wwPDB EM Validation Summary Report

Aug 22, 2022 – 04:17 pm BST

PDB ID	:	8A3T
EMDB ID	:	EMD-15123
Title	:	S. cerevisiae APC/C-Cdh1 complex
Authors	:	Barford, D.; Vazquez-Fernandez, E.; Zhang, Z.; Yang, J.
Deposited on	:	2022-06-09
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 ⓘ 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 ⓘ) were used in the production of this report:

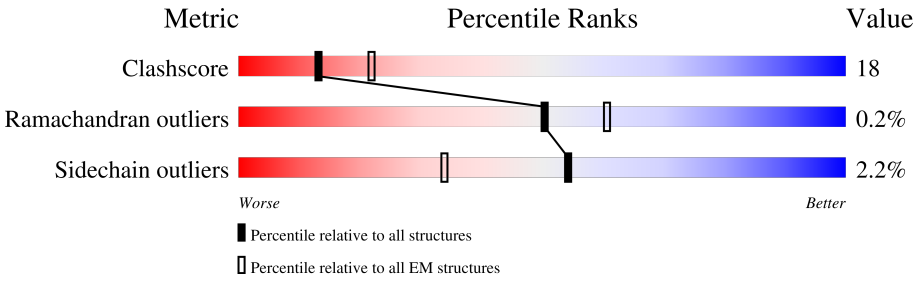
EMDB validation analysis	:	0.0.1.dev8
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.29

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	F	758	6% 44% 22% · 34%
1	H	758	29% 41% 24% · 33%
2	J	850	· 40% 19% · 40%
2	K	850	7% 35% 23% · 41%
3	G	124	9% 15% 13% 72%
3	W	124	20% 21% 9% 70%
4	E	265	24% 31% 18% · 51%
5	A	250	33% 50% 37% · 12%

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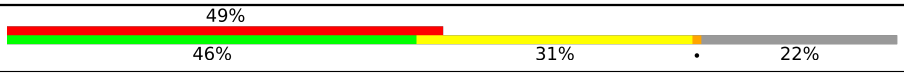
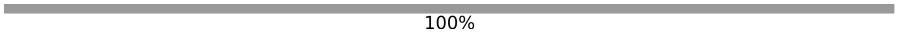
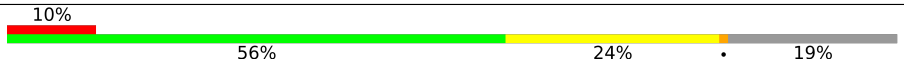
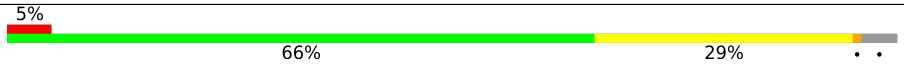
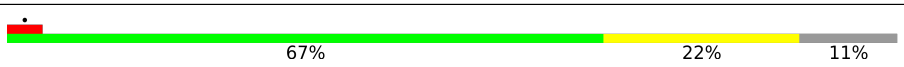
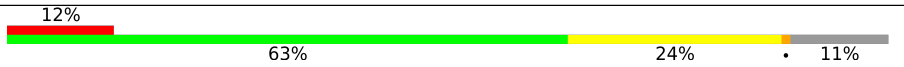
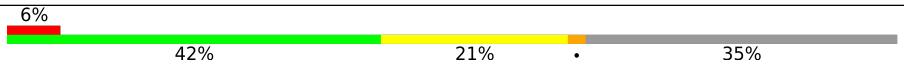
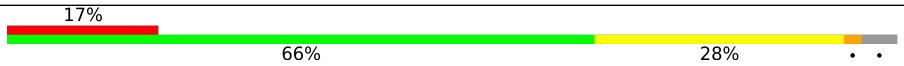
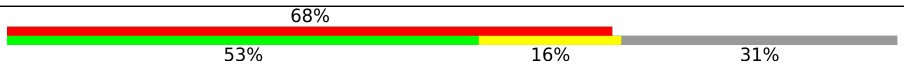
Mol	Chain	Length	Quality of chain
6	B	566	
7	S	1518	
8	C	1748	
9	O	685	
10	D	626	
10	P	626	
11	I	170	
12	N	368	
13	Q	652	
14	T	853	
15	U	165	

2 Entry composition (i)

There are 16 unique types of molecules in this entry. The entry contains 61351 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 CDC27.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	F	502	Total	C	N	O	S	0	0
			3991	2569	656	739	27		
1	H	505	Total	C	N	O	S	0	0
			4031	2593	664	747	27		

- Molecule 2 is a protein called Anaphase-promoting complex subunit CDC16.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	J	509	Total	C	N	O	S	0	0
			4128	2661	675	769	23		
2	K	505	Total	C	N	O	S	0	0
			4102	2642	673	764	23		

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	841	LYS	-	expression tag	UNP P09798
J	842	SER	-	expression tag	UNP P09798
J	843	SER	-	expression tag	UNP P09798
J	844	ILE	-	expression tag	UNP P09798
J	845	PRO	-	expression tag	UNP P09798
J	846	GLU	-	expression tag	UNP P09798
J	847	ASN	-	expression tag	UNP P09798
J	848	LEU	-	expression tag	UNP P09798
J	849	TYR	-	expression tag	UNP P09798
J	850	PHE	-	expression tag	UNP P09798
K	841	LYS	-	expression tag	UNP P09798
K	842	SER	-	expression tag	UNP P09798
K	843	SER	-	expression tag	UNP P09798
K	844	ILE	-	expression tag	UNP P09798
K	845	PRO	-	expression tag	UNP P09798
K	846	GLU	-	expression tag	UNP P09798
K	847	ASN	-	expression tag	UNP P09798

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Chain	Residue	Modelled	Actual	Comment	Reference
K	848	LEU	-	expression tag	UNP P09798
K	849	TYR	-	expression tag	UNP P09798
K	850	PHE	-	expression tag	UNP P09798

- Molecule 3 is a protein called Anaphase-promoting complex subunit CDC26.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	35	Total	C	N	O	S	0	0
			284	174	51	58	1		
3	W	37	Total	C	N	O	S	0	0
			300	184	54	61	1		

- Molecule 4 is a protein called Anaphase-promoting complex subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	130	Total	C	N	O	S	0	0
			1091	678	201	205	7		

- Molecule 5 is a protein called Anaphase-promoting complex subunit DOC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	A	219	Total	C	N	O	S	0	0
			1743	1118	304	311	10		

- Molecule 6 is a protein called CDH1 isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	B	440	Total	C	N	O	S	0	0
			3418	2143	602	660	13		

- Molecule 7 is a protein called HSL1 isoform 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	S	6	Total	C	N	O	0	0
			45	27	7	11		

- Molecule 8 is a protein called Anaphase-promoting complex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	C	1410	Total	C	N	O	S	0	0
			10863	7023	1756	2038	46		

- Molecule 9 is a protein called Anaphase-promoting complex subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	O	658	Total	C	N	O	S	0	0
			5288	3402	869	990	27		

- Molecule 10 is a protein called Anaphase-promoting complex subunit CDC23.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	D	560	Total	C	N	O	S	0	0
			4524	2925	729	844	26		
10	P	556	Total	C	N	O	S	0	0
			4518	2922	738	831	27		

- Molecule 11 is a protein called Anaphase-promoting complex subunit SWM1.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	I	111	Total	C	N	O	S	0	0
			906	568	158	176	4		

- Molecule 12 is a protein called Anaphase-promoting complex subunit MND2.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	N	96	Total	C	N	O	S	0	0
			784	504	138	139	3		

- Molecule 13 is a protein called Anaphase-promoting complex subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	Q	623	Total	C	N	O	S	0	0
			5083	3278	842	950	13		

- Molecule 14 is a protein called Anaphase-promoting complex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	T	645	Total	C	N	O	S	0	0
			5337	3466	871	976	24		

- Molecule 15 is a protein called Anaphase-promoting complex subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	U	114	Total	C	N	O	S	0	0
			912	574	164	162	12		

- Molecule 16 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

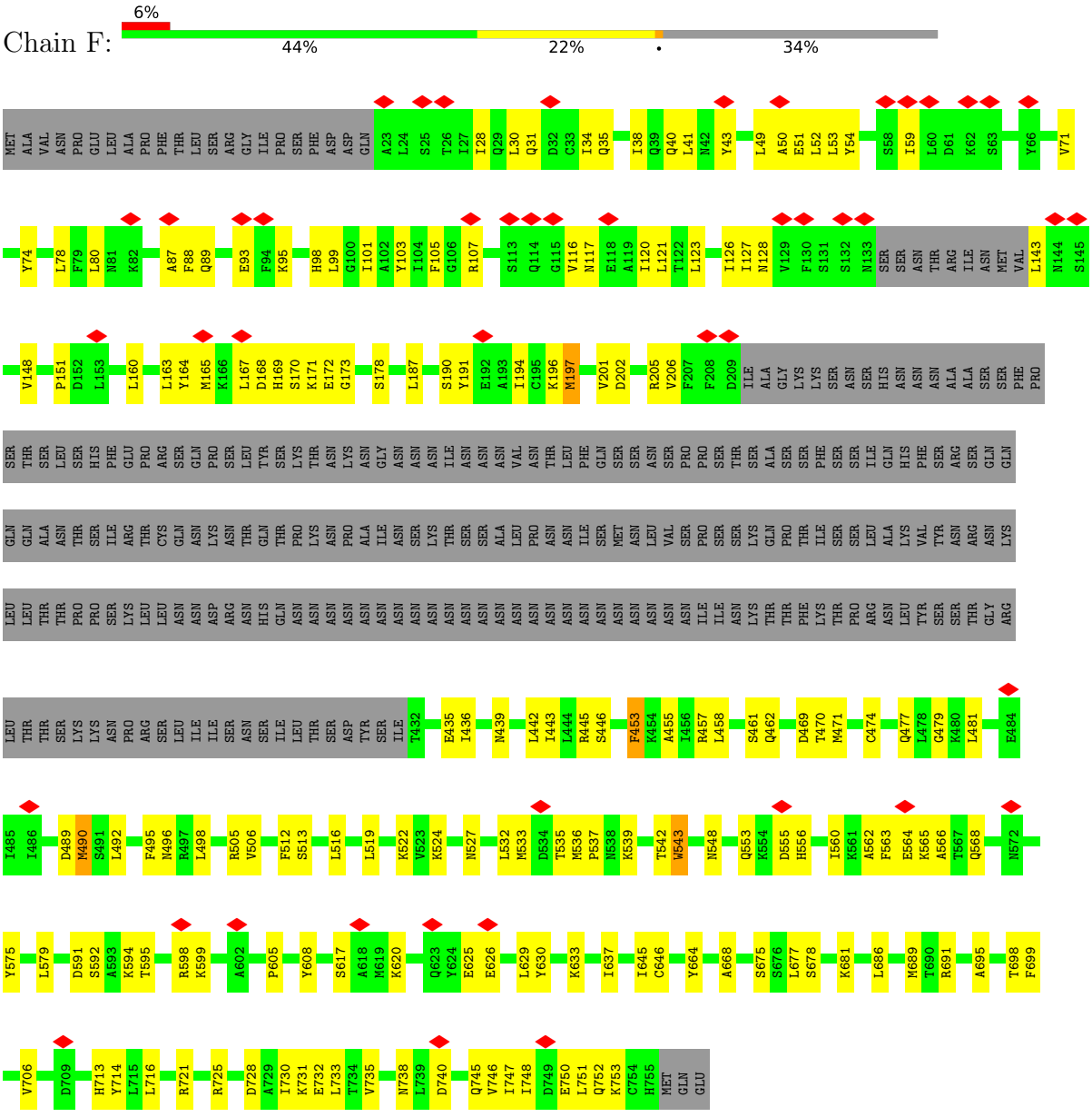
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
16	U	3	3	3	0

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.

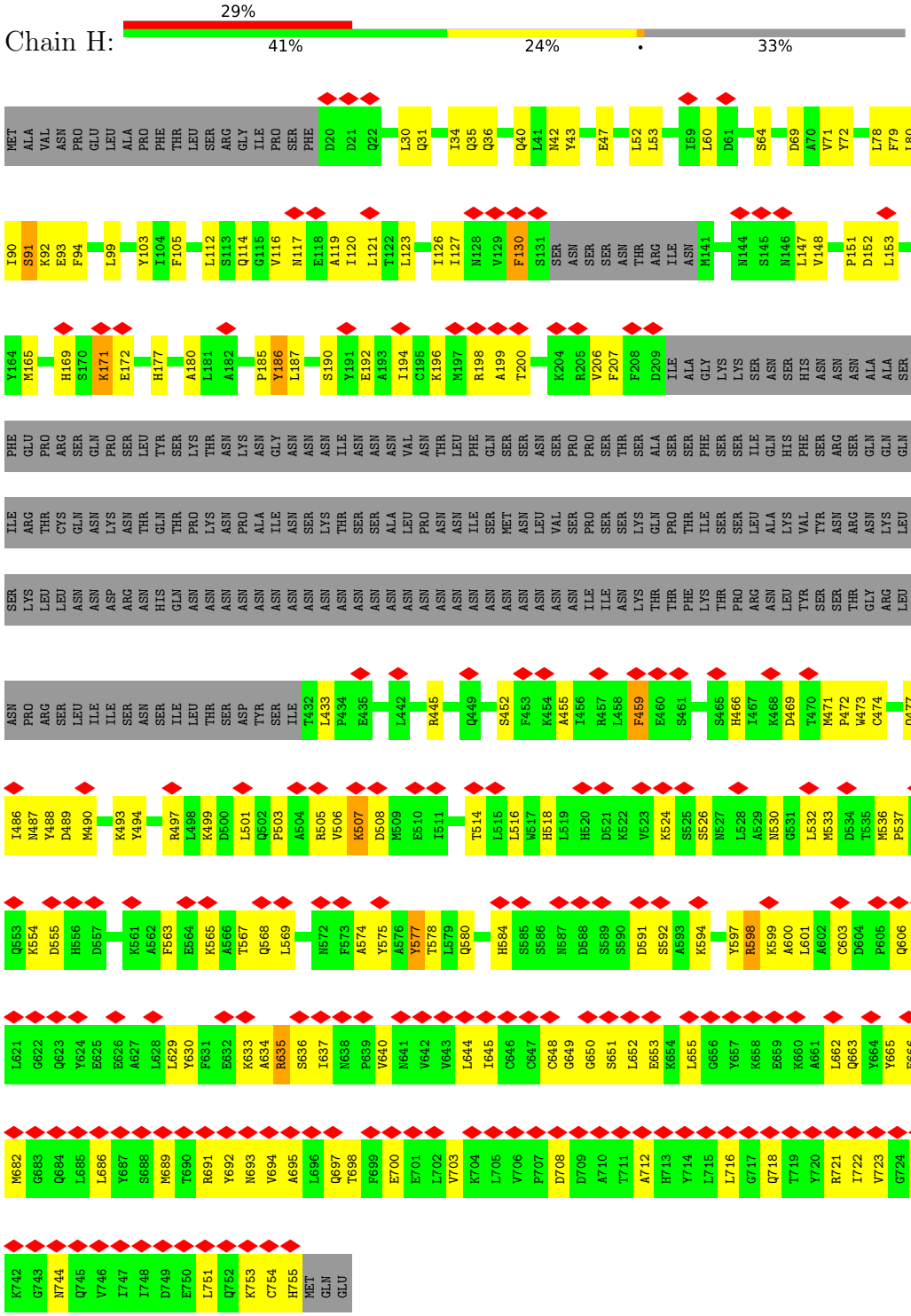
• Molecule 1: Anaphase-promoting complex subunit CDC27

Chain F:



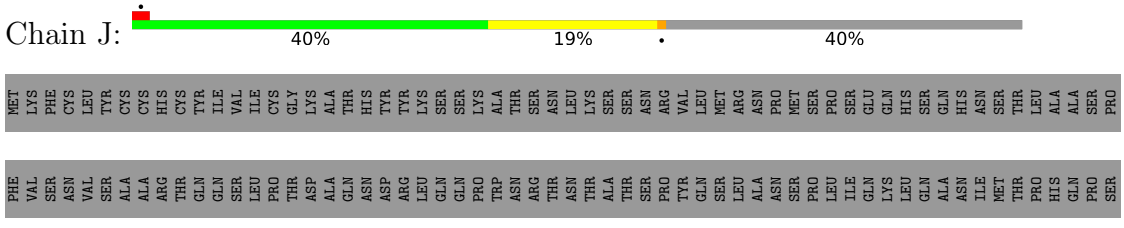
• Molecule 1: Anaphase-promoting complex subunit CDC27

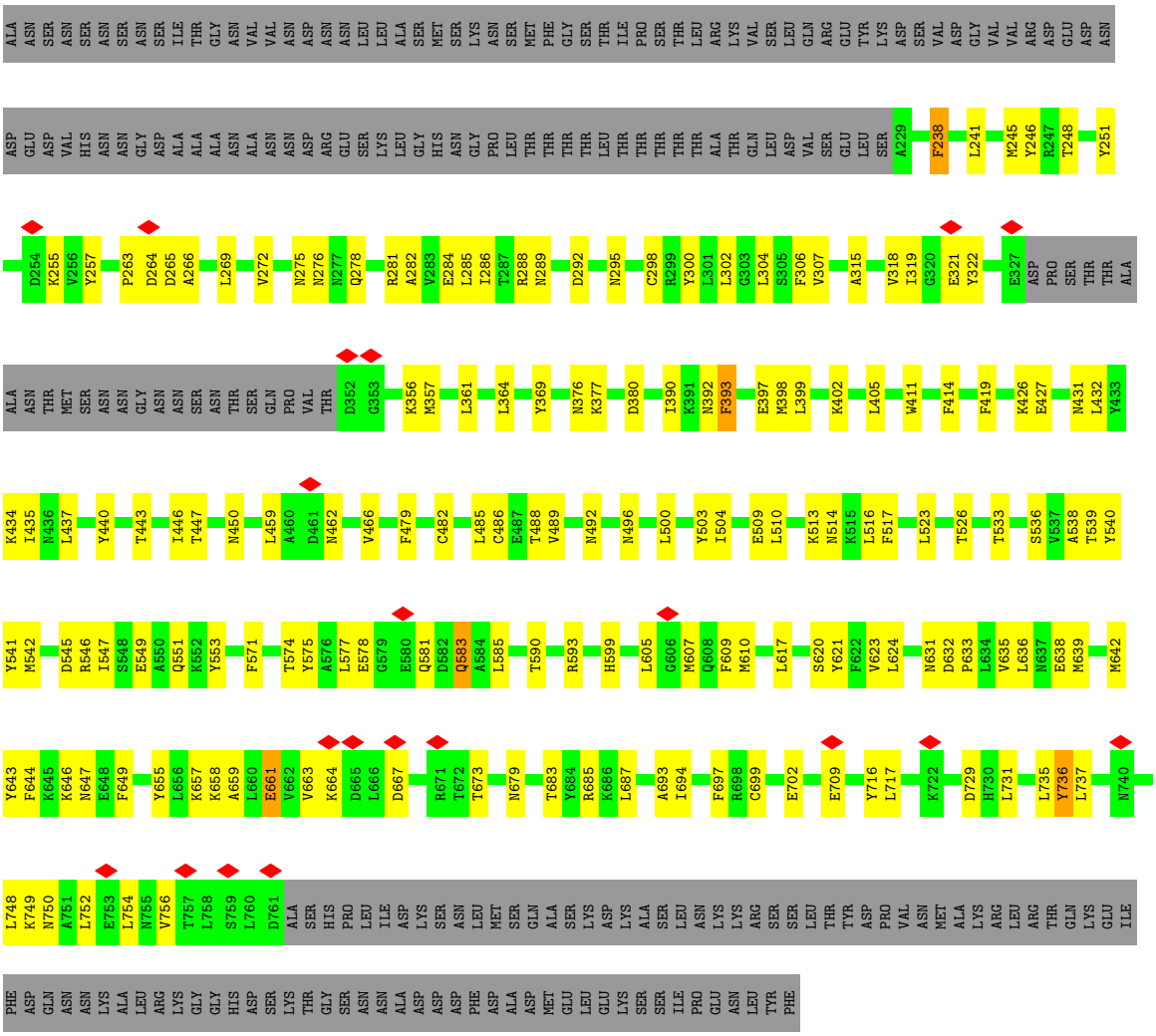
Chain H:



• Molecule 2: Anaphase-promoting complex subunit CDC16

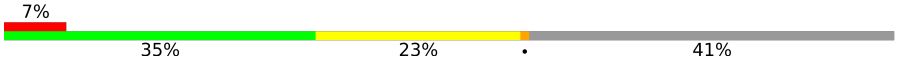
Chain J:

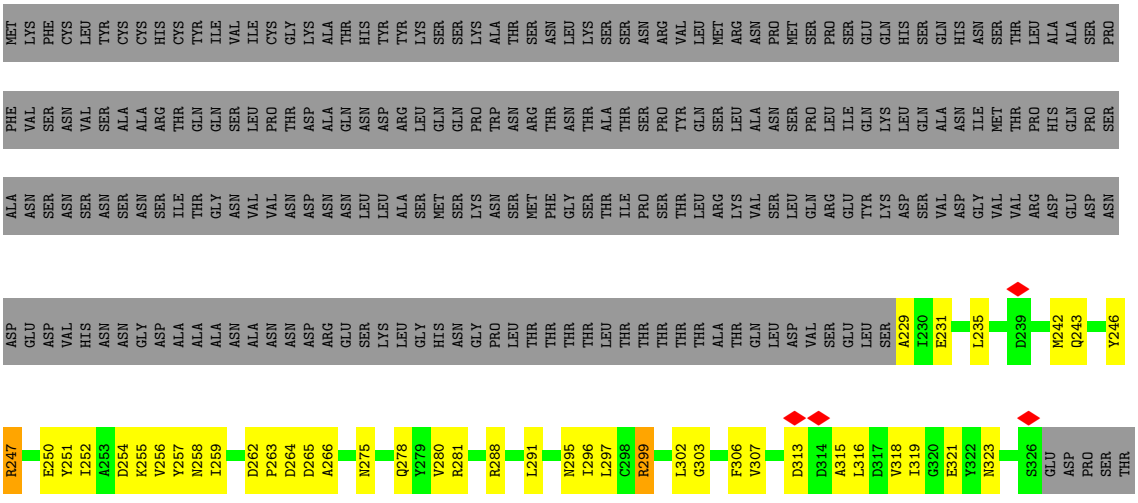


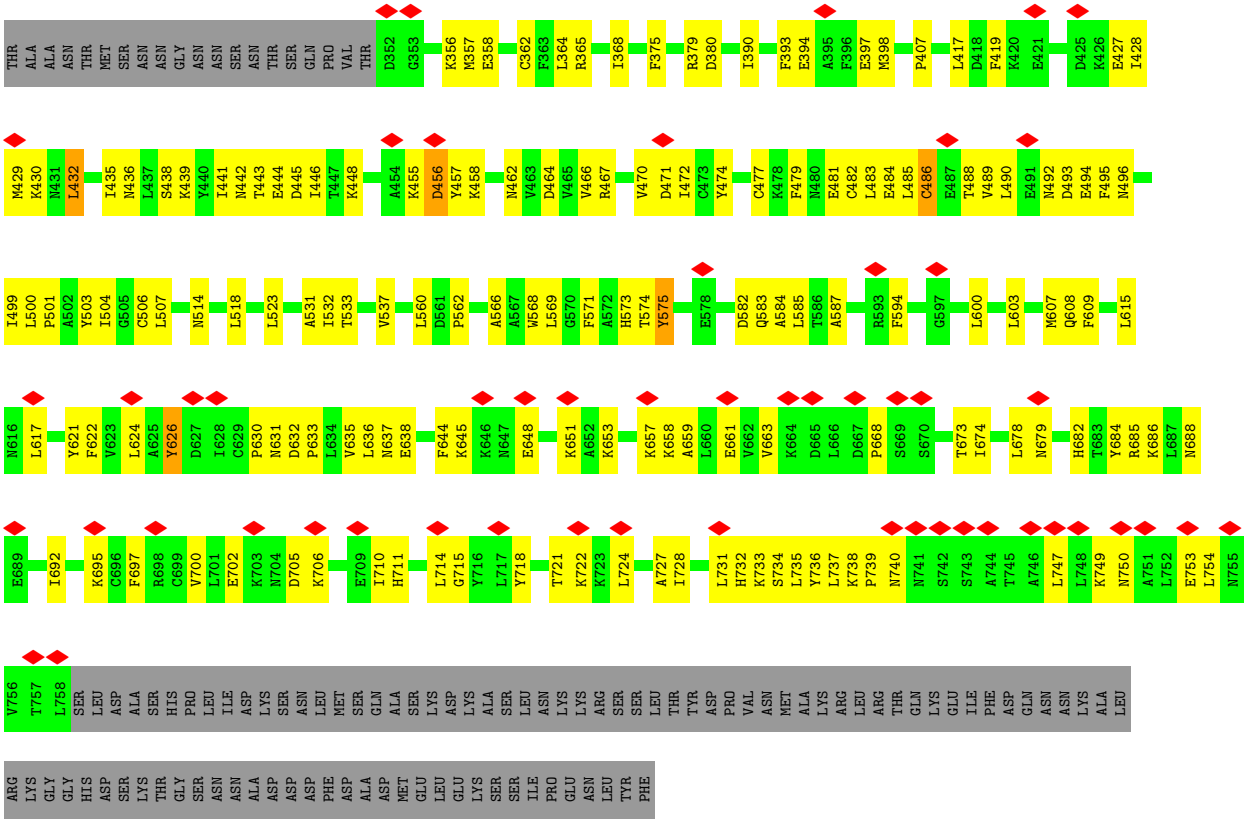


• Molecule 2: Anaphase-promoting complex subunit CDC16

Chain K:

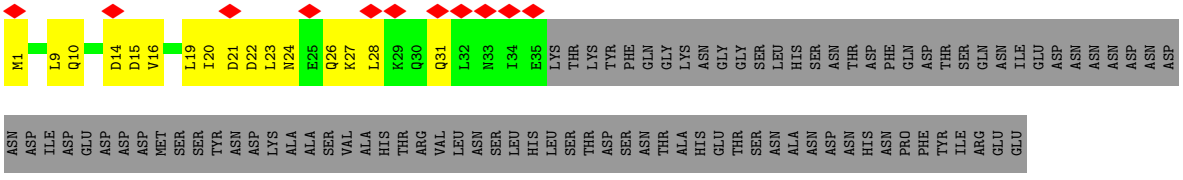






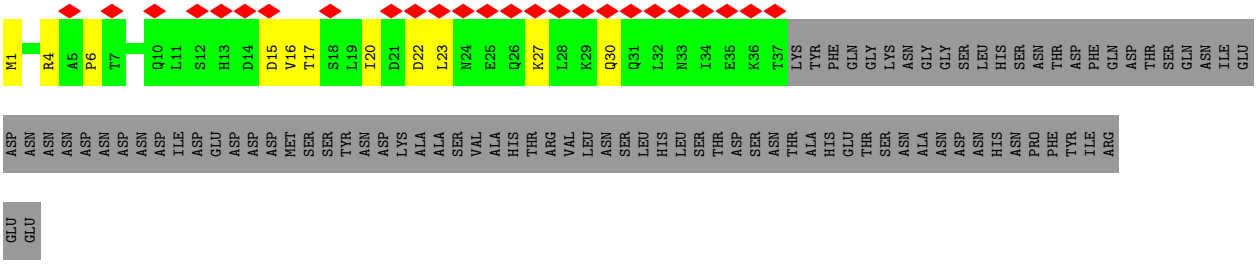
• Molecule 3: Anaphase-promoting complex subunit CDC26

Chain G:



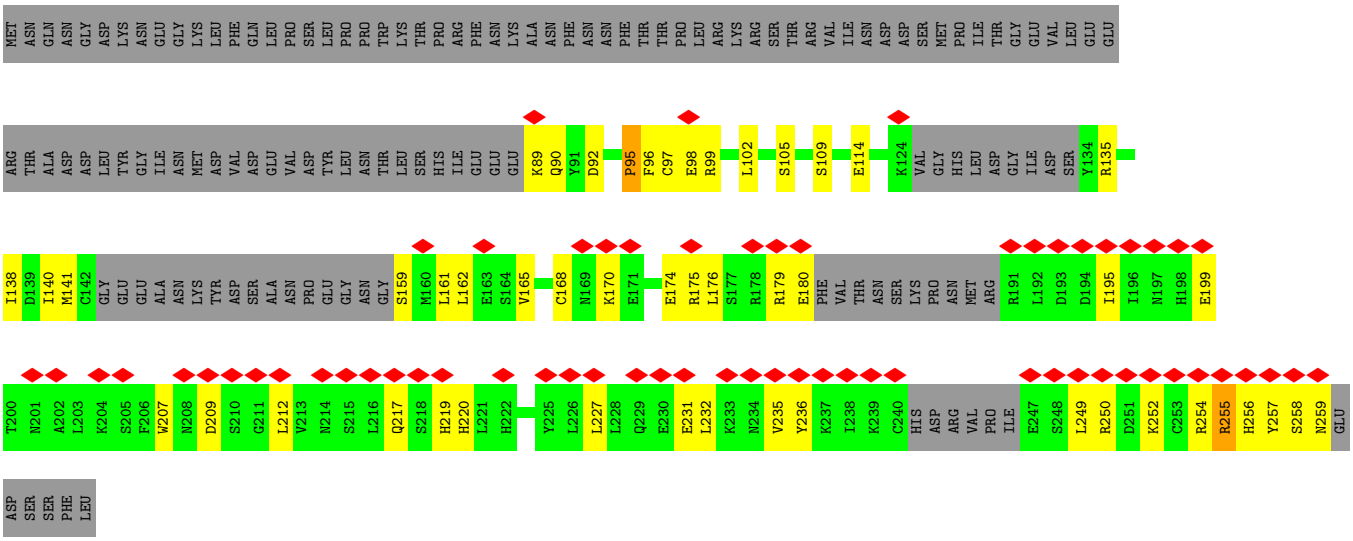
• Molecule 3: Anaphase-promoting complex subunit CDC26

Chain W:



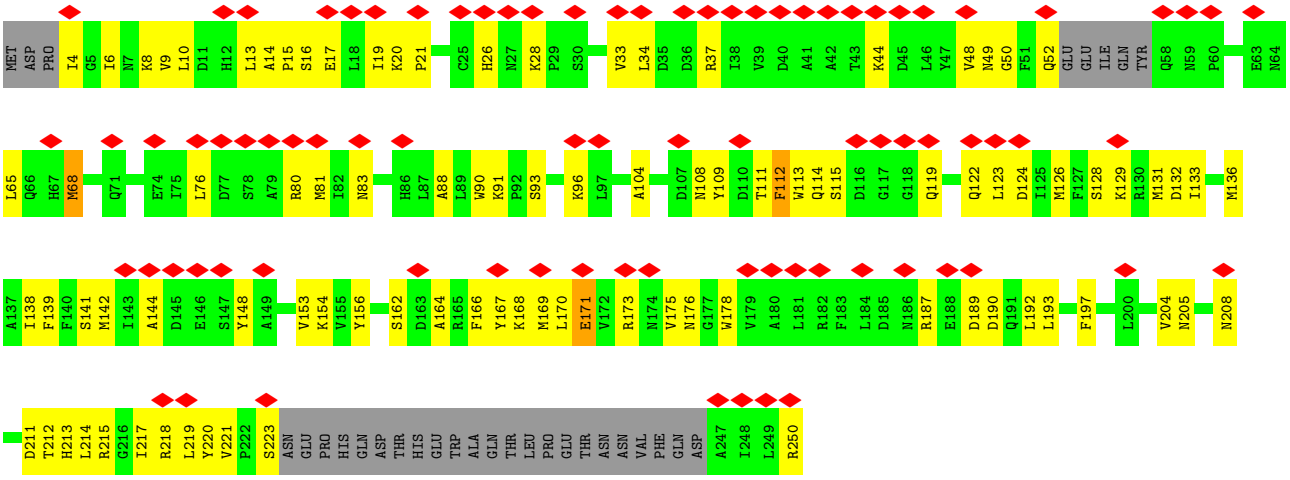
• Molecule 4: Anaphase-promoting complex subunit 9

Chain E:



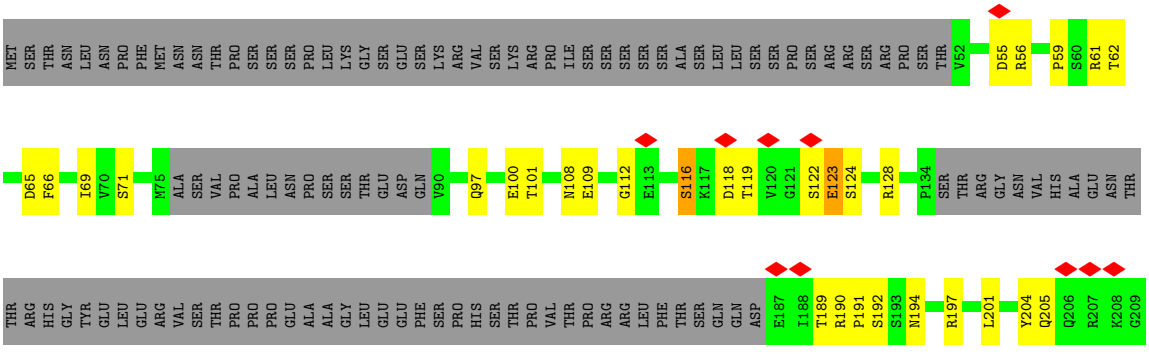
• Molecule 5: Anaphase-promoting complex subunit DOC1

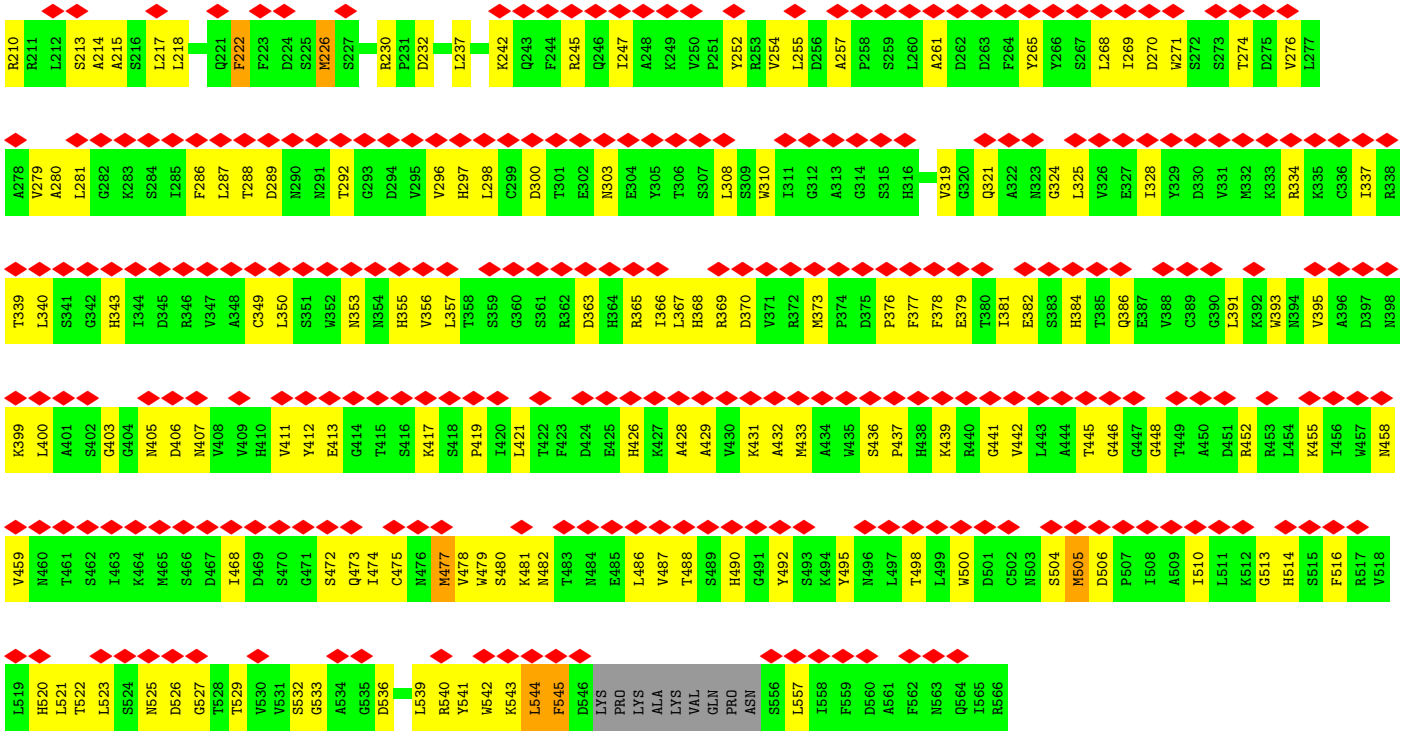
Chain A:



• Molecule 6: CDH1 isoform 1

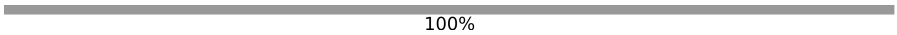
Chain B:

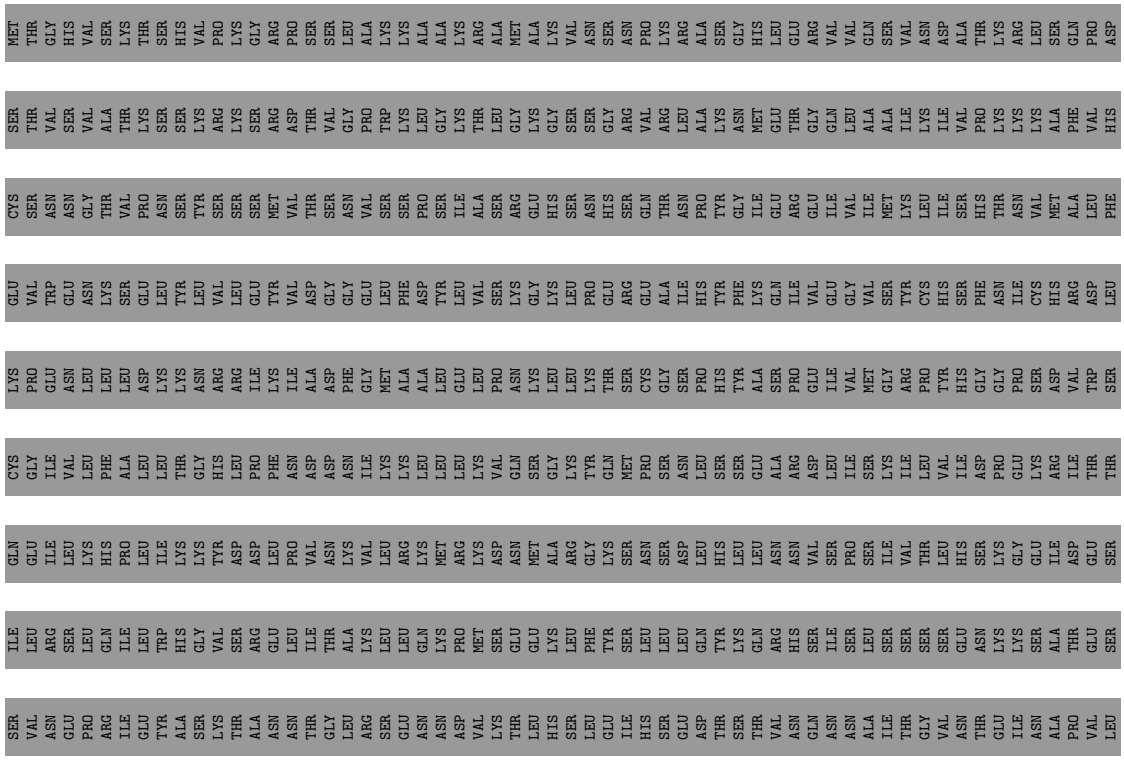


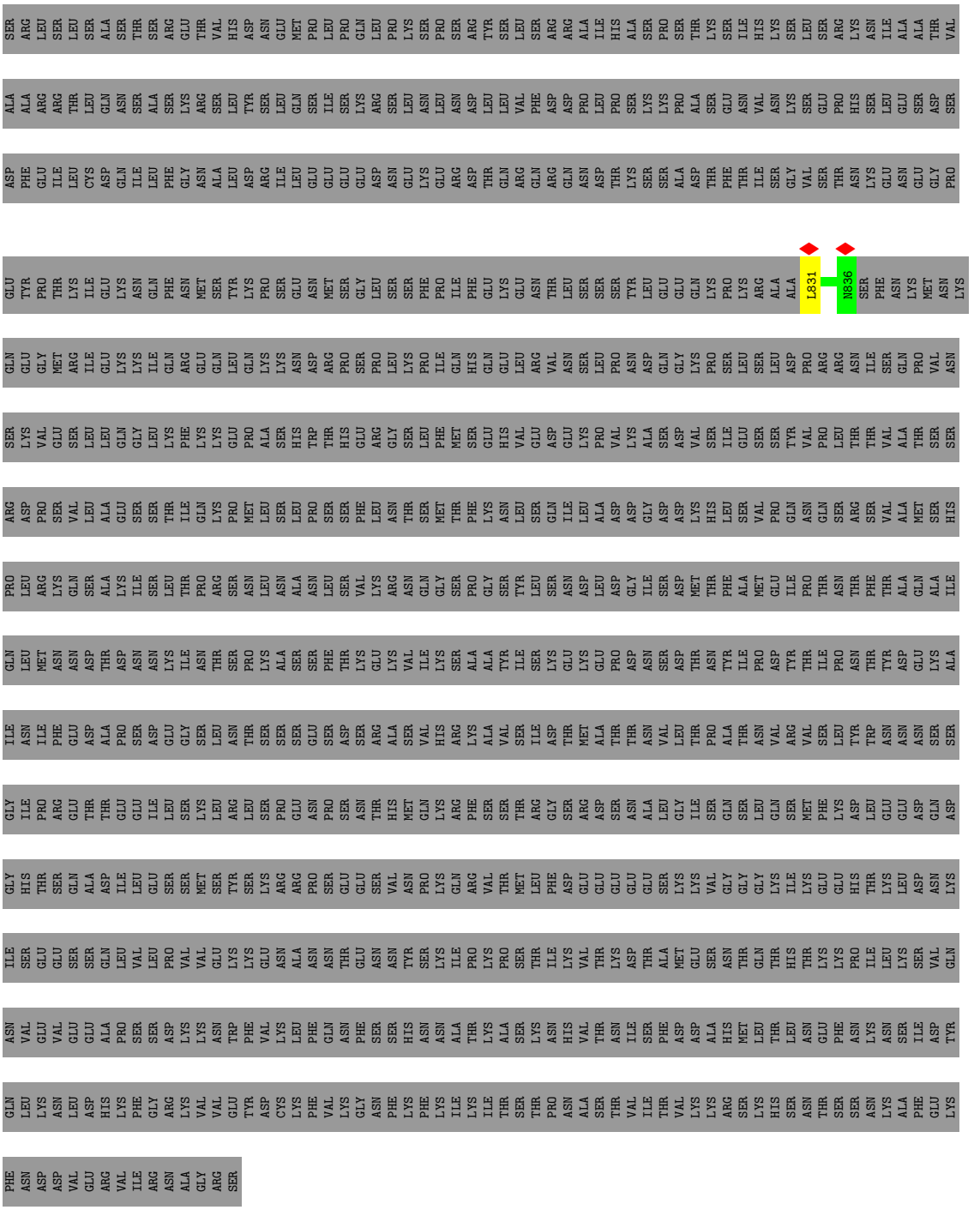


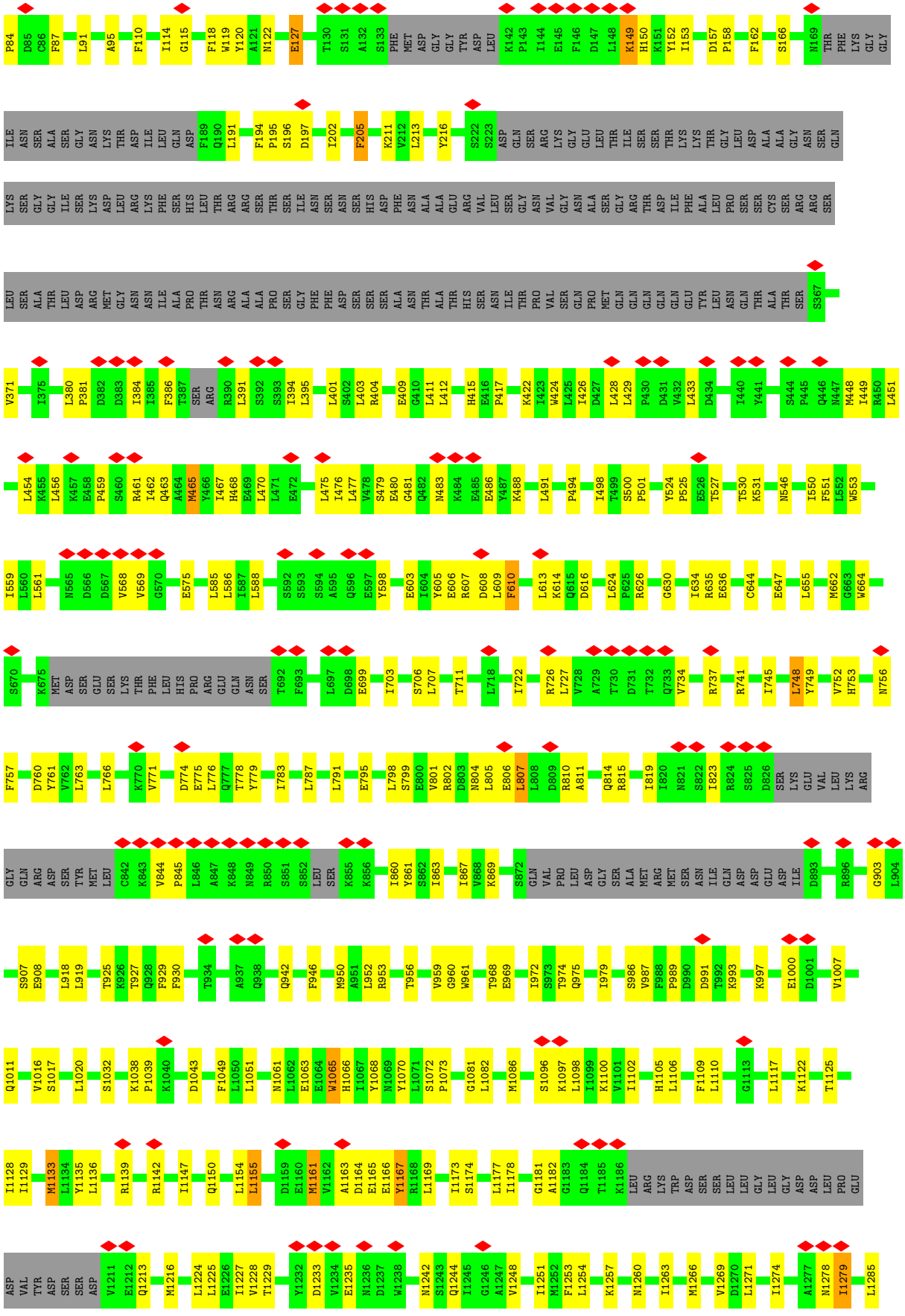
- Molecule 7: HSL1 isoform 1

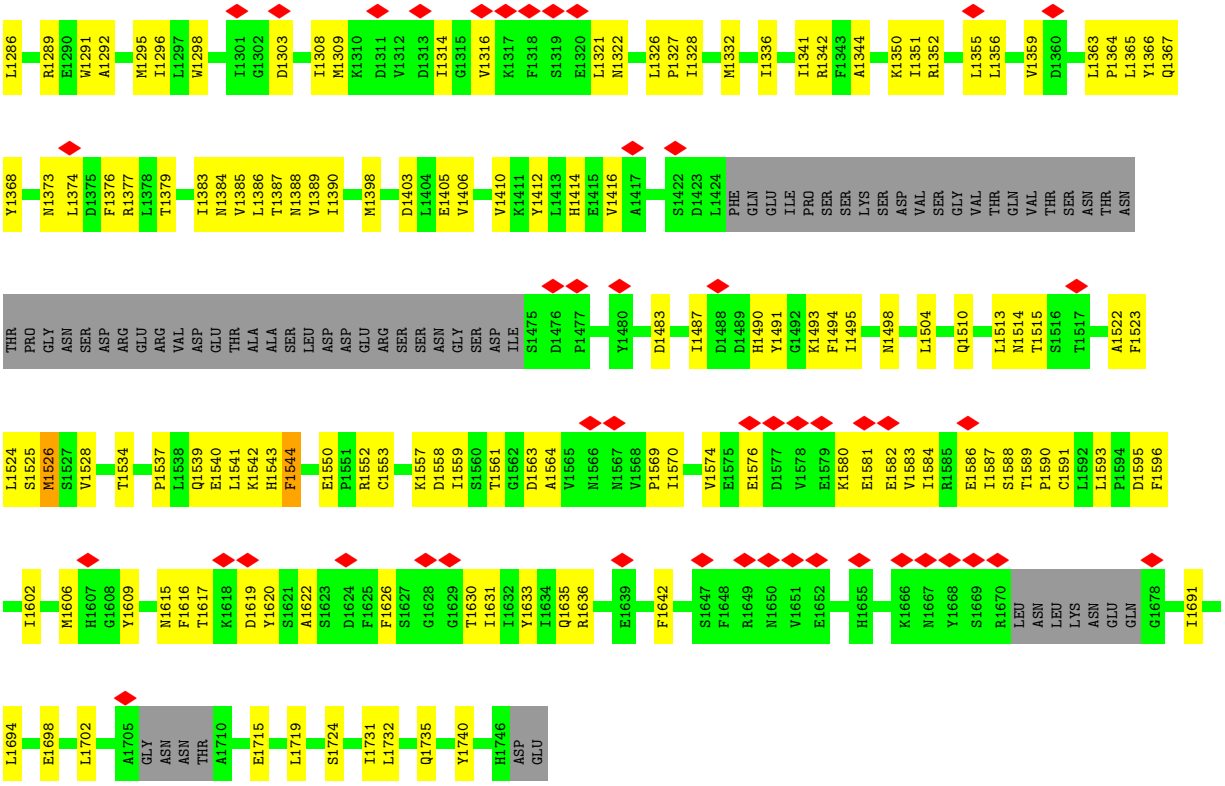
Chain S:





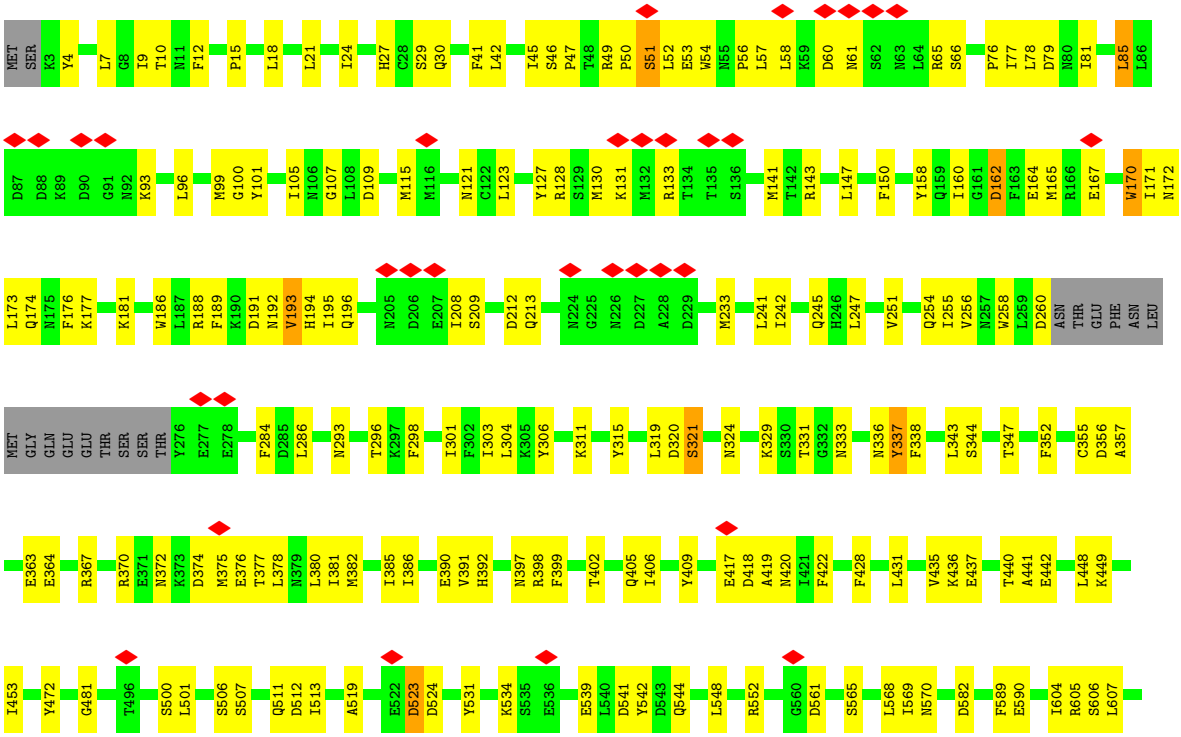

SER ARG LEU SER LEU SER ALA SER THR SER ARG GLU THR VAL HIS ASP ASN GLU MET PRO LEU PRO GLN LEU PRO LYS SER PRO SER ARG TYR SER LEU SER ARG ARG ALA ILE HIS ALA SER PRO SER THR LYS SER ILE HIS LYS SER LEU SER ARG LYS ASN ILE ALA ALA THR VAL
ALA ALA ARG ARG THR LEU GLN ASN SER ALA SER LYS ARG SER ILE SER LEU GLN LEU ASN LEU ASN ASP LEU LEU VAL PHE ASP ASP PRO LEU PRO SER LYS LYS PRO ALA SER GLU ASN VAL ASN LYS SER GLU PRO HIS SER LEU GLU GLU SER ASP SER
ASP PHE GLU ILE LEU CYS ASP GLN ILE LEU PHE GLY ASN ALA LEU ASP ARG ILE LEU GLU GLU GLU GLU ASP ASN GLU LYS GLU ARG ASP THR GLN ARG GLN ARG GLN ASN ASP THR LYS SER SER SER ALA ASP THR PHE THR ILE SER GLY VAL SER THR ASN LYS GLU ASN GLU GLY PRO
GLU TYR PRO THR LYS ILE GLU LYS ASN GLN PHE ASN MET SER TYR LYS PRO SER GLU ASN MET SER GLY LEU SER SER PHE PRO ILE PHE GLU LYS GLU ASN THR LEU SER SER SER TYR LEU GLU GLU GLN LYS PRO LYS ARG ALA ALA L831 N836 SER PHE ASN LYS MET ASN LYS
GLN GLU GLY MET ARG ILE GLU LYS LYS ILE GLN ARG GLU GLN LEU GLN LYS LYS LYS ASN ASP ARG PRO SER PRO LEU LYS PRO ILE GLN HIS GLN GLU LEU ARG VAL ASN SER LEU PRO ASN ASP GLN GLY LYS PRO SER LEU SER LEU ASP PRO ARG ARG ASN ILE SER GLN PRO VAL ASN
SER LYS VAL GLU SER LEU LEU GLN GLY LEU LYS PHE LYS LYS GLU PRO ALA SER HIS TRP THR HIS GLU ARG GLY SER LEU PHE MET SER GLU HIS VAL GLU ASP GLU LYS PRO VAL LYS ALA SER ASP VAL SER ILE GLU GLU SER SER TYR THR THR VAL ALA THR SER SER
ARG ASP PRO SER VAL ALA GLU GLN SER SER THR ILE GLN LYS PRO MET LEU SER LEU PRO SER SER PHE LEU ASN THR SER MET THR PHE LYS ASN LEU SER GLN ILE LEU ALA ASP ASP GLY ASP ASP LYS HIS LEU SER VAL PRO GLN ASN GLN SER ARG SER VAL ALA HIS SER
PRO LEU ARG LYS GLN SER ALA LYS ILE SER LEU THR PRO ARG SER ASN LEU ASN ALA ASN LEU SER VAL LYS ARG ASN GLN GLY SER PRO GLY SER TYR LEU SER ASN ASP LEU ASP GLY ILE SER ASP MET THR PHE ALA MET GLU ILE PRO THR ASN THR PHE THR ALA GLN ALA ILE
GLN LEU MET ASN ASN ASP THR ASP ASN ASN LYS ILE ASN THR SER PRO LYS ALA SER SER PHE THR LYS GLU LYS VAL ILE LYS SER ALA ALA TYR ILE SER GLU LYS GLU PRO ASP ASN SER ASP THR ASN TYR ILE PRO ASP TYR THR ILE PRO PRO ASN THR TYR ASP GLU LYS ALA
ILE ASN ILE PHE GLU ASP ALA PRO SER ASP SER ARG ALA SER VAL HIS ARG LYS ALA VAL LEU THR PRO ALA THR ASN VAL ARG VAL SER LEU TYR TRP ASN ASN ASN SER SER
GLY ILE PRO ARG GLU THR THR GLU GLU ILE LEU SER LYS LEU ARG LEU SER PRO GLU ASN PRO SER ASN THR HIS MET GLN LYS ARG PHE SER SER THR ARG GLY SER ARG ASP SER ASN ALA LEU GLY ILE SER LEU THR LEU GLN SER MET PHE LYS ASP LEU GLU GLU GLU ASP GLN ASP
GLY HIS THR SER GLN ALA ASP ILE LEU GLU SER SER MET SER TYR SER LYS ARG ARG PRO SER GLU GLU SER VAL ASN PRO LYS GLN ARG VAL THR MET LEU PHE ASP GLU GLU GLU GLU SER LYS LYS VAL GLY GLY LYS ILE LYS GLU GLU GLU HIS THR LYS LEU ASP ASN LYS
ILE SER GLU GLU SER SER GLN LEU VAL LEU PRO VAL VAL GLU LYS LYS GLU ASN ALA ASN ASN THR GLU ASN ASN TYR SER LYS ILE PRO LYS PRO SER THR ILE LYS VAL THR LYS ASP THR ALA MET GLU SER ASN THR GLN THR HIS THR ILE LYS LYS PRO ILE LEU LYS VAL SER SER VAL GLN
ASN VAL GLU VAL GLU GLU SER SER ASP LYS LYS ASN TRP PHE VAL LYS LEU PHE GLN ASN PHE SER SER HIS ASN ASN ALA THR LYS ALA SER LYS ASN HIS VAL THR ASN ILE SER PHE ASP ASP ALA HIS MET LEU THR LEU ASN GLU PHE ASN LYS ASN SER ILE ASP TYR
GLN LEU LYS ASN LEU ASP HIS LYS PHE GLY ARG LYS VAL ASP CYS LYS PHE VAL LYS GLY ASN PHE LYS PHE LYS ILE LYS ILE THR SER THR PRO ASN ALA SER THR VAL ILE THR VAL LYS LYS ARG SER LYS HIS SER ASN THR SER SER ASN LYS ALA PHE GLU LYS
PHE ASN ASP ASP VAL GLU ARG VAL ILE ARG ASN ALA GLY ARG SER
• Molecule 8: Anaphase-promoting complex subunit 1
Chain C:
10%
56%
24%
19%
MET THR SER LYS PRO SER THR ARG ASN ASP TYR LEU PRO ARG GLU THR HIS ASN GLY GLU TYR THR GLY ASP SER PRO E27 I32 N33 I34 T35 I38 G39 S48 R49 D50 V54 I58 E59 R64 Y68 I72 A75 G76 Y77 I78 D79 F80 E81 K82 T83

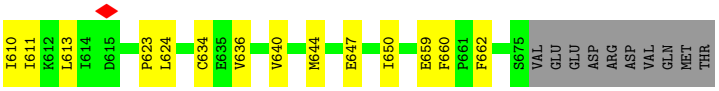

P84 D85 C86 F87 L91 A95 F110 I114 G115 F118 W119 Y120 A121 N122 E127 T130 S131 A132 S133 PHE MET ASP GLY GLY TYR ASP LEU K142 P143 I144 E145 F146 D147 L148 K149 H150 K151 Y152 I153 D157 P158 F162 S166 N169 THR PHE LYS GLY GLY
ILE ASN SER ALA SER GLY ASN LYS THR ASP ILE LEU GLN ASP F189 Q190 L191 F194 P195 S196 D197 I202 F205 K211 V212 L213 Y216 S222 S223 ASP GLN SER ARG LYS GLY GLU LEU THR ILE SER SER THR LYS LYS THR GLY LEU ASP ALA ALA GLY ASN SER GLN
LYS SER GLY GLY ILE SER LYS ASP LEU ARG LYS PHE SER HIS LEU THR ARG ARG ARG SER THR SER ILE ASN SER ASN SER HIS ASP PHE ASN ALA ALA GLU ARG VAL LEU SER GLY ASN VAL GLY ASN ALA SER GLY ARG THR ASP ILE PHE ALA LEU PRO SER SER CYS SER ARG ARG SER
LEU SER ALA THR LEU ASP ARG MET GLY ASN ASN ILE ALA PRO THR ASN ARG ALA ALA PRO SER GLY PHE PHE ASP SER SER SER ALA ASN THR ALA THR HIS SER ASN ILE THR PRO VAL SER GLN PRO MET GLN GLN GLN GLN GLU TYR LEU ASN GLN THR ALA THR SER S367
V371 I375 L380 P381 D382 D383 I384 I385 F386 T387 SER ARG R390 L391 S392 S393 I394 L395 L401 S402 L403 R404 E409 G410 L411 L412 H415 E416 P417 K422 I423 W424 L425 I426 D427 L428 L429 P430 D431 V432 L433 D434 I440 Y441 S444 P445 Q446 N447 M448 I449 R450 L451
L454 K455 L456 K457 E458 P459 S460 R461 I462 Q463 A464 M465 Y466 I467 H468 E469 L470 L471 E472 L475 I476 L477 V478 S479 E480 G481 Q482 N483 K484 E485 E486 Y487 K488 L491 P494 I498 T499 S500 P501 Y524 P525 E526 T527 T530 K531 N546 I550 F551 L552 W553
I559 L560 L561 N565 D566 D567 V568 V569 G570 E575 L585 L586 I587 L588 S592 S593 S594 A595 Q596 E597 Y598 E603 T604 Y605 E606 R607 D608 L609 F610 L613 K614 Q615 D616 L624 P625 R626 G630 I634 R635 E636 C644 E647 L655 M662 G663 W664
S670 K675 MET ASP SER GLU SER LYS THR PHE LEU HIS PRO ARG GLU GLN ASN SER T692 F693 L697 D698 E699 I703 S706 L707 T711 L718 I722 R726 L727 V728 A729 T730 D731 T732 Q733 V734 R737 R741 I745 L748 Y749 V752 H753 N756
F757 D760 Y761 V762 L763 L766 K770 V771 D774 E775 L776 Q777 T778 Y779 I783 L787 L791 E795 L798 S799 E800 V801 R802 D803 N804 L805 E806 L807 L808 D809 R810 A811 Q814 R815 I819 I820 N821 S822 I823 R824 S825 D826 SER LYS GLU VAL LEU LYS ARG
GLY GLN ARG ASP SER TYR MET LEU C842 K843 V844 P845 L846 A847 K848 N849 R850 S851 S852 LEU SER K855 K856 I860 Y861 S862 I863 I867 V868 K869 S872 GLN VAL PRO LEU ASP GLY SER ALA MET ARG MET SER ASN ILE GLN ASP ASP GLU ASP ILE D893 R896 G903 L904
S907 E908 L918 L919 T925 K926 T927 Q928 F929 F930 T934 A937 Q938 Q942 F946 M950 A951 L952 R953 T956 V959 G960 W961 T968 E969 I972 S973 T974 Q975 I979 S986 V987 F988 P989 D990 D991 T992 K993 K997 E1000 D1001 V1007
Q1011 V1016 S1017 L1020 S1032 K1038 P1039 K1040 D1043 F1049 L1050 L1051 N1061 L1062 E1063 E1064 W1065 H1066 I1067 Y1068 N1069 Y1070 L1071 S1072 P1073 G1081 L1082 M1086 S1096 K1097 L1098 I1099 K1100 V1101 I1102 H1105 L1106 F1109 L1110 G1113 L1117 K1122 T1125
I1128 I1129 M1133 L1134 Y1135 L1136 R1139 R1142 I1147 Q1150 L1154 L1155 D1159 E1160 M1161 V1162 A1163 D1164 E1165 E1166 Y1167 R1168 L1169 I1173 S1174 L1177 I1178 G1181 A1182 G1183 Q1184 T1185 K1186 LEU ARG LYS TRP ASP SER SER LEU LEU GLY LEU GLY ASP ASP LEU PRO GLU
ASP VAL TYR ASP SER SER ASP V1211 E1212 Q1213 M1216 L1224 L1225 E1226 I1227 V1228 T1229 Y1232 D1233 V1234 E1235 N1236 D1237 W1238 N1242 S1243 Q1244 I1245 G1246 A1247 V1248 I1251 M1252 F1253 L1254 K1257 N1260 I1263 M1266 V1269 D1270 L1271 I1274 A1277 N1278 I1279 L1285



• Molecule 9: Anaphase-promoting complex subunit 5

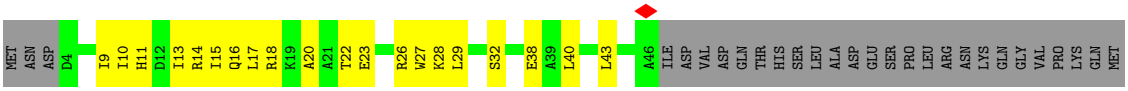
Chain O:

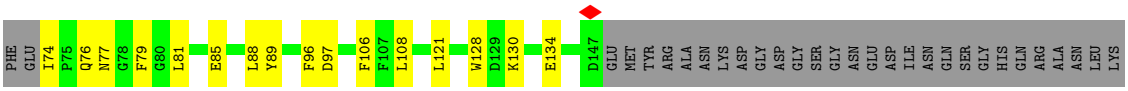


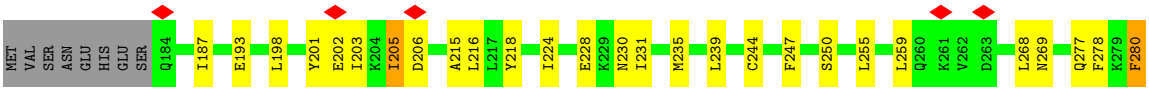


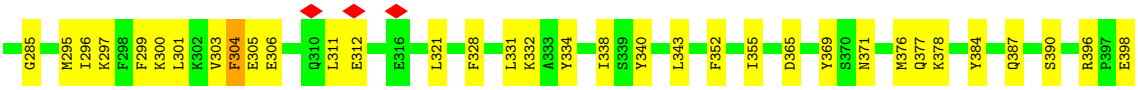
• Molecule 10: Anaphase-promoting complex subunit CDC23

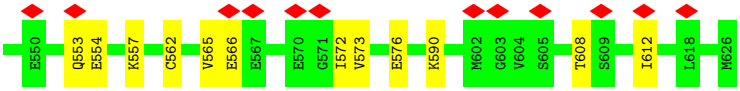
Chain D:





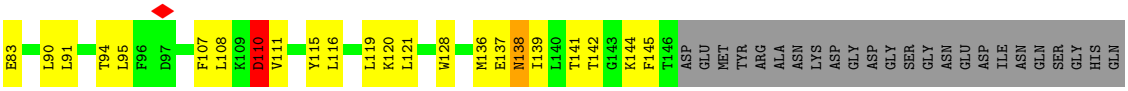


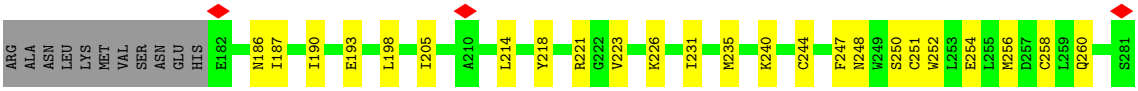


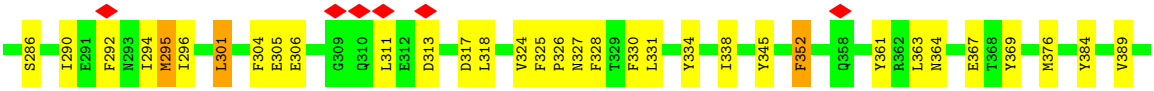


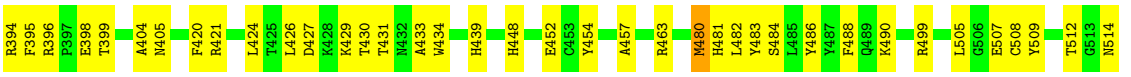
• Molecule 10: Anaphase-promoting complex subunit CDC23

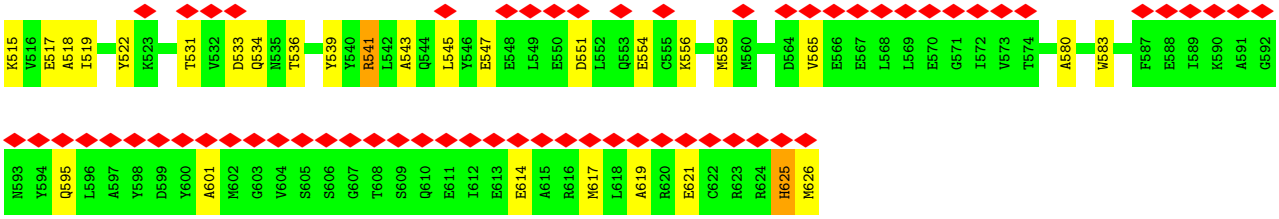
Chain P:





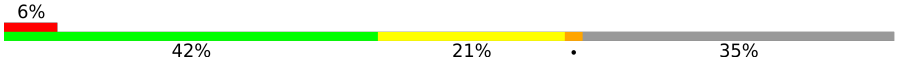


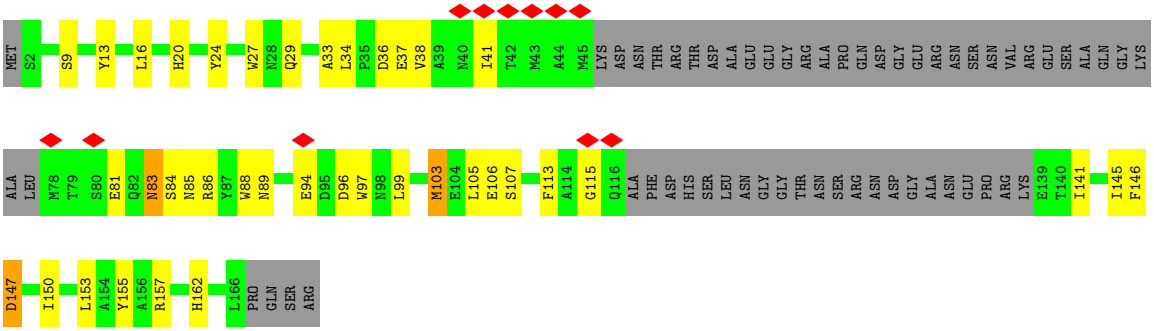




• Molecule 11: Anaphase-promoting complex subunit SWM1

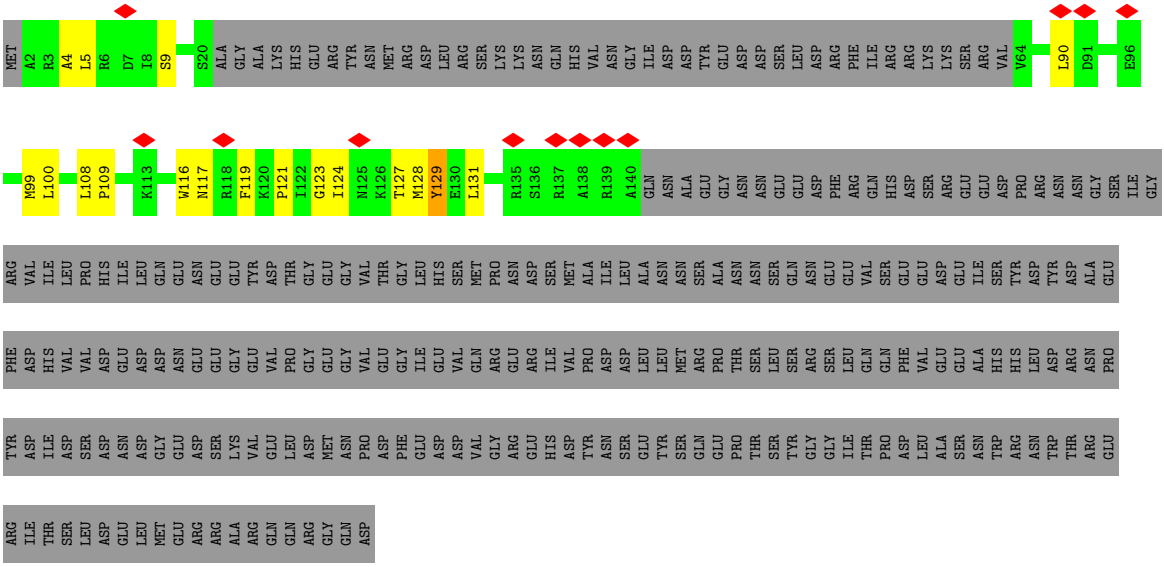
Chain I:





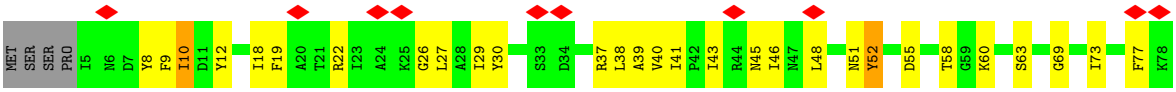
• Molecule 12: Anaphase-promoting complex subunit MND2

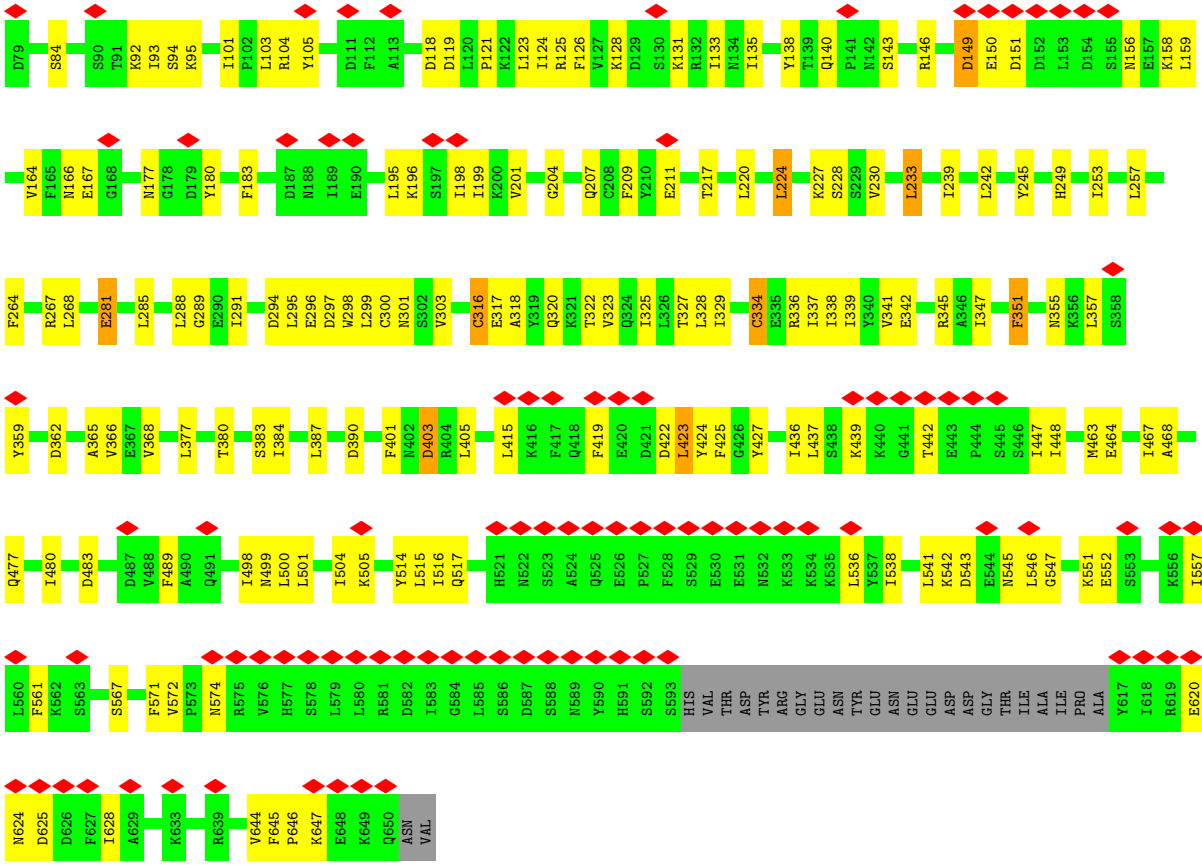
Chain N:



• Molecule 13: Anaphase-promoting complex subunit 4

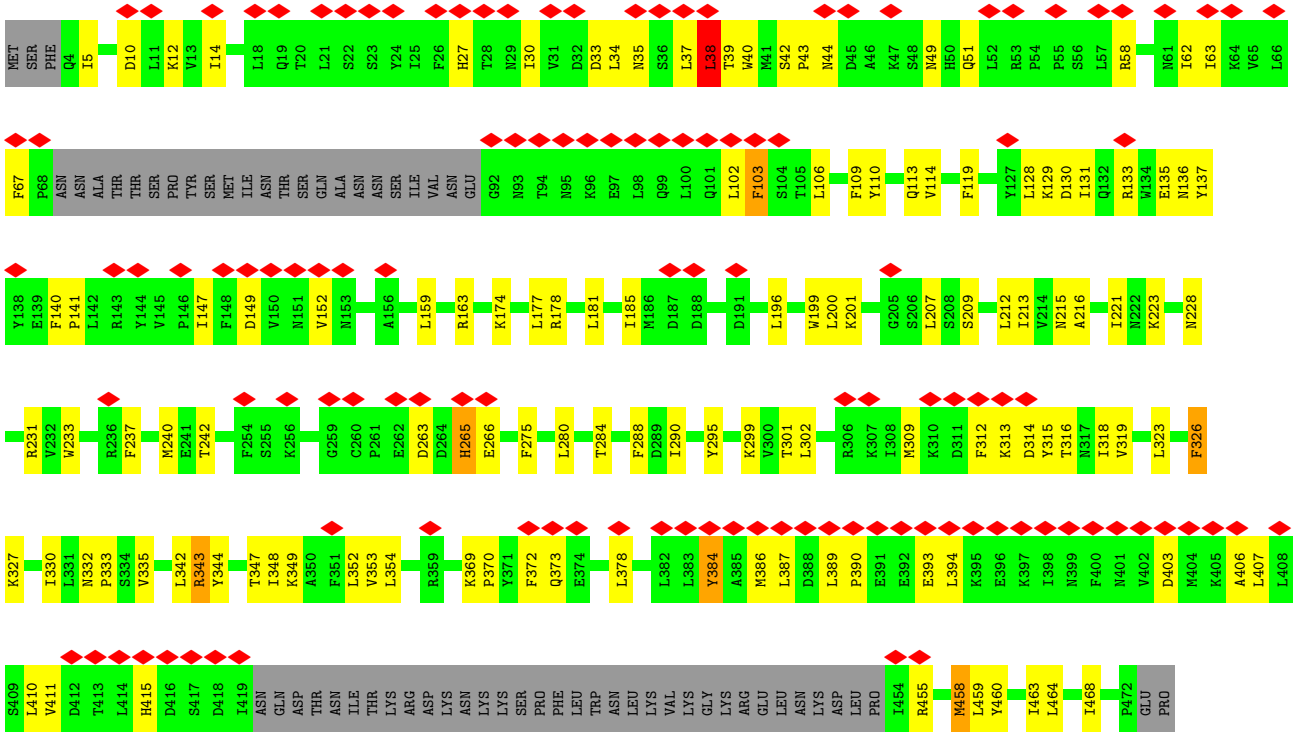
Chain Q:

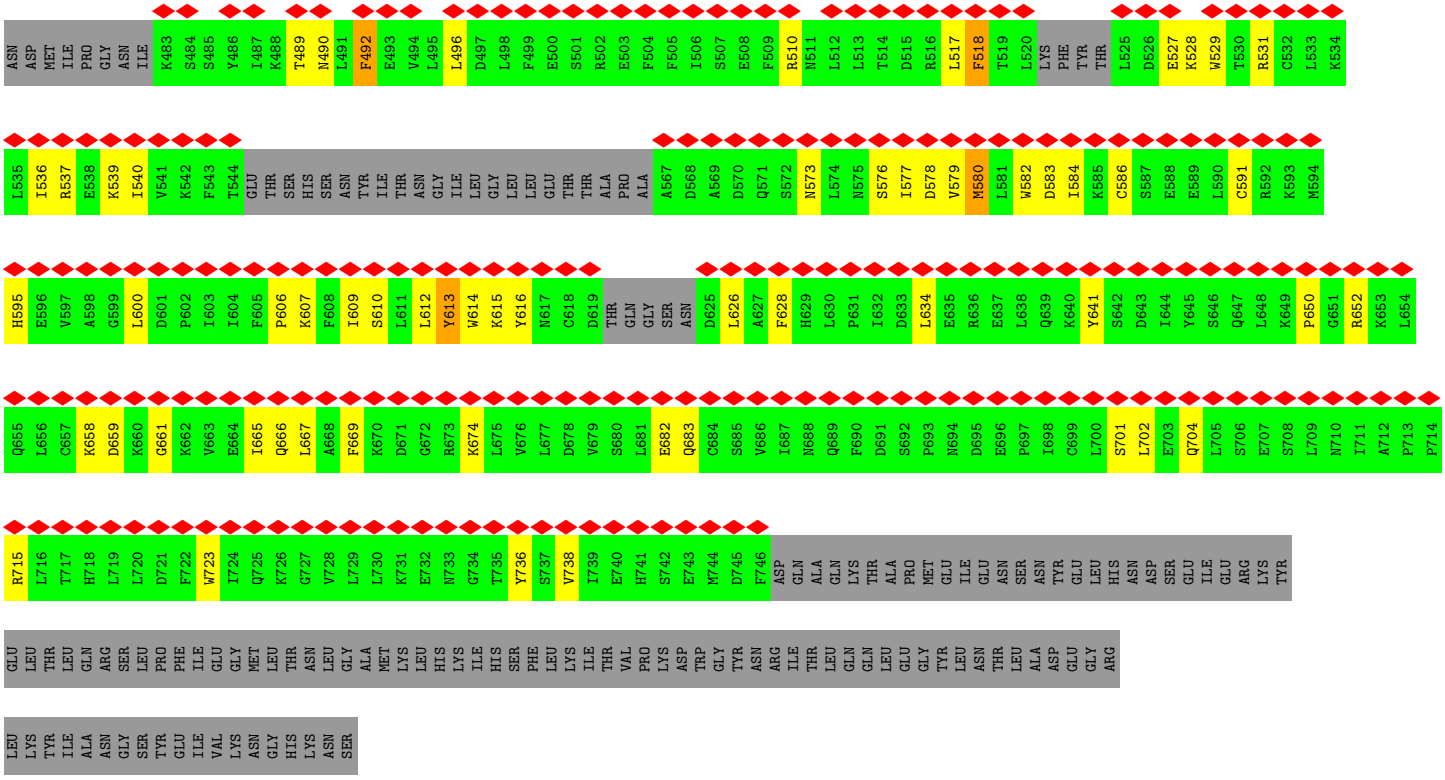




• Molecule 14: Anaphase-promoting complex subunit 2

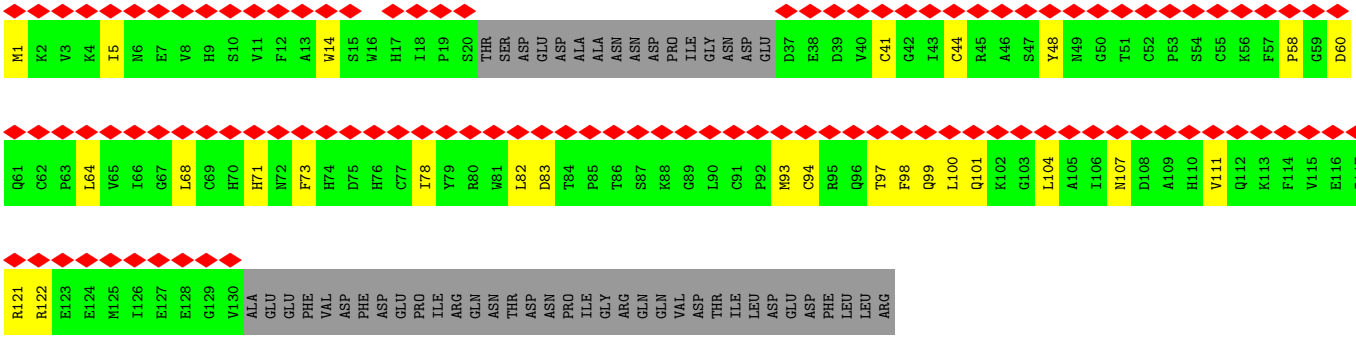
Chain T:





- Molecule 15: Anaphase-promoting complex subunit 11

Chain U:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	249193	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	59	Depositor
Minimum defocus (nm)	1600	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.287	Depositor
Minimum map value	-0.161	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.05	Depositor
Map size (Å)	353.28, 353.28, 353.28	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.38, 1.38, 1.38	Depositor

5 Model quality

5.1 Standard geometry

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	F	0.27	0/4079	0.53	1/5525 (0.0%)
1	H	0.27	0/4118	0.50	0/5574
2	J	0.28	0/4214	0.51	0/5692
2	K	0.30	0/4188	0.52	0/5657
3	G	0.28	0/285	0.68	0/384
3	W	0.25	0/301	0.59	0/405
4	E	0.75	1/1108 (0.1%)	0.73	2/1481 (0.1%)
5	A	0.25	0/1785	0.55	1/2418 (0.0%)
6	B	0.27	0/3487	0.53	0/4730
7	S	0.21	0/44	0.39	0/59
8	C	0.26	0/11088	0.50	3/15080 (0.0%)
9	O	0.27	0/5387	0.47	0/7291
10	D	0.26	0/4621	0.44	0/6243
10	P	0.28	0/4616	0.50	2/6228 (0.0%)
11	I	0.29	0/930	0.64	1/1263 (0.1%)
12	N	0.28	0/800	0.55	0/1076
13	Q	0.25	0/5190	0.49	0/7020
14	T	0.32	2/5455 (0.0%)	0.61	5/7387 (0.1%)
15	U	0.25	0/936	0.49	0/1265
All	All	0.29	3/62632 (0.0%)	0.52	15/84778 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	H	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	95	PRO	N-CD	23.35	1.80	1.47
14	T	650	PRO	CB-CG	-11.48	0.92	1.50
14	T	650	PRO	CG-CD	-6.54	1.29	1.50

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	T	650	PRO	CB-CG-CD	18.83	179.94	106.50
14	T	650	PRO	N-CD-CG	-18.79	75.01	103.20
4	E	95	PRO	CA-N-CD	-16.35	88.61	111.50
14	T	650	PRO	CA-CB-CG	-15.95	73.70	104.00
14	T	650	PRO	CA-N-CD	-9.06	98.81	111.50

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	H	635	ARG	Sidechain

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	F	3991	0	3947	171	0
1	H	4031	0	4003	204	0
2	J	4128	0	4096	176	0
2	K	4102	0	4065	230	0
3	G	284	0	293	20	0
3	W	300	0	313	17	0
4	E	1091	0	1058	67	0
5	A	1743	0	1714	82	0
6	B	3418	0	3307	184	0
7	S	45	0	43	1	0
8	C	10863	0	10672	373	0
9	O	5288	0	5299	176	0
10	D	4524	0	4391	132	0
10	P	4518	0	4410	189	0
11	I	906	0	813	61	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	N	784	0	784	20	0
13	Q	5083	0	5093	155	0
14	T	5337	0	5314	226	0
15	U	912	0	873	28	0
16	U	3	0	0	0	0
All	All	61351	0	60488	2228	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 18.

The worst 5 of 2228 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)
9:O:431:LEU:HD13	9:O:472:TYR:CZ	1.16	1.65
6:B:190:ARG:HB2	11:I:97:TRP:CZ3	1.32	1.62
10:P:27:TRP:CH2	10:P:115:TYR:CE1	1.85	1.61
9:O:170:TRP:CZ3	9:O:174:GLN:HG3	1.32	1.61
10:P:301:LEU:HD22	10:P:334:TYR:CE2	1.33	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	F	496/758 (65%)	475 (96%)	21 (4%)	0	100	100
1	H	499/758 (66%)	481 (96%)	16 (3%)	2 (0%)	34	72
2	J	505/850 (59%)	487 (96%)	18 (4%)	0	100	100
2	K	501/850 (59%)	488 (97%)	13 (3%)	0	100	100
3	G	33/124 (27%)	32 (97%)	1 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	W	35/124 (28%)	35 (100%)	0	0	100	100
4	E	120/265 (45%)	119 (99%)	1 (1%)	0	100	100
5	A	213/250 (85%)	201 (94%)	11 (5%)	1 (0%)	29	68
6	B	432/566 (76%)	404 (94%)	27 (6%)	1 (0%)	47	81
7	S	4/1518 (0%)	3 (75%)	1 (25%)	0	100	100
8	C	1384/1748 (79%)	1299 (94%)	81 (6%)	4 (0%)	41	75
9	O	654/685 (96%)	625 (96%)	25 (4%)	4 (1%)	25	64
10	D	554/626 (88%)	540 (98%)	13 (2%)	1 (0%)	47	81
10	P	550/626 (88%)	530 (96%)	20 (4%)	0	100	100
11	I	105/170 (62%)	98 (93%)	7 (7%)	0	100	100
12	N	92/368 (25%)	89 (97%)	3 (3%)	0	100	100
13	Q	619/652 (95%)	596 (96%)	22 (4%)	1 (0%)	47	81
14	T	631/853 (74%)	620 (98%)	11 (2%)	0	100	100
15	U	110/165 (67%)	107 (97%)	3 (3%)	0	100	100
All	All	7537/11956 (63%)	7229 (96%)	294 (4%)	14 (0%)	50	81

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	C	844	VAL
8	C	1279	ILE
9	O	193	VAL
10	D	205	ILE
1	H	507	LYS

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	F	433/684 (63%)	429 (99%)	4 (1%)	78	90
1	H	439/684 (64%)	428 (98%)	11 (2%)	47	75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	J	451/760 (59%)	443 (98%)	8 (2%)	59 81
2	K	448/760 (59%)	434 (97%)	14 (3%)	40 70
3	G	34/115 (30%)	33 (97%)	1 (3%)	42 71
3	W	36/115 (31%)	35 (97%)	1 (3%)	43 72
4	E	123/246 (50%)	120 (98%)	3 (2%)	49 76
5	A	190/226 (84%)	185 (97%)	5 (3%)	46 74
6	B	375/503 (75%)	362 (96%)	13 (4%)	36 67
7	S	6/1389 (0%)	6 (100%)	0	100 100
8	C	1180/1568 (75%)	1161 (98%)	19 (2%)	62 83
9	O	598/643 (93%)	583 (98%)	15 (2%)	47 75
10	D	477/560 (85%)	473 (99%)	4 (1%)	81 91
10	P	476/560 (85%)	464 (98%)	12 (2%)	47 75
11	I	95/144 (66%)	91 (96%)	4 (4%)	30 63
12	N	83/332 (25%)	82 (99%)	1 (1%)	71 87
13	Q	571/598 (96%)	555 (97%)	16 (3%)	43 72
14	T	605/804 (75%)	589 (97%)	16 (3%)	46 74
15	U	103/149 (69%)	103 (100%)	0	100 100
All	All	6723/10840 (62%)	6576 (98%)	147 (2%)	54 78

5 of 147 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
13	Q	52	TYR
14	T	492	PHE
13	Q	281	GLU
13	Q	546	LEU
6	B	222	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 27 such sidechains are listed below:

Mol	Chain	Res	Type
8	C	1543	HIS
10	D	77	ASN
13	Q	355	ASN
9	O	372	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
10	D	371	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

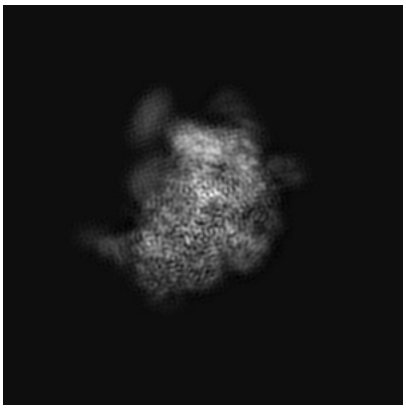
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-15123. These allow visual inspection of the internal detail of the map and identification of artifacts.

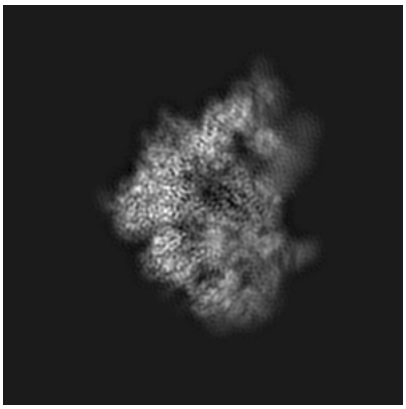
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

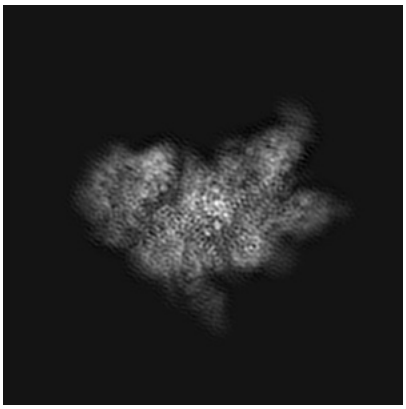
6.1.1 Primary map



X

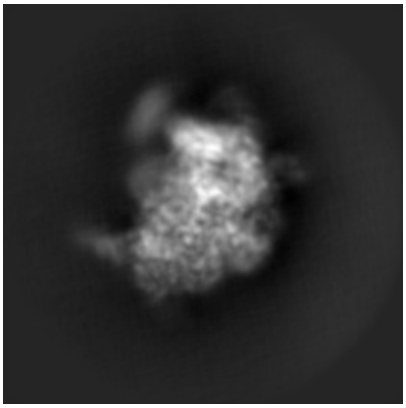


Y

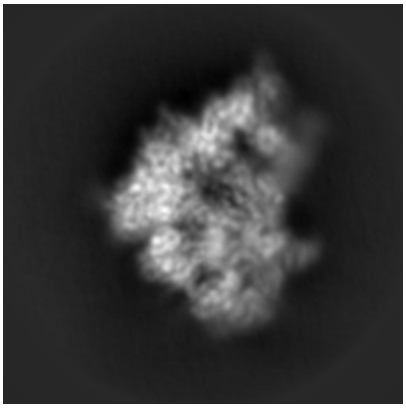


Z

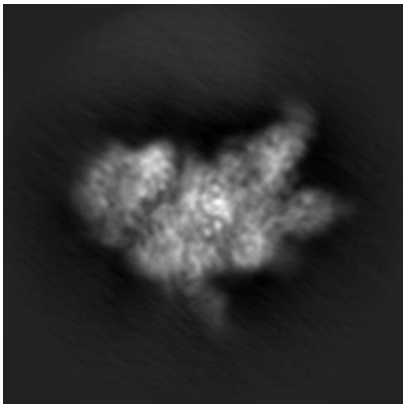
6.1.2 Raw map



X



Y

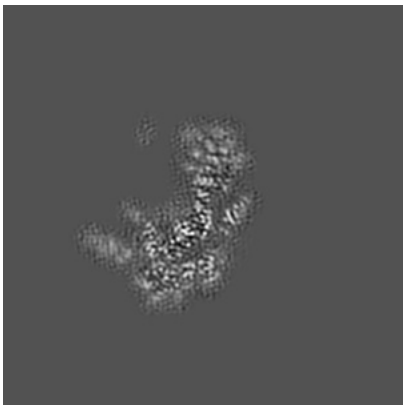


Z

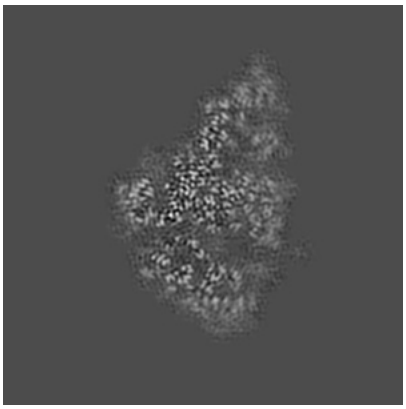
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

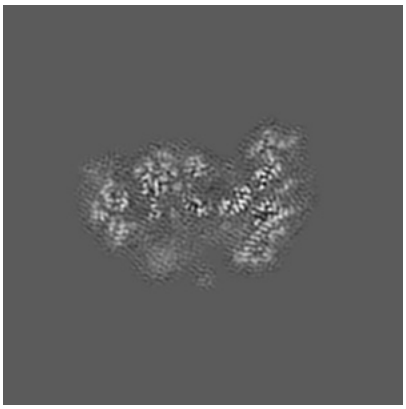
6.2.1 Primary map



X Index: 128

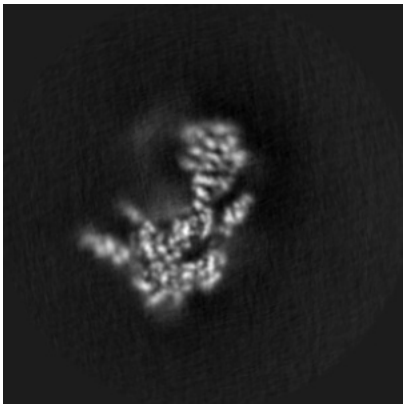


Y Index: 128

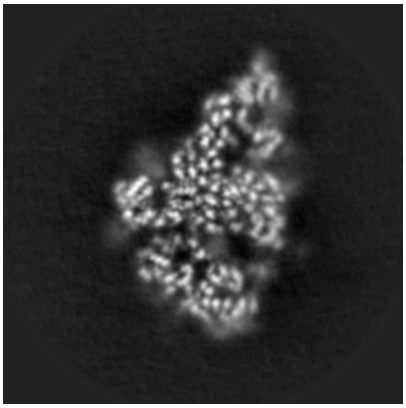


Z Index: 128

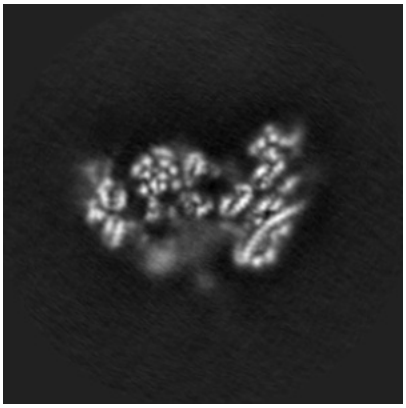
6.2.2 Raw map



X Index: 128



Y Index: 128

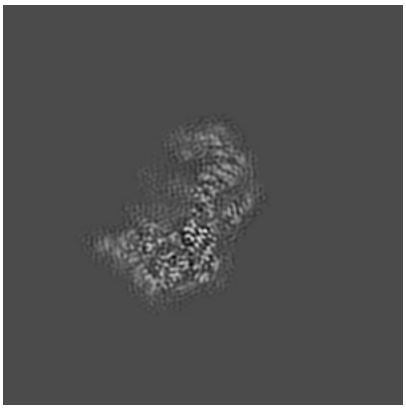


Z Index: 128

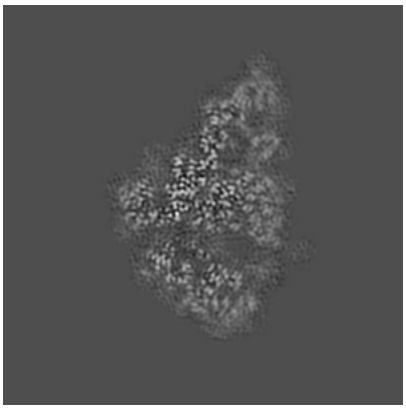
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

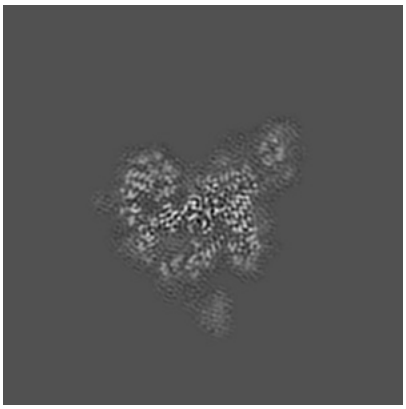
6.3.1 Primary map



X Index: 122

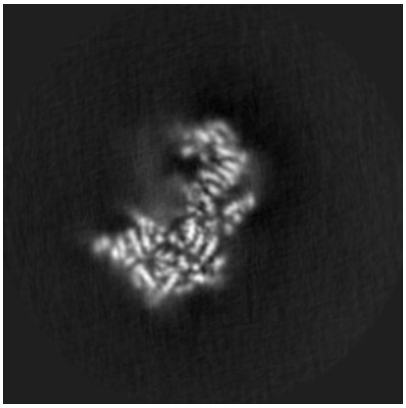


Y Index: 129

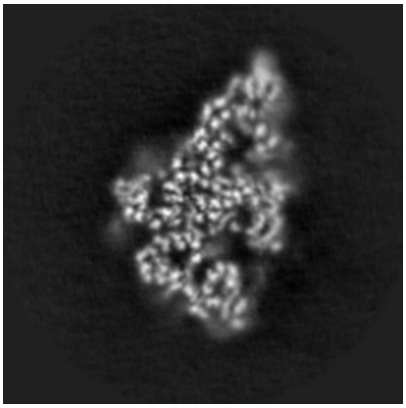


Z Index: 111

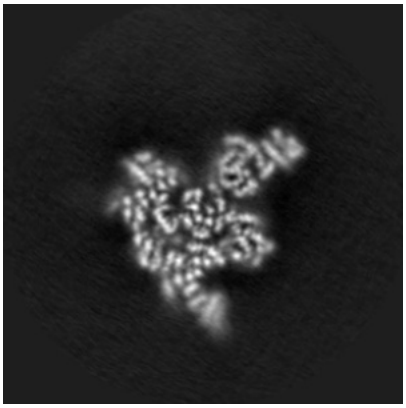
6.3.2 Raw map



X Index: 123



Y Index: 125



Z Index: 104

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

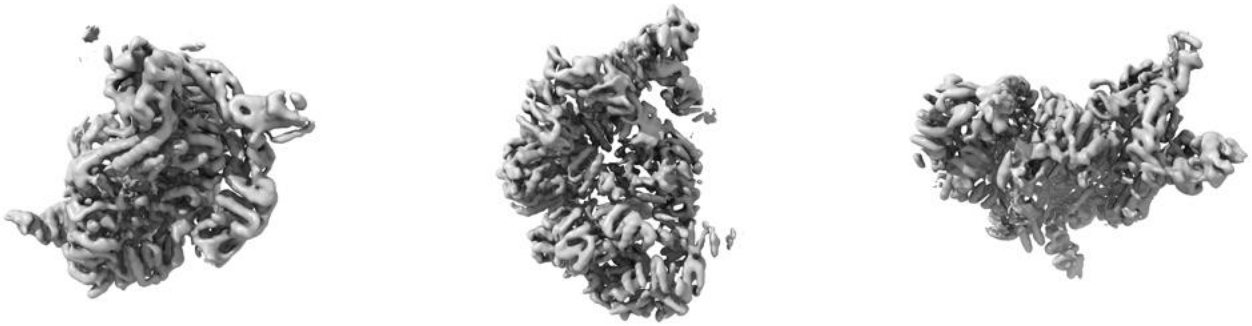
6.4 Orthogonal surface views (i)

6.4.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.05. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map



X Y Z

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

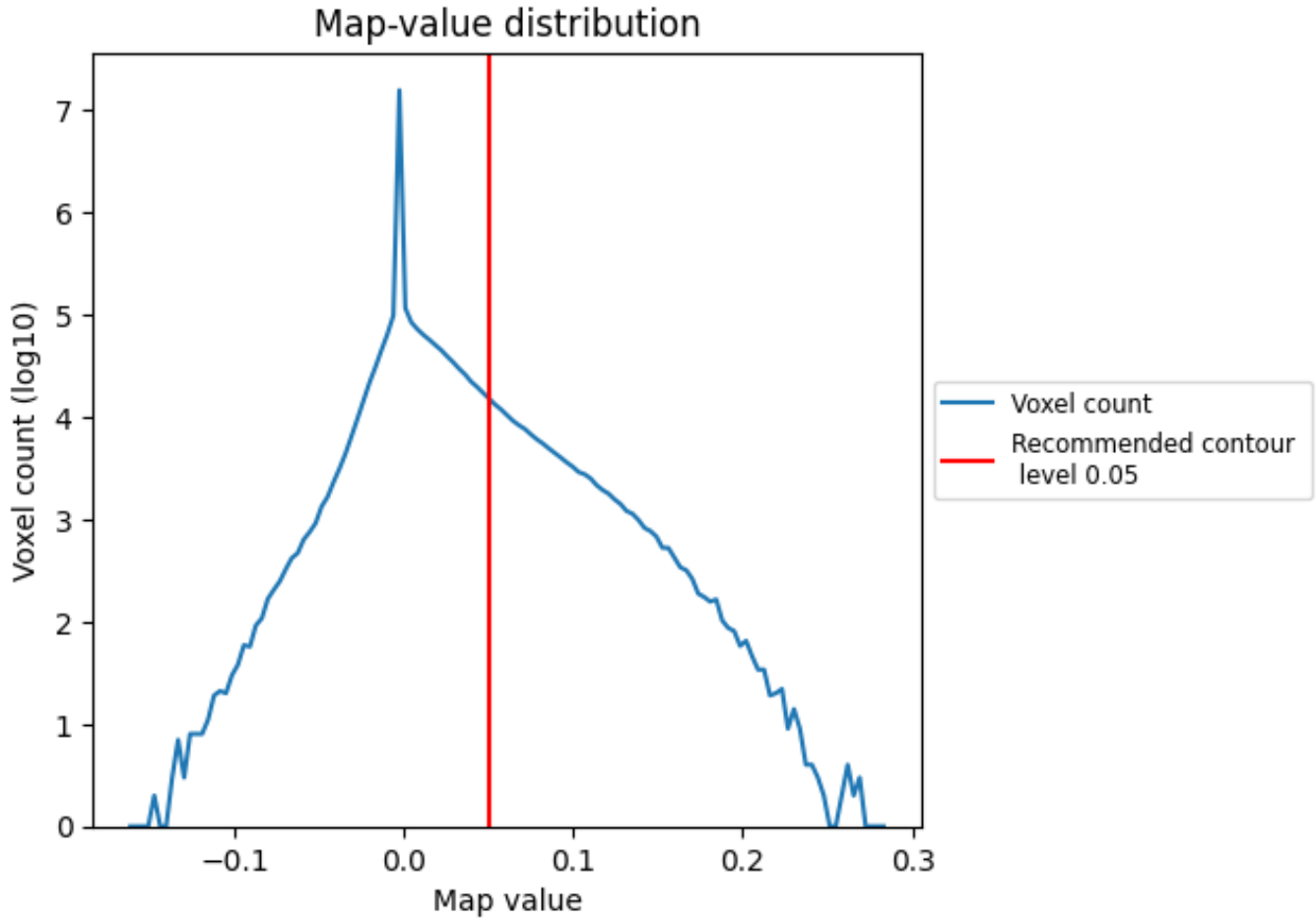
6.5 Mask visualisation (i)

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

7 Map analysis

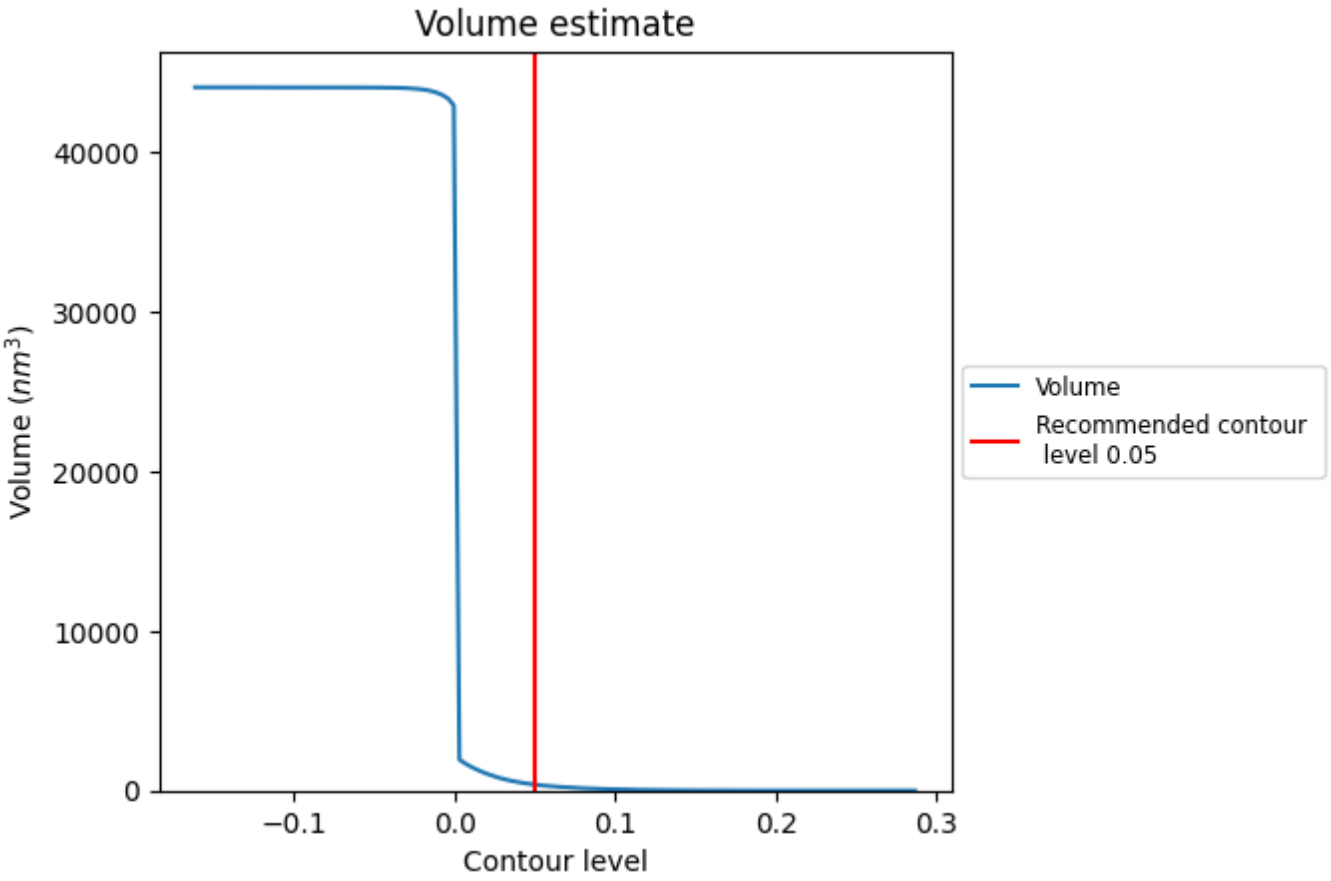
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

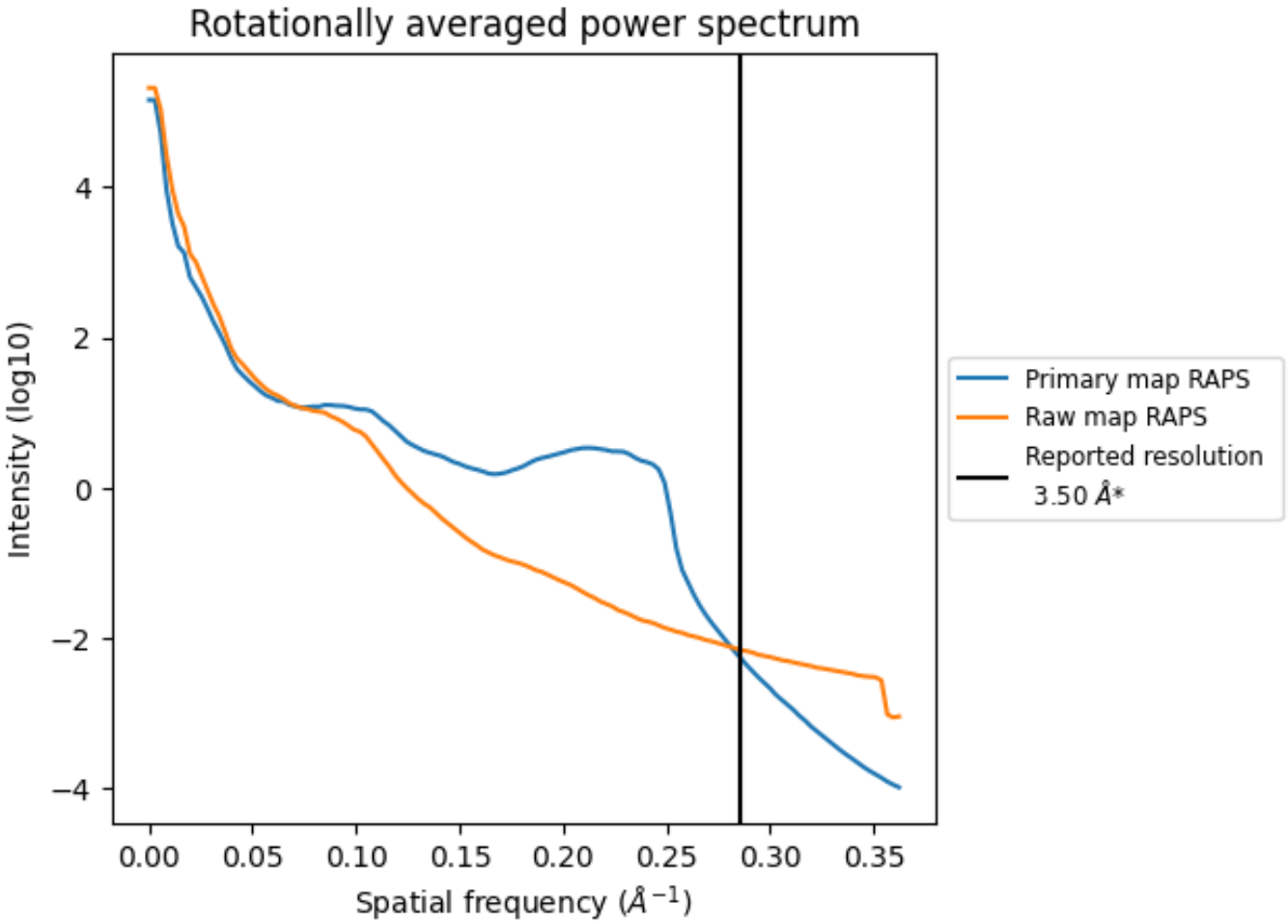
7.2 Volume estimate (i)



The volume at the recommended contour level is 376 nm^3; this corresponds to an approximate mass of 339 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)

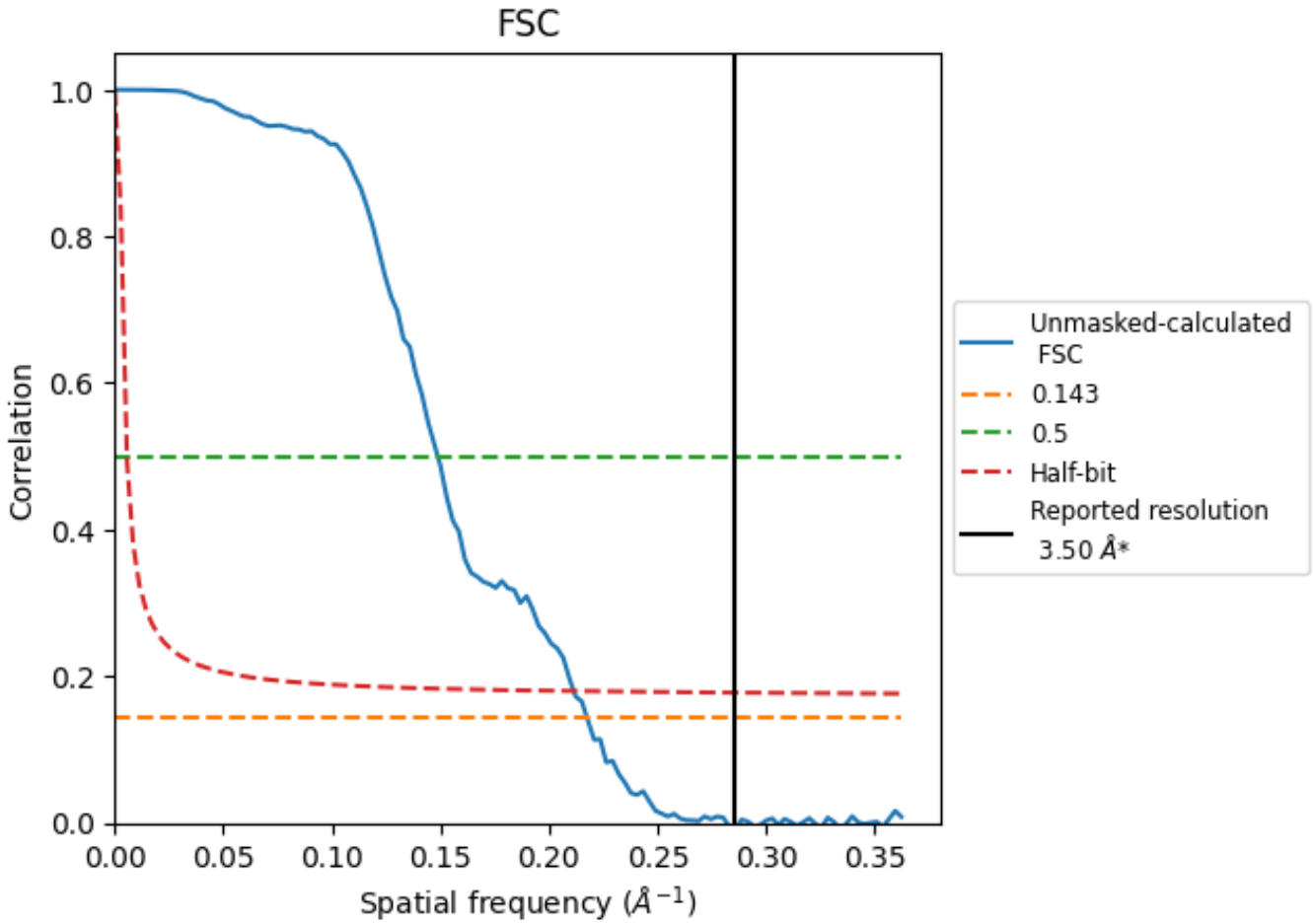


*Reported resolution corresponds to spatial frequency of 0.286 Å^{-1}

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.286 Å^{-1}

8.2 Resolution estimates (i)

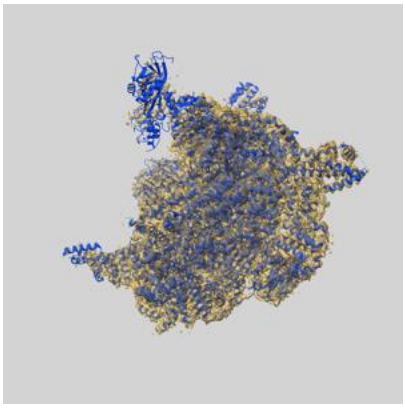
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.60	6.72	4.73

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.60 differs from the reported value 3.5 by more than 10 %

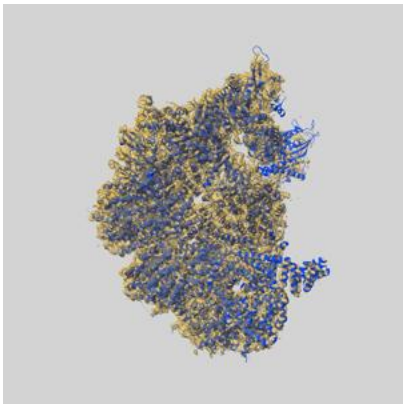
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-15123 and PDB model 8A3T. Per-residue inclusion information can be found in section 3 on page 8.

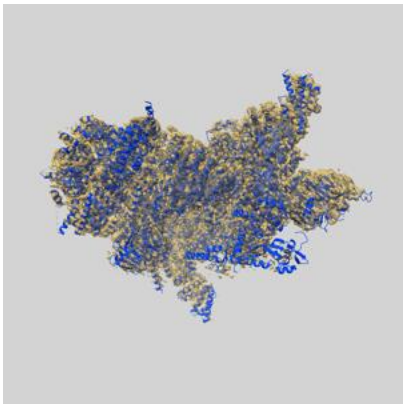
9.1 Map-model overlay



X



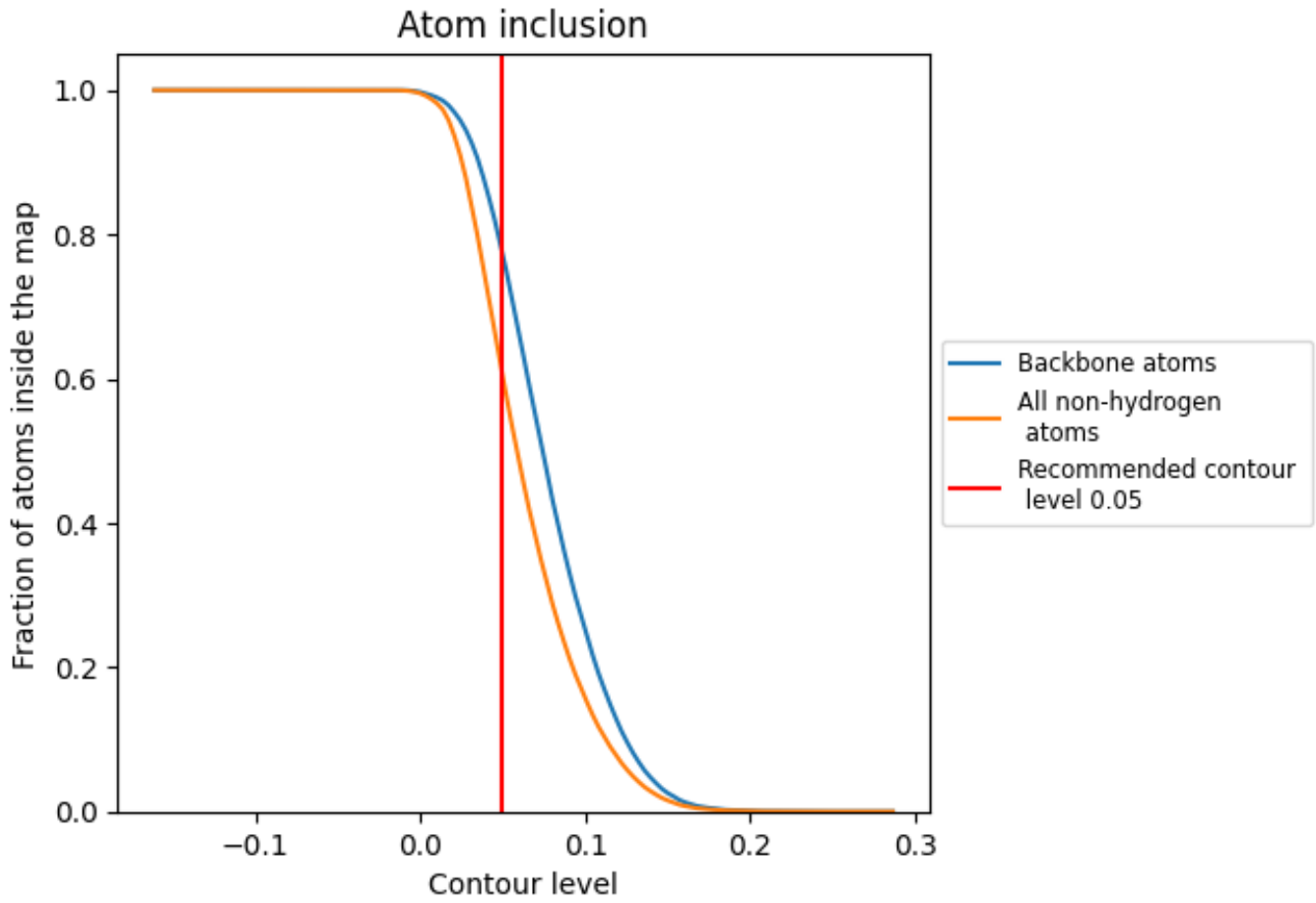
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.05 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 Atom inclusion (i)



At the recommended contour level, 77% of all backbone atoms, 60% of all non-hydrogen atoms, are inside the map.