



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Sep 2, 2019 – 07:43 PM EDT

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

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : 2.4

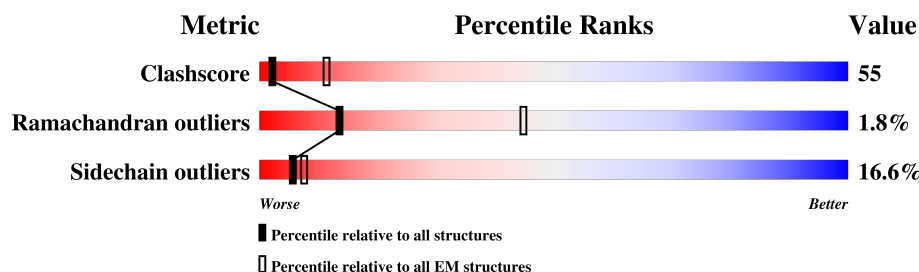
1 Overall quality at a glance

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.



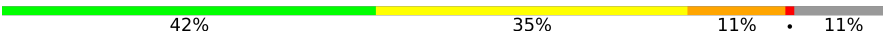
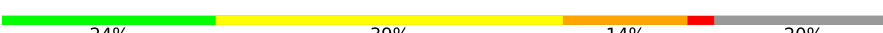
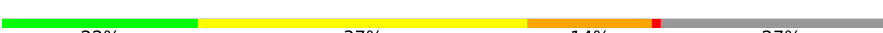



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531

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	
2	B	84	
3	C	597	
3	P	597	
4	D	121	
5	E	110	
6	F	824	
6	H	824	
7	G	85	

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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		

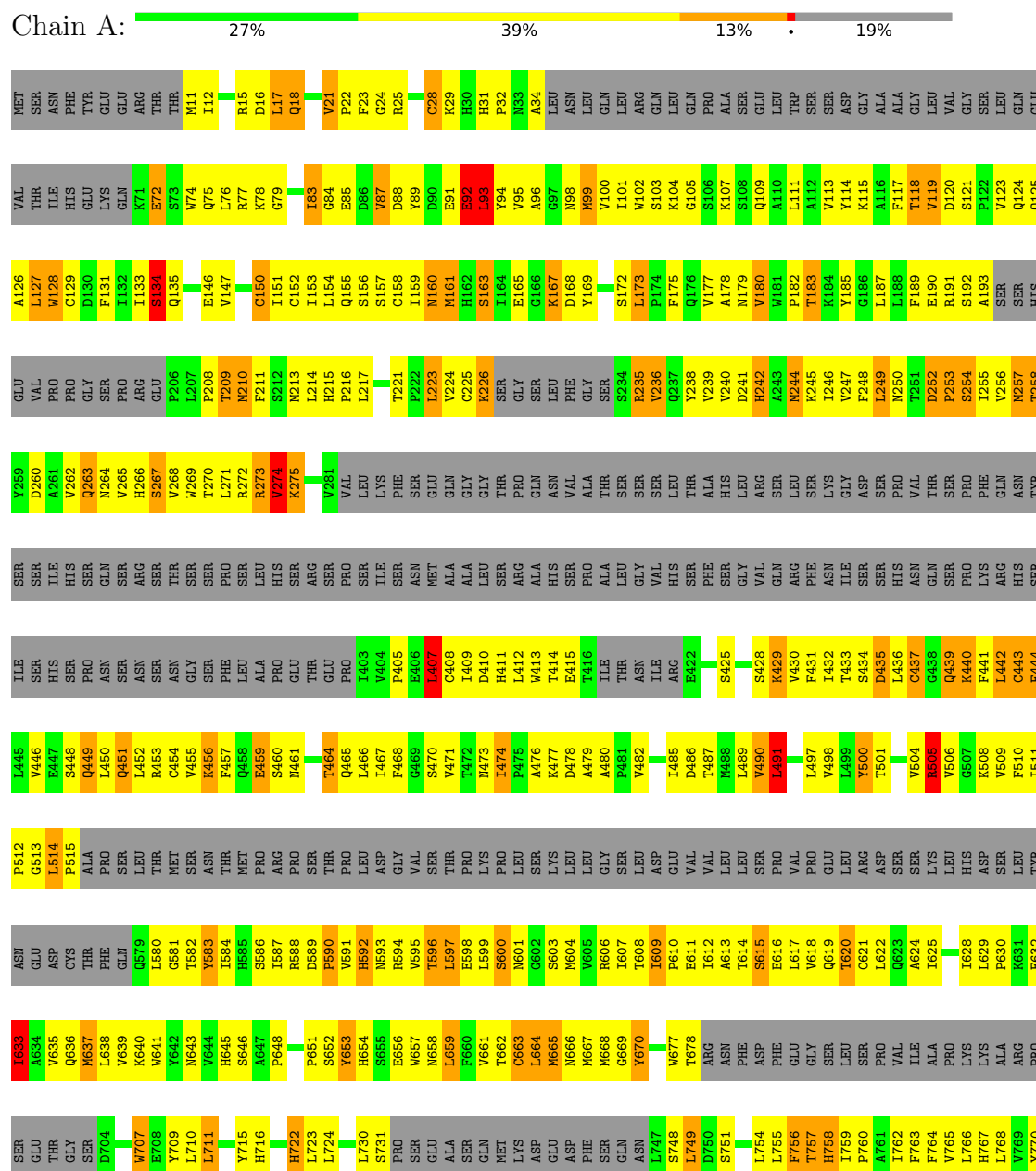
- Molecule 16 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

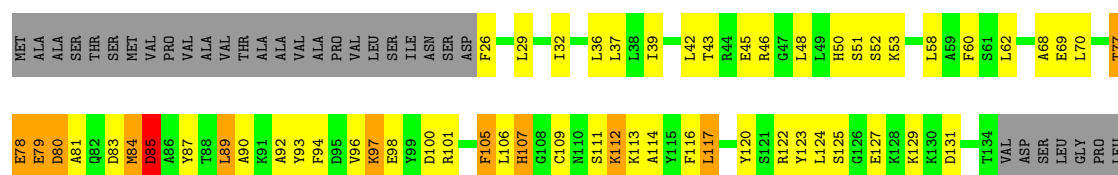
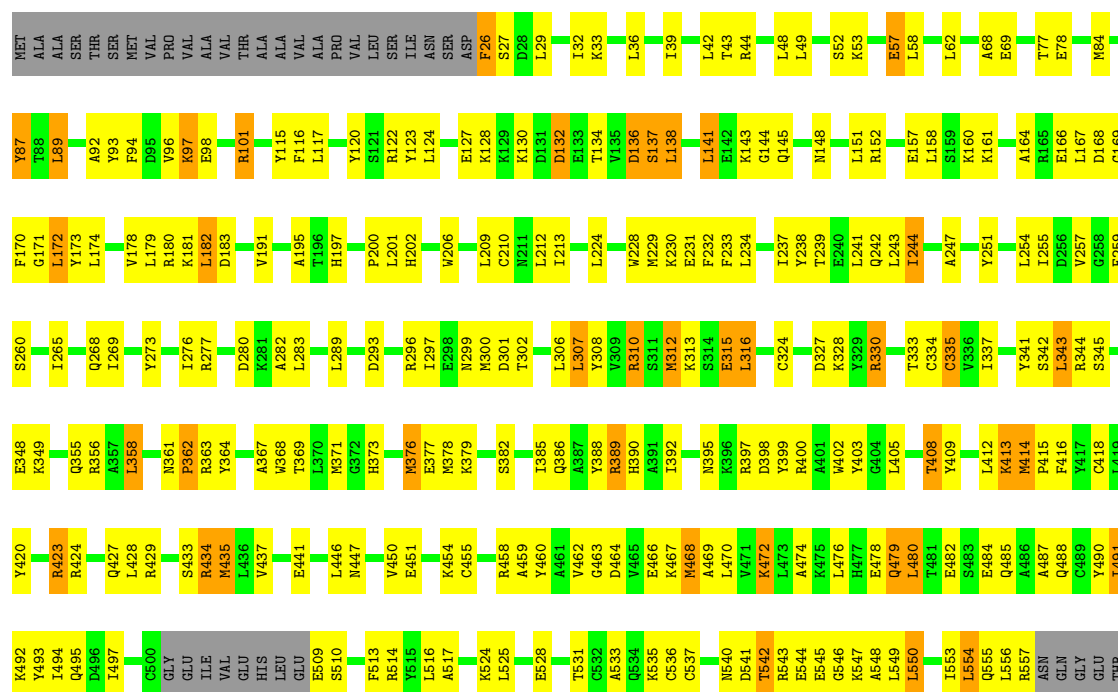
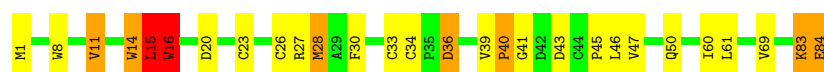
3 Residue-property plots

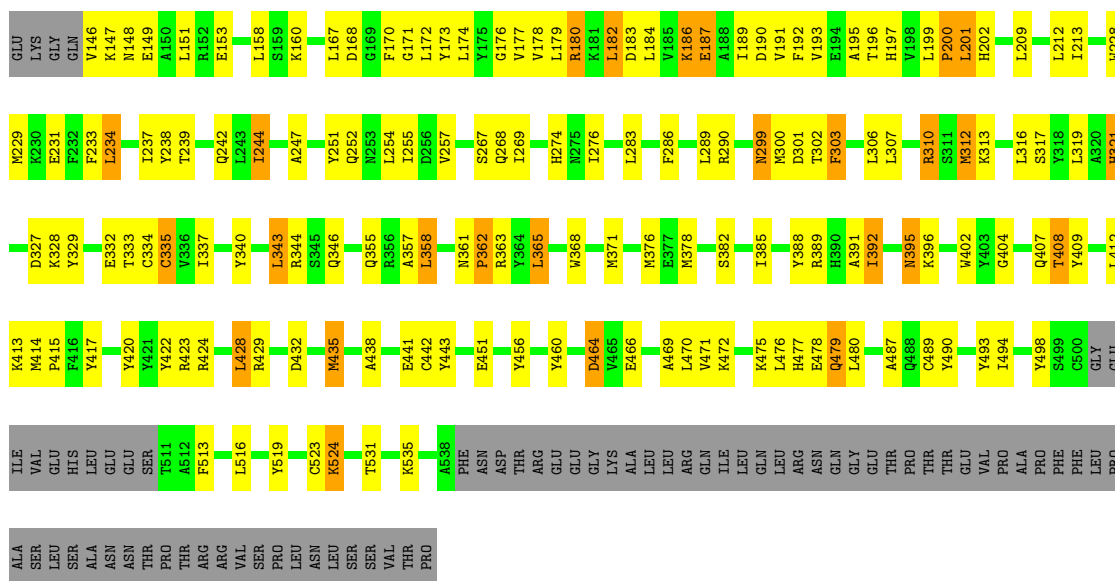
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according 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

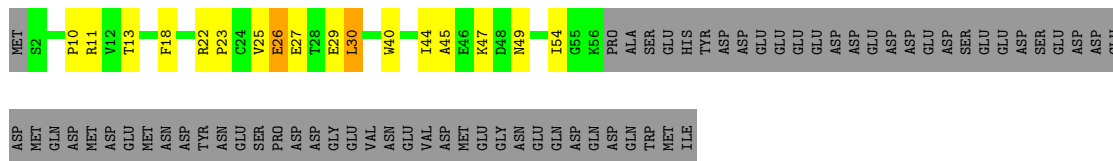


E1807	S1743	I1678	L1612	L1533	A1460	I1383	P1238	E1167	I1100	V1034	P966	I899	M831	E771
T1808	D1744	D1679	E1616	K1534	H1461	L1313	T1239	L1168	P1101	Q1035	P967	I900	H832	E772
E1810	P1745	L1680	P1615	V1536	Y1462	I1314	S1240	A1169	I1102	D1036	A967	I1E	H833	L773
L1811	A1746	T1684	R1617	L1536	Y1463	G1315	T1241	P1170	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	LEU	S1043	P971	LYS	F837	T777
K1815	A1751	L1690	P1621	L1395	L1395	M1321	N1249	L1176	GLN	A1044	V974	VAL	T838	L778
L1816	E1752	L1691	V1622	L1396	L1470	P1322	Q1250	M1177	GLN	A1046	L977	VAL	E840	G780
L1817	L1753	L1692	D1623	M1544	S1471	E1323	V1251	L1181	GLU	P1046	L978	GLN	P841	E781
L1818	F1754	S1692	V1624	K1545	L1472	Q1324	V1254	L1182	P1112	V1047	G979	GLN	P842	G782
L1819	C1755	K1693	D1625	L1546	G1473	L1325	V1255	G1183	P1113	K1048	R980	GLU	S843	G783
F1820	K1756	D1694	T1626	G1547	F1474	Y1326	V1255	H1184	R1114	V1049	Q981	GLU	I844	G784
F1821	P1757	G1695	N1627	M1550	F1475	Q1327	L1259	L1185	M1115	Q1053	Q982	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	D1119	E1056	S984	SER	W848	E788
S1825	K1761	L1701	A1632	F1554	N1481	H1333	T1264	N1193	L1120	L1057	X985	PHE	L789	L790
H1826	G1762	A1702	L1633	F1555	L1482	ARG	A1265	N1192	H1060	L1060	C988	HIS	L852	V791
Q1827	K1764	A1703	E1634	L1556	L1482	PHE	H1266	H1194	D1126	E1061	E989	SER	K853	Q792
L1830	L1768	Q1705	V1637	H1558	L1488	GLN	H1268	Y1196	D1127	F1062	P993	SER	M857	A794
H1833	D1769	L1706	Y1638	L1562	K1493	GLY	T1269	T1198	P1129	E1064	GLY	S924	P858	A795
P1834	F1771	S1707	G1640	G1563	D1494	MET	Y1272	L1199	N1130	E1065	LYS	S925	P859	D796
L1835	S1772	Y1708	K1649	L1564	F1495	HIS	L1274	H1201	M1131	K1066	LYS	L926	Y860	L797
L1836	Q1773	K1709	E1648	L1565	M1496	ARG	H1274	E1202	F1132	E1067	VAL	A927	P861	K798
G1837	S1774	E1710	Y1644	F1566	T1497	GLU	L1275	A1275	P1141	E1068	LEU	N934	Y862	L799
L1838	L1775	L1713	E1645	Q1570	Y1430	LYS	E1276	M1203	S1136	N1069	SER	R929	P864	G800
F1839	Y1776	G1714	Q1646	Q1571	P1431	LVS	T1277	T1204	F1137	L1071	SER	L930	P865	P801
R1840	E1777	L1715	K1648	Y1572	Q1432	LVS	G1278	S1205	H1138	L1071	ASP	V931	R866	Y803
S1841	Q1778	Y1716	E1649	S1573	I1433	LVS	R1279	T1206	N1139	Q1072	VAL	N933	C867	D804
L1842	V1779	S1717	E1650	L1574	I1434	HIS	P1281	G1207	G1140	L1073	PRO	N934	E868	H805
G1845	Q1780	L1718	E1651	L1574	Q1351	Q1351	P1281	L1208	V1141	C1074	SER	Y806	R869	Y806
P1846	E1782	L1719	M1652	T1507	L1352	L1352	G1282	Y1212	A1142	Q1075	GLY	F939	S870	Y807
L1847	T1783	Q1721	A1653	N1577	N1437	D1356	P1283	V1212	A1143	R1076	THR	N940	R871	R808
V1848	P1784	L1722	L1656	N1578	S1438	T1357	Y1287	A1215	G1144	T1077	GLU	T941	L872	D809
T1851	E1785	L1723	L1657	L1585	SER	L1358	Y1287	K1216	L1145	M1078	THR	L941	V873	Y810
L1852	L1786	Y1723	E1658	L1512	LEU	N1359	D1290	L1217	L1147	L1080	GLU	L944	I877	P811
D1853	L1787	A1724	P1659	E1513	SER	N1359	E1291	L1218	A1148	P1081	E1011	L945	A878	L813
N1854	T1791	N1726	L1660	G1515	GLU	V1360	E1292	G1219	P1149	V1082	E1012	T946	L879	Y814
D1857	A1792	R1727	H1661	V1518	ILE	C1364	S1293	M1220	A1150	G1063	D1014	L947	Y860	R815
Q1857	M1793	S1728	L1662	V1519	GLU	P1365	Y1294	L1224	S1151	R1084	G1015	P948	I881	T816
L1858	M1793	T1728	L1663	L1519	LEU	L1373	G1299	Q1152	Q1152	G1085	M1016	F949	L882	T817
W1859	D1794	E1729	K1664	L1520	PRO	N1374	L1300	T1225	I1153	M1086	D1018	G950	L882	Q818
L1860	Q1795	A1730	K1665	L1521	CYS	L1374	L1300	R1226	D1154	F1087	D1018	Y951	L887	Q819
Q1861	A1796	N1599	Q1665	S1522	SER	L1371	A1301	L1227	S1155	T1088	M1019	A952	VAL	V820
L1862	L1797	F1733	L1666	L1523	GLU	A1372	L1302	L1228	A1156	L1089	N1020	L953	SER	G821
G1863	R1798	K1734	K1669	A1524	ASP	M1373	G1303	L1229	W1157	F1090	M1024	R956	ASP	T822
L1864	P1799	P1735	M1670	M1525	L1452	L1374	L1304	I1230	I1158	H1093	S1025	D957	GLU	L823
L1865	L1800	E1736	L1672	V1526	N1453	Y1375	V1305	H1231	V1159	P1094	L1026	S892	S892	R824
L1866	G1801	T1737	R1673	M1527	L1454	L1376	C1306	H1232	V1160	V1094	L1026	S893	S893	P825
L1867	R1802	L1738	E1673	A1528	L1455	K1377	C1307	P1233	N1161	V1095	P1097	Y959	Q894	G826
C1867	S1739	S1739	W1674	G1529	T1456	T1378	G1308	A1234	K1162	P1096	E1030	Y960	Y895	Q827
L1868	E1804	A1740	E1675	S1530	L1457	N1379	H1309	A1234	P1163	T1097	E1030	H961	R896	Q827
H1869	M1805	F1741	L1676	G1531	L1458	N1379	H1309	L1235	P1163	T1097	D1031	H961	T897	T828
A1870	S1806	T1742	L1677	N1532	Q1459	N1380	S1311	L1236	K1164	E1098	L1032	C962	L896	G829
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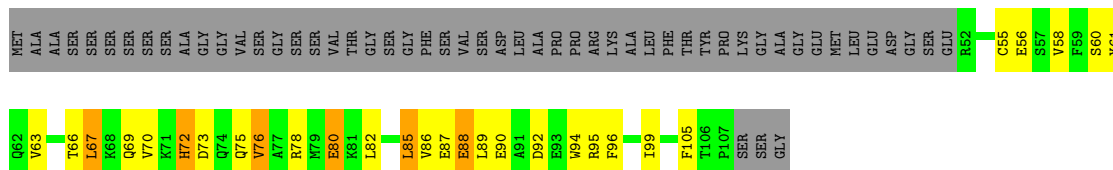




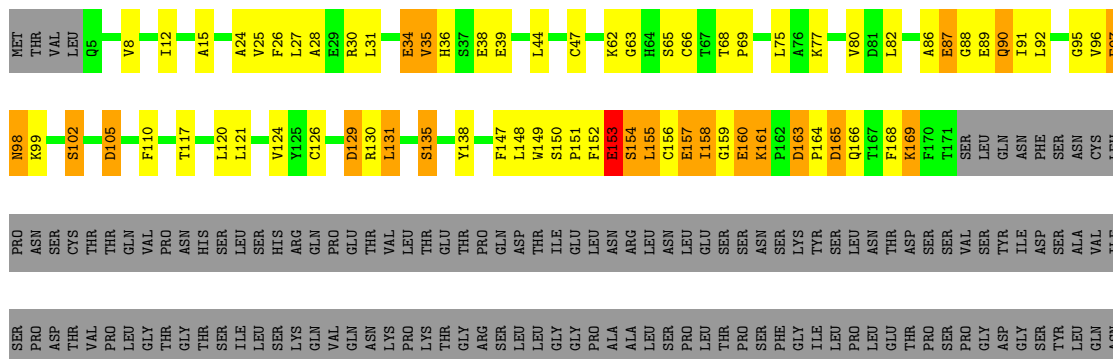
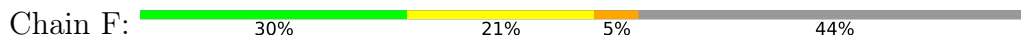
- Molecule 4: ANAPHASE-PROMOTING COMPLEX SUBUNIT 15

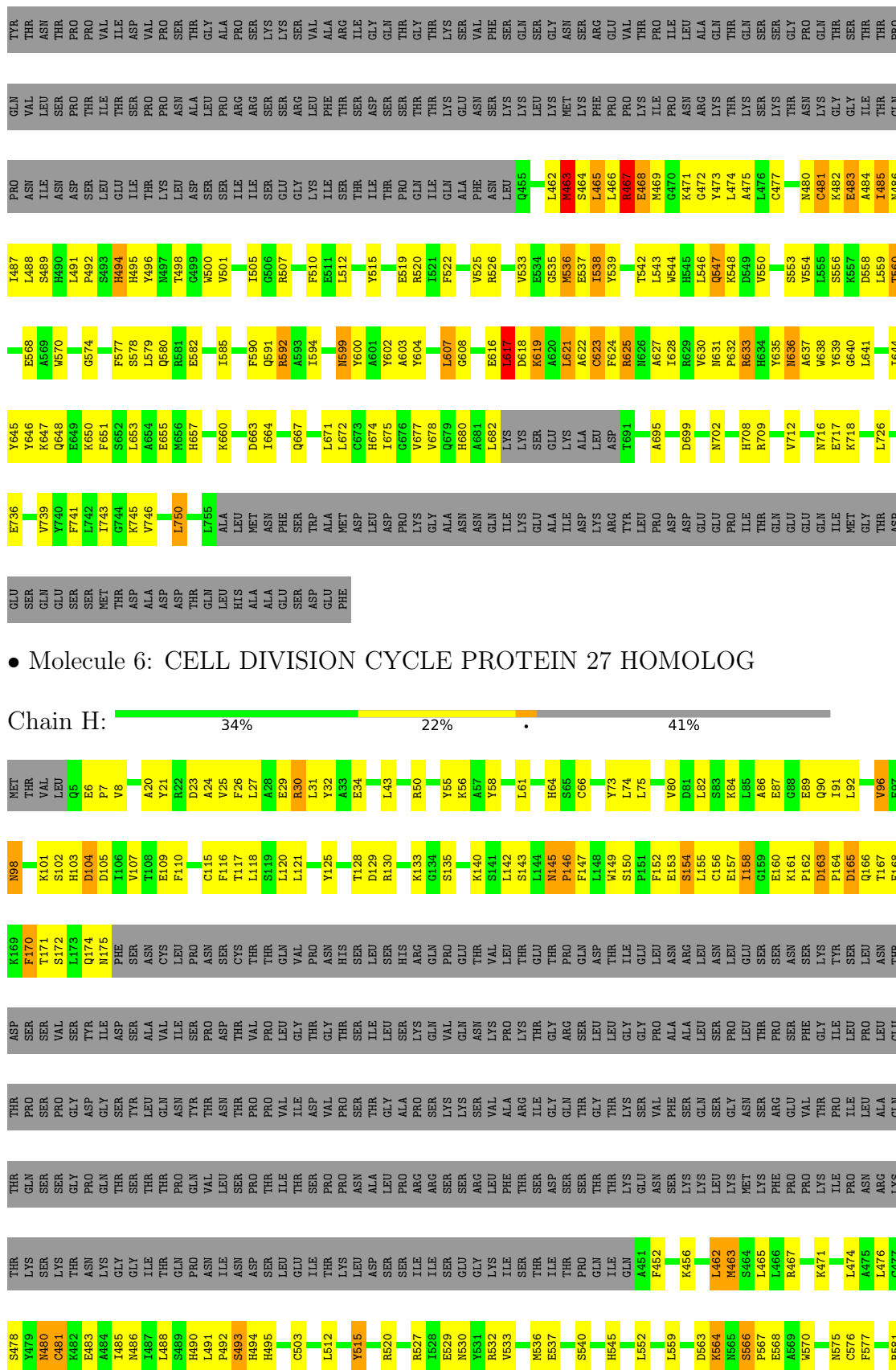


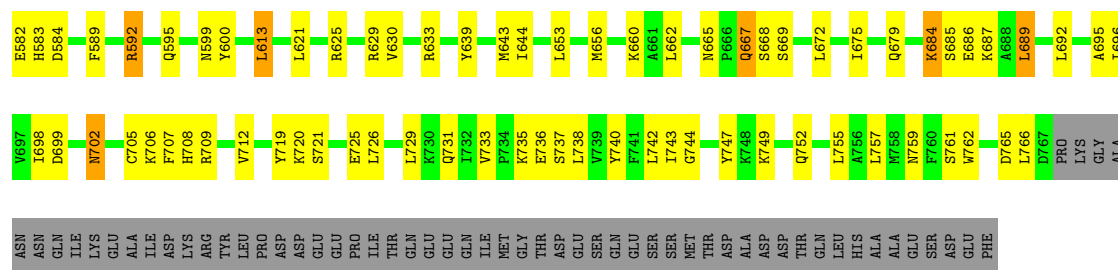
- Molecule 5: ANAPHASE-PROMOTING COMPLEX SUBUNIT 16



- Molecule 6: CELL DIVISION CYCLE PROTEIN 27 HOMOLOG

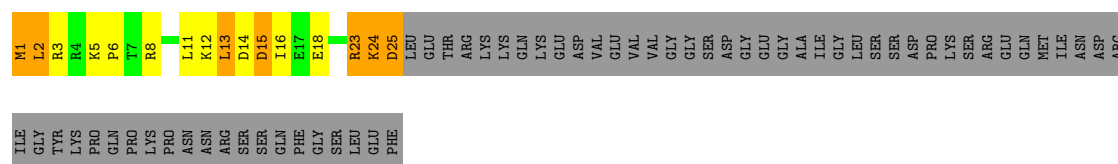






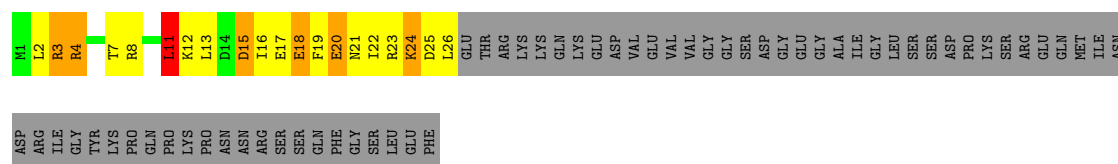
• Molecule 7: ANAPHASE-PROMOTING COMPLEX SUBUNIT CDC26

Chain G: 11% 11% 8% 71%



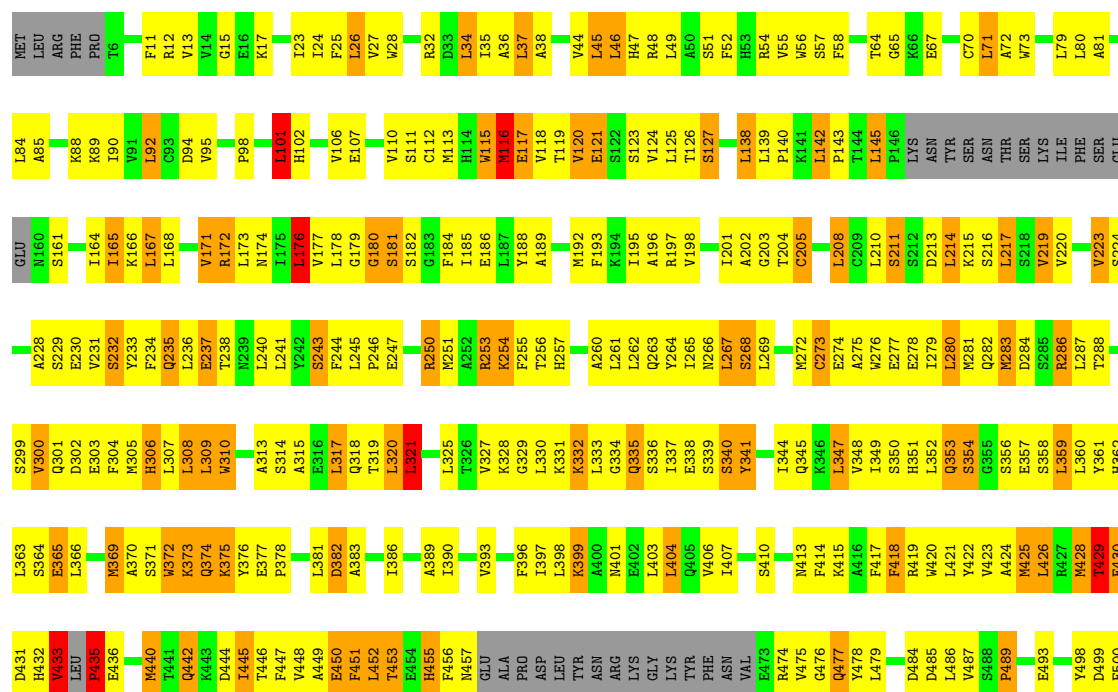
• Molecule 7: ANAPHASE-PROMOTING COMPLEX SUBUNIT CDC26

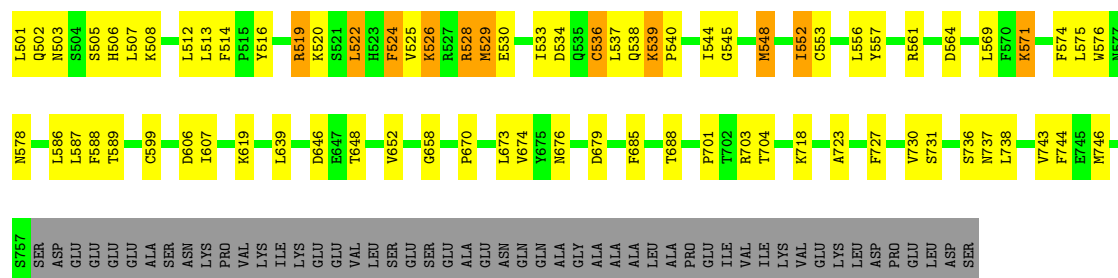
Chain W: 7% 15% 7% 69%



• Molecule 8: ANAPHASE-PROMOTING COMPLEX SUBUNIT 4

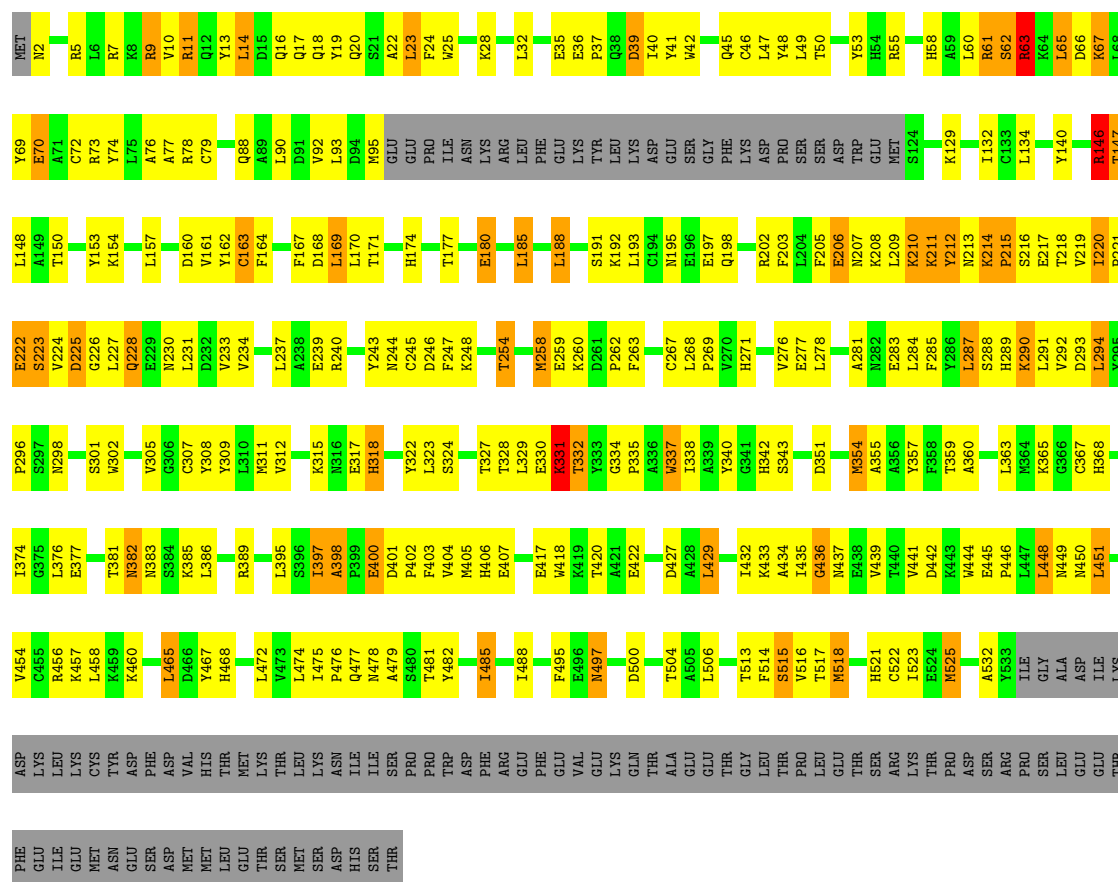
Chain I: 42% 35% 11% 11%





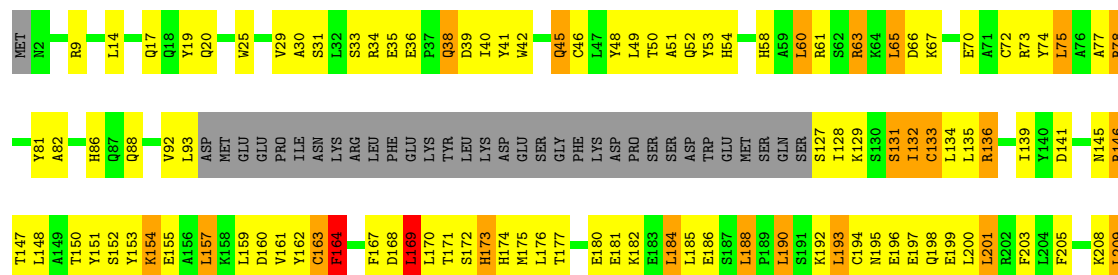
• Molecule 9: CELL DIVISION CYCLE PROTEIN 16 HOMOLOG

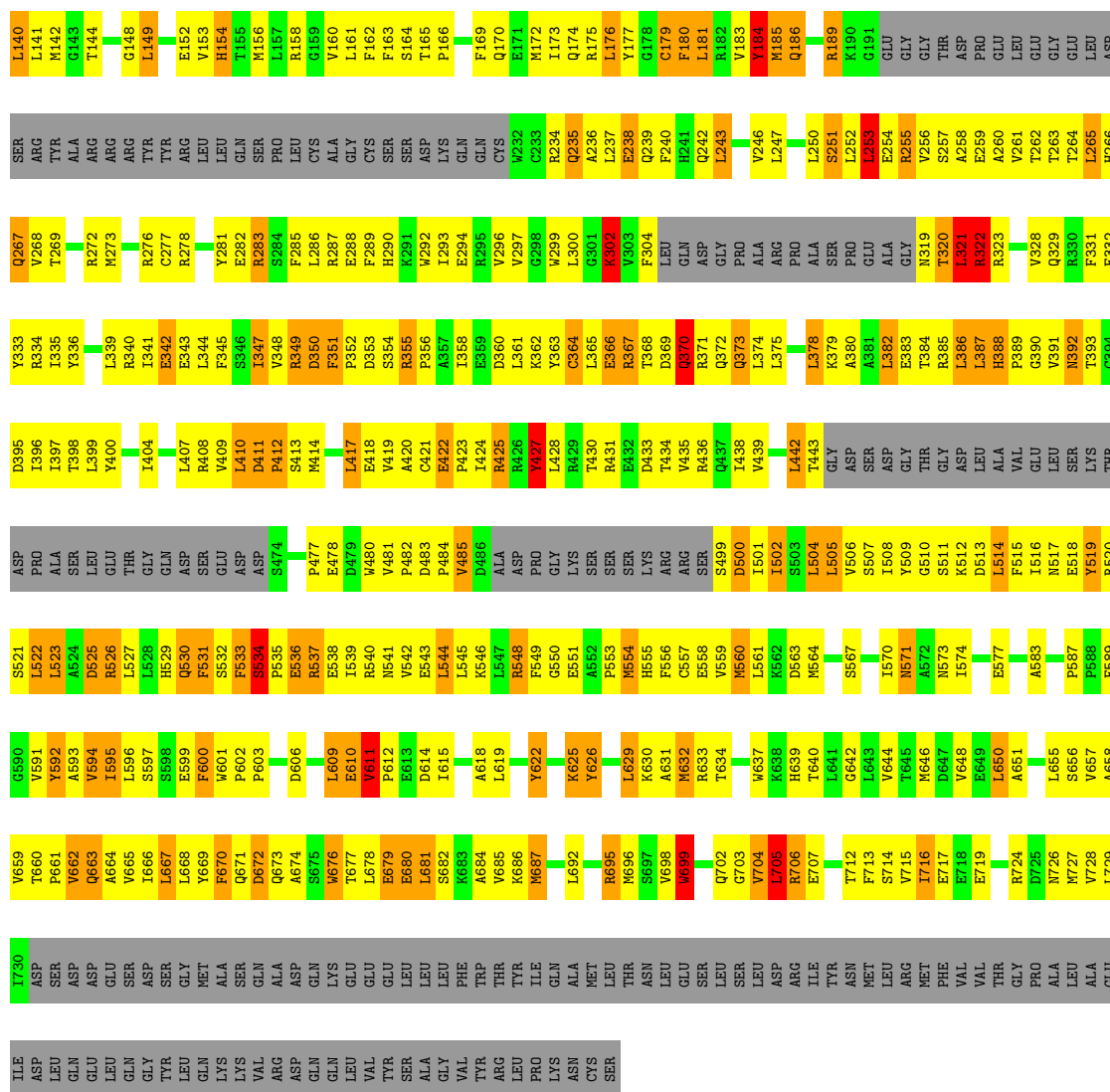
Chain J: 38% 35% 8% 19%



• Molecule 9: CELL DIVISION CYCLE PROTEIN 16 HOMOLOG

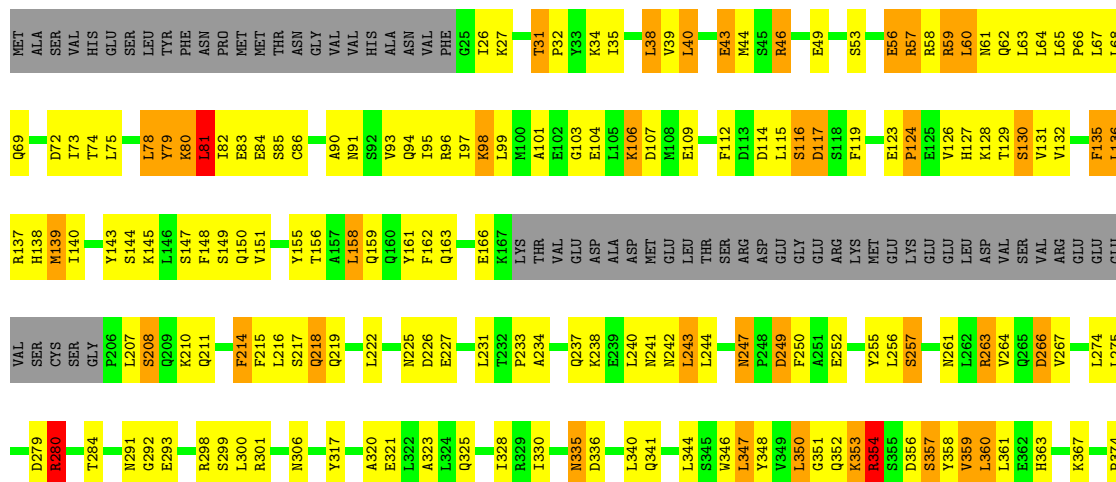
Chain K: 33% 38% 8% 20%

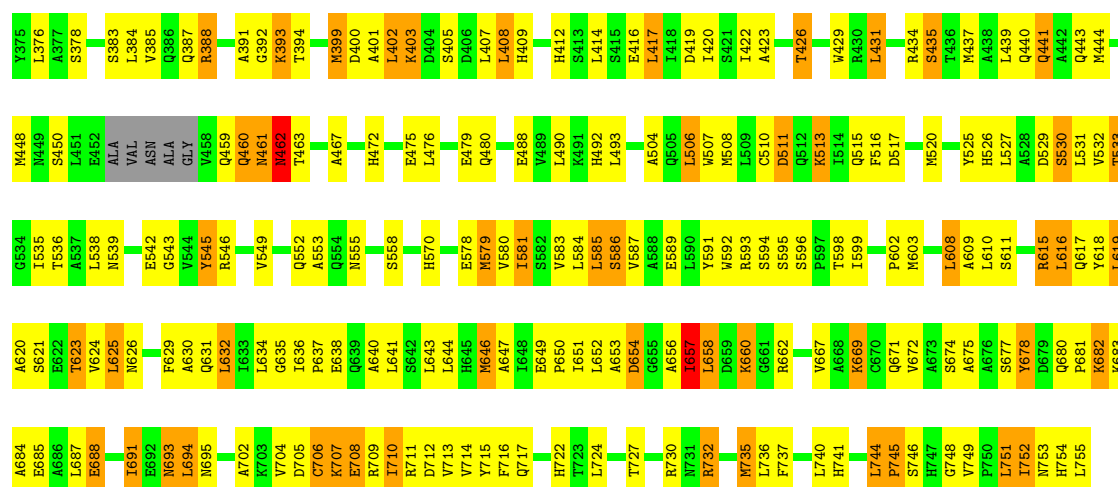




• Molecule 13: ANAPHASE-PROMOTING COMPLEX SUBUNIT 5

Chain O: 41% 37% 12% 9%





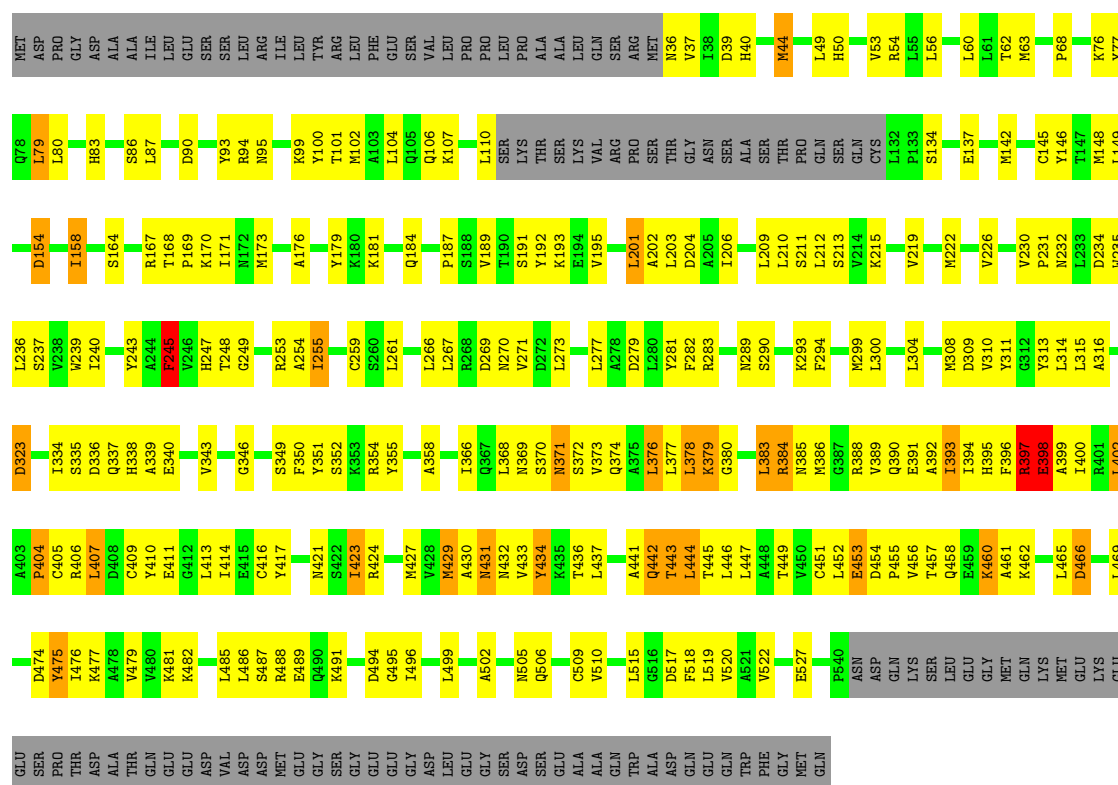
• Molecule 14: UNIDENTIFIED PEPTIDE

Chain T: 67% 27% 7%



• Molecule 15: ANAPHASE-PROMOTING COMPLEX SUBUNIT 7

Chain X: 41% 35% 5% 19%



• Molecule 15: ANAPHASE-PROMOTING COMPLEX SUBUNIT 7

Chain Y:  41% 35% 6% 17%

MET	ASP	PRO	GLY	ASP	ALA	ALA	ILE	LEU	GLU	SER	SER	LEU	ARG	ILE	LEU	TYR	ARG	LEU	PHE	GLU	SER	VAL	LEU	PRO	PRO	LEU	PRO	ALA	ALA	LEU	GLN	SER	ARG	MET	N36	V37	I38	D39	H40	V41	R42	D43	M44	A45	A46	A47	G48	L49	H50	S51	N52	V53	R54	L55	L56	S57	S58	L59	L60
L61	T62	M63	S64	N65	N66		L70	F71	S72	P73	Y77	Q78	L79		Y82	H83	A84	D85	S86	L87		D90	K91	E92	Y93	R94	N95	A96	V97	S98	K99	Y100	T101	M102	A103	L104	Q105	K106	K107		L110	SER	LYS	THR	SER	LYS	VAL	ARG	PRO	SER	THR	GLY	ASN	SER	ALA	THR	PRO		
GLN	SER	GLN	CYS	L132	P133	S134	E137	V138	K139		M142	C145	Y146	T147	M148	L149		D152	K153	D154	A155	I156	A157	I158	L159		I162	P163	S164	R167	T168	P169	K170	I171	L175	A176		Y179	R186	P187	S188	V189	T190	S191	Y192	K193	E194	V195	L196	R197	Q198	C199	P200	L201					
A202	L203	I206	L209		L212	S213	V214	K215	V219		N225	V226		T229	V230		W235	L236		W239	I240	K241	A242	Y243	A244	F245	V246	H247	T248	R253	A254	I255	D269	N270	V271	D272	L273	A278		Y281		D286	N289	S290	V291	L292	K293	F294	E295	Q296		W299							
L300	D301	P302	Y303	L304	I305	K306	G307	M308	D309	V310	Y311	G312	Y313	A316	D323	V324	E325	I334	S335	D336	Q337	H338	A339	L413	I414	P341	V342	V343	G346	C347	H348	S349	F350	Y351	S352	R353	Y355	S356	R357	A358	L359	Y360	L361	G362	A363	K364	A365	L366		N371	S372	V373	L376	L377					
L378	K379	A382	L383	R384	N385	M386	E391	I394	H395	E398	R401	L402	A403		R406	L407	D408	C409	Y410	E411	G412	L413	I414	E415	C416	Y417	L418	A419	I423	A426	M429	N432	V433	Y434	K435	T436	L437		T443	L444	T445	L446	L447	A448	T449	V450	C451	L452	E453	D454									
P455	V456	T457	Q458	E459	R460	A461	K462	L465	D466	L469	D474	Y475	L476	K477	A478	V479	V480	L485	L486	S487	R488	E489	Q490	K491	D494	G495	L496	A497	L498	L499	A502	L503	A504	N505	O506	S507	D508	C509	V510		L515	G516	D517	F518	L519	V520	A521	V522	Q526	E527									
Y532	S533	I534	L546	E547	G548	M549	Q550	K551	M552	GLU	LYS	GLU	GLU	SER	PRO	THR	ASP	ALA	GLN	THR	GLU	GLU	ASP	VAL	ASP	ASP	MET	GLU	GLY	SER	GLY	GLU	GLU	GLY	ASP	SER	GLU	ALA	ALA	GLN	TRP	ALA	ASP	GLN	GLU	GLN	TRP	PHE	GLY	MET	GLN								

4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	921993	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI POLARA 300	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	7/4861 (0.1%)	0.98	16/6585 (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	37/64540 (0.1%)	0.91	149/87457 (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	4686	1268	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	62108	6914	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 6914 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	30
2	B	83/84 (99%)	72 (87%)	7 (8%)	4 (5%)	2	22
3	C	518/597 (87%)	490 (95%)	23 (4%)	5 (1%)	17	57
3	P	486/597 (81%)	466 (96%)	16 (3%)	4 (1%)	21	62
4	D	53/121 (44%)	47 (89%)	5 (9%)	1 (2%)	9	43
5	E	54/110 (49%)	54 (100%)	0	0	100	100
6	F	454/824 (55%)	433 (95%)	19 (4%)	2 (0%)	36	75
6	H	484/824 (59%)	469 (97%)	10 (2%)	5 (1%)	17	57
7	G	23/85 (27%)	23 (100%)	0	0	100	100
7	W	24/85 (28%)	23 (96%)	0	1 (4%)	3	26
8	I	717/808 (89%)	682 (95%)	20 (3%)	15 (2%)	8	41
9	J	500/620 (81%)	468 (94%)	25 (5%)	7 (1%)	12	50
9	K	487/620 (78%)	456 (94%)	27 (6%)	4 (1%)	21	62
10	L	180/185 (97%)	169 (94%)	9 (5%)	2 (1%)	16	56
11	M	55/74 (74%)	49 (89%)	5 (9%)	1 (2%)	9	44
12	N	590/822 (72%)	547 (93%)	26 (4%)	17 (3%)	5	34
13	O	682/755 (90%)	643 (94%)	27 (4%)	12 (2%)	9	44
14	T	13/15 (87%)	11 (85%)	1 (8%)	1 (8%)	1	11
15	X	480/599 (80%)	463 (96%)	12 (2%)	5 (1%)	17	57
15	Y	492/599 (82%)	473 (96%)	15 (3%)	4 (1%)	21	62
All	All	7914/10368 (76%)	7410 (94%)	359 (4%)	145 (2%)	13	44

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	5
2	B	65/75 (87%)	54 (83%)	11 (17%)	2	13
3	C	452/520 (87%)	384 (85%)	68 (15%)	3	18
3	P	422/520 (81%)	368 (87%)	54 (13%)	5	23
4	D	46/115 (40%)	41 (89%)	5 (11%)	7	31
5	E	47/89 (53%)	35 (74%)	12 (26%)	0	3
6	F	371/727 (51%)	310 (84%)	61 (16%)	2	14
6	H	408/727 (56%)	368 (90%)	40 (10%)	9	35
7	G	25/77 (32%)	16 (64%)	9 (36%)	0	1
7	W	23/77 (30%)	15 (65%)	8 (35%)	0	1
8	I	607/730 (83%)	508 (84%)	99 (16%)	2	14
9	J	425/548 (78%)	363 (85%)	62 (15%)	3	19
9	K	423/548 (77%)	356 (84%)	67 (16%)	3	16
10	L	155/170 (91%)	139 (90%)	16 (10%)	8	33
11	M	52/67 (78%)	38 (73%)	14 (27%)	0	3
12	N	490/724 (68%)	372 (76%)	118 (24%)	1	4
13	O	573/650 (88%)	469 (82%)	104 (18%)	2	10
14	T	1/2 (50%)	1 (100%)	0	100	100
15	X	406/513 (79%)	370 (91%)	36 (9%)	11	40
15	Y	417/513 (81%)	373 (89%)	44 (11%)	7	32

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	6651/9112 (73%)	5547 (83%)	1104 (17%)	6 13

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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
13	O	2
3	C	1
12	N	1
9	K	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	N	563:ASP	C	564:MET	N	2.51
1	C	344:ARG	C	345:SER	N	2.01
1	K	219:VAL	C	220:ILE	N	2.00
1	O	116:SER	C	117:ASP	N	1.91
1	O	135:PHE	C	136:LEU	N	1.65