



wwPDB EM Map/Model Validation Report ⓘ

May 19, 2016 – 11:23 PM EDT

PDB ID : 5G04
EMDB ID: : EMD-3385
Title : Structure of the human APC-Cdc20-Hsl1 complex
Authors : Zhang, S.; Chang, L.; Alfieri, C.; Zhang, Z.; Yang, J.; Maslen, S.; Skehel, M.; Barford, D.
Deposited on : 2016-03-16
Resolution : 4.00 Å(reported)

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>

MolProbity : 4.02b-467
Mogul : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027457

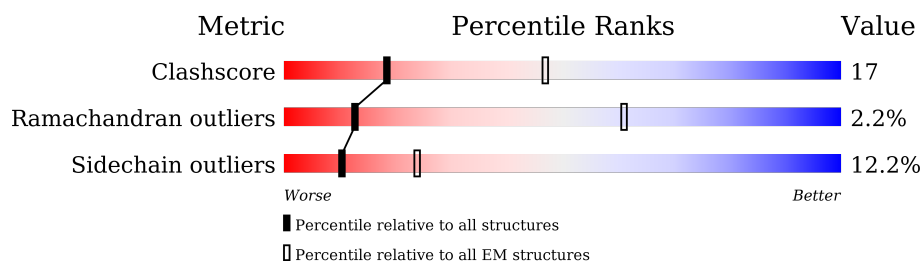
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.00 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.









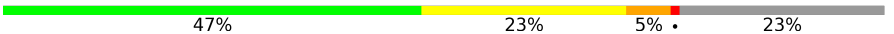


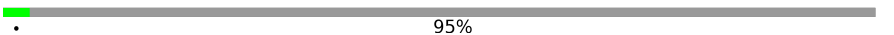


Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

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	41% 26% 6% • 26%
2	B	84	69% 23% 6% •
3	C	597	44% 34% 10% • 12%
3	P	597	53% 24% 5% 18%
4	D	121	26% 17% • 55%
5	E	110	35% 15% • 49%
6	F	824	41% 17% • 40%
6	H	824	41% 16% • 41%
7	G	85	19% 11% 71%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
7	W	85	 16% 13% 71%
8	I	808	 62% 26% • 10%
9	J	620	 50% 26% • 19%
9	K	620	 51% 24% • 20%
10	L	184	 59% 36% • •
11	M	74	 49% 20% 9% • 20%
12	N	822	 47% 23% 5% • 23%
13	O	755	 50% 33% 6% • 9%
14	R	499	 64% 9% • 26%
15	S	206	 • 95%
16	X	599	 55% 23% • 19%
16	Y	599	 56% 22% • 17%

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 65481 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	1437	Total	C	N	O	S	0	0
			10925	7025	1849	1977	74		

- 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	491	Total	C	N	O	S	0	0
			4039	2608	678	729	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	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		

- 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
			213	133	40	39	1		
7	W	25	Total	C	N	O	S	0	0
			213	133	40	39	1		

- 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		

- 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	2601	684	737	25		
9	K	493	Total	C	N	O	S	0	0
			3988	2563	672	729	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		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	.	-	ARG	DELETION	UNP Q9UM13

- 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
			493	310	79	102	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	N	631	Total	C	N	O	S	0	0
			4837	3067	880	868	22		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	O	685	Total	C	N	O	S	0	0
			5395	3440	940	987	28		

- Molecule 14 is a protein called CELL DIVISION CYCLE PROTEIN 20 HOMOLOG.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	R	370	Total	C	N	O	S	2	0
			2869	1801	524	532	12		

- Molecule 15 is a protein called PROBABLE SERINE/THREONINE-PROTEIN KINASE HSL1.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	S	10	Total	C	N	O	0	0
			72	42	14	16		

- Molecule 16 is a protein called ANAPHASE-PROMOTING COMPLEX SUBUNIT 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	X	484	Total	C	N	O	S	0	0
			3767	2390	649	704	24		
16	Y	496	Total	C	N	O	S	0	0
			3859	2444	666	724	25		

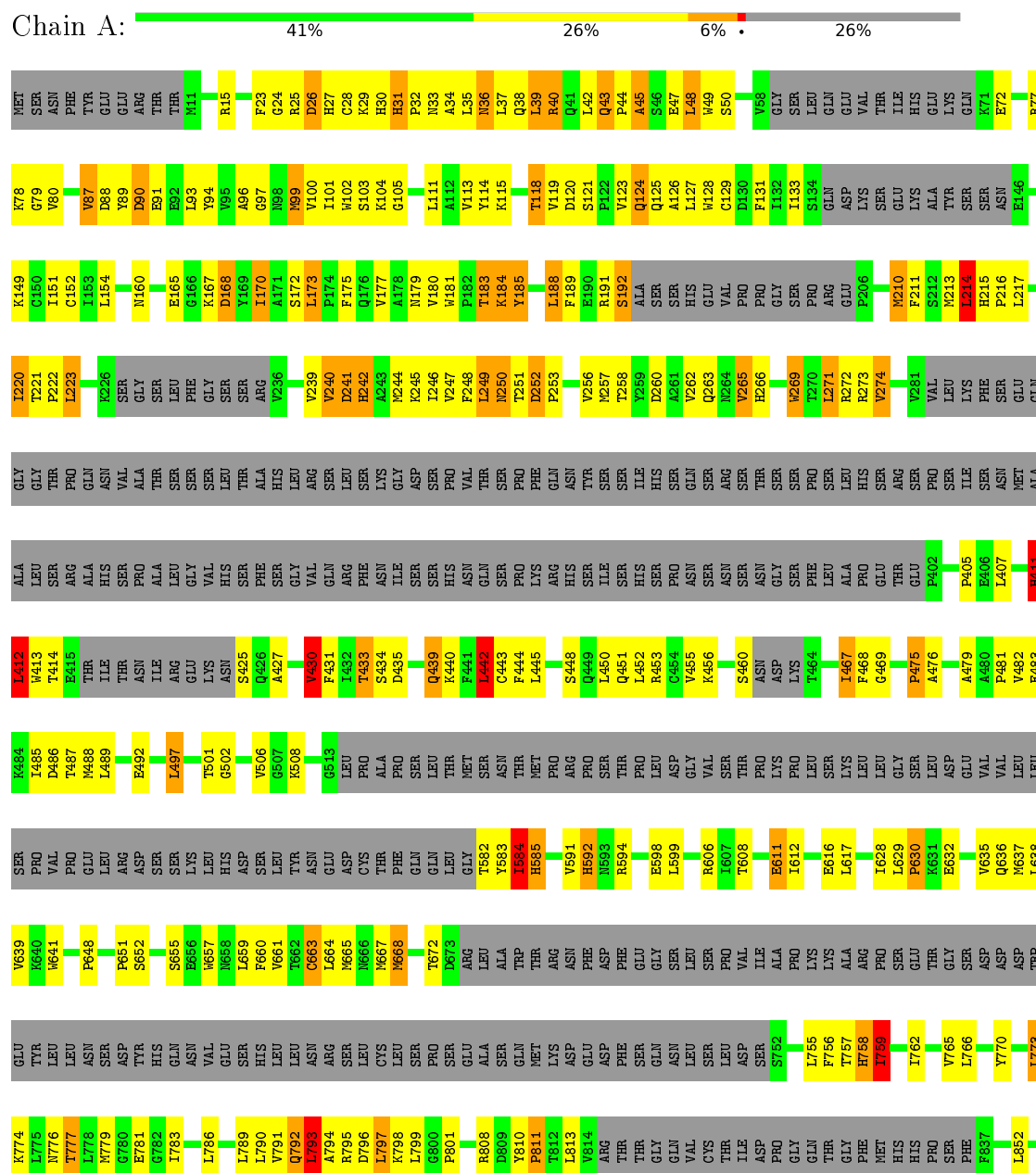
- Molecule 17 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
17	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 errors 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.

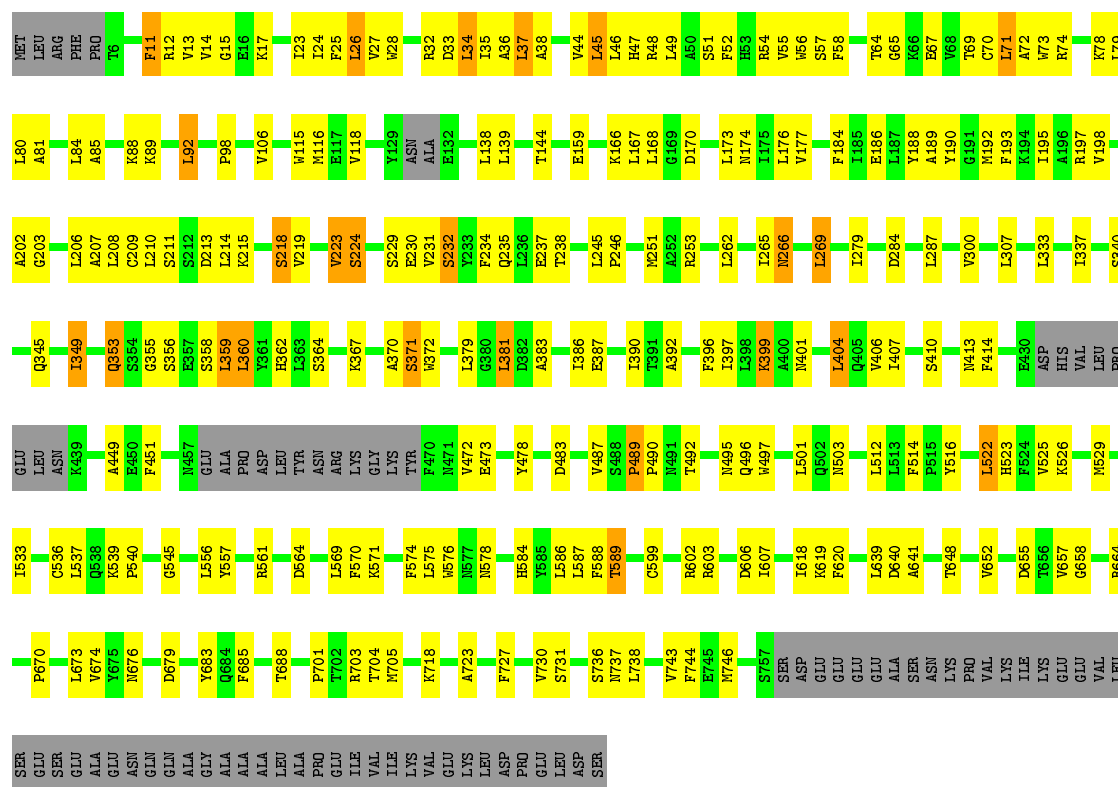
• Molecule 1: ANAPHASE-PROMOTING COMPLEX SUBUNIT 1





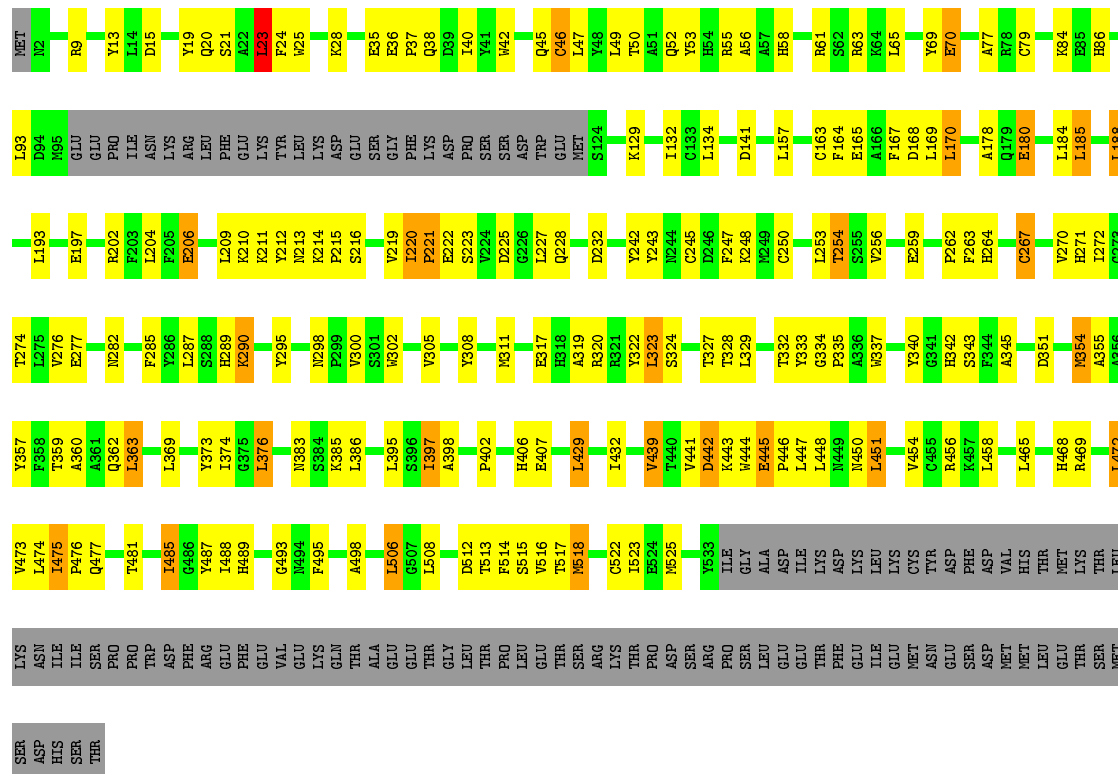
M1
W8
V11
W14
L15
W16
D20
G23
N28
A29
F30
S31
G32
C33
C34
P35
D36
V39
P40
G41
D42
D43
C44
P45
L46
V47
Q50
I60
L61
V69
K83
E84

Chain C: 44% 34% 10% 12%

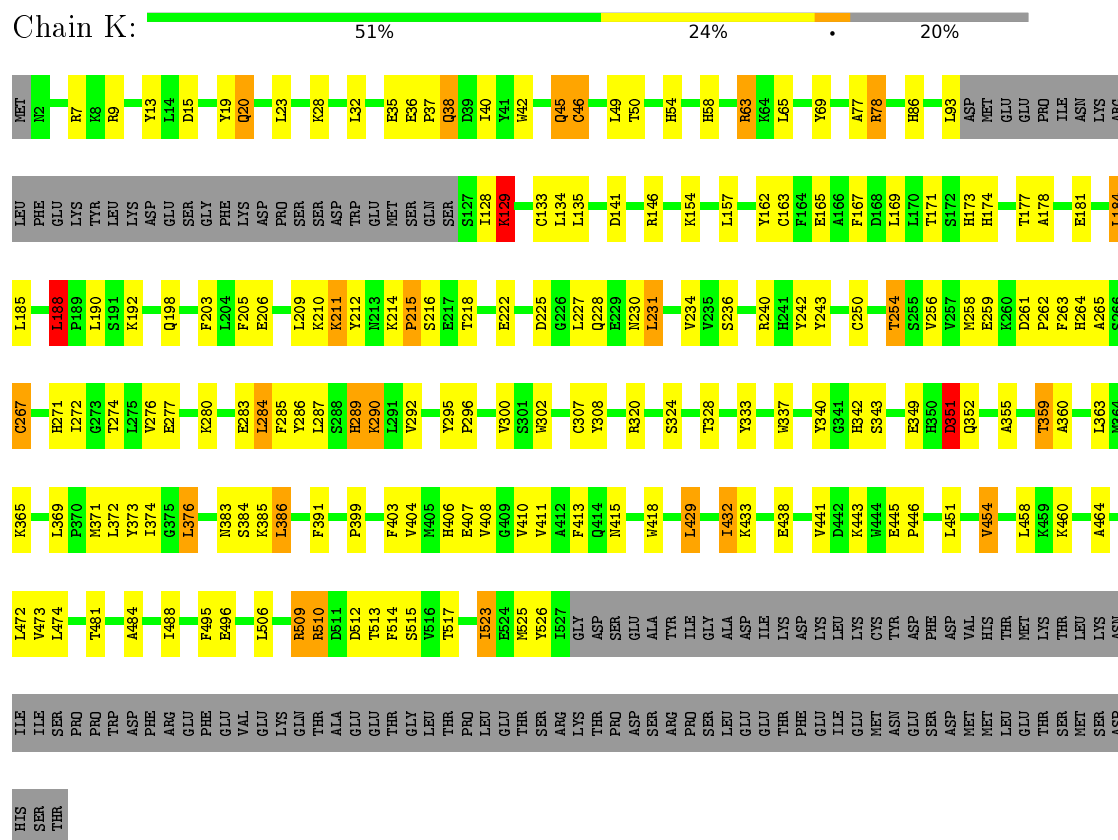


• Molecule 9: CELL DIVISION CYCLE PROTEIN 16 HOMOLOG

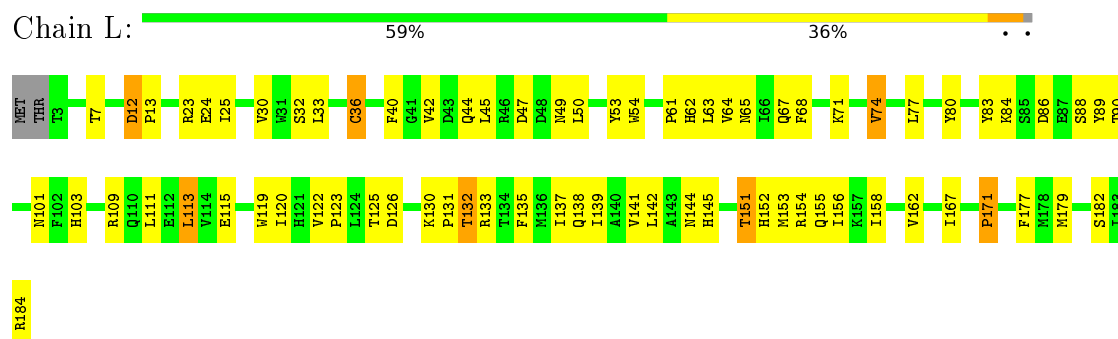
Chain J:  50%  26%  19%



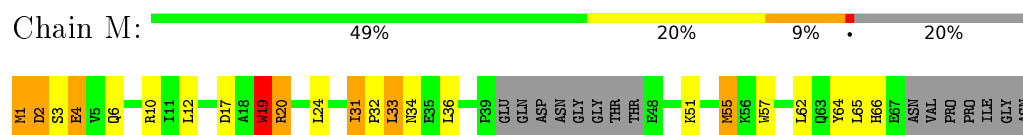
• Molecule 9: CELL DIVISION CYCLE PROTEIN 16 HOMOLOG



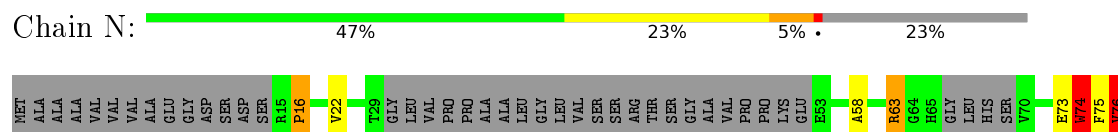
• Molecule 10: ANAPHASE-PROMOTING COMPLEX SUBUNIT 10

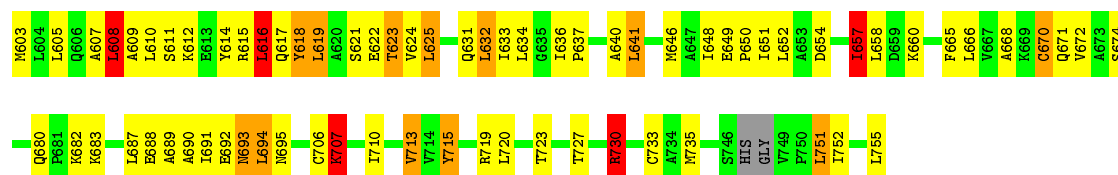


• Molecule 11: ANAPHASE-PROMOTING COMPLEX SUBUNIT 13



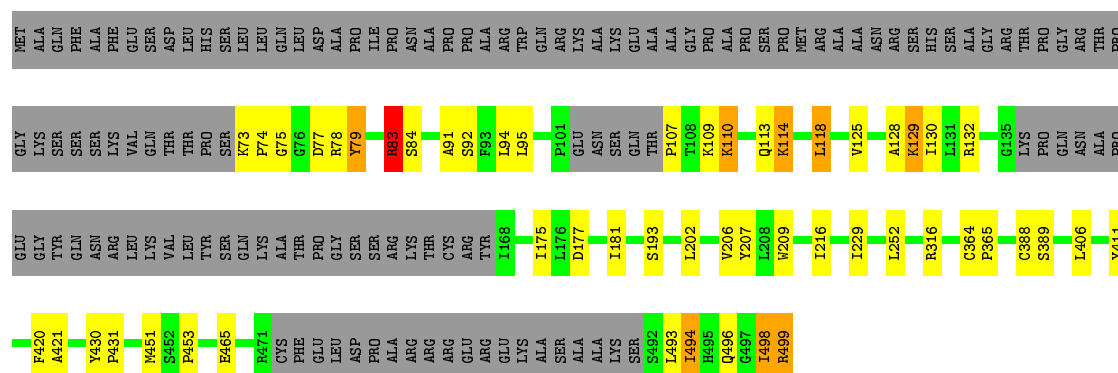
• Molecule 12: ANAPHASE-PROMOTING COMPLEX SUBUNIT 2





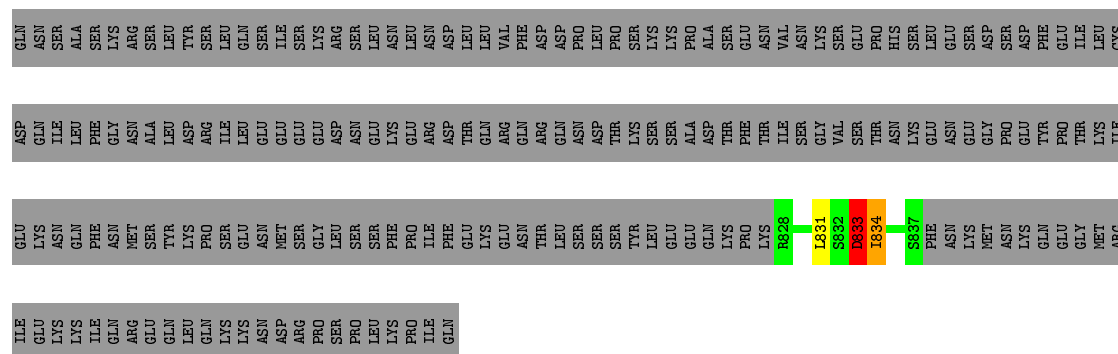
• Molecule 14: CELL DIVISION CYCLE PROTEIN 20 HOMOLOG

Chain R: 64% 9% 26%



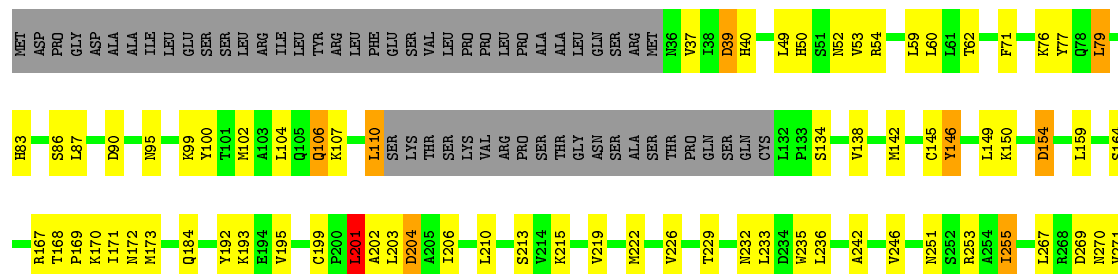
• Molecule 15: PROBABLE SERINE/THREONINE-PROTEIN KINASE HSL1

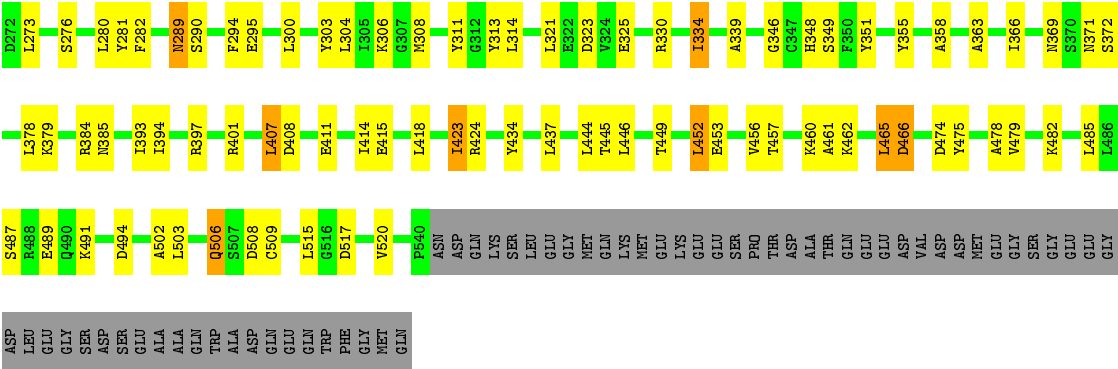
Chain S: 95%



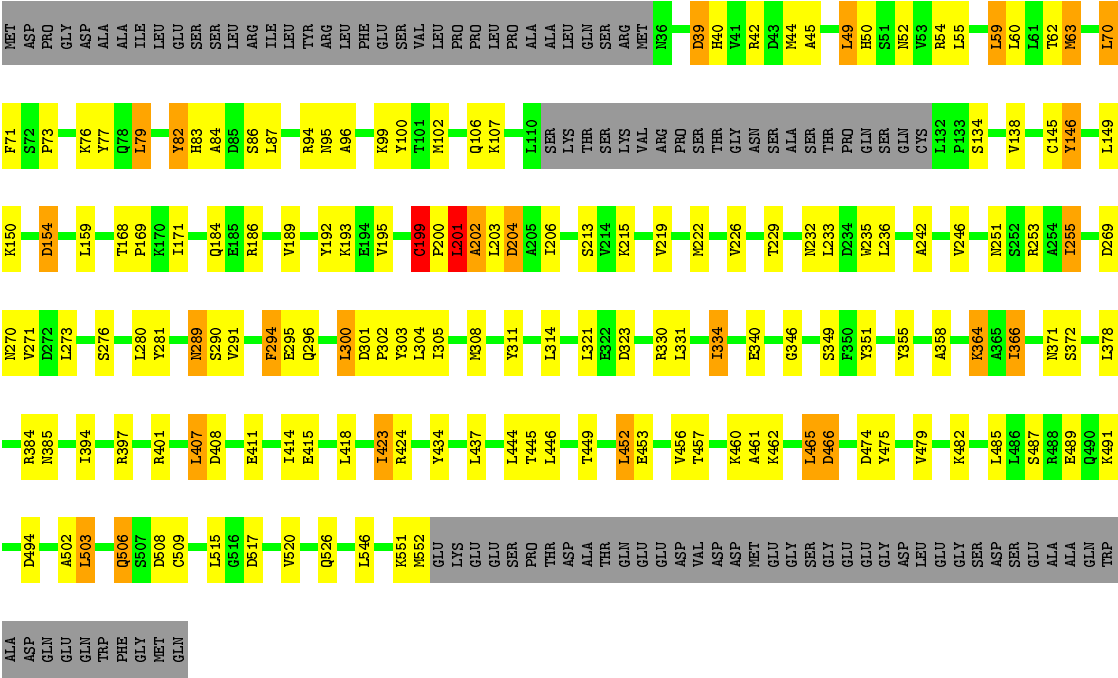
• Molecule 16: ANAPHASE-PROMOTING COMPLEX SUBUNIT 7

Chain X: 55% 23% 19%





• Molecule 16: ANAPHASE-PROMOTING COMPLEX SUBUNIT 7



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	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	0.58	0/11165	0.89	29/15204 (0.2%)
10	L	0.67	0/1468	0.88	1/1993 (0.1%)
11	M	0.63	1/502 (0.2%)	0.95	0/680
12	N	0.54	0/4915	0.88	15/6645 (0.2%)
13	O	0.61	1/5493 (0.0%)	0.92	14/7421 (0.2%)
14	R	0.54	2/2940 (0.1%)	0.72	1/3996 (0.0%)
15	S	0.50	0/71	1.09	1/95 (1.1%)
16	X	0.55	0/3826	0.80	6/5177 (0.1%)
16	Y	0.55	0/3919	0.82	10/5301 (0.2%)
2	B	0.67	0/674	0.91	0/913
3	C	0.65	0/4404	0.94	8/5945 (0.1%)
3	P	0.63	0/4134	0.91	7/5583 (0.1%)
4	D	0.58	0/446	0.85	1/610 (0.2%)
5	E	0.57	0/459	0.78	0/619
6	F	0.58	0/4013	0.83	4/5428 (0.1%)
6	H	0.59	0/3942	0.82	3/5326 (0.1%)
7	G	0.59	0/214	0.92	1/284 (0.4%)
7	W	0.64	0/214	0.86	0/284
8	I	0.65	0/5827	0.93	12/7899 (0.2%)
9	J	0.69	1/4146 (0.0%)	0.94	6/5616 (0.1%)
9	K	0.70	1/4086 (0.0%)	0.93	5/5534 (0.1%)
All	All	0.61	6/66858 (0.0%)	0.88	124/90553 (0.1%)

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
10	L	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
11	M	0	1
12	N	0	4
16	Y	0	1
3	P	0	1
6	F	0	1
6	H	0	1
8	I	0	3
9	J	0	1
All	All	0	15

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	O	268	PHE	CG-CD2	7.98	1.50	1.38
9	J	302	TRP	CB-CG	-6.32	1.38	1.50
14	R	79	TYR	CB-CG	5.73	1.60	1.51
11	M	19	TRP	CB-CG	5.53	1.60	1.50
14	R	79	TYR	CE1-CZ	5.37	1.45	1.38

The worst 5 of 124 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	P	358	LEU	CA-CB-CG	9.86	137.98	115.30
13	O	730	ARG	NE-CZ-NH1	9.15	124.88	120.30
3	C	440	GLY	N-CA-C	-8.87	90.94	113.10
9	K	351	ASP	CB-CG-OD1	8.76	126.19	118.30
1	A	1235	LEU	CA-CB-CG	8.41	134.65	115.30

There are no chirality outliers.

5 of 15 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	124	GLN	Peptide
6	F	565	ASN	Peptide
6	H	565	ASN	Peptide
8	I	489	PRO	Peptide
8	I	658	GLY	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	10925	0	10669	471	0
2	B	649	0	595	26	0
3	C	4306	0	4273	274	0
3	P	4039	0	3989	120	0
4	D	436	0	396	27	0
5	E	450	0	435	12	0
6	F	3923	0	3819	115	0
6	H	3853	0	3793	110	0
7	G	213	0	220	16	0
7	W	213	0	220	9	0
8	I	5709	0	5597	188	0
9	J	4047	0	3949	185	0
9	K	3988	0	3908	148	0
10	L	1435	0	1382	43	0
11	M	493	0	469	17	0
12	N	4837	0	4534	155	0
13	O	5395	0	5429	231	0
14	R	2869	0	2772	59	0
15	S	72	0	71	10	0
16	X	3767	0	3819	136	0
16	Y	3859	0	3908	150	0
17	B	3	0	0	0	0
All	All	65481	0	64247	2216	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 17.

The worst 5 of 2216 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)
12:N:362:LYS:HG3	12:N:410:LEU:CD2	1.38	1.52
9:J:223:SER:CB	9:J:228:GLN:HE21	1.29	1.44
12:N:362:LYS:CG	12:N:410:LEU:HD23	1.60	1.31
12:N:362:LYS:CB	12:N:410:LEU:HD21	1.67	1.24
14:R:177:ASP:OD2	15:S:834:ILE:HD11	1.30	1.23

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	A	1393/1944 (72%)	1186 (85%)	149 (11%)	58 (4%)	3	36
2	B	83/84 (99%)	72 (87%)	7 (8%)	4 (5%)	3	32
3	C	520/597 (87%)	489 (94%)	23 (4%)	8 (2%)	13	58
3	P	485/597 (81%)	460 (95%)	20 (4%)	5 (1%)	19	65
4	D	53/121 (44%)	45 (85%)	7 (13%)	1 (2%)	10	54
5	E	54/110 (49%)	54 (100%)	0	0	100	100
6	F	494/824 (60%)	461 (93%)	25 (5%)	8 (2%)	12	57
6	H	477/824 (58%)	448 (94%)	22 (5%)	7 (2%)	13	58
7	G	23/85 (27%)	23 (100%)	0	0	100	100
7	W	23/85 (27%)	23 (100%)	0	0	100	100
8	I	722/808 (89%)	683 (95%)	34 (5%)	5 (1%)	26	71
9	J	500/620 (81%)	467 (93%)	29 (6%)	4 (1%)	24	69
9	K	489/620 (79%)	459 (94%)	24 (5%)	6 (1%)	16	62
10	L	180/184 (98%)	165 (92%)	11 (6%)	4 (2%)	8	52
11	M	55/74 (74%)	42 (76%)	10 (18%)	3 (6%)	2	30
12	N	601/822 (73%)	497 (83%)	58 (10%)	46 (8%)	1	20
13	O	677/755 (90%)	619 (91%)	46 (7%)	12 (2%)	11	55
14	R	361/499 (72%)	338 (94%)	20 (6%)	3 (1%)	24	69
15	S	8/206 (4%)	6 (75%)	0	2 (25%)	0	1
16	X	478/599 (80%)	463 (97%)	12 (2%)	3 (1%)	30	73
16	Y	492/599 (82%)	474 (96%)	14 (3%)	4 (1%)	24	69
All	All	8168/11057 (74%)	7474 (92%)	511 (6%)	183 (2%)	13	52

5 of 183 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	45	ALA
1	A	241	ASP
1	A	274	VAL
1	A	411	HIS
1	A	413	TRP

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%)	970 (84%)	180 (16%)	3	24
2	B	65/75 (87%)	54 (83%)	11 (17%)	2	20
3	C	452/520 (87%)	357 (79%)	95 (21%)	1	11
3	P	421/520 (81%)	363 (86%)	58 (14%)	4	29
4	D	46/115 (40%)	37 (80%)	9 (20%)	1	14
5	E	47/89 (53%)	37 (79%)	10 (21%)	1	11
6	F	407/727 (56%)	369 (91%)	38 (9%)	11	46
6	H	408/727 (56%)	374 (92%)	34 (8%)	14	51
7	G	23/77 (30%)	22 (96%)	1 (4%)	35	72
7	W	23/77 (30%)	22 (96%)	1 (4%)	35	72
8	I	620/730 (85%)	584 (94%)	36 (6%)	25	64
9	J	424/548 (77%)	382 (90%)	42 (10%)	10	43
9	K	423/548 (77%)	379 (90%)	44 (10%)	9	40
10	L	155/169 (92%)	136 (88%)	19 (12%)	6	33
11	M	55/67 (82%)	42 (76%)	13 (24%)	1	8
12	N	460/724 (64%)	398 (86%)	62 (14%)	5	30
13	O	576/650 (89%)	478 (83%)	98 (17%)	2	20
14	R	304/411 (74%)	290 (95%)	14 (5%)	33	70
15	S	8/195 (4%)	8 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	X	406/513 (79%)	373 (92%)	33 (8%)	15	52
16	Y	416/513 (81%)	375 (90%)	41 (10%)	10	43
All	All	6889/9715 (71%)	6050 (88%)	839 (12%)	10	33

5 of 839 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	I	34	LEU
9	K	163	CYS
16	X	253	ARG
8	I	333	LEU
9	J	188	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 145 such sidechains are listed below:

Mol	Chain	Res	Type
9	J	38	GLN
9	K	198	GLN
16	X	371	ASN
9	J	58	HIS
9	J	342	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.