



wwPDB EM Validation Summary Report ⓘ

Aug 22, 2022 – 04:12 pm BST

PDB ID : 8A5Y
EMDB ID : EMD-15199
Title : S. cerevisiae apo unphosphorylated APC/C
Authors : Barford, D.; Fernandez-Vazquez, E.; Zhang, Z.; Yang, J.
Deposited on : 2022-06-16
Resolution : 4.90 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

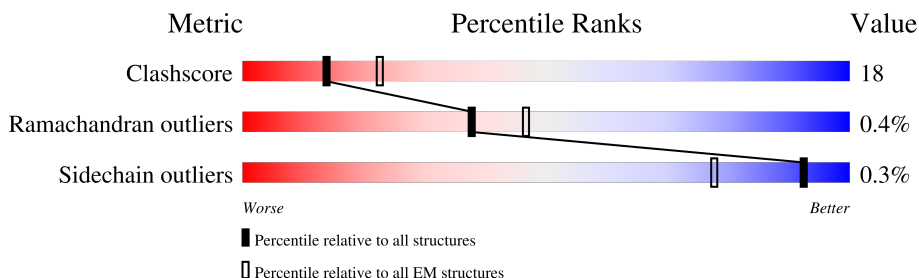
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.90 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 $\leq 5\%$. 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	
1	H	758	
2	J	850	
2	K	850	
3	G	124	
3	W	124	
4	E	265	
5	T	853	

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Mol	Chain	Length	Quality of chain
6	U	165	
7	C	1748	
8	O	685	
9	D	626	
9	P	626	
10	I	170	
11	N	368	
12	Q	652	
13	A	250	

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 57866 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
			4038	2599	664	748	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
			4124	2658	674	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	35	Total	C	N	O	S	0	0
			284	174	51	58	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 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	T	650	Total	C	N	O	S	0	0
			5362	3476	877	985	24		

- Molecule 6 is a protein called Anaphase-promoting complex subunit 11.

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

- Molecule 7 is a protein called Anaphase-promoting complex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	C	1406	Total	C	N	O	S	0	0
			10832	7003	1749	2034	46		

- Molecule 8 is a protein called Anaphase-promoting complex subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	O	658	Total	C	N	O	S	0	0
			5285	3399	869	990	27		

- Molecule 9 is a protein called Anaphase-promoting complex subunit CDC23.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	D	560	Total	C	N	O	S	0	0
			4524	2925	729	844	26		
9	P	556	Total	C	N	O	S	0	0
			4520	2923	738	832	27		

- Molecule 10 is a protein called Anaphase-promoting complex subunit SWM1.

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

- Molecule 11 is a protein called Anaphase-promoting complex subunit MND2.

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

- Molecule 12 is a protein called Anaphase-promoting complex subunit 4.

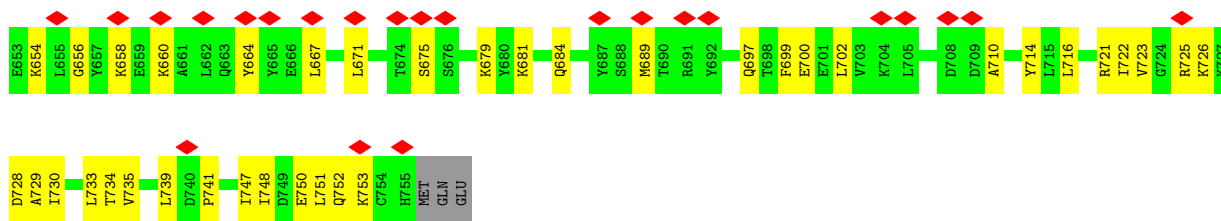
Mol	Chain	Residues	Atoms					AltConf	Trace
12	Q	623	Total	C	N	O	S	0	0
			5086	3279	842	952	13		

- Molecule 13 is a protein called Anaphase-promoting complex subunit DOC1.

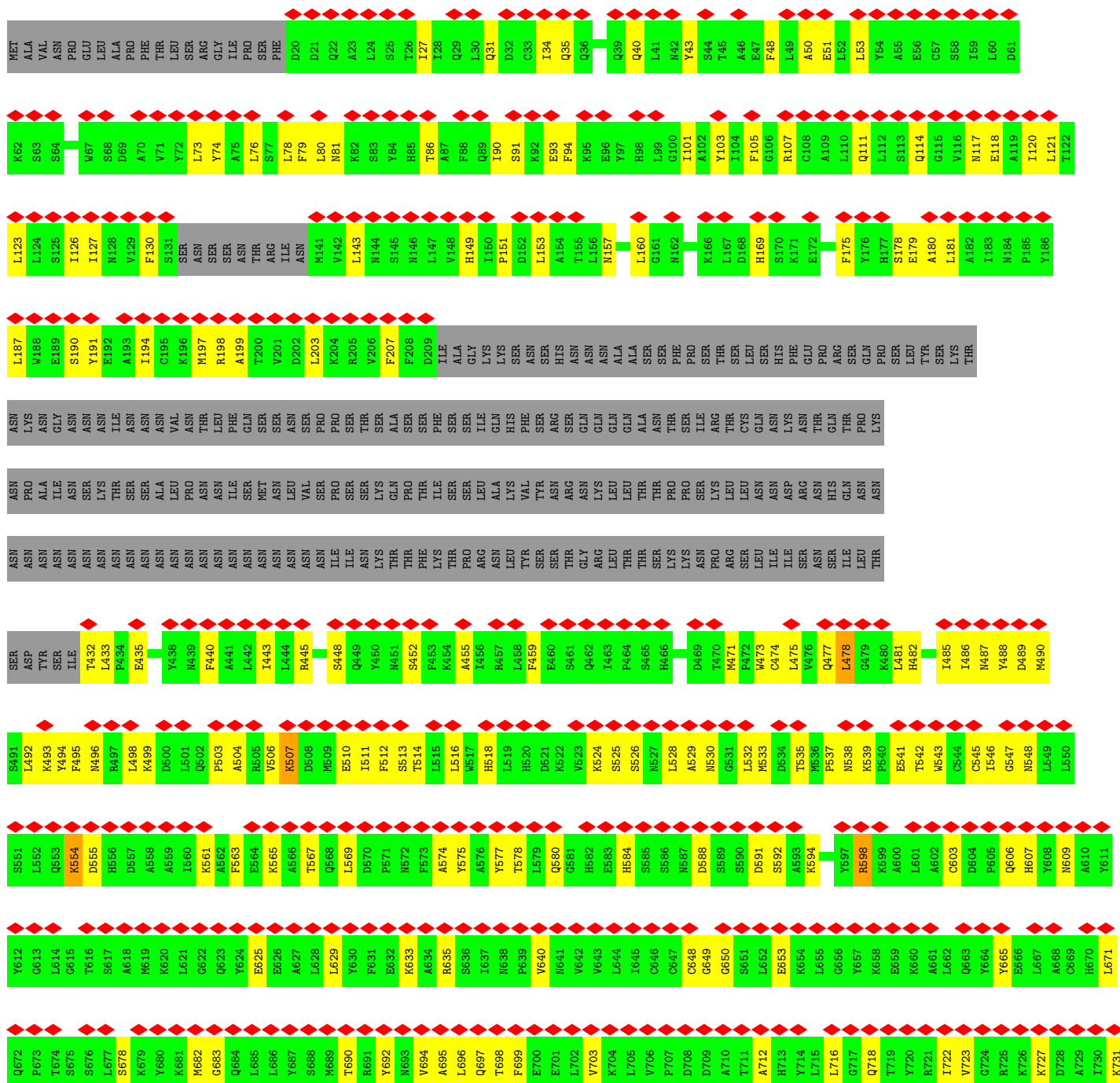
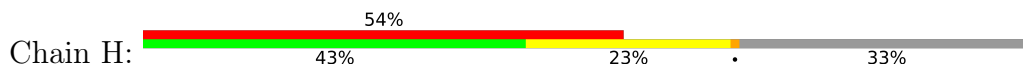
Mol	Chain	Residues	Atoms					AltConf	Trace
13	A	218	Total	C	N	O	S	0	0
			1738	1113	303	312	10		

- Molecule 14 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

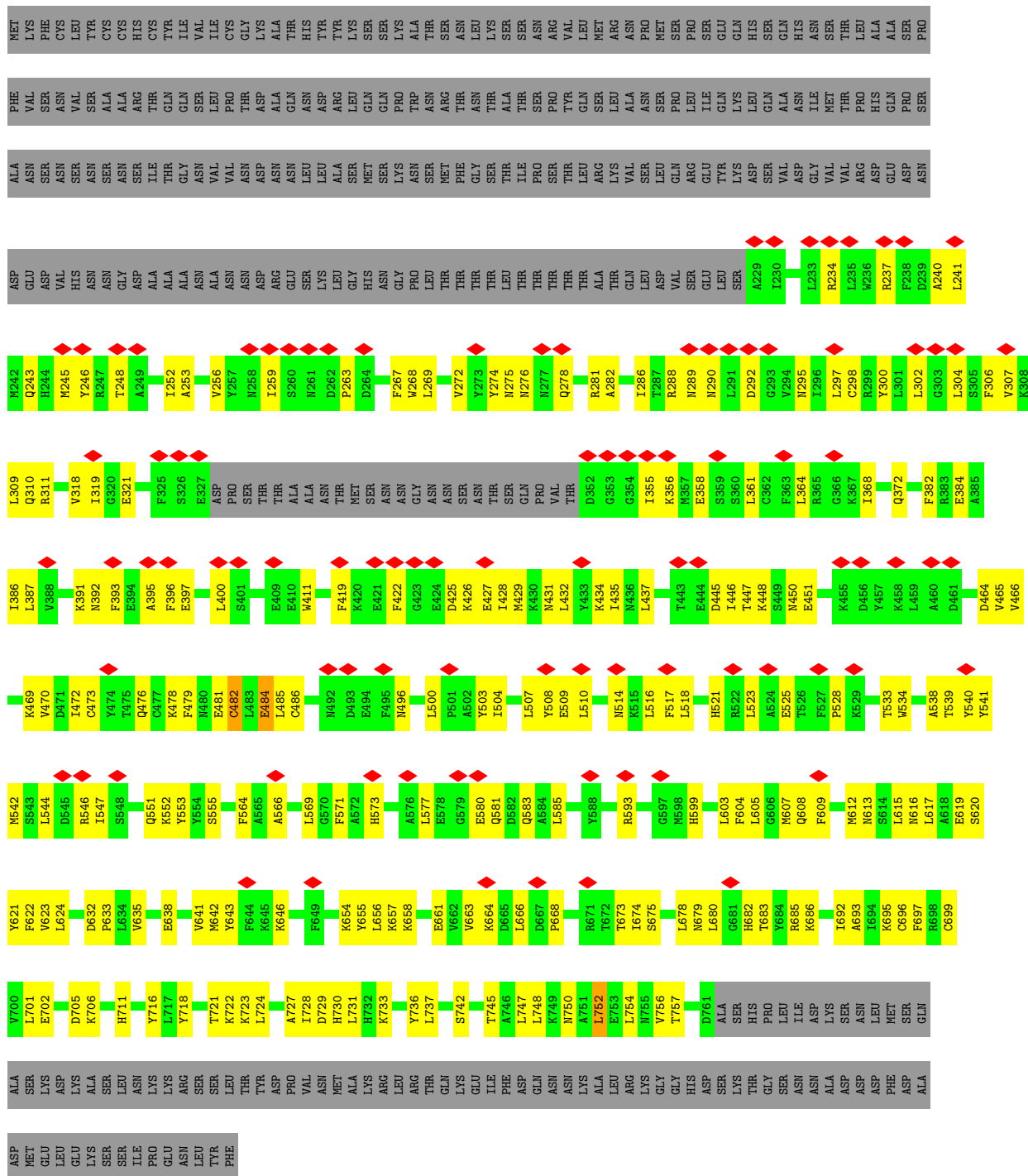
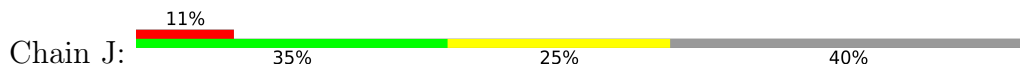


• Molecule 1: Anaphase-promoting complex subunit CDC27

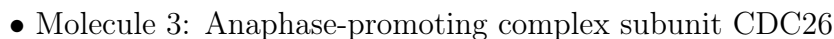


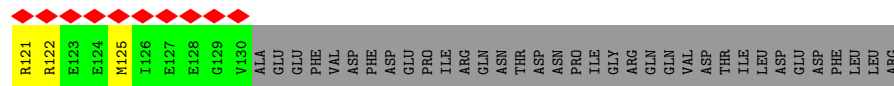


• Molecule 2: Anaphase-promoting complex subunit CDC16

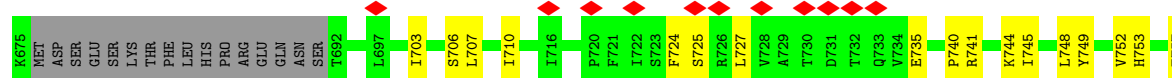
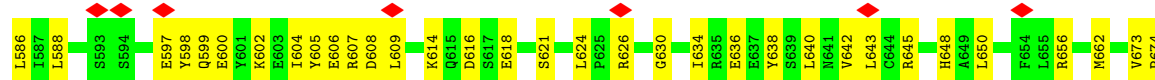
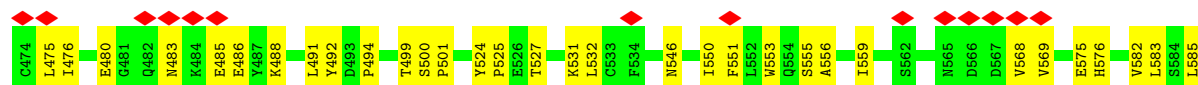
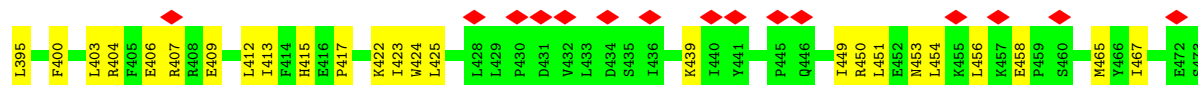
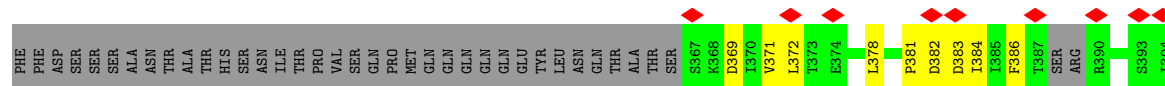
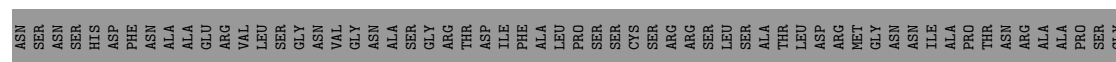
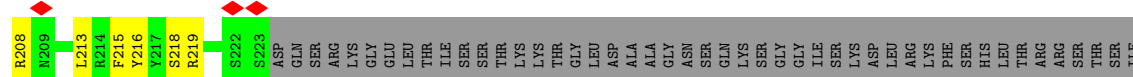
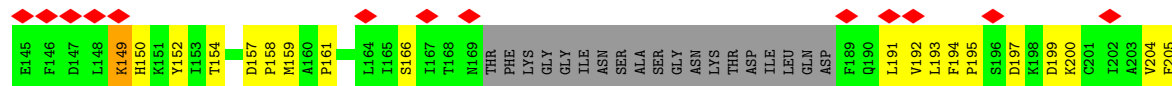


• Molecule 2: Anaphase-promoting complex subunit CDC16





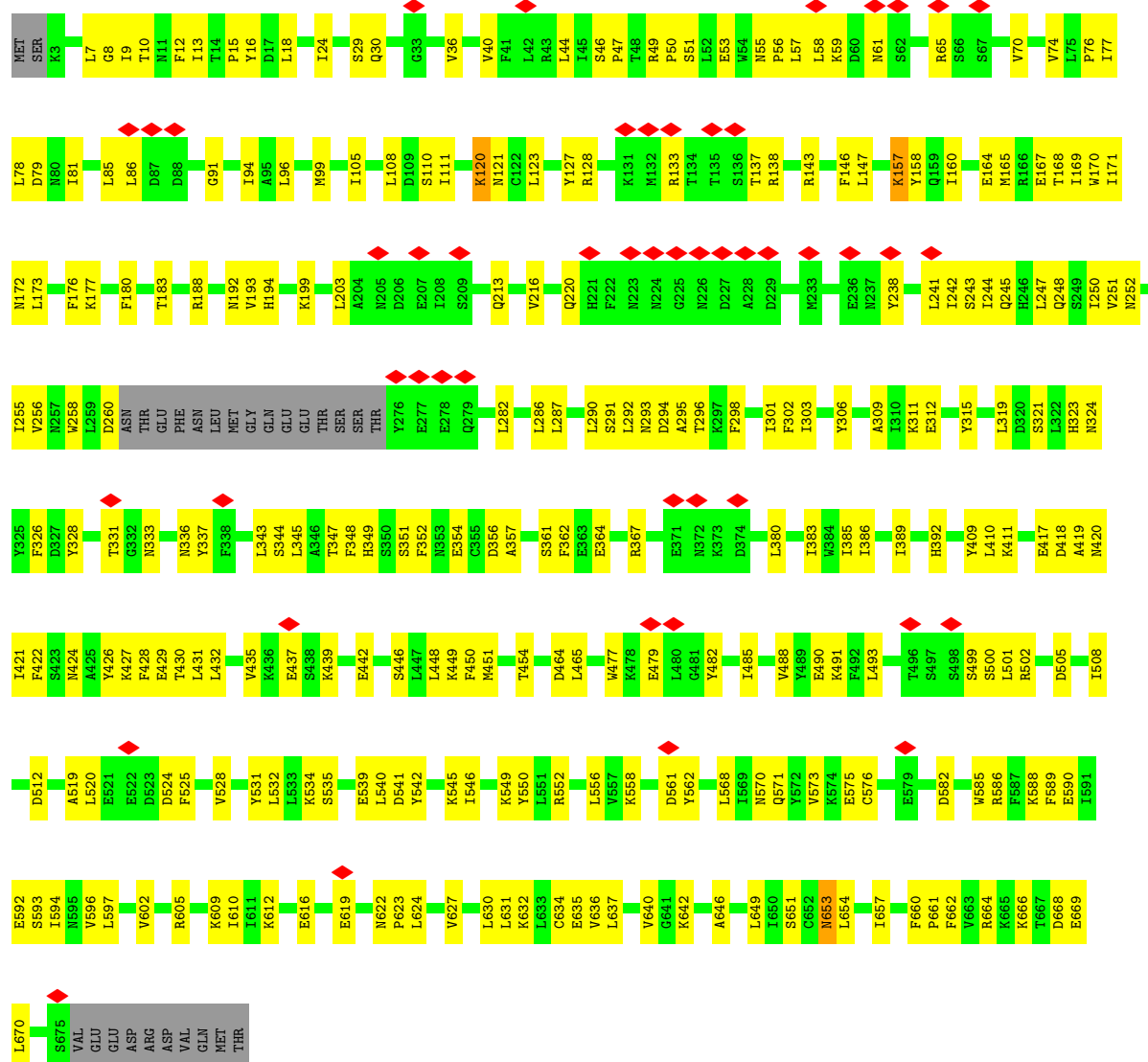
• Molecule 7: Anaphase-promoting complex subunit 1



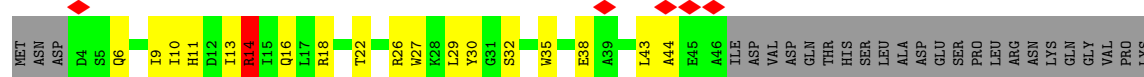
LEU	C942	C943	K843	V844	P845	L846	A847	K848	N849	R850	S851	S852	LEU	SER	K855	K856	P857	S858	D859	I860	Y861	S862	I863	L864	I867	V868	K869	S870	A871	S872	GLN	VAL	PRO	LEU	ASP	GLY	SER	ALA	MET	ARG	MET	SER	ASN	ILE	GLN	ASP	ASP	GLU	G995	R996	S997	L998	K999	L900	N901				
A902	G903	L904	I905	F906	S907	E908	D909	K910	R911	V915	V916	L919	Y922	R923	P924	T925	K926	T927	Q928	F929	F930	T931	T932	K933	T934	E935	Y936	A937	Q938	I939	L940	A941	Q942	K943	K944	Y945	F946	A947	K948	I949	M950	A951	L952	R953	T954	C955	T956	N957	G958	V959	G960	V961	G962	A963	V964	A965			
Y966	A967	T968	E969	K970	P971	T972	S973	T974	Q975	K976	Y977	Y978	Y979	L984	S985	S986	V987	F988	D989	D991	T992	K993	T994	T995	V996	K997	A998	P999	E1000	D1001	I1002	A1003	H1004	D1005	I1006	V1007	W1008	W1009	G1010	Q1011	F1012	H1013	G1019	L1020	R1021	I1022	S1023	K1024	L1025	A1026	T1027	G1028	T1029	T1030					
I1034	A1035	F1036	K1037	P1038	F1039	K1040	E1041	L1042	D1043	H1046	F1049	L1050	L1051	G1052	L1055	N1056	G1057	H1058	L1059	K1060	N1061	L1062	E1063	E1064	W1065	H1066	I1067	Y1068	N1069	Y1070	L1071	S1072	P1073	R1074	N1075	T1076	H1077	I1078	I1079	I1080	G1081	L1082	L1083	L1084	G1085	M1086	S1087	S1088	T1089	K1091	G1092	S1093	M1094	D1095	S1096				
K1097	L1098	I1099	K1100	V1101	I1102	S1103	V1104	H1105	L1106	V1107	A1108	F1109	L1110	P1111	S1112	G1113	S1114	S1115	D1116	L1117	M1118	I1119	L1120	L1121	K1122	L1123	Q1124	T1125	A1126	G1127	I1128	I1129	G1130	M1131	G1132	M1133	L1134	Y1135	L1136	M1137	S1138	R1139	H1140	K1141	R1142	M1143	G1144	D1145	S1146	I1147	F1148	A1149	Q1150	L1151	V1152	S1153	L1154	N1155	N1156
V1157	N1158	D1159	E1160	M1161	V1162	A1163	D1164	E1165	L1166	Y1167	R1168	L1169	A1170	A1171	G1172	I1173	S1174	L1175	G1176	L1177	L1180	G1181	A1182	G1183	Q1184	T1185	K1186	LEU	ARG	V1248	LYS	A1126	TRP	ASP	SER	SER	LEU	GLY	LEU	GLY	ASP	ASP	PRO	ASP	VAL	TYR	ASP	SER	ASP	VAL	GLU	Q1213	N1214	V1215	M1216	Y1217			
E1218	D1219	L1220	T1221	T1222	K1223	L1224	E1226	I1227	V1228	T1229	S1230	T1231	Y1232	D1233	V1234	E1235	N1236	D1237	W1238	I1239	P1240	E1241	G1183	N1242	Q1244	I1245	G1246	A1247	V1248	LYS	A1126	TRP	ASP	SER	SER	LEU	GLY	LEU	GLY	ASP	ASP	PRO	ASP	VAL	TYR	ASP	SER	ASP	VAL	GLU	Q1213	N1214	V1215	M1216	Y1217				
M1278	I1279	N1280	T1281	R1282	P1283	E1284	L1285	L1286	E1290	W1291	A1292	I1296	L1297	W1298	E1299	F1300	I1301	G1302	D1303	L1304	L1305	S1306	F1307	I1308	M1309	K1310	D1311	V1312	D1313	I1314	G1315	V1316	K1317	F1318	S1319	E1320	L1321	N1322	T1323	D1324	L1325	L1326	P1327	I1328	L1329	Y1330	T1331	M1332	G1333	G1334	R1335	L1336	L1337	M1338	G1340	I1341			
R1342	F1343	A1344	S1345	N1348	L1349	K1350	I1351	R1352	L1355	L1356	D1360	K1361	F1362	L1363	P1364	L1365	Y1366	Y1368	P1369	K1370	K1371	Q1372	N1373	K1374	D1375	F1376	T1379	I1380	I1383	N1384	V1385	L1386	T1387	N1388	V1389	Y1391	L1390	L1392	S1393	S1395	M1396	V1397	M1398	C1399	A1400	S1401	G1402	D1403	L1404	E1405	V1406	L1407							
R1408	E1409	V1410	K1411	Y1412	L1413	H1414	E1415	V1416	A1417	S1418	G1419	P1420	Y1421	S1422	D1423	L1424	PHE	GLN	ILE	PRO	SER	SER	LYS	SER	ASP	VAL	GLY	SER	VAL	THR	THR	THR	PRO	GLY	ASN	SER	ASP	ARG	GLU	VAL	ASP	GLU	ALA	ALA	SER	LEU	ASP	ASP	GLU	ARG									
SER	SER	ASN	GLY	SER	ASP	ILE	S1475	D1476	P1477	T1478	A1479	Y1480	L1481	E1482	D1483	K1484	K1485	D1486	I1487	D1488	D1489	H1490	Y1491	G1492	K1493	F1494	I1495	N1496	T1497	N1498	L1499	A1500	L1501	F1505	S1508	G1509	Q1510	Y1511	A1512	L1513	N1514	T1515	S1516	T1517	L1518	E1519	S1520	I1521	A1522	F1523	M1526	S1527	V1528	L1529	P1530	T1531			
Y1532	T1533	T1534	P1535	H1536	P1537	L1538	Q1539	E1540	L1541	K1542	H1543	F1544	W1545	V1549	E1550	P1551	R1552	I1556	K1557	D1558	I1559	D1563	N1566	N1567	V1568	P1569	L1572	V1573	V1574	E1575	E1576	D1577	V1578	E1579	K1580	E1581	E1582	V1583	I1584	R1585	E1586	I1587	S1588	T1589	P1590	C1591	D1595	F1596	S1601	T1602	L1605								
H1606	H1607	G1608	Y1609	F1610	P1611	N1615	F1616	T1617	K1618	D1619	V1620	S1621	A1622	S1623	D1624	F1625	F1626	S1627	G1628	G1629	T1630	I1631	Q1635	R1636	K1637	S1638	E1639	S1640	V1641	K1645	N1650	V1651	E1652	H1655	L1658	S1665	K1666	N1667	Y1668	S1669	L1670	LEU	ASN	LEU	LYS	ASN	GLU	GLN	G1678	N1679	Q1684								

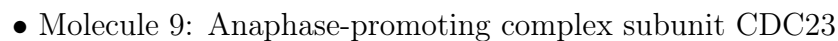


• Molecule 8: Anaphase-promoting complex subunit 5

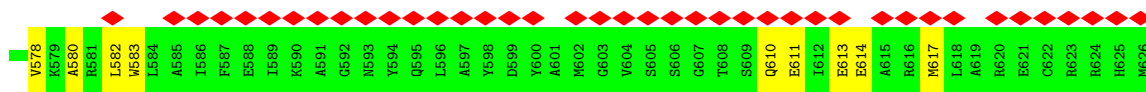


• Molecule 9: Anaphase-promoting complex subunit CDC23

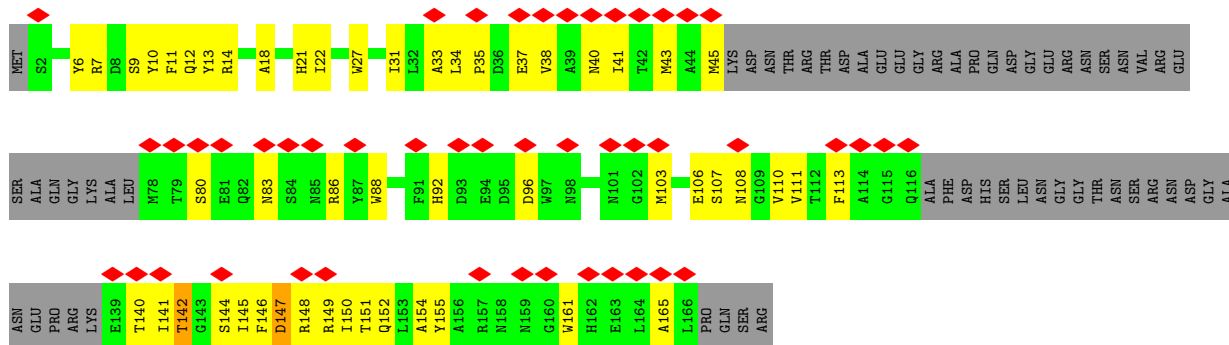




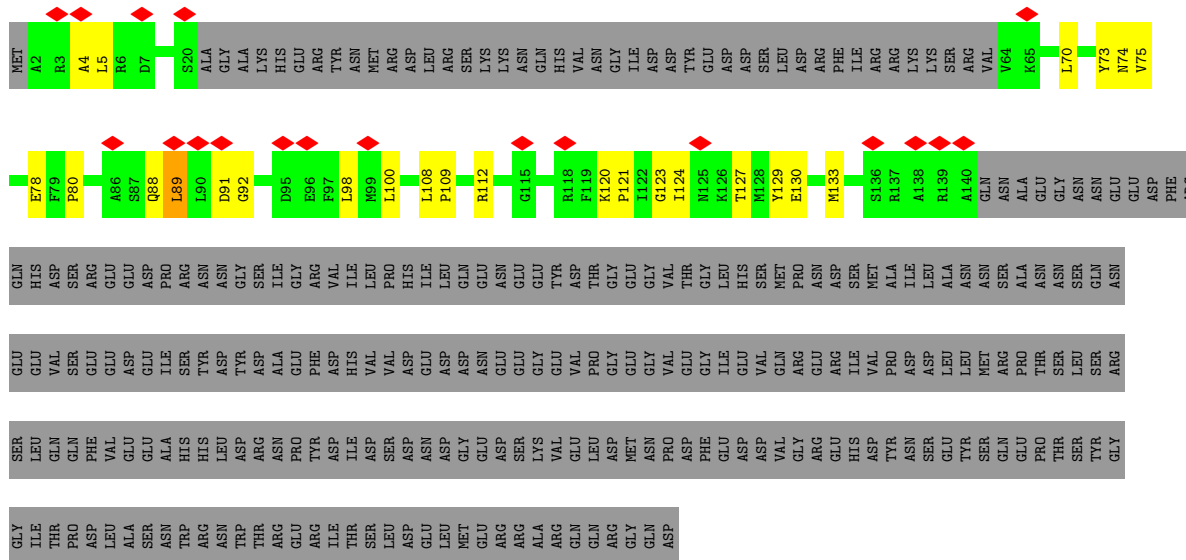
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S484	S242	LYS	ILE	ASN
R499	S243	ASP	P75	ASP
C508	C244	GLY	Q76	ASP
Y509	F247	GLY	F79	SER
T512	N248	GLY	G90	Q6
K515	W249	GLY	L81	H11
V516	S950	GLU	S82	D12
E517	C251	GLU	E83	I13
A518	W252	ASP	R14	R14
I519	L253	ILE	Y86	I15
K520	E254	GLN	D87	Q16
C521	L255	SER	L88	L17
Y522	Q260	GLY	Y89	R18
I526	Y406	GLY	L90	E23
S529	Y407	GLN	L91	W27
Q530	E414	ARG	L95	Y30
T531	K415	ALA	F96	Y30
V532	L272	ALA	ASN	Y30
D533	L272	LEU	D97	K34
Q534	S281	LYS	E100	W35
N535	E282	MET	G104	A36
I538	I294	VAL	V105	A37
Y539	M295	SER	F106	E38
Y541	F298	GLU	F107	A39
Q544	F299	HIS	L108	L40
L545	D427	GLU	K109	L43
E548	K428	E182	D110	A44
L549	K429	N186	N113	GLU
D551	T430	S189	P114	ALA
D551	T431	I190	Y115	ILE
E554	A432	N308	L116	ASP
D554	W434	S200	K117	VAL
D554	T435	G309	F118	ASP
E548	L436	Q310	L119	GLN
L549	M437	L311	K120	THR
D551	G438	E312	L121	HIS
D551	H439	D313	K130	SER
D551	I451	A210	K131	LEU
D551	E452	D211	S132	ALA
Q553	C453	L212	Q133	GLU
E554	Y454	N327	E134	SER
M559	R455	F328	E137	PRO
M559	R456	T329	E138	LEU
M560	I460	F330	N138	ARG
K561	C461	Y218	L139	ASN
C562	P462	Y219	L140	LYS
V563	R463	L220	L140	GLN
D564	Y475	V223	T146	GLY
V565	Y475	I224	ASP	VAL
E566	D479	N230	GLU	PRO
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			TYR	GLN
			ARG	TRP



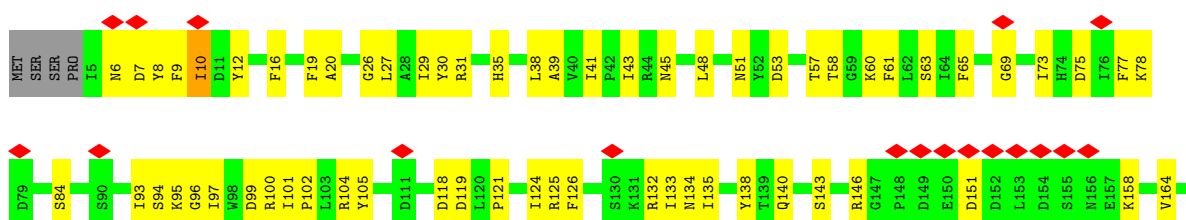
• Molecule 10: Anaphase-promoting complex subunit SWM1

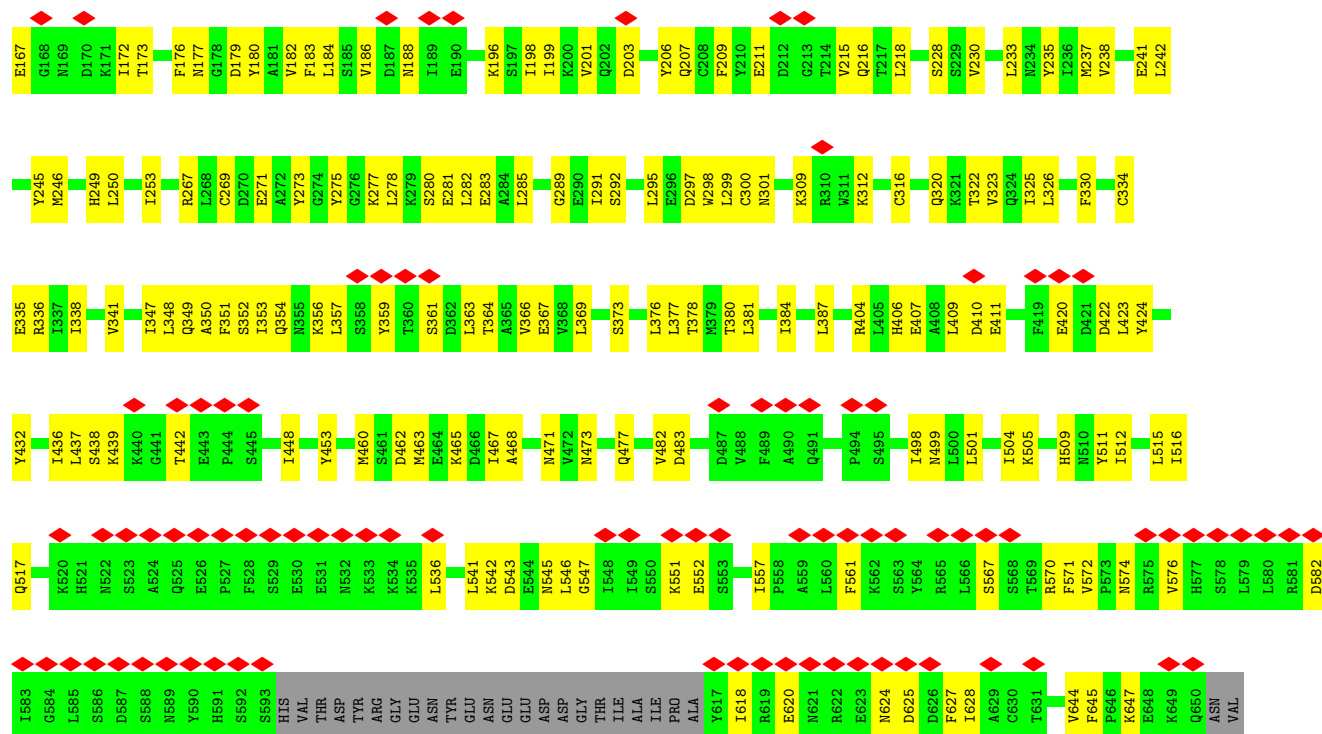


• Molecule 11: Anaphase-promoting complex subunit MND2

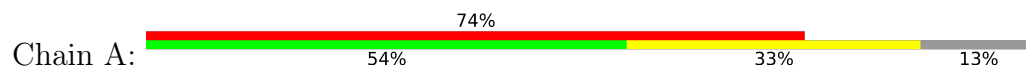


• Molecule 12: Anaphase-promoting complex subunit 4





• Molecule 13: Anaphase-promoting complex subunit DOC1



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	372535	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 ($e^-/\text{\AA}^2$)	59	Depositor
Minimum defocus (nm)	2600	Depositor
Maximum defocus (nm)	9000	Depositor
Magnification	59000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.214	Depositor
Minimum map value	-0.106	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.05	Depositor
Map size (\AA)	353.28, 353.28, 353.28	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	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	0.31	0/4079	0.60	7/5525 (0.1%)
1	H	0.28	0/4126	0.53	1/5585 (0.0%)
2	J	0.30	0/4210	0.61	5/5688 (0.1%)
2	K	0.30	0/4188	0.57	0/5657
3	G	0.28	0/285	0.76	0/384
3	W	0.27	0/285	0.58	0/384
4	E	0.29	0/1108	0.60	1/1481 (0.1%)
5	T	0.26	0/5479	0.53	1/7420 (0.0%)
6	U	0.26	0/936	0.57	0/1265
7	C	0.28	0/11057	0.58	4/15038 (0.0%)
8	O	0.29	0/5384	0.58	0/7287
9	D	0.28	0/4621	0.56	2/6243 (0.0%)
9	P	0.27	0/4618	0.55	0/6231
10	I	0.32	0/930	0.66	0/1263
11	N	0.27	0/800	0.64	1/1076 (0.1%)
12	Q	0.27	0/5193	0.53	0/7024
13	A	0.25	0/1780	0.56	0/2411
All	All	0.28	0/59079	0.57	22/79962 (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
5	T	0	4
7	C	0	1
All	All	0	5

There are no bond length outliers.

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	752	LEU	CB-CG-CD2	-7.79	97.76	111.00
7	C	1363	LEU	CA-CB-CG	6.89	131.16	115.30
2	J	482	CYS	CA-CB-SG	6.65	125.98	114.00
1	F	458	LEU	CA-CB-CG	6.61	130.51	115.30
1	F	181	LEU	CA-CB-CG	-6.18	101.08	115.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
7	C	1551	PRO	Peptide
5	T	620	THR	Peptide
5	T	621	GLN	Peptide
5	T	622	GLY	Peptide
5	T	623	SER	Peptide

5.2 Too-close contacts

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	183	0
1	H	4038	0	4010	141	0
2	J	4124	0	4085	186	0
2	K	4102	0	4065	184	0
3	G	284	0	293	19	0
3	W	284	0	293	21	0
4	E	1091	0	1058	38	0
5	T	5362	0	5336	157	0
6	U	912	0	873	31	0
7	C	10832	0	10637	435	0
8	O	5285	0	5290	235	0
9	D	4524	0	4391	139	0
9	P	4520	0	4415	143	0
10	I	906	0	813	60	0
11	N	784	0	784	24	0
12	Q	5086	0	5095	180	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	A	1738	0	1705	59	0
14	U	3	0	0	0	0
All	All	57866	0	57090	2031	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 2031 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)
5:T:463:ILE:HG12	7:C:1412:TYR:HE1	1.24	1.02
7:C:78:ILE:HD13	7:C:119:TRP:HD1	1.30	0.95
7:C:902:ALA:HA	7:C:905:ILE:HG12	1.49	0.92
9:P:95:LEU:HD11	9:P:104:CYS:HB2	1.53	0.91
2:K:453:LEU:HD12	2:K:459:LEU:HD23	1.52	0.90

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%)	479 (97%)	17 (3%)	0	100	100
1	H	499/758 (66%)	483 (97%)	13 (3%)	3 (1%)	25	65
2	J	505/850 (59%)	488 (97%)	17 (3%)	0	100	100
2	K	501/850 (59%)	487 (97%)	14 (3%)	0	100	100
3	G	33/124 (27%)	33 (100%)	0	0	100	100
3	W	33/124 (27%)	33 (100%)	0	0	100	100
4	E	120/265 (45%)	118 (98%)	2 (2%)	0	100	100
5	T	638/853 (75%)	613 (96%)	19 (3%)	6 (1%)	17	56

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	U	110/165 (67%)	108 (98%)	1 (1%)	1 (1%)	17	56
7	C	1380/1748 (79%)	1287 (93%)	87 (6%)	6 (0%)	34	72
8	O	654/685 (96%)	625 (96%)	26 (4%)	3 (0%)	29	68
9	D	554/626 (88%)	536 (97%)	15 (3%)	3 (0%)	29	68
9	P	550/626 (88%)	527 (96%)	23 (4%)	0	100	100
10	I	105/170 (62%)	94 (90%)	10 (10%)	1 (1%)	15	54
11	N	92/368 (25%)	89 (97%)	3 (3%)	0	100	100
12	Q	619/652 (95%)	597 (96%)	21 (3%)	1 (0%)	47	81
13	A	212/250 (85%)	203 (96%)	8 (4%)	1 (0%)	29	68
All	All	7101/9872 (72%)	6800 (96%)	276 (4%)	25 (0%)	38	72

5 of 25 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	588	ASP
5	T	621	GLN
5	T	624	ASN
5	T	745	ASP
7	C	844	VAL

5.3.2 Protein sidechains ⓘ

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%)	432 (100%)	1 (0%)	93	96
1	H	440/684 (64%)	439 (100%)	1 (0%)	93	96
2	J	450/760 (59%)	449 (100%)	1 (0%)	93	96
2	K	448/760 (59%)	445 (99%)	3 (1%)	84	90
3	G	34/115 (30%)	34 (100%)	0	100	100
3	W	34/115 (30%)	34 (100%)	0	100	100
4	E	123/246 (50%)	123 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	T	608/804 (76%)	606 (100%)	2 (0%)	92	95
6	U	103/149 (69%)	103 (100%)	0	100	100
7	C	1177/1568 (75%)	1174 (100%)	3 (0%)	92	95
8	O	597/643 (93%)	594 (100%)	3 (0%)	88	93
9	D	477/560 (85%)	475 (100%)	2 (0%)	91	94
9	P	477/560 (85%)	475 (100%)	2 (0%)	91	94
10	I	95/144 (66%)	93 (98%)	2 (2%)	53	72
11	N	83/332 (25%)	83 (100%)	0	100	100
12	Q	572/598 (96%)	572 (100%)	0	100	100
13	A	190/226 (84%)	188 (99%)	2 (1%)	73	85
All	All	6341/8948 (71%)	6319 (100%)	22 (0%)	92	95

5 of 22 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
9	D	14	ARG
9	P	371	ASN
9	P	138	ASN
10	I	147	ASP
5	T	143	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 29 such sidechains are listed below:

Mol	Chain	Res	Type
8	O	61	ASN
12	Q	320	GLN
8	O	333	ASN
9	P	535	ASN
8	O	220	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

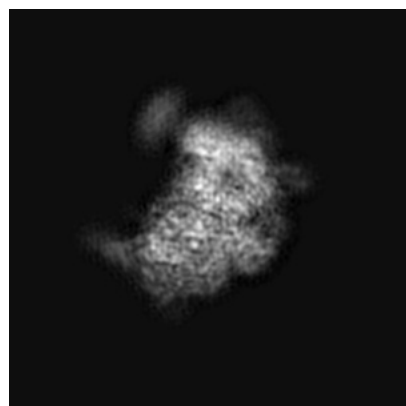
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-15199. These allow visual inspection of the internal detail of the map and identification of artifacts.

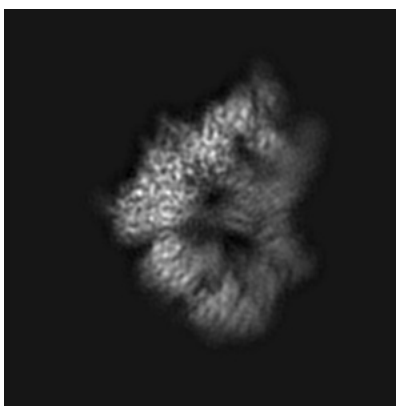
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

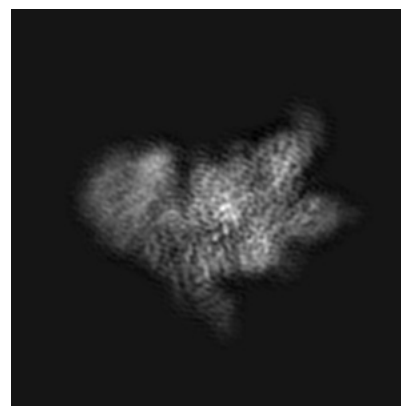
6.1.1 Primary map



X

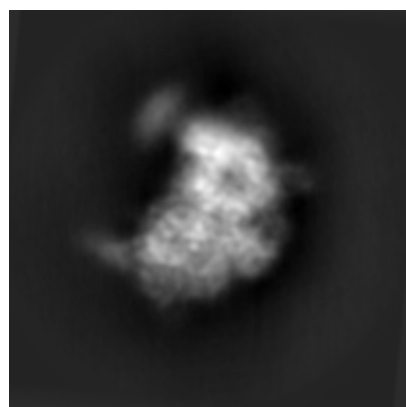


Y

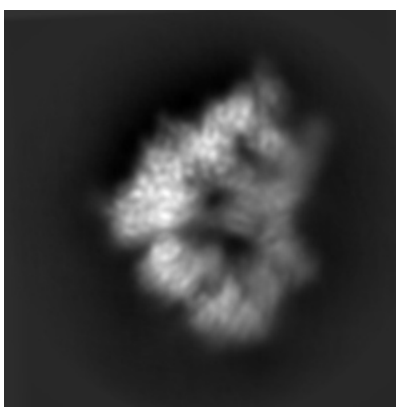


Z

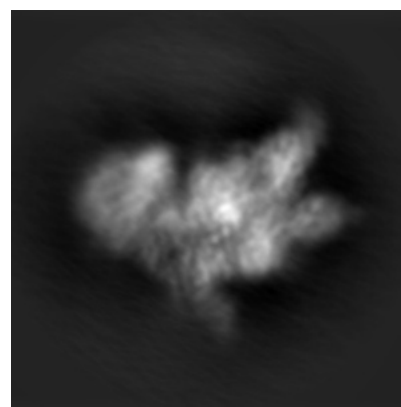
6.1.2 Raw map



X



Y

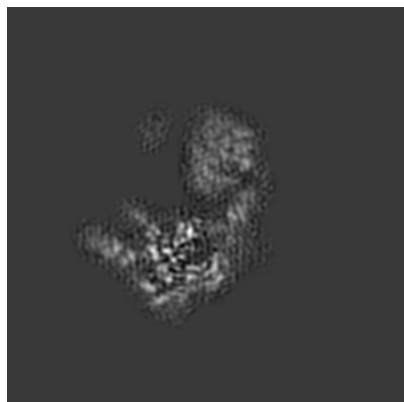


Z

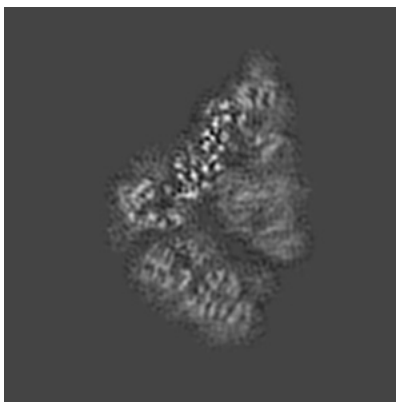
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

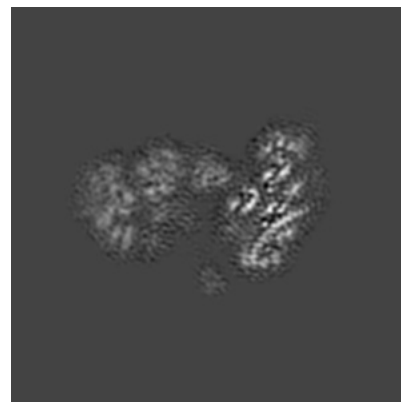
6.2.1 Primary map



X Index: 128

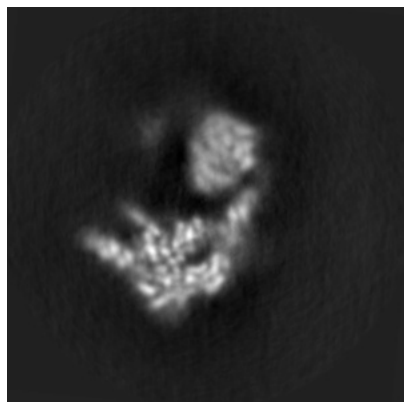


Y Index: 128

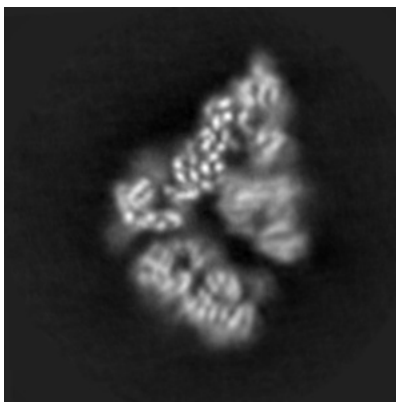


Z Index: 128

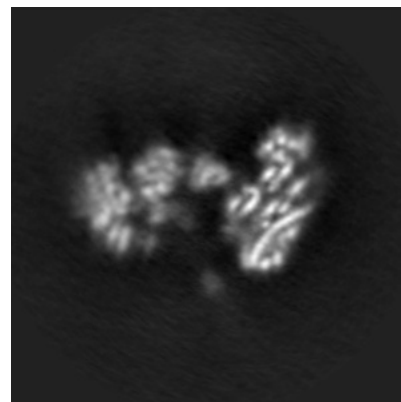
6.2.2 Raw map



X Index: 128



Y Index: 128



Z Index: 128

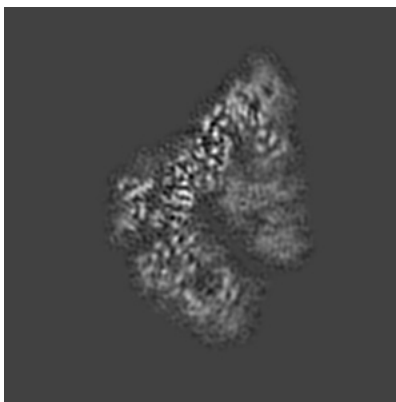
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

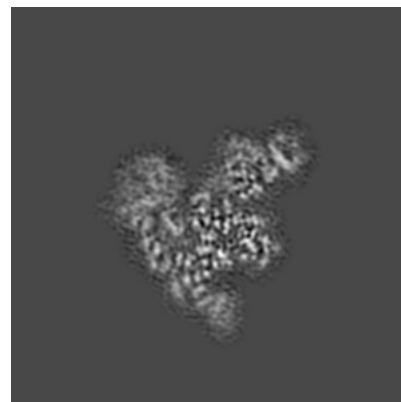
6.3.1 Primary map



X Index: 137

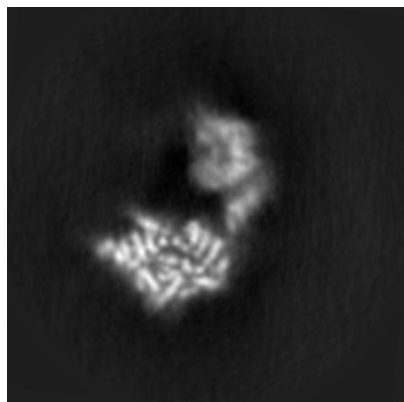


Y Index: 122

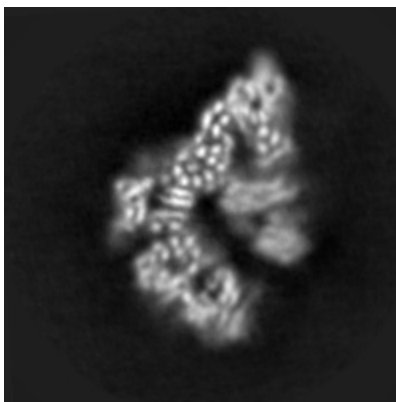


Z Index: 105

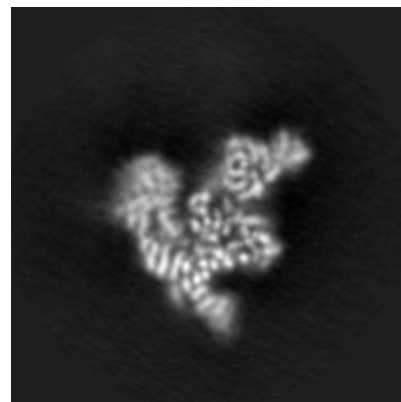
6.3.2 Raw map



X Index: 123



Y Index: 123



Z Index: 103

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

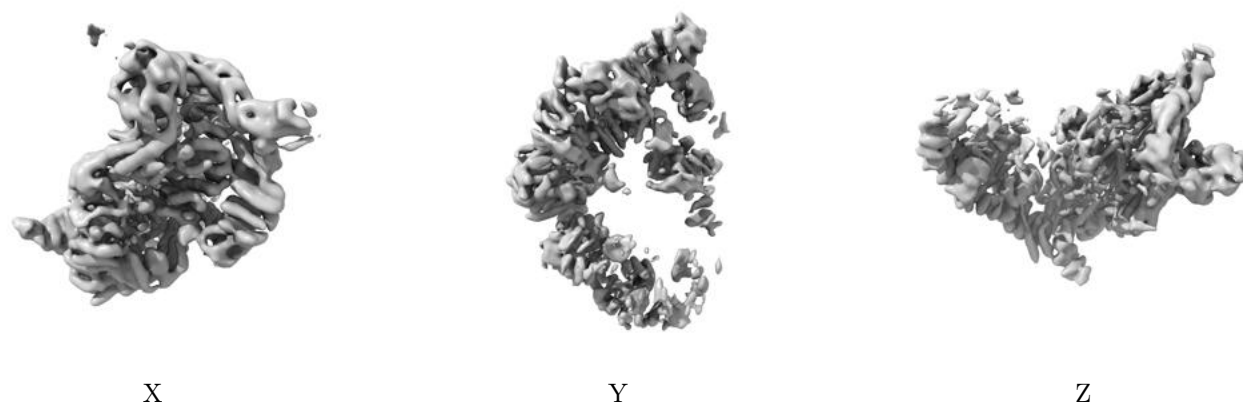
6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



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



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.

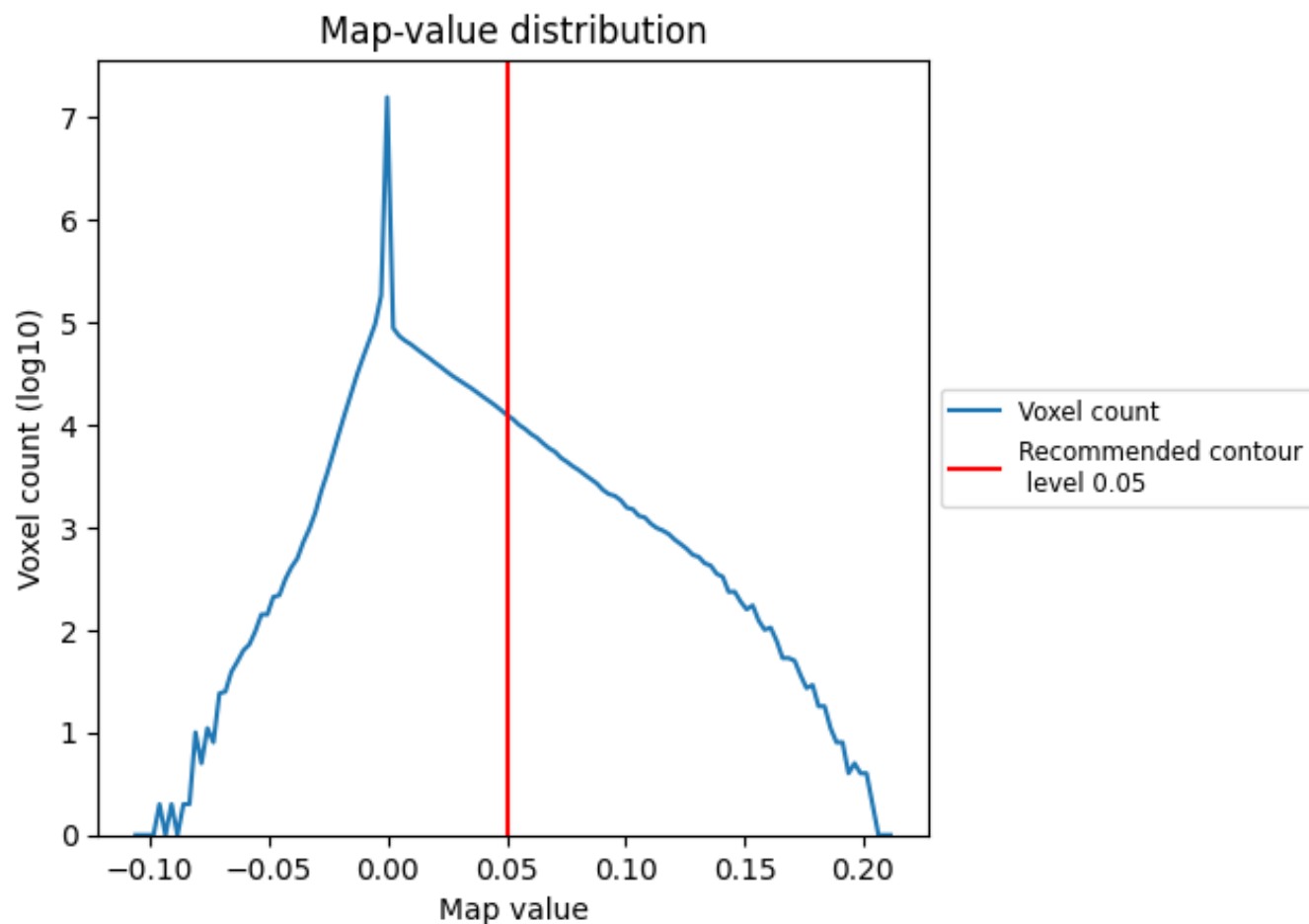
6.5 Mask visualisation [i](#)

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

7 Map analysis [i](#)

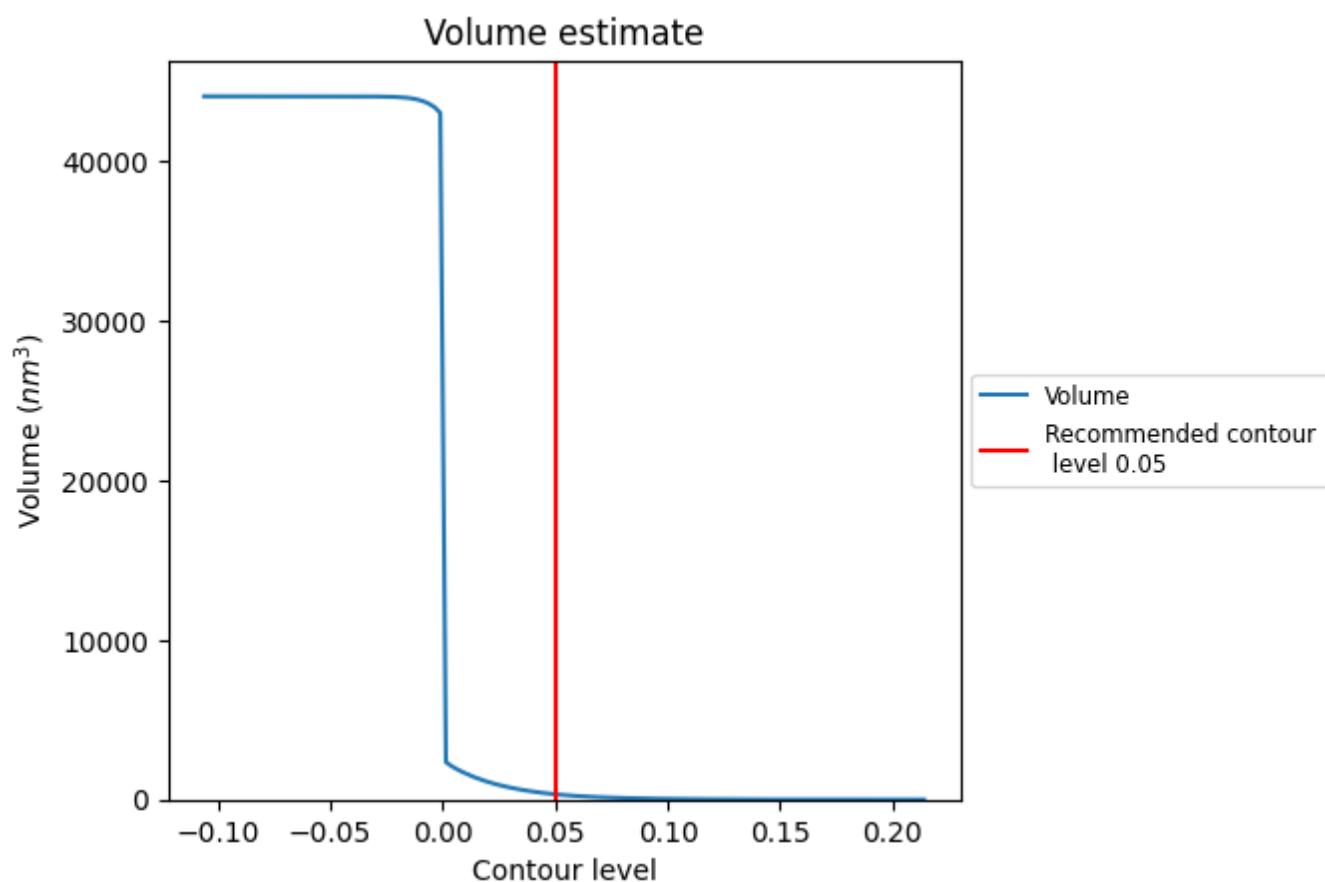
This section contains the results of statistical analysis of the map.

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.

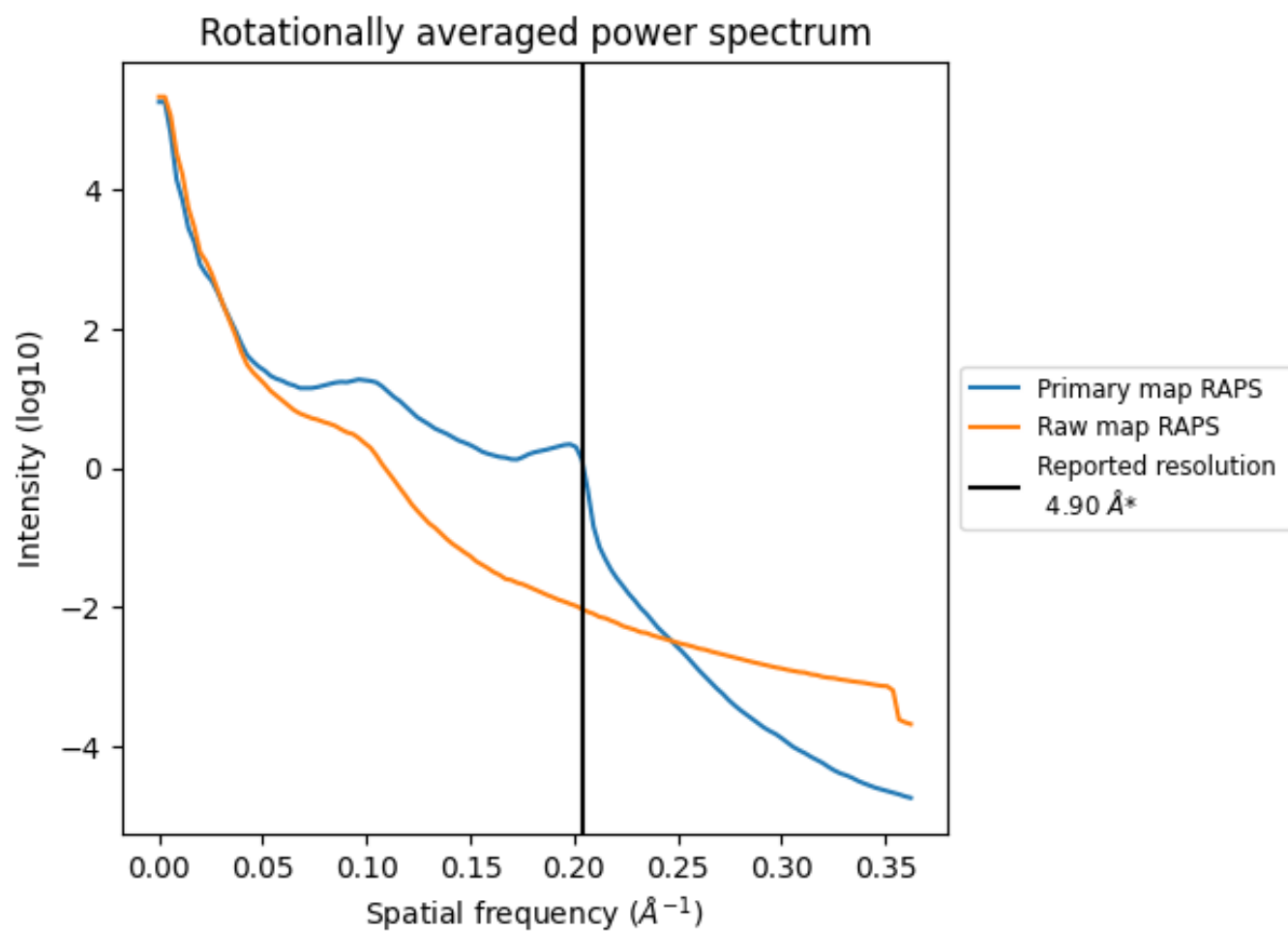
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 332 nm³; this corresponds to an approximate mass of 300 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 ⓘ

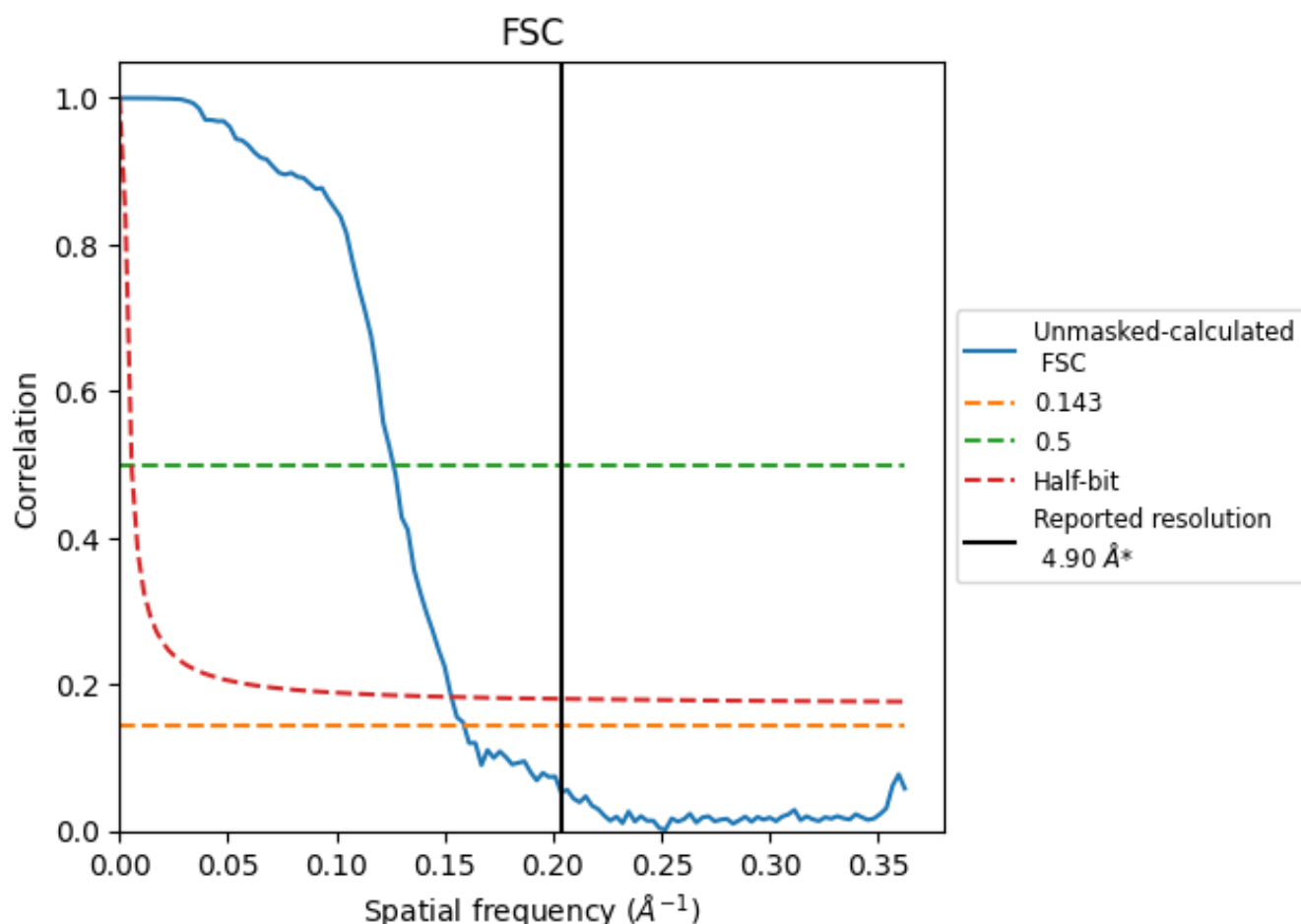


*Reported resolution corresponds to spatial frequency of 0.204 Å⁻¹

8 Fourier-Shell correlation [i](#)

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 [i](#)



*Reported resolution corresponds to spatial frequency of 0.204 Å⁻¹

8.2 Resolution estimates [i](#)

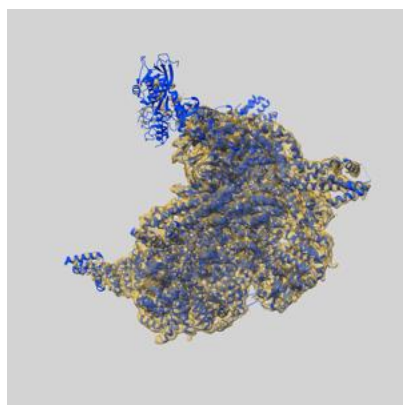
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.90	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	6.29	7.92	6.53

*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 6.29 differs from the reported value 4.9 by more than 10 %

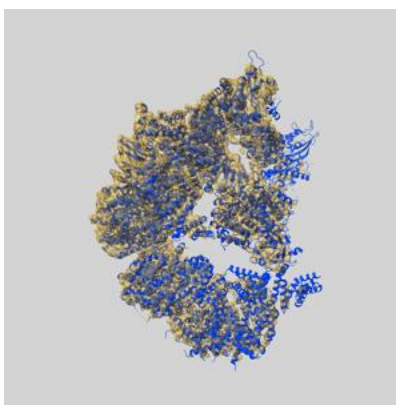
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-15199 and PDB model 8A5Y. Per-residue inclusion information can be found in section [3](#) on page [7](#).

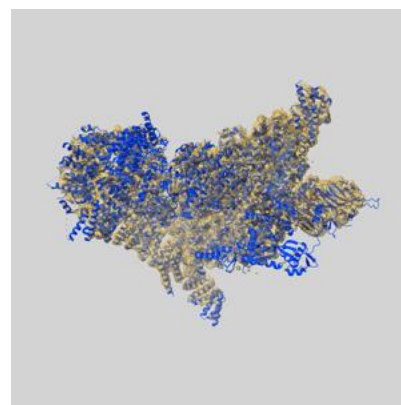
9.1 Map-model overlay [i](#)



X



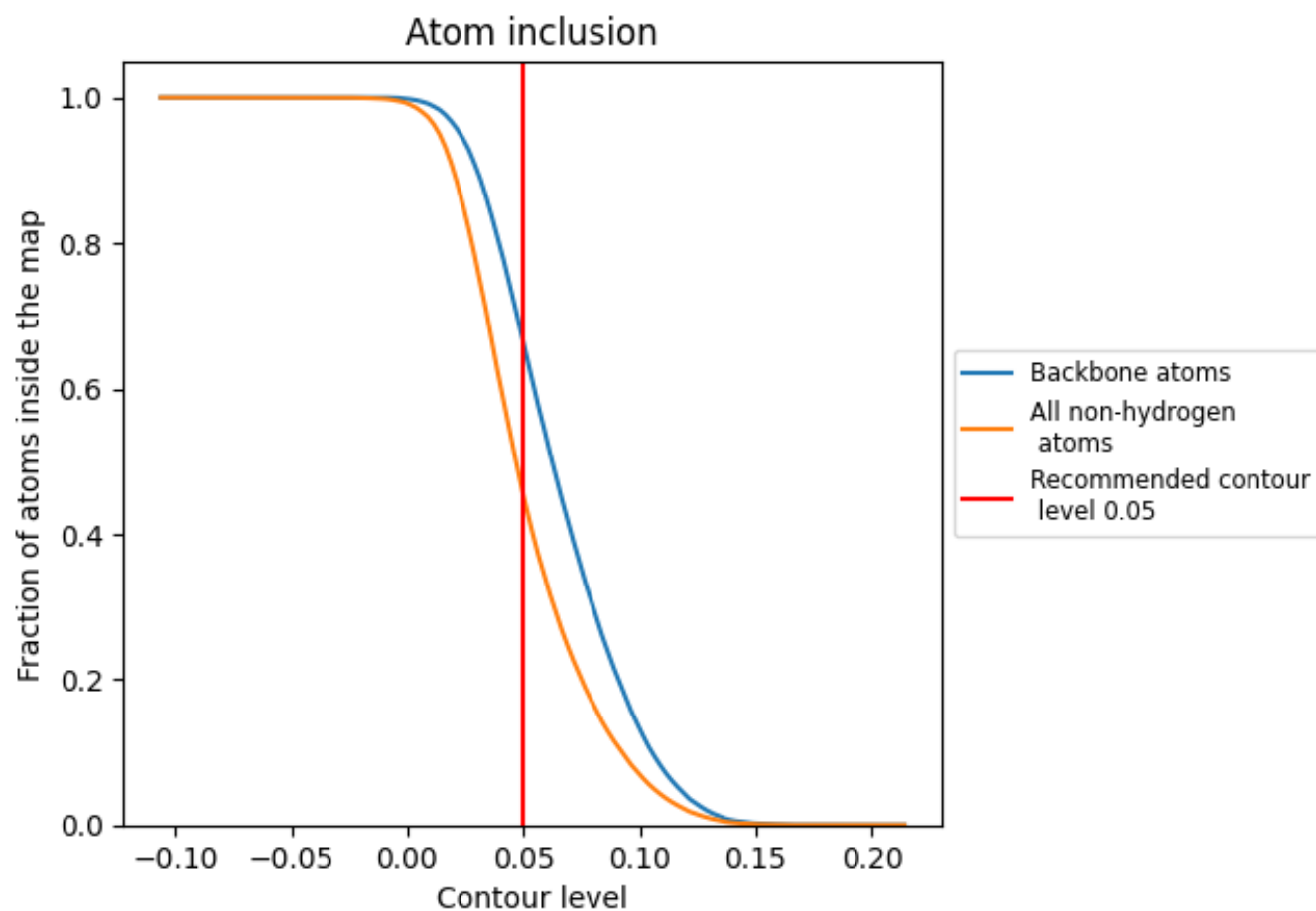
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.05 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, 66% of all backbone atoms, 45% of all non-hydrogen atoms, are inside the map.