wwPDB EM Validation Summary Report (i)

Sep 28, 2024 – 09:37 pm BST

PDB ID	:	5LCW
EMDB ID	:	EMD-4037
Title	:	Cryo-EM structure of the Anaphase-promoting complex/Cyclosome, in complex with the Mitotic checkpoint complex (APC/C-MCC) at 4.2 angstrom resolution
Authors	:	Alfieri, C.; Chang, L.; Zhang, Z.; Yang, J.; Maslen, S.; Skehel, M.; Barford, D.
Deposited on	:	2016-06-22
Resolution	:	4.20 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:

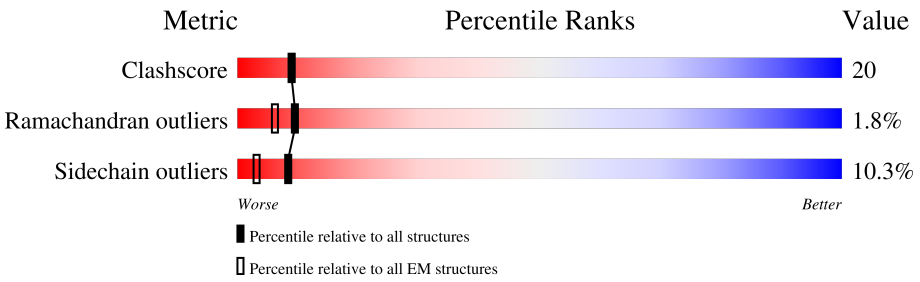
EMDB validation analysis	:	0.0.1.dev113
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 4.20 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	11%; 45%; 25%; •; 26%
2	B	84	79%; 40%; 42%; 8%; •; 6%
3	C	597	11%; 55%; 30%; •; 12%
3	P	597	8%; 54%; 24%; •; 18%
4	D	121	7%; 6%; 8%; •; 85%
5	E	110	•; 34%; 15%; •; 49%
6	F	824	•; 40%; 17%; •; 41%
6	H	824	40%; 17%; •; 41%

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Mol	Chain	Length	Quality of chain
7	G	85	16% 12% • 71%
7	W	85	• 18% 9% • 71%
8	I	808	19% 55% 33% • 9%
9	J	620	• 50% 26% 5% 19%
9	K	620	• 48% 28% • 20%
10	L	185	9% 61% 34% • •
11	M	74	15% 47% 28% • 20%
12	N	822	23% 48% 28% 7% • 14%
13	O	755	17% 57% 28% 6% 9%
14	Q	374	22% 74% 19% • 5%
15	R	499	15% 56% 19% • 23%
16	S	342	21% 47% 29% 5% 19%
17	X	599	13% 53% 26% • 19%
17	Y	599	7% 52% 27% • 17%
18	Z	205	26% 69% 21% • 5%

2 Entry composition (i)

There are 18 unique types of molecules in this entry. The entry contains 72075 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	1441	10949	7039	1853	1983	74	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	356	PHE	PRO	conflict	UNP Q9H1A4

- Molecule 2 is a protein called Anaphase-promoting complex subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	79	643	411	116	100	16	0	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	491	4043	2611	679	729	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	18	153	104	23	26	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	483	3849	2470	649	704	26	0	0
6	H	483	3853	2473	650	704	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	213	133	40	39	1	0	0
7	W	25	213	133	40	39	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	733	5716	3665	951	1067	33	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	4047	2601	684	737	25	0	0
9	K	493	3988	2563	672	729	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	493	310	79	102	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	703	5403	3436	971	971	25	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	685	5402	3446	940	988	28	0	0

- Molecule 14 is a protein called Cell division cycle protein 20 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	Q	354	2671	1676	488	496	11	0	0

- Molecule 15 is a protein called Cell division cycle protein 20 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	R	383	2953	1855	538	548	12	0	0

- Molecule 16 is a protein called Mitotic checkpoint serine/threonine-protein kinase BUB1 beta,Mitotic checkpoint serine/threonine-protein kinase BUB1 beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	S	277	2077	1292	380	400	5	0	0

- Molecule 17 is a protein called Anaphase-promoting complex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	X	484	3773	2393	652	704	24	0	0
17	Y	496	3868	2449	669	724	26	0	0

- Molecule 18 is a protein called Mitotic spindle assembly checkpoint protein MAD2A.

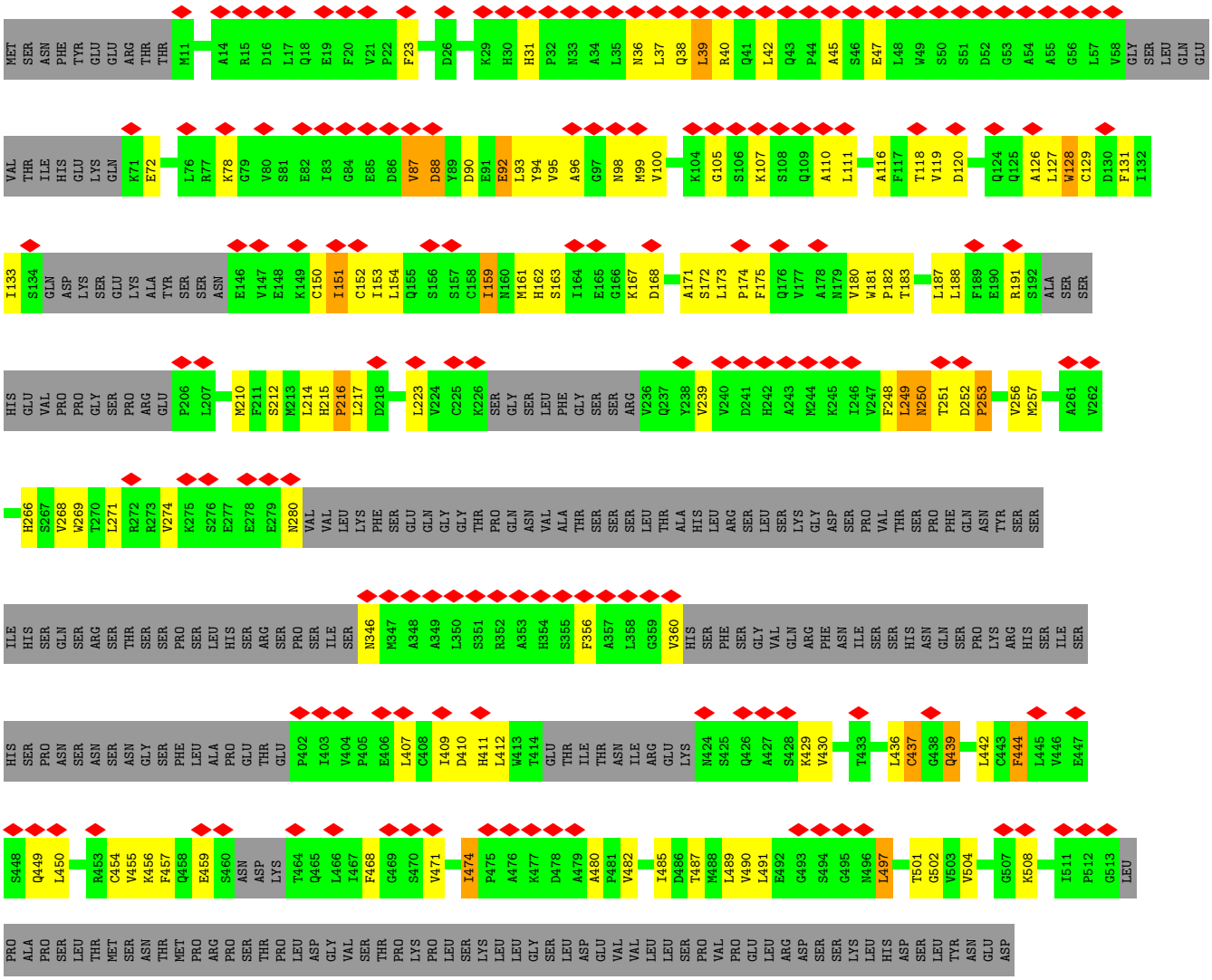
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	Z	195	1577	1012	256	305	4	0	0

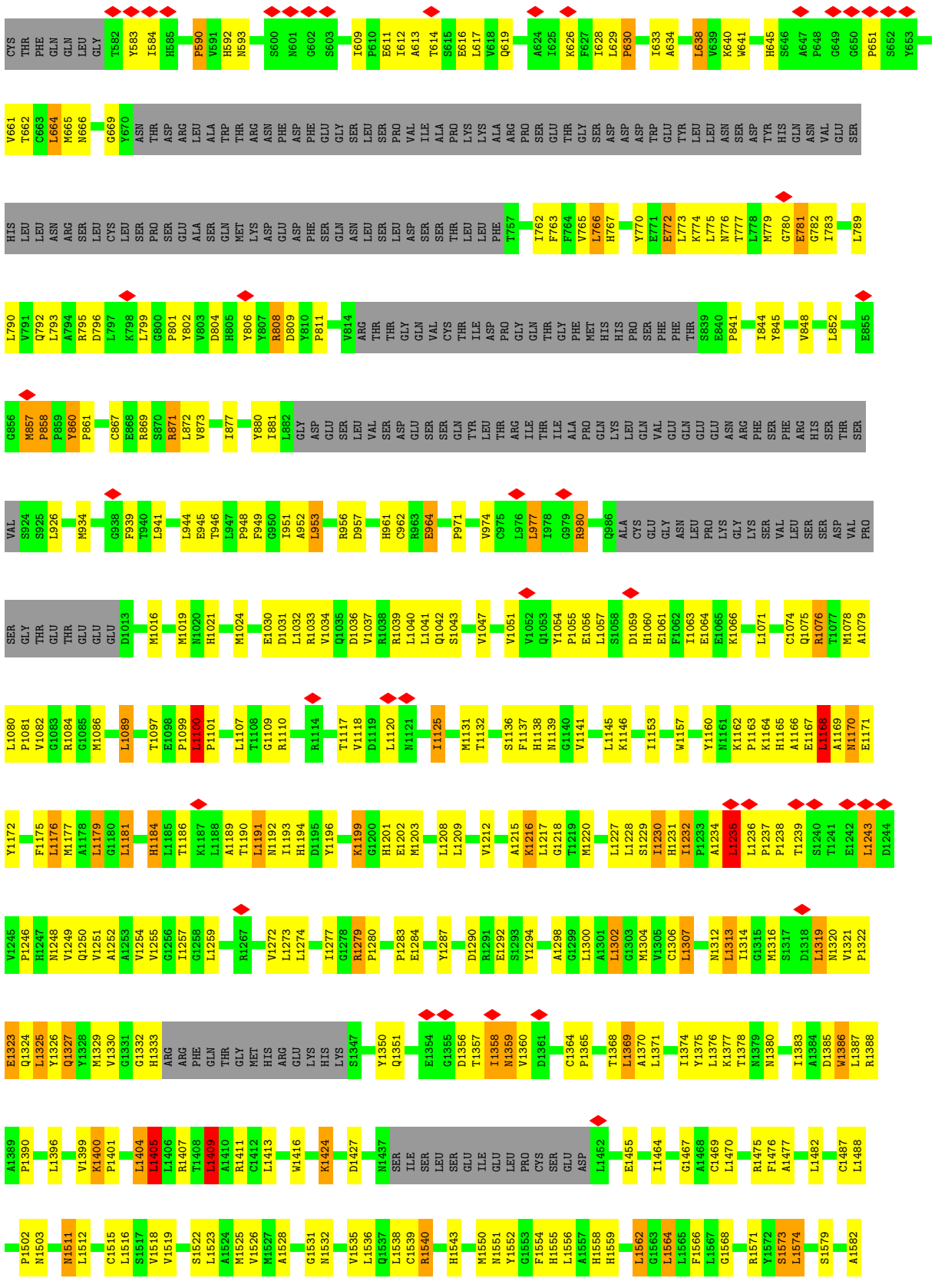
3 Residue-property plots (i)

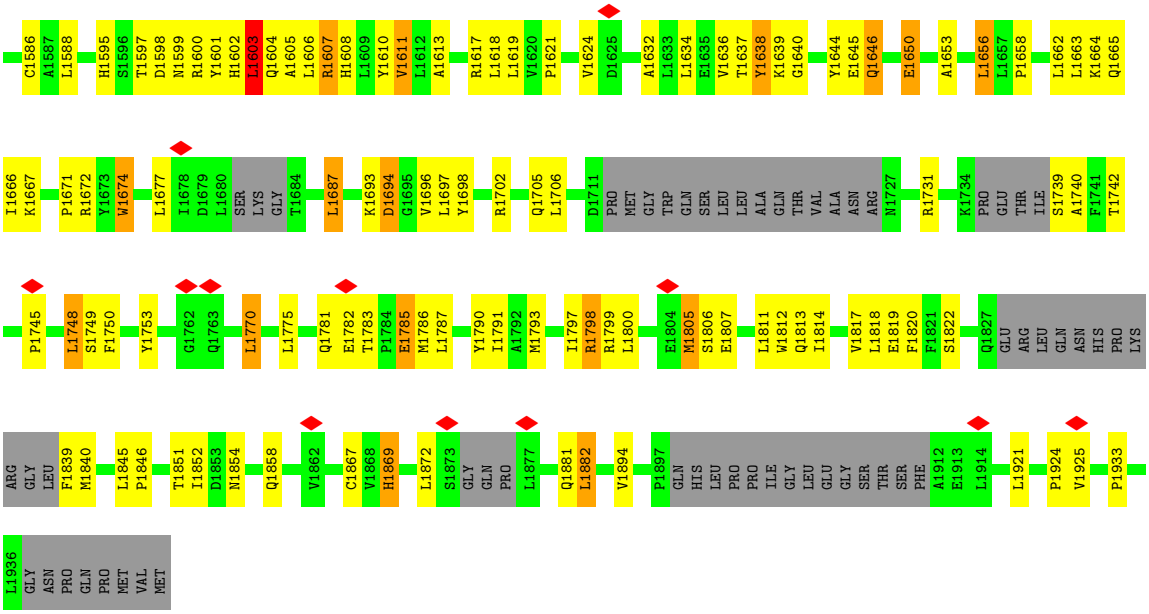
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Anaphase-promoting complex subunit 1

Chain A:

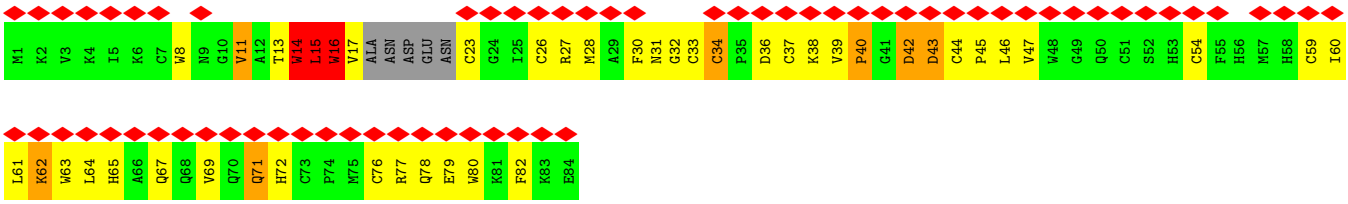



CYS THR PHE GLN GLN LEU GLY T582 Y583 I584 H585 P590 V591 H592 N593 S600 N601 G602 S603 I609 P610 E611 I612 A613 T614 S615 E616 L617 V618 Q619 A624 I625 K626 F627 I628 L629 P630 I633 A634 L638 V639 K640 W641 H645 S646 A647 P648 G649 G650 P651 S652 Y653
V661 T662 C663 L664 M665 N666 G669 Y670 ASN THR ASP ARG LEU ALA TRP THR ARG ASN PHE ASP PHE GLU GLY SER LEU SER PRO VAL ILE ALA PRO LYS LYS ALA ARG PRO SER GLU THR GLY SER ASP ASP TRP GLU TYR LEU LEU ASN SER ASP TYR HIS GLN ASN VAL GLU SER
HIS LEU LEU ASN ARG SER LEU CYS LEU SER PRO SER GLU ALA SER GLN MET LYS ASP GLU ASP PHE SER GLN ASN LEU LEU SER LEU ASP SER SER THR LEU LEU PHE T757 I762 F763 F764 V765 L766 H767 Y770 E771 E772 L773 K774 L775 N776 T777 L778 M779 G780 E781 G782 I783 L789
L790 V791 Q792 L793 A794 R795 D796 L797 K798 L799 G800 P801 Y802 V803 D804 H805 Y806 Y807 R808 D809 Y810 P811 V814 ARG THR THR GLY GLN VAL CYS THR ILE ASP PRO GLY GLN THR GLY PHE MET HIS HIS PRO SER PHE PHE THR S839 E840 P841 I844 Y845 V848 L852 E855
G856 M857 P858 P859 Y860 P861 C867 E868 R869 S870 R871 L872 V873 I877 Y880 I881 L882 GLY ASP GLU SER LEU VAL SER ASP GLU SER SER GLN TYR LEU THR ARG ILE THR ILE ALA PRO GLN LYS LEU GLN VAL GLU GLN GLU GLU ASN ARG PHE SER PHE ARG HIS SER THR SER
VAL S924 S925 L926 M934 G938 F939 T940 L941 L944 E945 T946 L947 P948 F949 G950 I951 A952 L953 R956 D957 H961 C962 R963 E964 P971 V974 C975 L976 L977 I978 G979 R980 Q986 ALA CYS GLU GLY ASN LEU PRO LYS GLY LYS SER VAL LEU SER SER ASP VAL PRO
SER GLY THR GLU THR GLU GLU GLU D1013 M1016 M1019 N1020 H1021 M1024 E1030 D1031 L1032 R1033 V1034 Q1035 D1036 V1037 R1038 R1039 L1040 L1041 Q1042 S1043 V1047 V1051 V1052 Q1053 Y1054 P1055 E1056 L1057 S1058 D1059 H1060 E1061 F1062 I1063 E1064 E1065 K1066 L1071 C1074 Q1075 R1076 T1077 M1078 A1079
L1080 P1081 V1082 G1083 R1084 G1085 M1086 L1089 T1097 E1098 P1099 L1100 P1101 L1107 T1108 G1109 R1110 R1114 T1117 V1118 D1119 L1120 N1121 I1125 M1131 T1132 S1136 F1137 H1138 N1139 G1140 V1141 L1145 K1146 I1153 W1157 Y1160 N1161 K1162 P1163 K1164 H1165 A1166 E1167 L1168 A1169 N1170 E1171
Y1172 F1175 L1176 M1177 A1178 L1179 G1180 L1181 H1184 L1185 T1186 K1187 L1188 A1189 T1190 L1191 N1192 I1193 H1194 D1195 Y1196 K1199 G1200 H1201 E1202 M1203 L1208 L1209 V1212 A1215 K1216 L1217 G1218 T1219 M1220 L1227 L1228 S1229 I1230 H1231 I1232 P1233 A1234 L1235 L1236 P1237 P1238 T1239 S1240 T1241 E1242 L1243 D1244
V1245 P1246 H1247 N1248 V1249 Q1250 V1251 A1252 A1253 V1254 V1255 G1256 I1257 G1258 L1259 R1267 V1272 L1273 L1274 I1277 G1278 R1279 P1280 P1283 E1284 Y1287 D1290 R1291 E1292 S1293 Y1294 A1298 G1299 L1300 A1301 L1302 G1303 M1304 V1305 C1306 L1307 N1312 L1313 I1314 G1315 M1316 S1317 D1318 L1319 N1320 V1321 P1322
E1323 Q1324 L1325 Y1326 Q1327 Y1328 M1329 V1330 G1331 G1332 H1333 ARG ARG PHE GLN THR GLY MET HIS ARG GLU LYS HIS LYS S1347 Y1350 Q1351 E1354 G1355 D1356 T1357 I1358 N1359 V1360 D1361 C1364 P1365 T1368 L1369 A1370 L1371 I1374 Y1375 L1376 K1377 T1378 N1379 N1380 I1383 A1384 D1385 W1386 L1387 R1388
A1389 P1390 L1396 V1399 K1400 P1401 L1404 L1405 L1406 R1407 T1408 L1409 A1410 R1411 C1412 L1413 W1416 K1424 D1427 N1437 SER ILE SER LEU SER GLU ILE GLU LEU PRO CYS SER GLU ASP L1452 E1455 I1464 G1467 A1468 C1469 L1470 R1475 F1476 A1477 L1482 C1487 L1488
P1502 N1503 N1511 L1512 C1515 L1516 S1517 V1518 V1519 S1522 L1523 A1524 M1525 V1526 M1527 A1528 G1531 N1532 V1535 L1536 G1537 L1538 C1539 R1540 H1543 M1550 N1551 Y1552 G1553 F1554 H1555 L1556 A1557 H1558 H1559 L1562 G1563 L1564 L1565 F1566 L1567 G1568 R1571 Y1572 S1573 L1574 S1579 A1582



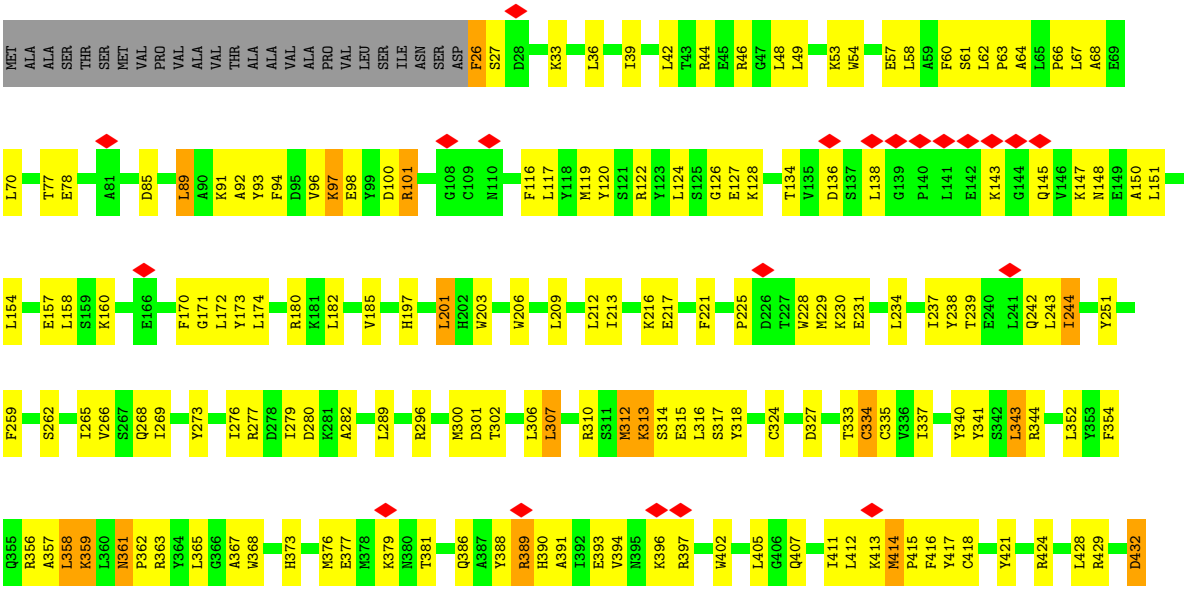
- Molecule 2: Anaphase-promoting complex subunit 11

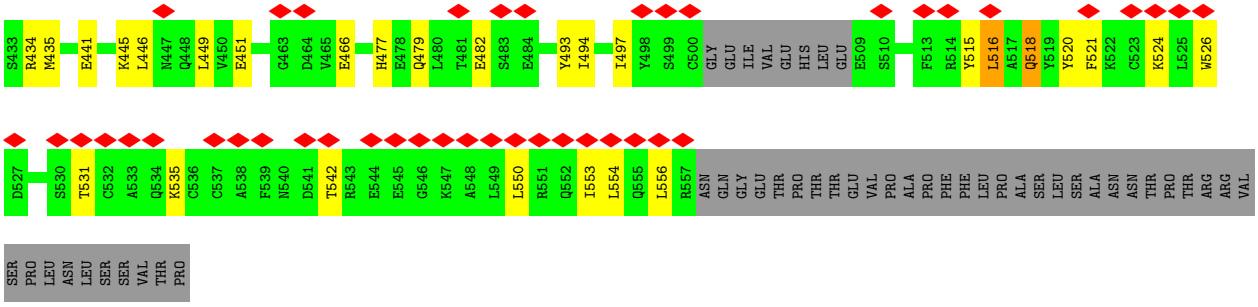
Chain B:



- Molecule 3: Cell division cycle protein 23 homolog

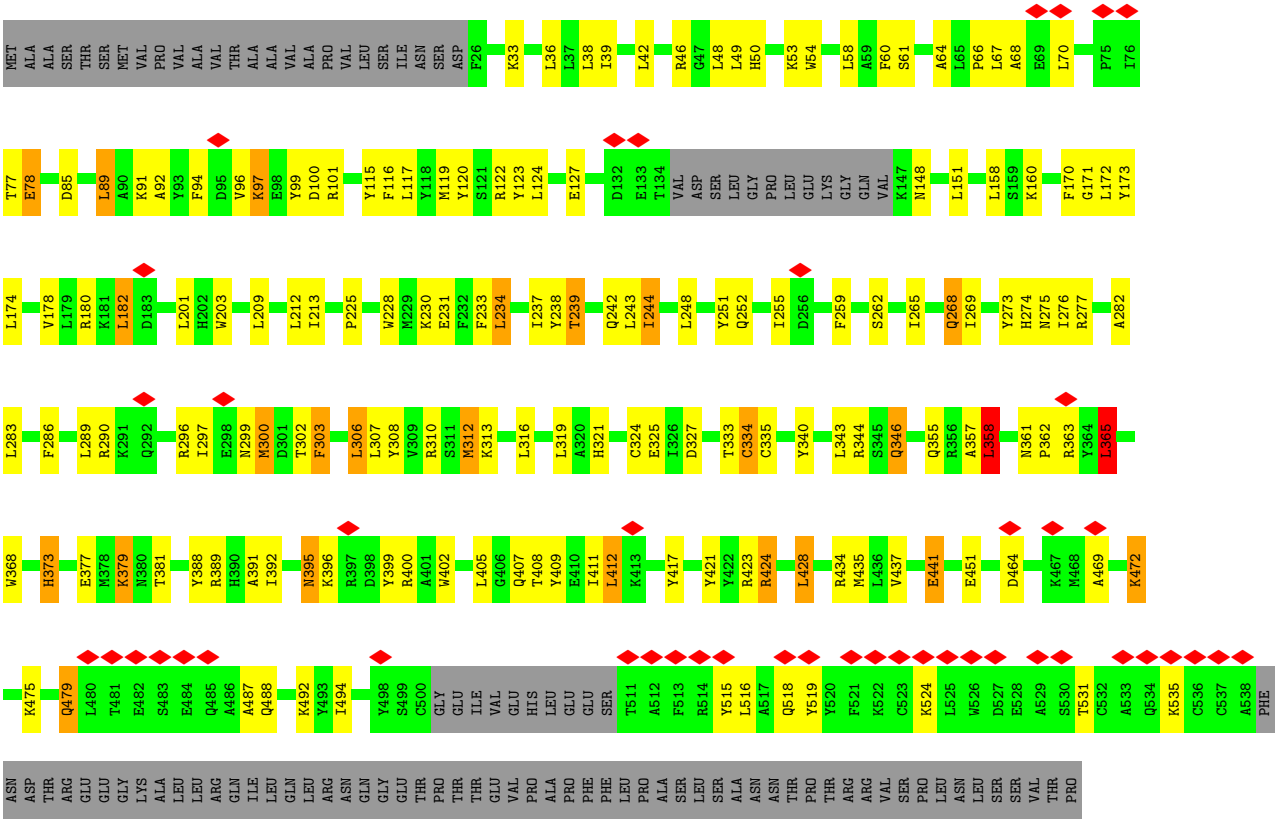
Chain C:





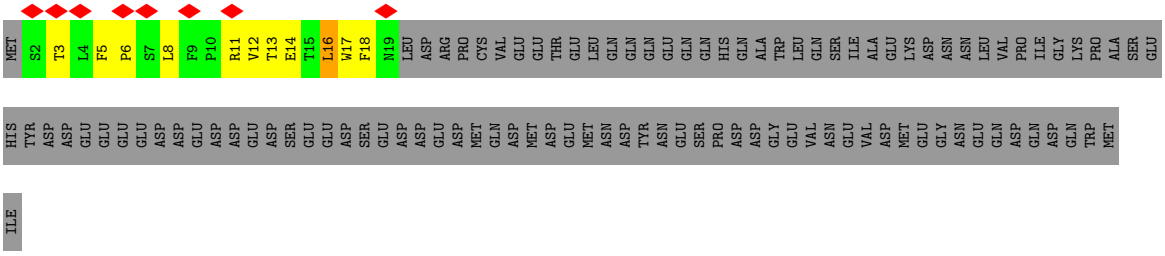
- Molecule 3: Cell division cycle protein 23 homolog

Chain P:



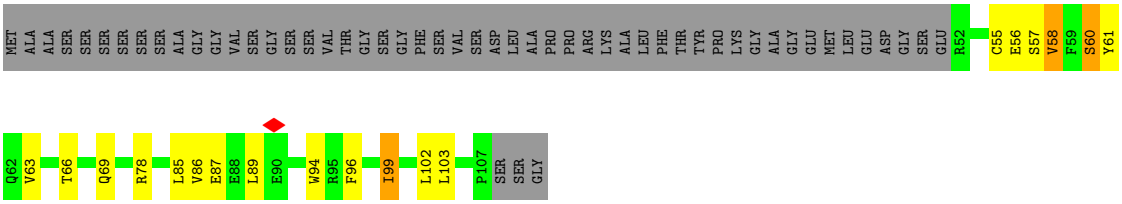
- Molecule 4: Anaphase-promoting complex subunit 15

Chain D:



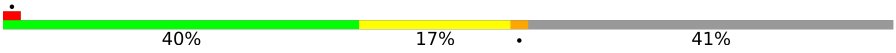
- Molecule 5: Anaphase-promoting complex subunit 16

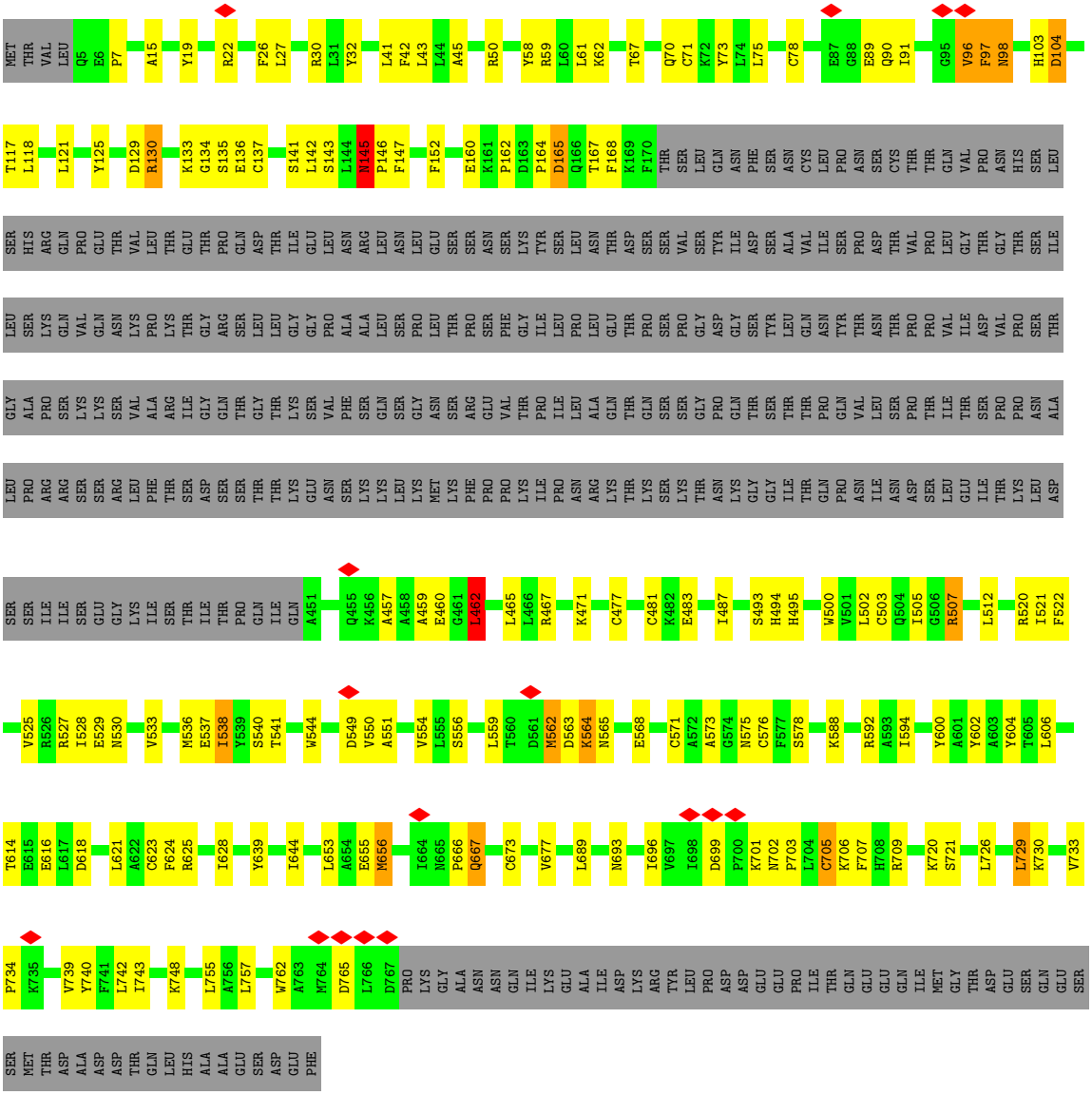
Chain E:



- Molecule 6: Cell division cycle protein 27 homolog

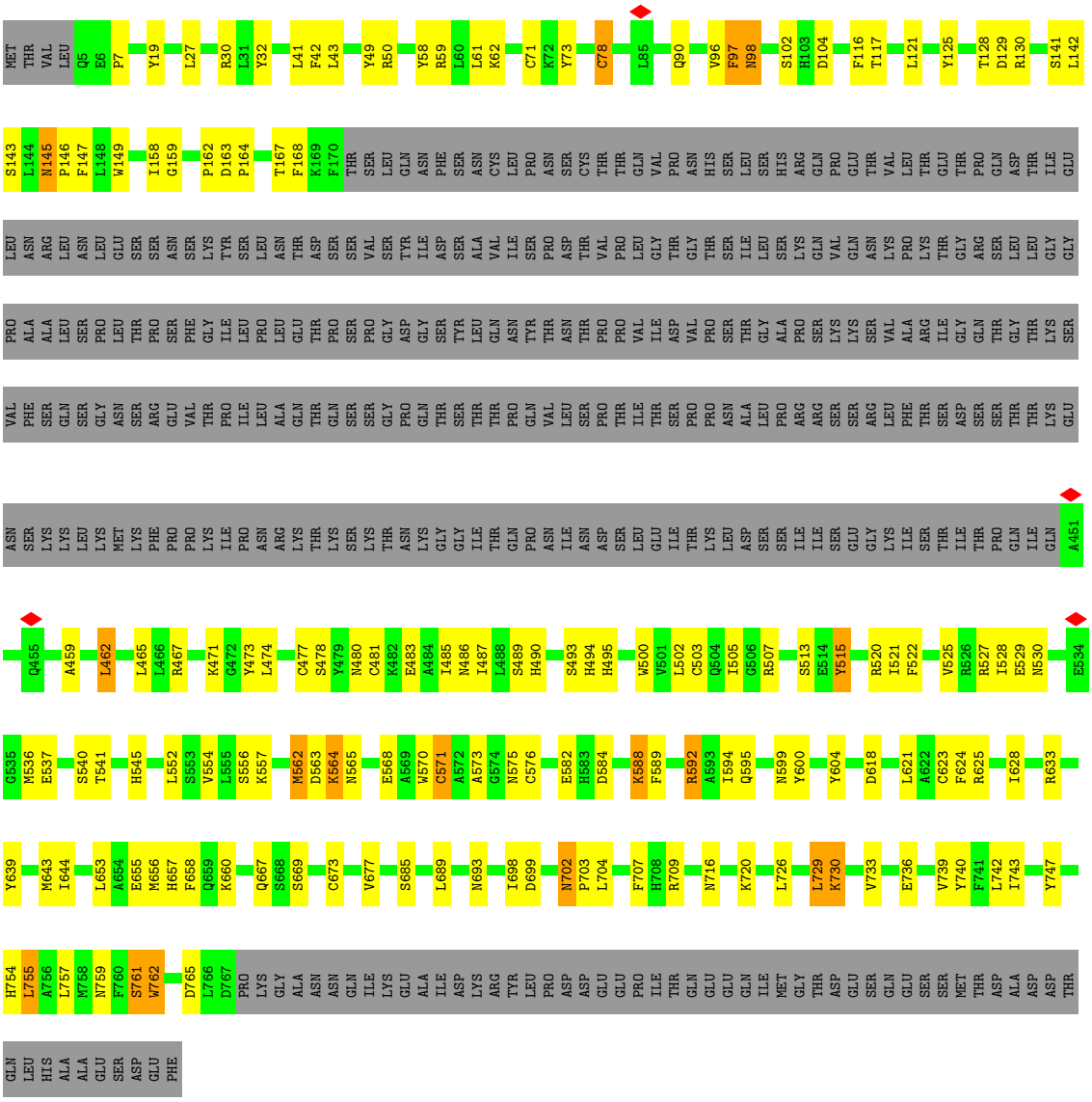
Chain F:





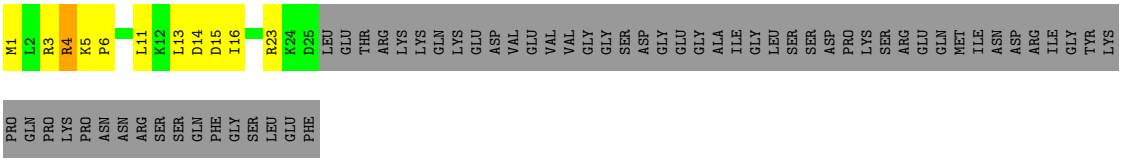
- Molecule 6: Cell division cycle protein 27 homolog

Chain H: 40% 17% • 41%



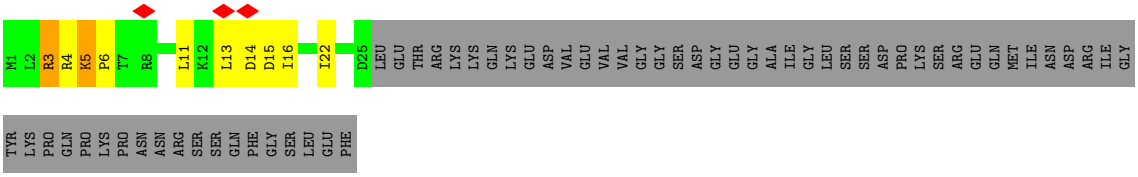
• Molecule 7: Anaphase-promoting complex subunit CDC26

Chain G: 16% 12% • 71%



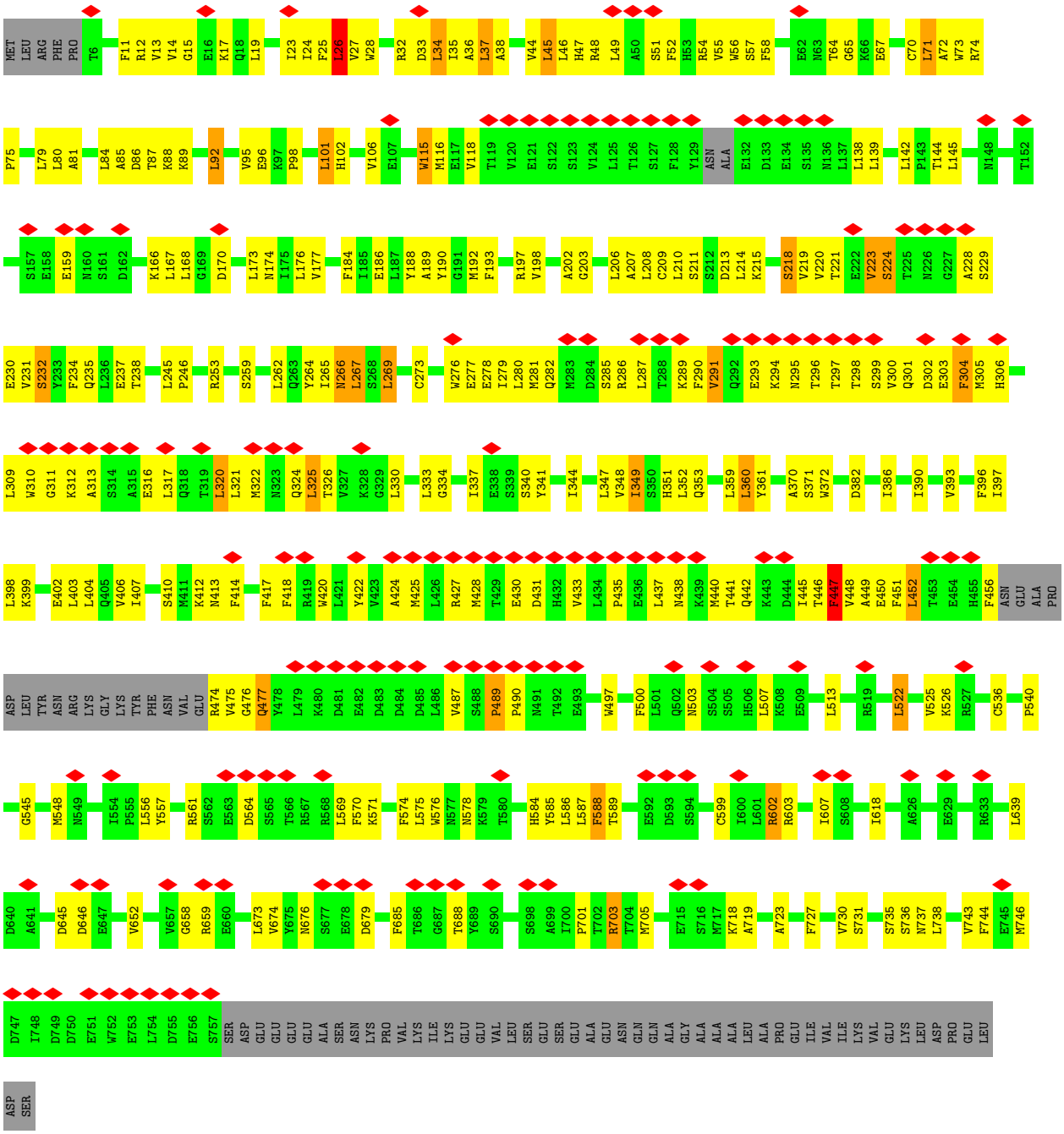
• Molecule 7: Anaphase-promoting complex subunit CDC26

Chain W: 18% 9% • 71%



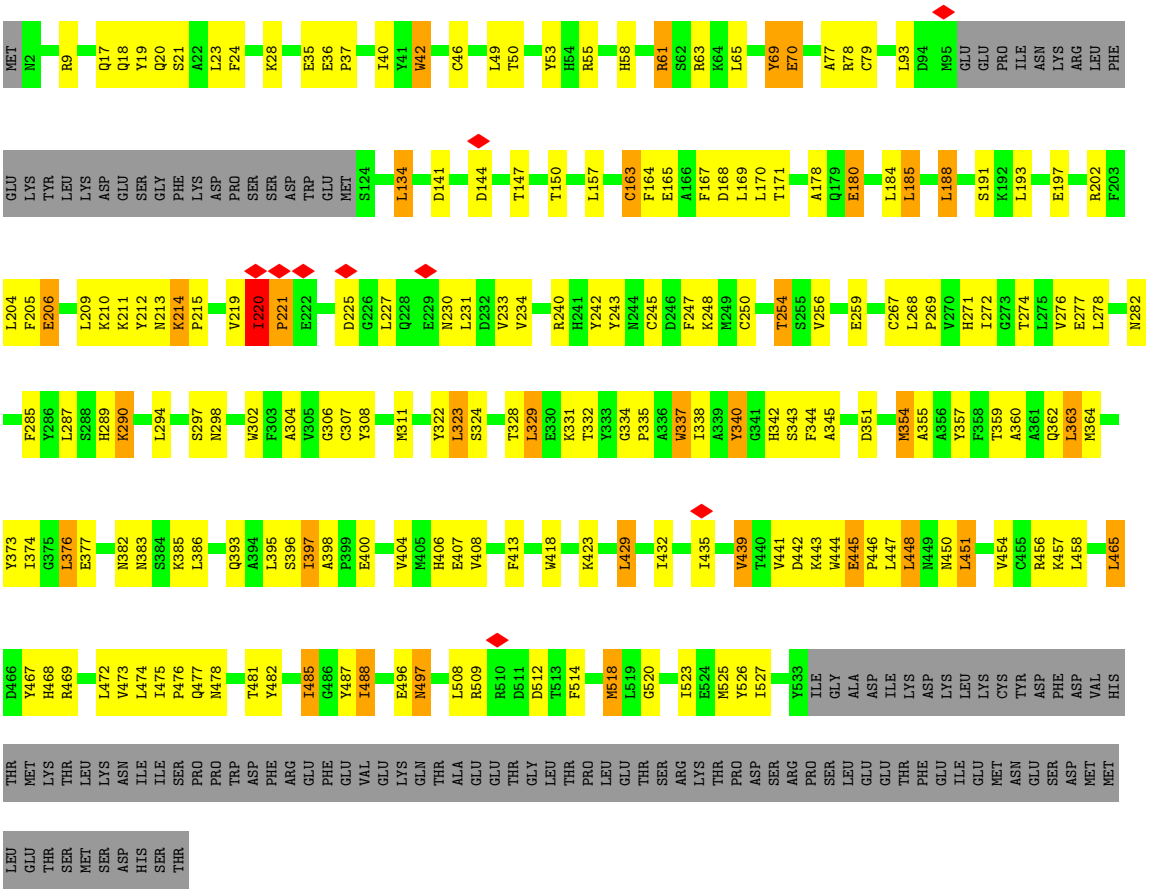
• Molecule 8: Anaphase-promoting complex subunit 4

Chain I:



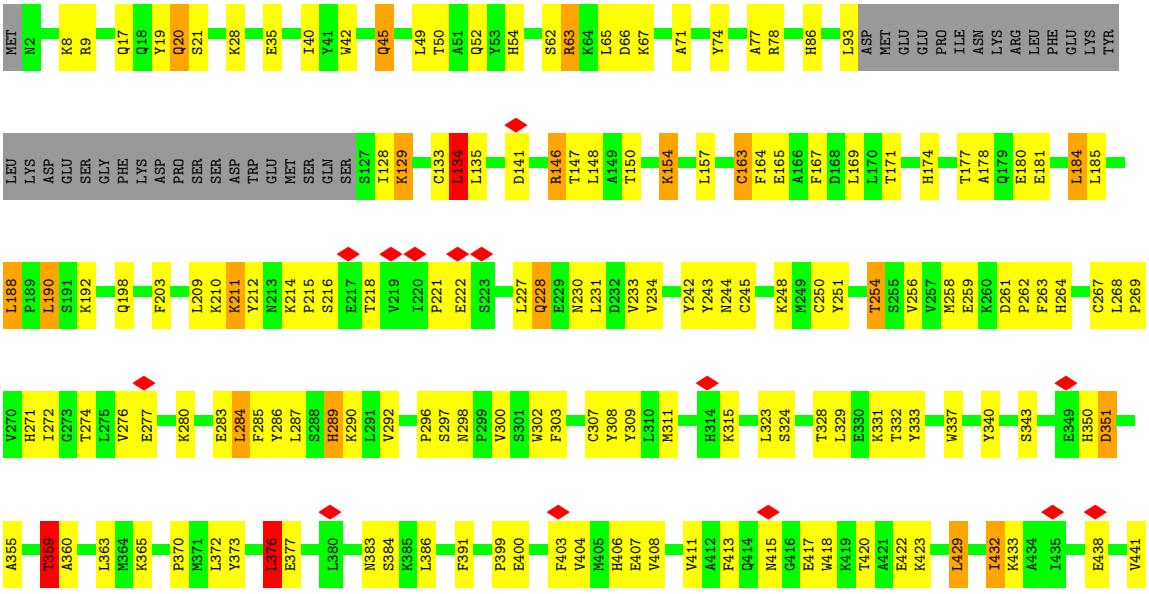
• Molecule 9: Cell division cycle protein 16 homolog

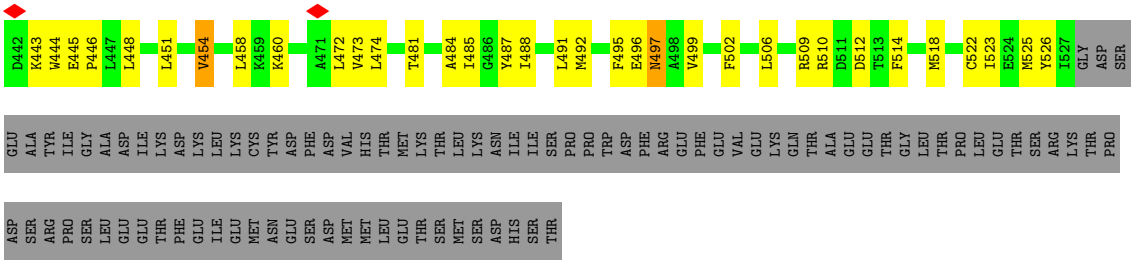
Chain J: 50% 26% 5% 19%



• Molecule 9: Cell division cycle protein 16 homolog

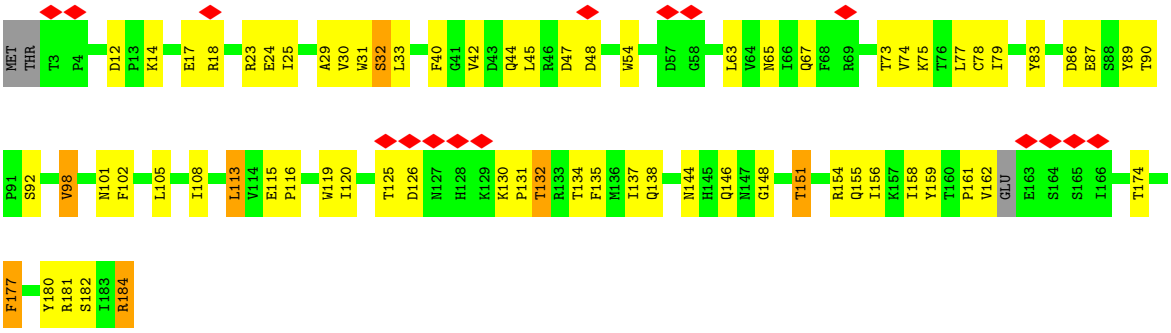
Chain K: 48% 28% • 20%





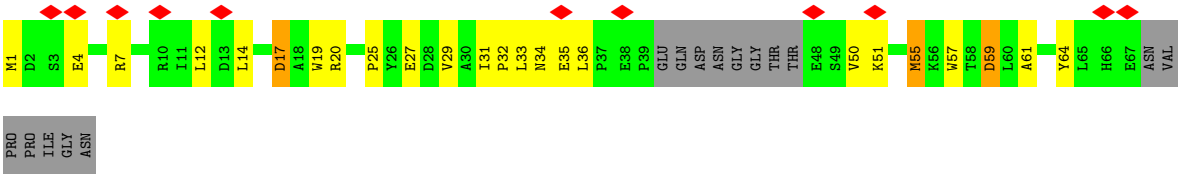
- Molecule 10: Anaphase-promoting complex subunit 10

Chain L:



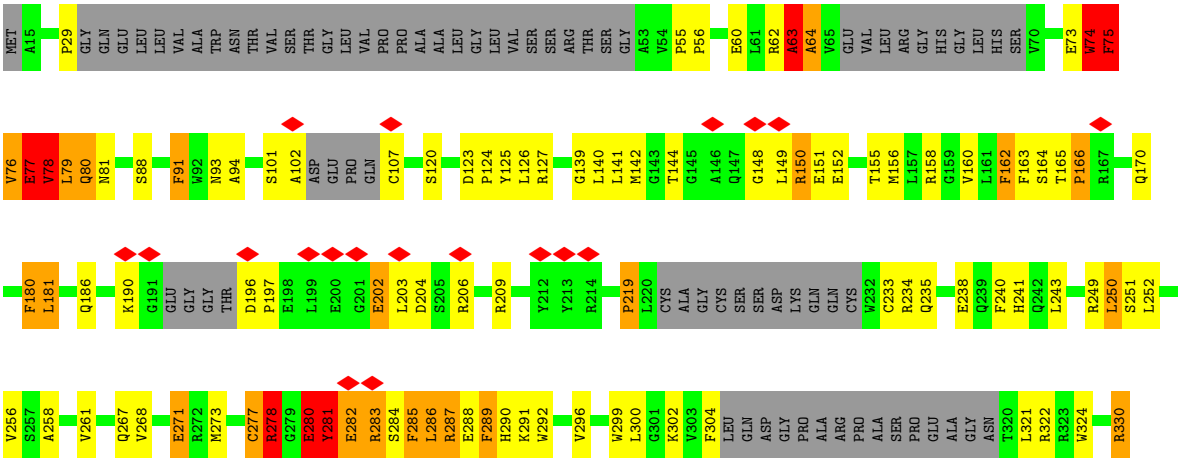
- Molecule 11: Anaphase-promoting complex subunit 13

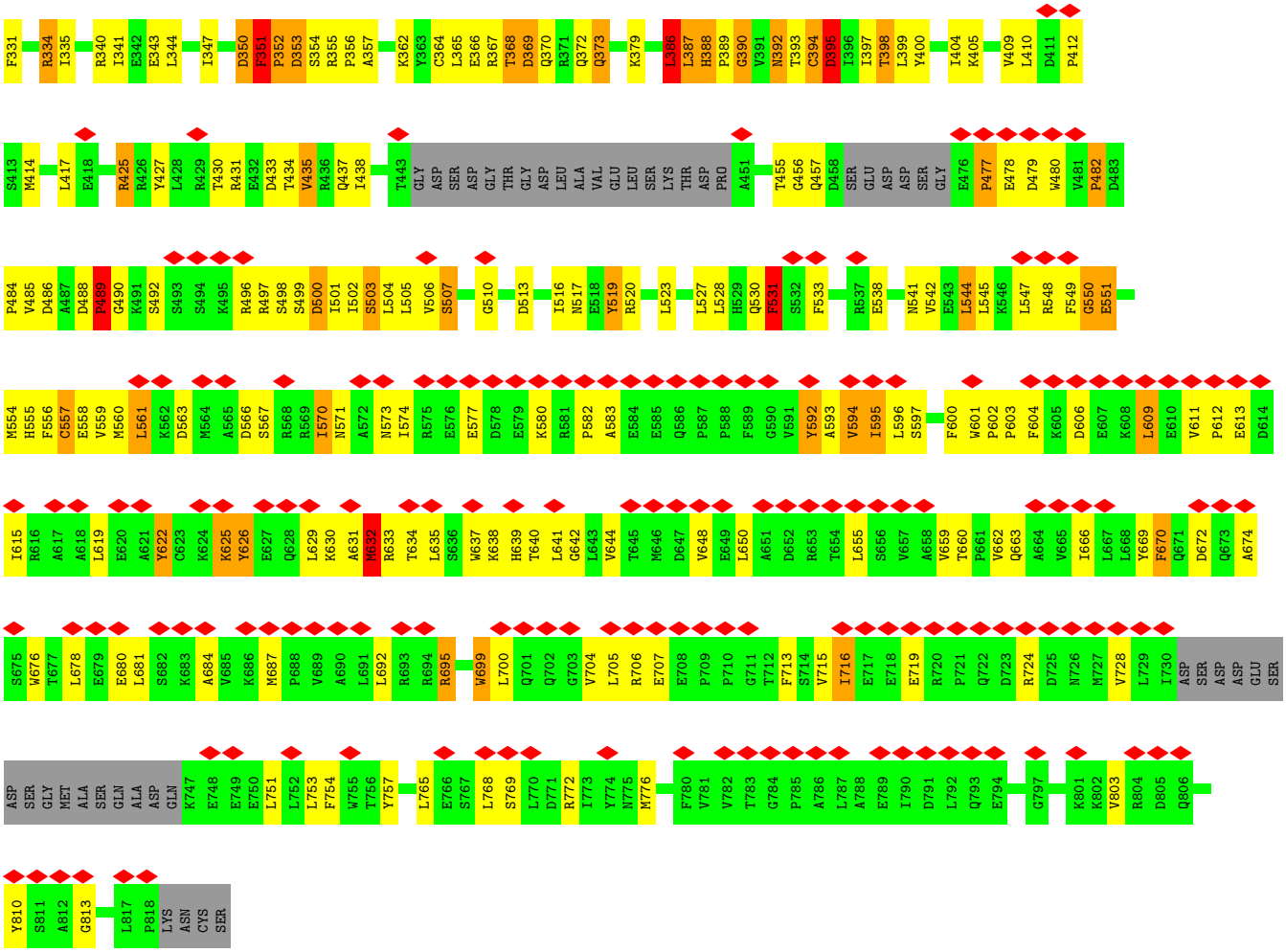
Chain M:



- Molecule 12: Anaphase-promoting complex subunit 2

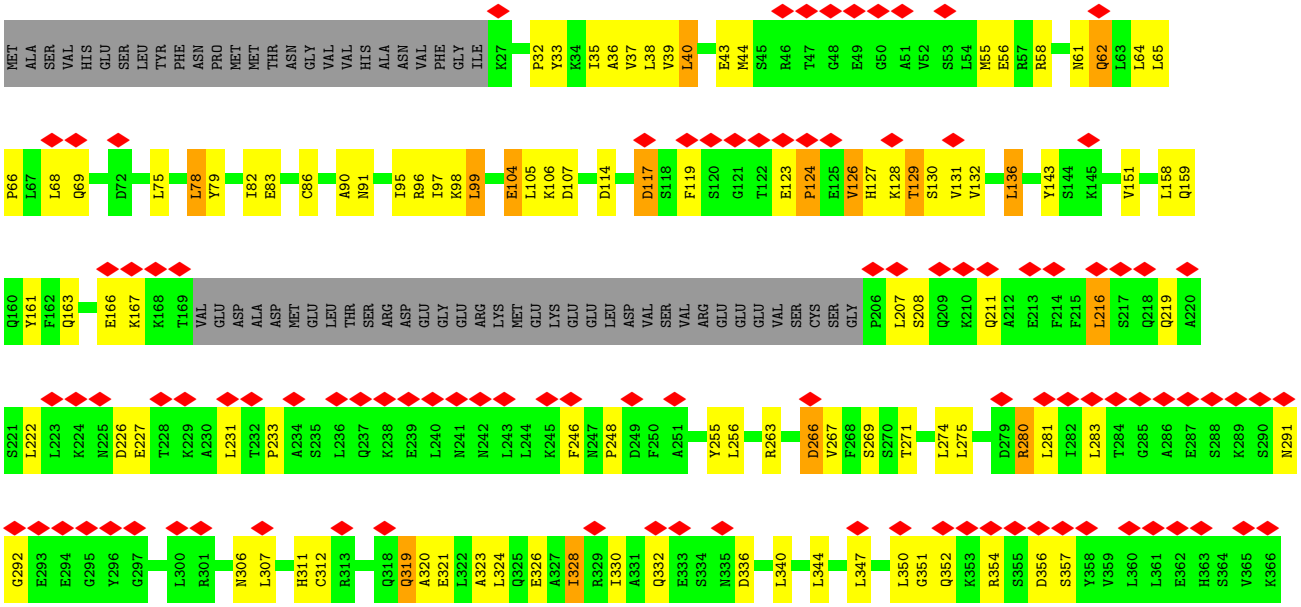
Chain N:

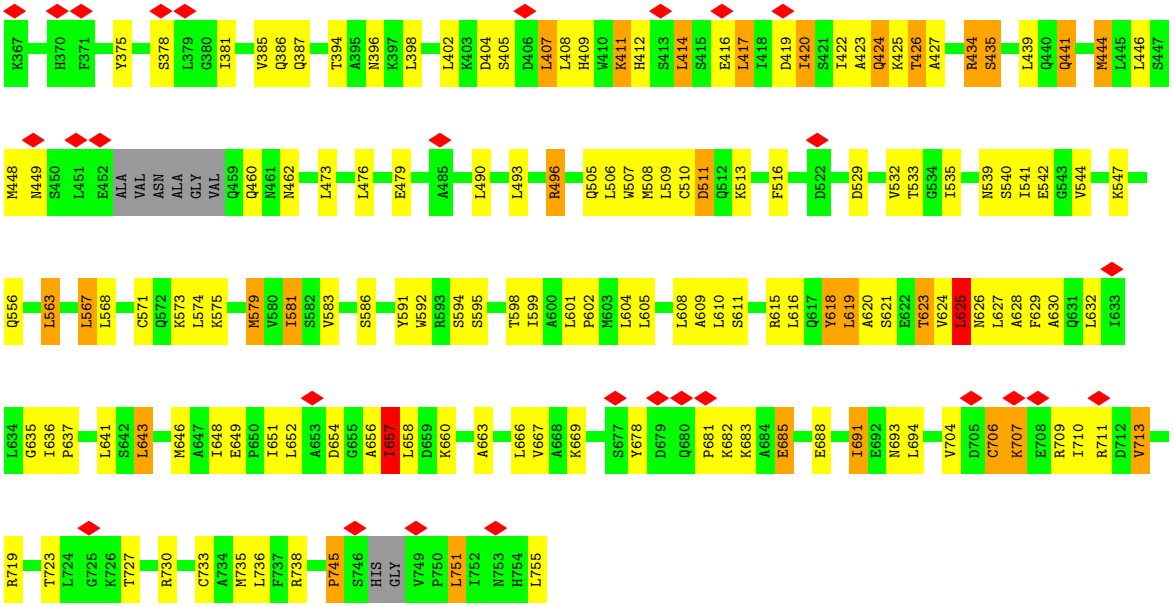




- Molecule 13: Anaphase-promoting complex subunit 5

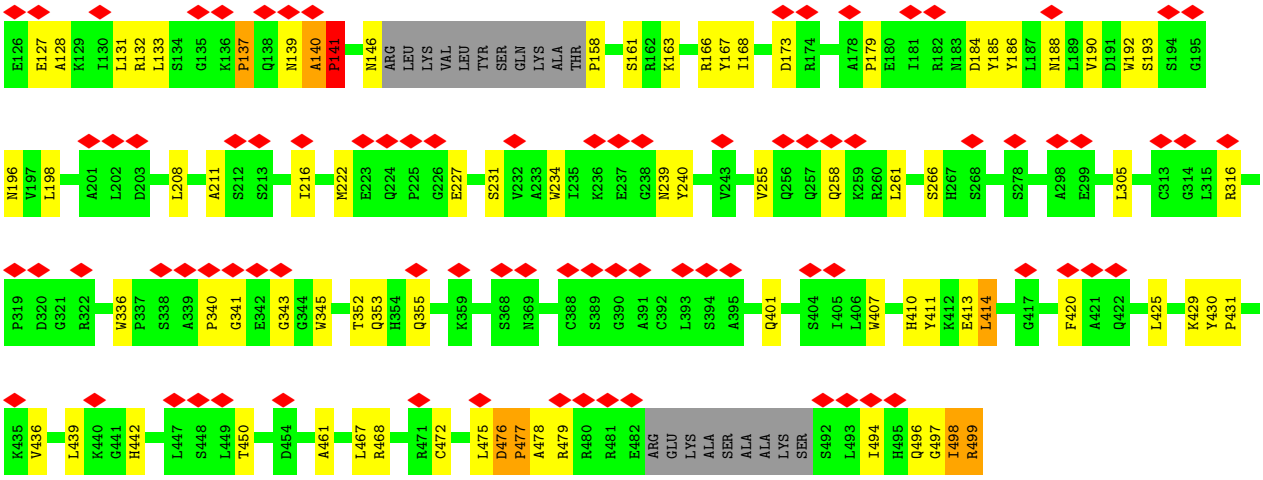
Chain O:





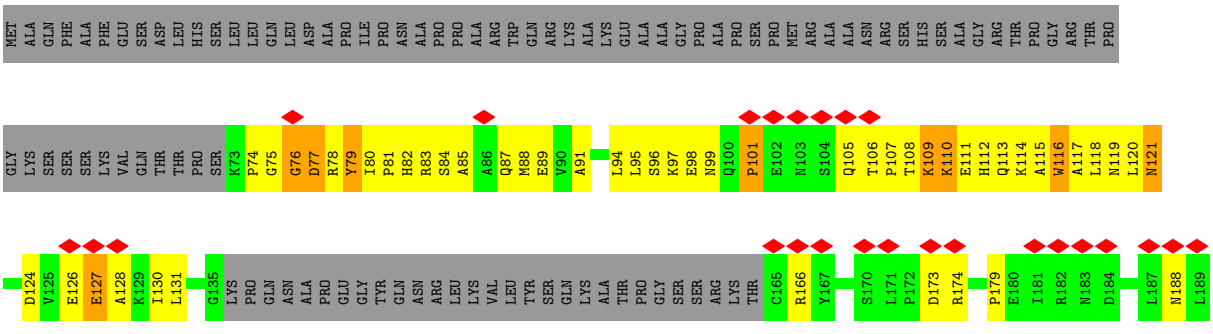
- Molecule 14: Cell division cycle protein 20 homolog

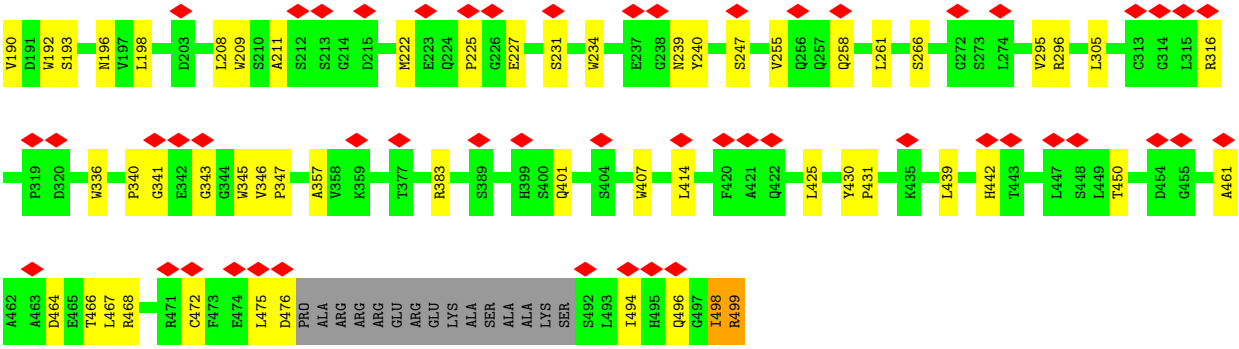
Chain Q:



- Molecule 15: Cell division cycle protein 20 homolog

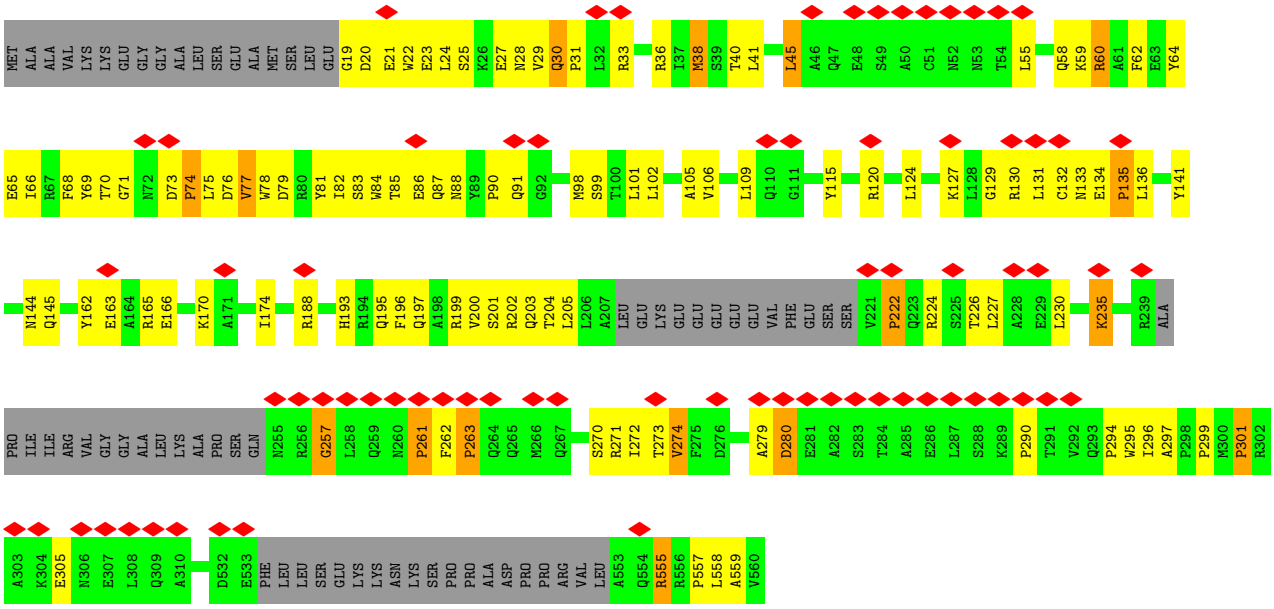
Chain R:





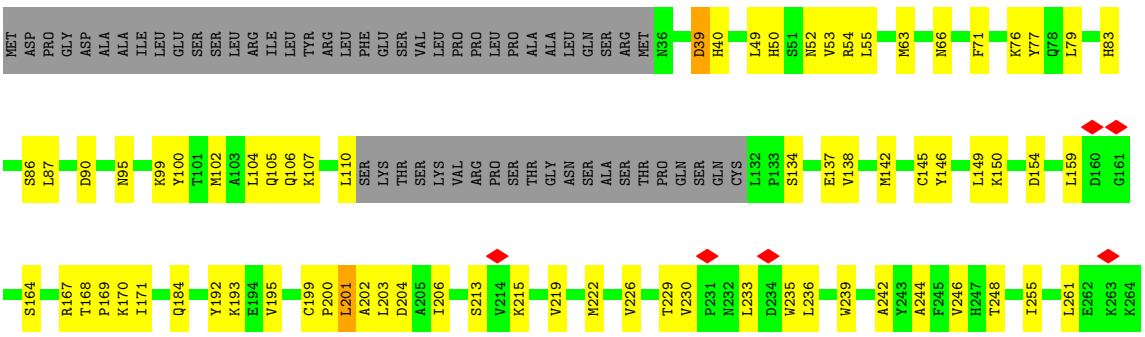
• Molecule 16: Mitotic checkpoint serine/threonine-protein kinase BUB1 beta,Mitotic checkpoint serine/threonine-protein kinase BUB1 beta

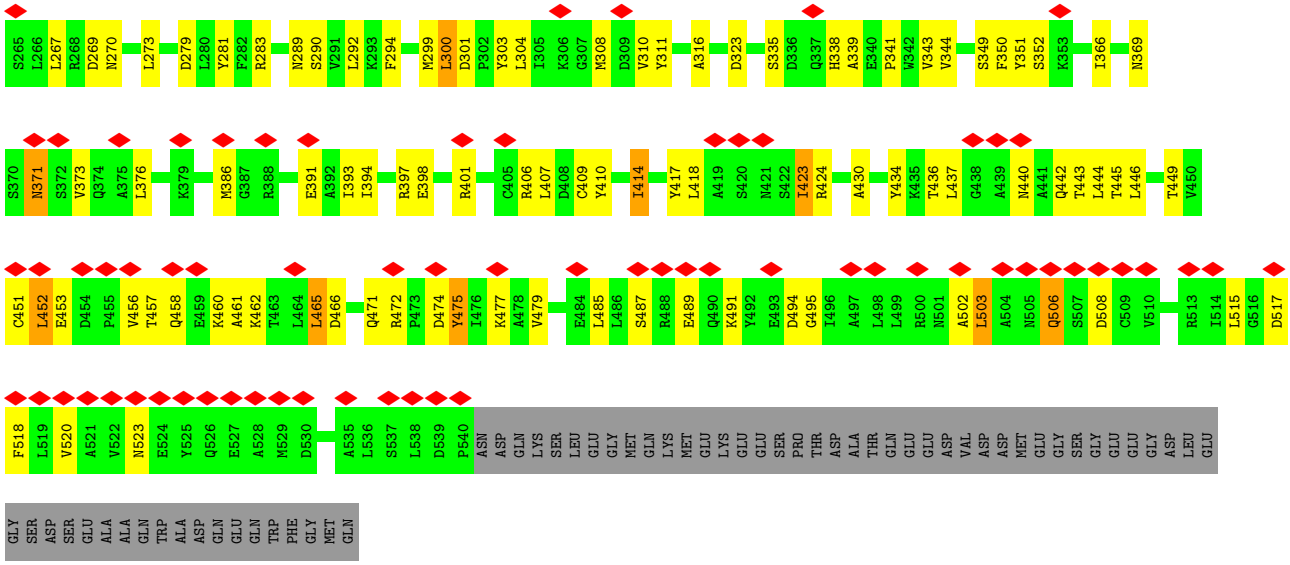
Chain S:



• Molecule 17: Anaphase-promoting complex subunit 7

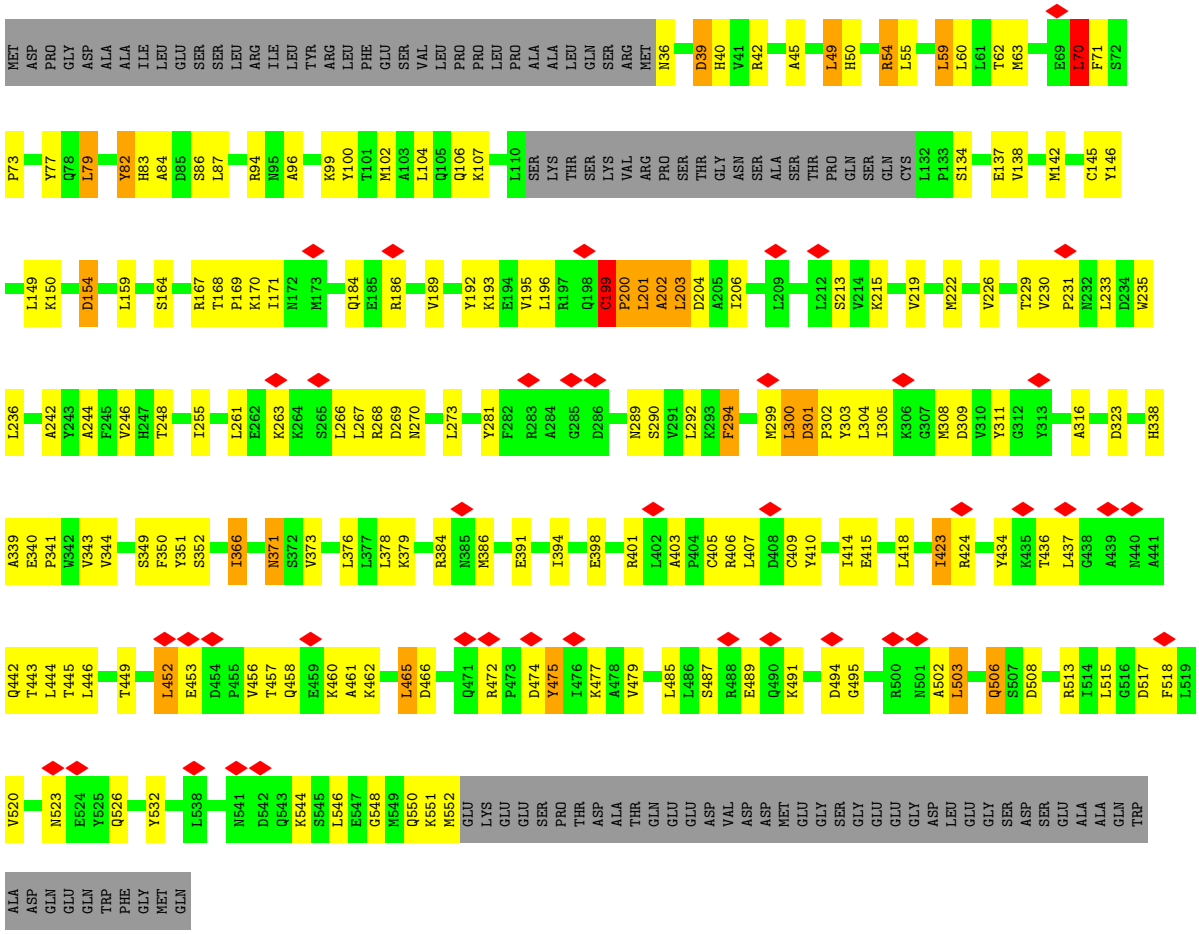
Chain X:





- Molecule 17: Anaphase-promoting complex subunit 7

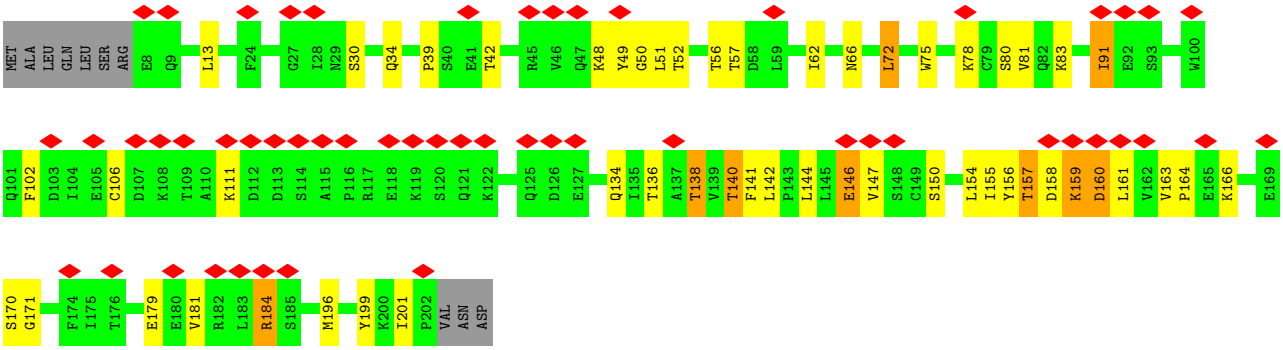
Chain Y:



- Molecule 18: Mitotic spindle assembly checkpoint protein MAD2A

Chain Z:

26%
69%
21%
5%


MET ALA LEU GLN LEU SER ARG E8 Q9 L13 F24 G27 I28 N29 S30 Q34 P39 S40 E41 T42 R45 V46 Q47 K48 Y49 G50 L51 T52 T56 T57 D58 L59 I62 N66 L72 W75 K78 C79 S80 V81 Q82 K83 I91 E92 S93 W100
Q101 F102 D103 I104 E105 C106 D107 K108 T109 A110 K111 D112 D113 S114 A115 P116 R117 E118 K119 S120 Q121 K122 Q125 D126 E127 Q134 I135 T136 A137 T138 V139 T140 F141 L142 P143 L144 L145 E146 V147 S148 G149 S150 L154 I155 Y156 T157 D158 K159 D160 L161 V162 V163 P164 E165 K166 E169
S170 G171 F174 I175 T176 E179 E180 V181 R182 L183 R184 S185 M196 Y199 K200 I201 P202 VAL ASN ASP

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	155263	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	27	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.292	Depositor
Minimum map value	-0.094	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.015	Depositor
Recommended contour level	0.08	Depositor
Map size (Å)	359.04, 359.04, 359.04	wwPDB
Map dimensions	264, 264, 264	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)

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	0.67	6/11190 (0.1%)	0.89	23/15236 (0.2%)
2	B	0.81	2/665 (0.3%)	0.98	2/896 (0.2%)
3	C	0.57	0/4404	0.83	4/5945 (0.1%)
3	P	0.60	0/4138	0.86	5/5587 (0.1%)
4	D	0.69	0/159	0.89	0/218
5	E	0.60	0/459	0.80	0/619
6	F	0.58	0/3939	0.82	3/5325 (0.1%)
6	H	0.61	2/3943 (0.1%)	0.82	2/5329 (0.0%)
7	G	0.63	0/214	1.02	1/284 (0.4%)
7	W	0.66	0/214	0.97	1/284 (0.4%)
8	I	0.66	1/5834 (0.0%)	0.92	11/7909 (0.1%)
9	J	0.71	2/4146 (0.0%)	0.95	5/5616 (0.1%)
9	K	0.73	1/4086 (0.0%)	0.93	7/5534 (0.1%)
10	L	0.54	0/1468	0.83	0/1993
11	M	0.66	0/502	0.95	0/680
12	N	0.63	3/5495 (0.1%)	0.94	18/7441 (0.2%)
13	O	0.58	0/5501	0.85	8/7432 (0.1%)
14	Q	0.72	0/2737	0.86	4/3732 (0.1%)
15	R	0.73	0/3029	0.86	2/4124 (0.0%)
16	S	0.66	0/2112	0.88	12/2863 (0.4%)
17	X	0.57	0/3833	0.82	3/5187 (0.1%)
17	Y	0.58	0/3928	0.84	9/5311 (0.2%)
18	Z	0.64	0/1605	0.79	2/2176 (0.1%)
All	All	0.64	17/73601 (0.0%)	0.88	122/99721 (0.1%)

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	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
9	J	0	1
12	N	0	16
16	S	0	1
All	All	0	21

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1030	GLU	CD-OE1	21.93	1.49	1.25
1	A	1030	GLU	CD-OE2	15.62	1.42	1.25
1	A	1199	LYS	CE-NZ	9.92	1.73	1.49
12	N	209	ARG	NE-CZ	9.66	1.45	1.33
1	A	1030	GLU	CG-CD	8.25	1.64	1.51

The worst 5 of 122 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	N	330	ARG	NE-CZ-NH2	-13.57	113.52	120.30
16	S	60	ARG	NE-CZ-NH1	9.25	124.92	120.30
9	K	351	ASP	CB-CG-OD1	8.97	126.37	118.30
1	A	1235	LEU	CB-CG-CD2	-8.77	96.09	111.00
3	P	358	LEU	CB-CG-CD1	-8.46	96.62	111.00

There are no chirality outliers.

5 of 21 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1191	LEU	Peptide
8	I	658	GLY	Peptide
8	I	727	PHE	Peptide
9	J	220	ILE	Peptide
12	N	62	ARG	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	10949	0	10690	418	0
2	B	643	0	617	80	0
3	C	4306	0	4272	161	0
3	P	4043	0	4000	137	0
4	D	153	0	148	8	0
5	E	450	0	435	10	0
6	F	3849	0	3783	108	0
6	H	3853	0	3794	128	0
7	G	213	0	220	11	0
7	W	213	0	220	12	0
8	I	5716	0	5587	345	0
9	J	4047	0	3949	185	0
9	K	3988	0	3908	174	0
10	L	1435	0	1382	55	0
11	M	493	0	469	24	0
12	N	5403	0	5103	276	0
13	O	5402	0	5436	221	0
14	Q	2671	0	2516	103	0
15	R	2953	0	2839	111	0
16	S	2077	0	1827	327	0
17	X	3773	0	3831	163	0
17	Y	3868	0	3925	169	0
18	Z	1577	0	1592	89	0
All	All	72075	0	70543	2914	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 20.

The worst 5 of 2914 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)
16:S:38:MET:CE	18:Z:181:VAL:HG23	1.22	1.65
16:S:22:TRP:CZ3	16:S:41:LEU:HB2	1.31	1.64
16:S:19:GLY:CA	18:Z:134:GLN:HE21	1.16	1.54
8:I:413:ASN:HA	8:I:447:PHE:CZ	1.38	1.53
1:A:1199:LYS:NZ	1:A:1199:LYS:CE	1.73	1.45

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	1397/1944 (72%)	1267 (91%)	106 (8%)	24 (2%)	7	37
2	B	75/84 (89%)	62 (83%)	8 (11%)	5 (7%)	1	15
3	C	520/597 (87%)	498 (96%)	20 (4%)	2 (0%)	30	67
3	P	485/597 (81%)	465 (96%)	20 (4%)	0	100	100
4	D	16/121 (13%)	14 (88%)	2 (12%)	0	100	100
5	E	54/110 (49%)	53 (98%)	1 (2%)	0	100	100
6	F	479/824 (58%)	458 (96%)	13 (3%)	8 (2%)	7	37
6	H	479/824 (58%)	459 (96%)	14 (3%)	6 (1%)	10	42
7	G	23/85 (27%)	23 (100%)	0	0	100	100
7	W	23/85 (27%)	23 (100%)	0	0	100	100
8	I	725/808 (90%)	683 (94%)	35 (5%)	7 (1%)	13	48
9	J	500/620 (81%)	467 (93%)	29 (6%)	4 (1%)	16	54
9	K	489/620 (79%)	456 (93%)	27 (6%)	6 (1%)	11	44
10	L	180/185 (97%)	165 (92%)	14 (8%)	1 (1%)	22	59
11	M	55/74 (74%)	46 (84%)	9 (16%)	0	100	100
12	N	679/822 (83%)	557 (82%)	68 (10%)	54 (8%)	1	11
13	O	677/755 (90%)	640 (94%)	29 (4%)	8 (1%)	11	44
14	Q	348/374 (93%)	317 (91%)	21 (6%)	10 (3%)	3	26
15	R	377/499 (76%)	344 (91%)	26 (7%)	7 (2%)	6	35
16	S	267/342 (78%)	237 (89%)	18 (7%)	12 (4%)	2	20
17	X	480/599 (80%)	464 (97%)	13 (3%)	3 (1%)	22	59
17	Y	492/599 (82%)	474 (96%)	13 (3%)	5 (1%)	13	48
18	Z	193/205 (94%)	186 (96%)	6 (3%)	1 (0%)	25	62
All	All	9013/11773 (77%)	8358 (93%)	492 (6%)	163 (2%)	9	36

5 of 163 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	274	VAL
1	A	630	PRO
1	A	857	MET
1	A	1125	ILE
1	A	1358	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	1151/1720 (67%)	1011 (88%)	140 (12%)	4	18
2	B	71/75 (95%)	59 (83%)	12 (17%)	1	11
3	C	452/520 (87%)	390 (86%)	62 (14%)	3	16
3	P	422/520 (81%)	374 (89%)	48 (11%)	4	19
4	D	18/115 (16%)	15 (83%)	3 (17%)	2	11
5	E	47/89 (53%)	37 (79%)	10 (21%)	1	5
6	F	407/727 (56%)	361 (89%)	46 (11%)	4	19
6	H	408/727 (56%)	368 (90%)	40 (10%)	6	23
7	G	23/77 (30%)	20 (87%)	3 (13%)	3	16
7	W	23/77 (30%)	21 (91%)	2 (9%)	8	28
8	I	617/730 (84%)	579 (94%)	38 (6%)	15	39
9	J	424/548 (77%)	373 (88%)	51 (12%)	4	18
9	K	423/548 (77%)	383 (90%)	40 (10%)	7	24
10	L	155/170 (91%)	137 (88%)	18 (12%)	4	19
11	M	55/67 (82%)	45 (82%)	10 (18%)	1	9
12	N	518/724 (72%)	448 (86%)	70 (14%)	3	16
13	O	577/650 (89%)	503 (87%)	74 (13%)	3	17
14	Q	271/310 (87%)	264 (97%)	7 (3%)	41	61
15	R	311/411 (76%)	293 (94%)	18 (6%)	17	40

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	S	186/293 (64%)	181 (97%)	5 (3%)	40	60
17	X	407/513 (79%)	376 (92%)	31 (8%)	11	33
17	Y	418/513 (82%)	381 (91%)	37 (9%)	8	27
18	Z	181/190 (95%)	170 (94%)	11 (6%)	15	39
All	All	7565/10314 (73%)	6789 (90%)	776 (10%)	8	22

5 of 776 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	M	7	ARG
13	O	419	ASP
12	N	77	GLU
10	L	184	ARG
12	N	519	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 162 such sidechains are listed below:

Mol	Chain	Res	Type
13	O	412	HIS
17	X	78	GLN
13	O	472	HIS
3	P	488	GLN
17	X	371	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 oligosaccharides 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)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
12	N	2
16	S	1
8	I	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	S	310:ALA	C	529:SER	N	39.42
1	N	92:TRP	C	93:ASN	N	3.29
1	N	563:ASP	C	564:MET	N	2.78
1	I	302:ASP	C	303:GLU	N	2.26

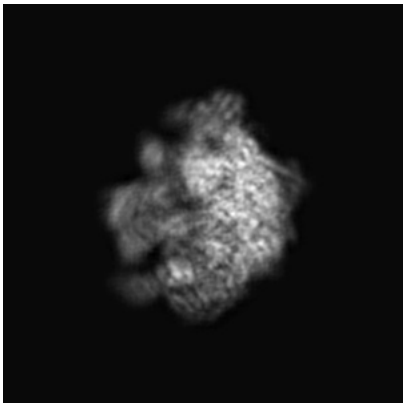
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-4037. These allow visual inspection of the internal detail of the map and identification of artifacts.

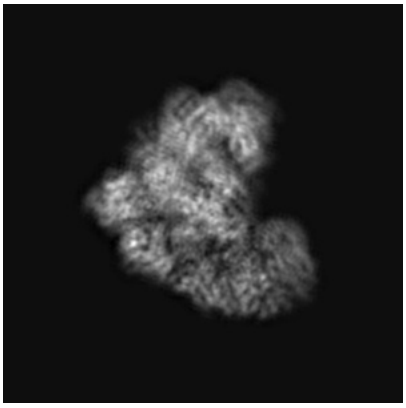
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

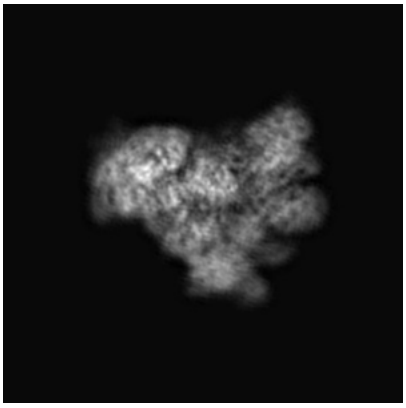
6.1.1 Primary map



X



Y

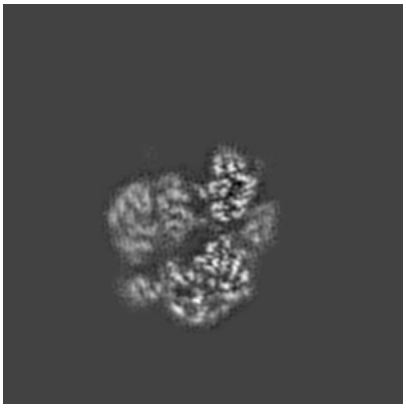


Z

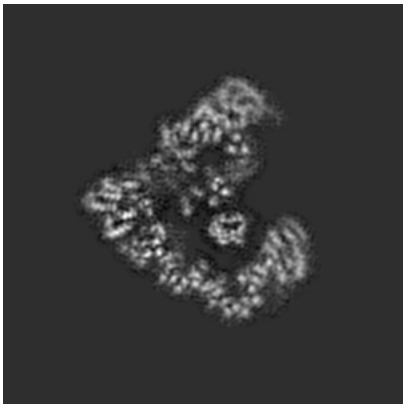
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

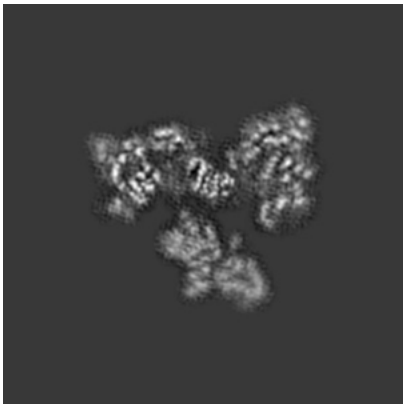
6.2.1 Primary map



X Index: 132



Y Index: 132

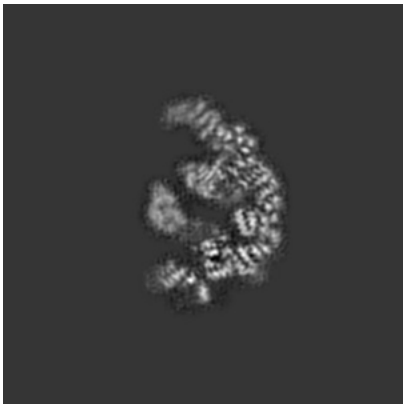


Z Index: 132

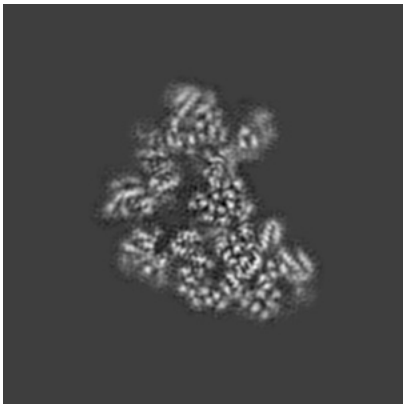
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

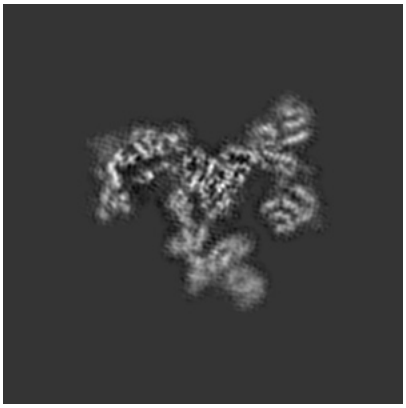
6.3.1 Primary map



X Index: 112



Y Index: 155

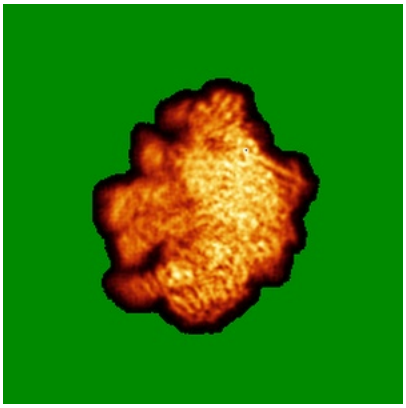


Z Index: 140

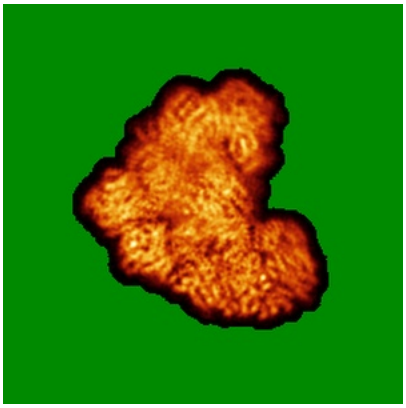
The images above show the largest variance slices of the map in three orthogonal directions.

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

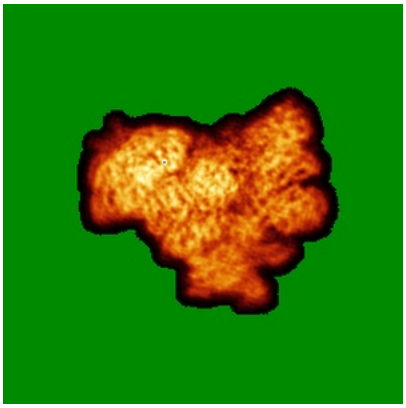
6.4.1 Primary map



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

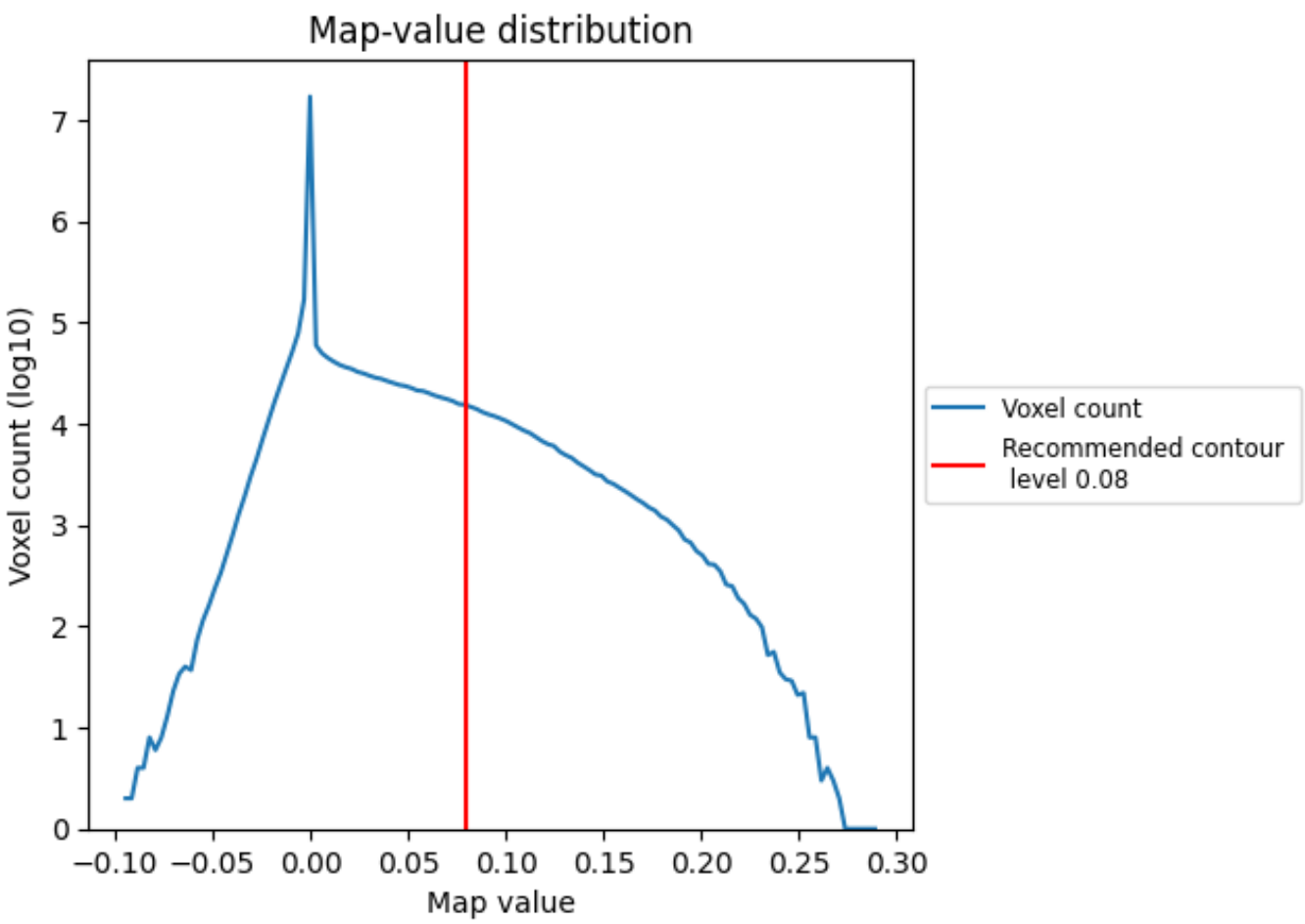
6.6 Mask visualisation (i)

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

7 Map analysis (i)

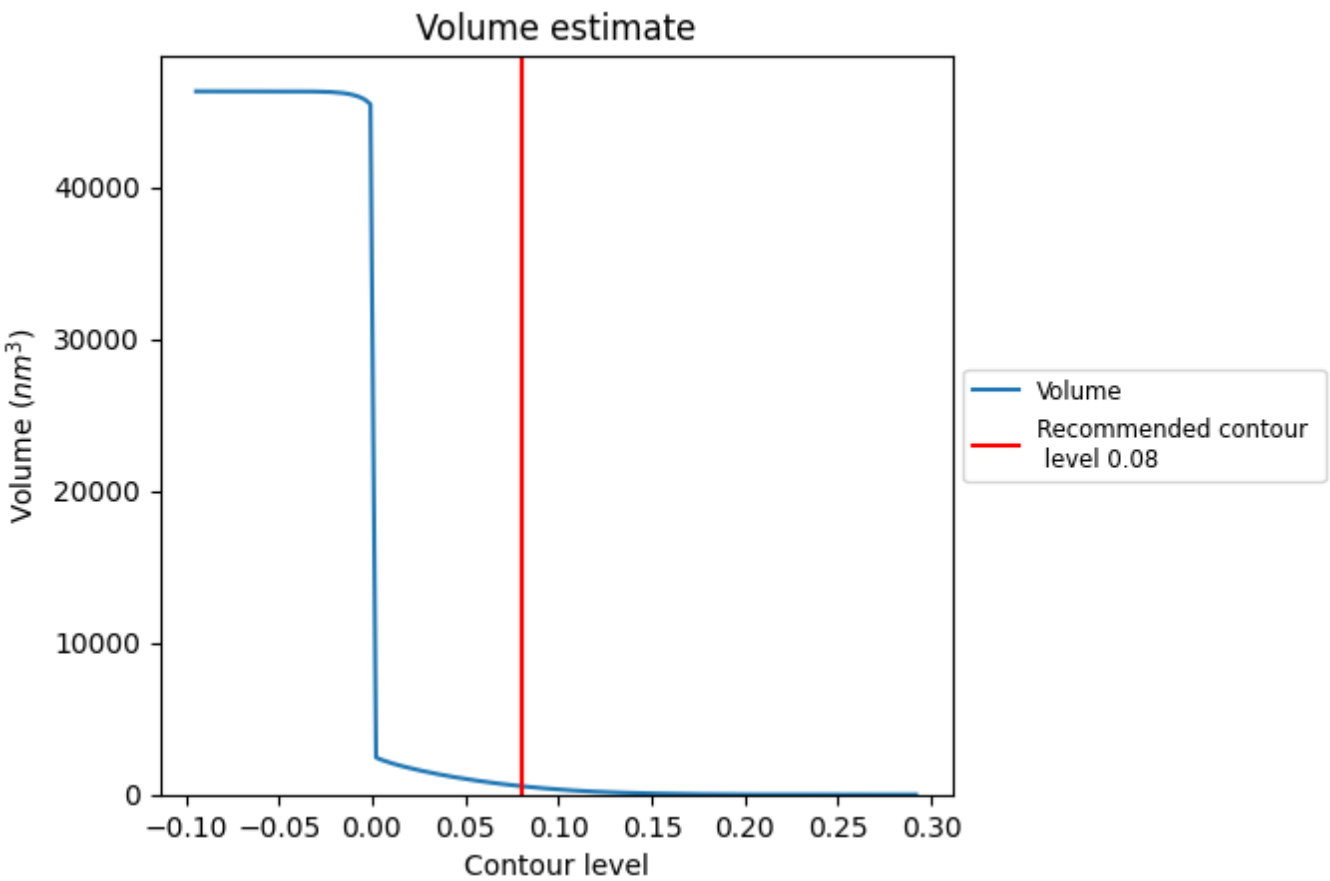
This section contains the results of statistical analysis of the map.

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.

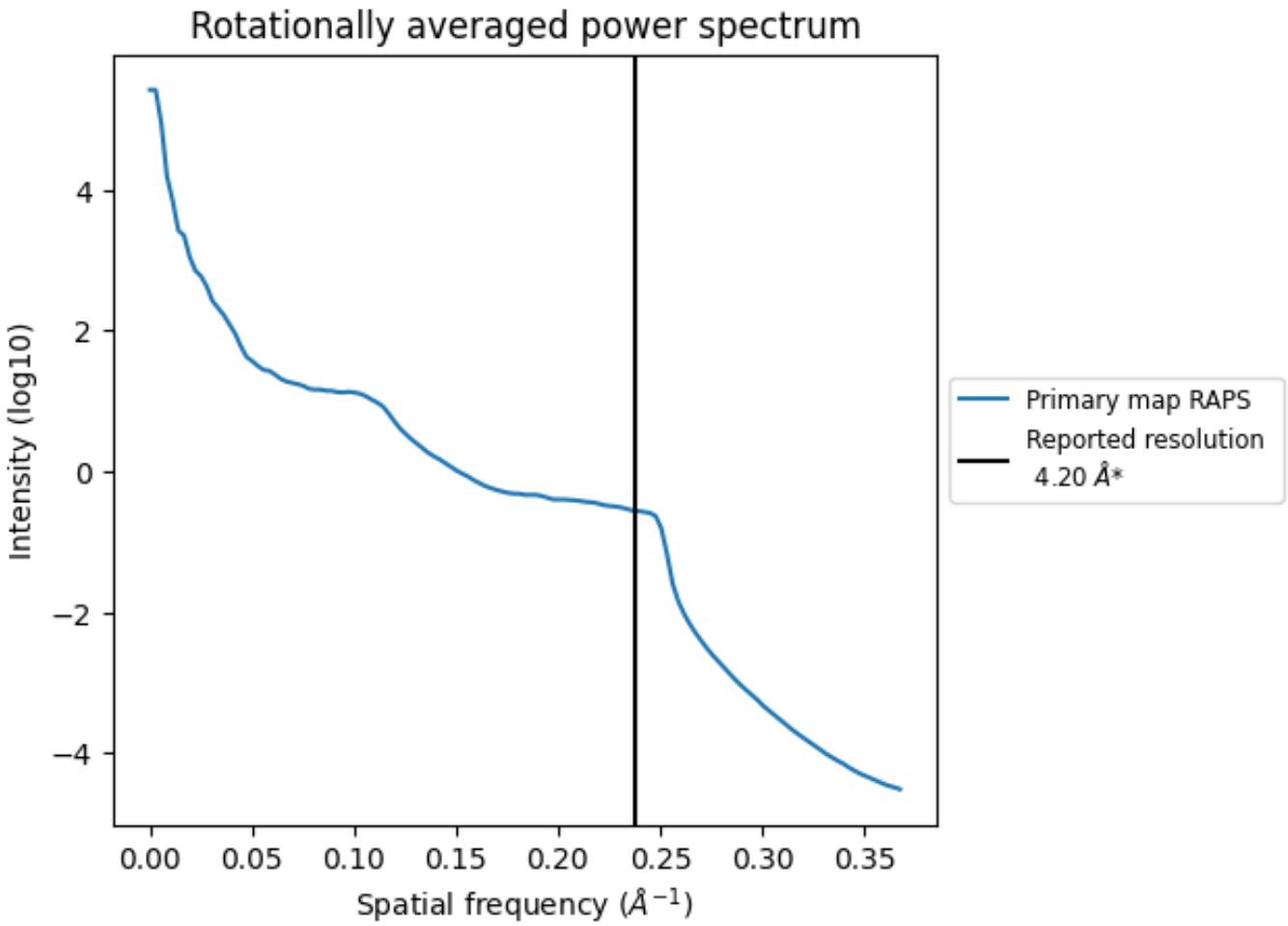
7.2 Volume estimate (i)



The volume at the recommended contour level is 554 nm^3; this corresponds to an approximate mass of 501 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 0.238 Å^{-1}

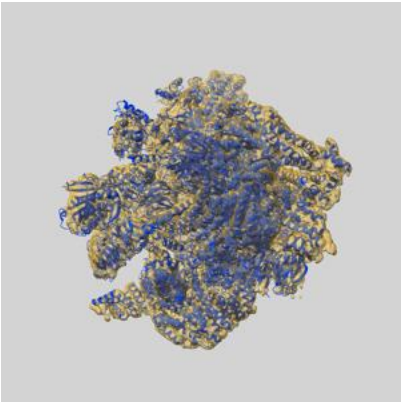
8 Fourier-Shell correlation (i)

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

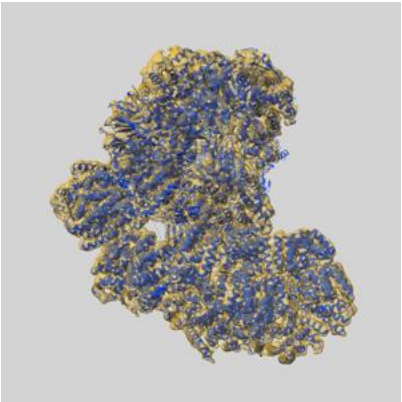
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-4037 and PDB model 5LCW. Per-residue inclusion information can be found in section 3 on page 7.

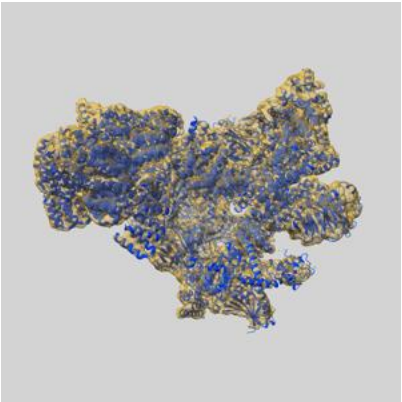
9.1 Map-model overlay (i)



X



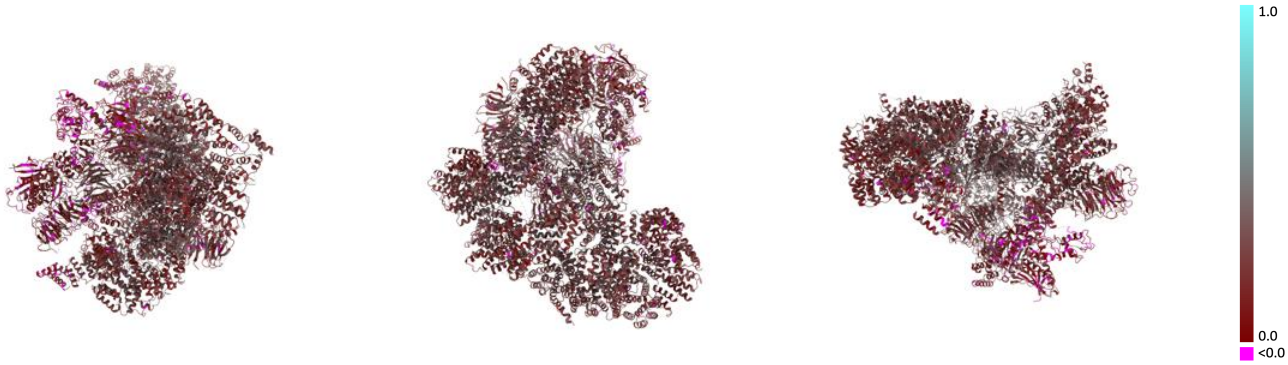
Y



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.

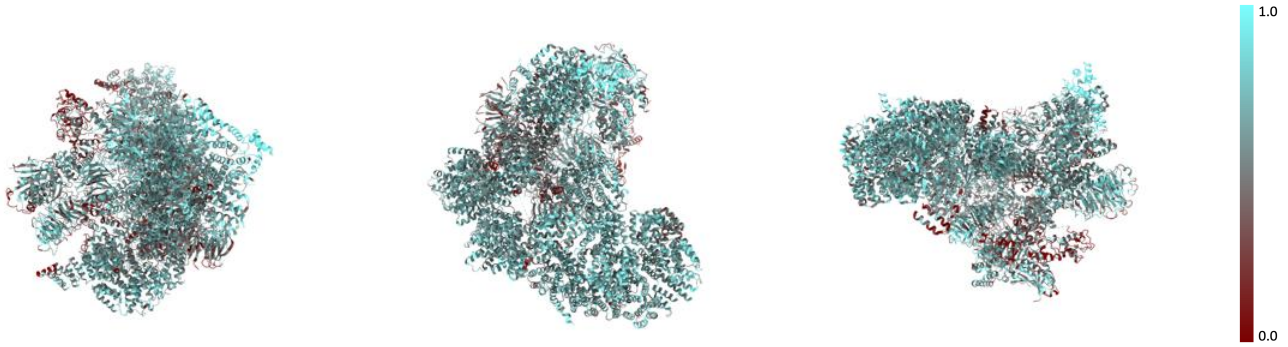
9.2 Q-score mapped to coordinate model (i)



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.

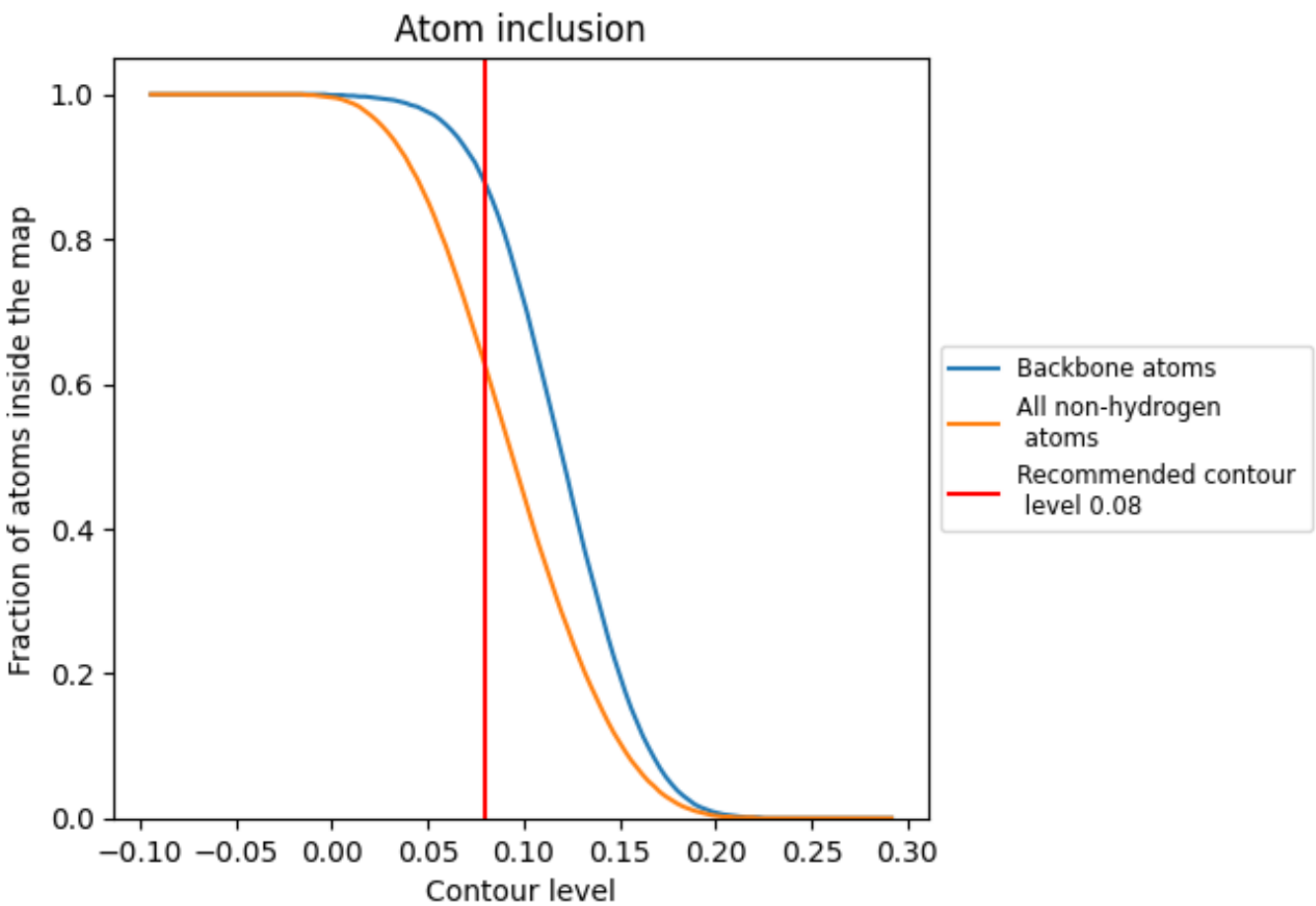
9.3 Atom inclusion mapped to coordinate model (i)



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, 88% of all backbone atoms, 62% 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	0.6250	0.2520
A	0.6230	0.3020
B	0.1260	0.0340
C	0.6190	0.2630
D	0.4400	0.3690
E	0.6760	0.3320
F	0.6860	0.2920
G	0.6240	0.3050
H	0.7130	0.3030
I	0.6010	0.2160
J	0.7110	0.2910
K	0.6910	0.2680
L	0.6840	0.3260
M	0.5570	0.3280
N	0.5600	0.1860
O	0.5680	0.2670
P	0.6460	0.2500
Q	0.6250	0.2000
R	0.6390	0.2310
S	0.5830	0.1970
W	0.5900	0.2950
X	0.6020	0.2040
Y	0.6430	0.2340
Z	0.5440	0.1520