



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Mar 2, 2017 – 12:32 pm GMT

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

This is a wwPDB/EMDataBank EM Map/Model Validation Summary Report
for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : recalc29047

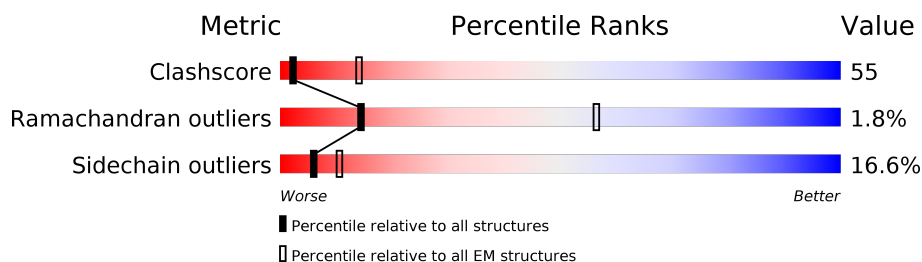
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 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.



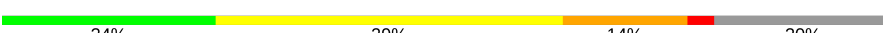
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	1944	27% 39% 13% 19%
2	B	84	67% 23% 8%
3	C	597	44% 37% 7% 12%
3	P	597	46% 30% 6% 18%
4	D	121	31% 12% 55%
5	E	110	25% 21% 5% 49%
6	F	824	30% 21% 5% 44%
6	H	824	34% 22% 41%
7	G	85	11% 11% 8% 71%

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Mol	Chain	Length	Quality of chain
7	W	85	
8	I	808	
9	J	620	
9	K	620	
10	L	185	
11	M	74	
12	N	822	
13	O	755	
14	T	15	
15	X	599	
15	Y	599	

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 63181 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called ANAPHASE-PROMOTING COMPLEX SUBUNIT 1.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 14 is a protein called UNIDENTIFIED PEPTIDE.

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

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

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

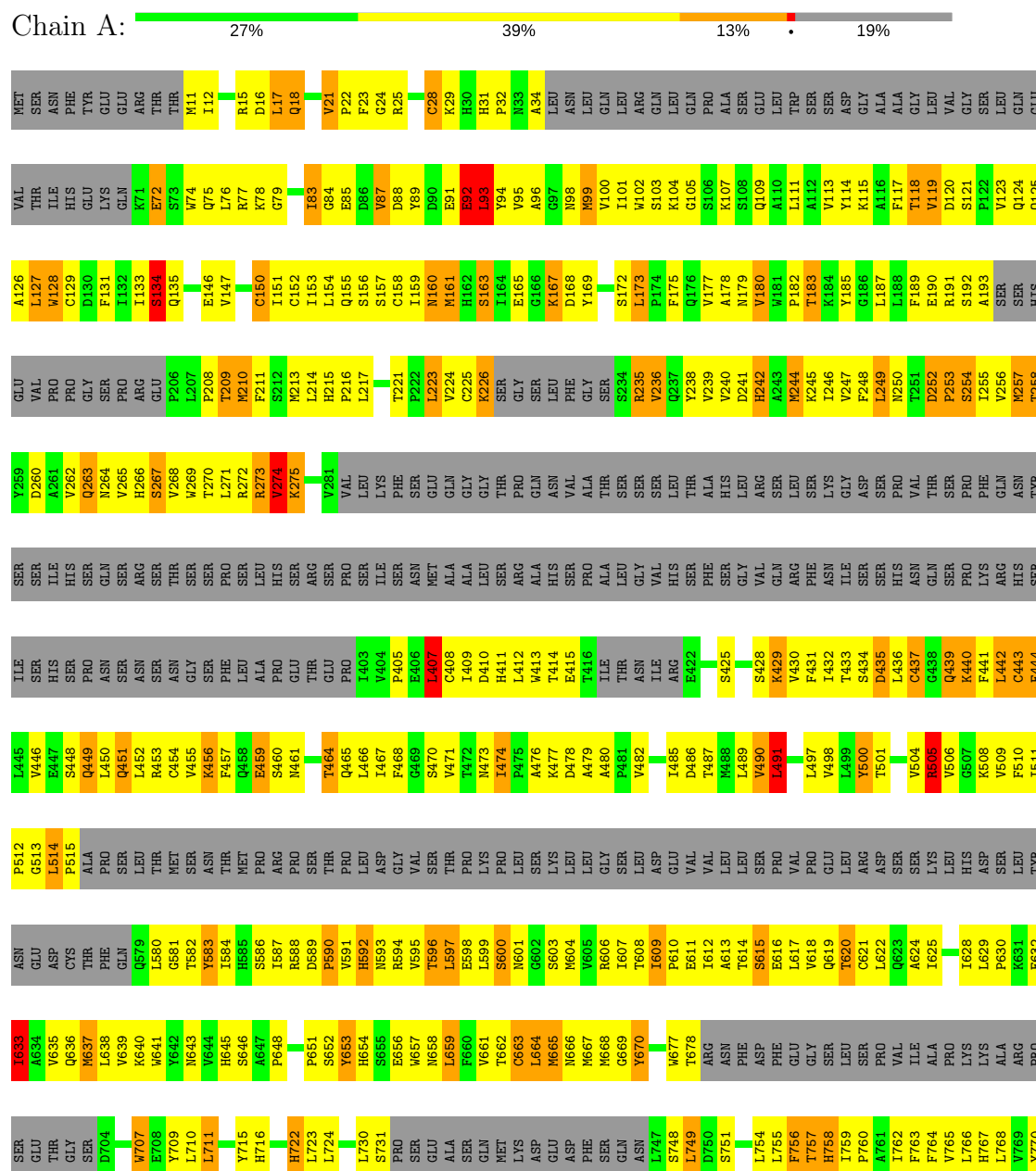
- Molecule 16 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

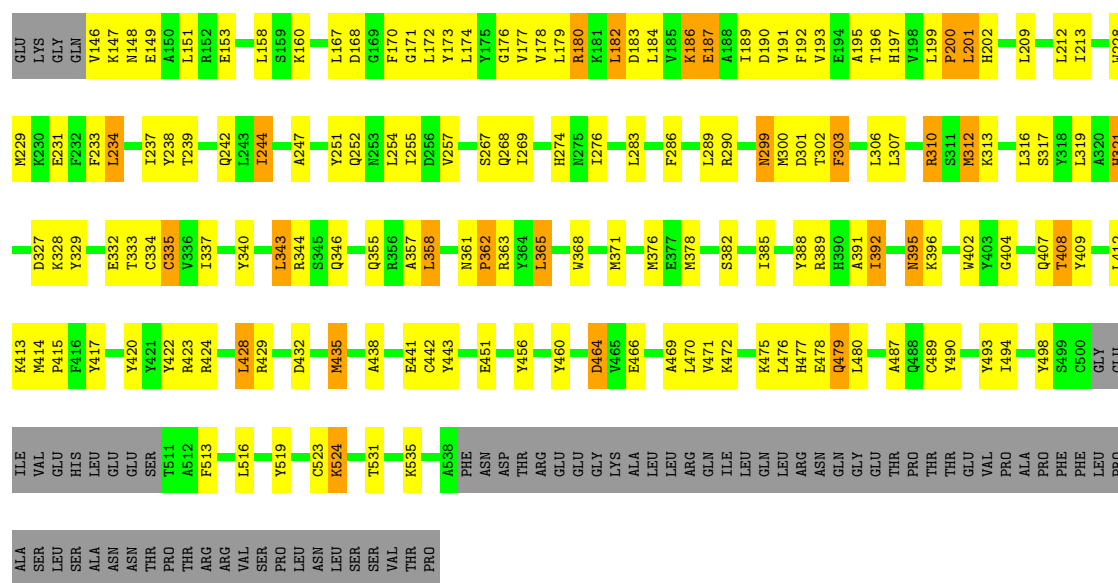
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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. 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. 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

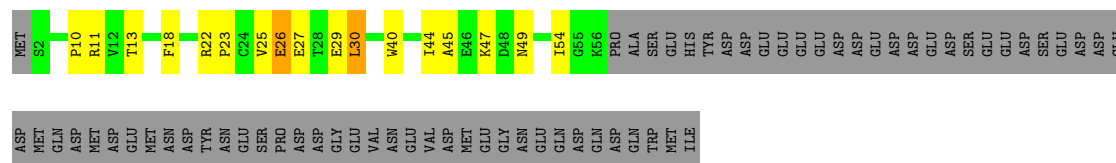


E1807	S1743	I1678	L1612	L1533	A1460	I1383	P1238	E1167	I1100	V1034	P966	I899	M831	E771
T1808	D1744	D1679	E1616	K1534	H1461	L1313	T1239	L1168	P1101	Q1035	P967	I900	H832	E772
E1810	P1745	L1680	P1615	V1536	Y1462	I1314	S1240	A1169	I1102	D1036	A967	I1E	H833	L773
L1811	A1746	T1684	R1617	L1536	Y1463	G1315	T1241	G1315	P1103	V1037	S968	ALA	P834	K774
L1812	L1747	G1685	L1618	Q1537	I1464	M1316	E1242	E1171	K1104	L1040	D969	PRO	S835	L775
Q1813	S1749	H1686	L1619	D1391	D1391	L1319	L1243	Y1172	L1107	L1040	N970	GLN	F836	L776
L1814	F1750	L1687	V1620	T1392	T1392	L1320	L1248	A1173	L1109	S1043	P971	LYS	F837	L777
K1815	A1751	L1690	P1621	L1395	L1395	M1321	N1249	L1176	GLN	A1044	V974	VAL	T838	L778
L1816	E1752	L1691	V1622	L1396	L1396	M1322	Q1250	M1177	GLN	A1046	P974	VAL	E840	G780
L1817	L1753	L1692	D1623	H1544	S1471	E1323	V1251	L1181	L977	P1046	L977	GLU	P841	E781
L1818	F1754	S1692	V1624	K1545	L1472	Q1324	Y1264	L1182	GLN	V1047	Y978	GLN	P842	G782
L1819	C1755	K1693	D1625	L1546	G1473	L1325	V1265	GL183	P1112	K1048	G979	GLU	S843	G783
F1820	K1756	D1694	T1626	G1547	F1474	Y1326	V1255	H1184	P1113	V1049	R980	GLU	I844	G784
F1821	P1757	G1695	N1627	M1550	F1475	Q1327	L1259	L1185	M1115	Q1053	Q981	ASN	Y845	S785
S1822	T1758	L1696	T1628	N1551	F1476	Y1328	L1260	T1186	T1116	Y1054	D982	ARG	Q846	L786
S1823	V1759	L1697	P1629	Y1552	F1477	M1329	Y1261	T1191	T1117	P1055	L983	PHE	W847	V787
L1824	N1760	V1698	G1630	G1553	E1480	G1332	Y1264	L1192	GLN	P1056	S984	SER	W848	E788
S1825	K1761	L1701	A1632	F1554	N1481	H1333	T1264	N1193	L1120	E1056	X985	PHE	L789	L789
H1826	G1762	A1702	L1633	F1555	L1482	ARG	A1265	N1192	H1060	L1057	C988	HIS	C851	L790
Q1827	K1764	A1703	E1634	L1556	L1482	ARG	H1266	N1193	SER	L852	E989	THR	L852	V791
L1830	L1768	Q1763	E1635	A1557	C1487	GLN	R1267	H1194	D1126	E1061	P993	THR	K853	Q792
H1833	L1769	Q1765	V1637	H1558	L1488	THR	T1269	Y1196	P1127	F1062	L993	SER	M857	A794
F1834	D1770	L1706	Y1638	L1562	K1493	GLY	Y1272	T1198	P1129	E1064	GLY	S924	P858	A795
P1834	F1771	S1707	G1640	G1563	D1494	MET	V1272	L1199	N1130	E1065	L993	S925	P859	D796
L1836	S1772	Y1708	L1644	L1564	F1495	HIS	L1273	G1200	VAL	L1066	L993	L926	Y860	L797
L1837	S1773	K1709	E1645	L1565	M1496	ARG	L1274	H1201	N1131	E1067	L993	VAL	P861	K798
L1838	F1774	E1710	Y1644	F1566	L1497	GLU	T1275	E1202	GLY	E1067	VAL	A927	Y862	L799
F1839	L1775	L1713	E1645	L1567	Y1498	LYS	E1276	M1203	S1136	N1068	L993	SER	P864	G800
L1840	Y1776	G1714	Q1646	L1571	L1499	LYS	T1277	T1204	F1137	R1069	SER	R929	P864	P801
L1841	C1778	L1715	K1648	Y1572	Q1432	HIS	G1278	S1205	N1138	L1071	ASP	V931	R865	Y802
S1842	Q1779	Q1716	E1649	S1573	N1503	LVS	R1279	T1206	N1139	Q1072	VAL	V932	R866	Y803
L1843	L1780	S1717	E1650	L1574	A1504	LYS	P1281	G1207	GLY	L1073	PRG	N933	R867	D804
P1846	Q1781	L1718	E1651	L1574	L1436	Q1351	G1282	L1208	V1141	C1074	SER	N934	R869	Y806
L1847	E1782	L1719	M1652	S1577	V1506	I1352	P1283	Y1212	A1142	Q1075	GLY	F939	S870	Y807
V1848	T1783	Q1721	A1653	N1578	T1507	I1352	Y1283	V1212	A1143	R1076	THR	F940	R871	R808
L1851	E1785	L1722	L1656	L1585	N1511	D1356	Y1287	A1215	GL144	T1077	GLY	T940	L872	D809
L1852	L1786	V1723	L1657	L1512	SER	T1357	Y1287	K1216	L1145	M1078	THR	L941	V873	Y810
D1853	L1787	A1724	E1658	E1513	LEU	N1358	D1290	L1217	K1146	A1079	GLY	L944	I877	P811
N1854	L1791	N1726	L1660	L1588	SER	N1359	E1291	G1218	A1148	P1081	E1011	L945	A878	L813
D1857	A1792	N1727	H1661	L1595	GLU	V1360	R1292	T1219	P1149	V1082	E1012	T946	L879	Y814
Q1857	M1793	L1728	H1662	V1518	ILE	C1364	S1293	M1220	A1150	G1063	D1014	L947	Y860	R815
L1859	M1799	S1728	L1663	L1519	GLU	P1365	Y1294	L1224	S1151	R1084	G1015	P948	I881	T816
L1860	Q1795	A1730	K1664	L1520	LEU	T1368	G1299	Q1152	Q1152	G1085	M1016	F949	L882	T817
Q1861	A1796	L1733	Q1665	L1522	PRO	N1373	L1300	T1225	I1153	M1086	M1017	G950	L882	Q818
L1862	L1797	F1733	L1666	L1524	SER	L1371	A1301	R1226	D1154	F1087	D1018	Y951	L882	Q819
G1863	R1798	K1734	K1669	A1524	ASP	A1372	L1302	L1228	S1155	T1089	M1019	A952	VAL	V820
L1864	L1800	P1735	M1525	L1524	L1452	L1374	G1303	L1229	W1157	F1090	ASP	L953	ASP	G821
L1865	G1801	E1736	L1672	M1526	N1453	L1375	L1304	T1230	I1158	H1093	GLU	R956	GLU	T822
L1866	L1802	T1738	R1673	V1527	N1454	Y1376	V1305	H1231	V1159	S1025	S892	D957	S892	R824
C1867	S1739	L1738	W1674	A1528	L1454	K1377	C1306	H1232	V1160	P1094	S893	A958	S893	P825
L1868	E1804	S1739	W1674	G1529	T1456	T1378	G1308	A1234	N1161	V1095	Q894	Y959	Q894	G826
H1869	M1805	F1741	L1676	S1530	L1457	L1379	H1309	A1234	K1162	P1096	E1030	Y960	Y895	Q827
A1870	S1806	T1742	L1677	G1531	L1458	N1379	H1309	T1235	P1163	T1097	D1031	H961	L896	T828
				N1532	Q1459	N1380	L1236	L1236	L1164	P1098	L1032	C962	T897	G829
							S1311	P1237		P1099	R1033	R963	R898	F830



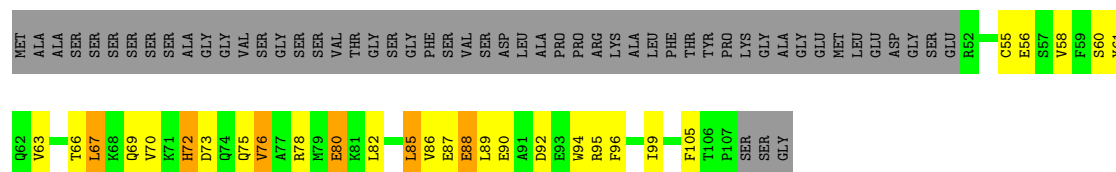
- Molecule 4: ANAPHASE-PROMOTING COMPLEX SUBUNIT 15

Chain D: 31% 12% . 55%



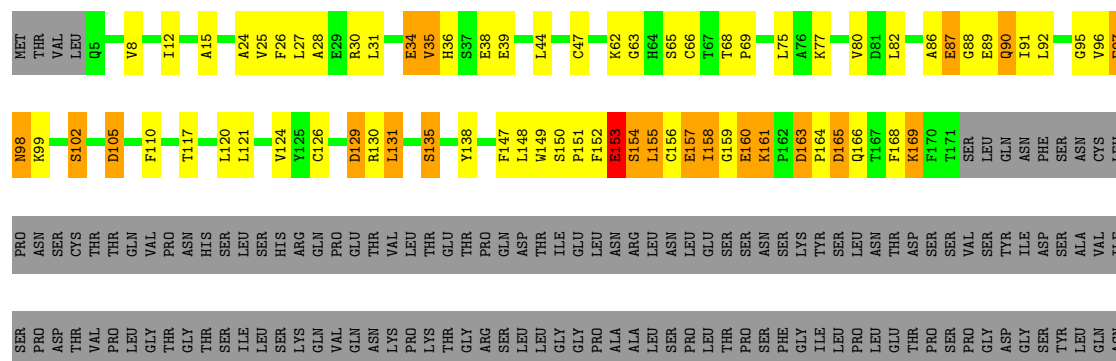
- Molecule 5: ANAPHASE-PROMOTING COMPLEX SUBUNIT 16

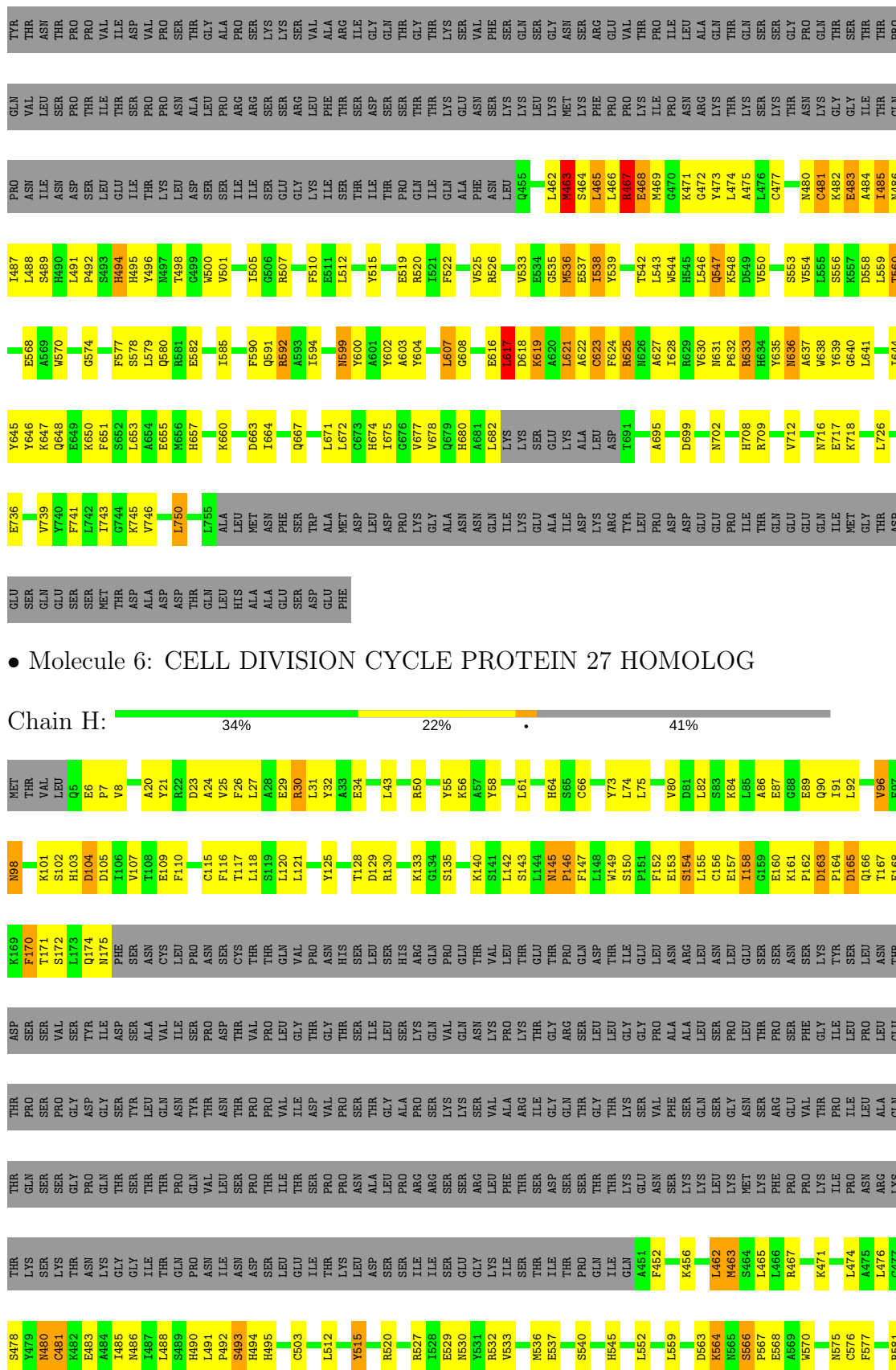
Chain E:  25% 21% 5% 49%

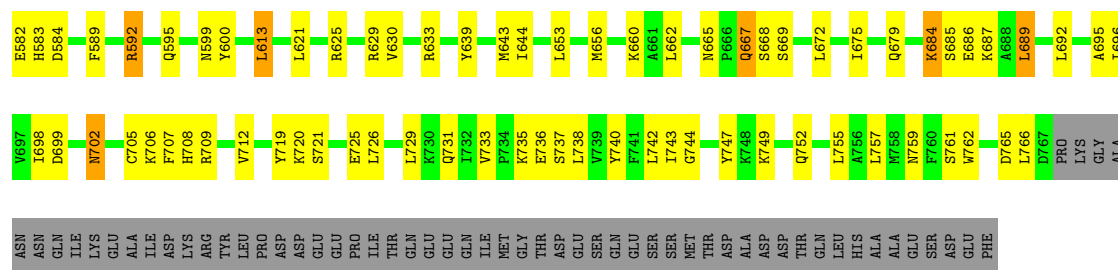


- Molecule 6: CELL DIVISION CYCLE PROTEIN 27 HOMOLOG

Chain F: 30% 21% 5% 44%

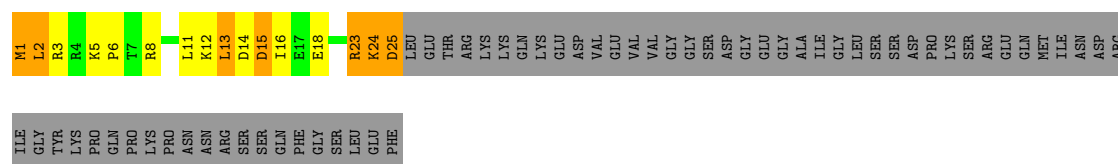






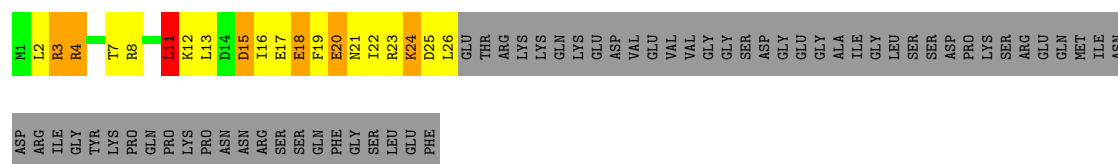
• Molecule 7: ANAPHASE-PROMOTING COMPLEX SUBUNIT CDC26

Chain G: 11% 11% 8% 71%



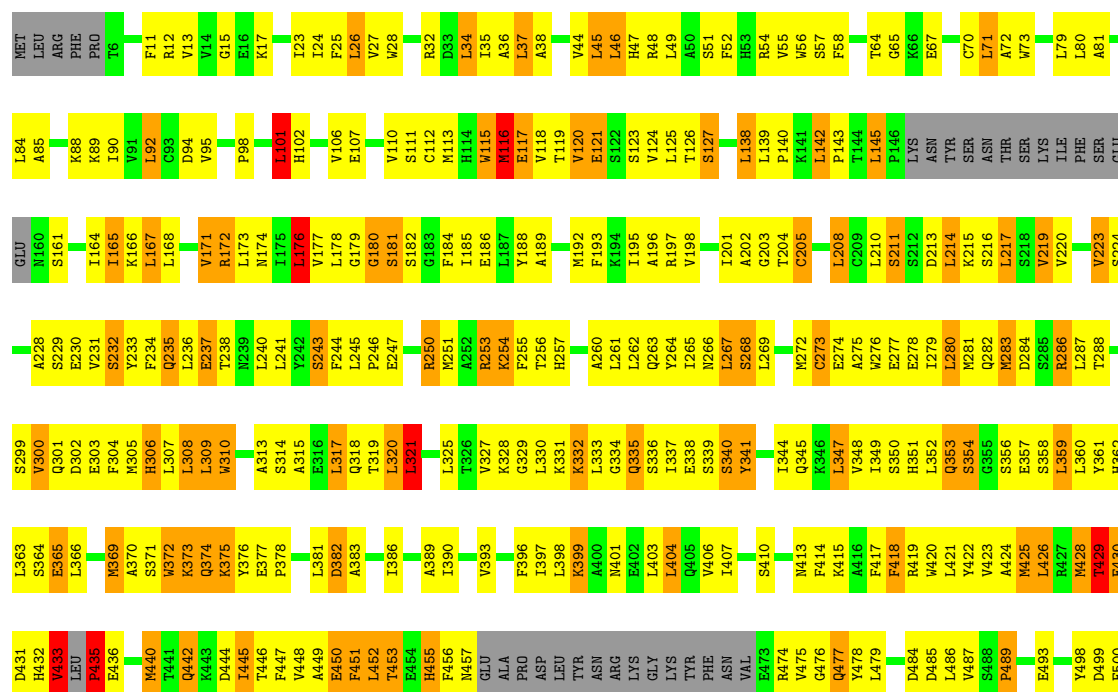
• Molecule 7: ANAPHASE-PROMOTING COMPLEX SUBUNIT CDC26

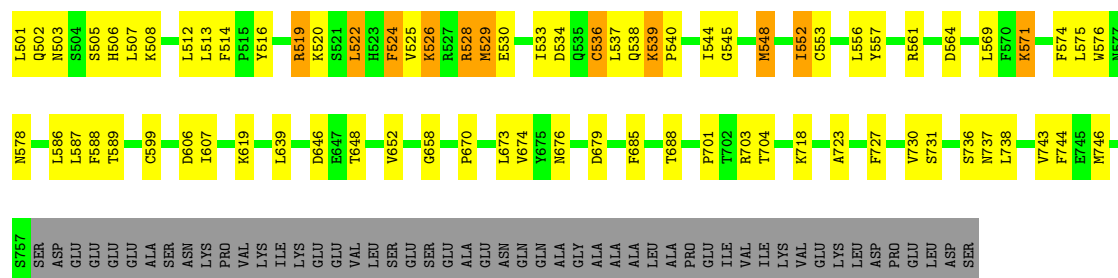
Chain W: 7% 15% 7% 69%



• Molecule 8: ANAPHASE-PROMOTING COMPLEX SUBUNIT 4

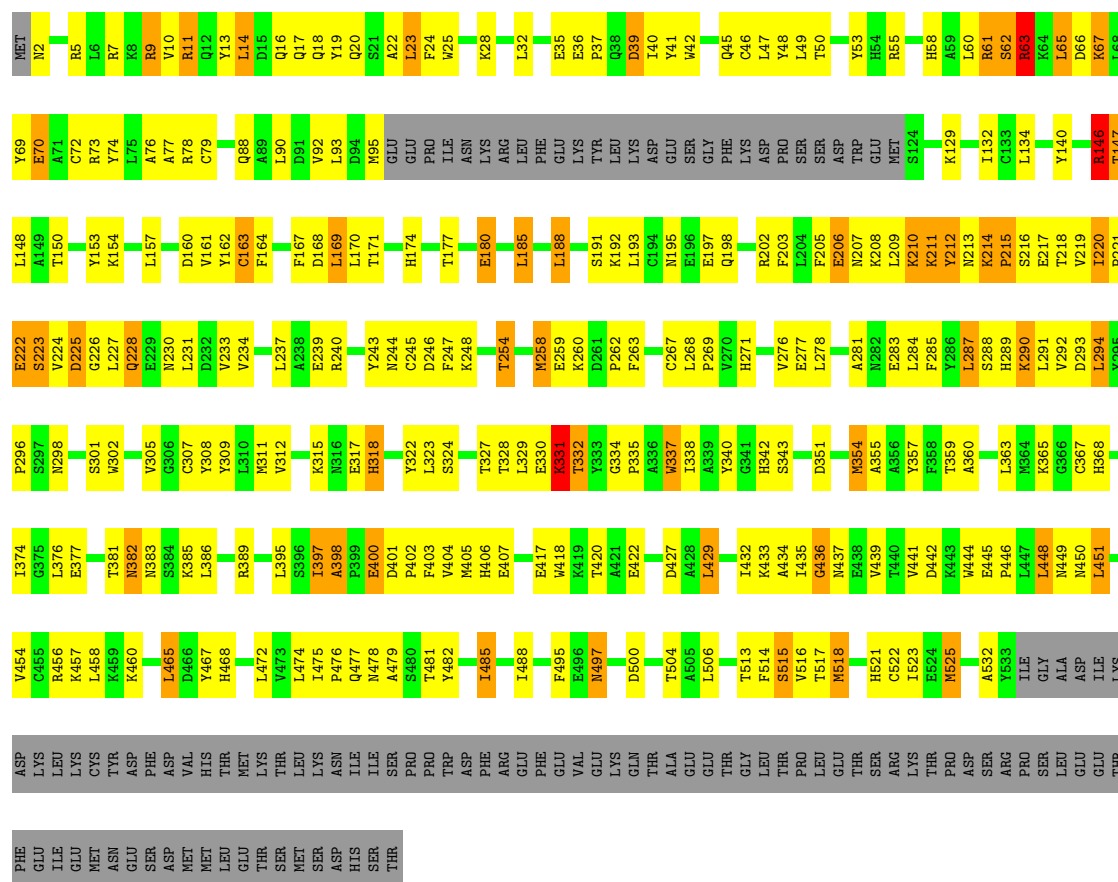
Chain I: 42% 35% 11% 11%





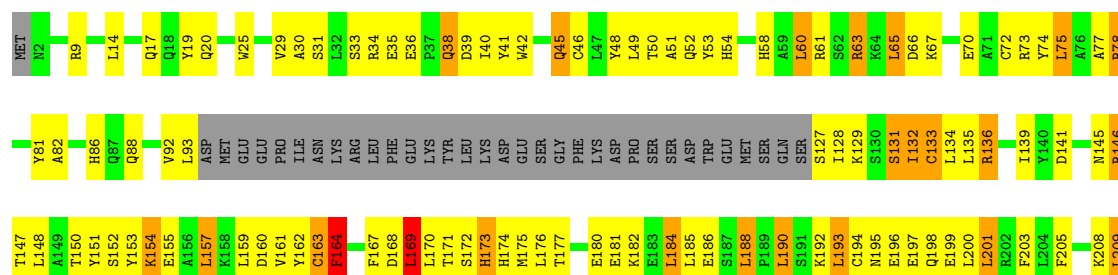
• Molecule 9: CELL DIVISION CYCLE PROTEIN 16 HOMOLOG

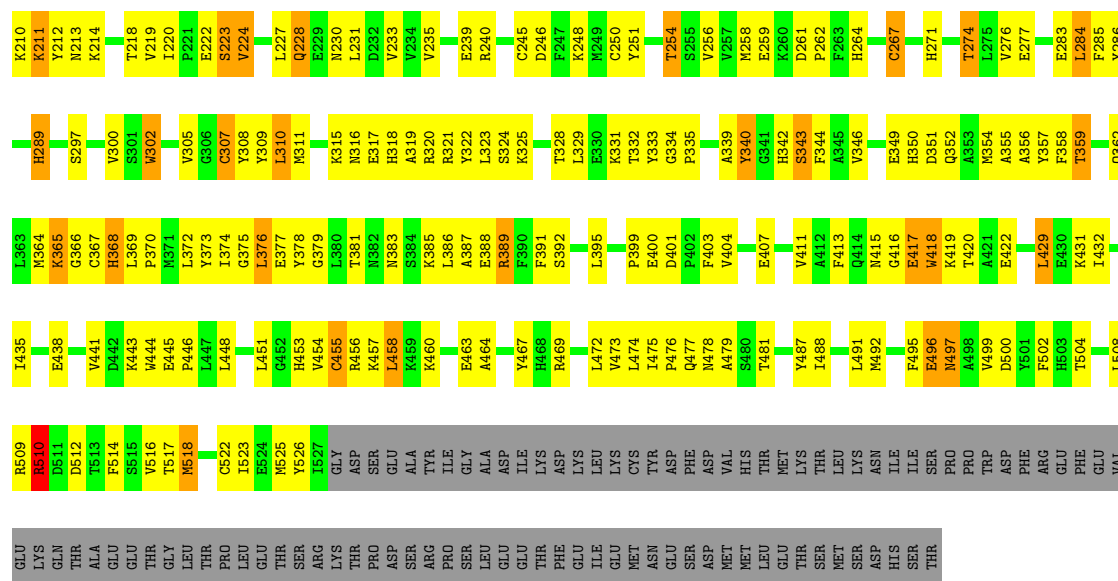
Chain J: 38% 35% 8% 19%



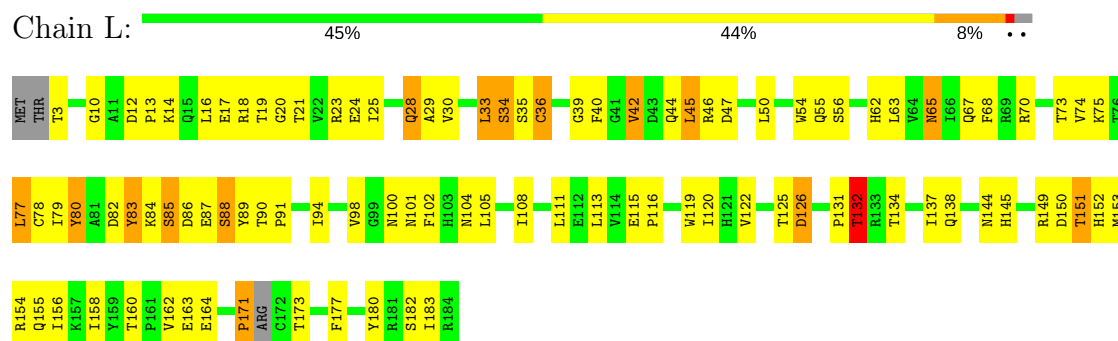
• Molecule 9: CELL DIVISION CYCLE PROTEIN 16 HOMOLOG

Chain K: 33% 38% 8% 20%

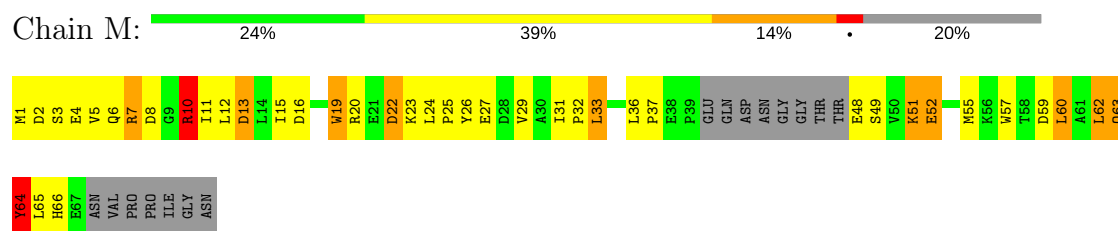




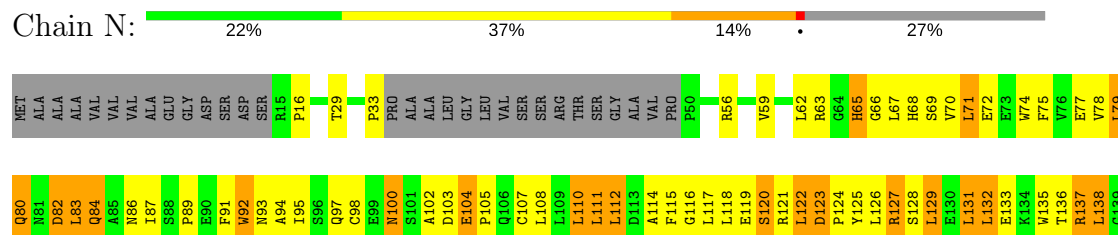
• Molecule 10: ANAPHASE-PROMOTING COMPLEX SUBUNIT 10



• Molecule 11: ANAPHASE-PROMOTING COMPLEX SUBUNIT 13



• Molecule 12: ANAPHASE-PROMOTING COMPLEX SUBUNIT 2

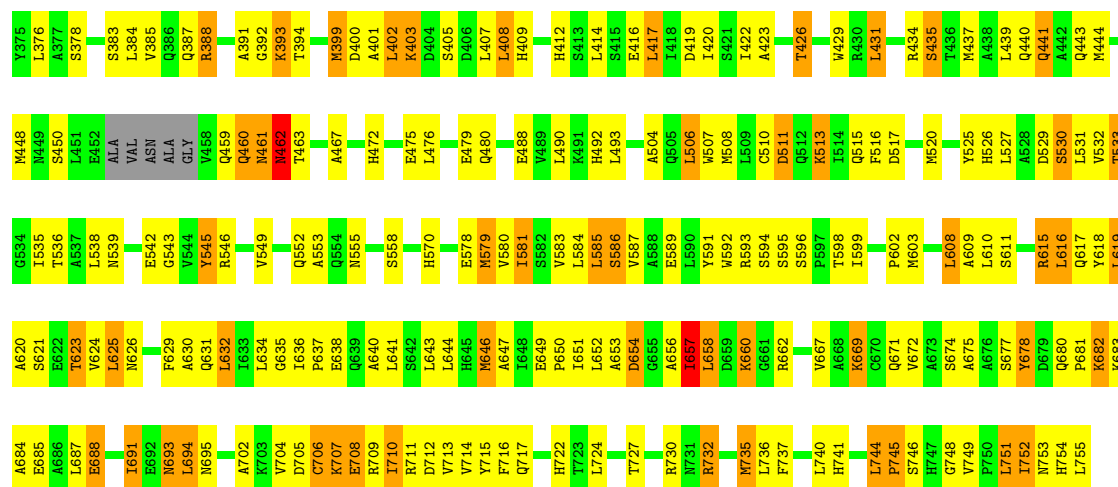


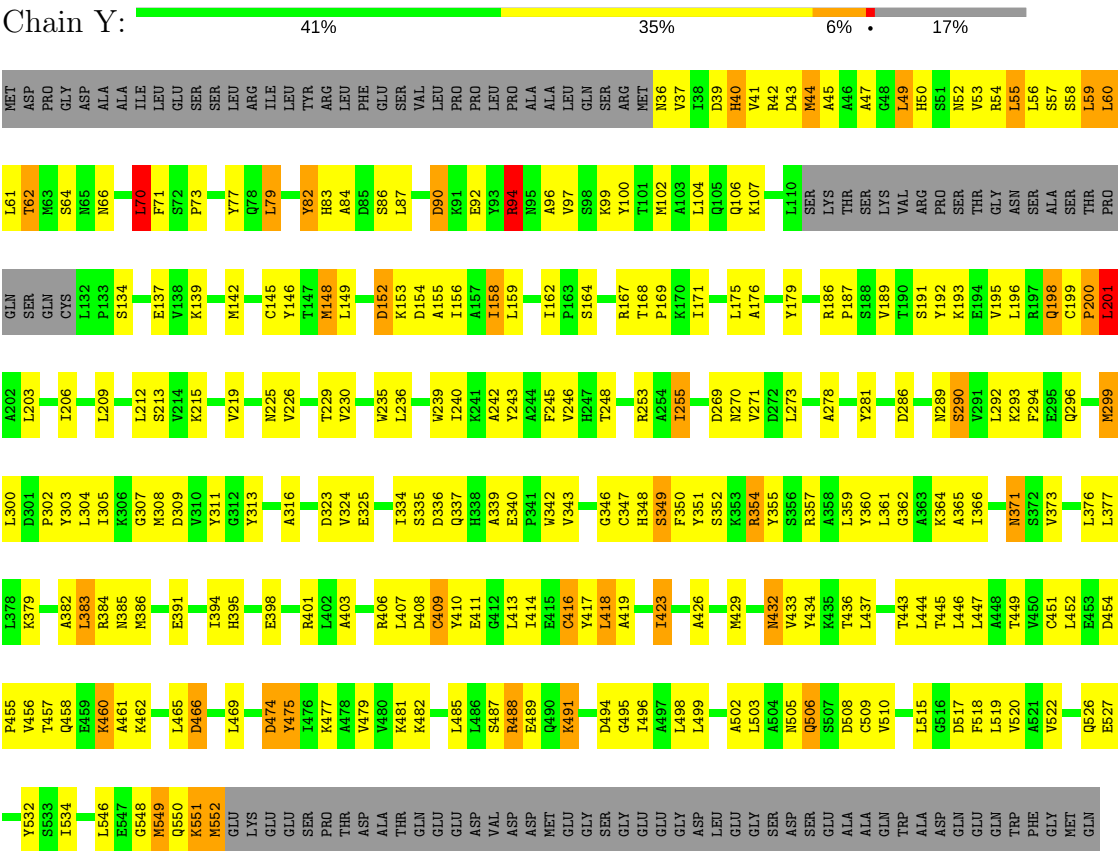
GLU	ILE	ASP	LEU	GLN	GLU	LEU	GLN	LYS	LYS	VAL	ARG	ASP	GLN	GLN	GLN	LYS	LEU	VAL	TYR	SER	ASN	CYS	SER																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																													
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• Molecule 13: ANAPHASE-PROMOTING COMPLEX SUBUNIT 5

Chain O:  41% 37% 12% 9%

MET	ALA	SER	VAL	HIS	GLU	SER	LEU	THR	PHE	ASN	PRO	MET	THR	ASN	ASN	GLY	VAL	HIS	ALA	ASN	VAL	PHE	G25	T26	K27	T31	P32	Y33	K34	I35	L38	V39	M108	E109	F112	D113	D114	L115	S116	D117	S118	F119	E123	P124	E125	V126	H127	K128	V129	S130	L131	V132	P135	L136	L68
Q69	D72	I73	T74	L75	L78	Y79	K80	L81	I82	E83	E84	S85	C86	A90	N91	S92	V93	Q94	I95	R96	I97	K98	L99	M100	A101	E102	G103	E104	L105	K106	D107	M108	E109	F112	D113	D114	L115	S116	D117	S118	F119	E123	P124	E125	V126	H127	K128	V129	S130	L131	V132	P135	L136	L68	
R137	H138	M139	I140	Y143	S144	L145	L146	F148	S149	Q150	V151	Y155	T156	A157	L158	Q159	Q160	Y161	F162	Q163	E166	K167	L168	T169	A170	E171	M172	I173	Q174	R175	L176	Y177	G178	C179	F180	L181	R182	Y184	M185	Q186	R189	G190	G191	GLY	GLY	GLY	THR	ASP	PRO	GLU	LEU	GLY	GLY	LEU	ASP
VAL	SER	CYS	SER	GLY	P206	L207	S208	Q209	Q210	Q211	F214	F215	L216	S217	Q218	Q219	L222	N225	D226	E227	L231	F232	P233	A234	Q237	K238	E239	L240	N241	N242	L243	L244	N247	P248	D249	F250	A251	E252	Y255	L256	S257	N261	L262	R263	V264	Q265	D266	V267	L274	L275	P374				
D279	R280	T284	N291	G292	E293	R298	S299	L300	R301	N306	Y317	A320	E321	A323	L322	Q324	Q325	T328	R329	I330	N335	D336	L340	Q341	L344	S345	W346	L347	Y348	V349	L350	G351	Q352	K353	S354	D355	S356	S357	Y358	V359	L360	L361	E362	H363	K367	P374									





4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	Not provided	Depositor
Microscope	OTHER	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	27	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	78000	Depositor
Image detector	FEI FALCON II (4K X 4K)	Depositor

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	$\# Z > 2$	RMSZ	$\# Z > 2$
1	A	0.73	11/12168 (0.1%)	0.93	35/16587 (0.2%)
10	L	0.74	1/1468 (0.1%)	0.93	3/1993 (0.2%)
11	M	0.65	1/490 (0.2%)	0.98	5/665 (0.8%)
12	N	0.75	7/4860 (0.1%)	0.98	16/6584 (0.2%)
13	O	0.87	3/5499 (0.1%)	0.95	12/7432 (0.2%)
14	T	0.70	0/78	1.02	0/107
15	X	0.64	2/3827 (0.1%)	0.87	6/5180 (0.1%)
15	Y	0.56	0/3922	0.83	9/5304 (0.2%)
2	B	0.63	0/674	0.95	2/913 (0.2%)
3	C	0.73	1/4403 (0.0%)	0.93	10/5942 (0.2%)
3	P	0.66	1/4141 (0.0%)	0.89	6/5593 (0.1%)
4	D	0.62	0/446	0.83	1/610 (0.2%)
5	E	0.56	0/459	0.68	0/619
6	F	0.68	1/3704 (0.0%)	0.82	4/5019 (0.1%)
6	H	0.71	1/3969 (0.0%)	0.85	2/5366 (0.0%)
7	G	0.56	0/221	0.93	1/292 (0.3%)
7	W	0.57	0/219	0.93	1/291 (0.3%)
8	I	0.72	3/5754 (0.1%)	0.96	20/7806 (0.3%)
9	J	0.72	3/4152 (0.1%)	0.97	10/5623 (0.2%)
9	K	0.71	2/4085 (0.0%)	0.90	6/5530 (0.1%)
All	All	0.71	37/64539 (0.1%)	0.91	149/87456 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
12	N	0	1
14	T	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
8	I	0	5
All	All	0	8

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

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

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

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

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

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

5.2 Too-close contacts

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

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	649	0	595	33	0
3	C	4306	0	4273	274	0
3	P	4046	0	3998	248	0
4	D	436	0	396	25	0
5	E	450	0	435	31	0
6	F	3618	0	3452	380	0
6	H	3879	0	3805	267	0
7	G	220	0	233	30	0
7	W	218	0	222	26	0
8	I	5634	0	5522	590	0
9	J	4053	0	3960	371	0
9	K	3988	0	3911	440	0
10	L	1435	0	1381	165	0
11	M	481	0	457	72	0
12	N	4767	0	4685	1269	0
13	O	5400	0	5416	464	0
14	T	79	0	77	8	0
15	X	3767	0	3820	438	0
15	Y	3862	0	3914	412	0
16	B	3	0	0	0	0
All	All	63181	0	62107	6915	0

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

The worst 5 of 6915 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

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

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1539/1944 (79%)	1372 (89%)	112 (7%)	55 (4%)	4	33
2	B	83/84 (99%)	72 (87%)	7 (8%)	4 (5%)	2	25
3	C	518/597 (87%)	490 (95%)	23 (4%)	5 (1%)	18	61
3	P	486/597 (81%)	466 (96%)	16 (3%)	4 (1%)	22	65
4	D	53/121 (44%)	47 (89%)	5 (9%)	1 (2%)	9	47
5	E	54/110 (49%)	54 (100%)	0	0	100	100
6	F	454/824 (55%)	433 (95%)	19 (4%)	2 (0%)	38	77
6	H	484/824 (59%)	469 (97%)	10 (2%)	5 (1%)	18	61
7	G	23/85 (27%)	23 (100%)	0	0	100	100
7	W	24/85 (28%)	23 (96%)	0	1 (4%)	3	28
8	I	717/808 (89%)	682 (95%)	20 (3%)	15 (2%)	8	45
9	J	500/620 (81%)	468 (94%)	25 (5%)	7 (1%)	13	53
9	K	487/620 (78%)	456 (94%)	27 (6%)	4 (1%)	22	65
10	L	180/185 (97%)	169 (94%)	9 (5%)	2 (1%)	17	59
11	M	55/74 (74%)	49 (89%)	5 (9%)	1 (2%)	10	48
12	N	590/822 (72%)	547 (93%)	26 (4%)	17 (3%)	5	38
13	O	682/755 (90%)	643 (94%)	27 (4%)	12 (2%)	10	48
14	T	13/15 (87%)	11 (85%)	1 (8%)	1 (8%)	1	13
15	X	480/599 (80%)	463 (96%)	12 (2%)	5 (1%)	18	61
15	Y	492/599 (82%)	473 (96%)	15 (3%)	4 (1%)	22	65
All	All	7914/10368 (76%)	7410 (94%)	359 (4%)	145 (2%)	14	48

5 of 145 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	274	VAL

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

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1243/1720 (72%)	967 (78%)	276 (22%)	1	6
2	B	65/75 (87%)	54 (83%)	11 (17%)	2	14
3	C	452/520 (87%)	384 (85%)	68 (15%)	3	19
3	P	422/520 (81%)	368 (87%)	54 (13%)	5	25
4	D	46/115 (40%)	41 (89%)	5 (11%)	7	33
5	E	47/89 (53%)	35 (74%)	12 (26%)	0	4
6	F	371/727 (51%)	310 (84%)	61 (16%)	2	15
6	H	408/727 (56%)	368 (90%)	40 (10%)	9	38
7	G	25/77 (32%)	16 (64%)	9 (36%)	0	1
7	W	23/77 (30%)	15 (65%)	8 (35%)	0	2
8	I	607/730 (83%)	508 (84%)	99 (16%)	3	15
9	J	425/548 (78%)	363 (85%)	62 (15%)	3	20
9	K	423/548 (77%)	356 (84%)	67 (16%)	3	17
10	L	155/170 (91%)	139 (90%)	16 (10%)	8	36
11	M	52/67 (78%)	38 (73%)	14 (27%)	0	3
12	N	489/724 (68%)	371 (76%)	118 (24%)	1	4
13	O	573/650 (88%)	469 (82%)	104 (18%)	2	11
14	T	1/2 (50%)	1 (100%)	0	100	100
15	X	406/513 (79%)	370 (91%)	36 (9%)	11	43
15	Y	417/513 (81%)	373 (89%)	44 (11%)	8	35

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	6650/9112 (73%)	5546 (83%)	1104 (17%)	6 15

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

Mol	Chain	Res	Type
8	I	165	ILE
9	J	294	LEU
7	W	15	ASP
8	I	254	LYS
8	I	450	GLU

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

Mol	Chain	Res	Type
8	I	477	GLN
9	K	318	HIS
15	X	371	ASN
9	J	38	GLN
9	J	406	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates 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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.