wwPDB EM Validation Summary Report (i)

Dec 10, 2022 – 10:52 am GMT

PDB ID	:	5G05
EMDB ID	:	EMD-3388
Title	:	Cryo-EM structure of combined apo phosphorylated APC
Authors	:	Zhang, S.; Chang, L.; Alfieri, C.; Zhang, Z.; Yang, J.; Maslen, S.; Skehel, M.; Barford, D.
Deposited on	:	2016-03-16
Resolution	:	3.50 Å(reported)

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

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

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

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

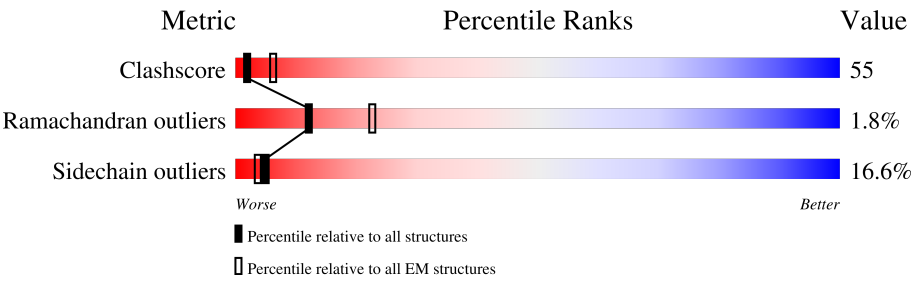
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	A	1944	27% 39% 13% • 19%
2	B	84	82% 67% 23% 8% •
3	C	597	44% 37% 7% 12%
3	P	597	5% 46% 30% 6% 18%
4	D	121	31% 12% • 55%
5	E	110	25% 21% 5% 49%
6	F	824	6% 30% 21% 5% 44%
6	H	824	34% 22% • 41%

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Mol	Chain	Length	Quality of chain
7	G	85	11% 11% 8% 71%
7	W	85	7% 15% 7% • 69%
8	I	808	5% 42% 35% 11% • 11%
9	J	620	• 38% 35% 8% 19%
9	K	620	• 33% 38% 8% 20%
10	L	185	6% 45% 44% 8% • •
11	M	74	8% 24% 39% 14% • 20%
12	N	822	13% 22% 37% 14% • 27%
13	O	755	• 41% 37% 12% • 9%
14	T	15	13% 67% 27% 7%
15	X	599	11% 41% 35% 5% • 19%
15	Y	599	7% 41% 35% 6% • 17%

2 Entry composition (i)

There are 16 unique types of molecules in this entry. The entry contains 63181 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 ANAPHASE-PROMOTING COMPLEX SUBUNIT 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1569	11890	7656	2014	2140	80	0	0

- Molecule 2 is a protein called ANAPHASE-PROMOTING COMPLEX SUBUNIT 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	84	649	416	117	99	17	1	0

- Molecule 3 is a protein called CELL DIVISION CYCLE PROTEIN 23 HOMOLOG.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	524	4306	2774	727	781	24	0	0
3	P	492	4046	2613	679	730	24	0	0

- Molecule 4 is a protein called ANAPHASE-PROMOTING COMPLEX SUBUNIT 15.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	D	55	436	277	73	86	0	0

- Molecule 5 is a protein called ANAPHASE-PROMOTING COMPLEX SUBUNIT 16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	56	450	290	74	85	1	0	0

- Molecule 6 is a protein called CELL DIVISION CYCLE PROTEIN 27 HOMOLOG.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	460	3618	2320	608	666	24	0	0
6	H	488	3879	2489	655	709	26	0	0

- Molecule 7 is a protein called ANAPHASE-PROMOTING COMPLEX SUBUNIT CDC26.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	G	25	220	137	41	41	1	0	0
7	W	26	218	136	41	40	1	0	0

- Molecule 8 is a protein called ANAPHASE-PROMOTING COMPLEX SUBUNIT 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	I	723	5634	3619	940	1041	34	0	0

- Molecule 9 is a protein called CELL DIVISION CYCLE PROTEIN 16 HOMOLOG.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	J	504	4053	2604	687	737	25	0	0
9	K	493	3988	2564	672	728	24	0	0

- Molecule 10 is a protein called ANAPHASE-PROMOTING COMPLEX SUBUNIT 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	L	182	1435	898	263	268	6	0	0

- Molecule 11 is a protein called ANAPHASE-PROMOTING COMPLEX SUBUNIT 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	M	59	481	304	79	96	2	0	0

- Molecule 12 is a protein called ANAPHASE-PROMOTING COMPLEX SUBUNIT 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	N	604	4767	3053	851	841	22	0	0

- Molecule 13 is a protein called ANAPHASE-PROMOTING COMPLEX SUBUNIT 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	O	688	5400	3443	940	989	28	0	0

- Molecule 14 is a protein called UNIDENTIFIED PEPTIDE.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
14	T	15	79	47	16	16	0	0

- Molecule 15 is a protein called ANAPHASE-PROMOTING COMPLEX SUBUNIT 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	X	484	3767	2390	649	704	24	0	0
			Total	C	N	O	S		
15	Y	496	3862	2446	666	724	26	0	0

- Molecule 16 is ZINC ION (three-letter code: ZN) (formula: Zn).

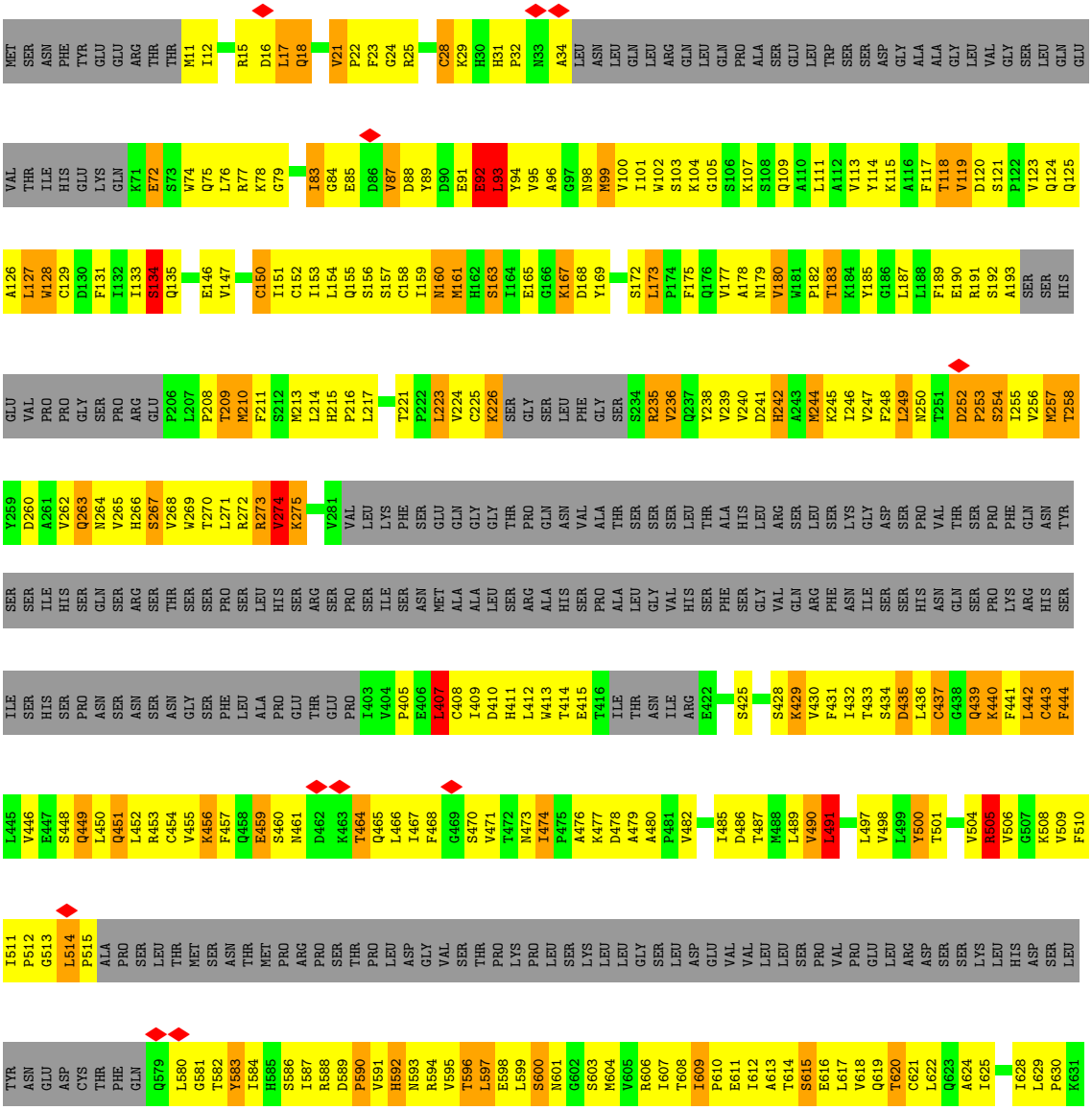
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
16	B	3	3	3	0

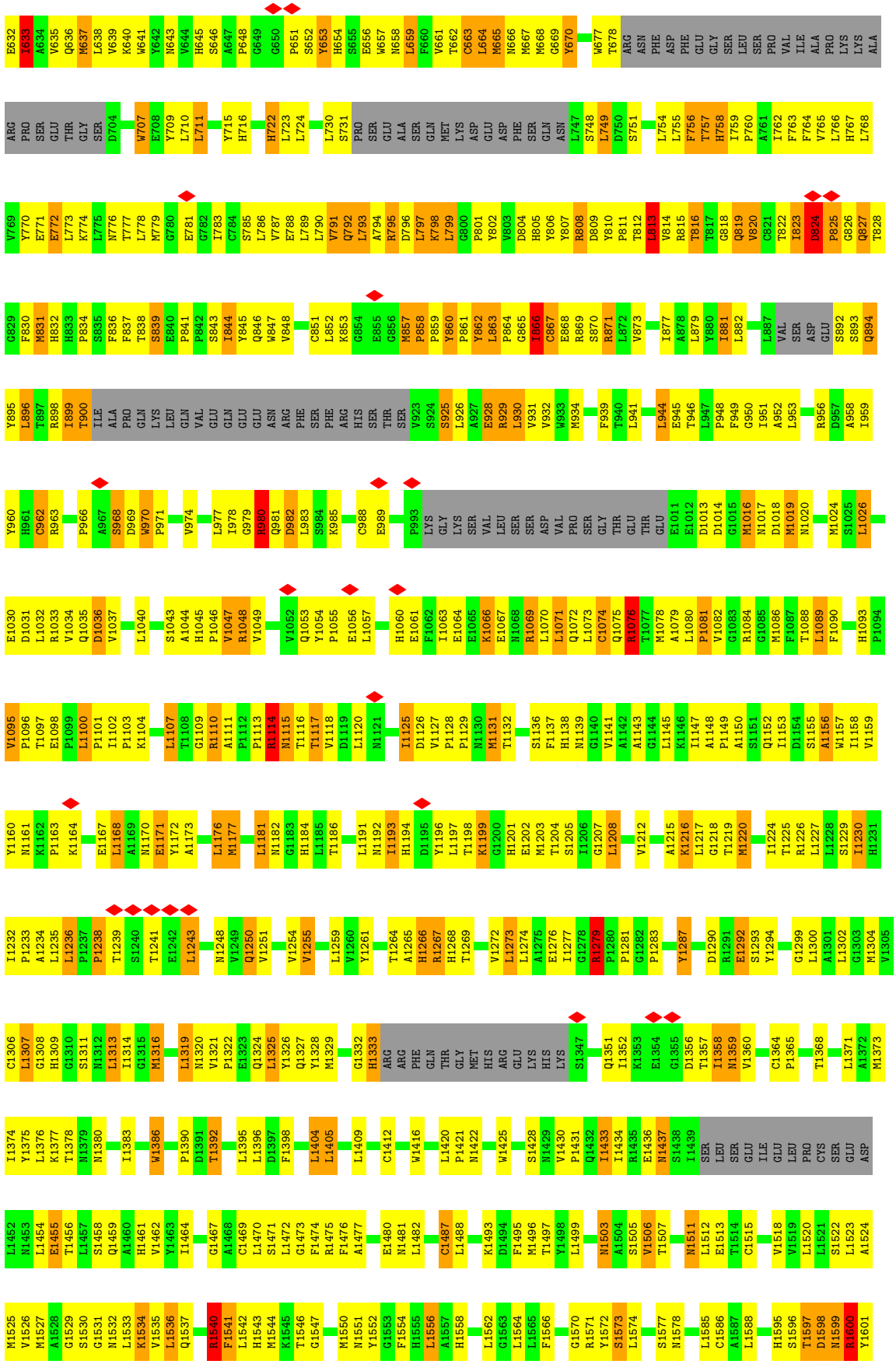
3 Residue-property plots (i)

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: ANAPHASE-PROMOTING COMPLEX SUBUNIT 1

Chain A: 27% 39% 13% 19%

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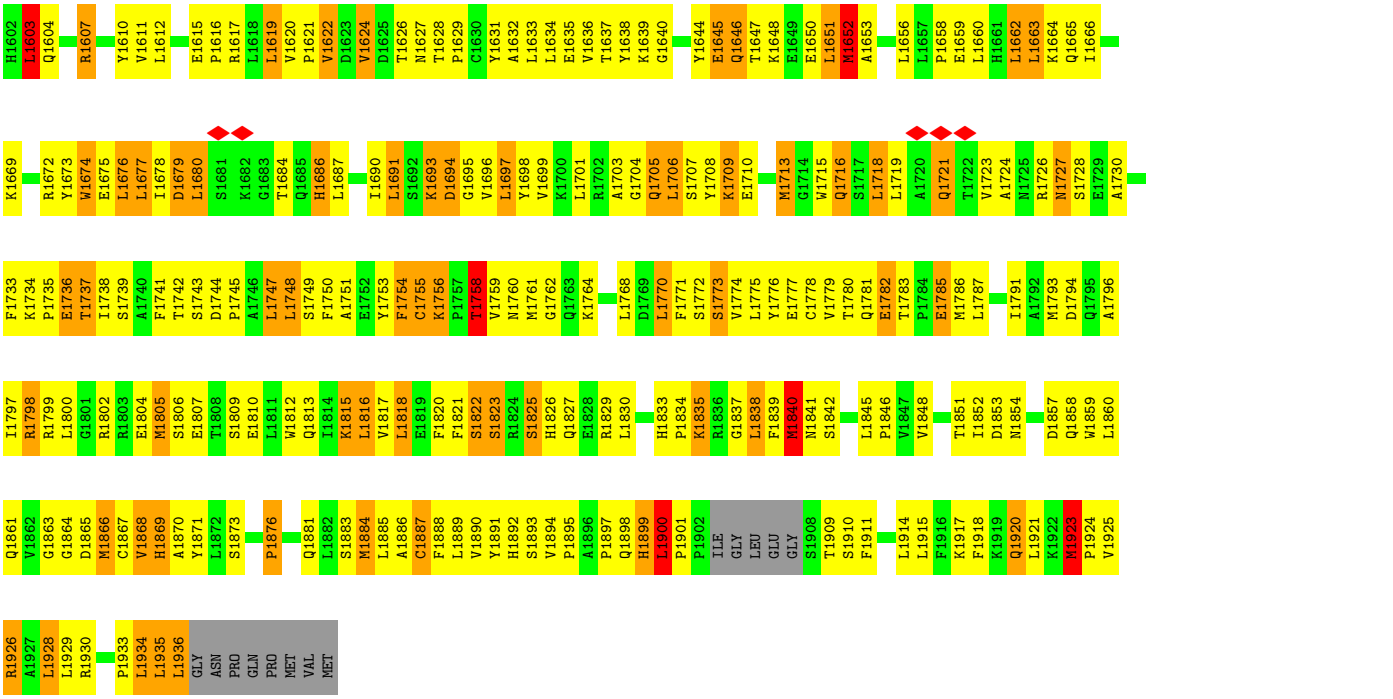
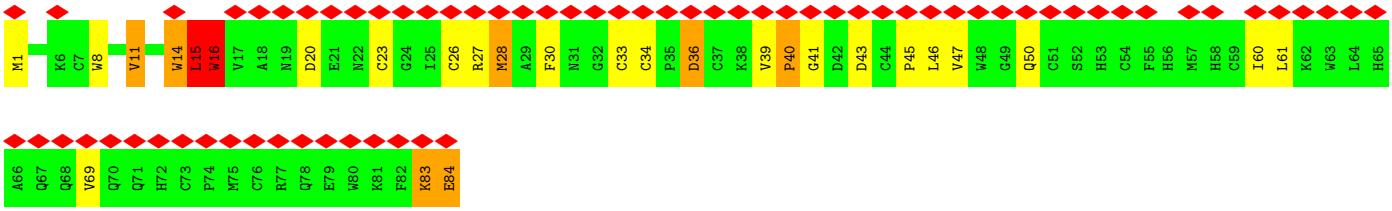
ARG PRO SER GLU THR GLY SER D704 W707 E708 Y709 L710 L711 Y715 H716 H722 L723 L724 L730 S731 PRO SER GLU ALA SER GLN MET LYS ASP GLU ASP PHE SER GLN ASN L747 S748 L749 D750 S751 L754 L755 F756 T757 H758 I759 P760 A761 I762 F763 F764 V765 L766 H767 L768
V769 Y770 E771 E772 L773 K774 L775 N776 T777 L778 M779 G780 E781 G782 I783 C784 S785 L786 V787 E788 L789 L790 V791 Q792 L793 A794 R795 D796 L797 K798 L799 G800 P801 Y802 W803 D804 H805 Y806 Y807 R808 D809 Y810 P811 T812 L813 V814 R815 T816 T817 G818 Q819 V820 C821 T822 I823 D824 P825 G826 Q827 T828
G829 F830 M831 H832 H833 P834 S835 F836 F837 T838 S839 E840 P841 P842 S843 I844 Y845 Q846 W847 V848 C851 L852 K853 G854 E855 G856 M857 P858 P859 Y860 P861 Y862 L863 P864 G865 I866 C867 E868 R869 S870 R871 L872 V873 I877 A878 L879 Y880 I881 L882 L887 VAL SER ASP GLU S892 S893 Q894
Y895 L896 T897 R898 I899 T900 ILE ALA PRO GLN LYS LEU GLN VAL GLU GLN GLU GLU ASN ARG PHE SER PHE ARG HIS SER THR SER V923 S924 S925 L926 A927 E928 R929 L930 V931 V932 W933 M934 F939 T940 L941 L944 E945 T946 L947 P948 F949 G950 I951 A952 L953 R956 D957 A958 I959
Y960 H961 C962 R963 P966 A967 S968 D969 W970 P971 V974 L977 I978 G979 R980 Q981 D982 L983 S984 K985 G988 E989 P993 LYS GLY LYS SER VAL LEU SER SER ASP VAL PRO SER GLY THR GLU THR GLU E1011 E1012 D1013 D1014 G1015 M1016 N1017 D1018 M1019 N1020 M1024 S1025 L1026
E1030 D1031 L1032 R1033 V1034 Q1035 D1036 V1037 L1040 S1043 A1044 H1045 P1046 V1047 R1048 V1049 V1052 Q1053 Y1054 P1055 E1056 L1057 H1060 E1061 F1062 I1063 E1064 E1065 K1066 E1067 N1068 R1069 L1070 L1071 Q1072 L1073 C1074 Q1075 R1076 T1077 M1078 A1079 L1080 P1081 V1082 G1083 R1084 G1085 M1086 F1087 T1088 L1089 F1090 H1093 P1094
V1095 P1096 T1097 E1098 P1099 L1100 P1101 I1102 P1103 K1104 L1107 T1108 G1109 R1110 A1111 P1112 P1113 R1114 N1115 T1116 T1117 V1118 D1119 L1120 N1121 I1125 D1126 V1127 P1128 P1129 N1130 M1131 T1132 S1136 F1137 H1138 N1139 G1140 V1141 A1142 A1143 G1144 L1145 K1146 I1147 A1148 P1149 A1150 S1151 Q1152 I1153 D1154 S1155 A1156 W1157 I1158 V1159
Y1160 N1161 K1162 P1163 K1164 E1167 L1168 A1169 N1170 E1171 Y1172 A1173 L1176 M1177 L1181 N1182 G1183 H1184 L1185 T1186 L1191 N1192 I1193 H1194 D1195 Y1196 L1197 T1198 K1199 G1200 H1201 E1202 M1203 T1204 S1205 I1206 G1207 L1208 V1212 A1215 K1216 L1217 G1218 T1219 M1220 I1224 T1225 R1226 L1227 L1228 S1229 I1230 H1231
I1232 P1233 A1234 L1235 L1236 P1237 P1238 T1239 S1240 T1241 E1242 L1243 N1248 V1249 Q1250 V1251 V1254 V1255 L1259 V1260 Y1261 T1264 A1265 H1266 R1267 H1268 T1269 V1272 L1273 L1274 A1275 E1276 I1277 G1278 R1279 P1280 P1281 G1282 P1283 Y1287 D1290 R1291 E1292 S1293 Y1294 G1299 L1300 A1301 L1302 G1303 M1304 V1305
C1306 L1307 G1308 H1309 G1310 S1311 N1312 L1313 I1314 G1315 M1316 L1319 N1320 V1321 P1322 E1323 Q1324 L1325 Q1327 Y1328 M1329 G1332 H1333 ARG ARG PHE GLN THR GLY MET HIS HIS ARG GLU LYS HIS LYS S1347 Q1351 I1352 K1353 E1354 G1355 D1356 T1357 I1358 N1359 V1360 C1364 P1365 T1368 L1371 A1372 M1373
I1374 Y1375 L1376 K1377 T1378 N1379 N1380 I1383 W1386 P1390 D1391 T1392 L1395 L1396 D1397 F1398 L1404 L1405 L1409 C1412 W1416 L1420 P1421 N1422 W1425 S1428 N1429 V1430 P1431 Q1432 I1433 I1434 R1435 E1436 N1437 S1438 I1439 SER LEU SER GLU ILE GLU LEU PRO CYS SER GLU ASP
L1452 N1453 L1454 E1455 T1456 L1457 S1458 Q1459 A1460 H1461 V1462 Y1463 I1464 G1467 A1468 C1469 L1470 S1471 L1472 G1473 F1474 R1475 F1476 A1477 E1480 N1481 L1482 C1487 L1488 K1493 D1494 F1495 M1496 T1497 Y1498 L1499 N1503 A1504 S1505 V1506 T1507 N1511 L1512 E1513 T1514 C1515 V1518 Y1519 L1520 L1521 S1522 L1523 A1524
M1525 V1526 M1527 A1528 G1529 S1530 G1531 N1532 L1533 K1534 V1535 L1536 Q1537 R1540 F1541 L1542 H1543 M1544 K1545 T1546 G1547 M1550 N1551 Y1552 G1553 F1554 H1555 L1556 A1557 H1558 L1562 G1563 L1564 L1565 F1566 G1570 R1571 Y1572 S1573 L1574 S1577 N1578 L1585 C1586 A1587 L1588 H1595 S1596 T1597 D1598 N1599 R1600 Y1601



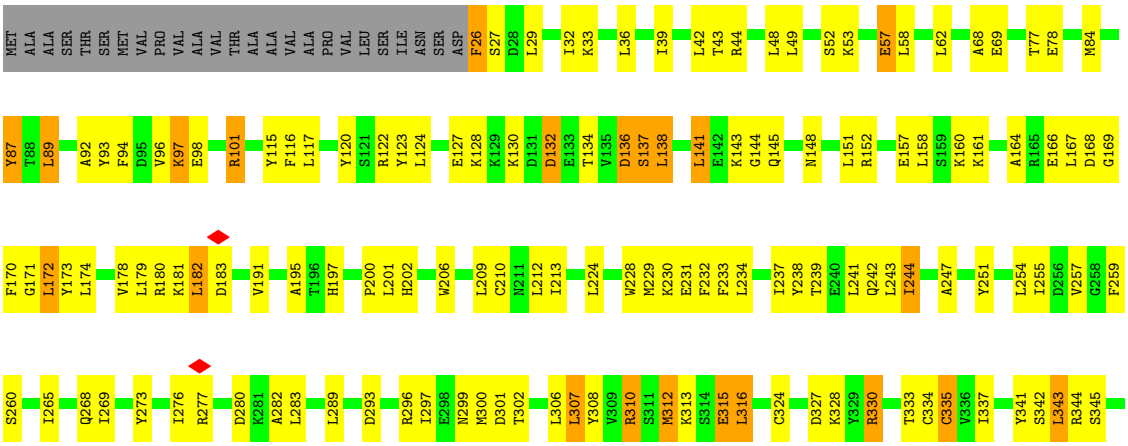
- Molecule 2: ANAPHASE-PROMOTING COMPLEX SUBUNIT 11

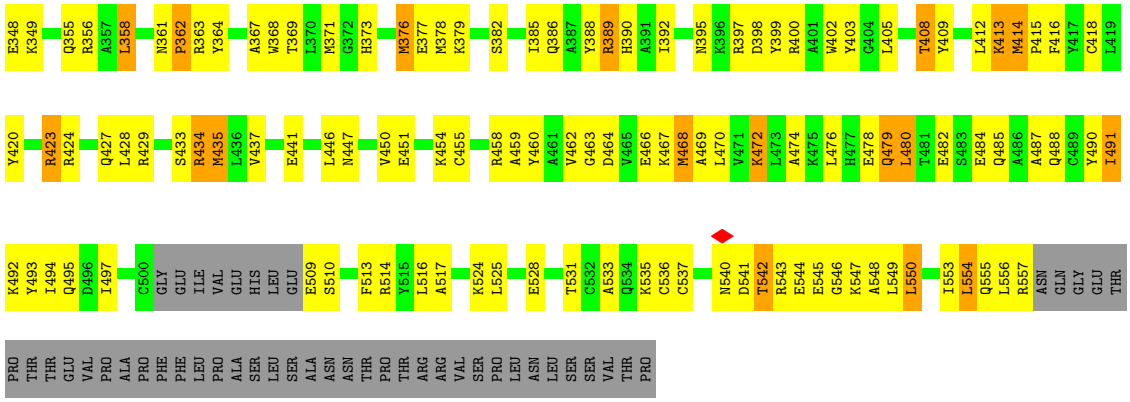
Chain B:



- Molecule 3: CELL DIVISION CYCLE PROTEIN 23 HOMOLOG

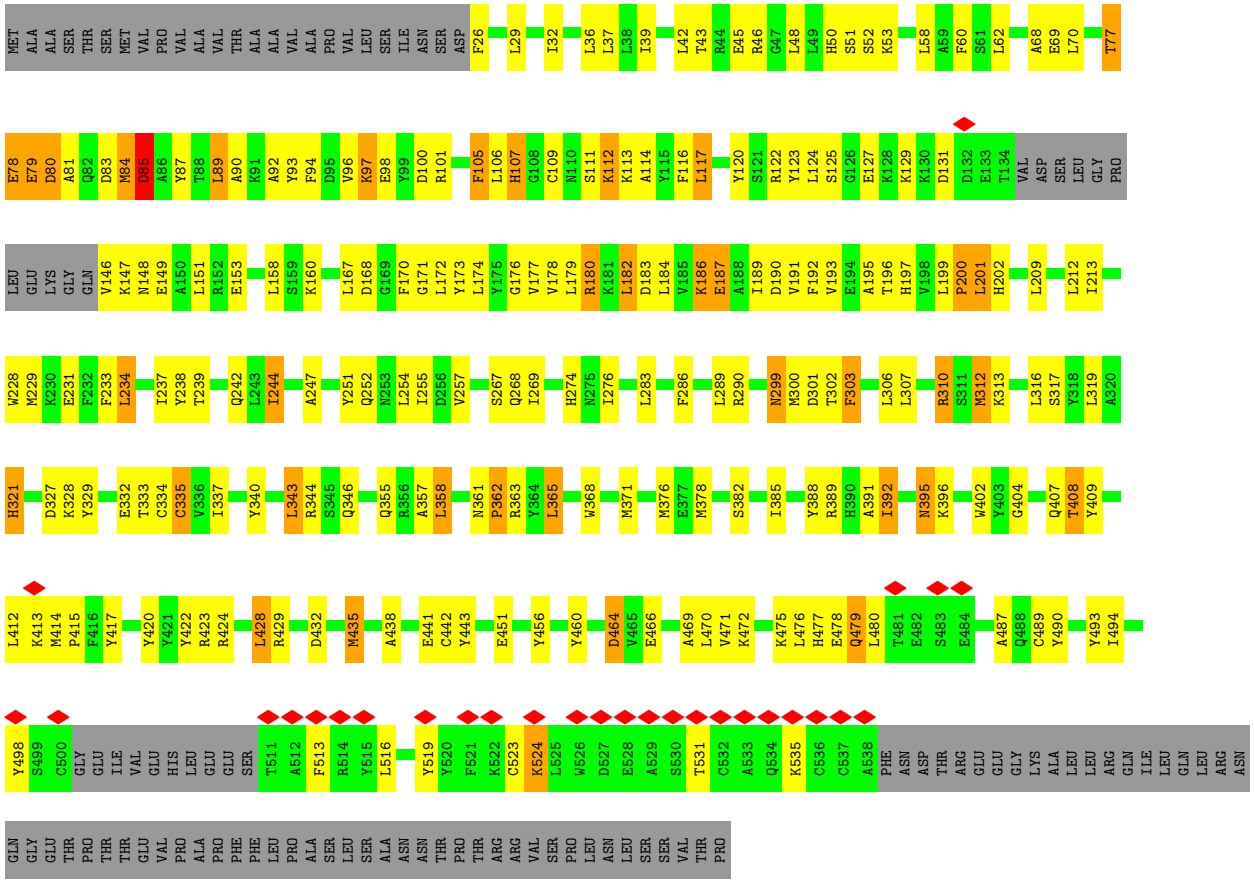
Chain C:





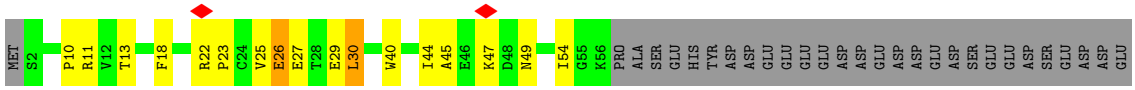
• Molecule 3: CELL DIVISION CYCLE PROTEIN 23 HOMOLOG

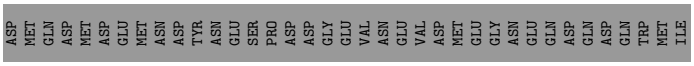
Chain P: 5% 46% 30% 6% 18%



• Molecule 4: ANAPHASE-PROMOTING COMPLEX SUBUNIT 15

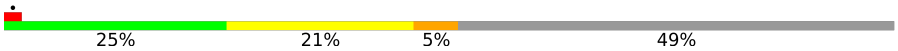
Chain D: 31% 12% • 55%

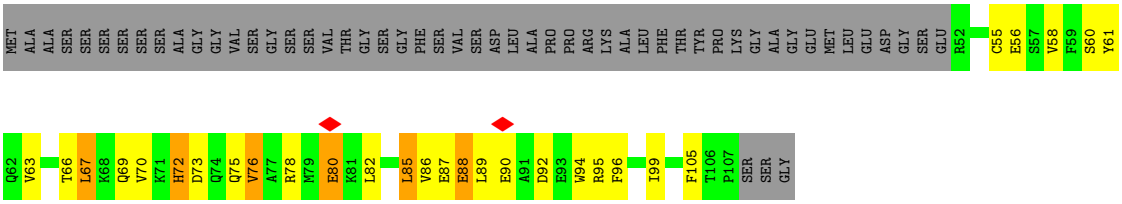




- Molecule 5: ANAPHASE-PROMOTING COMPLEX SUBUNIT 16

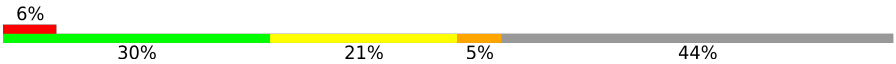
Chain E:

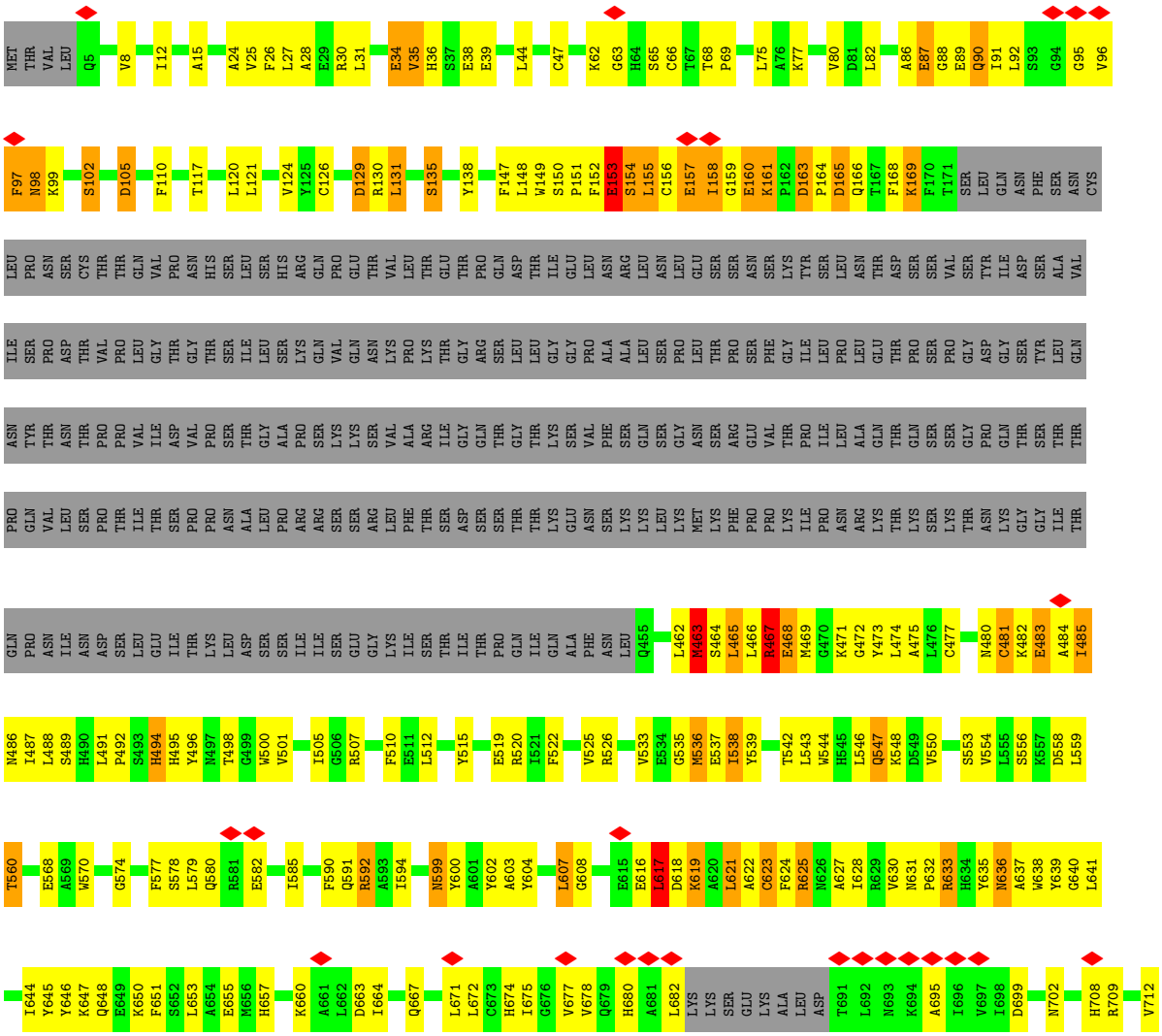


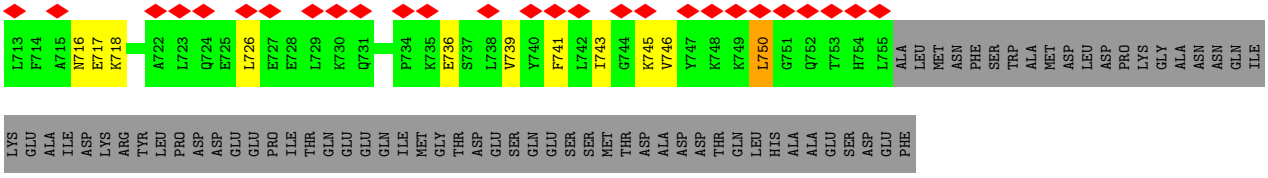


- Molecule 6: CELL DIVISION CYCLE PROTEIN 27 HOMOLOG

Chain F:

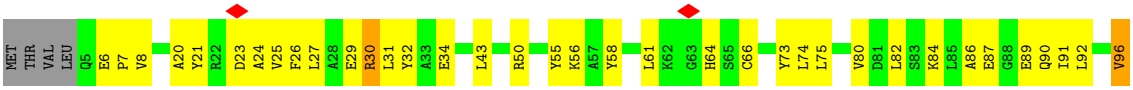


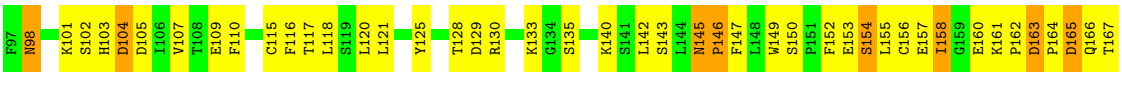


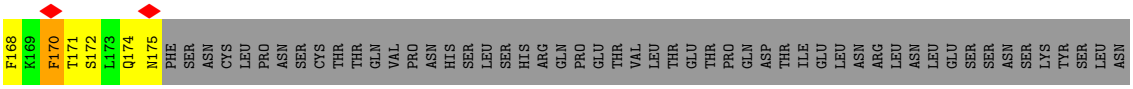


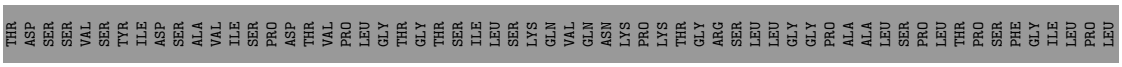
- Molecule 6: CELL DIVISION CYCLE PROTEIN 27 HOMOLOG

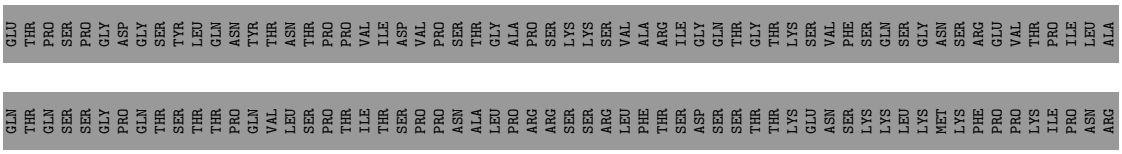
Chain H:

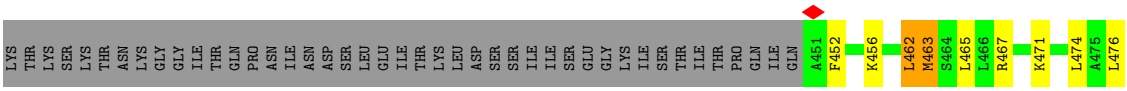


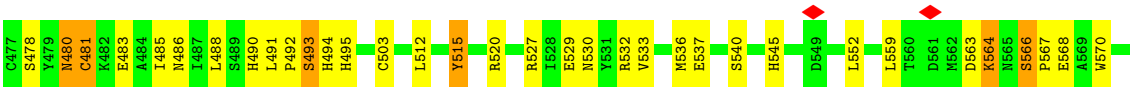


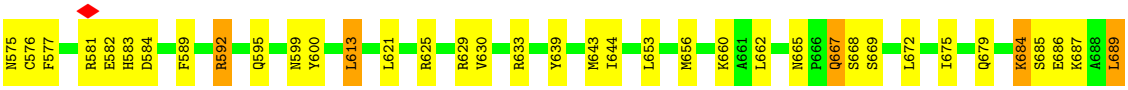


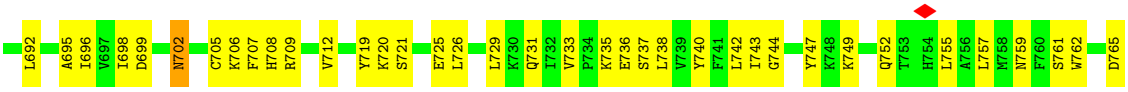


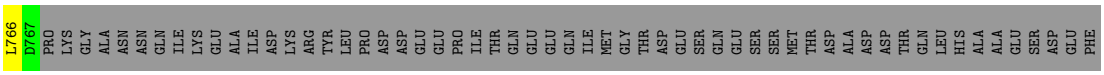






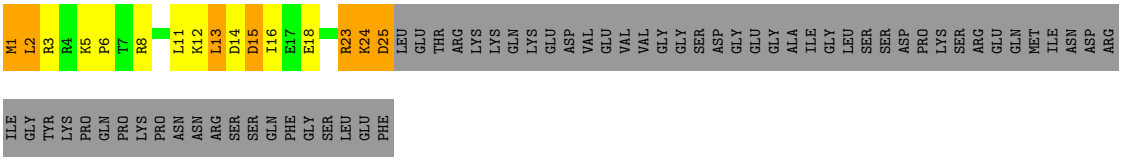






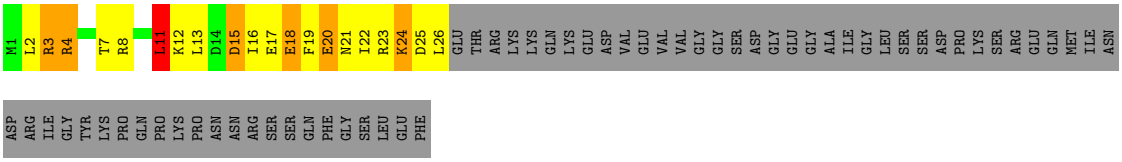
- Molecule 7: ANAPHASE-PROMOTING COMPLEX SUBUNIT CDC26

Chain G:



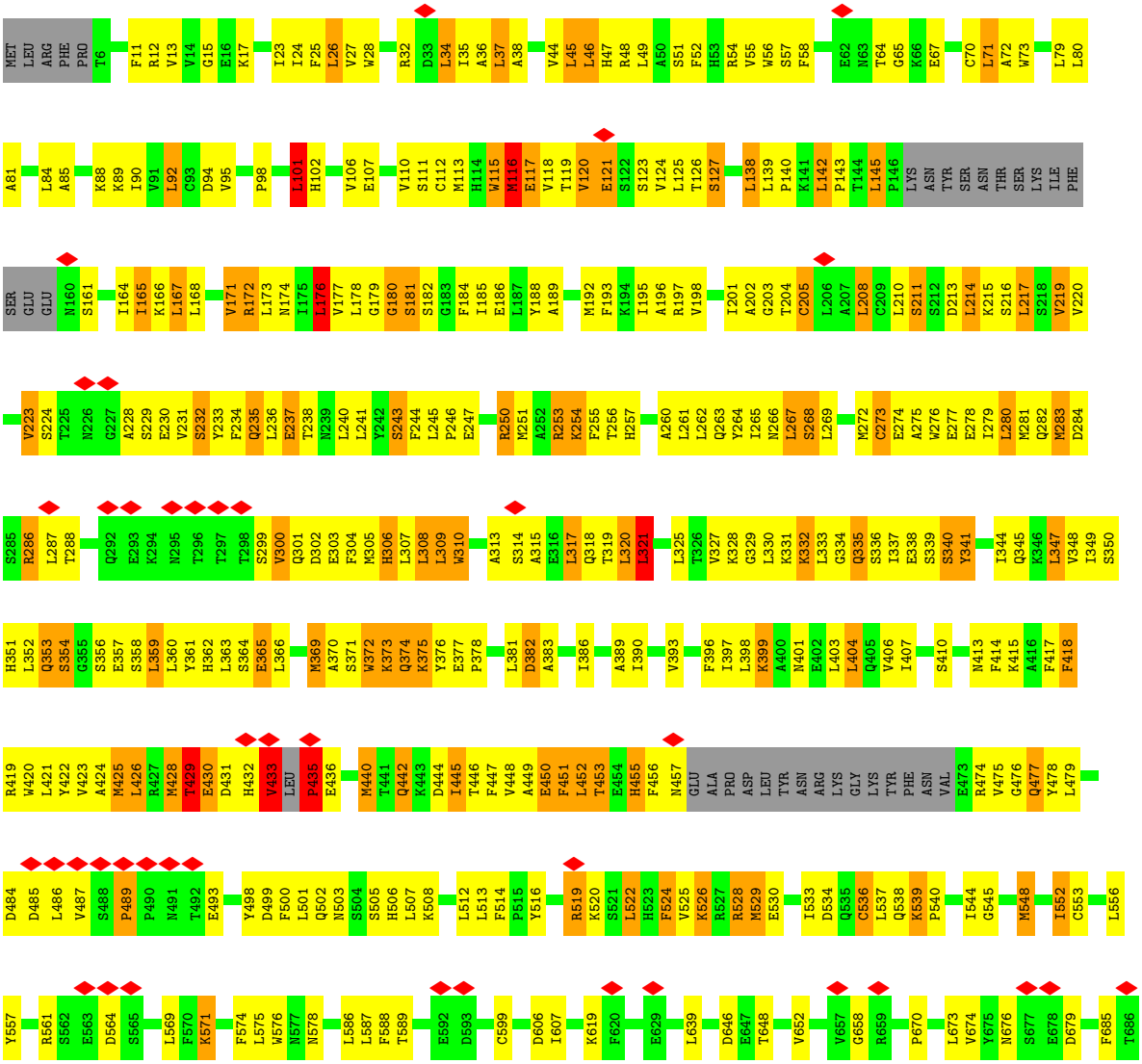
• Molecule 7: ANAPHASE-PROMOTING COMPLEX SUBUNIT CDC26

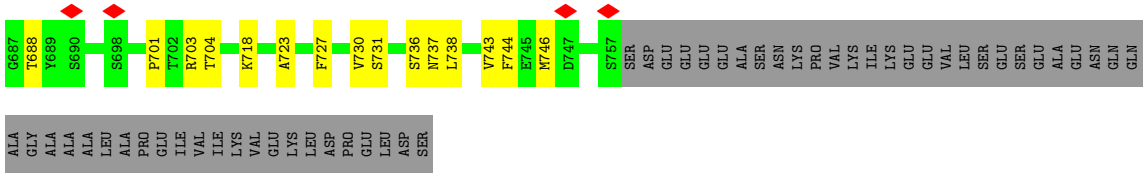
Chain W: 7% 15% 7% • 69%



• Molecule 8: ANAPHASE-PROMOTING COMPLEX SUBUNIT 4

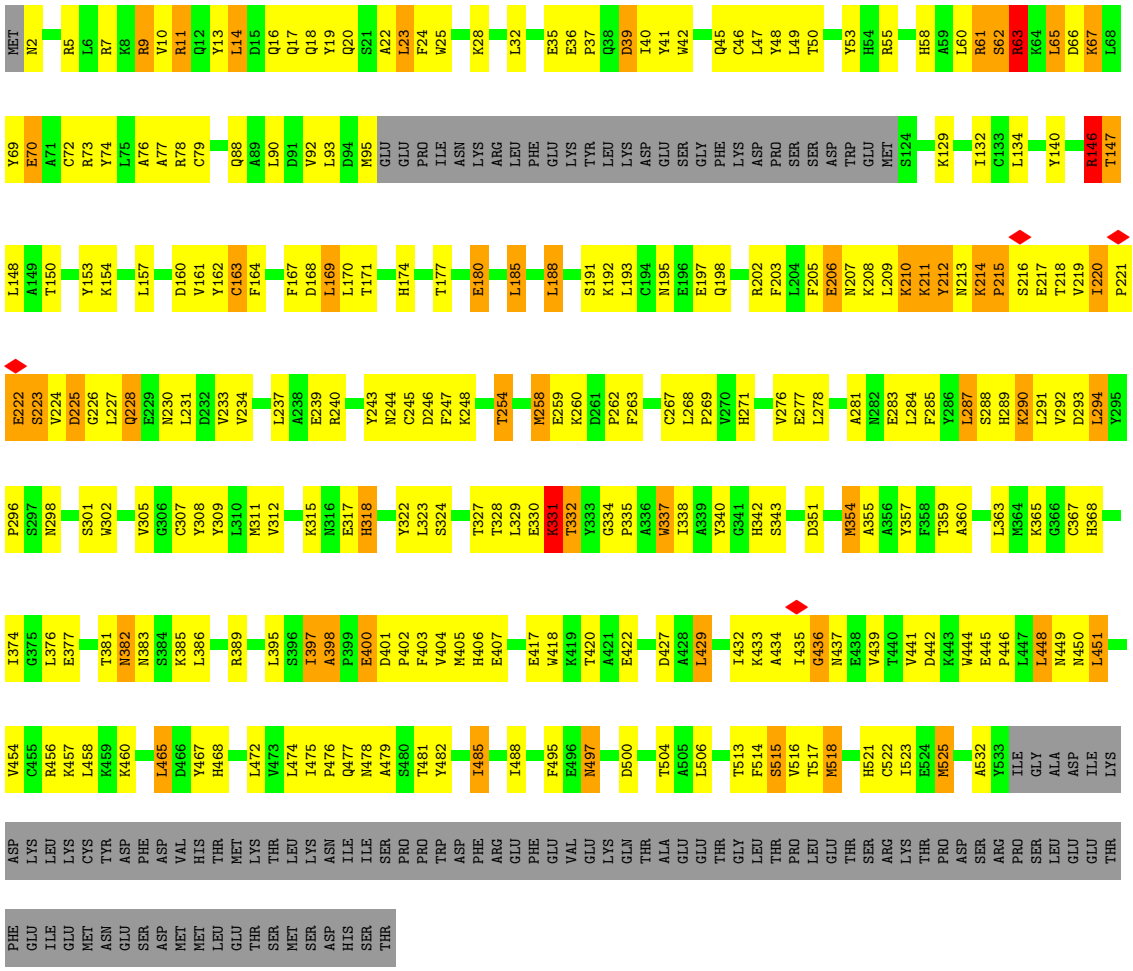
Chain I: 5% 42% 35% 11% • 11%





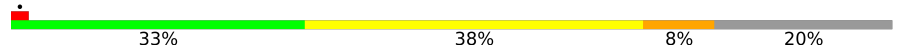
• Molecule 9: CELL DIVISION CYCLE PROTEIN 16 HOMOLOG

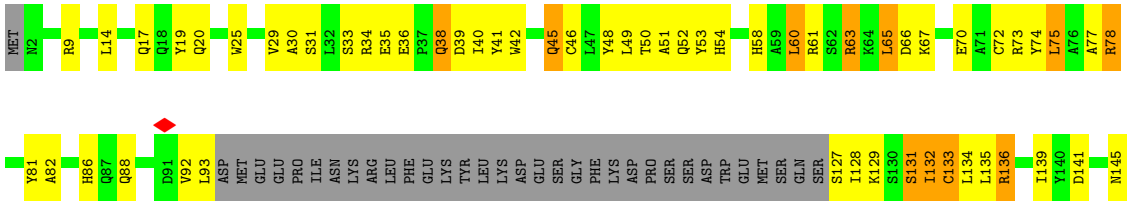
Chain J:

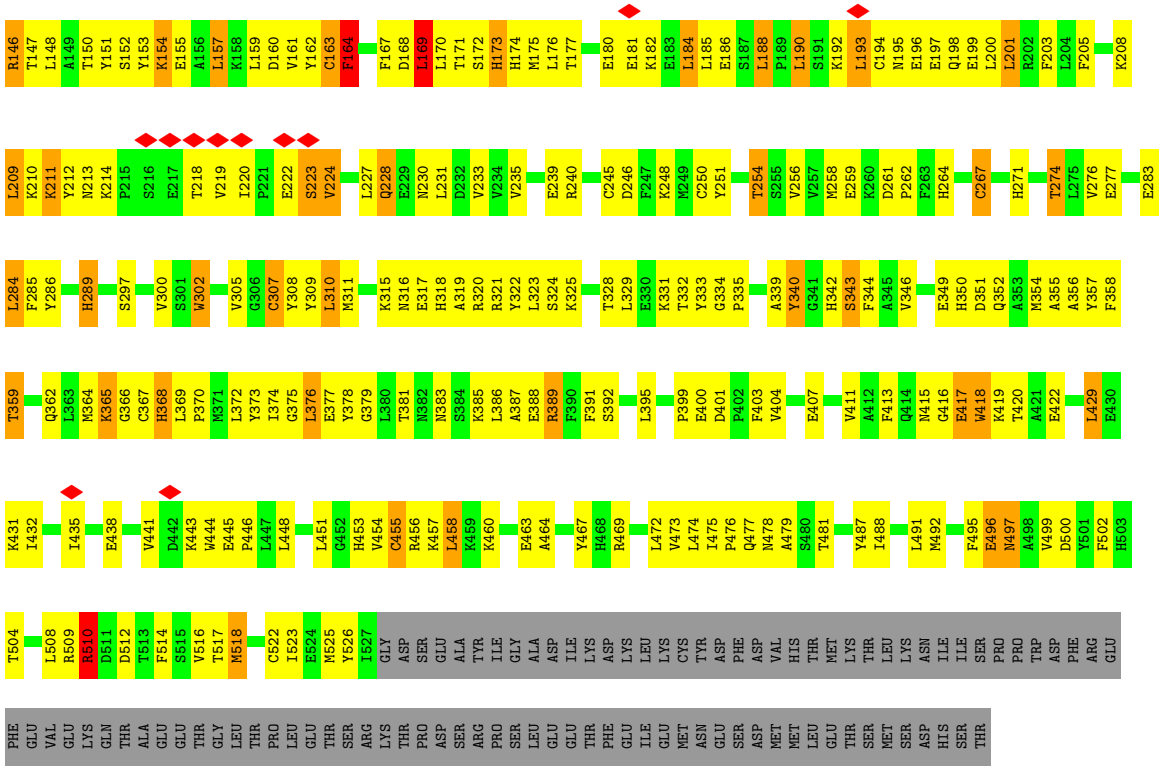


• Molecule 9: CELL DIVISION CYCLE PROTEIN 16 HOMOLOG

Chain K:

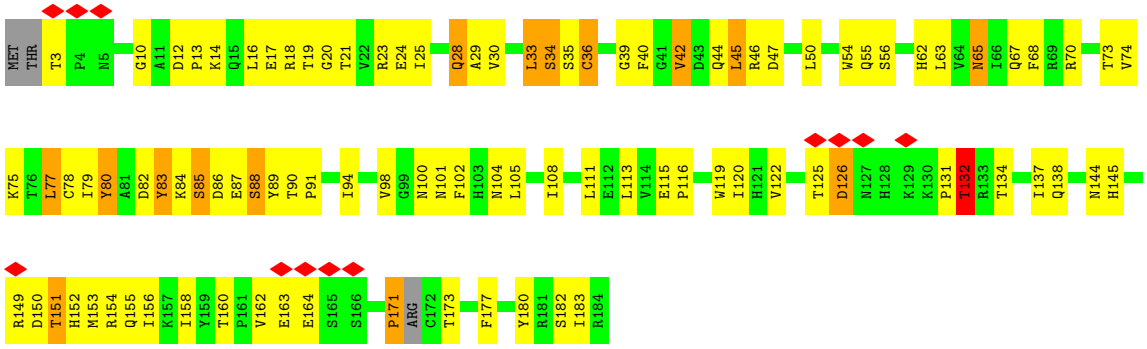






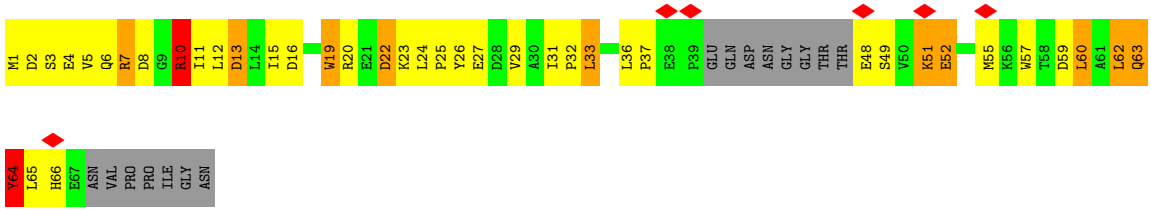
- Molecule 10: ANAPHASE-PROMOTING COMPLEX SUBUNIT 10

Chain L:



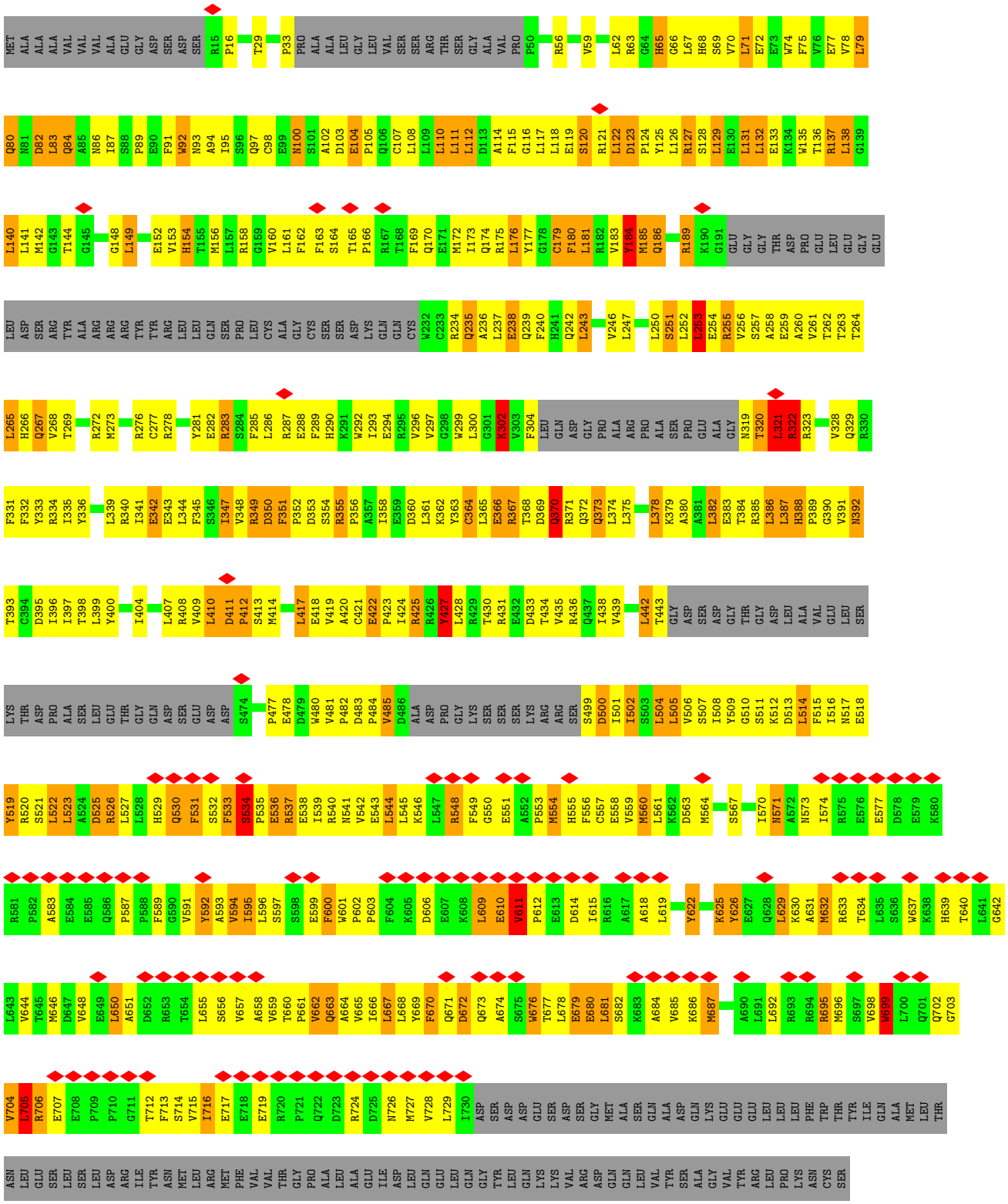
- Molecule 11: ANAPHASE-PROMOTING COMPLEX SUBUNIT 13

Chain M:



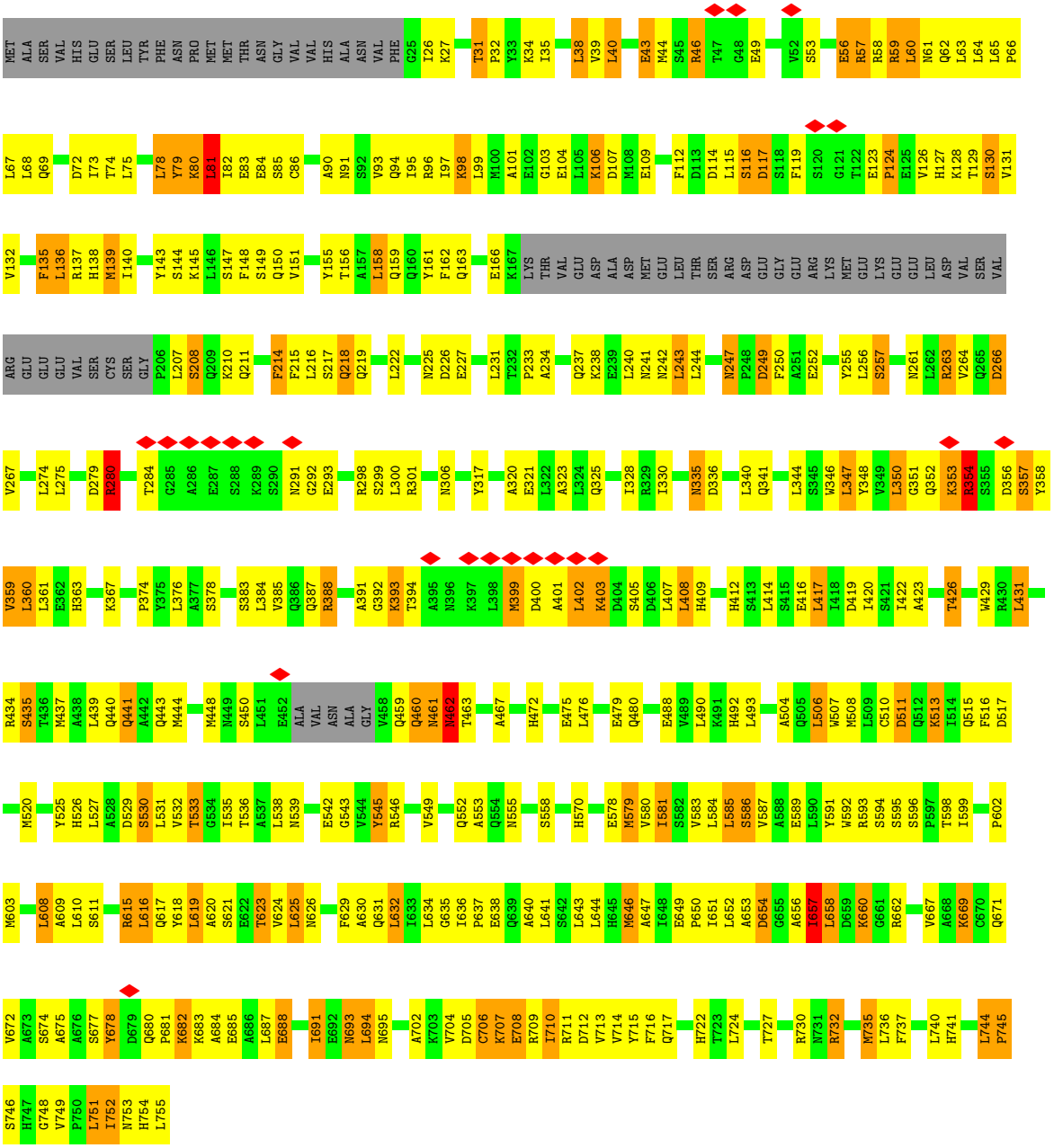
- Molecule 12: ANAPHASE-PROMOTING COMPLEX SUBUNIT 2

Chain N: 13% 22% 37% 14% • 27%



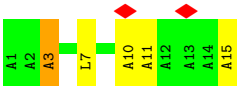
• Molecule 13: ANAPHASE-PROMOTING COMPLEX SUBUNIT 5

Chain O: • 41% 37% 12% • 9%



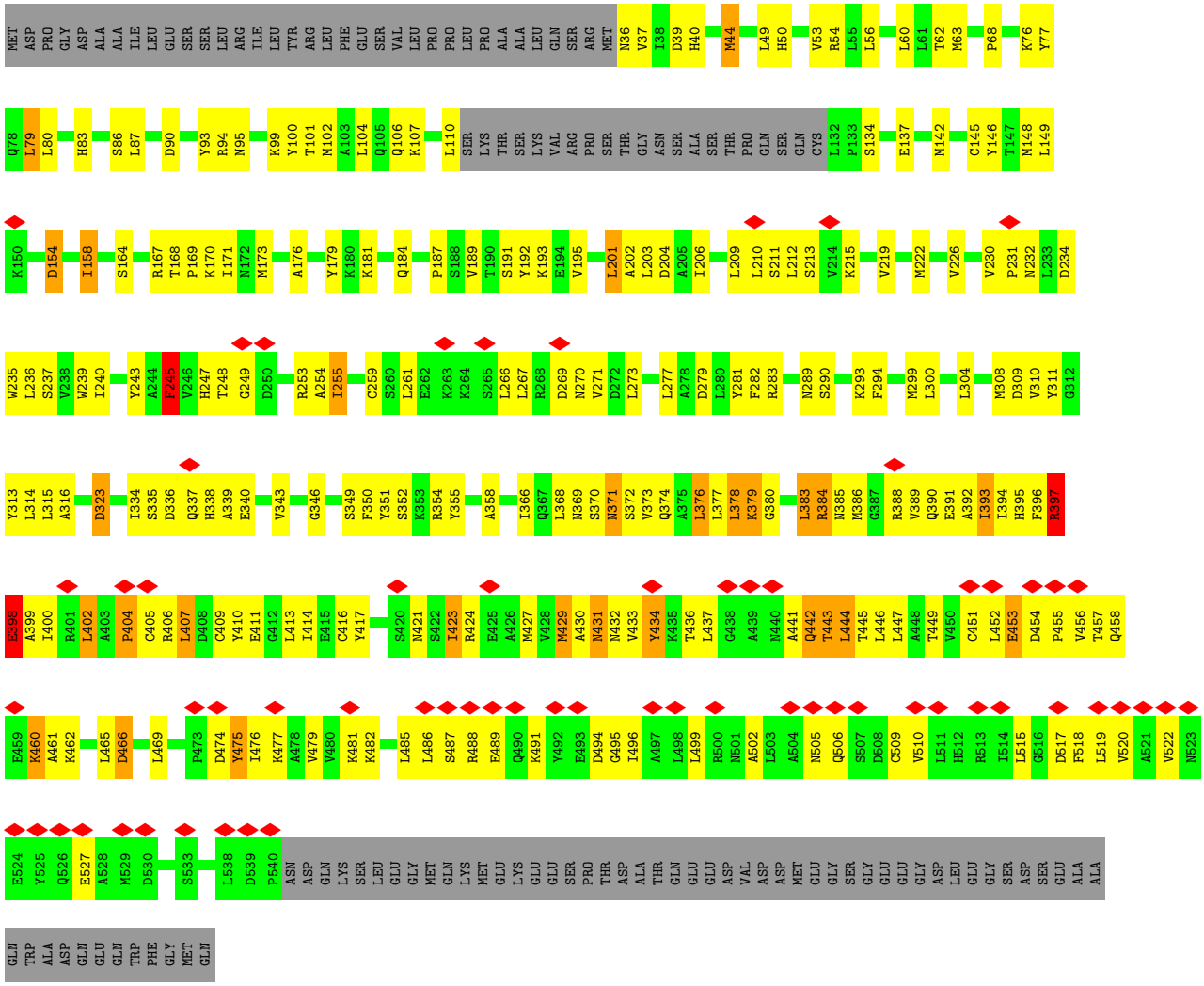
- Molecule 14: UNIDENTIFIED PEPTIDE

Chain T:



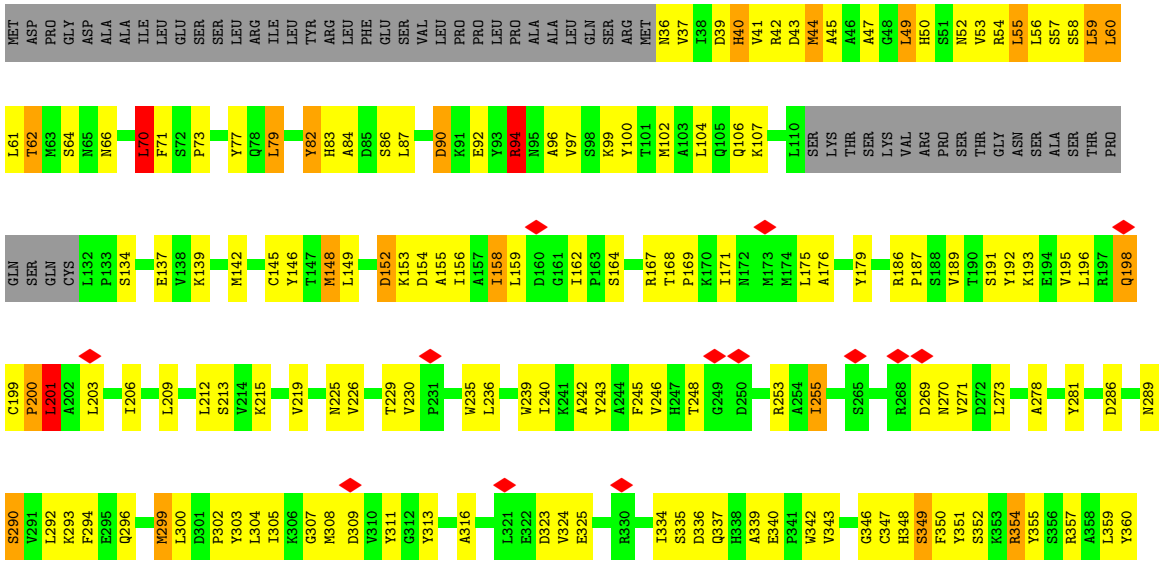
- Molecule 15: ANAPHASE-PROMOTING COMPLEX SUBUNIT 7

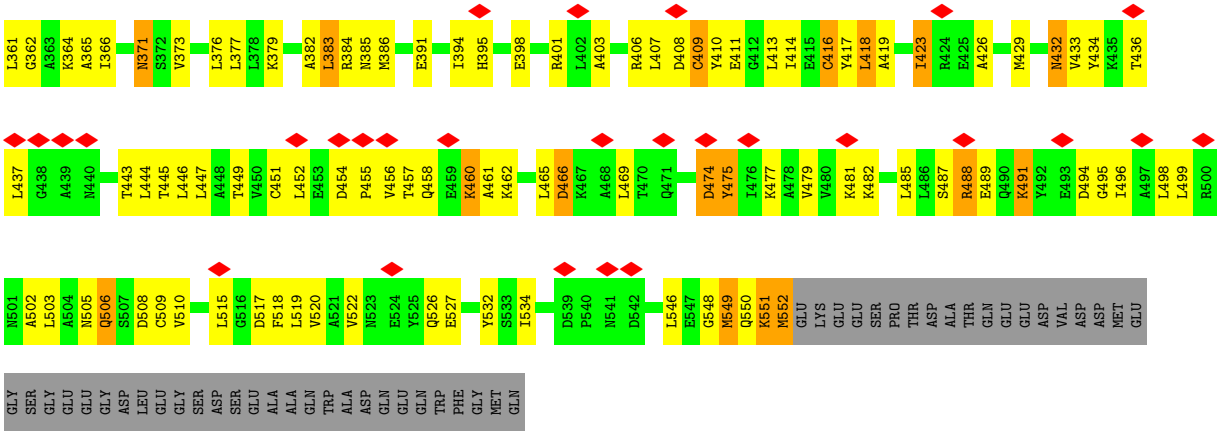
Chain X:



• Molecule 15: ANAPHASE-PROMOTING COMPLEX SUBUNIT 7

Chain Y:




L361 G362 A363 K364 A365 I366 N371 S372 V373 L376 L377 L378 K379 A382 L383 R384 N385 M386 E391 I394 H395 E398 R401 L402 A403 R406 L407 D408 C409 Y410 E411 G412 L413 I414 E415 C416 Y417 L418 A419 I423 R424 E425 A426 M429 N432 V433 Y434 K435 T436
L437 G438 A439 N440 T443 L444 T445 L446 L447 A448 T449 V450 C451 L452 E453 D454 P455 V456 T457 Q458 E459 K460 A461 K462 L465 D466 K467 A468 L469 T470 Q471 D474 Y475 I476 K477 A478 V479 V480 K481 K482 L485 L486 S487 R488 E489 Q490 K491 Y492 E493 D494 G495 I496 A497 L498 L499 R500
N501 A502 L503 A504 N505 Q506 S507 D508 C509 V510 L515 G516 D517 F518 L519 V520 A521 V522 N523 E524 Y525 Q526 E527 Y532 S533 I534 D539 P540 N541 D542 L546 E547 G548 M549 Q550 K551 M552 GLU LYS GLU GLU SER PRO THR ASP ALA THR GLN GLU GLU ASP VAL ASP ASP MET GLU
GLY SER GLY GLU GLU GLY ASP LEU GLU GLY SER ASP SER GLU ALA ALA GLN TRP ALA ASP GLN GLU GLN TRP PHE GLY MET GLN

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	921993	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	27	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	78000	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.440	Depositor
Minimum map value	-0.185	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.015	Depositor
Recommended contour level	0.08	Depositor
Map size (Å)	386.24, 386.24, 386.24	wwPDB
Map dimensions	284, 284, 284	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.36, 1.36, 1.36	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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	0.73	11/12168 (0.1%)	0.93	35/16587 (0.2%)
2	B	0.63	0/674	0.95	2/913 (0.2%)
3	C	0.73	1/4403 (0.0%)	0.93	10/5942 (0.2%)
3	P	0.66	1/4141 (0.0%)	0.89	6/5593 (0.1%)
4	D	0.62	0/446	0.83	1/610 (0.2%)
5	E	0.56	0/459	0.68	0/619
6	F	0.68	1/3704 (0.0%)	0.82	4/5019 (0.1%)
6	H	0.71	1/3969 (0.0%)	0.85	2/5366 (0.0%)
7	G	0.56	0/221	0.93	1/292 (0.3%)
7	W	0.57	0/219	0.93	1/291 (0.3%)
8	I	0.72	3/5754 (0.1%)	0.96	20/7806 (0.3%)
9	J	0.72	3/4152 (0.1%)	0.97	10/5623 (0.2%)
9	K	0.71	2/4085 (0.0%)	0.90	6/5530 (0.1%)
10	L	0.74	1/1468 (0.1%)	0.93	3/1993 (0.2%)
11	M	0.65	1/490 (0.2%)	0.98	5/665 (0.8%)
12	N	0.75	7/4861 (0.1%)	0.98	16/6585 (0.2%)
13	O	0.87	3/5499 (0.1%)	0.95	12/7432 (0.2%)
14	T	0.70	0/78	1.02	0/107
15	X	0.64	2/3827 (0.1%)	0.87	6/5180 (0.1%)
15	Y	0.56	0/3922	0.83	9/5304 (0.2%)
All	All	0.71	37/64540 (0.1%)	0.91	149/87457 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
8	I	0	5
12	N	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
14	T	0	1
All	All	0	8

The worst 5 of 37 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	O	116	SER	C-N	24.88	1.91	1.34
13	O	135	PHE	C-N	13.64	1.65	1.34
12	N	427	TYR	CG-CD2	-9.69	1.26	1.39
12	N	600	PHE	CG-CD1	-9.42	1.24	1.38
1	A	236	VAL	N-CA	8.96	1.64	1.46

The worst 5 of 149 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	I	433	VAL	O-C-N	-16.78	89.22	121.10
1	A	505	ARG	NE-CZ-NH1	11.43	126.01	120.30
9	J	61	ARG	NE-CZ-NH2	-11.40	114.60	120.30
13	O	388	ARG	NE-CZ-NH2	-10.83	114.89	120.30
9	J	61	ARG	NE-CZ-NH1	10.42	125.51	120.30

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1652	MET	Peptide
8	I	429	THR	Mainchain
8	I	433	VAL	Mainchain,Peptide
8	I	658	GLY	Peptide
8	I	727	PHE	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11890	0	11555	1834	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	649	0	595	33	0
3	C	4306	0	4273	274	0
3	P	4046	0	3998	248	0
4	D	436	0	396	25	0
5	E	450	0	435	31	0
6	F	3618	0	3452	380	0
6	H	3879	0	3805	267	0
7	G	220	0	233	30	0
7	W	218	0	222	26	0
8	I	5634	0	5522	590	0
9	J	4053	0	3960	371	0
9	K	3988	0	3911	440	0
10	L	1435	0	1381	165	0
11	M	481	0	457	72	0
12	N	4767	0	4686	1268	0
13	O	5400	0	5416	464	0
14	T	79	0	77	8	0
15	X	3767	0	3820	438	0
15	Y	3862	0	3914	412	0
16	B	3	0	0	0	0
All	All	63181	0	62108	6914	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 55.

The worst 5 of 6914 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:89:LEU:HD11	3:P:105:PHE:CE2	1.34	1.62
12:N:184:TYR:CZ	12:N:302:LYS:HE2	1.22	1.62
15:Y:104:LEU:HD11	15:Y:142:MET:CE	1.20	1.59
3:P:89:LEU:HD11	3:P:105:PHE:CD2	1.37	1.58
1:A:948:PRO:CB	1:A:1813:GLN:HE22	1.12	1.57

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1539/1944 (79%)	1372 (89%)	112 (7%)	55 (4%)	3	26
2	B	83/84 (99%)	72 (87%)	7 (8%)	4 (5%)	2	20
3	C	518/597 (87%)	490 (95%)	23 (4%)	5 (1%)	15	54
3	P	486/597 (81%)	466 (96%)	16 (3%)	4 (1%)	19	58
4	D	53/121 (44%)	47 (89%)	5 (9%)	1 (2%)	8	40
5	E	54/110 (49%)	54 (100%)	0	0	100	100
6	F	454/824 (55%)	433 (95%)	19 (4%)	2 (0%)	34	72
6	H	484/824 (59%)	469 (97%)	10 (2%)	5 (1%)	15	54
7	G	23/85 (27%)	23 (100%)	0	0	100	100
7	W	24/85 (28%)	23 (96%)	0	1 (4%)	3	23
8	I	717/808 (89%)	682 (95%)	20 (3%)	15 (2%)	7	38
9	J	500/620 (81%)	468 (94%)	25 (5%)	7 (1%)	11	46
9	K	487/620 (78%)	456 (94%)	27 (6%)	4 (1%)	19	58
10	L	180/185 (97%)	169 (94%)	9 (5%)	2 (1%)	14	52
11	M	55/74 (74%)	49 (89%)	5 (9%)	1 (2%)	8	41
12	N	590/822 (72%)	547 (93%)	26 (4%)	17 (3%)	4	31
13	O	682/755 (90%)	643 (94%)	27 (4%)	12 (2%)	8	41
14	T	13/15 (87%)	11 (85%)	1 (8%)	1 (8%)	1	10
15	X	480/599 (80%)	463 (96%)	12 (2%)	5 (1%)	15	54
15	Y	492/599 (82%)	473 (96%)	15 (3%)	4 (1%)	19	58
All	All	7914/10368 (76%)	7410 (94%)	359 (4%)	145 (2%)	12	41

5 of 145 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	274	VAL

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Mol	Chain	Res	Type
1	A	514	LEU
1	A	723	LEU
1	A	813	LEU
1	A	823	ILE

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	1243/1720 (72%)	967 (78%)	276 (22%)	1	5
2	B	65/75 (87%)	54 (83%)	11 (17%)	2	12
3	C	452/520 (87%)	384 (85%)	68 (15%)	3	17
3	P	422/520 (81%)	368 (87%)	54 (13%)	4	22
4	D	46/115 (40%)	41 (89%)	5 (11%)	6	29
5	E	47/89 (53%)	35 (74%)	12 (26%)	0	3
6	F	371/727 (51%)	310 (84%)	61 (16%)	2	13
6	H	408/727 (56%)	368 (90%)	40 (10%)	8	33
7	G	25/77 (32%)	16 (64%)	9 (36%)	0	1
7	W	23/77 (30%)	15 (65%)	8 (35%)	0	1
8	I	607/730 (83%)	508 (84%)	99 (16%)	2	13
9	J	425/548 (78%)	363 (85%)	62 (15%)	3	18
9	K	423/548 (77%)	356 (84%)	67 (16%)	2	15
10	L	155/170 (91%)	139 (90%)	16 (10%)	7	32
11	M	52/67 (78%)	38 (73%)	14 (27%)	0	3
12	N	490/724 (68%)	372 (76%)	118 (24%)	0	4
13	O	573/650 (88%)	469 (82%)	104 (18%)	1	9
14	T	1/2 (50%)	1 (100%)	0	100	100
15	X	406/513 (79%)	370 (91%)	36 (9%)	9	37
15	Y	417/513 (81%)	373 (89%)	44 (11%)	6	30

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	6651/9112 (73%)	5547 (83%)	1104 (17%)	5 13

5 of 1104 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
13	O	585	LEU
13	O	693	ASN
13	O	581	ILE
15	X	383	LEU
6	F	129	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 190 such sidechains are listed below:

Mol	Chain	Res	Type
11	M	53	GLN
13	O	503	HIS
12	N	267	GLN
13	O	219	GLN
13	O	741	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
13	O	2
12	N	1
3	C	1
9	K	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	N	563:ASP	C	564:MET	N	2.51
1	C	344:ARG	C	345:SER	N	2.01
1	K	219:VAL	C	220:ILE	N	2.00
1	O	116:SER	C	117:ASP	N	1.91
1	O	135:PHE	C	136:LEU	N	1.65

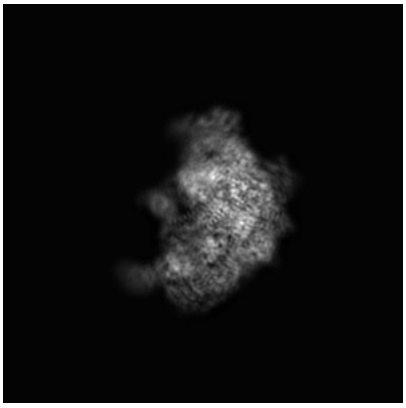
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-3388. These allow visual inspection of the internal detail of the map and identification of artifacts.

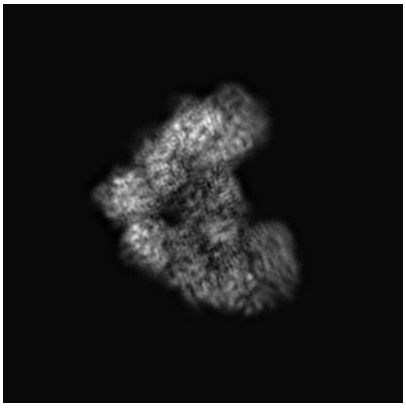
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

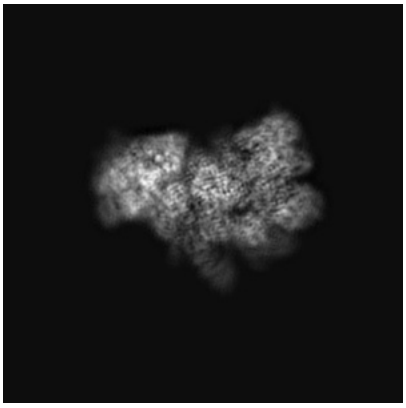
6.1.1 Primary map



X



Y

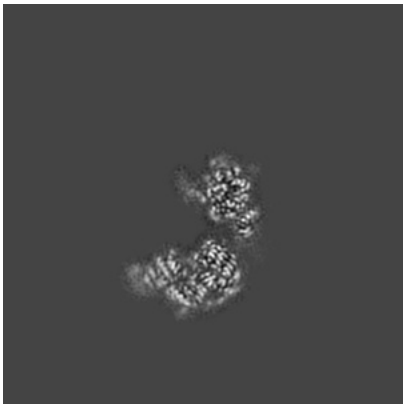


Z

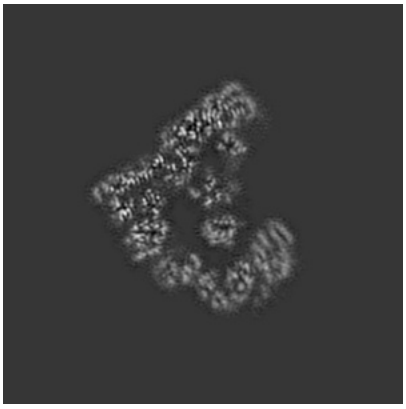
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

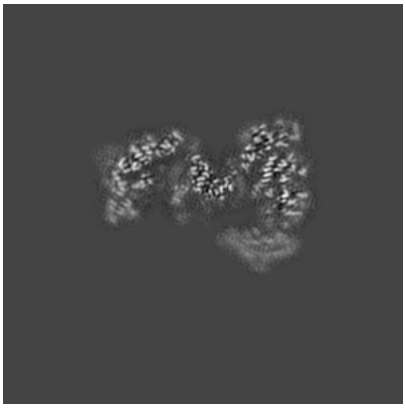
6.2.1 Primary map



X Index: 142



Y Index: 142

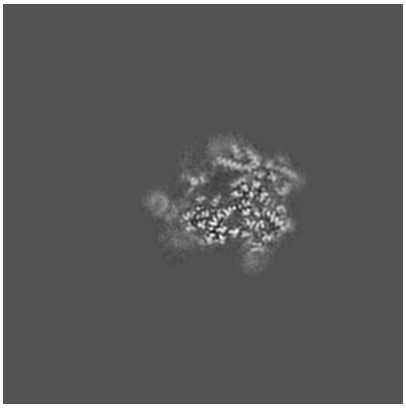


Z Index: 142

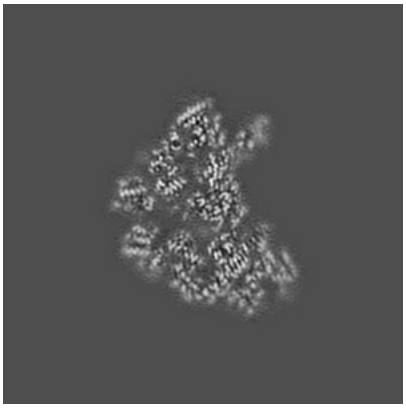
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

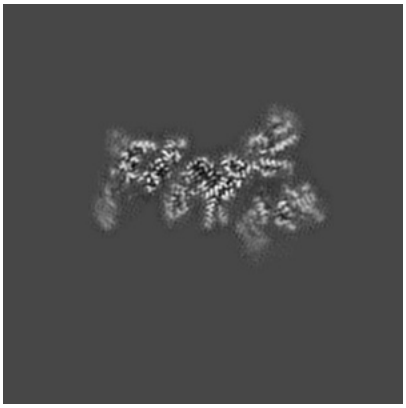
6.3.1 Primary map



X Index: 191



Y Index: 163



Z Index: 154

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map

X

Y

Z

The images above show the 3D surface view of the map at the recommended contour level 0.08. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

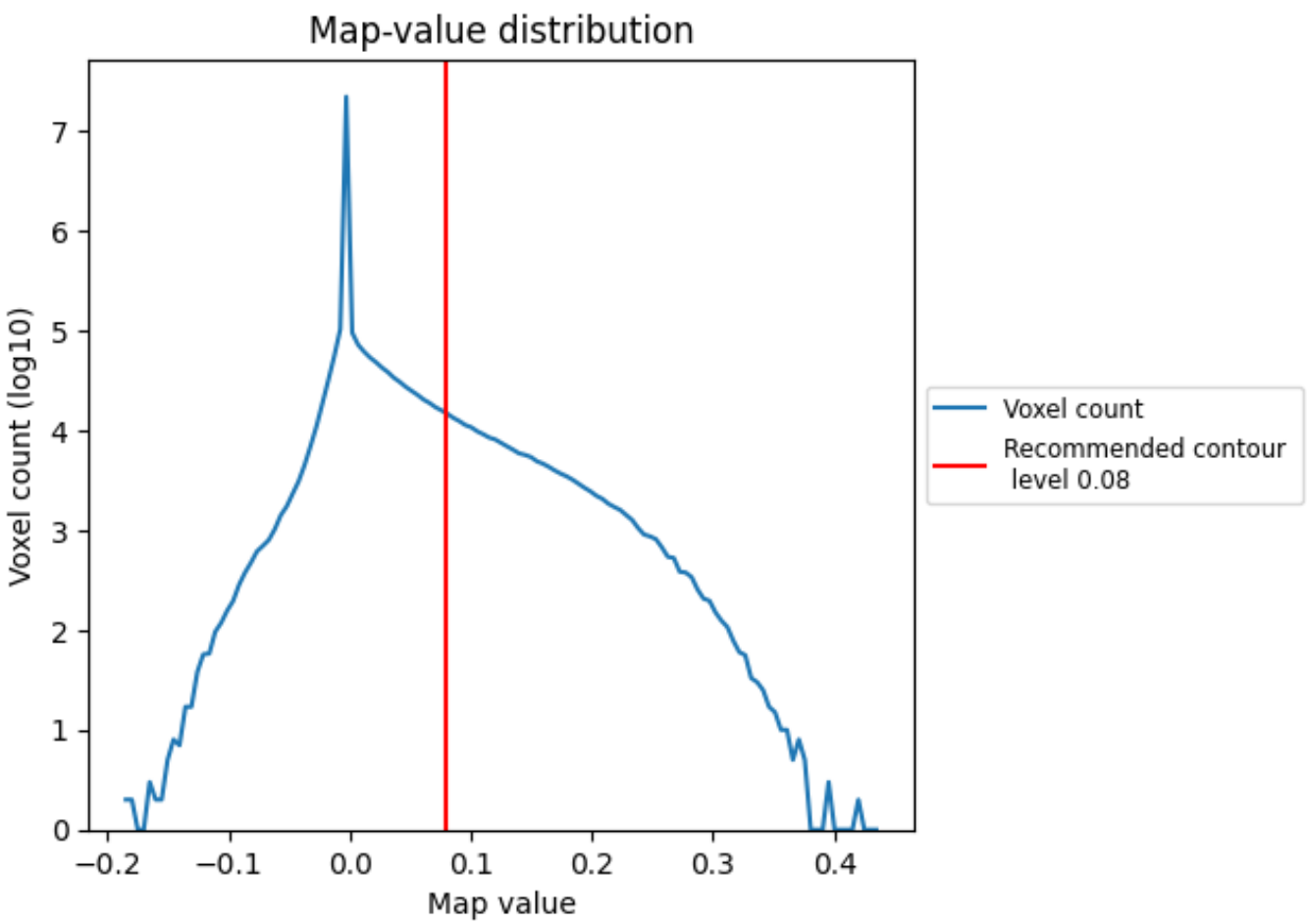
6.5 Mask visualisation (i)

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

7 Map analysis (i)

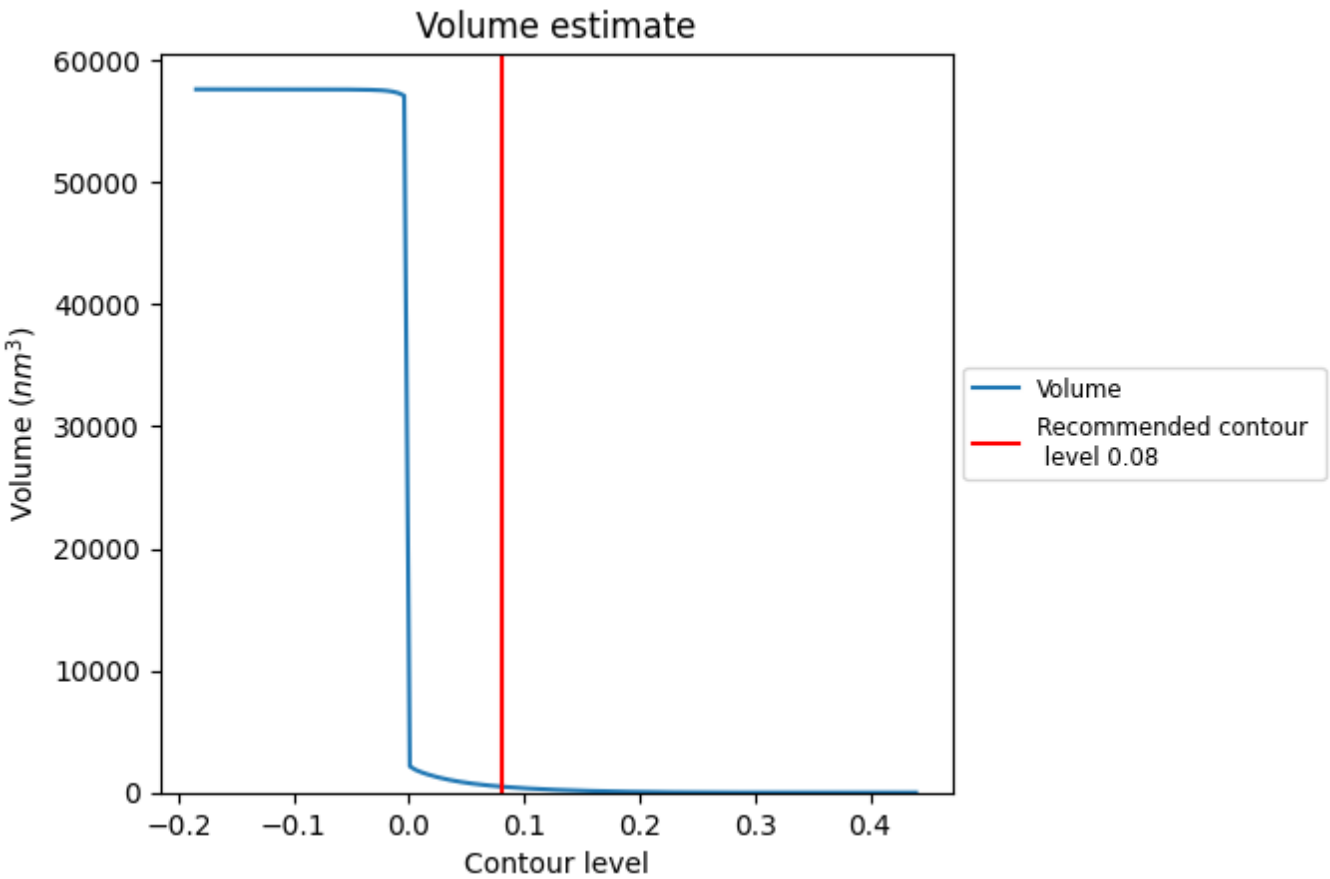
This section contains the results of statistical analysis of the map.

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.

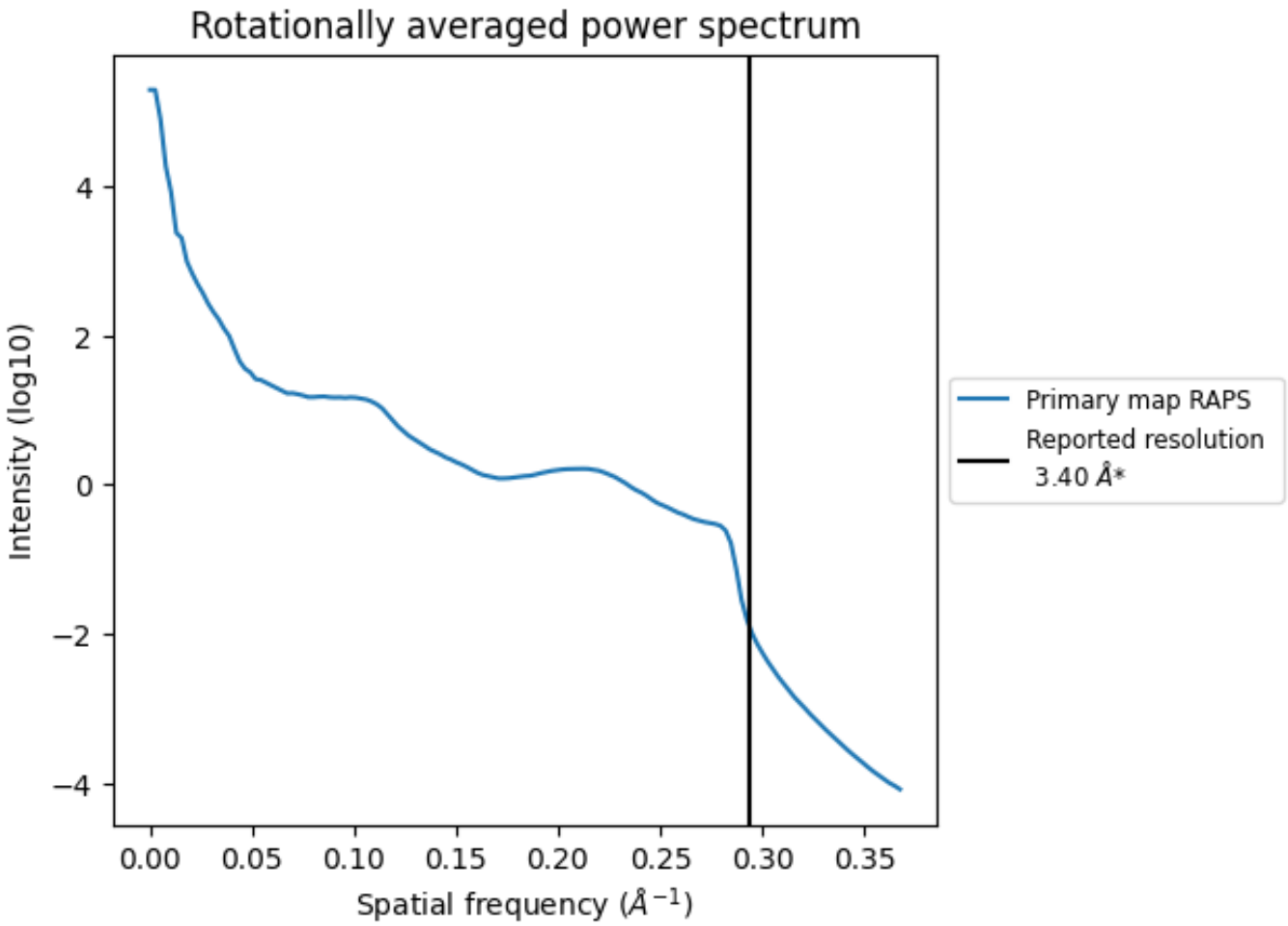
7.2 Volume estimate (i)



The volume at the recommended contour level is 488 nm^3; this corresponds to an approximate mass of 441 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 0.294 Å^{-1}

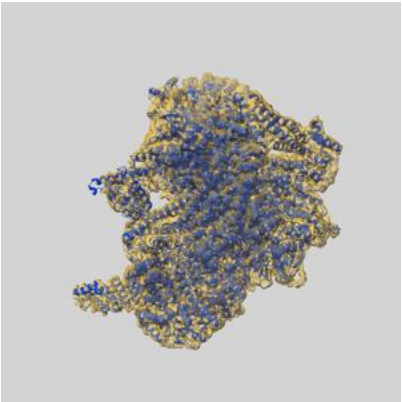
8 Fourier-Shell correlation (i)

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

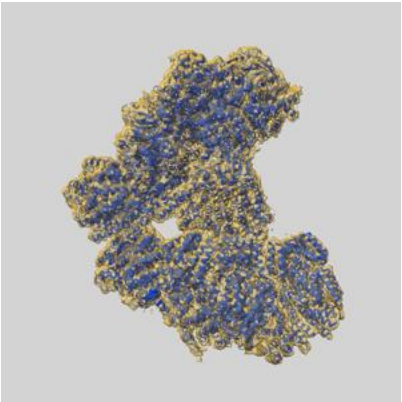
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-3388 and PDB model 5G05. Per-residue inclusion information can be found in section 3 on page 7.

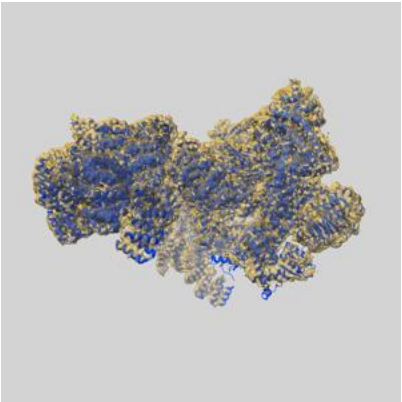
9.1 Map-model overlay (i)



X



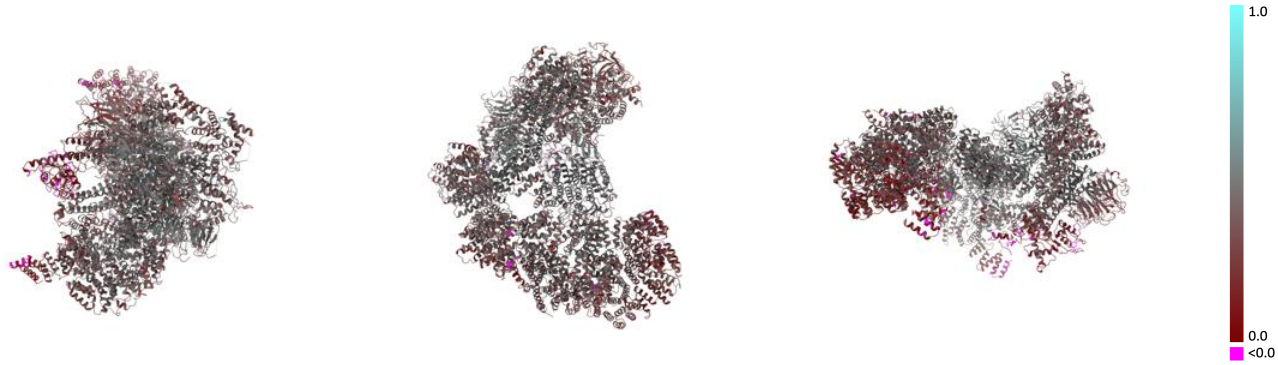
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.08 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.

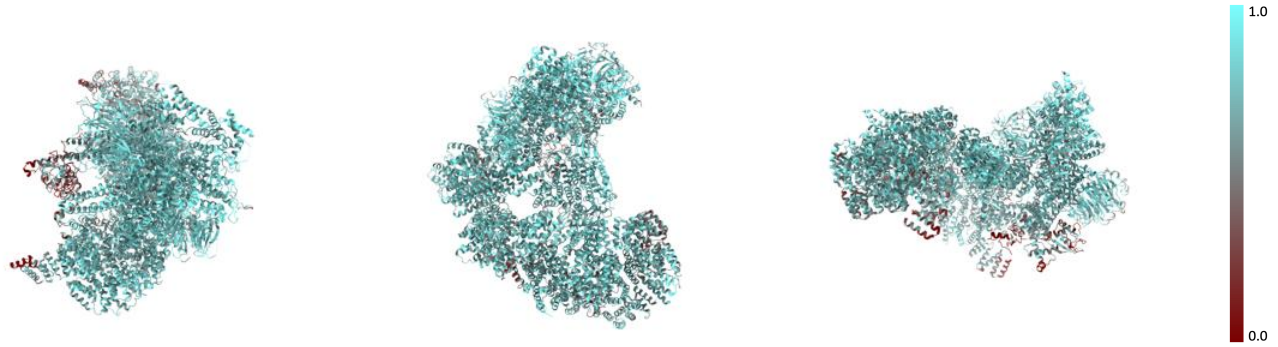
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

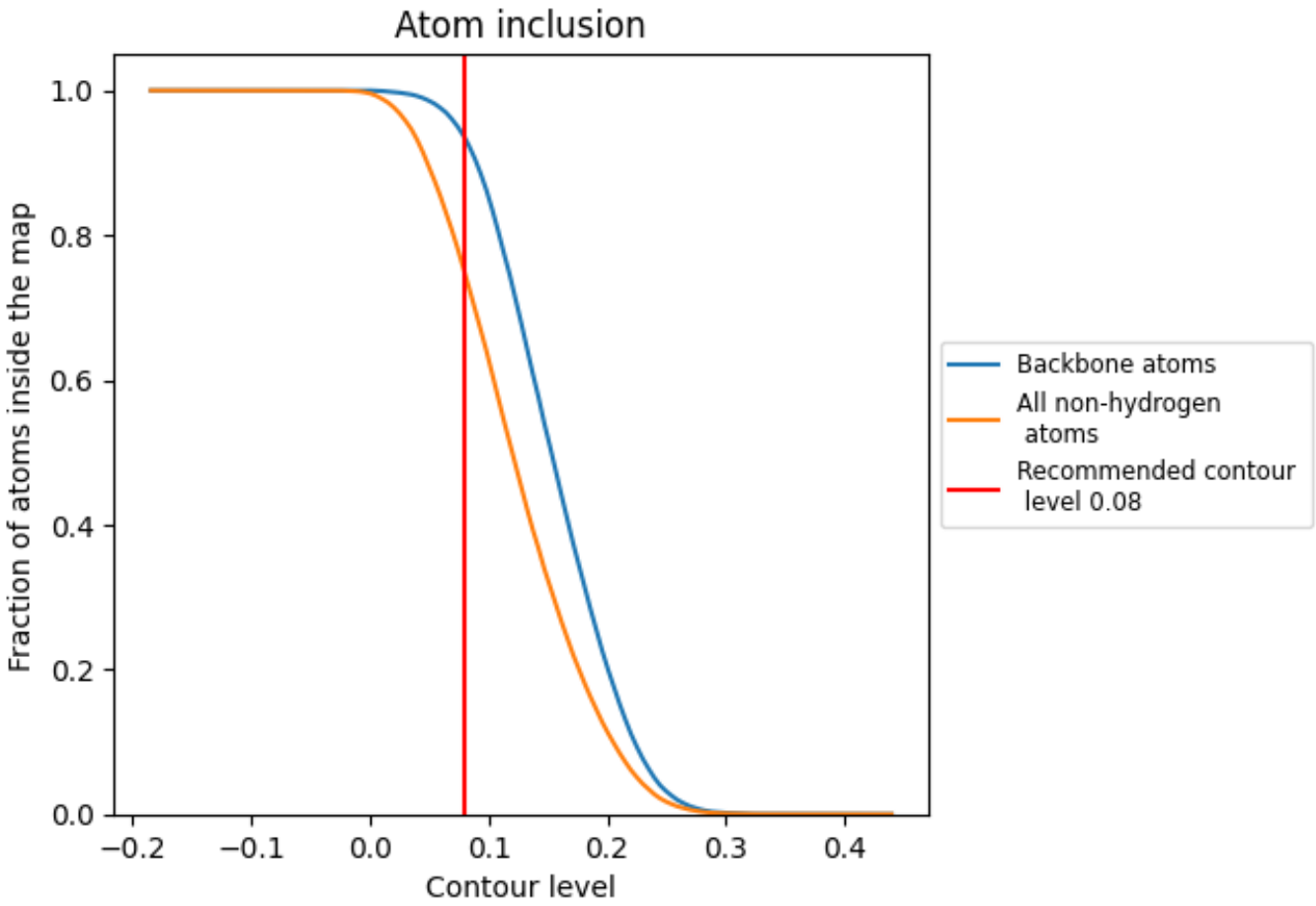
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.08).

9.4 Atom inclusion (i)



At the recommended contour level, 93% of all backbone atoms, 75% 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 (0.08) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7475	0.3750
A	0.8153	0.4400
B	0.1774	0.0870
C	0.7972	0.4190
D	0.7523	0.4040
E	0.7410	0.4040
F	0.7080	0.3510
G	0.7453	0.3740
H	0.7830	0.4030
I	0.7660	0.3820
J	0.7854	0.3650
K	0.7787	0.3950
L	0.7404	0.3790
M	0.6603	0.4070
N	0.6334	0.2980
O	0.8009	0.4350
P	0.7479	0.3480
T	0.7722	0.4360
W	0.7476	0.4360
X	0.6436	0.2640
Y	0.6604	0.2730