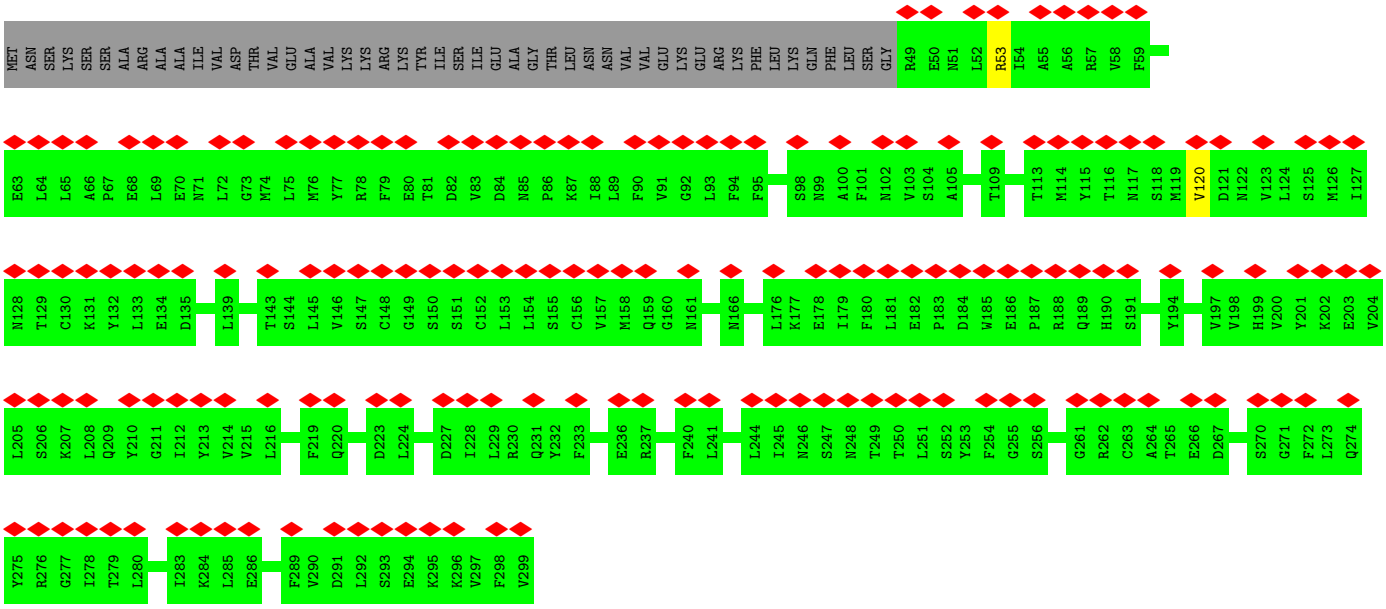
- Molecule 3: Small capsomere-interacting protein

Chain 4:



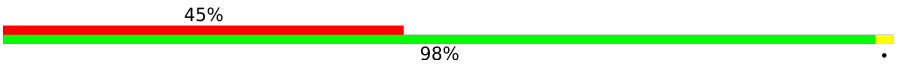
- Molecule 4: Triplex capsid protein 1

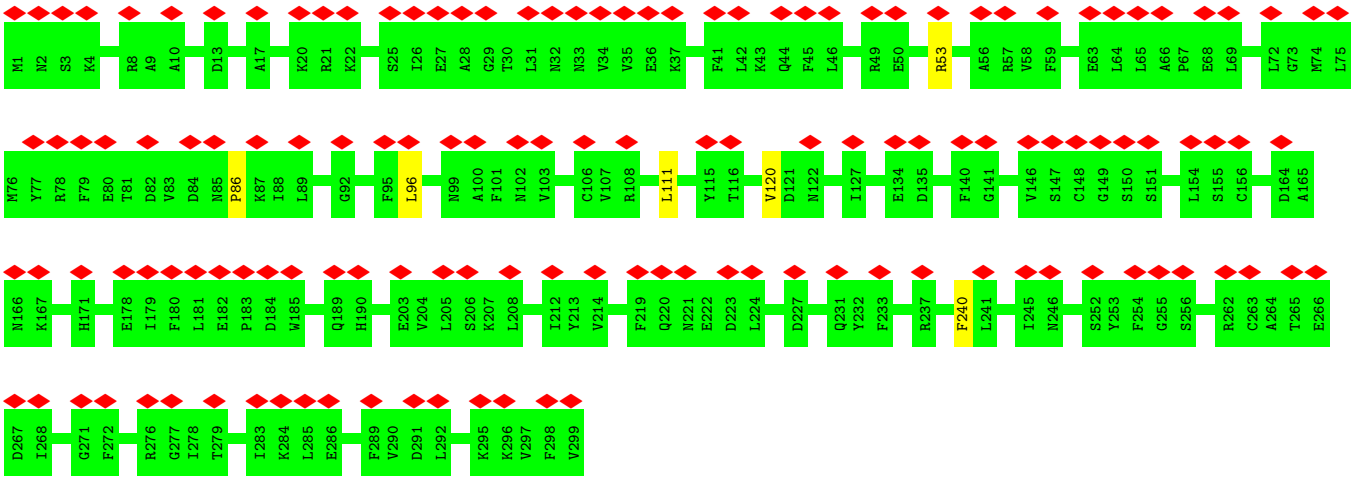
Chain 5:



- Molecule 4: Triplex capsid protein 1

Chain S:





- Molecule 4: Triplex capsid protein 1

Chain T: 57% 99%

M1 N2 S3 K4 S5 S6 A7 R8 A9 A10 D13 A17 V18 K19 K20 R21 K22 Y23 I26 E27 A28 G29 T30 L31 N32 N33 E36 K37 E38 R39 K40 L46 R49 E50 N51 L52 R53 I54 R57 E63 L64 L65 A66 P67 E68 L69 E70 N71 L72 L75 M76

Y77 R78 F79 E80 T81 D82 V83 D84 N85 P86 K87 I88 V91 G92 L93 F94 F95 L96 C97 A100 F101 N102 V103 S104 A105 C106 V107 R108 T113 M114 Y115 T116 N117 S118 M119 L124 I127 N128 T129 C130 K131 E134 D135 L139 F140 G141 V142 T143 S144 L145 V146 S147 C148

G149 S150 S151 C152 L153 L154 S155 C156 V157 D164 A165 N166 K167 I170 H171 G172 I179 F180 L181 E182 P183 D184 W185 E186 P187 R188 Q189 H190 S191 Y194 V195 Y196 H199 V200 Y201 L205 S206 K207 Y210 G211 I212 Y213 V214 V215 L216 F219 Q220 N221 E222 D223 L224

D227 I228 L229 R230 Q231 Y232 F233 R237 F238 L241 N242 Y243 N246 S247 N248 T249 T250 L251 S252 Y253 F254 R259 I260 G261 R262 C263 A264 T265 E266 D267 I268 K269 S270 G271 F272 L273 Q274 Y275 R276 G277 I278 T279 K284 L285 E286 F289 V290 D291 E294 K295 K296 V297 F298

V299

- Molecule 4: Triplex capsid protein 1

Chain U: 48% 97%

M1 N2 S3 K4 S5 S6 A9 A10 D13 A17 R21 E27 A28 G29 T30 L31 N32 N33 V34 V35 E36 K37 E38 R39 K40 F41 L42 K43 R49 E50 N51 L52 R53 I54 A55 A56 R57 V58 F59 C62 E63 L64 L65 A66 P67 E68 L69 E70 N71 L72 G73 M74

Y77 R78 F79 E80 T81 D82 V83 D84 N85 P86 K87 I88 L89 G92 L93 F94 F95 N99 A100 V103 C106 V107 R108 Y115 T116 M119 V120 M126 I127 N128 T129 C130 K131 E134 D135 L139 F140 G141 L145 V146 S147 C148 G149 S150 S151 L154 S155 C156 V157

M158 Q159 G160 N161 D164 A165 N166 K167 E168 N169 I170 H171 E178 I179 D184 R188 Q189 Y194 V195 Y196 H199 V200 Y201 L205 S206 K207 Y210 G211 V214 V215 L216 F219 D223 L224 D227 Q231 Y232 F233 R237 F238 L241 N242 Y243 L244 I245

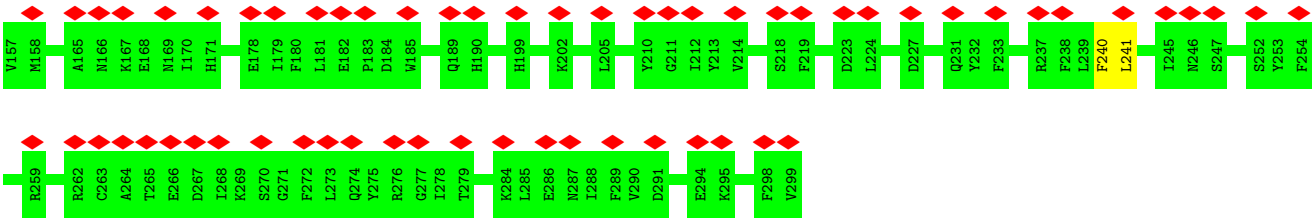
N248 T249 T250 L251 S252 Y253 F254 G255 R259 I260 G261 R262 C263 A264 T265 E266 D267 S270 G271 F272 R276 G277 I278 T279 K284 D291 E294 F298 V299

- Molecule 4: Triplex capsid protein 1

Chain V: 47% 97%

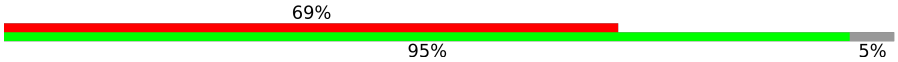
M1 N2 S3 K4 S5 S6 A7 R8 A9 A10 D13 E16 A17 K20 R21 K22 Y23 I24 S25 I26 E27 A28 G29 T30 L31 N32 N33 V34 V35 E36 K37 E38 R39 K40 F41 L42 K43 Q44 F45 R49 E50 N51 L52 R53 I54 A55 A56 R57 E63 L64 L65 A66 P67 E68 L69

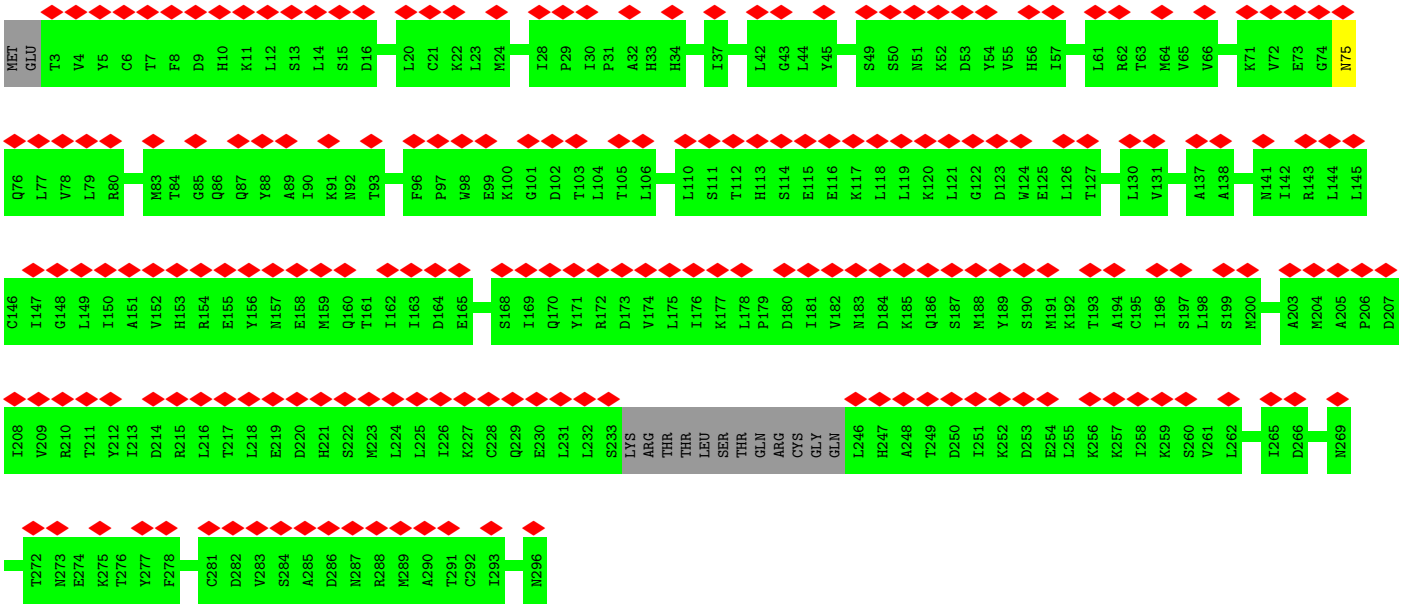
E70 N71 L72 G73 M74 R78 F79 E80 T81 D82 V83 D84 N85 P86 K87 I88 L89 F90 V91 G92 L93 F94 F95 A100 F101 N102 V103 S104 A105 C106 Y115 T116 N117 V120 M126 T129 C130 K131 E134 D135 K136 G141 S147 S150 S151 C152 L153 L154 S155 C156



• Molecule 5: Triplex capsid protein 2

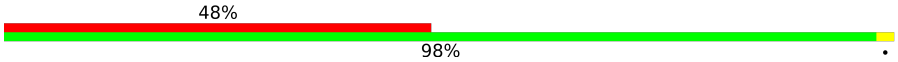
Chain 6:

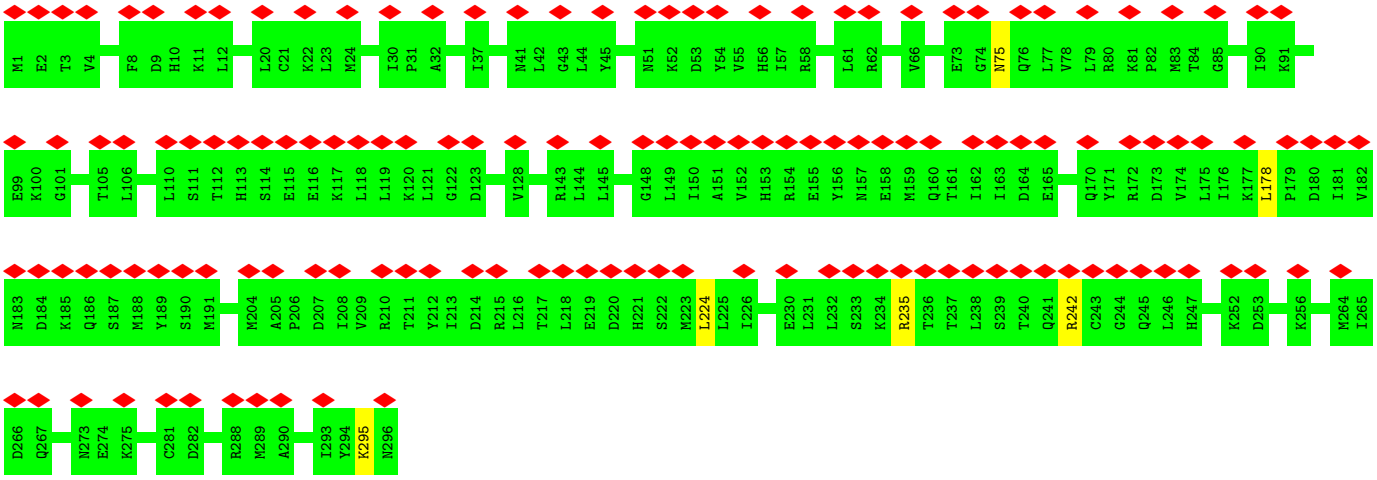




• Molecule 5: Triplex capsid protein 2

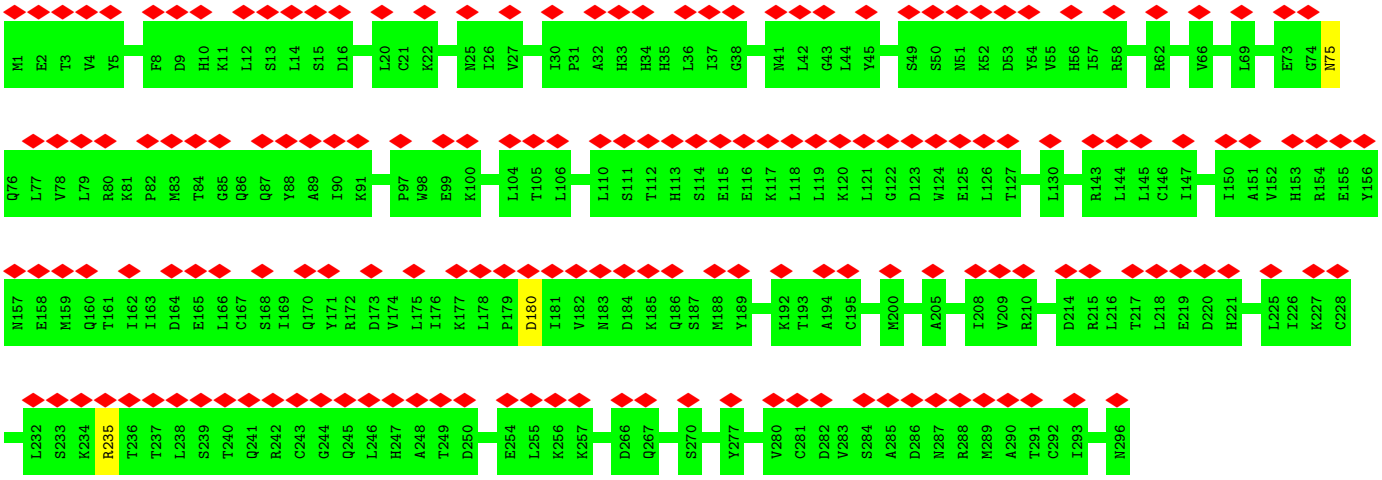
Chain W:





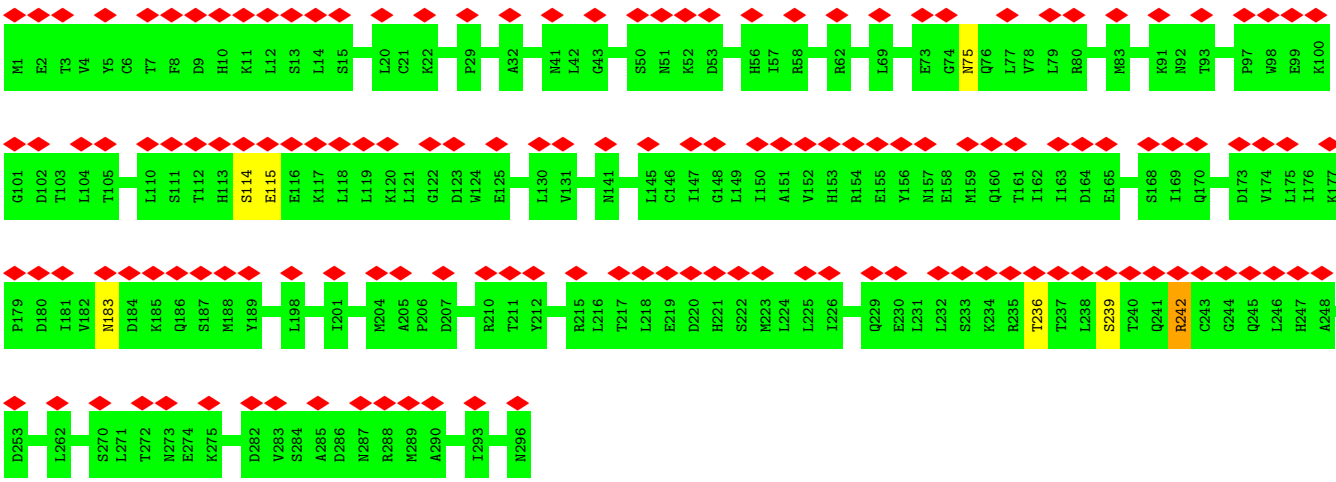
• Molecule 5: Triplex capsid protein 2

Chain X: 58% 99%



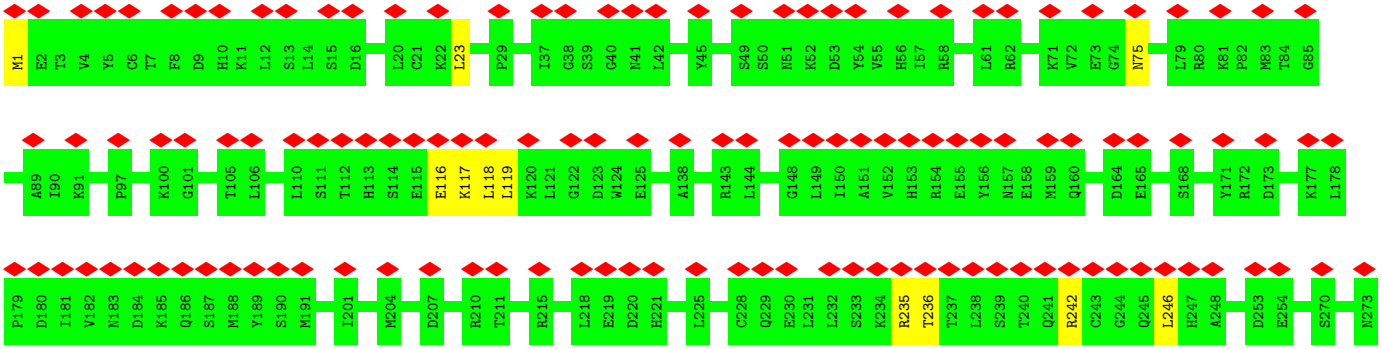
- Molecule 5: Triplex capsid protein 2

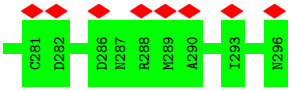
Chain Y: 50% 98%



- Molecule 5: Triplex capsid protein 2

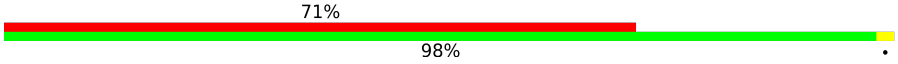
Chain Z: 46% 96%

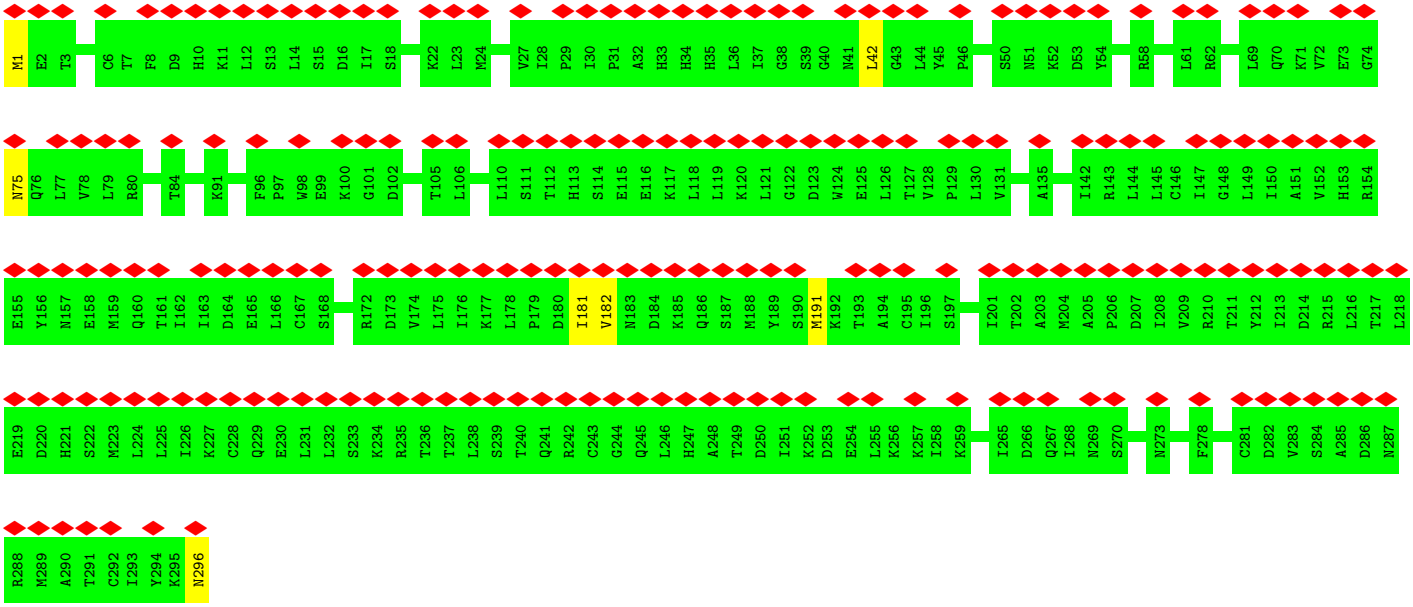




• Molecule 5: Triplex capsid protein 2

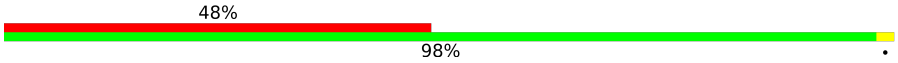
Chain 7:

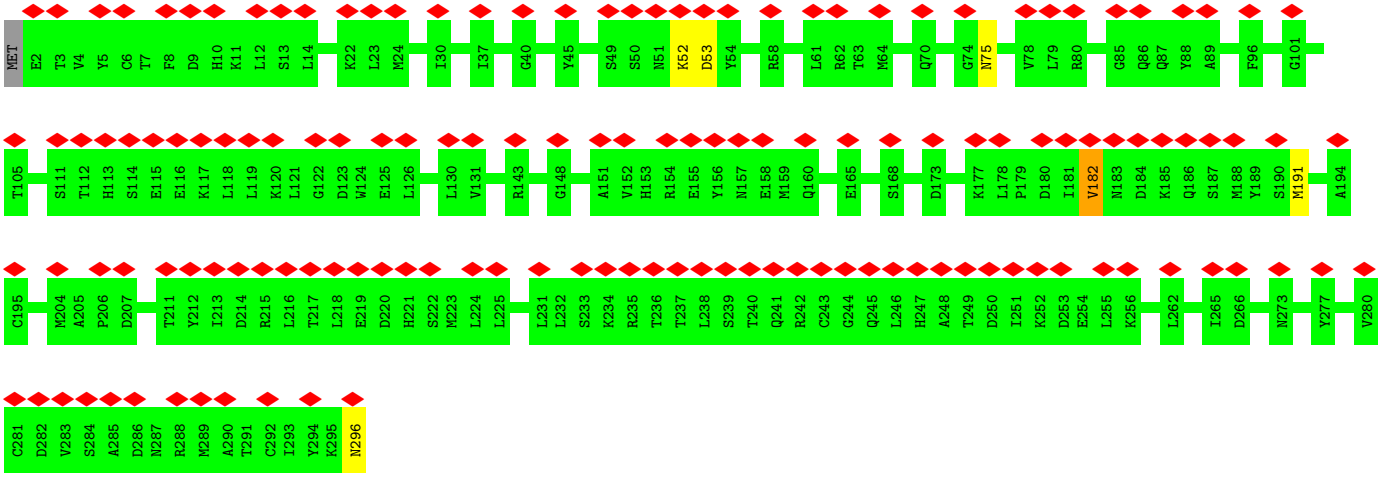




• Molecule 5: Triplex capsid protein 2

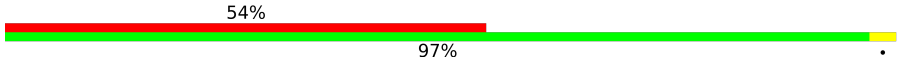
Chain a:

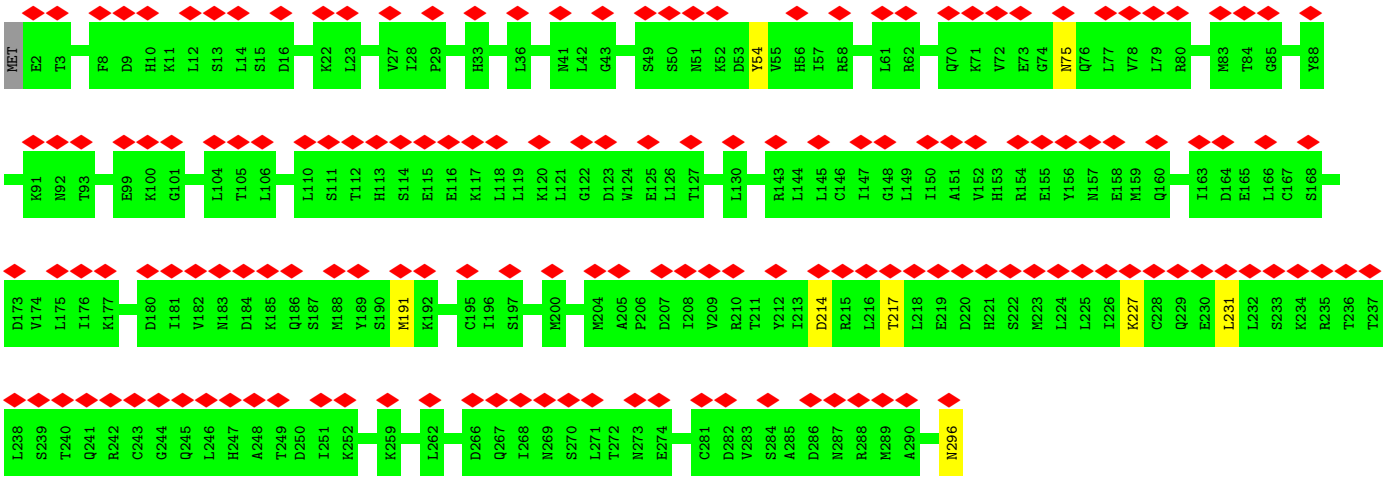




• Molecule 5: Triplex capsid protein 2

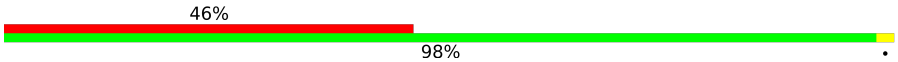
Chain b:

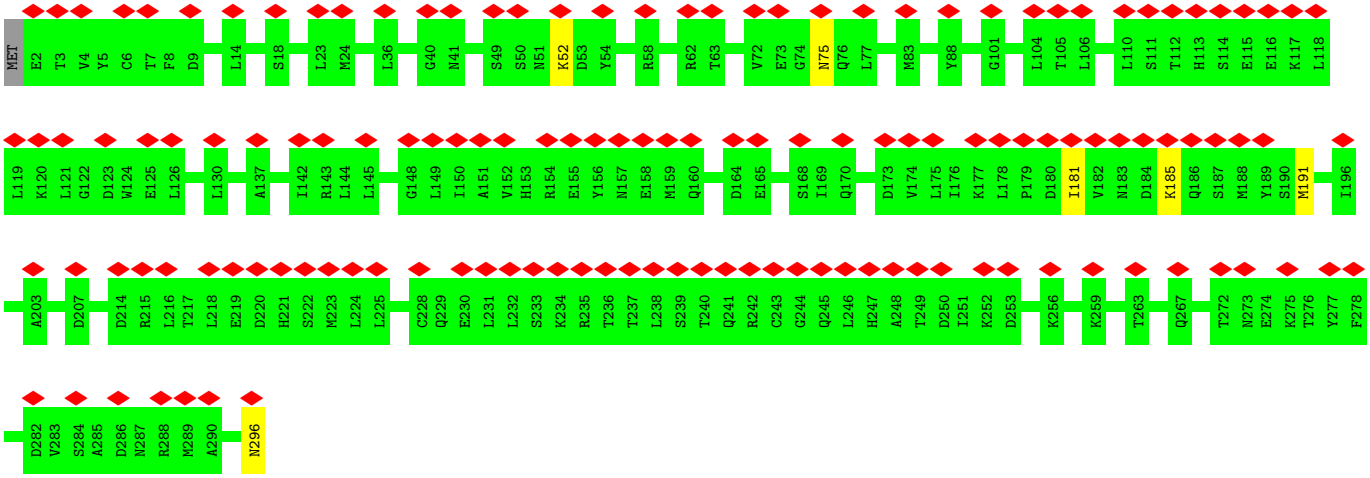




- Molecule 5: Triplex capsid protein 2

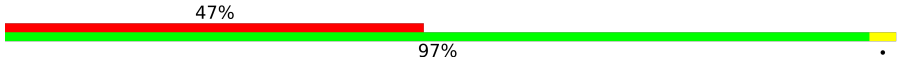
Chain c:

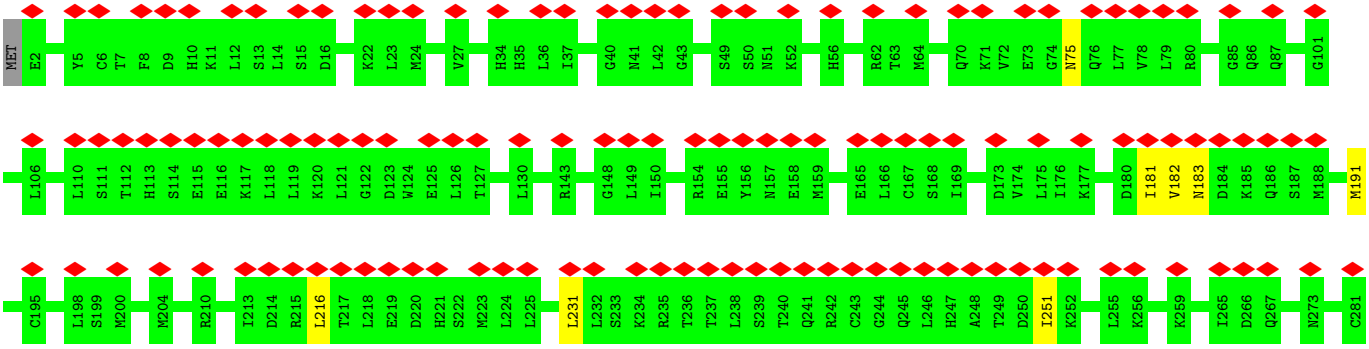


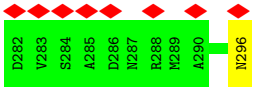


- Molecule 5: Triplex capsid protein 2

Chain d:






D282
V283
S284
A285
D286
N287
R288
M289
A290
N296

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	6443	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	23	Depositor
Minimum defocus (nm)	2200	Depositor
Maximum defocus (nm)	3200	Depositor
Magnification	64000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.125	Depositor
Minimum map value	-0.077	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.012	Depositor
Recommended contour level	0.036	Depositor
Map size (Å)	1388.8, 1388.8, 1388.8	wwPDB
Map dimensions	640, 640, 640	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.17, 2.17, 2.17	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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	0.51	0/10927	0.68	0/14860
1	B	0.46	0/10927	0.66	0/14860
1	C	0.46	0/10793	0.63	0/14676
1	D	0.46	0/10927	0.64	1/14860 (0.0%)
1	E	0.50	0/10927	0.66	0/14860
1	F	0.42	0/10927	0.65	0/14860
1	G	0.42	1/10927 (0.0%)	0.66	0/14860
1	H	0.50	0/10927	0.66	0/14860
1	I	0.47	0/10927	0.64	0/14860
1	q	0.42	0/10550	0.64	0/14349
1	r	0.38	0/10927	0.62	0/14860
1	s	0.39	0/10927	0.64	0/14860
1	t	0.40	0/10927	0.63	0/14860
1	u	0.38	0/10935	0.62	0/14870
1	v	0.38	0/10566	0.62	0/14366
1	w	0.38	0/10161	0.66	1/13814 (0.0%)
2	e	0.32	0/2272	0.54	0/3084
2	f	0.34	0/2272	0.62	0/3084
2	g	0.35	0/2272	0.62	0/3084
2	h	0.31	0/2272	0.56	0/3084
2	i	0.32	0/2272	0.63	0/3084
2	j	0.32	0/2272	0.59	0/3084
2	k	0.33	0/2272	0.58	0/3084
2	l	0.32	0/2272	0.57	1/3084 (0.0%)
2	m	0.36	0/2272	0.60	1/3084 (0.0%)
2	n	0.34	0/2272	0.63	1/3084 (0.0%)
2	o	0.40	0/2272	0.66	0/3084
2	p	0.34	0/2272	0.60	0/3084
3	1	0.29	0/490	0.44	0/656
3	2	0.29	0/490	0.44	0/656
3	3	0.28	0/490	0.44	0/656
3	4	0.29	0/463	0.44	0/621
3	J	0.28	0/490	0.44	0/656
3	K	0.28	0/490	0.44	0/656

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
3	L	0.29	0/490	0.44	0/656
3	M	0.29	0/490	0.44	0/656
3	N	0.29	0/490	0.44	0/656
3	O	0.29	0/490	0.44	0/656
3	P	0.29	0/490	0.44	0/656
3	Q	0.28	0/490	0.44	0/656
3	R	0.29	0/490	0.44	0/656
3	x	0.29	0/490	0.44	0/656
3	y	0.29	0/490	0.44	0/656
3	z	0.29	0/490	0.44	0/656
4	5	0.39	0/2062	0.67	0/2793
4	S	0.49	0/2440	0.67	0/3297
4	T	0.48	0/2440	0.70	0/3297
4	U	0.41	0/2440	0.67	0/3297
4	V	0.41	0/2440	0.66	0/3297
5	6	0.39	0/2262	0.67	0/3069
5	7	0.33	0/2374	0.66	0/3219
5	W	0.42	0/2374	0.68	0/3219
5	X	0.38	0/2374	0.62	0/3219
5	Y	0.39	0/2374	0.68	0/3219
5	Z	0.41	0/2374	0.72	0/3219
5	a	0.44	0/2366	0.73	0/3209
5	b	0.44	0/2366	0.73	0/3209
5	c	0.52	0/2366	0.77	0/3209
5	d	0.41	0/2366	0.75	0/3209
All	All	0.42	1/243697 (0.0%)	0.64	5/330985 (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
2	o	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	1115	GLU	C-N	-5.30	1.21	1.34

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	w	563	LEU	C-N-CD	-8.35	102.23	120.60
2	l	181	ASP	N-CA-C	5.66	126.28	111.00
2	m	154	ALA	N-CA-C	5.37	125.51	111.00
2	n	179	ILE	N-CA-C	-5.11	97.21	111.00
1	D	255	LEU	CA-CB-CG	5.01	126.82	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	o	7	SER	Mainchain

5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	1341/1345 (100%)	1238 (92%)	102 (8%)	1 (0%)	51	86
1	B	1341/1345 (100%)	1251 (93%)	87 (6%)	3 (0%)	47	81
1	C	1321/1345 (98%)	1239 (94%)	80 (6%)	2 (0%)	47	81
1	D	1341/1345 (100%)	1248 (93%)	89 (7%)	4 (0%)	41	77
1	E	1341/1345 (100%)	1243 (93%)	94 (7%)	4 (0%)	41	77
1	F	1341/1345 (100%)	1243 (93%)	96 (7%)	2 (0%)	51	86
1	G	1341/1345 (100%)	1253 (93%)	83 (6%)	5 (0%)	34	72
1	H	1341/1345 (100%)	1253 (93%)	84 (6%)	4 (0%)	41	77
1	I	1341/1345 (100%)	1242 (93%)	98 (7%)	1 (0%)	51	86
1	q	1292/1345 (96%)	1190 (92%)	99 (8%)	3 (0%)	47	81

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	r	1341/1345 (100%)	1235 (92%)	103 (8%)	3 (0%)	47	81
1	s	1341/1345 (100%)	1246 (93%)	93 (7%)	2 (0%)	51	86
1	t	1341/1345 (100%)	1240 (92%)	98 (7%)	3 (0%)	47	81
1	u	1342/1345 (100%)	1234 (92%)	106 (8%)	2 (0%)	51	86
1	v	1299/1345 (97%)	1204 (93%)	89 (7%)	6 (0%)	29	69
1	w	1240/1345 (92%)	1141 (92%)	98 (8%)	1 (0%)	51	86
2	e	267/858 (31%)	254 (95%)	13 (5%)	0	100	100
2	f	267/858 (31%)	248 (93%)	16 (6%)	3 (1%)	14	52
2	g	267/858 (31%)	255 (96%)	9 (3%)	3 (1%)	14	52
2	h	267/858 (31%)	248 (93%)	19 (7%)	0	100	100
2	i	267/858 (31%)	245 (92%)	17 (6%)	5 (2%)	8	38
2	j	267/858 (31%)	249 (93%)	16 (6%)	2 (1%)	22	63
2	k	267/858 (31%)	249 (93%)	17 (6%)	1 (0%)	34	72
2	l	267/858 (31%)	247 (92%)	19 (7%)	1 (0%)	34	72
2	m	267/858 (31%)	248 (93%)	18 (7%)	1 (0%)	34	72
2	n	267/858 (31%)	244 (91%)	18 (7%)	5 (2%)	8	38
2	o	267/858 (31%)	247 (92%)	16 (6%)	4 (2%)	10	46
2	p	267/858 (31%)	249 (93%)	18 (7%)	0	100	100
3	1	59/89 (66%)	52 (88%)	7 (12%)	0	100	100
3	2	59/89 (66%)	52 (88%)	7 (12%)	0	100	100
3	3	59/89 (66%)	52 (88%)	7 (12%)	0	100	100
3	4	56/89 (63%)	49 (88%)	7 (12%)	0	100	100
3	J	59/89 (66%)	51 (86%)	7 (12%)	1 (2%)	9	42
3	K	59/89 (66%)	52 (88%)	7 (12%)	0	100	100
3	L	59/89 (66%)	52 (88%)	7 (12%)	0	100	100
3	M	59/89 (66%)	52 (88%)	7 (12%)	0	100	100
3	N	59/89 (66%)	52 (88%)	7 (12%)	0	100	100
3	O	59/89 (66%)	52 (88%)	7 (12%)	0	100	100
3	P	59/89 (66%)	52 (88%)	7 (12%)	0	100	100
3	Q	59/89 (66%)	52 (88%)	7 (12%)	0	100	100
3	R	59/89 (66%)	52 (88%)	7 (12%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	x	59/89 (66%)	52 (88%)	7 (12%)	0	100	100
3	y	59/89 (66%)	52 (88%)	7 (12%)	0	100	100
3	z	59/89 (66%)	52 (88%)	7 (12%)	0	100	100
4	5	249/299 (83%)	226 (91%)	23 (9%)	0	100	100
4	S	297/299 (99%)	269 (91%)	27 (9%)	1 (0%)	41	77
4	T	297/299 (99%)	275 (93%)	21 (7%)	1 (0%)	41	77
4	U	297/299 (99%)	267 (90%)	29 (10%)	1 (0%)	41	77
4	V	297/299 (99%)	268 (90%)	27 (9%)	2 (1%)	22	63
5	6	278/296 (94%)	260 (94%)	18 (6%)	0	100	100
5	7	294/296 (99%)	259 (88%)	32 (11%)	3 (1%)	15	55
5	W	294/296 (99%)	277 (94%)	17 (6%)	0	100	100
5	X	294/296 (99%)	273 (93%)	20 (7%)	1 (0%)	41	77
5	Y	294/296 (99%)	269 (92%)	22 (8%)	3 (1%)	15	55
5	Z	294/296 (99%)	274 (93%)	19 (6%)	1 (0%)	41	77
5	a	293/296 (99%)	262 (89%)	28 (10%)	3 (1%)	15	55
5	b	293/296 (99%)	268 (92%)	24 (8%)	1 (0%)	41	77
5	c	293/296 (99%)	259 (88%)	33 (11%)	1 (0%)	41	77
5	d	293/296 (99%)	258 (88%)	30 (10%)	5 (2%)	9	42
All	All	29747/37695 (79%)	27475 (92%)	2177 (7%)	95 (0%)	44	77

All (95) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	55	GLY
1	F	19	ILE
1	G	810	TYR
1	H	21	ASN
1	H	818	ASP
1	v	148	ILE
1	v	810	TYR
1	v	818	ASP
1	w	564	PRO
2	f	178	ASN
2	g	10	PHE
2	i	108	ASN
2	j	149	TYR

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Mol	Chain	Res	Type
2	n	178	ASN
2	o	10	PHE
4	U	85	ASN
4	V	85	ASN
5	X	180	ASP
5	Y	242	ARG
5	Z	116	GLU
5	7	182	VAL
5	a	182	VAL
5	d	182	VAL
1	r	55	GLY
2	i	105	ASN
2	i	150	VAL
4	S	86	PRO
4	T	86	PRO
5	7	191	MET
5	a	52	LYS
5	b	191	MET
5	c	191	MET
5	d	191	MET
1	E	549	GLU
1	G	1120	SER
1	H	549	GLU
1	I	549	GLU
2	f	105	ASN
2	g	11	ALA
2	n	104	LEU
2	n	105	ASN
2	o	149	TYR
3	J	26	GLU
5	a	191	MET
5	d	251	ILE
1	A	549	GLU
1	B	549	GLU
1	C	549	GLU
1	D	549	GLU
1	D	845	VAL
1	E	23	ILE
1	E	948	GLY
1	E	1275	GLU
1	F	549	GLU
1	G	549	GLU

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Mol	Chain	Res	Type
1	G	1119	PRO
1	G	1275	GLU
1	H	1275	GLU
1	q	549	GLU
1	r	1275	GLU
1	t	549	GLU
1	u	549	GLU
1	v	549	GLU
1	v	1275	GLU
2	i	178	ASN
2	n	49	ARG
2	o	144	PRO
5	Y	114	SER
5	Y	115	GLU
1	D	1041	VAL
1	D	1275	GLU
1	r	549	GLU
1	s	549	GLU
1	s	1275	GLU
1	u	1275	GLU
2	i	148	PRO
2	j	148	PRO
2	l	110	GLU
2	m	146	ASP
2	n	12	TRP
5	d	183	ASN
1	q	1275	GLU
1	t	716	PRO
1	t	1275	GLU
2	f	104	LEU
4	V	3	SER
1	B	715	CYS
1	v	147	VAL
1	B	812	GLU
5	7	181	ILE
5	d	181	ILE
2	g	143	VAL
2	o	145	ILE
1	q	716	PRO
2	k	143	VAL

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	1218/1220 (100%)	1202 (99%)	16 (1%)	69	81
1	B	1218/1220 (100%)	1201 (99%)	17 (1%)	67	80
1	C	1204/1220 (99%)	1191 (99%)	13 (1%)	73	84
1	D	1218/1220 (100%)	1197 (98%)	21 (2%)	60	78
1	E	1218/1220 (100%)	1200 (98%)	18 (2%)	65	80
1	F	1218/1220 (100%)	1198 (98%)	20 (2%)	62	79
1	G	1218/1220 (100%)	1199 (98%)	19 (2%)	62	79
1	H	1218/1220 (100%)	1197 (98%)	21 (2%)	60	78
1	I	1218/1220 (100%)	1204 (99%)	14 (1%)	73	84
1	q	1180/1220 (97%)	1168 (99%)	12 (1%)	76	86
1	r	1218/1220 (100%)	1204 (99%)	14 (1%)	73	84
1	s	1218/1220 (100%)	1202 (99%)	16 (1%)	69	81
1	t	1218/1220 (100%)	1207 (99%)	11 (1%)	78	87
1	u	1219/1220 (100%)	1205 (99%)	14 (1%)	73	84
1	v	1180/1220 (97%)	1170 (99%)	10 (1%)	81	89
1	w	1133/1220 (93%)	1123 (99%)	10 (1%)	78	87
2	e	253/761 (33%)	247 (98%)	6 (2%)	49	69
2	f	253/761 (33%)	253 (100%)	0	100	100
2	g	253/761 (33%)	246 (97%)	7 (3%)	43	65
2	h	253/761 (33%)	249 (98%)	4 (2%)	62	79
2	i	253/761 (33%)	245 (97%)	8 (3%)	39	61
2	j	253/761 (33%)	246 (97%)	7 (3%)	43	65
2	k	253/761 (33%)	246 (97%)	7 (3%)	43	65
2	l	253/761 (33%)	246 (97%)	7 (3%)	43	65
2	m	253/761 (33%)	249 (98%)	4 (2%)	62	79
2	n	253/761 (33%)	247 (98%)	6 (2%)	49	69

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	o	253/761 (33%)	247 (98%)	6 (2%)	49	69
2	p	253/761 (33%)	248 (98%)	5 (2%)	55	74
3	1	52/77 (68%)	51 (98%)	1 (2%)	57	75
3	2	52/77 (68%)	51 (98%)	1 (2%)	57	75
3	3	52/77 (68%)	51 (98%)	1 (2%)	57	75
3	4	49/77 (64%)	48 (98%)	1 (2%)	55	74
3	J	52/77 (68%)	49 (94%)	3 (6%)	20	45
3	K	52/77 (68%)	51 (98%)	1 (2%)	57	75
3	L	52/77 (68%)	50 (96%)	2 (4%)	33	57
3	M	52/77 (68%)	51 (98%)	1 (2%)	57	75
3	N	52/77 (68%)	51 (98%)	1 (2%)	57	75
3	O	52/77 (68%)	51 (98%)	1 (2%)	57	75
3	P	52/77 (68%)	51 (98%)	1 (2%)	57	75
3	Q	52/77 (68%)	51 (98%)	1 (2%)	57	75
3	R	52/77 (68%)	51 (98%)	1 (2%)	57	75
3	x	52/77 (68%)	51 (98%)	1 (2%)	57	75
3	y	52/77 (68%)	51 (98%)	1 (2%)	57	75
3	z	52/77 (68%)	51 (98%)	1 (2%)	57	75
4	5	232/273 (85%)	230 (99%)	2 (1%)	78	87
4	S	273/273 (100%)	268 (98%)	5 (2%)	59	77
4	T	273/273 (100%)	271 (99%)	2 (1%)	84	90
4	U	273/273 (100%)	265 (97%)	8 (3%)	42	64
4	V	273/273 (100%)	266 (97%)	7 (3%)	46	66
5	6	261/274 (95%)	260 (100%)	1 (0%)	91	94
5	7	274/274 (100%)	270 (98%)	4 (2%)	65	80
5	W	274/274 (100%)	268 (98%)	6 (2%)	52	71
5	X	274/274 (100%)	272 (99%)	2 (1%)	84	90
5	Y	274/274 (100%)	269 (98%)	5 (2%)	59	77
5	Z	274/274 (100%)	264 (96%)	10 (4%)	35	59
5	a	273/274 (100%)	269 (98%)	4 (2%)	65	80
5	b	273/274 (100%)	266 (97%)	7 (3%)	46	66

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
5	c	273/274 (100%)	268 (98%)	5 (2%)	59 77
5	d	273/274 (100%)	269 (98%)	4 (2%)	65 80
All	All	27226/33989 (80%)	26822 (98%)	404 (2%)	66 80

All (404) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	ARG
1	A	139	LEU
1	A	140	GLU
1	A	244	ASN
1	A	691	ASN
1	A	743	ARG
1	A	746	ASN
1	A	772	ASN
1	A	831	LEU
1	A	839	MET
1	A	950	PHE
1	A	1029	ARG
1	A	1032	THR
1	A	1075	ASN
1	A	1134	ASN
1	A	1250	LYS
1	B	139	LEU
1	B	244	ASN
1	B	397	LEU
1	B	439	ARG
1	B	691	ASN
1	B	702	VAL
1	B	712	ARG
1	B	715	CYS
1	B	743	ARG
1	B	746	ASN
1	B	769	ARG
1	B	772	ASN
1	B	839	MET
1	B	1029	ARG
1	B	1075	ASN
1	B	1118	ASN
1	B	1250	LYS
1	C	244	ASN

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Mol	Chain	Res	Type
1	C	691	ASN
1	C	743	ARG
1	C	746	ASN
1	C	769	ARG
1	C	772	ASN
1	C	839	MET
1	C	854	GLN
1	C	855	LEU
1	C	950	PHE
1	C	1029	ARG
1	C	1075	ASN
1	C	1250	LYS
1	D	244	ASN
1	D	307	MET
1	D	397	LEU
1	D	691	ASN
1	D	702	VAL
1	D	709	PHE
1	D	729	LYS
1	D	743	ARG
1	D	746	ASN
1	D	754	ARG
1	D	769	ARG
1	D	772	ASN
1	D	809	PHE
1	D	831	LEU
1	D	839	MET
1	D	856	PHE
1	D	950	PHE
1	D	1029	ARG
1	D	1042	THR
1	D	1075	ASN
1	D	1250	LYS
1	E	244	ASN
1	E	439	ARG
1	E	691	ASN
1	E	702	VAL
1	E	743	ARG
1	E	746	ASN
1	E	769	ARG
1	E	772	ASN
1	E	831	LEU

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Mol	Chain	Res	Type
1	E	947	ASP
1	E	1029	ARG
1	E	1032	THR
1	E	1075	ASN
1	E	1130	PHE
1	E	1133	ILE
1	E	1135	LYS
1	E	1201	THR
1	E	1250	LYS
1	F	18	ASN
1	F	201	VAL
1	F	244	ASN
1	F	439	ARG
1	F	546	ARG
1	F	691	ASN
1	F	702	VAL
1	F	743	ARG
1	F	746	ASN
1	F	769	ARG
1	F	772	ASN
1	F	815	ILE
1	F	818	ASP
1	F	822	GLN
1	F	839	MET
1	F	1029	ARG
1	F	1035	ILE
1	F	1075	ASN
1	F	1118	ASN
1	F	1250	LYS
1	G	18	ASN
1	G	20	PHE
1	G	139	LEU
1	G	244	ASN
1	G	439	ARG
1	G	691	ASN
1	G	702	VAL
1	G	743	ARG
1	G	746	ASN
1	G	769	ARG
1	G	772	ASN
1	G	808	LEU
1	G	818	ASP

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Mol	Chain	Res	Type
1	G	830	VAL
1	G	831	LEU
1	G	839	MET
1	G	1029	ARG
1	G	1075	ASN
1	G	1250	LYS
1	H	36	ARG
1	H	53	LEU
1	H	244	ASN
1	H	439	ARG
1	H	464	MET
1	H	691	ASN
1	H	724	ASN
1	H	743	ARG
1	H	746	ASN
1	H	769	ARG
1	H	772	ASN
1	H	818	ASP
1	H	831	LEU
1	H	839	MET
1	H	1029	ARG
1	H	1032	THR
1	H	1075	ASN
1	H	1125	LEU
1	H	1230	CYS
1	H	1250	LYS
1	H	1255	MET
1	I	244	ASN
1	I	255	LEU
1	I	439	ARG
1	I	691	ASN
1	I	743	ARG
1	I	746	ASN
1	I	769	ARG
1	I	772	ASN
1	I	1029	ARG
1	I	1075	ASN
1	I	1126	ASN
1	I	1201	THR
1	I	1216	LEU
1	I	1250	LYS
1	q	90	LYS

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Mol	Chain	Res	Type
1	q	139	LEU
1	q	244	ASN
1	q	691	ASN
1	q	746	ASN
1	q	769	ARG
1	q	772	ASN
1	q	831	LEU
1	q	832	MET
1	q	1029	ARG
1	q	1075	ASN
1	q	1250	LYS
1	r	3	ASN
1	r	18	ASN
1	r	36	ARG
1	r	244	ASN
1	r	439	ARG
1	r	691	ASN
1	r	743	ARG
1	r	746	ASN
1	r	769	ARG
1	r	772	ASN
1	r	839	MET
1	r	1029	ARG
1	r	1075	ASN
1	r	1250	LYS
1	s	18	ASN
1	s	36	ARG
1	s	204	LYS
1	s	244	ASN
1	s	439	ARG
1	s	691	ASN
1	s	743	ARG
1	s	746	ASN
1	s	769	ARG
1	s	772	ASN
1	s	839	MET
1	s	860	ILE
1	s	1029	ARG
1	s	1075	ASN
1	s	1129	THR
1	s	1250	LYS
1	t	36	ARG

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Mol	Chain	Res	Type
1	t	244	ASN
1	t	439	ARG
1	t	691	ASN
1	t	743	ARG
1	t	746	ASN
1	t	772	ASN
1	t	839	MET
1	t	1029	ARG
1	t	1075	ASN
1	t	1250	LYS
1	u	1	MET
1	u	36	ARG
1	u	200	LYS
1	u	244	ASN
1	u	691	ASN
1	u	743	ARG
1	u	746	ASN
1	u	769	ARG
1	u	772	ASN
1	u	839	MET
1	u	1029	ARG
1	u	1036	LEU
1	u	1075	ASN
1	u	1250	LYS
1	v	244	ASN
1	v	691	ASN
1	v	743	ARG
1	v	746	ASN
1	v	769	ARG
1	v	772	ASN
1	v	839	MET
1	v	1075	ASN
1	v	1118	ASN
1	v	1250	LYS
1	w	45	ARG
1	w	104	ASN
1	w	231	ASN
1	w	241	ARG
1	w	439	ARG
1	w	563	LEU
1	w	745	ARG
1	w	832	MET

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Mol	Chain	Res	Type
1	w	1164	LYS
1	w	1206	THR
2	e	33	ASN
2	e	62	ASN
2	e	96	ASN
2	e	138	ARG
2	e	163	ASN
2	e	255	ARG
2	g	33	ASN
2	g	62	ASN
2	g	96	ASN
2	g	99	LEU
2	g	106	LYS
2	g	132	ARG
2	g	163	ASN
2	h	33	ASN
2	h	62	ASN
2	h	96	ASN
2	h	163	ASN
2	i	33	ASN
2	i	44	ASN
2	i	49	ARG
2	i	96	ASN
2	i	112	MET
2	i	138	ARG
2	i	163	ASN
2	i	171	MET
2	j	33	ASN
2	j	60	LEU
2	j	62	ASN
2	j	96	ASN
2	j	105	ASN
2	j	163	ASN
2	j	255	ARG
2	k	33	ASN
2	k	62	ASN
2	k	96	ASN
2	k	99	LEU
2	k	106	LYS
2	k	132	ARG
2	k	163	ASN
2	l	31	LEU

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Mol	Chain	Res	Type
2	l	33	ASN
2	l	62	ASN
2	l	96	ASN
2	l	108	ASN
2	l	163	ASN
2	l	180	ASN
2	m	33	ASN
2	m	62	ASN
2	m	96	ASN
2	m	163	ASN
2	n	33	ASN
2	n	60	LEU
2	n	62	ASN
2	n	96	ASN
2	n	132	ARG
2	n	163	ASN
2	o	10	PHE
2	o	31	LEU
2	o	33	ASN
2	o	96	ASN
2	o	132	ARG
2	o	163	ASN
2	p	33	ASN
2	p	62	ASN
2	p	96	ASN
2	p	108	ASN
2	p	163	ASN
3	J	26	GLU
3	J	27	LYS
3	J	76	MET
3	K	76	MET
3	L	23	LYS
3	L	76	MET
3	M	76	MET
3	N	76	MET
3	O	76	MET
3	P	76	MET
3	Q	76	MET
3	R	76	MET
3	x	76	MET
3	y	76	MET
3	z	76	MET

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Mol	Chain	Res	Type
3	1	76	MET
3	2	76	MET
3	3	76	MET
3	4	76	MET
4	5	53	ARG
4	5	120	VAL
4	S	53	ARG
4	S	96	LEU
4	S	111	LEU
4	S	120	VAL
4	S	240	PHE
4	T	53	ARG
4	T	180	PHE
4	U	31	LEU
4	U	32	ASN
4	U	34	VAL
4	U	53	ARG
4	U	85	ASN
4	U	120	VAL
4	U	184	ASP
4	U	241	LEU
4	V	31	LEU
4	V	32	ASN
4	V	34	VAL
4	V	53	ARG
4	V	120	VAL
4	V	240	PHE
4	V	241	LEU
5	6	75	ASN
5	W	75	ASN
5	W	178	LEU
5	W	224	LEU
5	W	235	ARG
5	W	242	ARG
5	W	295	LYS
5	X	75	ASN
5	X	235	ARG
5	Y	75	ASN
5	Y	183	ASN
5	Y	236	THR
5	Y	239	SER
5	Y	242	ARG

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Mol	Chain	Res	Type
5	Z	1	MET
5	Z	23	LEU
5	Z	75	ASN
5	Z	117	LYS
5	Z	118	LEU
5	Z	119	LEU
5	Z	235	ARG
5	Z	236	THR
5	Z	242	ARG
5	Z	246	LEU
5	7	1	MET
5	7	42	LEU
5	7	75	ASN
5	7	296	ASN
5	a	53	ASP
5	a	75	ASN
5	a	182	VAL
5	a	296	ASN
5	b	54	TYR
5	b	75	ASN
5	b	214	ASP
5	b	217	THR
5	b	227	LYS
5	b	231	LEU
5	b	296	ASN
5	c	52	LYS
5	c	75	ASN
5	c	181	ILE
5	c	185	LYS
5	c	296	ASN
5	d	75	ASN
5	d	216	LEU
5	d	231	LEU
5	d	296	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (534) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	244	ASN
1	A	260	ASN
1	A	294	GLN
1	A	432	ASN

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Mol	Chain	Res	Type
1	A	435	GLN
1	A	438	GLN
1	A	477	GLN
1	A	691	ASN
1	A	727	ASN
1	A	772	ASN
1	A	791	ASN
1	A	863	ASN
1	A	888	GLN
1	A	892	HIS
1	A	896	ASN
1	A	977	ASN
1	A	1000	GLN
1	A	1006	HIS
1	A	1111	HIS
1	B	155	ASN
1	B	211	GLN
1	B	244	ASN
1	B	294	GLN
1	B	387	GLN
1	B	432	ASN
1	B	543	GLN
1	B	581	HIS
1	B	691	ASN
1	B	746	ASN
1	B	772	ASN
1	B	847	ASN
1	B	891	GLN
1	B	896	ASN
1	B	1000	GLN
1	B	1110	HIS
1	B	1111	HIS
1	B	1118	ASN
1	B	1143	HIS
1	B	1159	ASN
1	B	1271	ASN
1	C	244	ASN
1	C	311	ASN
1	C	337	GLN
1	C	432	ASN
1	C	438	GLN
1	C	477	GLN

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Mol	Chain	Res	Type
1	C	543	GLN
1	C	691	ASN
1	C	746	ASN
1	C	772	ASN
1	C	854	GLN
1	C	896	ASN
1	C	1000	GLN
1	C	1168	ASN
1	C	1239	ASN
1	C	1320	GLN
1	C	1325	HIS
1	D	244	ASN
1	D	331	ASN
1	D	435	GLN
1	D	581	HIS
1	D	691	ASN
1	D	739	GLN
1	D	746	ASN
1	D	772	ASN
1	D	891	GLN
1	D	896	ASN
1	D	1000	GLN
1	D	1053	ASN
1	D	1105	ASN
1	D	1111	HIS
1	D	1159	ASN
1	D	1194	HIS
1	D	1325	HIS
1	E	18	ASN
1	E	202	HIS
1	E	244	ASN
1	E	260	ASN
1	E	294	GLN
1	E	378	ASN
1	E	387	GLN
1	E	432	ASN
1	E	435	GLN
1	E	438	GLN
1	E	534	HIS
1	E	543	GLN
1	E	691	ASN
1	E	772	ASN

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Mol	Chain	Res	Type
1	E	791	ASN
1	E	946	ASN
1	E	1000	GLN
1	E	1089	ASN
1	E	1101	ASN
1	E	1111	HIS
1	E	1134	ASN
1	E	1159	ASN
1	E	1239	ASN
1	E	1325	HIS
1	F	18	ASN
1	F	203	ASN
1	F	244	ASN
1	F	294	GLN
1	F	378	ASN
1	F	387	GLN
1	F	432	ASN
1	F	438	GLN
1	F	473	HIS
1	F	543	GLN
1	F	581	HIS
1	F	691	ASN
1	F	746	ASN
1	F	772	ASN
1	F	822	GLN
1	F	847	ASN
1	F	891	GLN
1	F	896	ASN
1	F	938	ASN
1	F	1000	GLN
1	F	1057	HIS
1	F	1097	HIS
1	F	1101	ASN
1	F	1105	ASN
1	F	1111	HIS
1	F	1118	ASN
1	F	1143	HIS
1	G	5	GLN
1	G	18	ASN
1	G	123	HIS
1	G	138	HIS
1	G	155	ASN

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Mol	Chain	Res	Type
1	G	203	ASN
1	G	244	ASN
1	G	294	GLN
1	G	387	GLN
1	G	432	ASN
1	G	438	GLN
1	G	543	GLN
1	G	581	HIS
1	G	691	ASN
1	G	740	ASN
1	G	746	ASN
1	G	772	ASN
1	G	847	ASN
1	G	863	ASN
1	G	888	GLN
1	G	891	GLN
1	G	896	ASN
1	G	938	ASN
1	G	964	GLN
1	G	1000	GLN
1	G	1097	HIS
1	G	1111	HIS
1	G	1134	ASN
1	G	1143	HIS
1	H	244	ASN
1	H	331	ASN
1	H	387	GLN
1	H	435	GLN
1	H	581	HIS
1	H	691	ASN
1	H	724	ASN
1	H	739	GLN
1	H	740	ASN
1	H	746	ASN
1	H	772	ASN
1	H	888	GLN
1	H	896	ASN
1	H	964	GLN
1	H	1000	GLN
1	H	1101	ASN
1	H	1111	HIS
1	H	1159	ASN

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Mol	Chain	Res	Type
1	I	244	ASN
1	I	294	GLN
1	I	432	ASN
1	I	438	GLN
1	I	543	GLN
1	I	581	HIS
1	I	691	ASN
1	I	746	ASN
1	I	772	ASN
1	I	896	ASN
1	I	964	GLN
1	I	1000	GLN
1	I	1101	ASN
1	I	1111	HIS
1	I	1126	ASN
1	I	1159	ASN
1	I	1325	HIS
1	q	203	ASN
1	q	211	GLN
1	q	244	ASN
1	q	294	GLN
1	q	432	ASN
1	q	438	GLN
1	q	543	GLN
1	q	581	HIS
1	q	691	ASN
1	q	746	ASN
1	q	772	ASN
1	q	791	ASN
1	q	891	GLN
1	q	942	HIS
1	q	1000	GLN
1	q	1111	HIS
1	q	1168	ASN
1	q	1182	HIS
1	r	3	ASN
1	r	5	GLN
1	r	21	ASN
1	r	138	HIS
1	r	155	ASN
1	r	244	ASN
1	r	294	GLN

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Mol	Chain	Res	Type
1	r	387	GLN
1	r	432	ASN
1	r	435	GLN
1	r	438	GLN
1	r	543	GLN
1	r	581	HIS
1	r	658	ASN
1	r	691	ASN
1	r	746	ASN
1	r	772	ASN
1	r	847	ASN
1	r	888	GLN
1	r	891	GLN
1	r	1000	GLN
1	r	1111	HIS
1	r	1168	ASN
1	r	1241	GLN
1	r	1325	HIS
1	s	18	ASN
1	s	119	HIS
1	s	138	HIS
1	s	244	ASN
1	s	294	GLN
1	s	378	ASN
1	s	382	ASN
1	s	387	GLN
1	s	432	ASN
1	s	435	GLN
1	s	438	GLN
1	s	543	GLN
1	s	560	ASN
1	s	672	HIS
1	s	691	ASN
1	s	746	ASN
1	s	772	ASN
1	s	847	ASN
1	s	891	GLN
1	s	1000	GLN
1	s	1105	ASN
1	s	1111	HIS
1	s	1168	ASN
1	s	1252	ASN

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Mol	Chain	Res	Type
1	t	145	ASN
1	t	150	GLN
1	t	244	ASN
1	t	294	GLN
1	t	387	GLN
1	t	432	ASN
1	t	438	GLN
1	t	543	GLN
1	t	581	HIS
1	t	691	ASN
1	t	746	ASN
1	t	772	ASN
1	t	847	ASN
1	t	891	GLN
1	t	892	HIS
1	t	1000	GLN
1	t	1111	HIS
1	t	1168	ASN
1	t	1338	GLN
1	u	244	ASN
1	u	294	GLN
1	u	304	HIS
1	u	387	GLN
1	u	432	ASN
1	u	435	GLN
1	u	438	GLN
1	u	543	GLN
1	u	560	ASN
1	u	581	HIS
1	u	672	HIS
1	u	691	ASN
1	u	746	ASN
1	u	772	ASN
1	u	891	GLN
1	u	892	HIS
1	u	896	ASN
1	u	1000	GLN
1	u	1097	HIS
1	u	1101	ASN
1	u	1111	HIS
1	u	1168	ASN
1	v	155	ASN

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Mol	Chain	Res	Type
1	v	211	GLN
1	v	244	ASN
1	v	294	GLN
1	v	331	ASN
1	v	432	ASN
1	v	435	GLN
1	v	438	GLN
1	v	543	GLN
1	v	659	HIS
1	v	691	ASN
1	v	746	ASN
1	v	772	ASN
1	v	888	GLN
1	v	891	GLN
1	v	892	HIS
1	v	1000	GLN
1	v	1111	HIS
1	v	1118	ASN
1	v	1241	GLN
1	v	1325	HIS
1	w	104	ASN
1	w	119	HIS
1	w	141	ASN
1	w	202	HIS
1	w	387	GLN
1	w	432	ASN
1	w	466	ASN
1	w	477	GLN
1	w	514	ASN
1	w	617	HIS
1	w	746	ASN
1	w	847	ASN
1	w	854	GLN
1	w	863	ASN
1	w	879	GLN
1	w	881	HIS
1	w	934	GLN
1	w	964	GLN
1	w	1088	GLN
1	w	1097	HIS
1	w	1182	HIS
1	w	1297	ASN

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Mol	Chain	Res	Type
1	w	1318	ASN
2	e	33	ASN
2	e	71	HIS
2	e	96	ASN
2	f	33	ASN
2	f	71	HIS
2	f	82	ASN
2	f	105	ASN
2	f	163	ASN
2	f	194	ASN
2	f	248	GLN
2	g	33	ASN
2	g	44	ASN
2	g	71	HIS
2	g	92	GLN
2	g	115	ASN
2	g	122	GLN
2	g	163	ASN
2	g	194	ASN
2	h	27	ASN
2	h	30	ASN
2	h	33	ASN
2	h	71	HIS
2	h	92	GLN
2	h	122	GLN
2	h	194	ASN
2	h	237	ASN
2	i	27	ASN
2	i	33	ASN
2	i	39	HIS
2	i	44	ASN
2	i	71	HIS
2	i	96	ASN
2	i	194	ASN
2	j	33	ASN
2	j	71	HIS
2	j	96	ASN
2	j	105	ASN
2	j	163	ASN
2	j	248	GLN
2	k	30	ASN
2	k	33	ASN

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Mol	Chain	Res	Type
2	k	44	ASN
2	k	71	HIS
2	k	92	GLN
2	k	108	ASN
2	k	163	ASN
2	k	239	ASN
2	l	33	ASN
2	l	71	HIS
2	l	92	GLN
2	l	108	ASN
2	l	142	ASN
2	l	163	ASN
2	l	180	ASN
2	l	237	ASN
2	m	33	ASN
2	m	62	ASN
2	m	71	HIS
2	m	92	GLN
2	n	62	ASN
2	n	71	HIS
2	n	92	GLN
2	n	96	ASN
2	n	248	GLN
2	n	254	GLN
2	o	27	ASN
2	o	33	ASN
2	o	44	ASN
2	o	62	ASN
2	o	71	HIS
2	o	92	GLN
2	o	111	ASN
2	p	27	ASN
2	p	30	ASN
2	p	33	ASN
2	p	71	HIS
2	p	108	ASN
2	p	115	ASN
2	p	142	ASN
2	p	186	ASN
3	J	46	HIS
3	J	59	GLN
3	J	60	ASN

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Mol	Chain	Res	Type
3	K	46	HIS
3	K	59	GLN
3	K	60	ASN
3	L	46	HIS
3	L	59	GLN
3	L	60	ASN
3	M	46	HIS
3	M	59	GLN
3	M	60	ASN
3	N	46	HIS
3	N	59	GLN
3	N	60	ASN
3	O	46	HIS
3	O	59	GLN
3	O	60	ASN
3	P	46	HIS
3	P	59	GLN
3	P	60	ASN
3	Q	46	HIS
3	Q	59	GLN
3	Q	60	ASN
3	R	46	HIS
3	R	59	GLN
3	R	60	ASN
3	x	46	HIS
3	x	59	GLN
3	x	60	ASN
3	y	46	HIS
3	y	59	GLN
3	y	60	ASN
3	z	46	HIS
3	z	59	GLN
3	z	60	ASN
3	1	46	HIS
3	1	59	GLN
3	1	60	ASN
3	2	46	HIS
3	2	59	GLN
3	2	60	ASN
3	3	59	GLN
3	3	60	ASN
3	4	46	HIS

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Mol	Chain	Res	Type
3	4	59	GLN
3	4	60	ASN
4	S	193	GLN
4	T	220	GLN
4	T	242	ASN
4	U	122	ASN
4	V	122	ASN
4	V	161	ASN
5	6	34	HIS
5	6	75	ASN
5	6	170	GLN
5	W	34	HIS
5	W	75	ASN
5	W	170	GLN
5	W	221	HIS
5	X	34	HIS
5	X	75	ASN
5	X	170	GLN
5	X	186	GLN
5	X	247	HIS
5	Y	34	HIS
5	Y	75	ASN
5	Y	153	HIS
5	Y	170	GLN
5	Y	183	ASN
5	Y	221	HIS
5	Y	269	ASN
5	Z	34	HIS
5	Z	75	ASN
5	Z	76	GLN
5	Z	153	HIS
5	Z	170	GLN
5	Z	221	HIS
5	Z	269	ASN
5	7	75	ASN
5	7	76	GLN
5	7	113	HIS
5	7	229	GLN
5	7	296	ASN
5	a	51	ASN
5	a	75	ASN
5	a	76	GLN

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Mol	Chain	Res	Type
5	a	87	GLN
5	a	92	ASN
5	a	229	GLN
5	a	296	ASN
5	b	56	HIS
5	b	75	ASN
5	b	87	GLN
5	b	92	ASN
5	b	229	GLN
5	b	267	GLN
5	b	296	ASN
5	c	75	ASN
5	c	113	HIS
5	c	153	HIS
5	c	229	GLN
5	c	247	HIS
5	c	296	ASN
5	d	75	ASN
5	d	87	GLN
5	d	92	ASN
5	d	113	HIS
5	d	157	ASN
5	d	221	HIS
5	d	245	GLN
5	d	247	HIS
5	d	296	ASN

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.

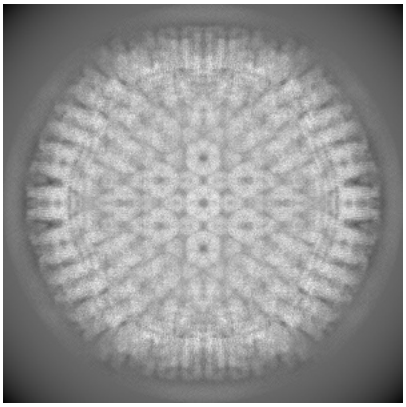
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-20557. These allow visual inspection of the internal detail of the map and identification of artifacts.

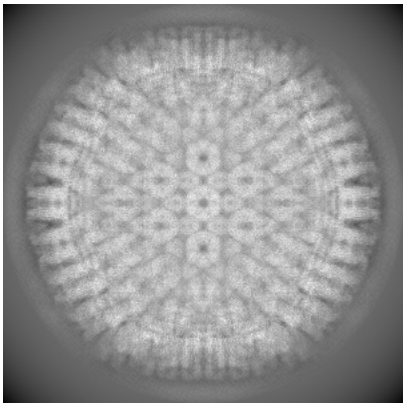
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

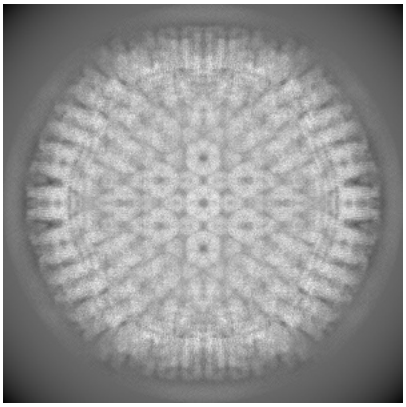
6.1.1 Primary map



X



Y

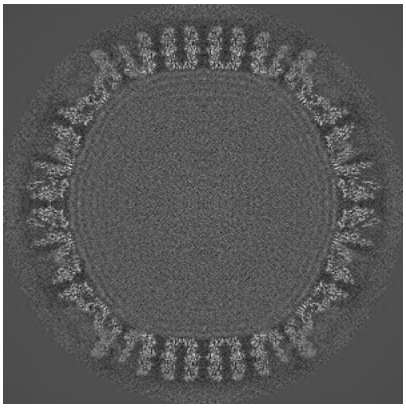


Z

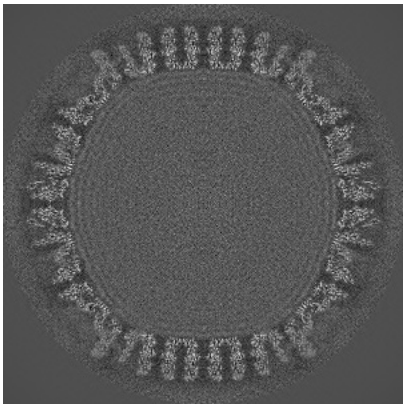
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

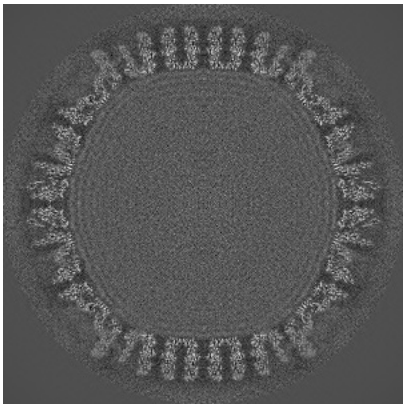
6.2.1 Primary map



X Index: 320



Y Index: 320

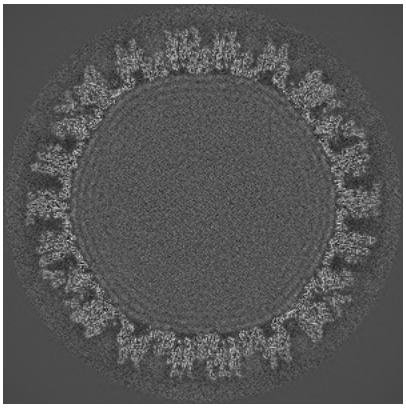


Z Index: 320

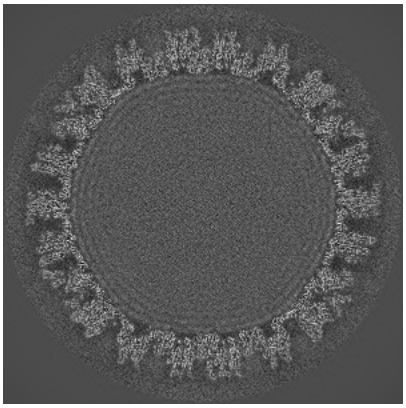
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

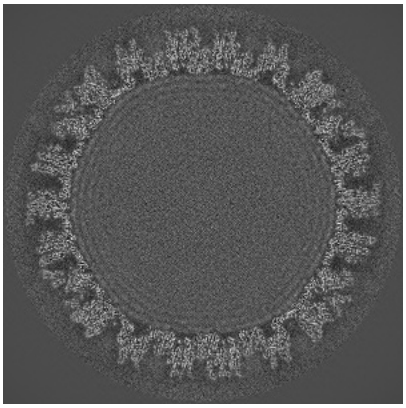
6.3.1 Primary map



X Index: 266



Y Index: 266

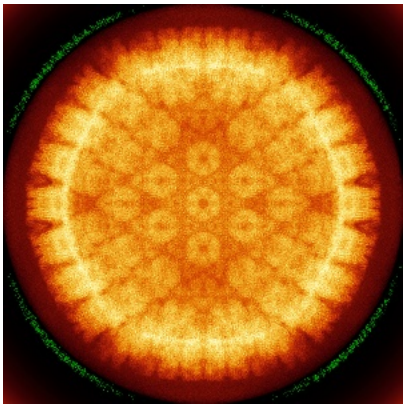


Z Index: 266

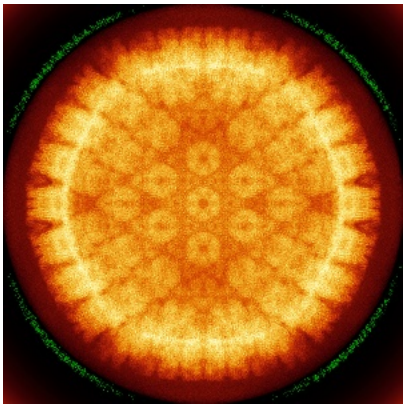
The images above show the largest variance slices of the map in three orthogonal directions.

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

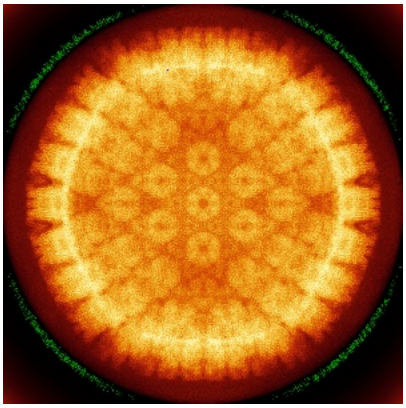
6.4.1 Primary map



X



Y



Z

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 0.036. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

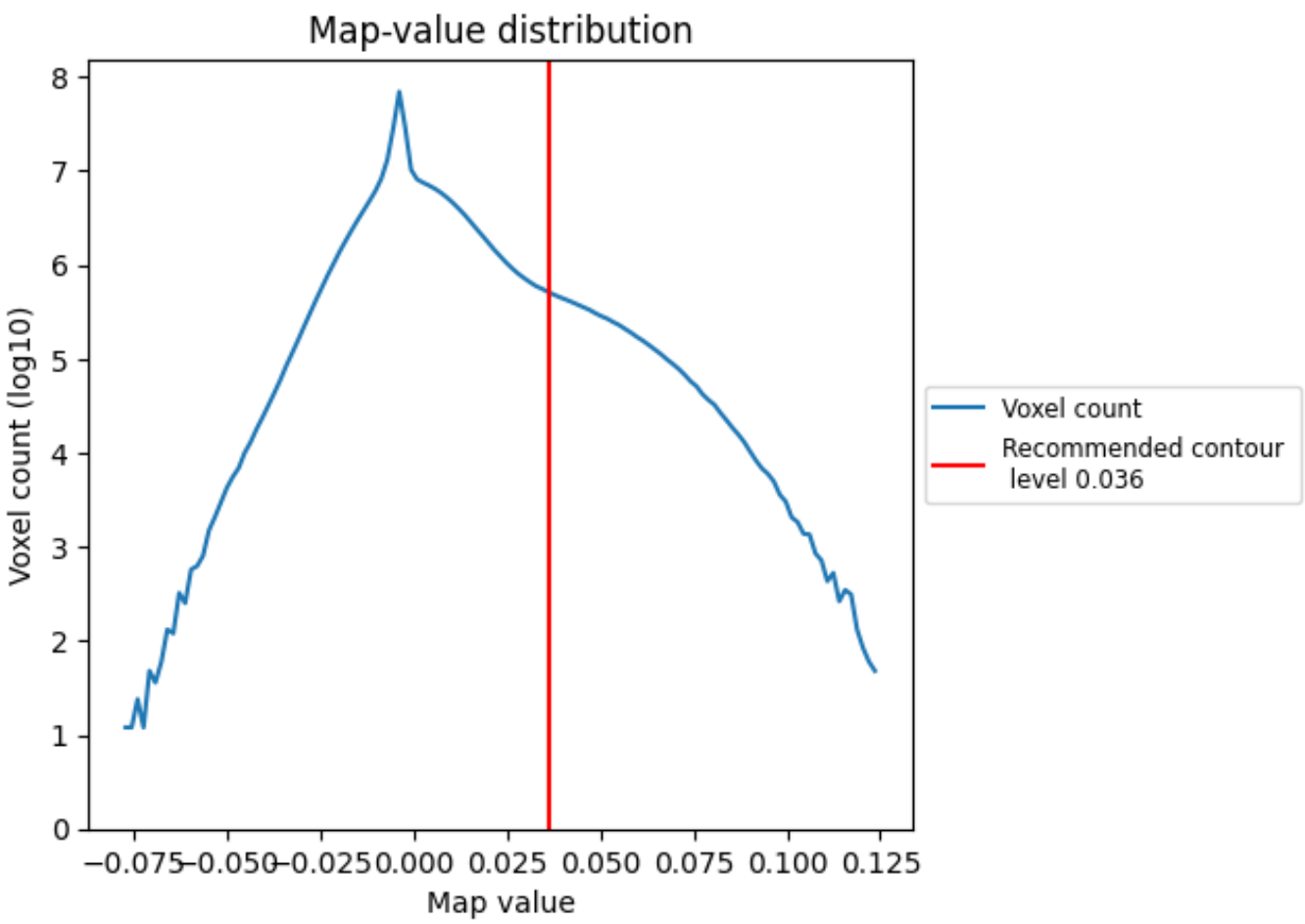
6.6 Mask visualisation (i)

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

7 Map analysis (i)

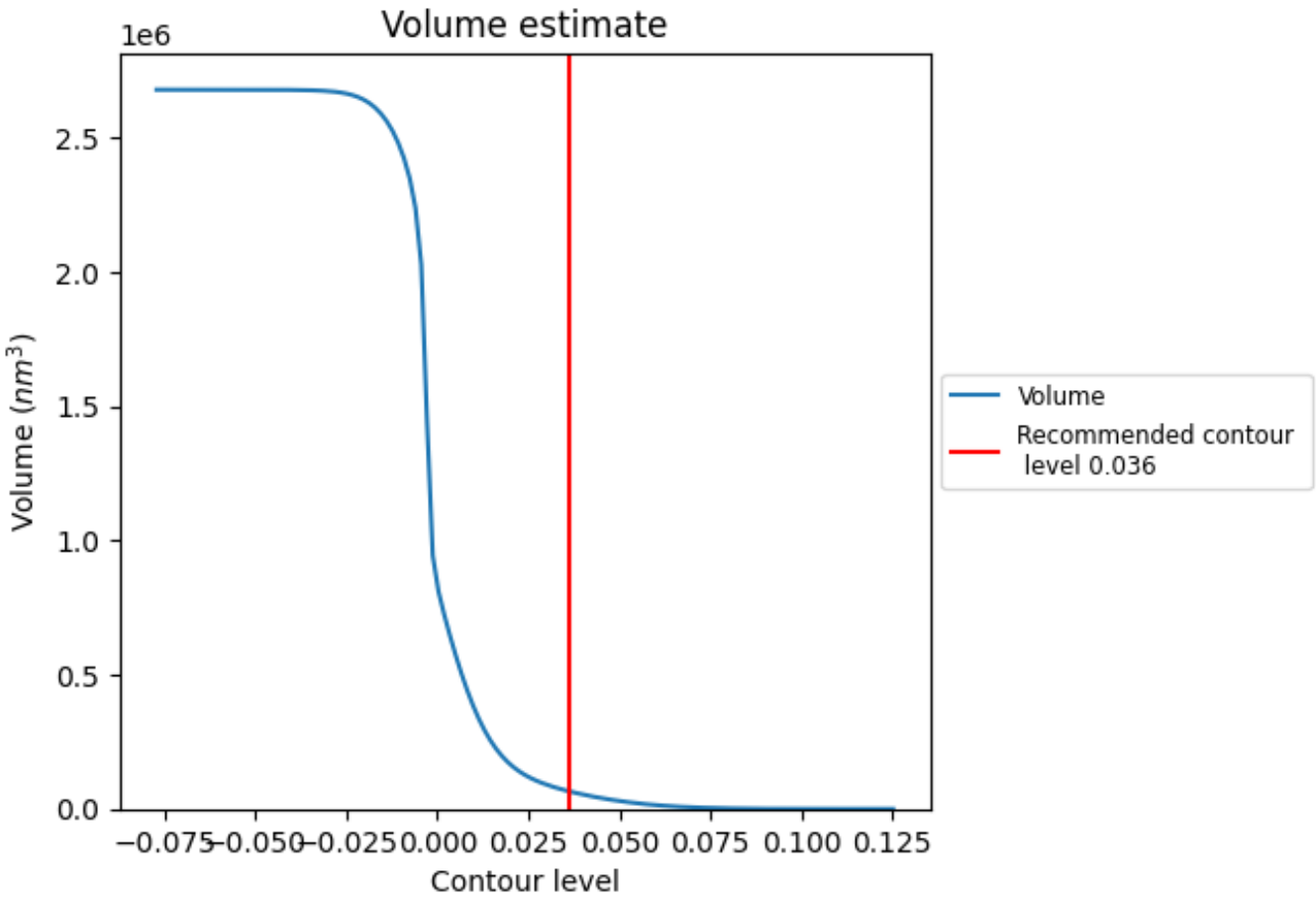
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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.

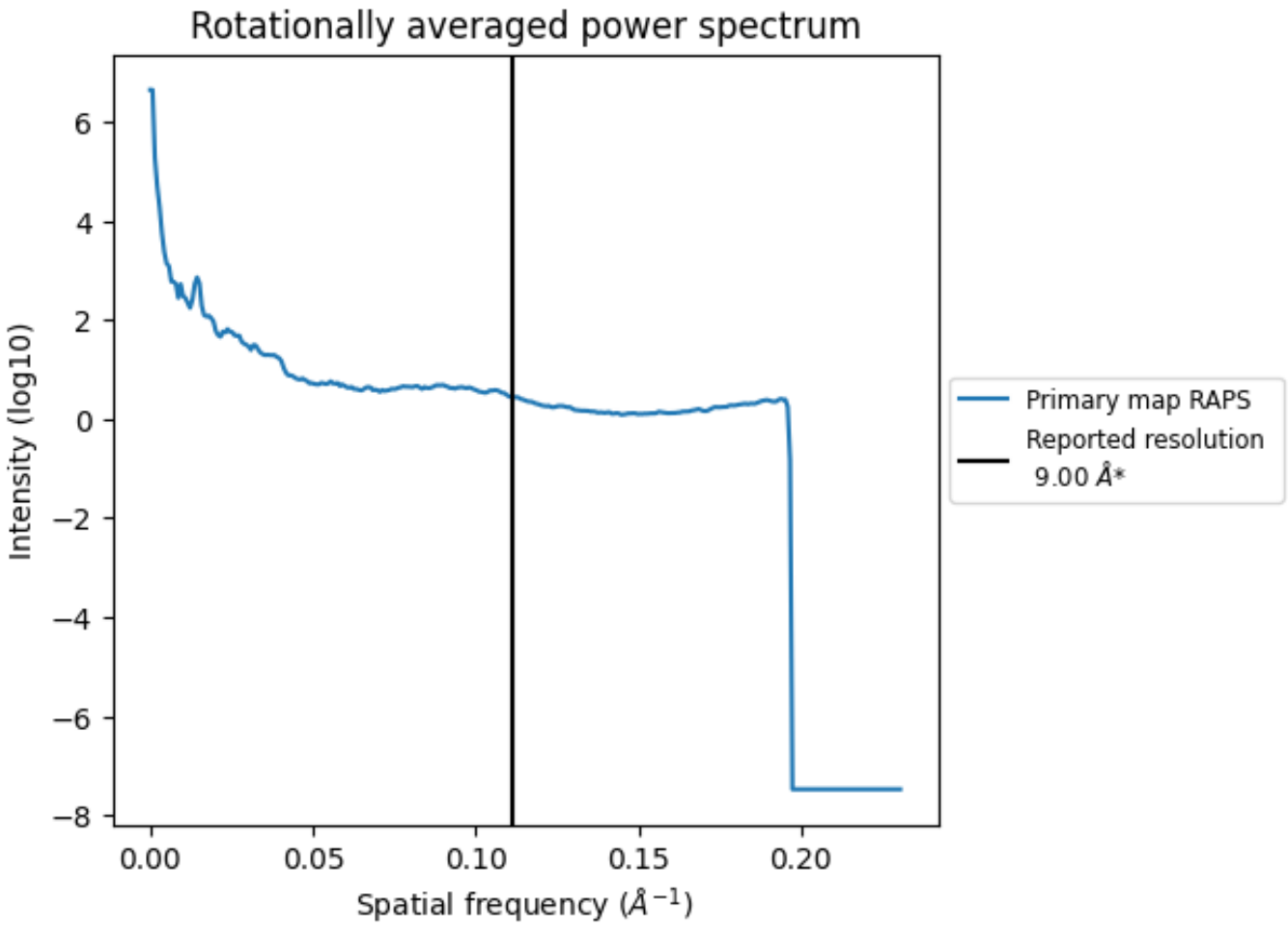
7.2 Volume estimate (i)



The volume at the recommended contour level is 66298 nm^3; this corresponds to an approximate mass of 59889 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 0.111 Å^{-1}

8 Fourier-Shell correlation (i)

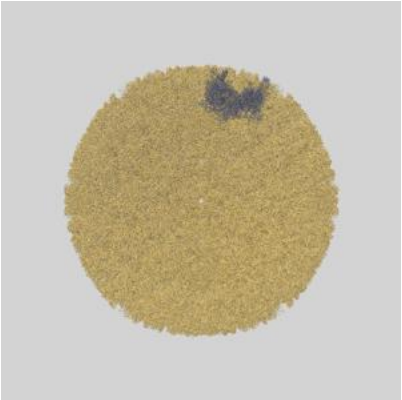
This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit (i)

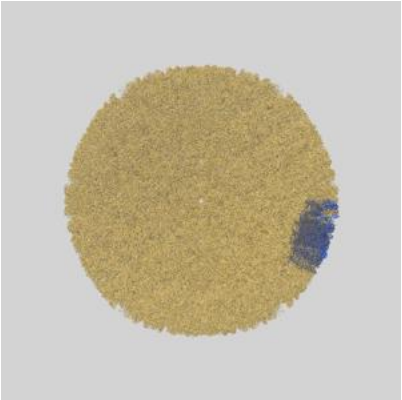
This section contains information regarding the fit between EMDB map EMD-20557 and PDB model 6Q1F. Per-residue inclusion information can be found in section 3 on page 9.

9.1 Map-model overlays

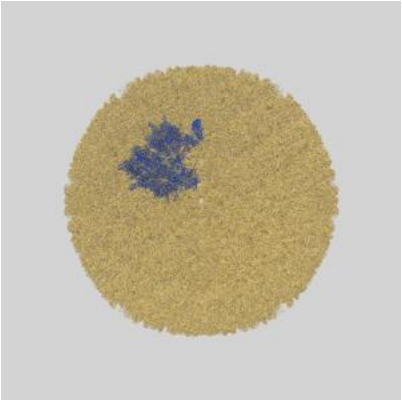
9.1.1 Map-model overlay (i)



X

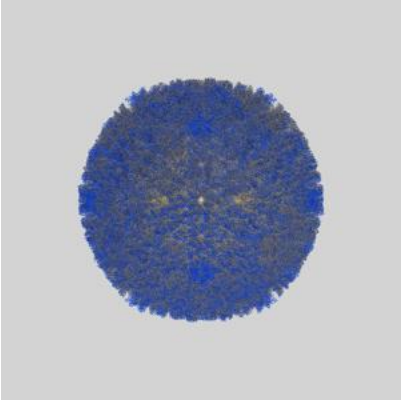


Y

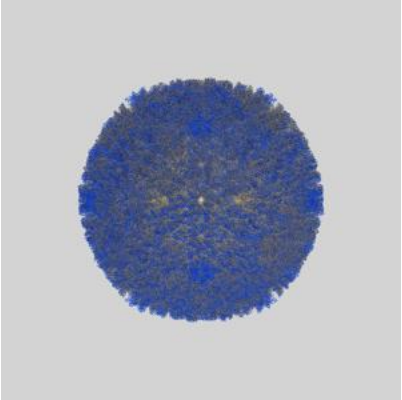


Z

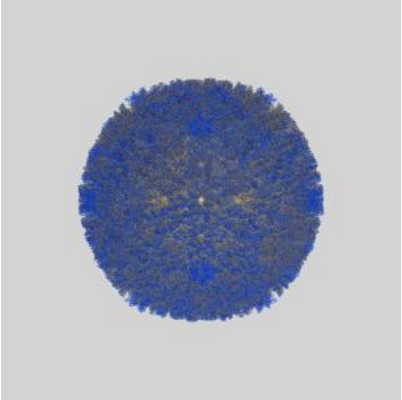
9.1.2 Map-model assembly overlay (i)



X



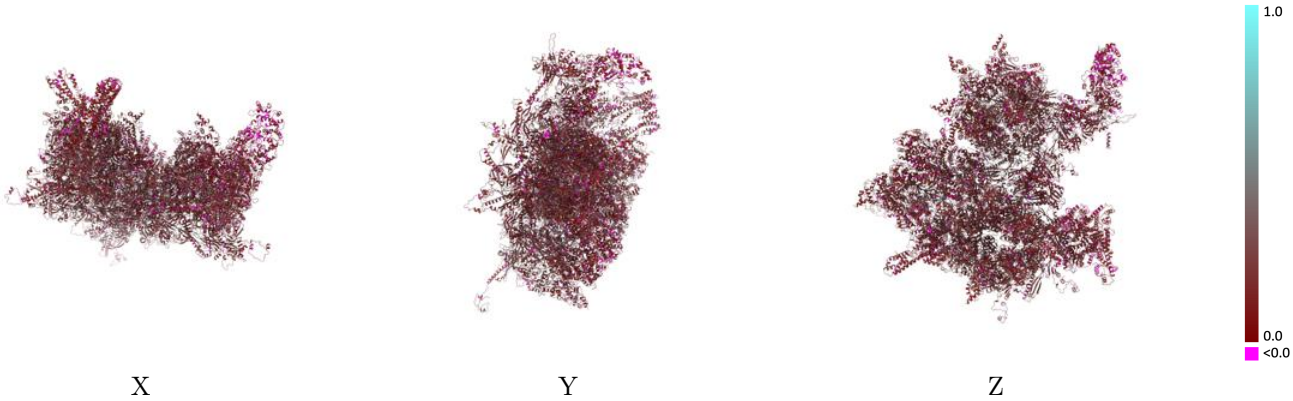
Y



Z

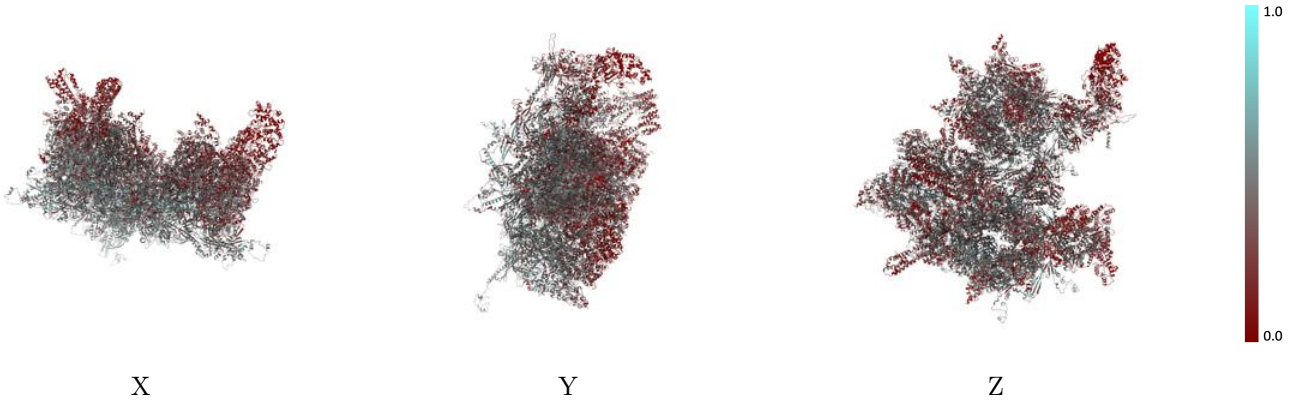
The images above show the 3D surface view of the map at the recommended contour level 0.036 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



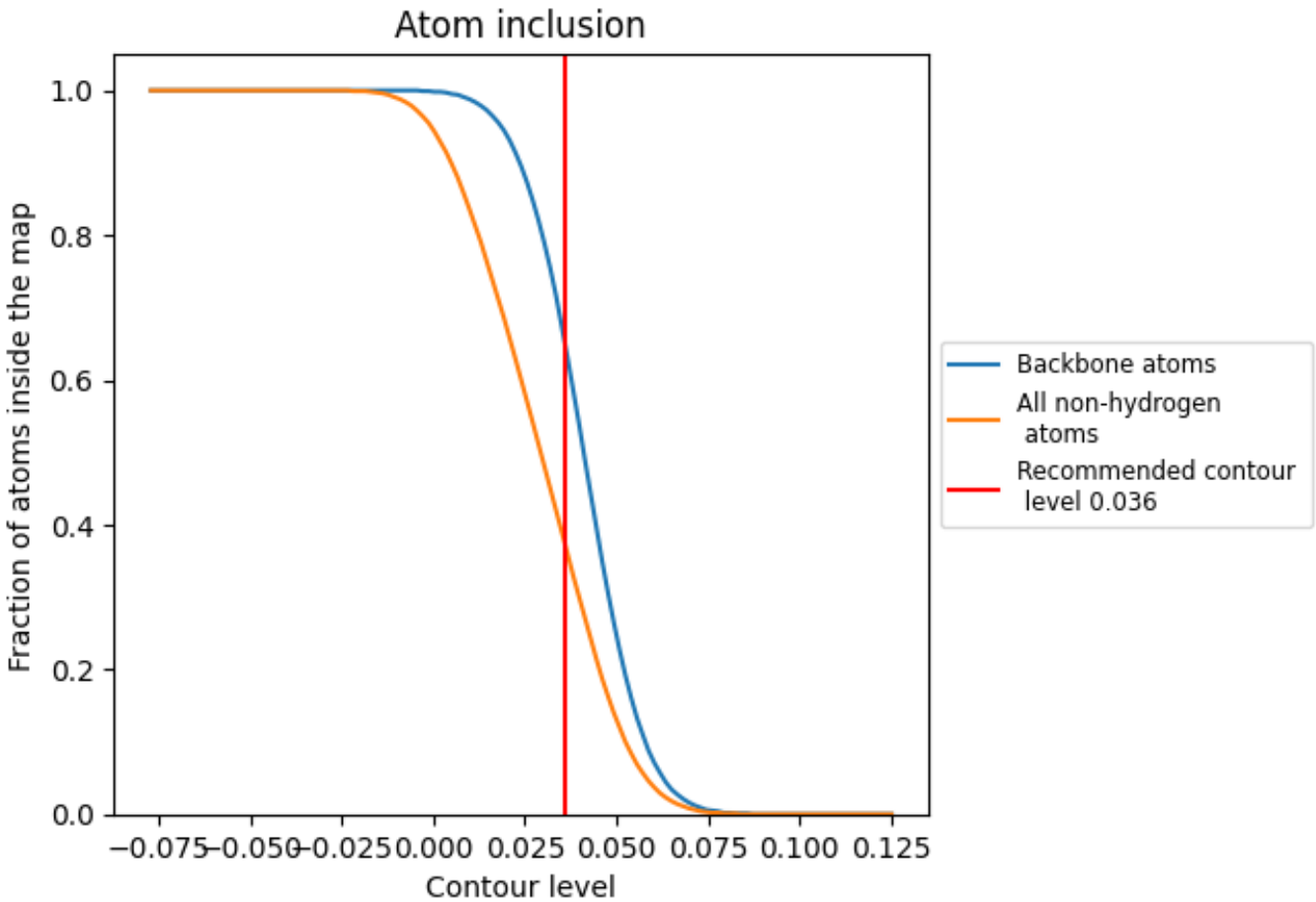
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (i)



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 (0.036).

9.4 Atom inclusion (i)



At the recommended contour level, 65% of all backbone atoms, 37% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.036) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.3730	0.2130
1	0.3130	0.1980
2	0.2630	0.1960
3	0.1550	0.1720
4	0.0020	0.1250
5	0.3020	0.2000
6	0.2610	0.1820
7	0.2510	0.1770
A	0.4450	0.2310
B	0.4320	0.2250
C	0.4360	0.2330
D	0.4520	0.2340
E	0.4520	0.2330
F	0.4260	0.2240
G	0.4410	0.2260
H	0.4620	0.2370
I	0.4430	0.2290
J	0.2860	0.1930
K	0.2750	0.2050
L	0.2460	0.2050
M	0.2900	0.1910
N	0.2610	0.2000
O	0.2160	0.2160
P	0.2900	0.1820
Q	0.2480	0.1880
R	0.2790	0.1850
S	0.4240	0.2310
T	0.3590	0.2160
U	0.4060	0.2300
V	0.4190	0.2280
W	0.3780	0.2090
X	0.3300	0.2030
Y	0.3680	0.2050
Z	0.3840	0.2100
a	0.3800	0.2150

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Chain	Atom inclusion	Q-score
b	0.3540	0.2050
c	0.3910	0.2110
d	0.3850	0.2110
e	0.1900	0.1650
f	0.1630	0.1710
g	0.2110	0.1730
h	0.1070	0.1560
i	0.1960	0.1750
j	0.1240	0.1680
k	0.2250	0.1540
l	0.1050	0.1590
m	0.2480	0.1690
n	0.2660	0.1640
o	0.2990	0.1730
p	0.2170	0.1740
q	0.3610	0.2130
r	0.4000	0.2230
s	0.4050	0.2190
t	0.4220	0.2250
u	0.4020	0.2170
v	0.3810	0.2120
w	0.1810	0.1650
x	0.1410	0.1800
y	0.1680	0.1790
z	0.2250	0.1960