

wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Jul 24, 2017 – 01:47 PM EDT

PDB ID : 4UI9
EMDB ID: : EMD-2924
Title : Atomic structure of the human Anaphase-Promoting Complex
Authors : Chang, L.; Zhang, Z.; Yang, J.; McLaughlin, S.H.; Barford, D.
Deposited on : unknown
Resolution : 3.60 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) : rb-20029824

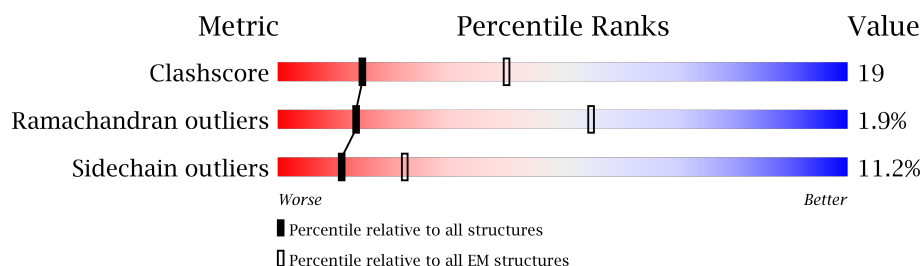
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.60 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	
2	B	84	
3	C	591	
3	P	591	
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
8	I	808	
9	J	620	
10	K	620	
11	L	183	
12	M	74	
13	N	822	
14	O	756	
15	R	493	
16	S	447	
17	T	21	
18	U	24	
19	W	85	
20	X	565	
20	Y	565	

2 Entry composition [i](#)

There are 21 unique types of molecules in this entry. The entry contains 66453 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	1441	Total	C	N	O	S	0	0
			10947	7043	1853	1977	74		

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	291	PHE	THR	conflict	UNP Q9H1A4
A	940	ILE	THR	conflict	UNP Q9H1A4
A	1059	GLU	ASP	conflict	UNP Q9H1A4
A	1358	LEU	ILE	conflict	UNP Q9H1A4
A	1637	LEU	THR	conflict	UNP Q9H1A4
A	1880	PRO	LEU	conflict	UNP Q9H1A4
A	1881	LEU	GLU	conflict	UNP Q9H1A4

- 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
			650	418	117	98	17		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	13	LEU	THR	conflict	UNP Q9NYG5

- 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
			4305	2774	726	781	24		
3	P	491	Total	C	N	O	S	0	0
			4042	2611	678	729	24		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	161	LEU	LYS	conflict	UNP Q9UJX2
P	161	LEU	LYS	conflict	UNP Q9UJX2

- 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
			437	277	73	87		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	5	TYR	PHE	conflict	UNP P60006

- 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	498	Total	C	N	O	S	0	0
			3923	2514	664	719	26		
6	H	483	Total	C	N	O	S	0	0
			3853	2473	650	704	26		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	403	GLU	LYS	conflict	UNP P30260
F	475	SER	ALA	conflict	UNP P30260
F	484	SER	ALA	conflict	UNP P30260
H	403	GLU	LYS	conflict	UNP P30260
H	475	SER	ALA	conflict	UNP P30260
H	484	SER	ALA	conflict	UNP P30260

- 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
			214	134	40	39	1		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	14	GLU	ASP	conflict	UNP Q8NHZ8

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	730	Total	C	N	O	S	0	0
			5709	3660	950	1066	33		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	430	ASP	GLU	conflict	UNP Q9UJX5

- 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
			4047	2602	685	735	25		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	225	ASN	ASP	conflict	UNP Q13042
J	228	GLU	GLN	conflict	UNP Q13042
J	229	LYS	GLU	conflict	UNP Q13042

- Molecule 10 is a protein called CELL DIVISION CYCLE PROTEIN 16 HOMOLOG.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	493	Total	C	N	O	S	0	0
			3988	2565	673	726	24		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	228	GLU	GLN	conflict	UNP Q13042

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Chain	Residue	Modelled	Actual	Comment	Reference
K	229	LYS	GLU	conflict	UNP Q13042
K	265	LYS	ALA	conflict	UNP Q13042

- Molecule 11 is a protein called ANAPHASE-PROMOTING COMPLEX SUBUNIT 10.

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	?	-	GLU	deletion	UNP Q9UM13

- Molecule 12 is a protein called ANAPHASE-PROMOTING COMPLEX SUBUNIT 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	M	59	Total	C	N	O	S	0	0
			493	310	79	102	2		

- Molecule 13 is a protein called ANAPHASE-PROMOTING COMPLEX SUBUNIT 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	N	631	Total	C	N	O	S	0	0
			4831	3064	877	868	22		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
N	410	ILE	LEU	conflict	UNP Q9UJX6

- Molecule 14 is a protein called ANAPHASE-PROMOTING COMPLEX SUBUNIT 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	O	685	Total	C	N	O	S	0	0
			5396	3439	939	991	27		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	42	SER	ASN	conflict	UNP Q9UJX4

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Chain	Residue	Modelled	Actual	Comment	Reference
O	55	VAL	MET	conflict	UNP Q9UJX4
O	63	GLN	LEU	conflict	UNP Q9UJX4
O	75	VAL	LEU	conflict	UNP Q9UJX4
O	79	LEU	TYR	conflict	UNP Q9UJX4
O	164	SER	ASN	conflict	UNP Q9UJX4
O	165	ASP	GLY	conflict	UNP Q9UJX4
O	167	ASN	-	insertion	UNP Q9UJX4

- Molecule 15 is a protein called FIZZY-RELATED PROTEIN HOMOLOG.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	R	387	Total	C	N	O	S	0	0
			3003	1895	541	557	10		

- Molecule 16 is a protein called F-BOX ONLY PROTEIN 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	S	94	Total	C	N	O	S	0	0
			648	396	119	124	9		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S	323	ILE	THR	conflict	UNP Q9UKT4
S	326	LYS	ALA	conflict	UNP Q9UKT4

- Molecule 17 is a protein called PEPTIDE.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	T	21	Total	C	N	O	0	0
			109	65	22	22		

- Molecule 18 is a protein called PEPTIDE.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	U	24	Total	C	N	O	0	0
			120	72	24	24		

- Molecule 19 is a protein called ANAPHASE-PROMOTING COMPLEX SUBUNIT CDC26.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	W	25	Total	C	N	O	S	0	0
			213	133	40	39	1		

- Molecule 20 is a protein called ANAPHASE-PROMOTING COMPLEX SUBUNIT 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	X	484	Total	C	N	O	S	0	0
			3770	2394	650	705	21		
20	Y	496	Total	C	N	O	S	0	0
			3865	2450	667	725	23		

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	63	LEU	MET	conflict	UNP Q9UJX3
X	142	LEU	MET	conflict	UNP Q9UJX3
X	148	VAL	MET	conflict	UNP Q9UJX3
X	466	ASN	ASP	conflict	UNP Q9UJX3
X	472	GLU	ARG	conflict	UNP Q9UJX3
Y	63	LEU	MET	conflict	UNP Q9UJX3
Y	142	LEU	MET	conflict	UNP Q9UJX3
Y	148	VAL	MET	conflict	UNP Q9UJX3
Y	466	ASN	ASP	conflict	UNP Q9UJX3
Y	472	GLU	ARG	conflict	UNP Q9UJX3

- Molecule 21 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
21	B	3	Total	Zn	0
			3	3	
21	S	2	Total	Zn	0
			2	2	

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.

Chain A: 45% 25% 26%

ASP	GLU	SER	LEU	VAL	SER	ASP	GLU	SER	GLN	TYR	LEU	THR	ARG	ILE	THR	ILE	ALA	PRO	GLN	LYS	LEU	GLN	VAL	GLU	GLN	GLU	ASN	ARG	PHE	SER	PHE	ARG	HIS	SER	THR	SER	VAL	S924	S925	H934	F939	L944	E945	T946	L947	P948	Y951	A952	L953	R956	Y960										
H961	C962	R963	E964			P971					R980	Q981				Q986	ALA	CYS	GLU	GLY	ASN	LEU	PRO	LYS	GLY	SER	VAL	LEU	SER	ASP	VAL	PRO	SER	HIS	GLY	THR	THR	GLU	GLU	S924	S925	H934	F939	L944	E945	T946	L947	P948	Y951	A952	L953	R956	Y960								
Y1054	E1056	L1057				H1060	E1061				F1062	I1063	E1064			Q1075	R1076	T1077	M1078	A1079	P1081	V1082	G1083	R1084	G1085	M1086	L1089	T1097	E1098	P1099	L1100	P1101			L1105	H1106	L1107	T1108	G1109	R1110			R1114	M1115	T1116	T1117	L1120	L1125	W1134	S1135	F1137	H1138	M1139	Q1053							
V1141	L1145	K1146				Y1160	M1161	P1162	P1163		L1168	A1169	M1170	E1171	Y1172			F1175	L1176	M1177	A1178	L1179	G1180	L1181			H1184	L1185	T1186			E1202	M1203	T1204	S1205			L1208	L1209			G1218	M1219			L1212	A1215	K1216	L1217	G1218	M1219	L1220	L1227	I1230	M1231	P1232	S1233	A1234	M1235	L1236	L1239
T1239	S1240	T1241	E1242	L1243		H1248	V1249	Q1250	V1251		V1254	V1255			L1259			Q1262	G1263	T1264	A1265	H1266	R1267			V1272	L1273	L1274	A1275	E1276			R1279	P1280	P1281	G1282	P1283			Y1287	D1290	R1291	E1292	S1293	Y1294			A1298	L1302	G1303	M1304	L1307	G1308	T1309	M1312	L1313	I1314	G1315	M1316	L1319	L1239
H1320	V1321	P1322	E1323	Q1324	L1325		G1332	H1333	ARG	ARG	PHE	GLN	THR	GLY	MET	HIS	ARG	G1363	GLU	LYS	HIS	LYS	S1347	P1348			Q1351	I1352	T1357	L1358	M1359	C1364	P1365			L1369			Y1375	L1376	K1377	T1378	H1379	M1380			T1383	W1386	L1387	P1390	D1391	T1392	L1396	V1399	L1404	L1405	L1406				
L1409	C1412		H1416			L1420	P1421	M1422	S1423	K1424		D1427		V1430		H1437	SER	ILE	SER	LEU	SER	ILE	GLU	PRO	CYS	SER	GLU	ASP	L1452	V1462	Y1463			G1467			M1468	C1469	L1470	S1471	L1472			R1475	F1476	A1477	E1480	M1481	L1482	C1487	L1488	K1493	D1494	F1495	L1496	T1497	Y1498				
L1499	P1502	M1503				M1511	L1512	E1513		V1518	S1522	V1526	M1527			G1531	M1532	L1533	K1534	V1535	C1536	Q1537	L1538	C1539	R1540	H1543	M1544	L1545	T1546	G1547	Y1552	G1553	F1554	H1555	L1556			L1562	G1563	L1564	L1565	F1566			R1571	Y1572	S1573	L1574	S1575	T1576	S1577	S1580	L1585	L1588	S1596						
T1597	R1600	L1603				R1607	Y1610	V1611		E1615	P1616	R1617		P1621		V1622	D1623	M1624	P1629	C1630	Y1631	A1632		L1637	G1640	Y1644	E1645	Q1646		E1650	L1651	M1652	A1653	H1655	L1656			L1662	G1663	Q1664	L1666			R1672	Y1673	M1674	E1675	L1676	K1677	L1678	L1679	L1680	SER	LYS	GLY						
T1684	L1687	K1688				K1693	D1694	L1697	V1698	V1699	L1701	L1706			D1711	PRO	MET	TRP	GLN	SER	LEU	ALA	THR	VAL	ALA	ASN	ARG	M1727	R1734		K1737	PRO	GLU	THR	ILE			S1742	A1743			D1747	L1750	L1751	E1755	Y1756	F1757	C1758	K1759	L1771	D1772	L1773	F1774								
L1778	Y1782	T1783	Q1784	E1785	T1786	P1787	M1789			I1794	A1795	M1796	D1797		I1800	R1801	R1802	L1803		M1808	S1809		L1814	H1815	L1817	K1818	L1819	V1820	L1821	E1822	F1823	F1824	S1825			S1828	H1829	Q1830	GLU	ARG	LEU	GLN	ASN	HIS	LYS	ARG	GLY	F1842	M1843	K1852	C1853	T1854	I1855	Q1861							
G1867	C1870	H1871	A1872	A1873	L1874	L1875	V1876	GLY	PRO	F1880	L1881	Q1884	L1885	S1886	V1887	L1888	F1891	H1895	S1896	V1897	P1900	GLN	HIS	LEU	PRO	PRO	ILE	GLY	LEU	GLU	GLY	S1911	L1924	P1927	A1935	PRO	LEU	LEU	LEU	GLY	ASN	PRO	GLN	PRO	MET	VAL	MET														

• Molecule 2: ANAPHASE-PROMOTING COMPLEX SUBUNIT 11

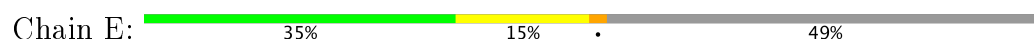
Chain B:  64% 25% 8%

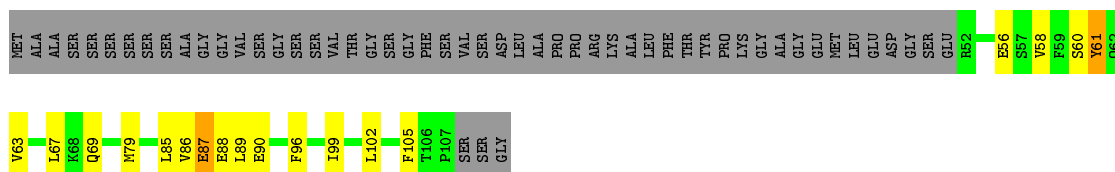
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• Molecule 3: CELL DIVISION CYCLE PROTEIN 23 HOMOLOG

Chain C:  61% 24% 11%

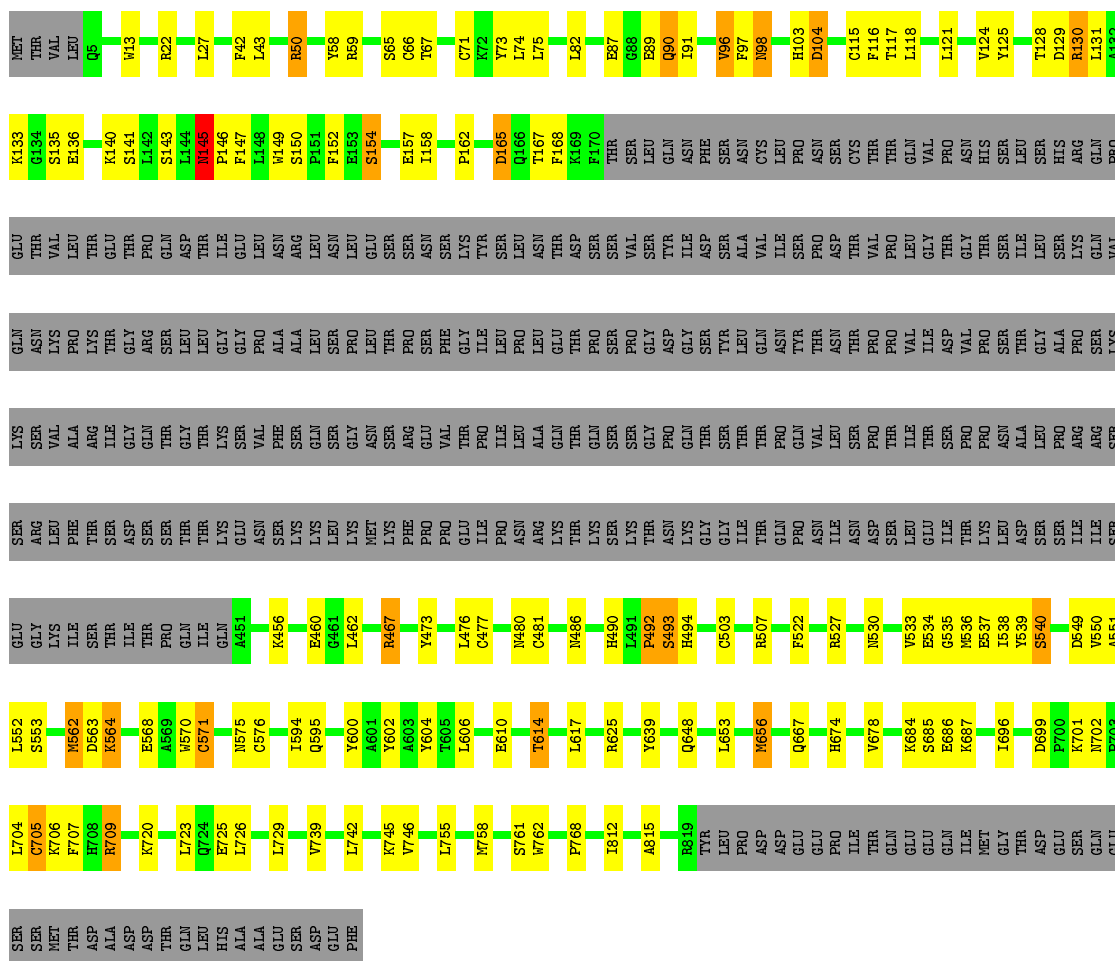
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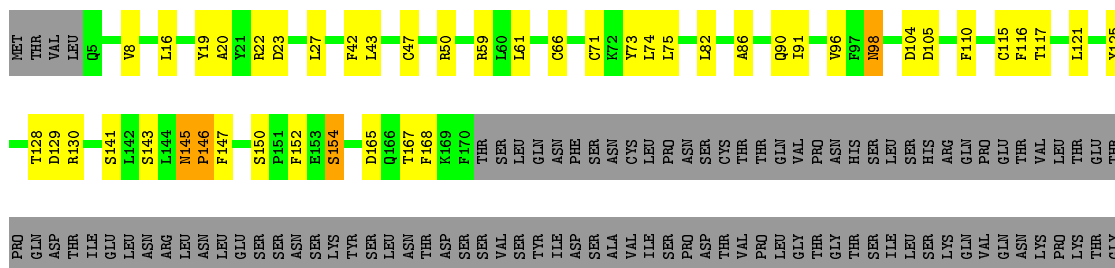
• Molecule 6: CELL DIVISION CYCLE PROTEIN 27 HOMOLOG

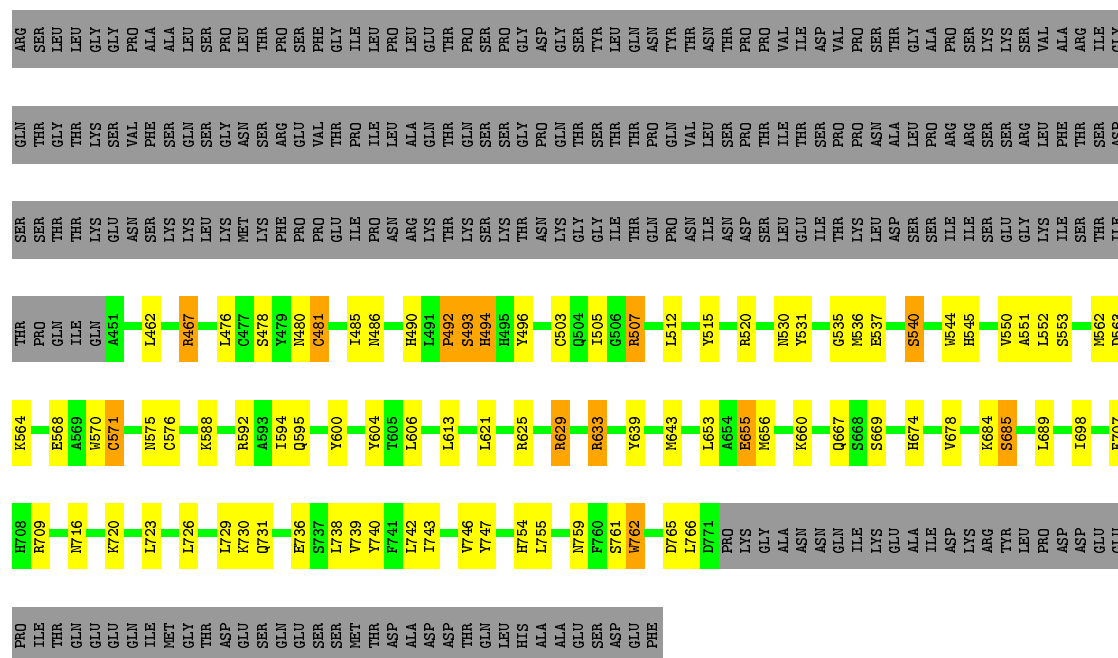
Chain F: 43% 15% 40%



• Molecule 6: CELL DIVISION CYCLE PROTEIN 27 HOMOLOG

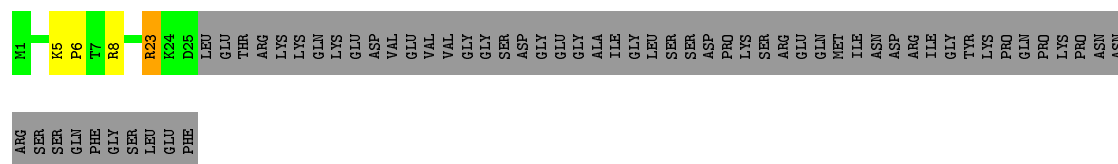
Chain H: 42% 14% 41%





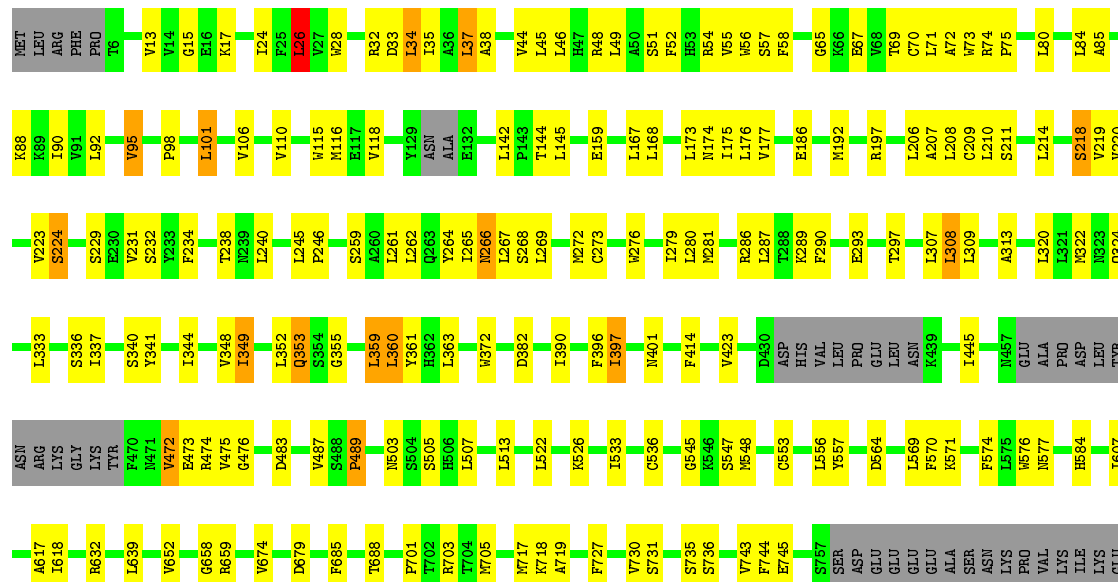
• Molecule 7: ANAPHASE-PROMOTING COMPLEX SUBUNIT CDC26

Chain G: 25% 71%



• Molecule 8: ANAPHASE-PROMOTING COMPLEX SUBUNIT 4

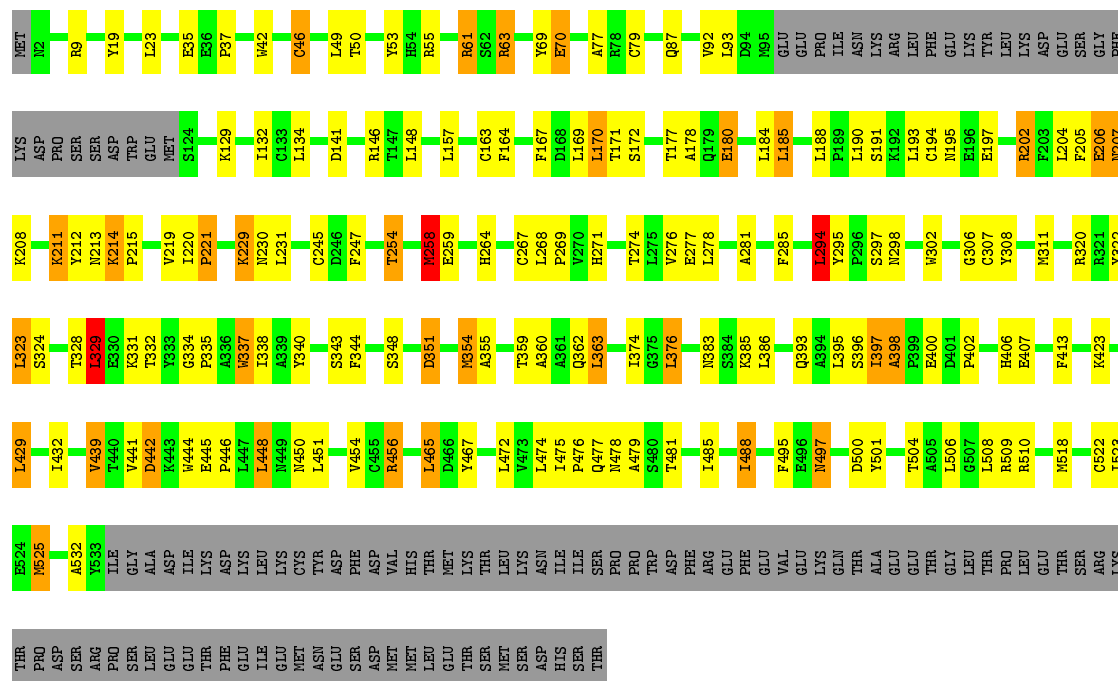
Chain I: 67% 21% 10%



GLU VAL LEU SER SER SER GLU ALA GLU ASN GLN GLN ALA GLY ALA ALA ALA LEU LEU ALA PRO GLU ILE VAL ILE LYS VAL GLU LYS LEU ASP PRO GLU LEU ASP SER

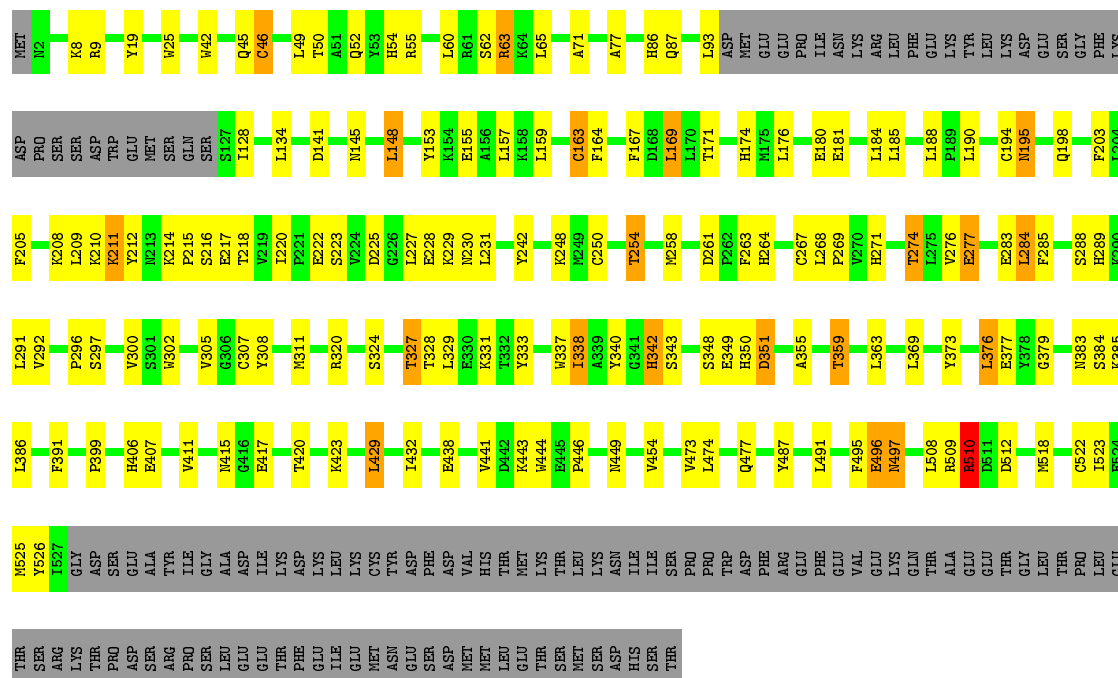
• Molecule 9: CELL DIVISION CYCLE PROTEIN 16 HOMOLOG

Chain J: 55% 21% 5% 19%



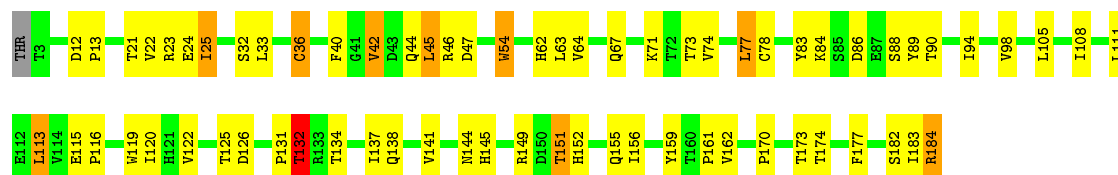
• Molecule 10: CELL DIVISION CYCLE PROTEIN 16 HOMOLOG

Chain K: 54% 22% 20%



• Molecule 11: ANAPHASE-PROMOTING COMPLEX SUBUNIT 10

Chain L: 



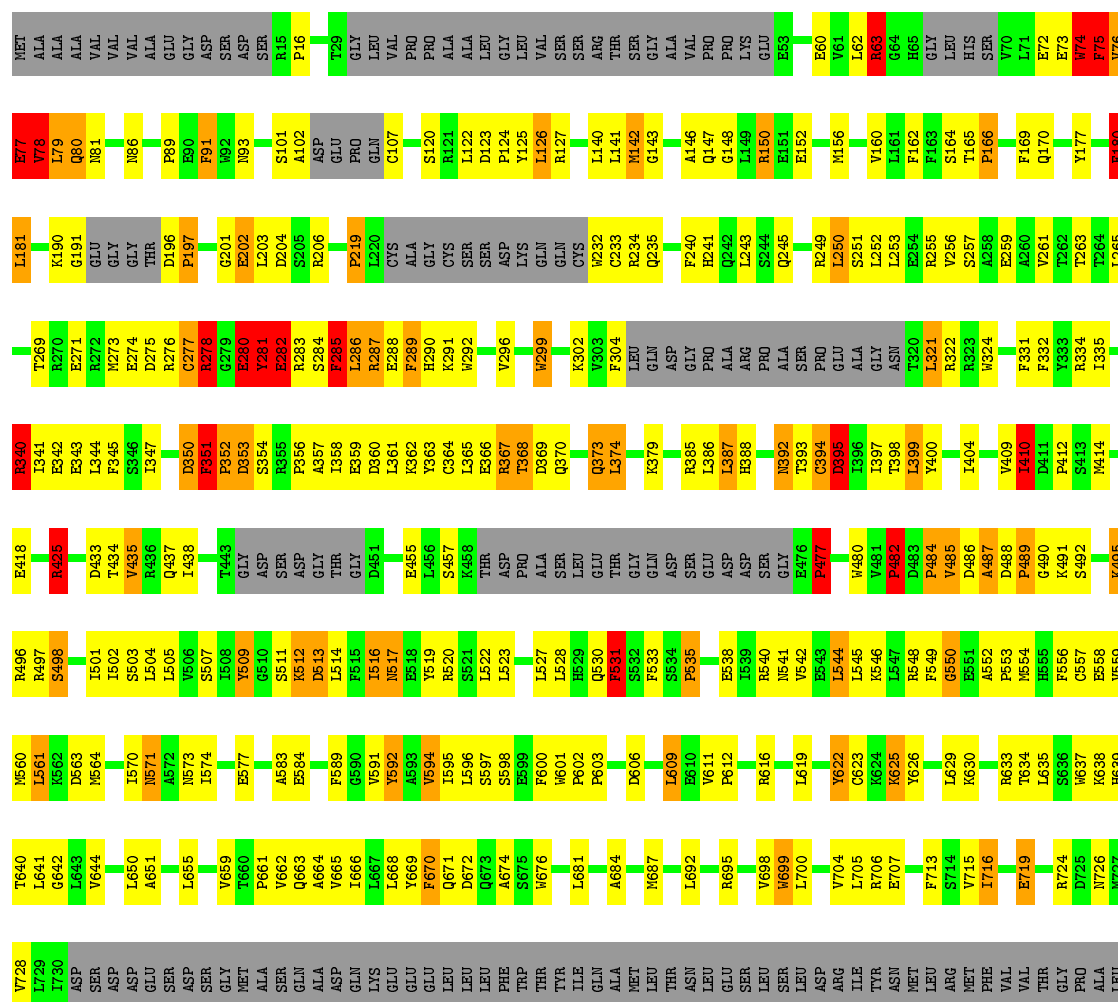
• Molecule 12: ANAPHASE-PROMOTING COMPLEX SUBUNIT 13

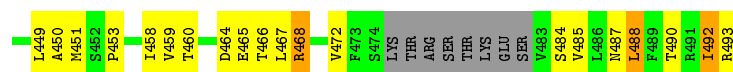
Chain M: 



• Molecule 13: ANAPHASE-PROMOTING COMPLEX SUBUNIT 2

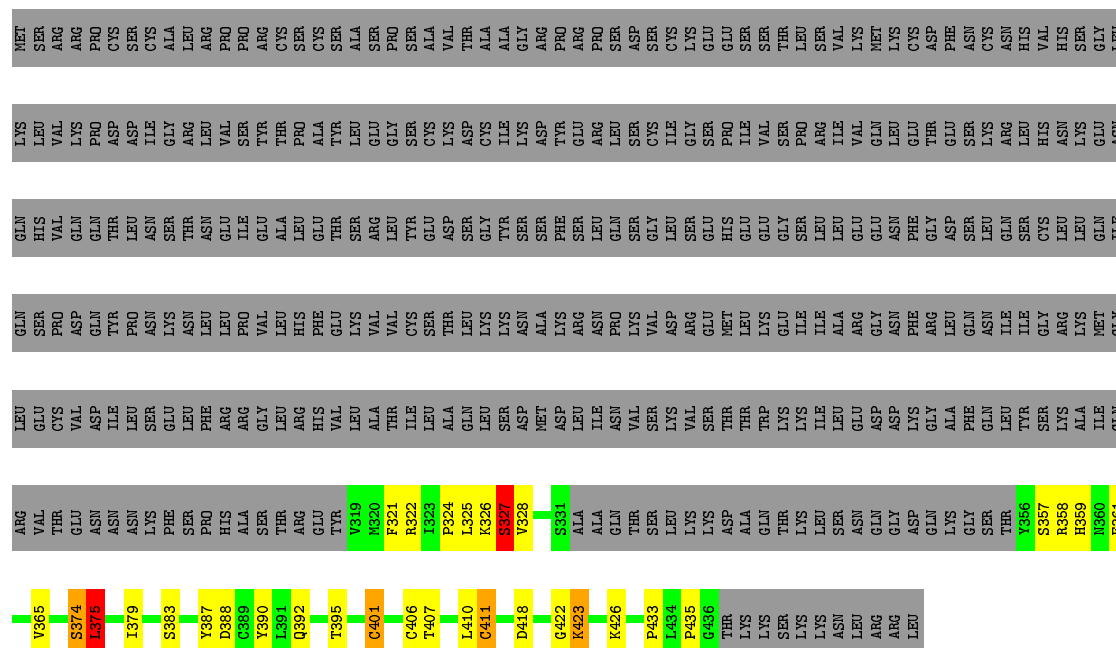
Chain N: 





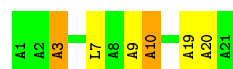
- Molecule 16: F-BOX ONLY PROTEIN 5

Chain S:  14% 6% 79%

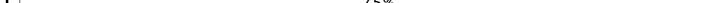


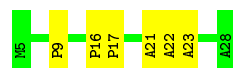
- Molecule 17: PEPTIDE

Chain T: 71% 19% 10%



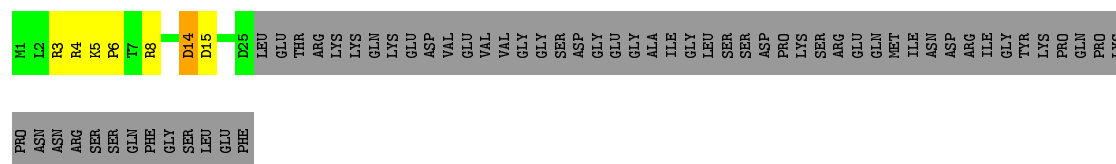
- Molecule 18: PEPTIDE

Chain U:  75% 25%



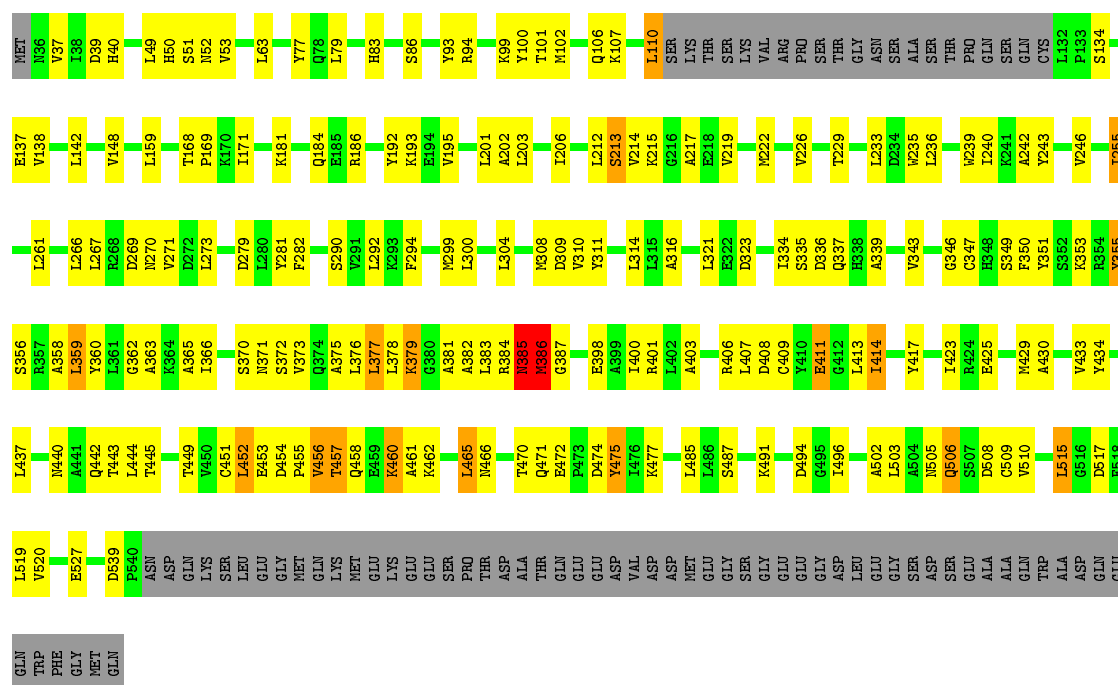
- Molecule 19: ANAPHASE-PROMOTING COMPLEX SUBUNIT CDC26

Chain W:  21% 7% 71%



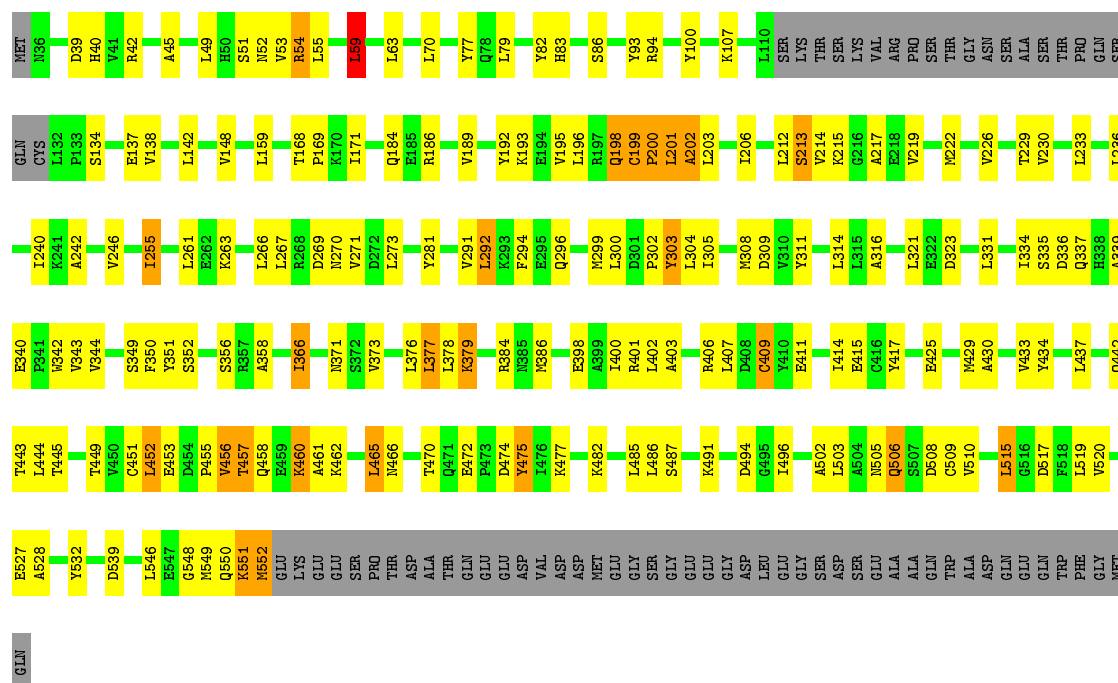
- Molecule 20: ANAPHASE-PROMOTING COMPLEX SUBUNIT 7

Chain X:  53% 29% . 14%



- Molecule 20: ANAPHASE-PROMOTING COMPLEX SUBUNIT 7

Chain Y:  56% 27% • 12%



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	202084	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TECNAI F30	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	0.75	0/11190	0.99	21/15238 (0.1%)
10	K	0.89	3/4086 (0.1%)	0.96	5/5532 (0.1%)
11	L	0.71	0/1468	0.96	5/1993 (0.3%)
12	M	0.73	0/502	1.05	1/680 (0.1%)
13	N	0.63	1/4913 (0.0%)	1.01	18/6650 (0.3%)
14	O	0.73	5/5494 (0.1%)	0.96	5/7425 (0.1%)
15	R	2.23	11/3068 (0.4%)	2.62	75/4162 (1.8%)
16	S	0.54	0/654	0.81	3/880 (0.3%)
17	T	1.02	0/108	1.11	0/149
18	U	0.91	0/119	1.10	3/165 (1.8%)
19	W	0.64	0/214	1.02	0/284
2	B	0.52	0/675	0.86	1/914 (0.1%)
20	X	0.60	4/3830 (0.1%)	0.84	6/5187 (0.1%)
20	Y	0.54	0/3925	0.85	4/5311 (0.1%)
3	C	0.75	1/4403 (0.0%)	0.95	9/5945 (0.2%)
3	P	0.70	1/4137 (0.0%)	0.92	3/5587 (0.1%)
4	D	0.71	0/447	0.98	1/612 (0.2%)
5	E	0.65	0/459	0.86	0/619
6	F	0.70	3/4013 (0.1%)	0.90	7/5428 (0.1%)
6	H	0.70	2/3943 (0.1%)	0.90	4/5329 (0.1%)
7	G	0.62	0/215	1.03	1/285 (0.4%)
8	I	0.58	0/5827	0.85	3/7899 (0.0%)
9	J	0.75	3/4146 (0.1%)	0.97	9/5615 (0.2%)
All	All	0.83	34/67836 (0.1%)	1.07	184/91889 (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	9
13	N	0	26
15	R	0	5
17	T	0	1
20	X	0	1
8	I	0	2
9	J	0	1
All	All	0	45

The worst 5 of 34 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	R	431	PRO	N-CD	53.78	2.23	1.47
15	R	392	PRO	N-CD	50.89	2.19	1.47
15	R	302	PRO	N-CD	48.99	2.16	1.47
15	R	301	PRO	N-CD	47.51	2.14	1.47
10	K	229	LYS	CB-CG	33.09	2.42	1.52

The worst 5 of 184 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	R	431	PRO	O-C-N	-52.04	39.44	122.70
15	R	310	GLN	O-C-N	-29.51	73.03	123.20
15	R	240	ARG	NE-CZ-NH2	-25.22	107.69	120.30
15	R	307	ARG	NE-CZ-NH2	-25.20	107.70	120.30
15	R	313	ARG	NE-CZ-NH2	-25.18	107.71	120.30

There are no chirality outliers.

5 of 45 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	11	MET	Peptide
1	A	124	GLN	Peptide
1	A	14	ALA	Peptide
1	A	83	ILE	Peptide
1	A	86	ASP	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	10947	0	10690	367	0
2	B	650	0	600	33	0
3	C	4305	0	4273	121	0
3	P	4042	0	3998	137	0
4	D	437	0	396	14	0
5	E	450	0	435	12	0
6	F	3923	0	3813	95	0
6	H	3853	0	3788	95	0
7	G	214	0	222	2	0
8	I	5709	0	5597	124	0
9	J	4047	0	3956	138	0
10	K	3988	0	3917	126	0
11	L	1435	0	1382	69	0
12	M	493	0	469	28	0
13	N	4831	0	4527	292	0
14	O	5396	0	5425	160	0
15	R	3003	0	2951	432	0
16	S	648	0	543	31	0
17	T	109	0	107	9	0
18	U	120	0	80	1	0
19	W	213	0	220	8	0
20	X	3770	0	3829	254	0
20	Y	3865	0	3925	168	0
21	B	3	0	0	0	0
21	S	2	0	0	0	0
All	All	66453	0	65143	2494	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 19.

The worst 5 of 2494 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)
15:R:404:ASN:CB	15:R:449:LEU:HD21	1.22	1.60
15:R:404:ASN:HB2	15:R:449:LEU:CD2	1.35	1.53
15:R:292:MET:CE	15:R:309:LEU:HD21	1.42	1.47
20:X:358:ALA:HB3	20:X:382:ALA:CB	1.43	1.46
20:X:355:TYR:CD2	20:X:386:MET:N	1.83	1.46

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	1399/1944 (72%)	1260 (90%)	107 (8%)	32 (2%)	7	46
2	B	83/84 (99%)	72 (87%)	7 (8%)	4 (5%)	2	27
3	C	520/591 (88%)	495 (95%)	23 (4%)	2 (0%)	38	77
3	P	485/591 (82%)	460 (95%)	24 (5%)	1 (0%)	51	85
4	D	53/121 (44%)	46 (87%)	6 (11%)	1 (2%)	9	50
5	E	54/110 (49%)	54 (100%)	0	0	100	100
6	F	494/824 (60%)	477 (97%)	11 (2%)	6 (1%)	15	59
6	H	479/824 (58%)	462 (96%)	12 (2%)	5 (1%)	18	62
7	G	23/85 (27%)	23 (100%)	0	0	100	100
8	I	722/808 (89%)	690 (96%)	28 (4%)	4 (1%)	28	70
9	J	500/620 (81%)	467 (93%)	28 (6%)	5 (1%)	18	62
10	K	489/620 (79%)	458 (94%)	26 (5%)	5 (1%)	18	62
11	L	180/183 (98%)	170 (94%)	8 (4%)	2 (1%)	17	61
12	M	55/74 (74%)	46 (84%)	9 (16%)	0	100	100
13	N	609/822 (74%)	501 (82%)	50 (8%)	58 (10%)	1	11
14	O	677/756 (90%)	644 (95%)	25 (4%)	8 (1%)	15	59
15	R	375/493 (76%)	343 (92%)	25 (7%)	7 (2%)	9	50
16	S	88/447 (20%)	68 (77%)	15 (17%)	5 (6%)	2	23
17	T	19/21 (90%)	14 (74%)	3 (16%)	2 (10%)	0	9
18	U	22/24 (92%)	19 (86%)	2 (9%)	1 (4%)	3	29
19	W	23/85 (27%)	23 (100%)	0	0	100	100
20	X	480/565 (85%)	462 (96%)	15 (3%)	3 (1%)	28	70
20	Y	492/565 (87%)	471 (96%)	16 (3%)	5 (1%)	18	62
All	All	8321/11257 (74%)	7725 (93%)	440 (5%)	156 (2%)	14	50

5 of 156 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	274	VAL
1	A	630	PRO
1	A	857	MET
1	A	860	TYR
1	A	1125	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	1150/1720 (67%)	988 (86%)	162 (14%)	4	26
2	B	65/75 (87%)	55 (85%)	10 (15%)	3	22
3	C	452/516 (88%)	399 (88%)	53 (12%)	6	34
3	P	422/516 (82%)	373 (88%)	49 (12%)	6	34
4	D	46/115 (40%)	42 (91%)	4 (9%)	12	47
5	E	47/89 (53%)	37 (79%)	10 (21%)	1	8
6	F	407/729 (56%)	367 (90%)	40 (10%)	9	42
6	H	408/729 (56%)	372 (91%)	36 (9%)	12	47
7	G	23/77 (30%)	21 (91%)	2 (9%)	12	47
8	I	620/730 (85%)	572 (92%)	48 (8%)	15	52
9	J	424/548 (77%)	368 (87%)	56 (13%)	5	29
10	K	423/549 (77%)	381 (90%)	42 (10%)	9	41
11	L	155/168 (92%)	140 (90%)	15 (10%)	9	42
12	M	55/67 (82%)	44 (80%)	11 (20%)	1	10
13	N	459/724 (63%)	403 (88%)	56 (12%)	6	31
14	O	578/652 (89%)	491 (85%)	87 (15%)	3	23
15	R	324/428 (76%)	306 (94%)	18 (6%)	25	63
16	S	56/404 (14%)	43 (77%)	13 (23%)	1	6
17	T	1/2 (50%)	1 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	W	23/77 (30%)	22 (96%)	1 (4%)	33	71
20	X	407/484 (84%)	378 (93%)	29 (7%)	17	55
20	Y	418/484 (86%)	382 (91%)	36 (9%)	12	48
All	All	6963/9883 (70%)	6185 (89%)	778 (11%)	11	36

5 of 778 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	I	473	GLU
10	K	194	CYS
20	X	184	GLN
8	I	718	LYS
9	J	323	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 142 such sidechains are listed below:

Mol	Chain	Res	Type
8	I	740	HIS
10	K	271	HIS
20	X	151	GLN
9	J	18	GLN
9	J	393	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 5 ligands modelled in this entry, 5 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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
13	N	2
16	S	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	S	419:CYS	C	420:SER	N	27.15
1	N	92:TRP	C	93:ASN	N	3.02
1	N	563:ASP	C	564:MET	N	2.52