Full wwPDB EM Validation Report (i)

Apr 29, 2024 – 10:33 pm BST

PDB ID	:	5L9T
EMDB ID	:	EMD-3433
Title	:	Model of human Anaphase-promoting complex/Cyclosome (APC/C-CDH1) with E2 UBE2S poised for polyubiquitination where UBE2S, APC2, and APC11 are modeled into low resolution density
Authors	:	Brown, N.G.; VanderLinden, R.; Dube, P.; Haselbach, D.; Peters, J.M.; Stark, H.; Schulman, B.A.
Deposited on	:	2016-06-11
Resolution	:	6.40 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:

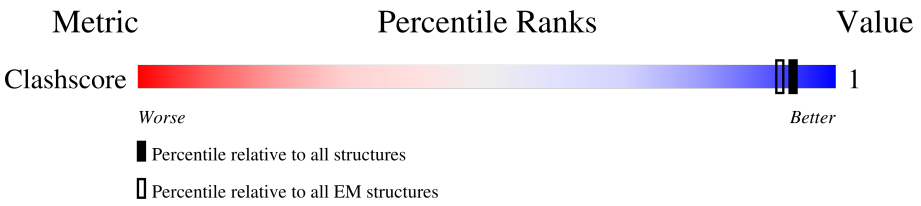
EMDB validation analysis	:	0.0.1.dev92
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 6.40 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

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	35% 71% 29%
2	B	84	21% 81% 19%
3	C	597	29% 79% 20%
3	P	597	39% 74% 26%
4	D	121	34% 45% 55%
5	E	110	29% 51% 49%
6	F	824	28% 58% 42%
6	H	824	29% 59% 41%
7	G	85	27% 29% 71%
7	W	85	11% 29% 71%

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Mol	Chain	Length	Quality of chain
8	I	818	40% 89% 11%
9	J	620	35% 81% 19%
9	K	620	21% 80% 20%
10	L	185	36% 91% • 8%
11	M	74	35% 57% 43%
12	N	822	37% 66% 34%
13	O	755	45% 90% 9%
14	R	493	36% 77% • 22%
15	S	108	48% 78% 22%
16	T	185	25% 52% 48%
17	X	565	38% 70% 30%
17	Y	565	34% 74% 26%

2 Entry composition (i)

There are 17 unique types of molecules in this entry. The entry contains 8038 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		
1	A	1380	1380	1380	0	1380

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

Mol	Chain	Residues	Atoms		AltConf	Trace
			Total	C		
2	B	68	68	68	0	68

- Molecule 3 is a protein called Cell division cycle protein 23 homolog.

Mol	Chain	Residues	Atoms		AltConf	Trace
			Total	C		
3	C	475	475	475	0	475
3	P	443	443	443	0	443

- Molecule 4 is a protein called Anaphase-promoting complex subunit 15.

Mol	Chain	Residues	Atoms		AltConf	Trace
			Total	C		
4	D	55	55	55	0	55

- Molecule 5 is a protein called Anaphase-promoting complex subunit 16.

Mol	Chain	Residues	Atoms		AltConf	Trace
			Total	C		
5	E	56	56	56	0	56

- Molecule 6 is a protein called Cell division cycle protein 27 homolog.

Mol	Chain	Residues	Atoms		AltConf	Trace
			Total	C		
6	F	482	482	482	0	482
			Total	C		
6	H	483	483	483	0	483

- Molecule 7 is a protein called Anaphase-promoting complex subunit CDC26.

Mol	Chain	Residues	Atoms		AltConf	Trace
			Total	C		
7	G	25	25	25	0	25
			Total	C		
7	W	25	25	25	0	25

- Molecule 8 is a protein called Anaphase-promoting complex subunit 4.

Mol	Chain	Residues	Atoms		AltConf	Trace
			Total	C		
8	I	727	727	727	0	727

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	809	GLY	-	expression tag	UNP Q9UJX5
I	810	GLY	-	expression tag	UNP Q9UJX5
I	811	SER	-	expression tag	UNP Q9UJX5
I	812	LEU	-	expression tag	UNP Q9UJX5
I	813	GLU	-	expression tag	UNP Q9UJX5
I	814	VAL	-	expression tag	UNP Q9UJX5
I	815	LEU	-	expression tag	UNP Q9UJX5
I	816	PHE	-	expression tag	UNP Q9UJX5
I	817	GLN	-	expression tag	UNP Q9UJX5
I	818	GLY	-	expression tag	UNP Q9UJX5

- Molecule 9 is a protein called Cell division cycle protein 16 homolog.

Mol	Chain	Residues	Atoms		AltConf	Trace
			Total	C		
9	J	504	504	504	0	504
			Total	C		
9	K	493	493	493	0	493

- Molecule 10 is a protein called Anaphase-promoting complex subunit 10.

Mol	Chain	Residues	Atoms	AltConf	Trace
10	L	170	Total C 170 170	0	170

- Molecule 11 is a protein called Anaphase-promoting complex subunit 13.

Mol	Chain	Residues	Atoms	AltConf	Trace
11	M	42	Total C 42 42	0	42

- Molecule 12 is a protein called Anaphase-promoting complex subunit 2.

Mol	Chain	Residues	Atoms	AltConf	Trace
12	N	546	Total C 546 546	0	546

- Molecule 13 is a protein called Anaphase-promoting complex subunit 5.

Mol	Chain	Residues	Atoms	AltConf	Trace
13	O	685	Total C 685 685	0	685

- Molecule 14 is a protein called Fizzy-related protein homolog.

Mol	Chain	Residues	Atoms	AltConf	Trace
14	R	385	Total C 385 385	0	385

- Molecule 15 is a protein called Ubiquitin_variant-Hsl1(substrate) fusion.

Mol	Chain	Residues	Atoms	AltConf	Trace
15	S	84	Total C 84 84	0	84

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S	-4	GLY	-	expression tag	UNP P0CG47
S	-3	SER	-	expression tag	UNP P0CG47
S	-2	GLY	-	expression tag	UNP P0CG47
S	-1	GLY	-	expression tag	UNP P0CG47
S	0	SER	-	expression tag	UNP P0CG47
S	4	LEU	PHE	engineered mutation	UNP P0CG47

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Chain	Residue	Modelled	Actual	Comment	Reference
S	8	PRO	LEU	engineered mutation	UNP P0CG47
S	9	ARG	THR	engineered mutation	UNP P0CG47
S	11	CYS	LYS	engineered mutation	UNP P0CG47
S	42	ILE	ARG	engineered mutation	UNP P0CG47
S	44	PHE	ILE	engineered mutation	UNP P0CG47
S	47	VAL	GLY	engineered mutation	UNP P0CG47
S	49	ARG	GLN	engineered mutation	UNP P0CG47
S	64	LYS	GLU	engineered mutation	UNP P0CG47
S	66	SER	THR	engineered mutation	UNP P0CG47
S	68	LEU	HIS	engineered mutation	UNP P0CG47
S	70	ALA	VAL	engineered mutation	UNP P0CG47
S	71	MET	LEU	engineered mutation	UNP P0CG47
S	73	VAL	LEU	engineered mutation	UNP P0CG47
S	74	PRO	ARG	engineered mutation	UNP P0CG47
S	815	LYS	GLY	engineered mutation	UNP P0CG47
S	817	LYS	-	linker	UNP P0CG47

- Molecule 16 is a protein called Ubiquitin-conjugating enzyme E2 S.

Mol	Chain	Residues	Atoms		AltConf	Trace
			Total	C		
16	T	97	97	97	0	97

There are 46 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
T	-3	GLY	-	expression tag	UNP Q16763
T	-2	PRO	-	expression tag	UNP Q16763
T	-1	GLY	-	expression tag	UNP Q16763
T	0	SER	-	expression tag	UNP Q16763
T	118	PHE	CYS	conflict	UNP Q16763
T	?	-	GLY	deletion	UNP Q16763
T	?	-	PRO	deletion	UNP Q16763
T	?	-	SER	deletion	UNP Q16763
T	?	-	GLY	deletion	UNP Q16763
T	?	-	ARG	deletion	UNP Q16763
T	?	-	ALA	deletion	UNP Q16763
T	?	-	GLU	deletion	UNP Q16763
T	?	-	ALA	deletion	UNP Q16763
T	?	-	GLY	deletion	UNP Q16763
T	?	-	ARG	deletion	UNP Q16763
T	?	-	ALA	deletion	UNP Q16763

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Chain	Residue	Modelled	Actual	Comment	Reference
T	?	-	LEU	deletion	UNP Q16763
T	?	-	ALA	deletion	UNP Q16763
T	?	-	SER	deletion	UNP Q16763
T	?	-	GLY	deletion	UNP Q16763
T	?	-	THR	deletion	UNP Q16763
T	?	-	GLU	deletion	UNP Q16763
T	?	-	ALA	deletion	UNP Q16763
T	?	-	SER	deletion	UNP Q16763
T	?	-	SER	deletion	UNP Q16763
T	?	-	THR	deletion	UNP Q16763
T	?	-	ASP	deletion	UNP Q16763
T	?	-	PRO	deletion	UNP Q16763
T	?	-	GLY	deletion	UNP Q16763
T	?	-	ALA	deletion	UNP Q16763
T	?	-	PRO	deletion	UNP Q16763
T	?	-	GLY	deletion	UNP Q16763
T	?	-	GLY	deletion	UNP Q16763
T	?	-	PRO	deletion	UNP Q16763
T	?	-	GLY	deletion	UNP Q16763
T	?	-	GLY	deletion	UNP Q16763
T	?	-	ALA	deletion	UNP Q16763
T	?	-	GLU	deletion	UNP Q16763
T	?	-	GLY	deletion	UNP Q16763
T	?	-	PRO	deletion	UNP Q16763
T	?	-	MET	deletion	UNP Q16763
T	?	-	ALA	deletion	UNP Q16763
T	?	-	LYS	deletion	UNP Q16763
T	?	-	LYS	deletion	UNP Q16763
T	?	-	HIS	deletion	UNP Q16763
T	?	-	ALA	deletion	UNP Q16763

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

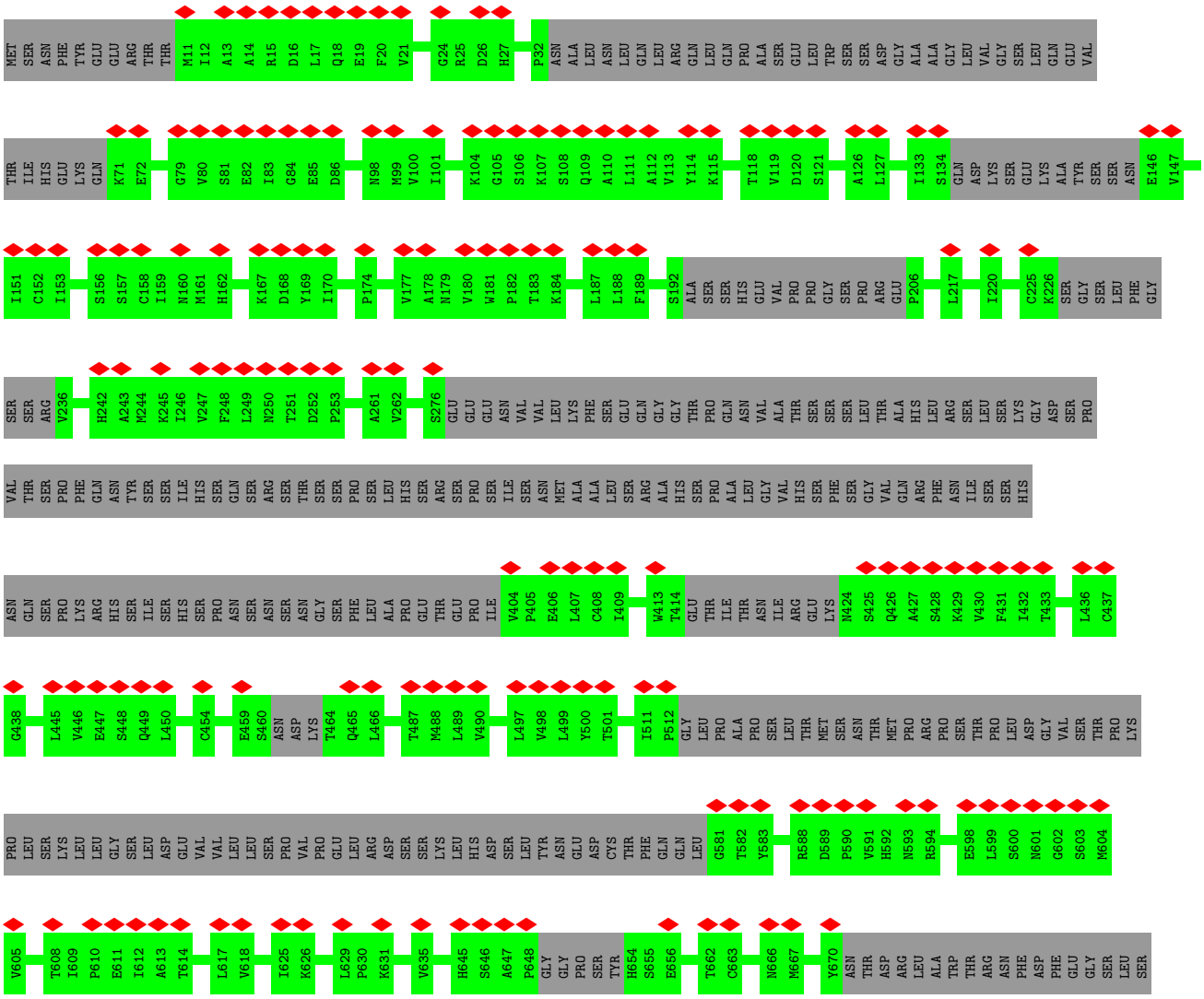
Mol	Chain	Residues	Atoms		AltConf	Trace
			Total	C		
17	X	397	397	397	0	397
			Total	C		
17	Y	416	416	416	0	416

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:



PRO VAL ILE ALA PRO LYS LYS ALA ARG PRO SER GLU THR GLY SER D704 N718 H722 L723 L724 L728 S731 PRO SER GLU ALA SER GLN MET LYS ASP GLU ASP PHE SER GLN ASN LEU SER LEU ASP SER SER THR LEU LEU PHE T757 P760 A761 I762 F763 F764 V765 L766

H767 L768 V769 W779 G780 E781 G782 I783 C784 S785 L786 V787 E788 L789 L790 V791 Q792 L793 D796 L797 G800 P801 Y802 V803 Y806 P811 T812 L813 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 P842 S843 I844 Y845 Q846 W847 V848 G854 P859 Y860 L863 P864 G865 I866 C867 E868 R869 L872 V873 V874 L875 S876 I877 A878 L879 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 GLU ASN ARG PHE SER PHE ARG HIS SER THR SER VAL S924 R929 L930 V931 V932 T935 N936 V937 G938 F939 T940 L941 R942 D943 L944 E945 T946 L947 P948 F949 G950 I951 A952 L953 P954 I955 R956 D957 A958 I959 Y960 H961 C962 R963 E964 A967 S968 P971 E972 A973 V974 C975

L976 L977 I978 G979 R980 Q981 S984 K985 Q986 ALA CYS GLU 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 M1019 N1020 H1021 E1022 V1023 M1024 S1025 L1026 E1030 D1031 L1032 Q1035 D1036 R1039 L1040 L1041 V1047 R1048

V1049 N1050 V1051 Y1054 P1055 E1056 L1057 S1058 D1059 H1060 E1061 F1062 I1063 E1064 E1065 N1068 Y1092 H1093 P1094 T1097 E1098 P1099 L1100 P1101 K1104 L1105 N1106 L1107 T1108 G1109 R1110 A1111 P1112 P1113 R1114 N1115 T1116 T1117 V1118 D1119 L1120 N1121 S1122 G1123 N1124 I1125 D1126 V1127 P1128 P1129 N1130 L1145 K1146

Q1152 I1153 N1161 H1165 A1166 E1167 L1168 A1169 N1170 M1177 A1178 L1181 N1182 G1183 H1184 L1188 A1189 T1190 I1193 L1197 T1198 K1199 G1200 H1201 E1202 M1203 I1206 G1207 L1210 G1211 A1214 L1217 G1218 T1224 T1225 L1228 I1232 P1233 A1234 L1235 L1236 P1237 P1238 T1239 S1240 T1241

E1242 L1243 D1244 V1245 P1246 H1247 N1248 V1251 A1252 A1253 V1254 V1255 G1256 L1259 Q1262 G1263 R1267 A1270 L1274 I1277 G1278 R1279 P1280 P1281 G1282 P1283 E1284 M1285 C1288 T1289 D1290 R1291 E1292 L1296 A1297 L1300 M1304 L1307 G1308 M1316 S1317 P1322 E1323 Y1326

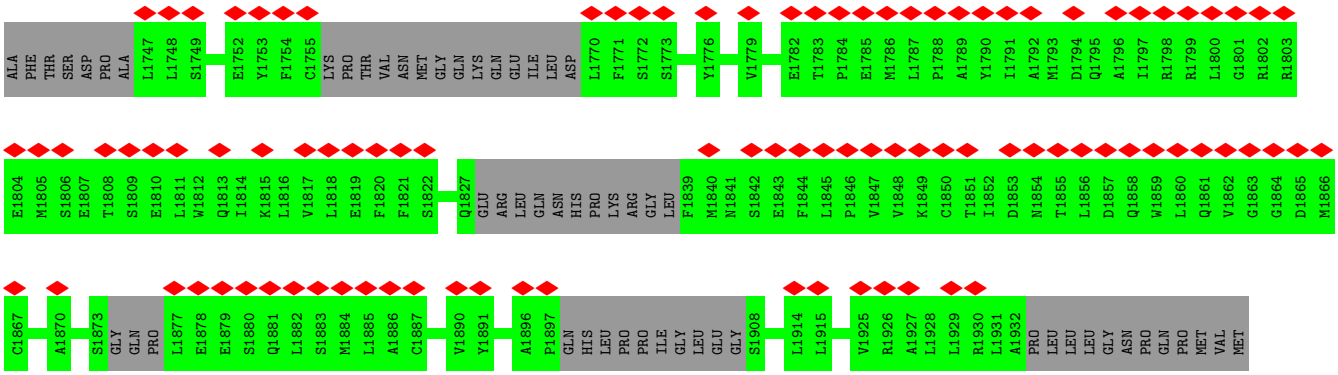
M1329 V1330 G1331 G1332 H1333 ARG ARG PHE GLN THR GLY MET HIS ARG GLU LYS HIS LYS S1347 P1348 S1349 Y1350 Q1351 I1352 K1353 E1354 G1355 D1356 T1357 I1358 N1359 V1360 D1361 C1364 P1365 G1366 L1369 A1370 L1371 A1372 M1373 R1381 D1385 R1388 A1389 T1392 M1393 Y1394 L1395 L1396 D1397 F1398 V1399 K1400

P1401 E1402 C1412 N1422 S1423 K1424 D1427 S1428 N1429 V1430 R1435 E1436 N1437 SER ILE SER LEU SER GLU ILE GLU LEU PRO CYS SER GLU ASP L1452 N1453 L1454 E1455 S1458 V1462 I1465 A1466 C1469 L1472 G1473 F1476 E1480 N1481 L1482 K1493 D1494 T1497 S1500

A1501 P1502 N1503 A1504 S1505 V1506 P1509 L1512 E1513 L1516 S1517 V1518 V1519 L1520 L1523 A1524 M1525 V1526 M1527 G1531 F1541 M1544 K1545 T1546 G1547 G1548 E1549 M1550 N1551 H1559 L1562 G1563 L1564 L1565 F1566 G1569 G1570 R1571 L1574 S1575 T1576 S1577 S1580 I1581 L1584 L1585 C1586

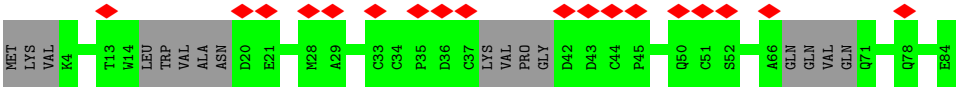
A1587 L1588 Y1589 P1590 H1591 A1594 H1595 D1598 N1599 R1600 Y1601 Q1604 R1607 H1608 L1609 Y1610 V1611 L1612 A1613 A1614 L1618 L1619 V1620 P1621 V1622 D1623 V1624 D1625 T1626 N1627 T1628 P1629 C1630 Y1631 A1632 L1633 Y1644 E1645 E1649 E1650 L1651 M1652 L1656 L1657 P1658 E1659 L1663 K1669 G1670 P1671

R1672 L1676 L1677 I1678 D1679 L1680 SER LYS GLY T1684 L1687 S1692 K1693 D1694 G1695 V1696 K1700 L1701 R1702 A1703 G1704 GLN LEU SER TYR LYS GLU ASP PRO MET GLY TRP GLN SER LEU LEU ALA GLN THR VAL ALA ASN ARG ASN SER GLU ALA ARG ALA PHE LYS PRO GLU THR ILE SER



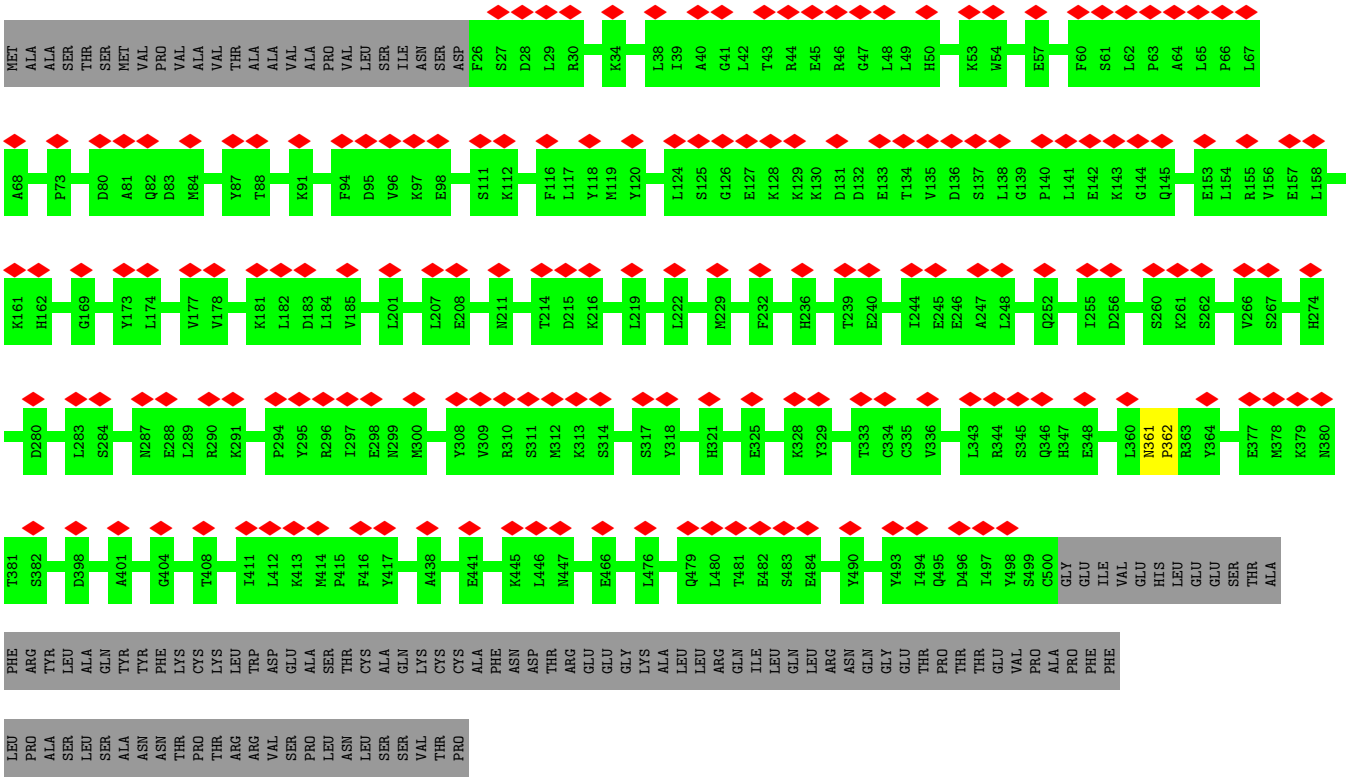
• Molecule 2: Anaphase-promoting complex subunit 11

Chain B:



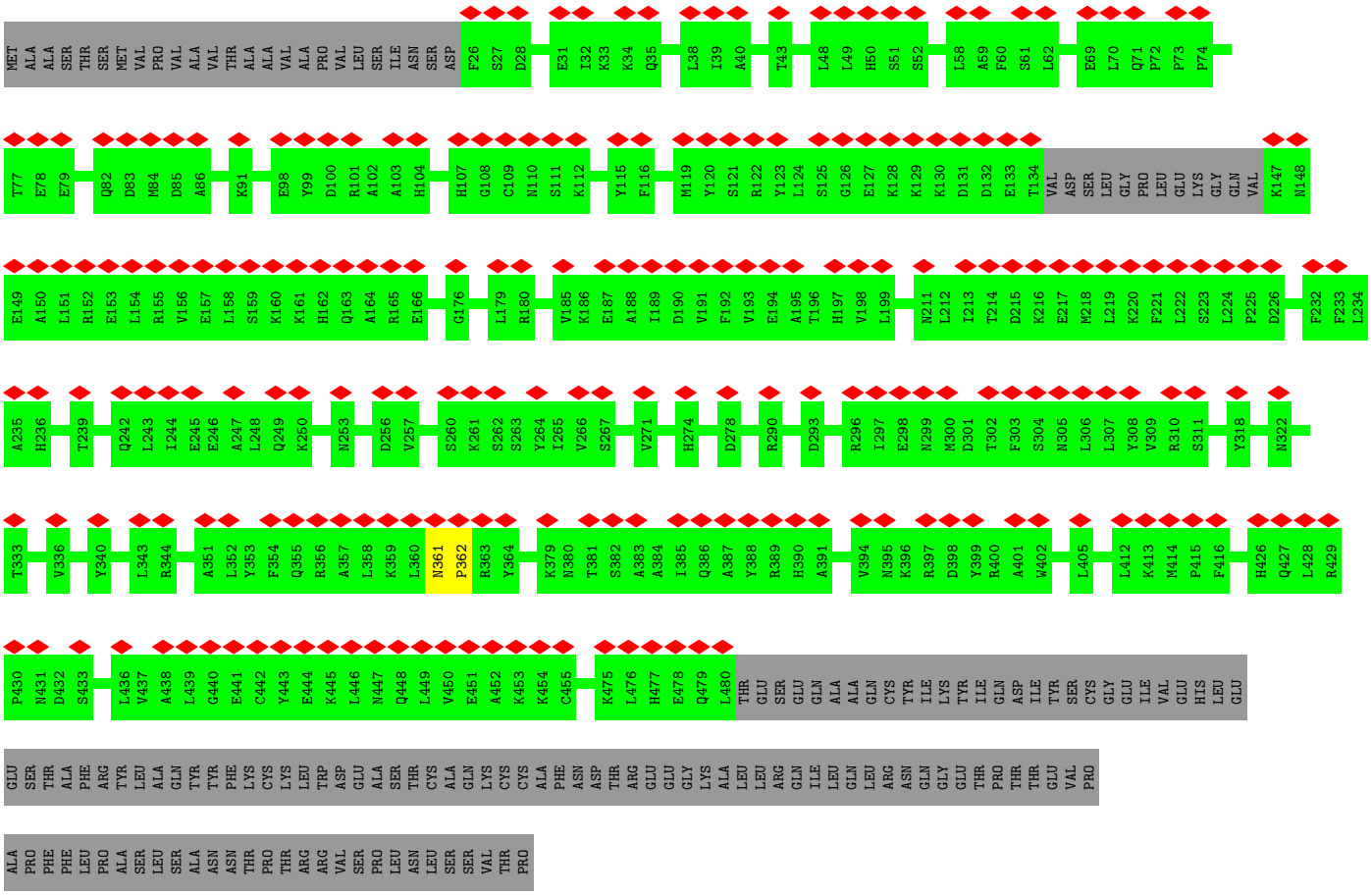
• Molecule 3: Cell division cycle protein 23 homolog

Chain C:



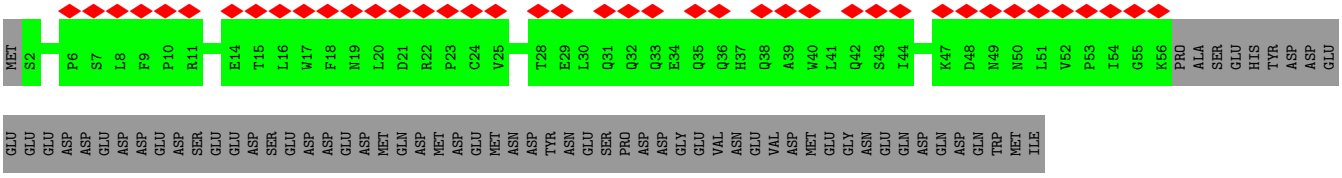
• Molecule 3: Cell division cycle protein 23 homolog

Chain P:



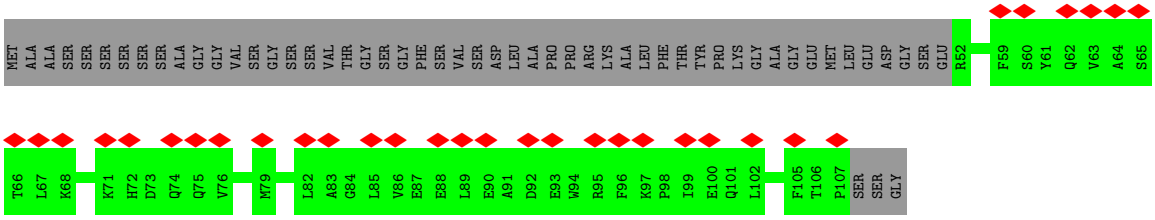
- Molecule 4: Anaphase-promoting complex subunit 15

Chain D:



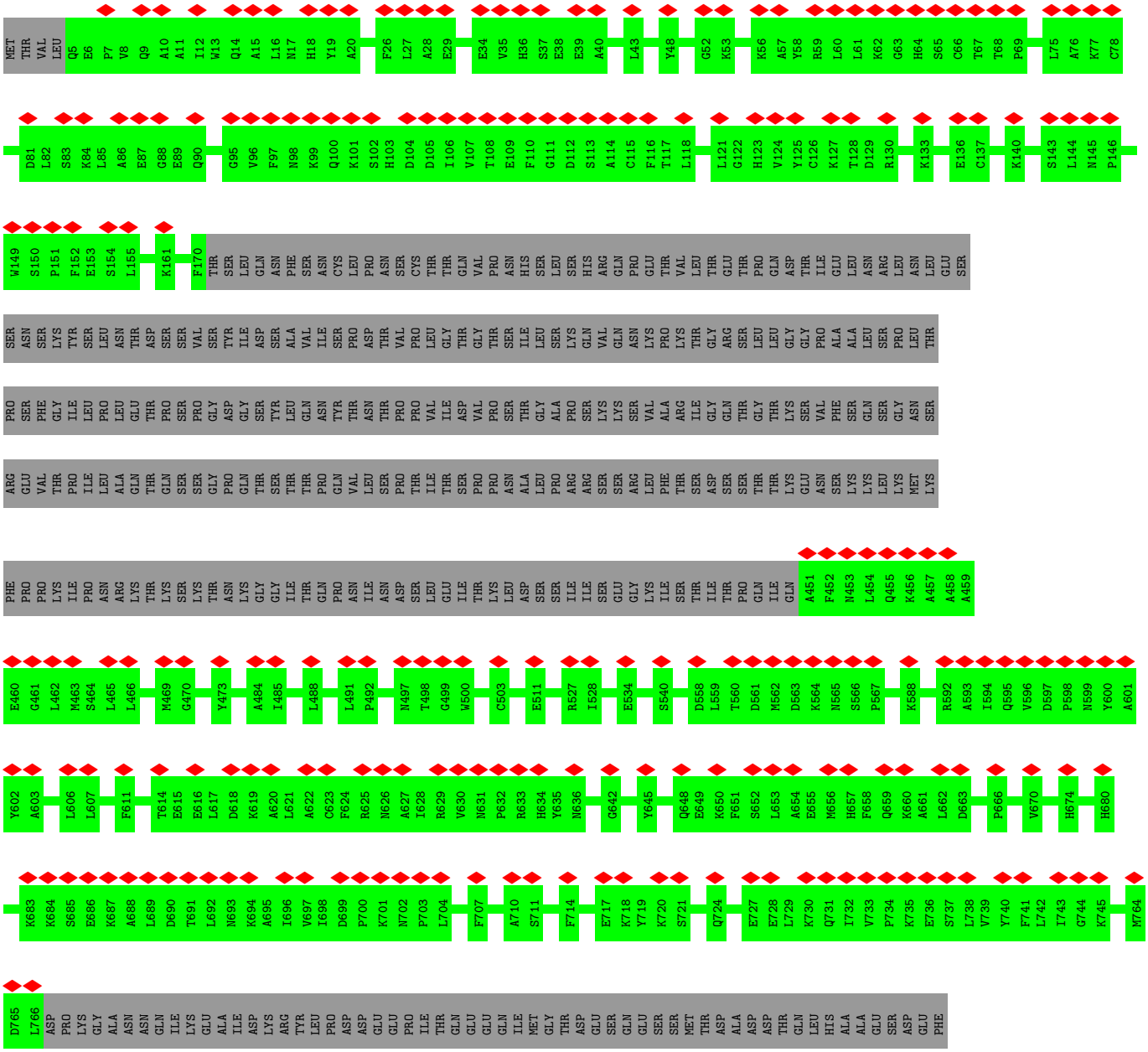
- Molecule 5: Anaphase-promoting complex subunit 16

Chain E:



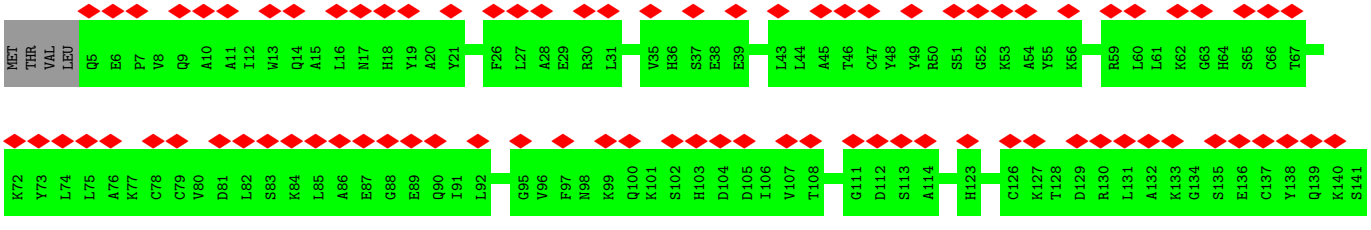
- Molecule 6: Cell division cycle protein 27 homolog

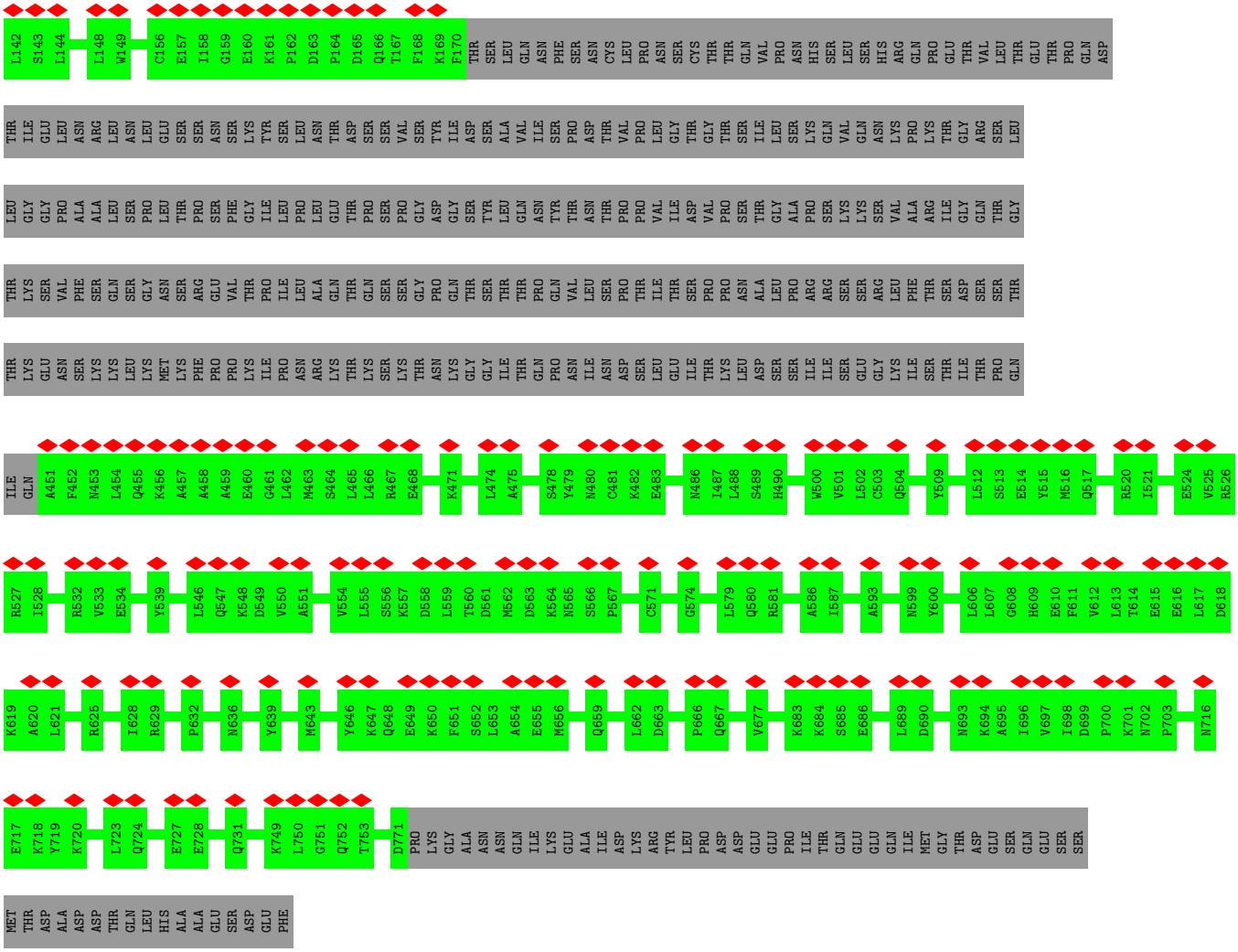
Chain F: 28% 58% 42%



- Molecule 6: Cell division cycle protein 27 homolog

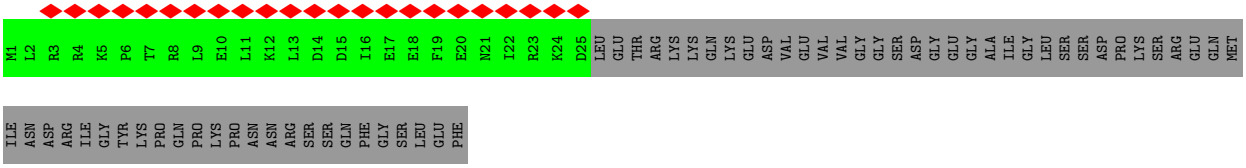
Chain H: 29% 59% 41%





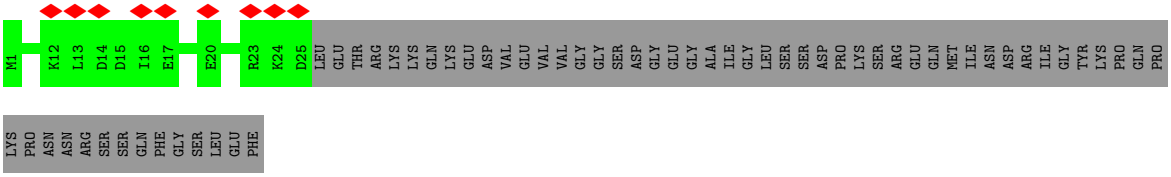
- Molecule 7: Anaphase-promoting complex subunit CDC26

Chain G:



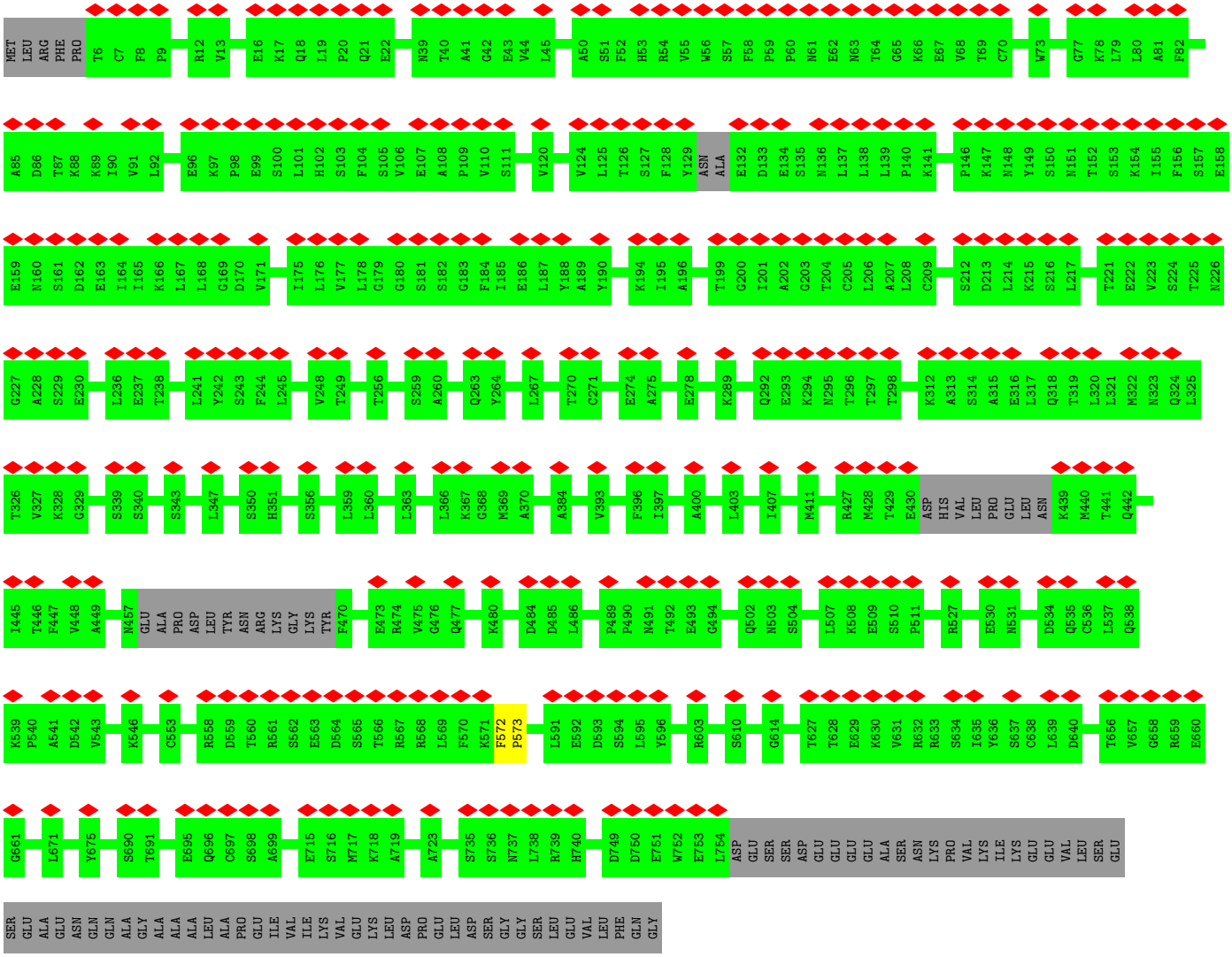
- Molecule 7: Anaphase-promoting complex subunit CDC26

Chain W:



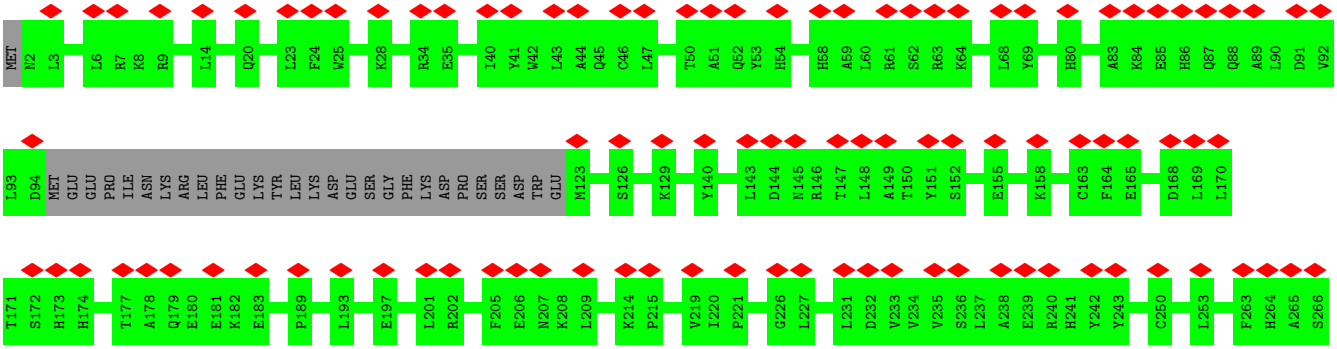
- Molecule 8: Anaphase-promoting complex subunit 4

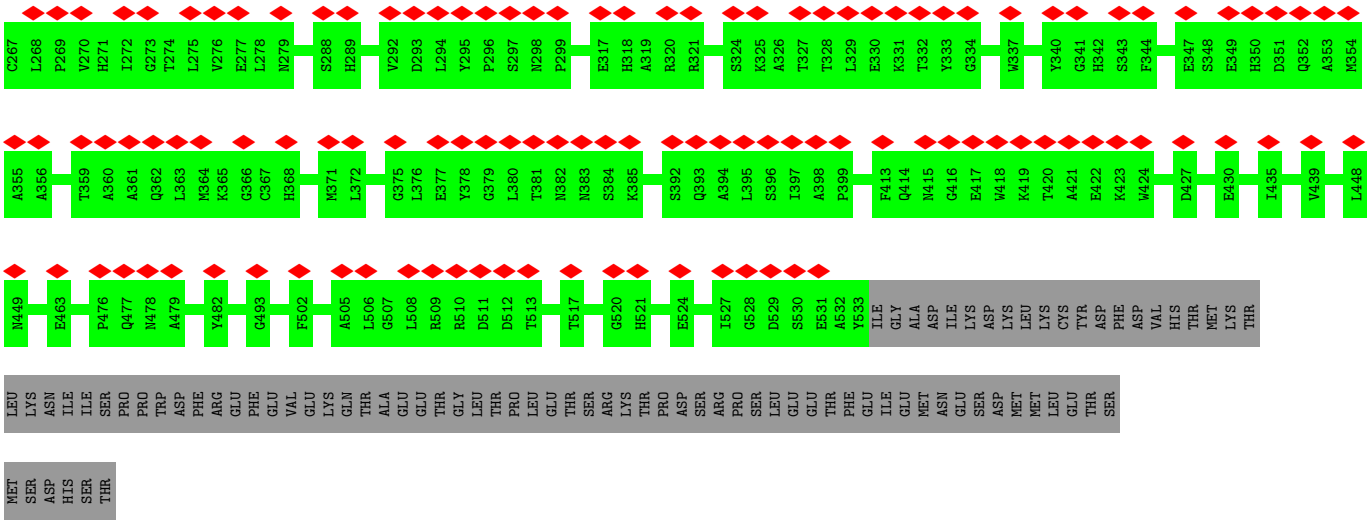
Chain I:



- Molecule 9: Cell division cycle protein 16 homolog

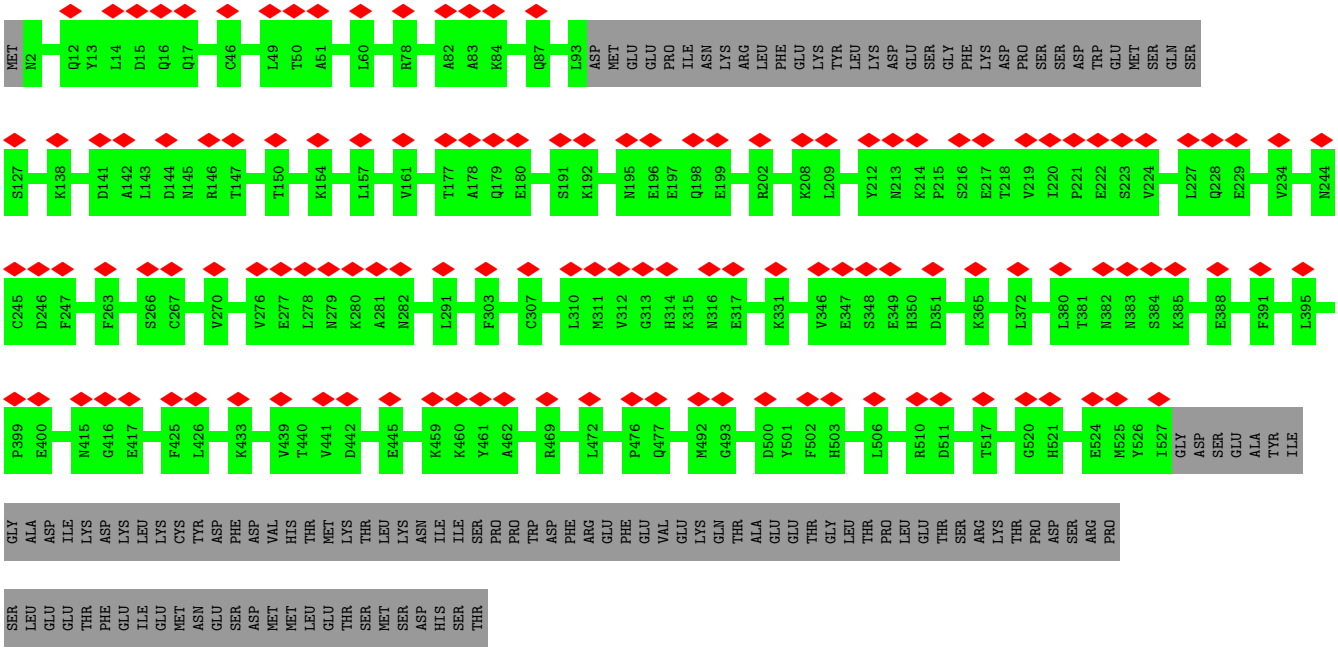
Chain J:





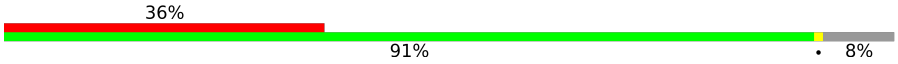
- Molecule 9: Cell division cycle protein 16 homolog

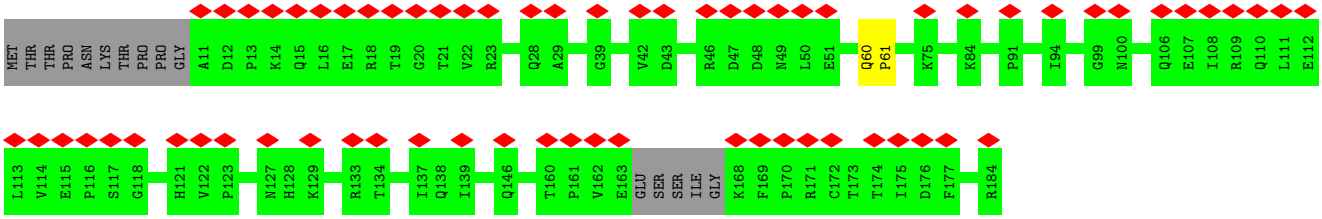
Chain K:



- Molecule 10: Anaphase-promoting complex subunit 10

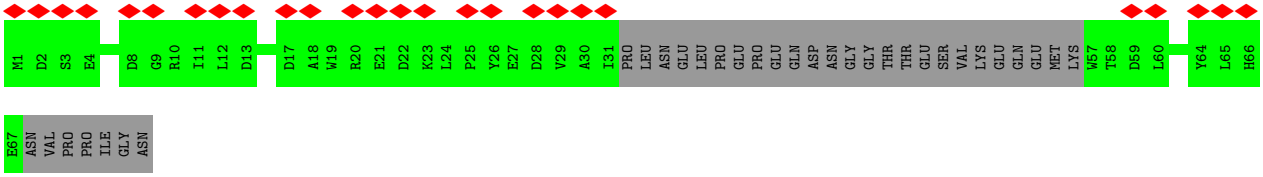
Chain L:





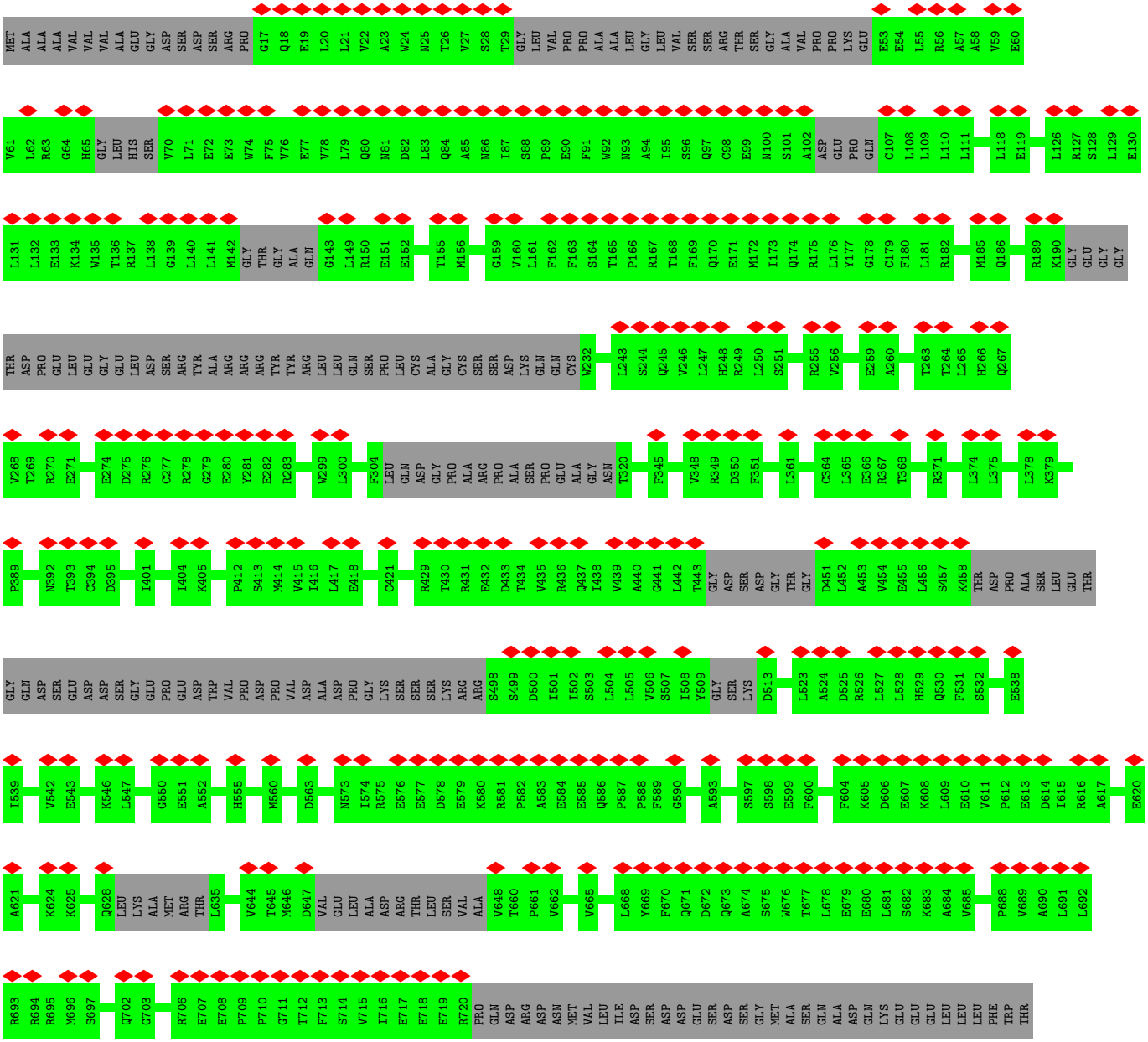
- Molecule 11: Anaphase-promoting complex subunit 13

Chain M:



- Molecule 12: Anaphase-promoting complex subunit 2

Chain N:



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

LEU PRO LYS ASN CYS SER

- Molecule 13: Anaphase-promoting complex subunit 5

Chain O: 45% 90% 9%

MET ALA SER VAL HIS GLU SER LEU TYR PHE ASN PRO MET MET THR ASN GLY VAL VAL HIS ALA ASN VAL PHE GLY ILE K27 D28 W29 V30 T31 P32 Y33 K34 I35 A36 V37 L38 V39 L40 L41 N42 E43 M44 S45 R46 T47 G48 E49 G50 M61 Q62 L63 L64 L65 P66 L67 L68 Q69

G70 P71 L75 S76 K77 L81 S85 Q88 S92 V93 Q94 I95 L105 M108 F111 F112 D113 D114 L115 S116 D117 S118 F119 S120 G121 T122 E123 P124 H127 K128 L134 F135 L136 R137 H138 M139 I140 Y143 S144 K145 L146 S147 F148 S149 Q150 V151 F152 T169

VAL GLU ASP ALA ASP MET GLU LEU THR SER ARG ASP GLU GLY GLU ARG LYS MET GLU LYS GLU GLU LEU ASP VAL SER VAL ARG GLU GLU GLU VAL SER CYS SER GLY P206 Q209 K210 E213 F214 F215 L216 S217 Q218 Q219 A220 S221 K224 N225 K229 A230 L231 T232 P233

L236 Q237 K238 E239 L240 L243 F246 N247 P248 D249 F250 A251 E252 A253 L259 L262 V267 T271 L274 F278 D279 R280 L281 I282 L283 T284 G285 A286 E287 S288 K289 S290 N291 G292 E293 E294 G295 Y296 G297 L305 A308 A309 C312 Y317 A320 E321

L324 E333 S334 N335 D336 H337 Q341 L344 S345 Y348 Q352 K353 R354 V359 V369 H370 F371 G372 L373 P374 Y375 S378 L379 G380 I381 L384 V385 R388 A389 T394 A395 N396 K397 L398 M399 D400 A401 L402 K403 D404 S405 D406 L407 L408 H409 W410 K411 H412 S413

L414 S415 E416 I422 K425 I428 W429 Y432 T436 M437 Q441 L445 L446 S447 M448 N449 S450 L451 E452 ALA VAL ASN ALA GLY VAL Q459 Q460 N461 N462 T463 E464 S465 F466 A467 V468 A469 H472 L473 A474 E475 L476 H477 Q480 A486 E495 R496 F497 N500

S501 Q502 L506 W507 D511 Q512 K513 I514 Q515 F516 D517 N521 D522 G523 K524 L527 S530 T536 A537 L538 N539 S540 I541 E542 G543 V544 Y545 R546 K547 A548 V549 V550 L551 Q552 A553 M557 S558 E559 A560 H561 K562 L563 L564 L567 L574 K575 N576 T577 E578 M579 V580

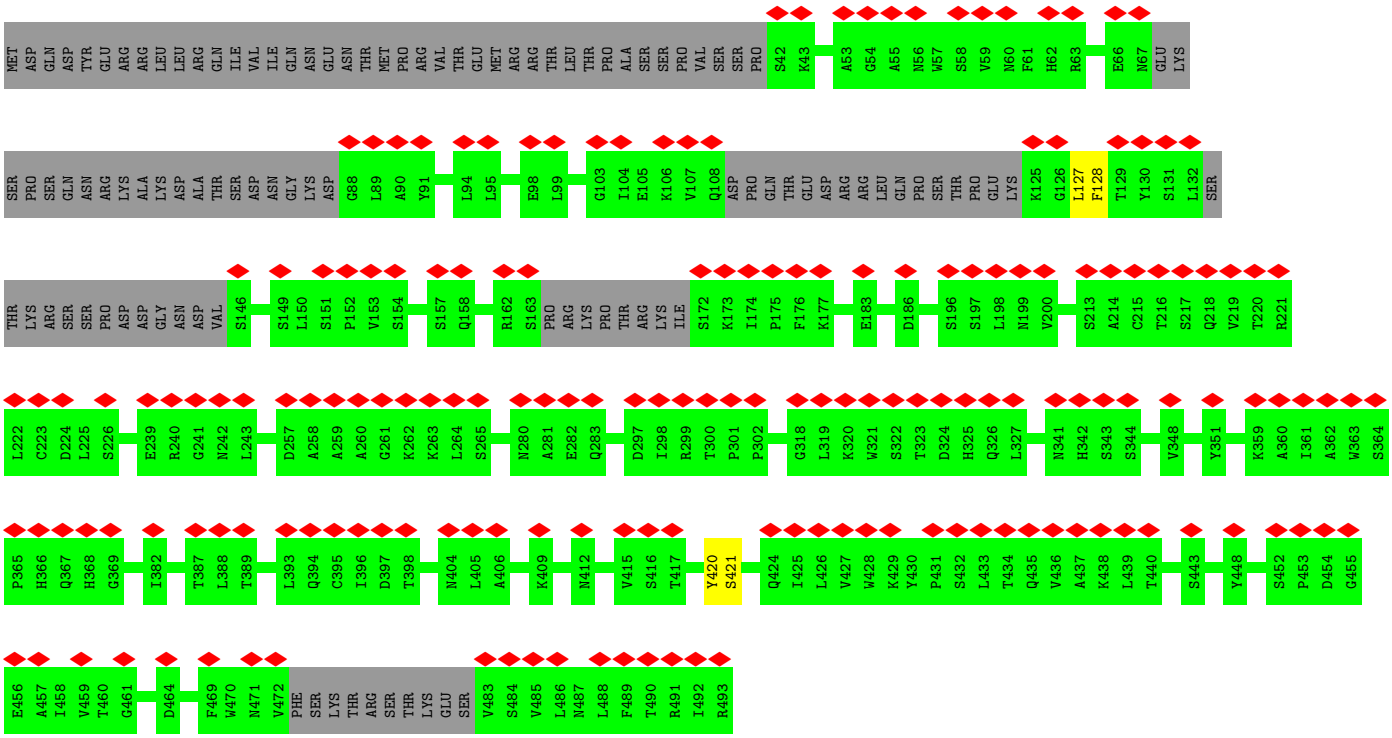
I581 S582 L585 S586 V587 A588 E589 L590 Y591 W592 R593 S594 S595 T598 I599 A600 L601 L605 L608 K612 E613 Y614 R615 L616 Q617 A620 S621 V624 F629 I633 E638 S642 H645 M646 D654 G655 A656 I657 K660 G661 M664 S674 Q680

P681 K682 K683 A684 E685 A686 L687 E688 A689 A690 I691 E692 N693 L694 N695 E696 A697 K698 N699 Y700 F701 A702 K703 V704 D705 C706 Y715 A718 R719 L720 Y721 L724 G725 K726 T727 Q728 E729 R730 N731 R732 C733 A734 M735 L736 F737 R738 Q739 L740 H741 Q742 E743 L744 P745 S746 HIS GLY V749

P750 L751 I752 N753 H754 L755

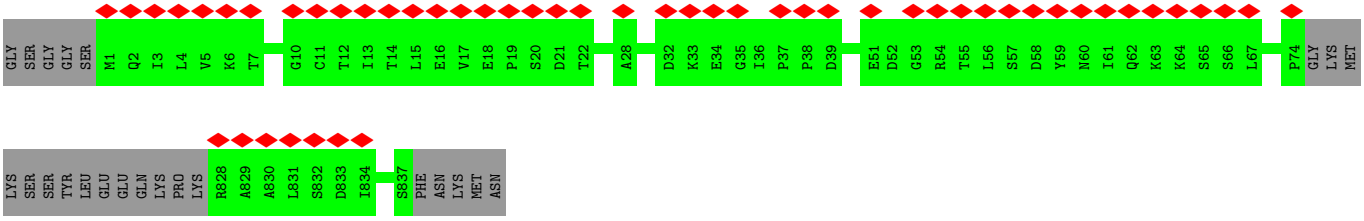
- Molecule 14: Fizzy-related protein homolog

Chain R: 36% 77% 22%



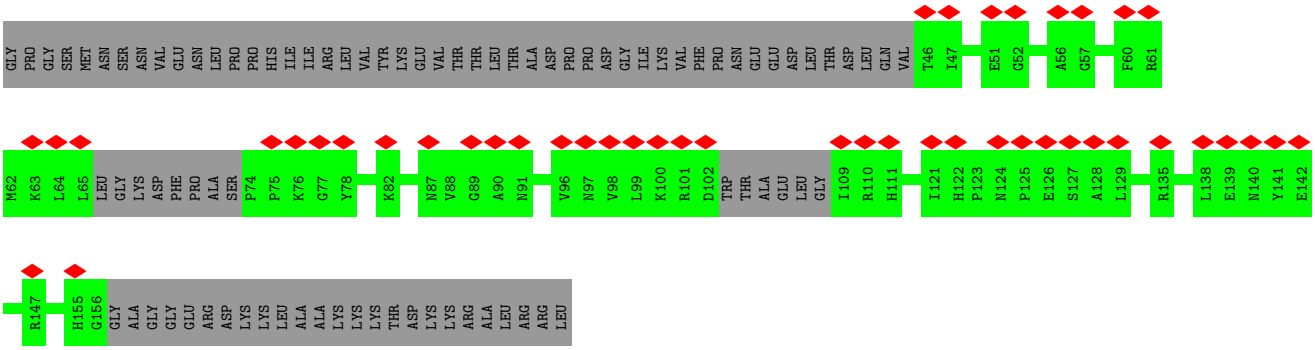
- Molecule 15: Ubiquitin_variant-Hsl1(substrate) fusion

Chain S:



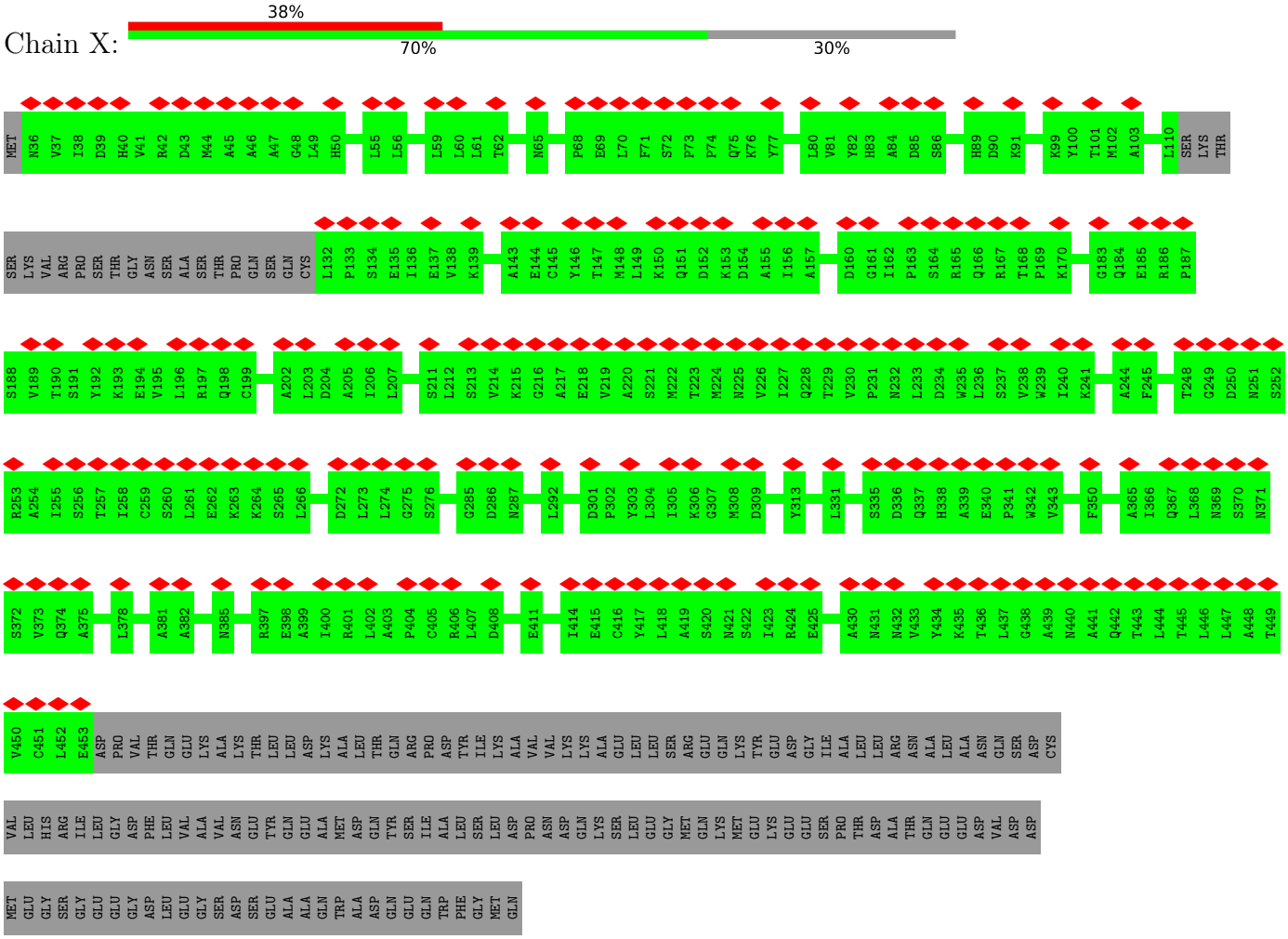
- Molecule 16: Ubiquitin-conjugating enzyme E2 S

Chain T:



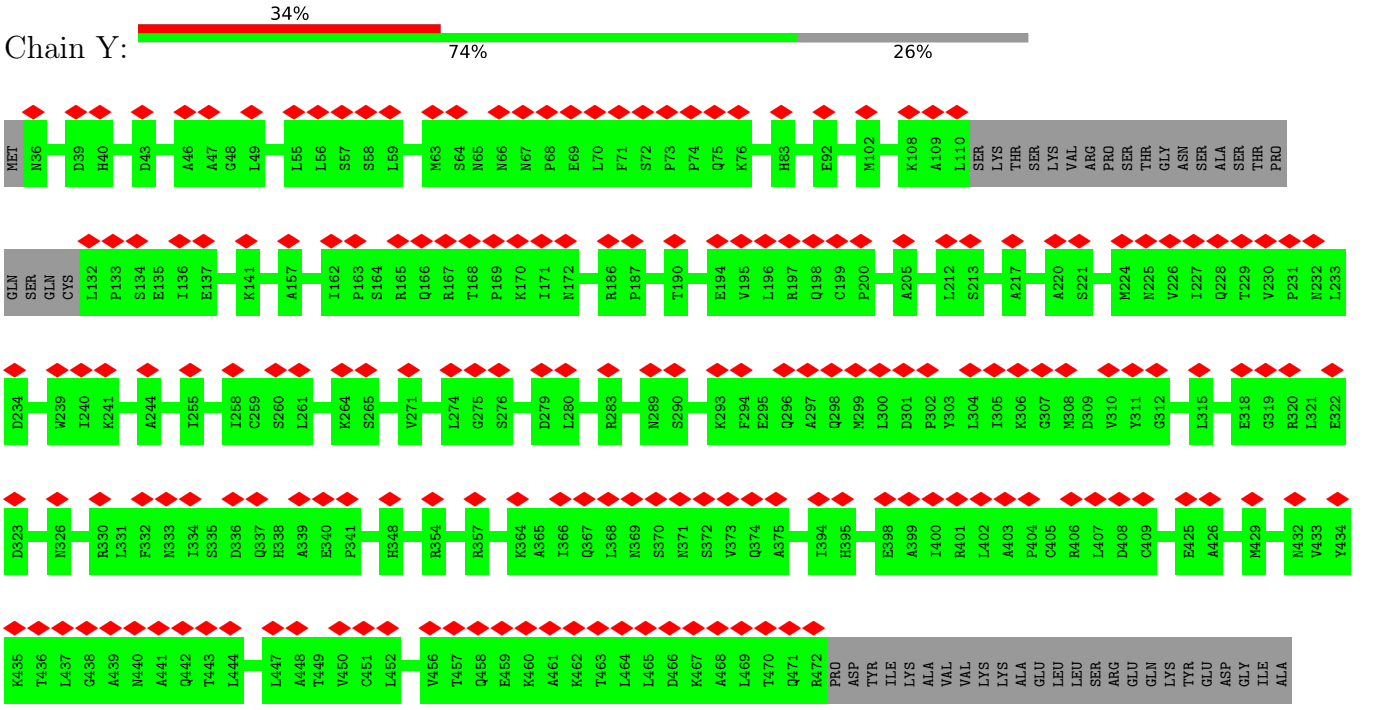
- Molecule 17: Anaphase-promoting complex subunit 7

Chain X:



- Molecule 17: Anaphase-promoting complex subunit 7

Chain Y:



LEU LEU ARG ASN ALA LEU ALA ASN GLN SER ASP CYS VAL LEU HIS ARG ILE LEU GLY ASP PHE LEU VAL ALA VAL ASN GLU TYR GLN GLU ALA MET ASP GLN TYR SER ILE ALA LEU SER LEU ASP PRO ASN ASP GLN LYS SER LEU GLU GLY MET GLN LYS MET 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, Not provided	
Number of particles used	135578	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 ($e^-/Å^2$)	40	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	0.206	Depositor
Minimum map value	-0.089	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.013	Depositor
Recommended contour level	0.065	Depositor
Map size (Å)	401.92, 401.92, 401.92	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.57, 1.57, 1.57	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).

There are no protein, RNA or DNA chains available to summarize Z scores of covalent bonds and angles.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	1380	0	0	3	0
2	B	68	0	0	0	0
3	C	475	0	0	1	0
3	P	443	0	0	1	0
4	D	55	0	0	0	0
5	E	56	0	0	0	0
6	F	482	0	0	0	0
6	H	483	0	0	0	0
7	G	25	0	0	0	0
7	W	25	0	0	0	0
8	I	727	0	0	1	0
9	J	504	0	0	0	0
9	K	493	0	0	0	0
10	L	170	0	0	1	0
11	M	42	0	0	0	0
12	N	546	0	0	0	0
13	O	685	0	0	1	0
14	R	385	0	0	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	S	84	0	0	0	0
16	T	97	0	0	0	0
17	X	397	0	0	0	0
17	Y	416	0	0	0	0
All	All	8038	0	0	10	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 1.

All (10) 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)
14:R:420:TYR:CA	14:R:421:SER:CA	2.81	0.59
1:A:1670:GLY:CA	1:A:1671:PRO:CA	2.84	0.54
14:R:127:LEU:CA	14:R:128:PHE:CA	2.92	0.48
3:P:361:ASN:CA	3:P:362:PRO:CA	2.92	0.47
1:A:1100:LEU:CA	1:A:1101:PRO:CA	2.93	0.46
10:L:60:GLN:CA	10:L:61:PRO:CA	2.93	0.46
3:C:361:ASN:CA	3:C:362:PRO:CA	2.97	0.43
8:I:572:PHE:CA	8:I:573:PRO:CA	2.96	0.42
13:O:123:GLU:CA	13:O:124:PRO:CA	2.99	0.41
1:A:1112:PRO:CA	1:A:1113:PRO:CA	2.99	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains (i)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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.

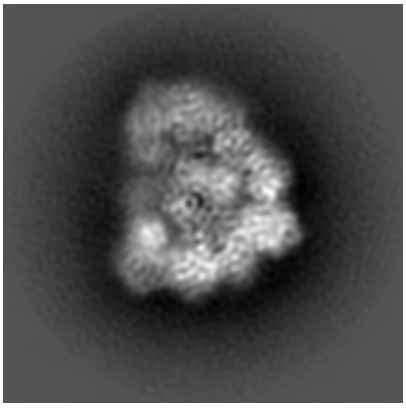
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-3433. These allow visual inspection of the internal detail of the map and identification of artifacts.

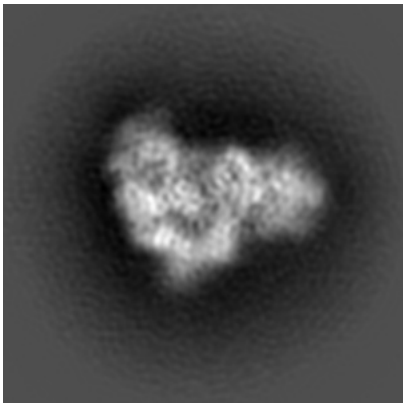
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

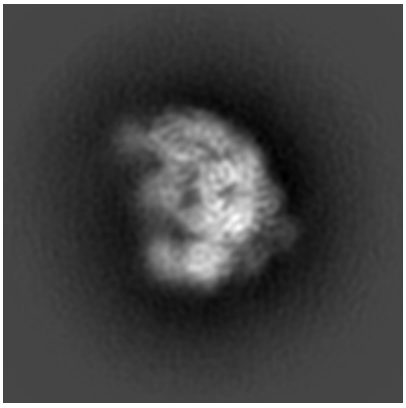
6.1.1 Primary map



X



Y

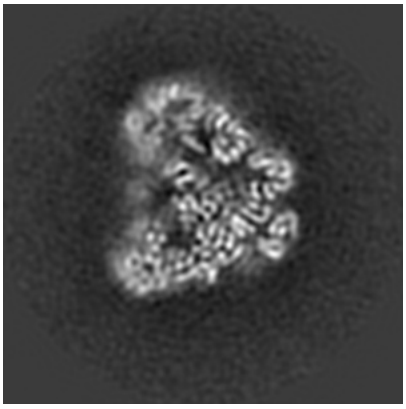


Z

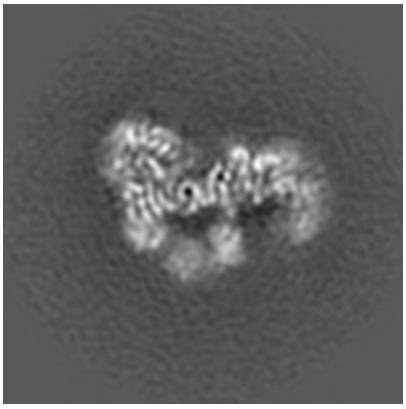
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

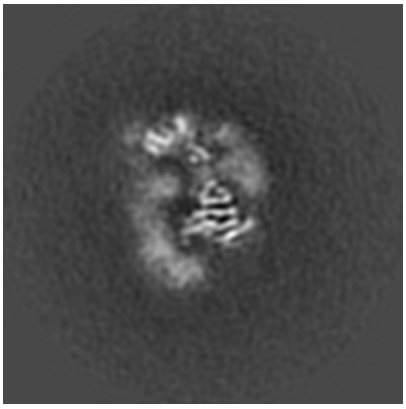
6.2.1 Primary map



X Index: 128



Y Index: 128

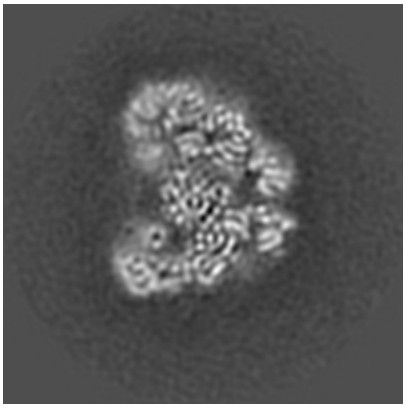


Z Index: 128

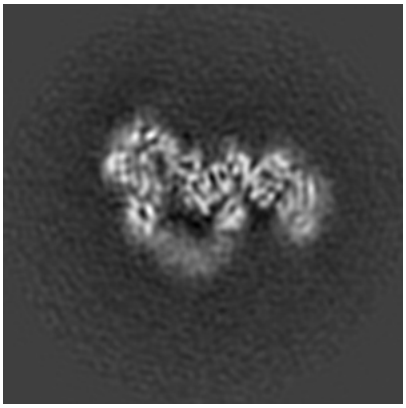
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

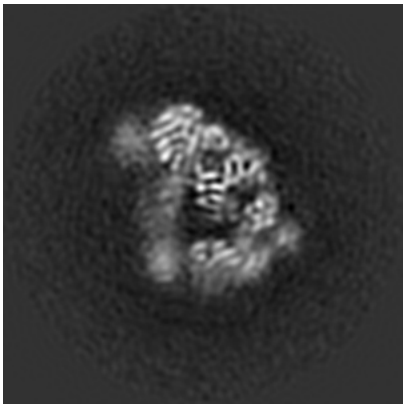
6.3.1 Primary map



X Index: 134



Y Index: 121

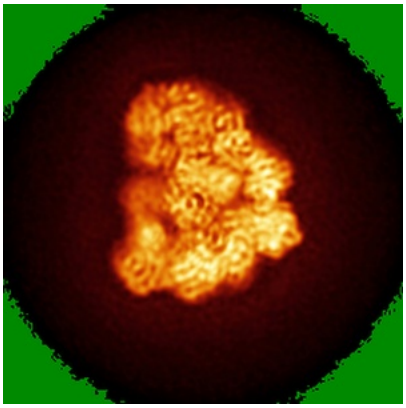


Z Index: 104

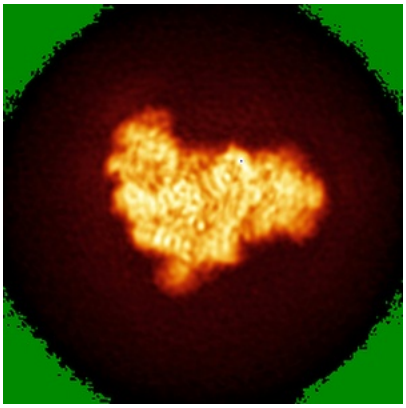
The images above show the largest variance slices of the map in three orthogonal directions.

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

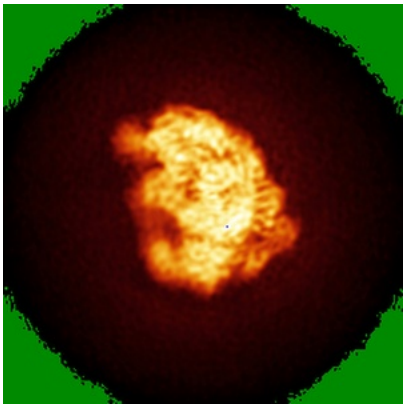
6.4.1 Primary map



X



Y

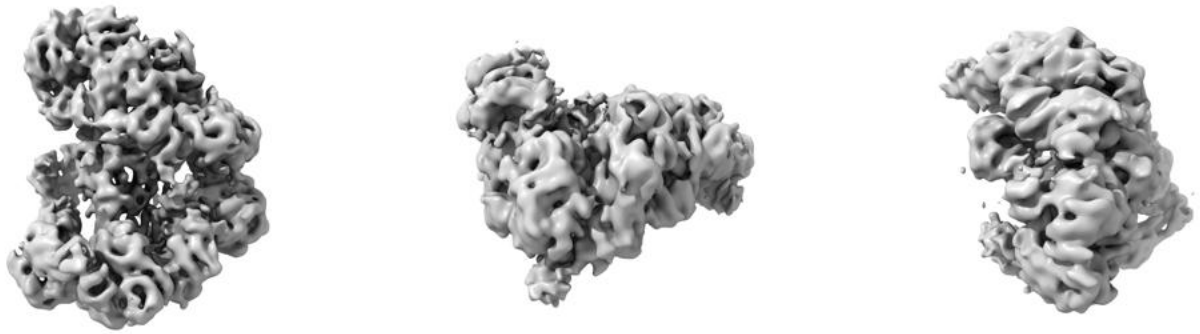


Z

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

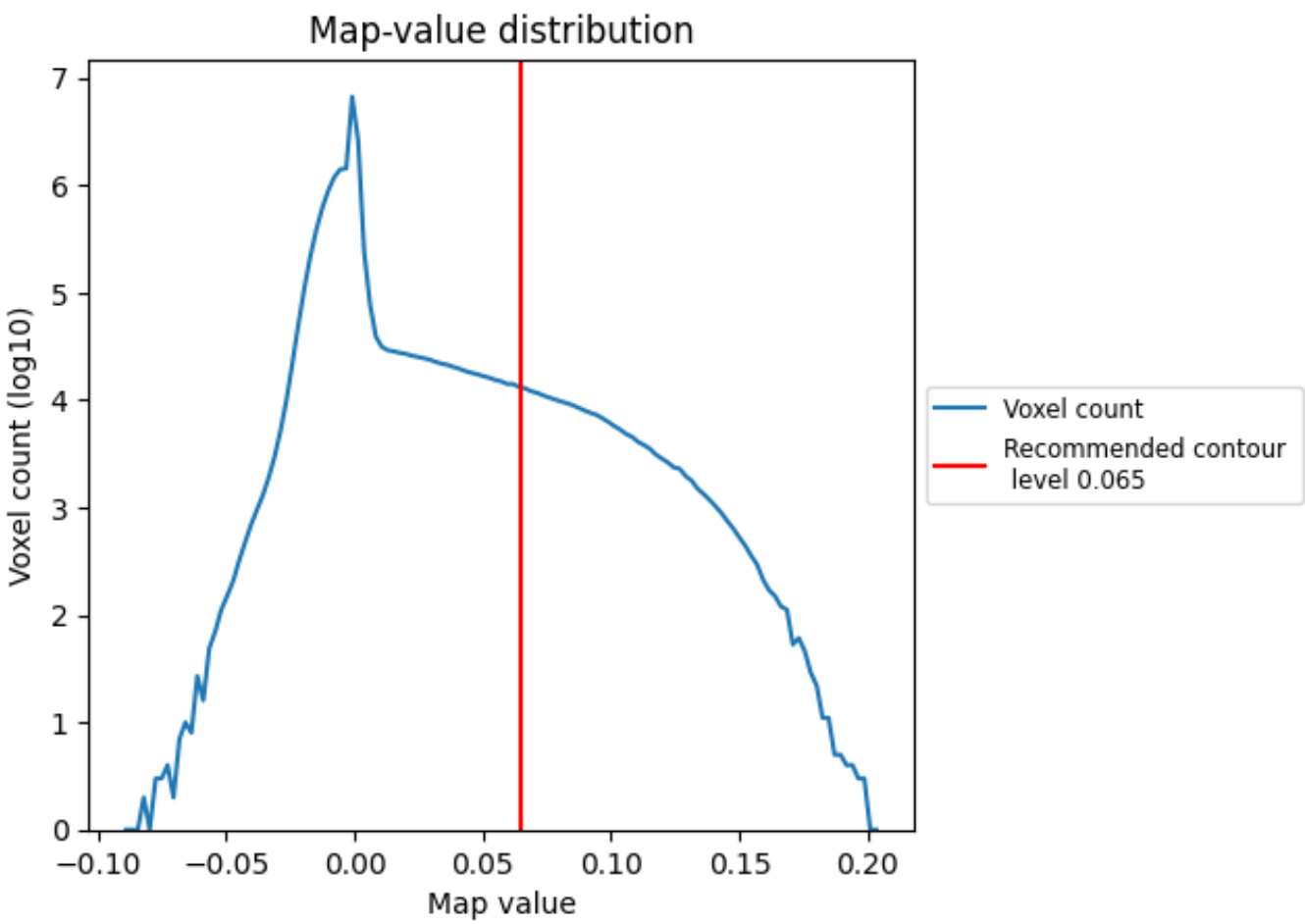
6.6 Mask visualisation (i)

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

7 Map analysis (i)

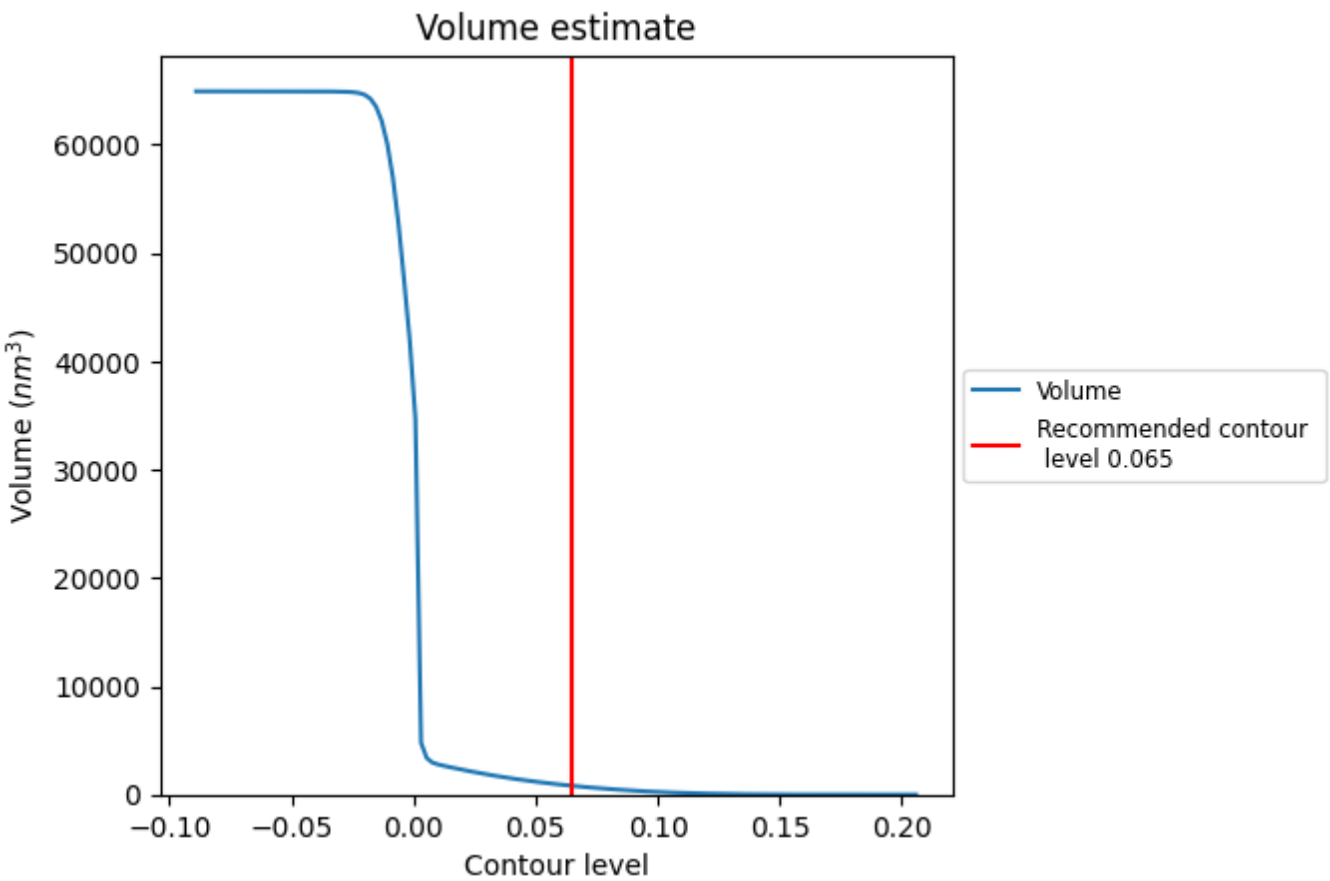
This section contains the results of statistical analysis of the map.

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.

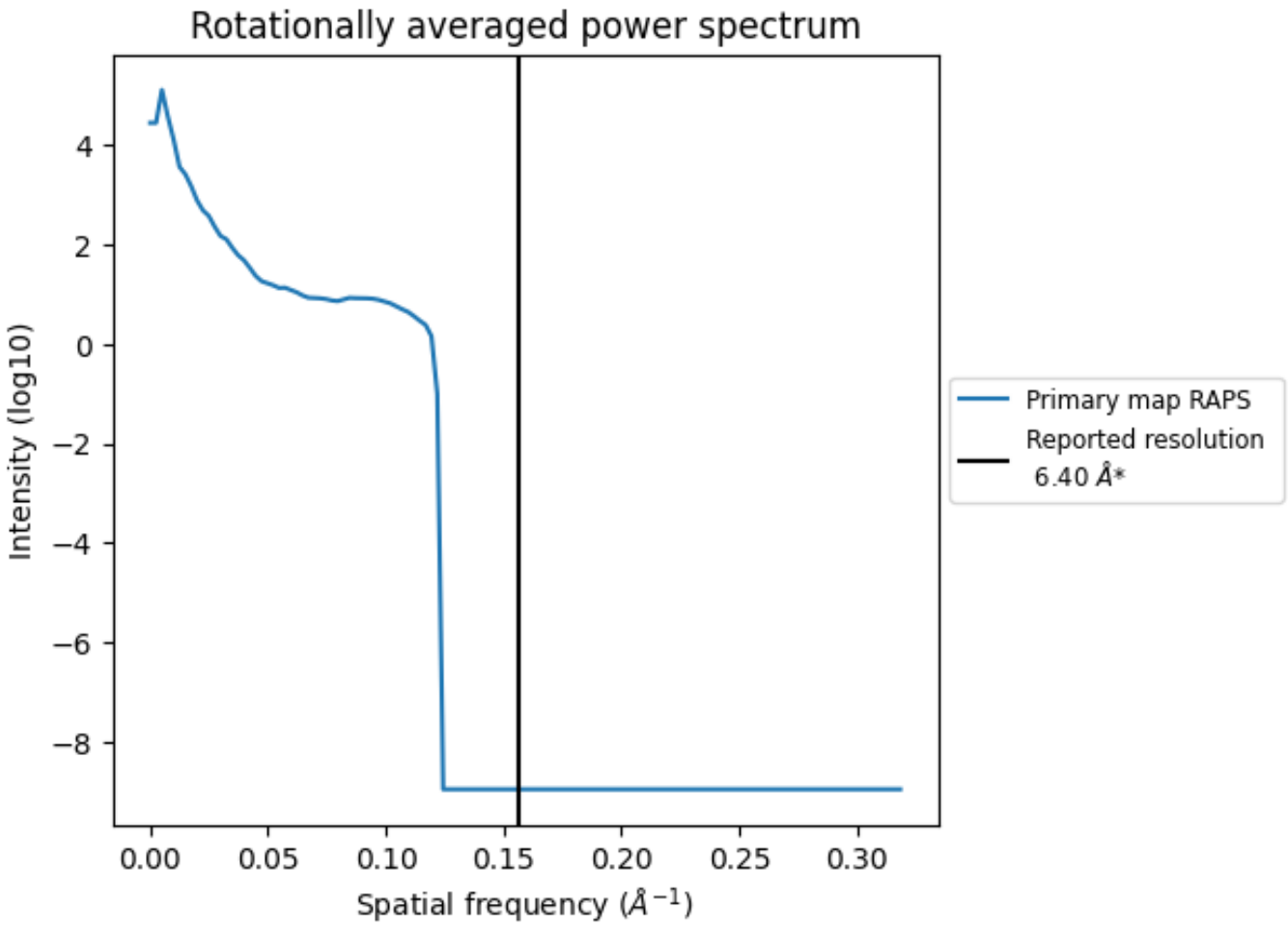
7.2 Volume estimate (i)



The volume at the recommended contour level is 807 nm^3; this corresponds to an approximate mass of 729 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 0.156 Å^{-1}

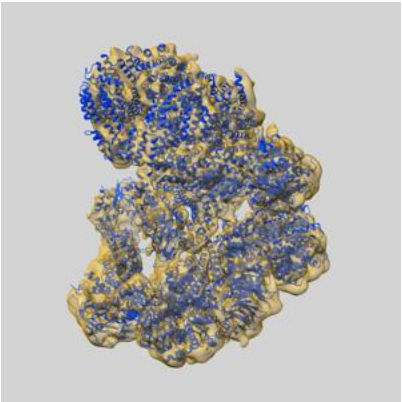
8 Fourier-Shell correlation (i)

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

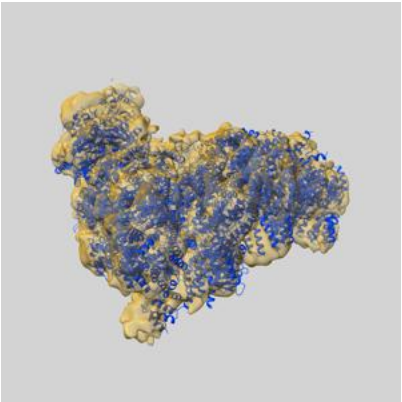
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-3433 and PDB model 5L9T. Per-residue inclusion information can be found in section 3 on page 9.

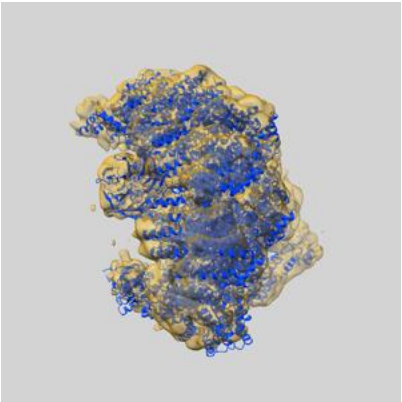
9.1 Map-model overlay (i)



X



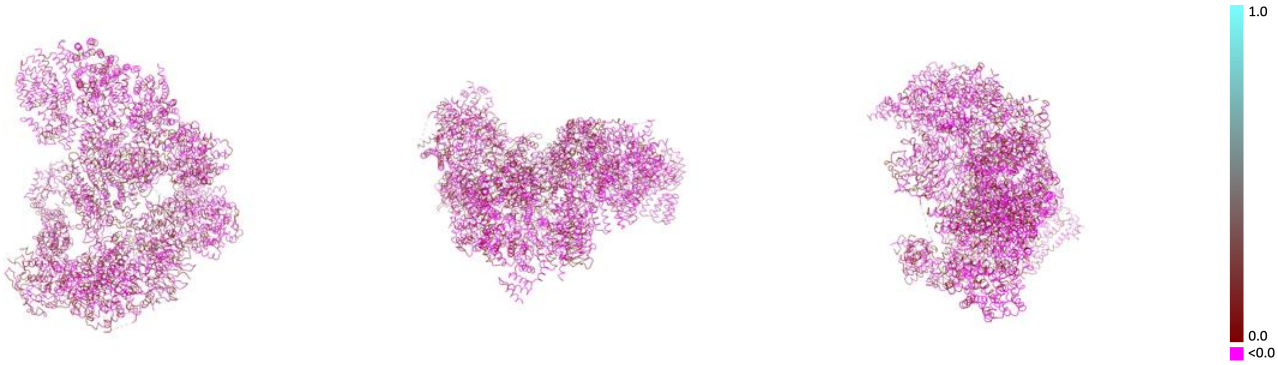
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.065 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.

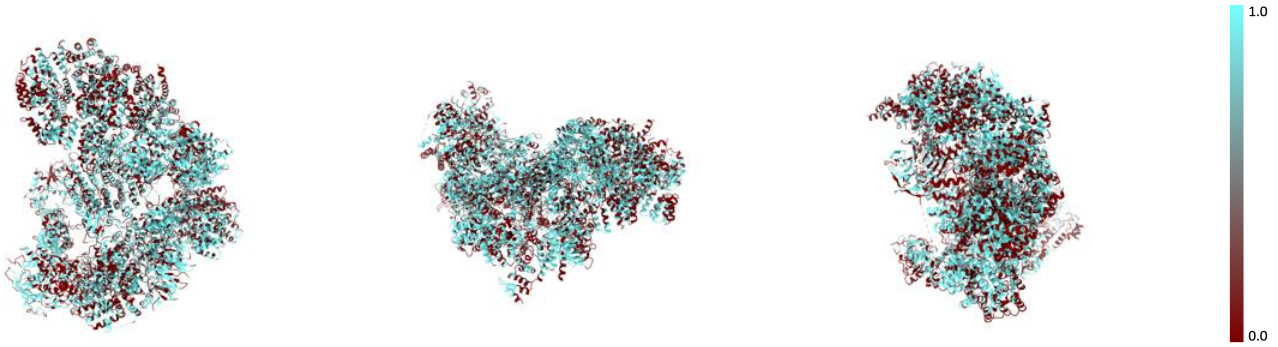
9.2 Q-score mapped to coordinate model (i)



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.

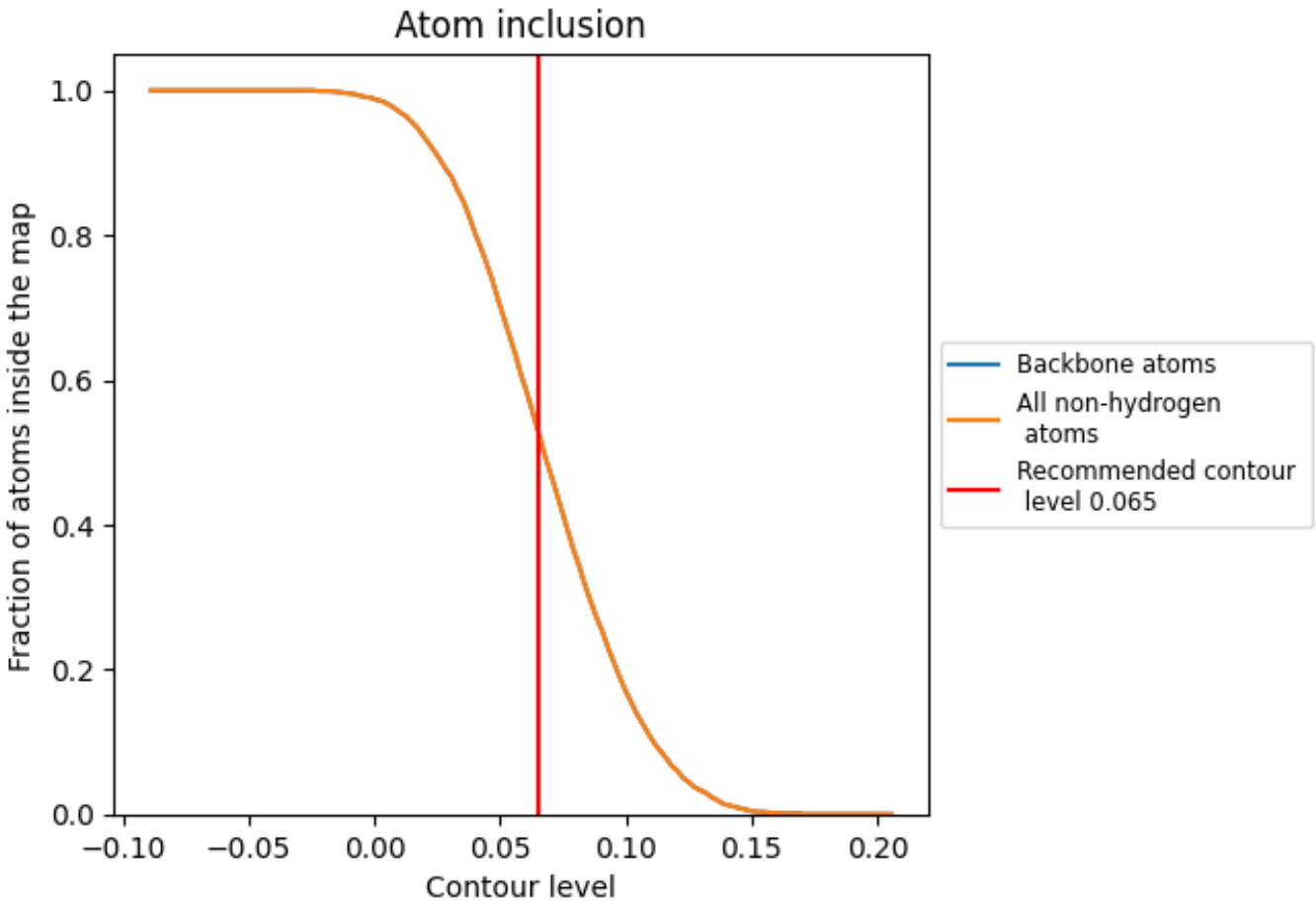
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.065).

9.4 Atom inclusion (i)



At the recommended contour level, 53% of all backbone atoms, 53% 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 (0.065) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5300	0.0200
A	0.5030	0.0460
B	0.7350	0.0960
C	0.6290	0.0360
D	0.2550	0.0010
E	0.4290	-0.0170
F	0.5210	-0.0290
G	0.0800	-0.1230
H	0.5050	-0.0140
I	0.5520	0.0420
J	0.5690	-0.0200
K	0.7380	0.0700
L	0.6060	0.0710
M	0.3810	0.0660
N	0.4380	0.0370
O	0.5040	0.0180
P	0.4810	-0.0420
R	0.5400	0.0320
S	0.3810	0.0450
T	0.5260	0.0410
W	0.6400	0.1460
X	0.4560	-0.0220
Y	0.5430	-0.0000