wwPDB EM Validation Summary Report (i)

May 13, 2024 – 09:20 pm BST

PDB ID	:	7QE7
EMDB ID	:	EMD-13931
Title	:	High-resolution structure of the Anaphase-promoting complex/cyclosome (APC/C) bound to co-activator Cdh1
Authors	:	Hoefler, A.; Yu, J.; Chang, L.; Zhang, Z.; Yang, J.; Boland, A.; Barford, D.
Deposited on	:	2021-12-01
Resolution	:	2.90 Å(reported)
Based on initial model	:	4UI9

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

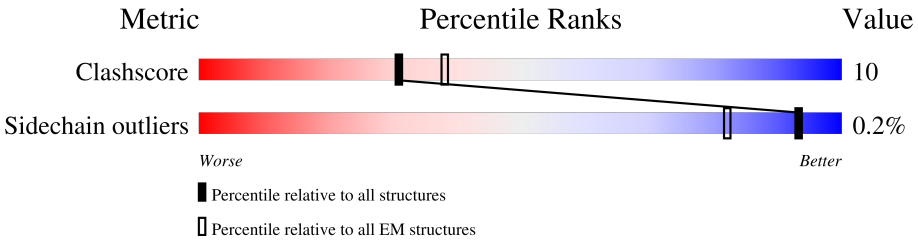
EMDB validation analysis	:	0.0.1.dev92
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain
1	L	185	75% 24% .
2	D	121	43% . 54%
3	A	1944	66% 19% 15%
4	N	822	58% 24% 17%
5	I	814	69% 22% 9%
6	O	755	75% 19% 6%
7	S	447	12% 7% 80%
8	K	620	72% 14% 14%
8	Q	620	65% 16% 18%
9	G	85	27% 5% 68%

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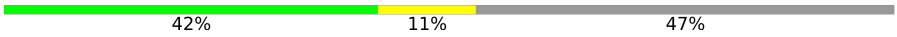
Mol	Chain	Length	Quality of chain
9	W	85	
10	M	74	
11	H	110	
12	J	824	
12	P	824	
13	Y	599	
13	Z	599	
14	U	597	
14	V	597	
15	R	496	
16	C	84	

2 Entry composition (i)

There are 17 unique types of molecules in this entry. The entry contains 71208 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 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	L	183	Total	C	N	O	S	0	0
			1479	926	268	278	7		

- Molecule 2 is a protein called Anaphase-promoting complex subunit 15.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	56	Total	C	N	O	S	1	0
			470	299	81	89	1		

- Molecule 3 is a protein called Anaphase-promoting complex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	1648	Total	C	N	O	S	0	0
			12968	8284	2191	2407	86		

- Molecule 4 is a protein called Anaphase-promoting complex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	N	682	Total	C	N	O	S	0	0
			5505	3484	973	1021	27		

- Molecule 5 is a protein called Anaphase-promoting complex subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	742	Total	C	N	O	S	0	0
			5925	3793	989	1109	34		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	809	GLU	-	expression tag	UNP Q9UJX5
I	810	ASN	-	expression tag	UNP Q9UJX5
I	811	LEU	-	expression tag	UNP Q9UJX5

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Chain	Residue	Modelled	Actual	Comment	Reference
I	812	TYR	-	expression tag	UNP Q9UJX5
I	813	PHE	-	expression tag	UNP Q9UJX5
I	814	GLN	-	expression tag	UNP Q9UJX5

- Molecule 6 is a protein called Anaphase-promoting complex subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	O	707	Total	C	N	O	S	0	0
			5593	3567	972	1024	30		

- Molecule 7 is a protein called F-box only protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	S	88	Total	C	N	O	S	0	0
			692	428	131	125	8		

- Molecule 8 is a protein called Cell division cycle protein 16 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	K	531	Total	C	N	O	S	0	0
			4323	2775	726	794	28		
8	Q	506	Total	C	N	O	S	1	0
			4103	2630	694	754	25		

- Molecule 9 is a protein called Anaphase-promoting complex subunit CDC26.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	G	27	Total	C	N	O	S	0	0
			233	146	43	43	1		
9	W	26	Total	C	N	O	S	0	0
			225	142	42	40	1		

- Molecule 10 is a protein called Anaphase-promoting complex subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	M	68	Total	C	N	O	S	0	0
			553	342	91	118	2		

- Molecule 11 is a protein called Anaphase-promoting complex subunit 16.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	H	58	Total	C	N	O	S	0	0
			475	304	79	90	2		

- Molecule 12 is a protein called Cell division cycle protein 27 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	J	510	Total	C	N	O	S	1	0
			4097	2632	691	748	26		
12	P	496	Total	C	N	O	S	0	0
			3994	2569	671	728	26		

- Molecule 13 is a protein called Anaphase-promoting complex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	Y	502	Total	C	N	O	S	0	0
			3922	2480	682	731	29		
13	Z	488	Total	C	N	O	S	1	0
			3830	2426	664	714	26		

- Molecule 14 is a protein called Cell division cycle protein 23 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	U	540	Total	C	N	O	S	0	0
			4442	2859	747	810	26		
14	V	534	Total	C	N	O	S	1	0
			4380	2817	732	805	26		

- Molecule 15 is a protein called Fizzy-related protein homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	R	432	Total	C	N	O	S	0	0
			3375	2120	612	632	11		

- Molecule 16 is a protein called Anaphase-promoting complex subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	C	83	Total	C	N	O	S	0	0
			618	393	109	102	14		

- Molecule 17 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

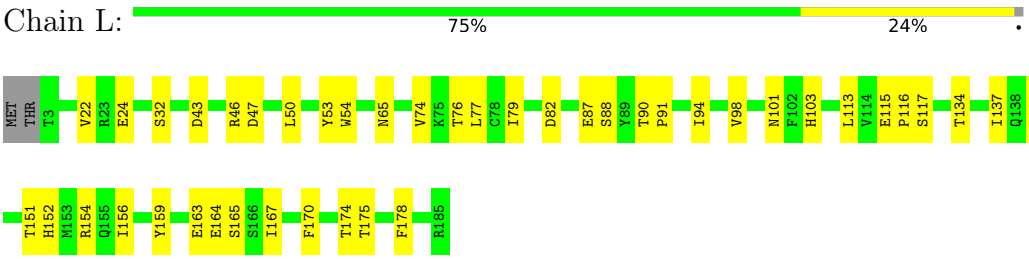
Mol	Chain	Residues	Atoms	AltConf
17	N	1	Total Zn 1 1	0
17	S	2	Total Zn 2 2	0
17	C	3	Total Zn 3 3	0

3 Residue-property plots (i)

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

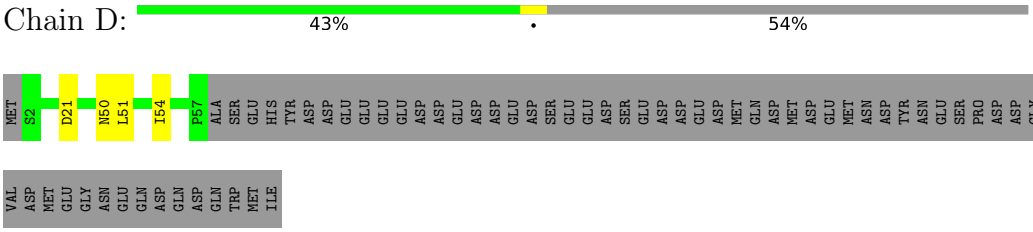
- Molecule 1: Anaphase-promoting complex subunit 10

Chain L:



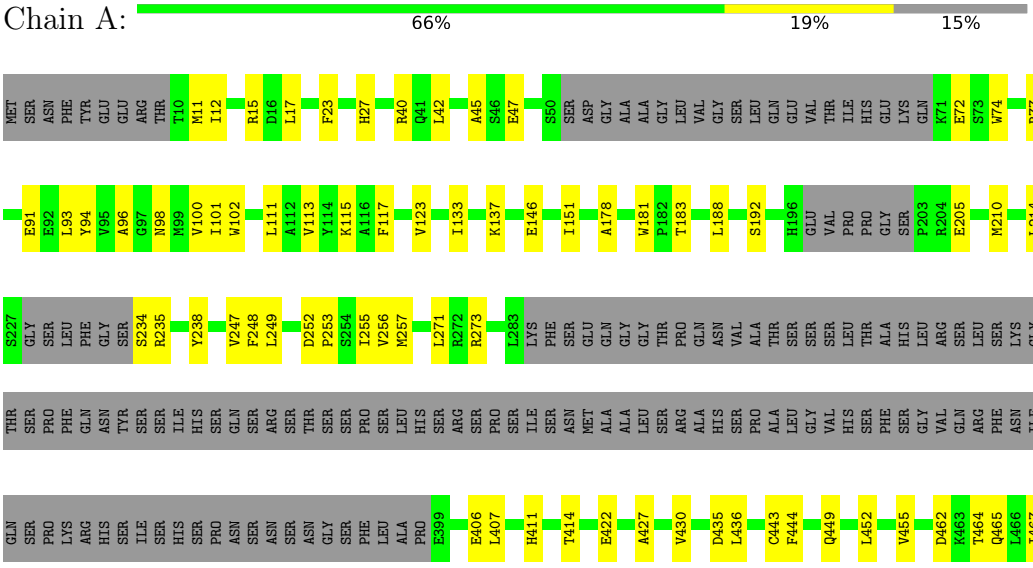
- Molecule 2: Anaphase-promoting complex subunit 15

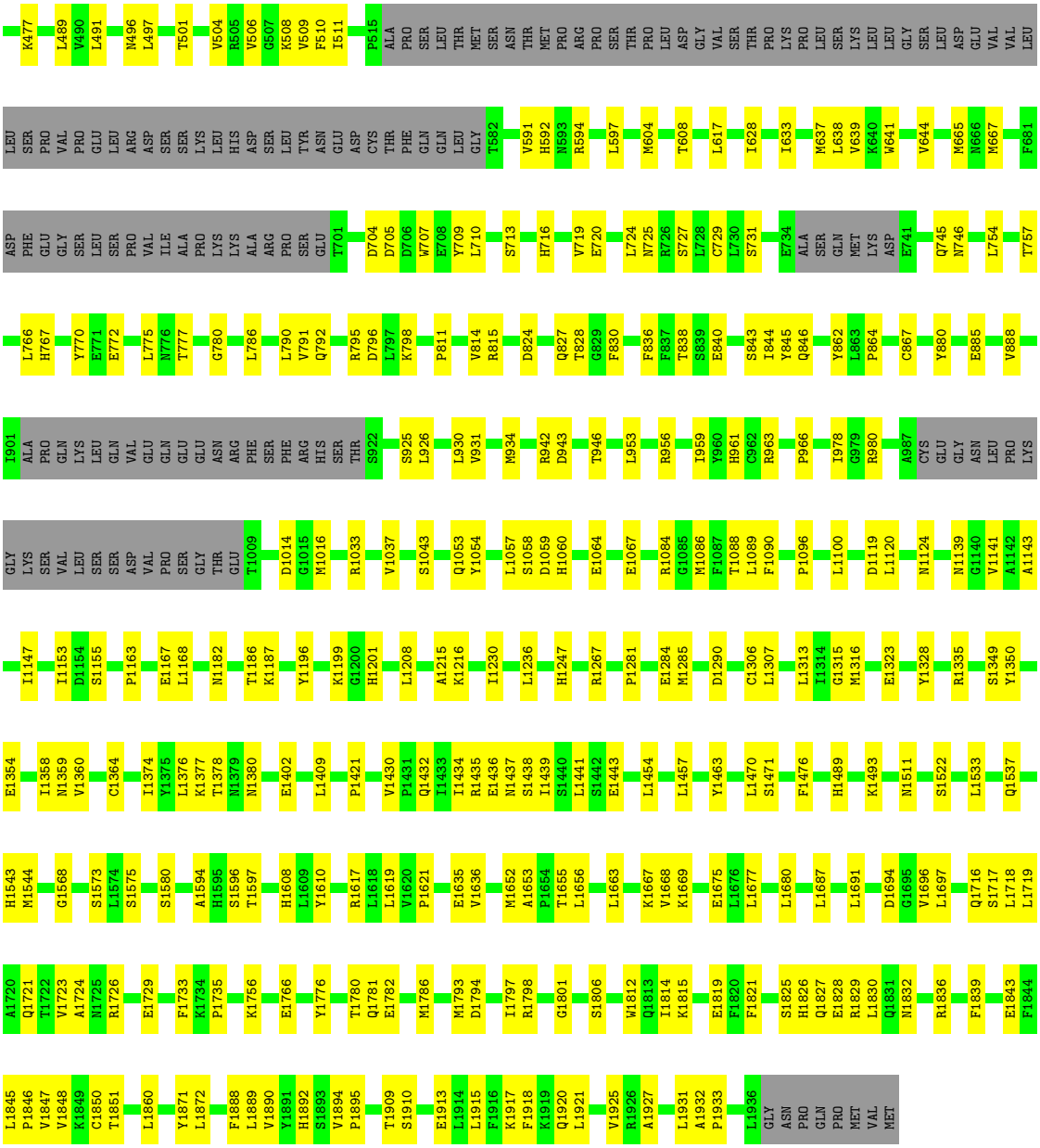
Chain D:



- Molecule 3: Anaphase-promoting complex subunit 1

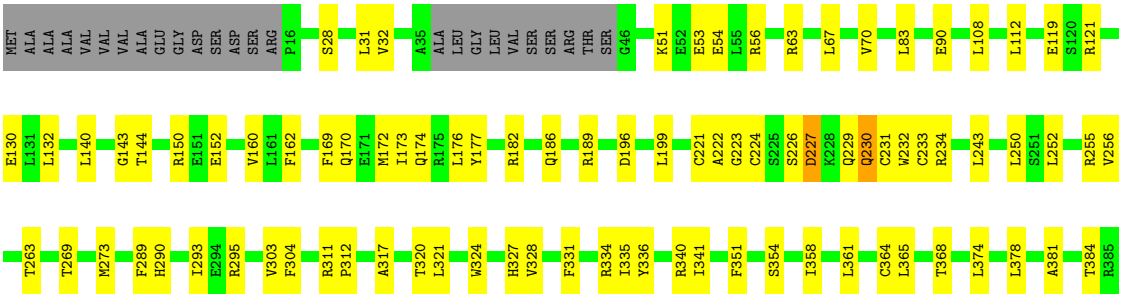
Chain A:

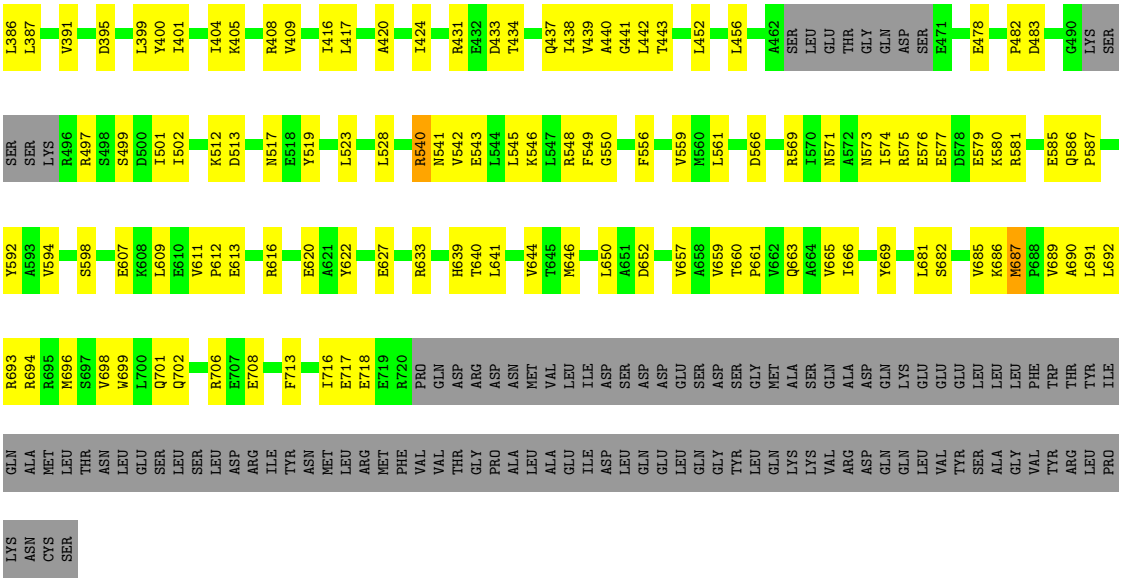




• Molecule 4: Anaphase-promoting complex subunit 2

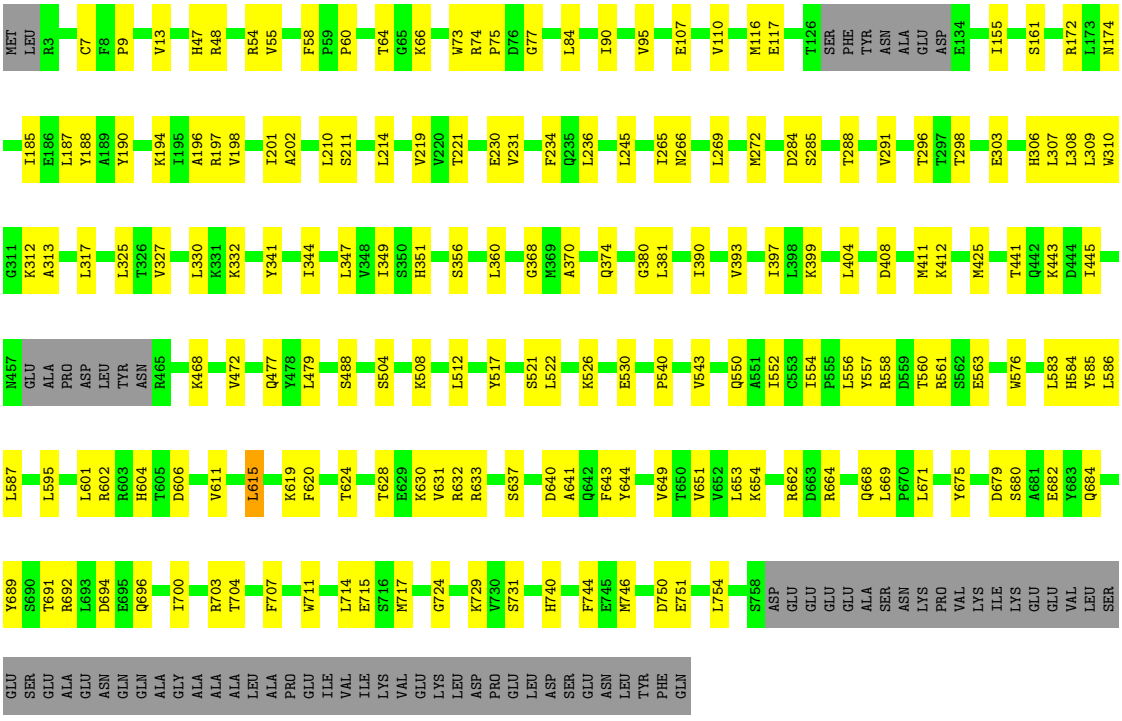
Chain N:





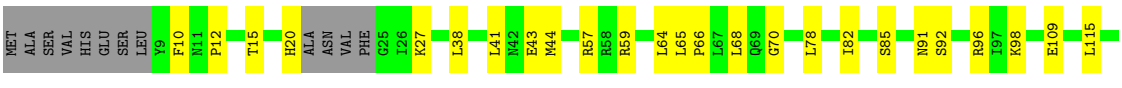
• Molecule 5: Anaphase-promoting complex subunit 4

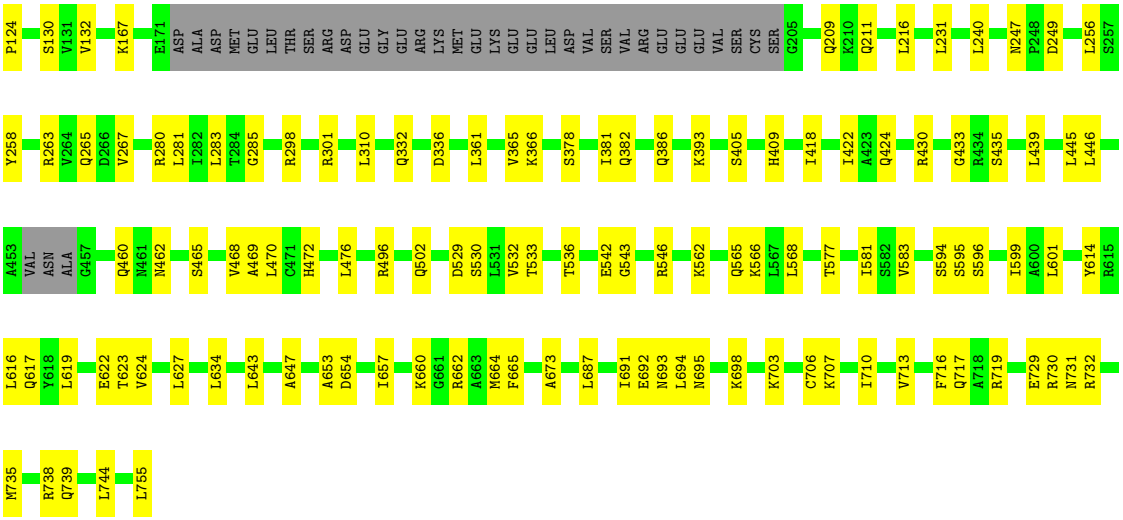
Chain I:



• Molecule 6: Anaphase-promoting complex subunit 5

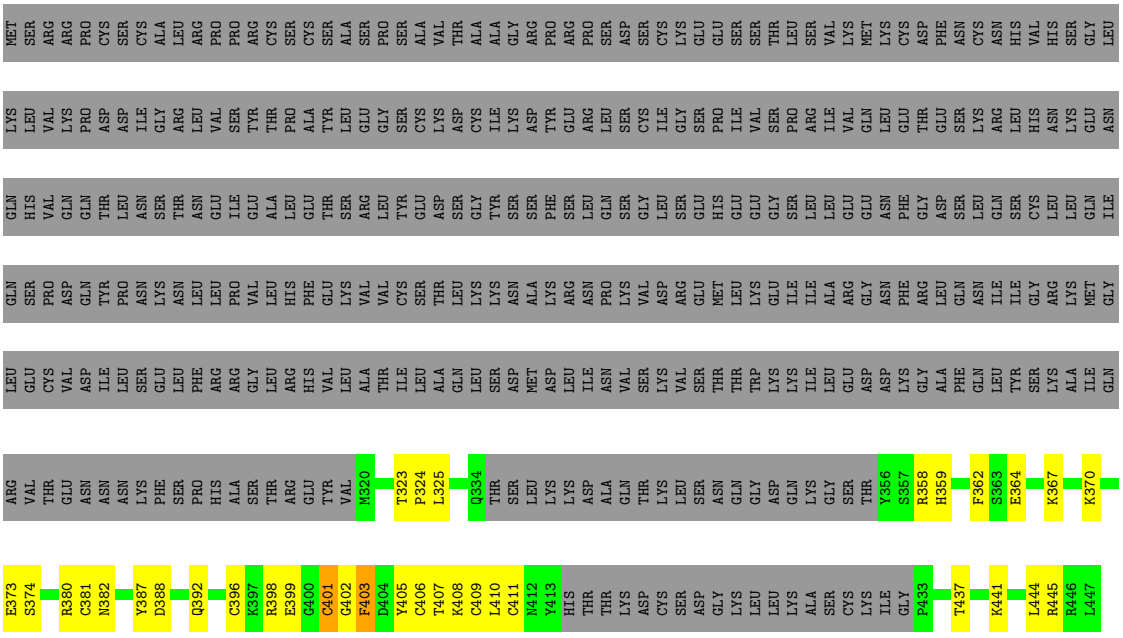
Chain O:





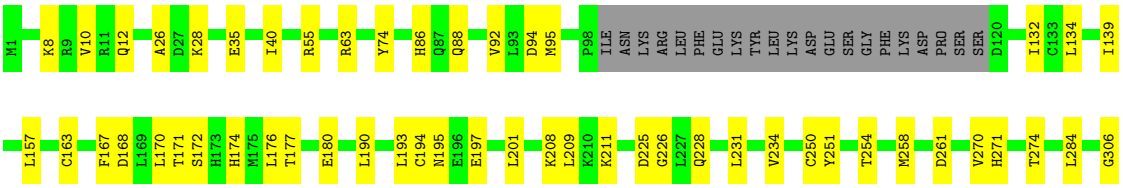
• Molecule 7: F-box only protein 5

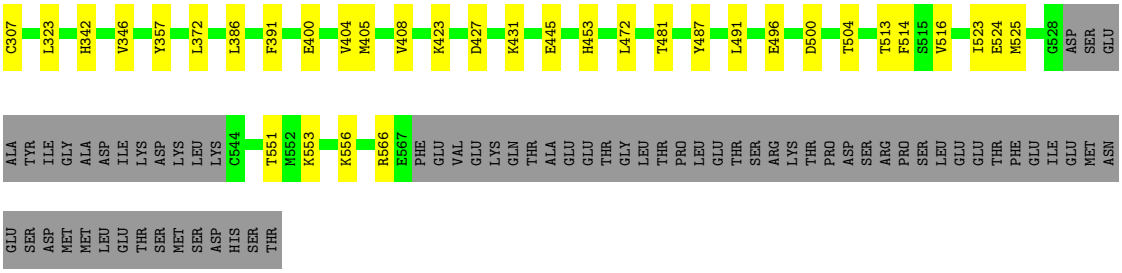
Chain S:



• Molecule 8: Cell division cycle protein 16 homolog

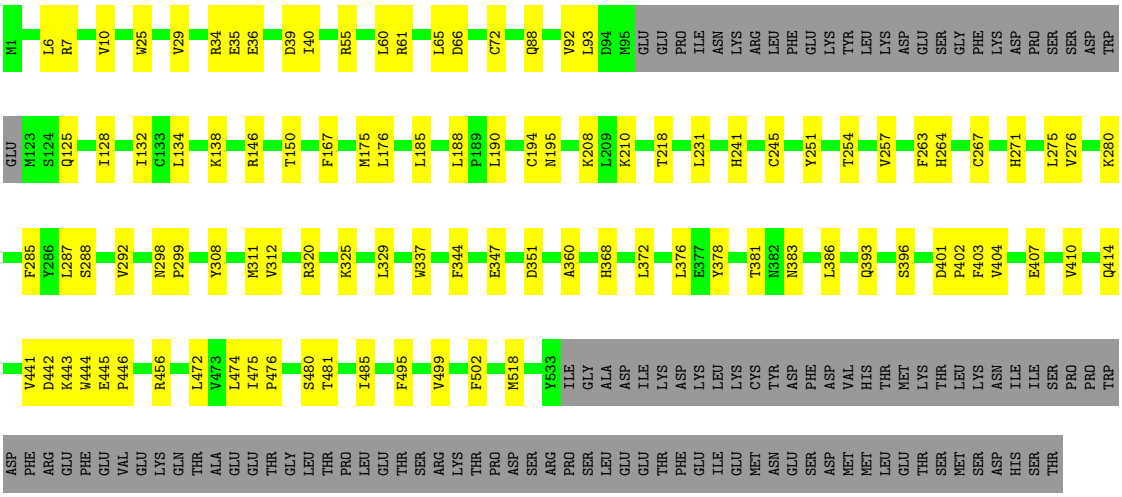
Chain K:





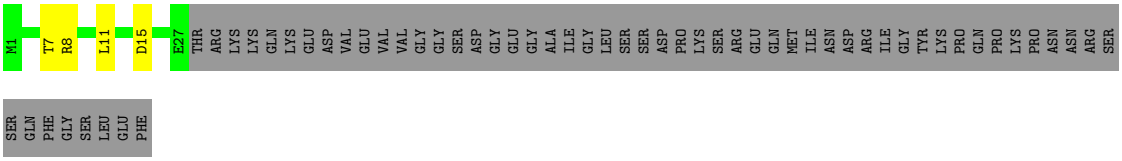
• Molecule 8: Cell division cycle protein 16 homolog

Chain Q:



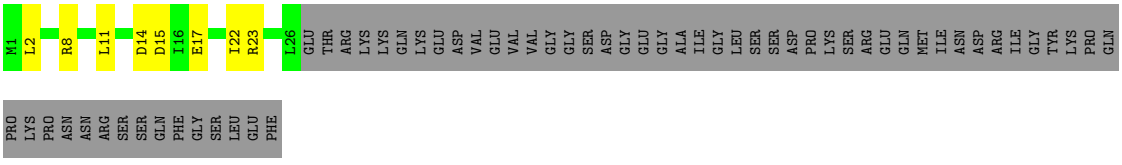
• Molecule 9: Anaphase-promoting complex subunit CDC26

Chain G:



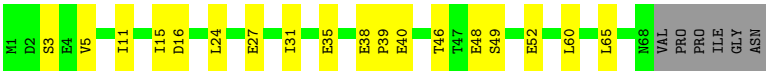
• Molecule 9: Anaphase-promoting complex subunit CDC26

Chain W:



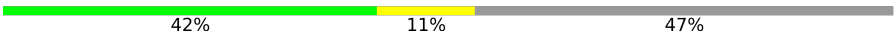
• Molecule 10: Anaphase-promoting complex subunit 13

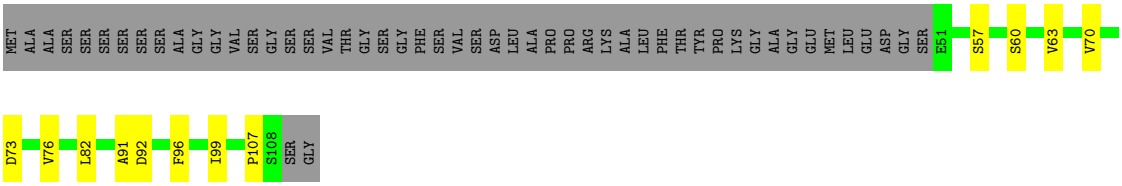
Chain M:



• Molecule 11: Anaphase-promoting complex subunit 16

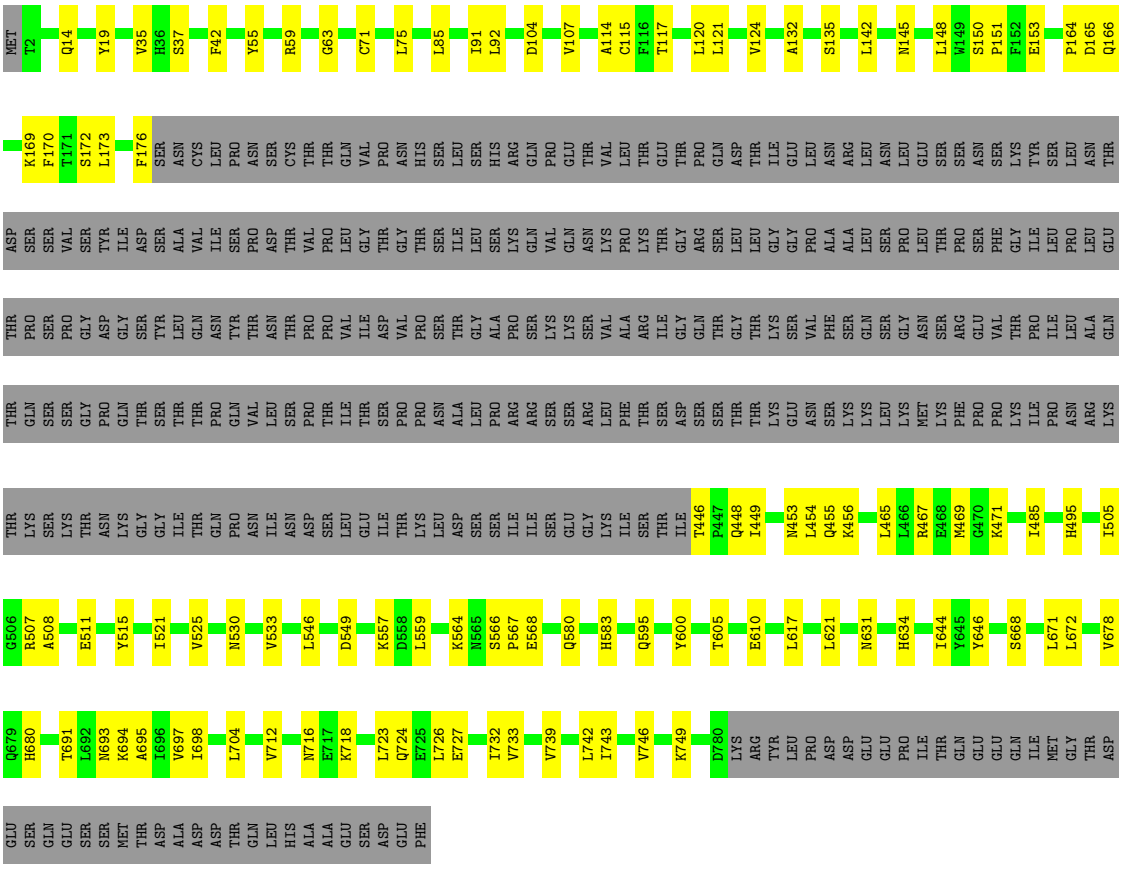
Chain H:





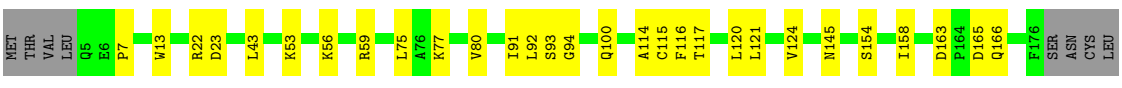
• Molecule 12: Cell division cycle protein 27 homolog

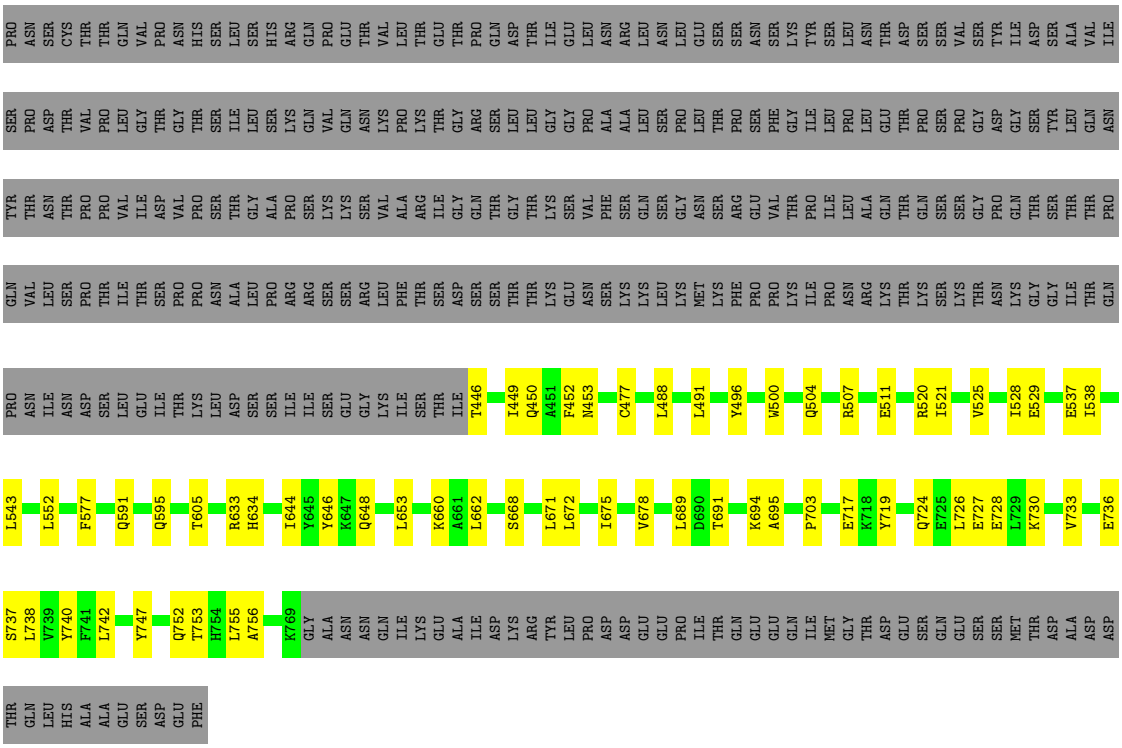
Chain J:



• Molecule 12: Cell division cycle protein 27 homolog

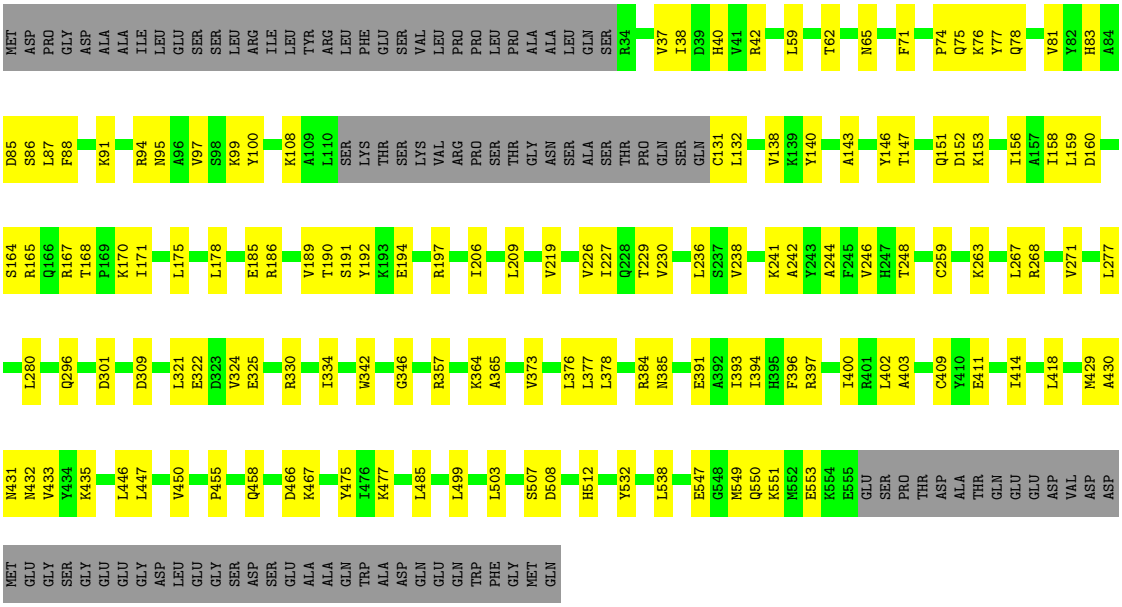
Chain P:





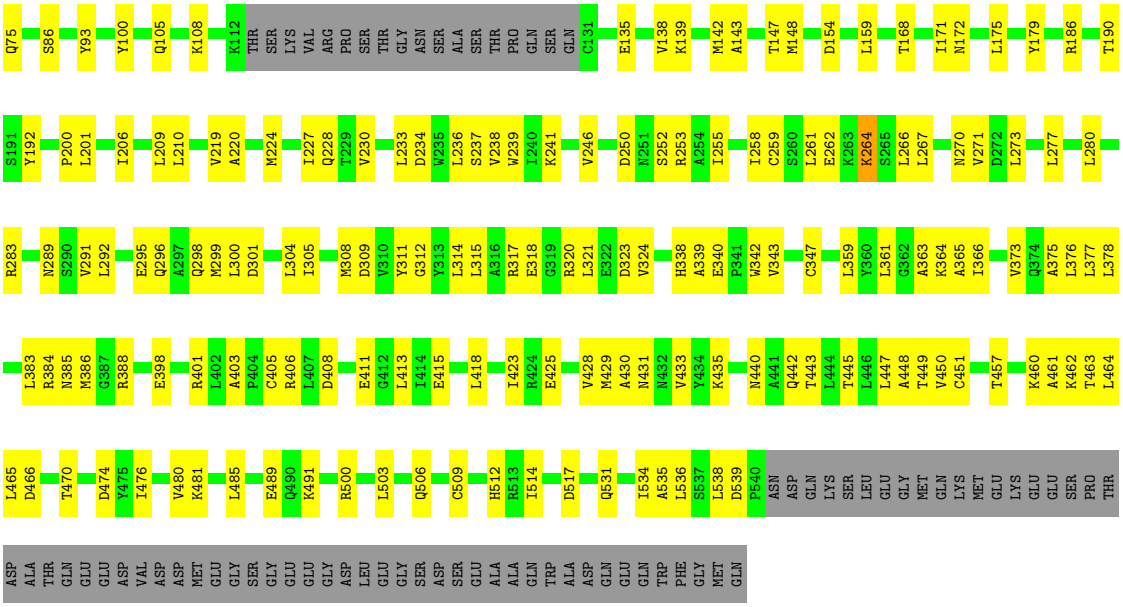
• Molecule 13: Anaphase-promoting complex subunit 7

Chain Y:



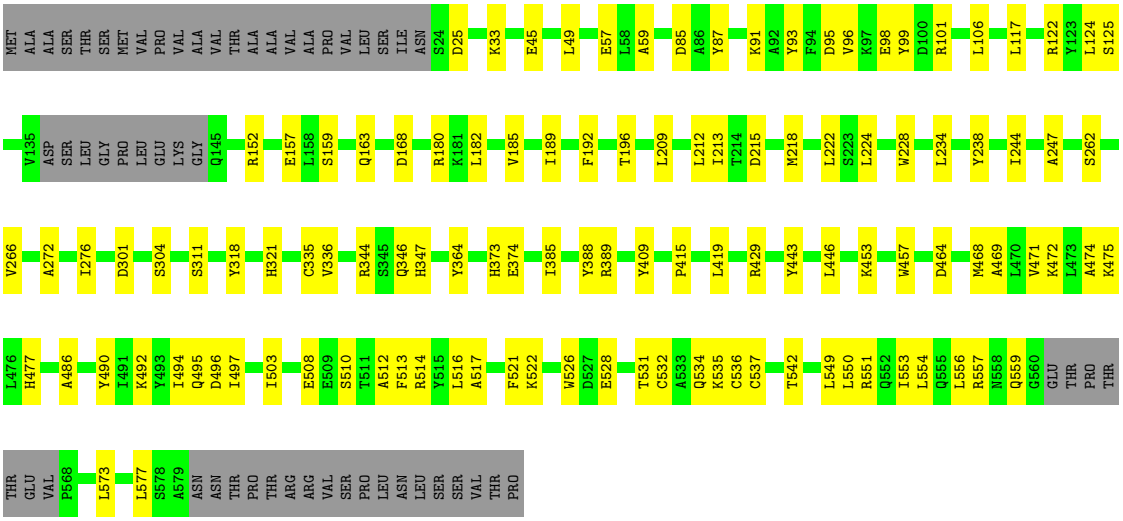
• Molecule 13: Anaphase-promoting complex subunit 7

Chain Z:



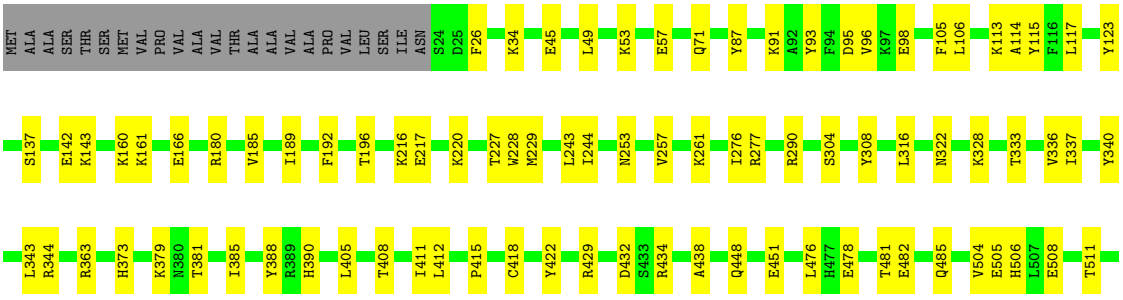
• Molecule 14: Cell division cycle protein 23 homolog

Chain U:



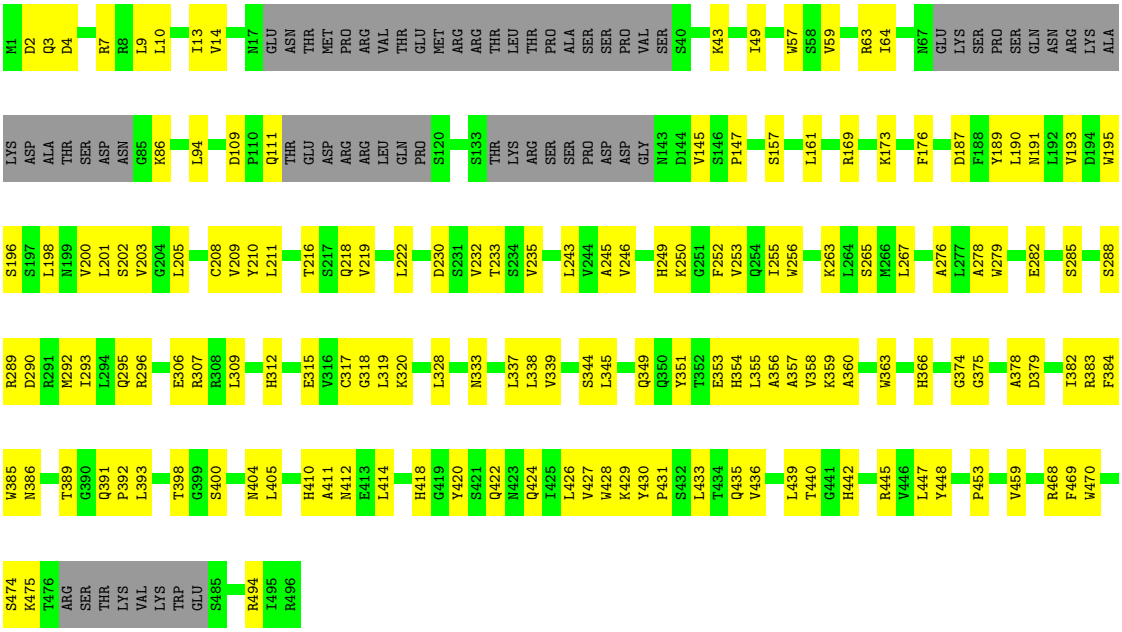
• Molecule 14: Cell division cycle protein 23 homolog

Chain V:



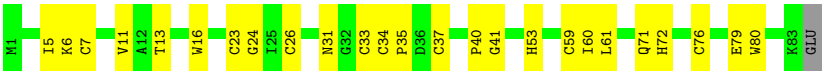
• Molecule 15: Fizzy-related protein homolog

Chain R:



• Molecule 16: Anaphase-promoting complex subunit 11

Chain C:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	364331	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (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	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	L	0.30	0/1514	0.47	0/2051
2	D	0.29	0/485	0.45	0/662
3	A	0.32	0/13269	0.45	0/18041
4	N	0.28	0/5618	0.46	0/7605
5	I	0.29	0/6050	0.45	0/8188
6	O	0.32	0/5697	0.43	0/7694
7	S	0.35	0/701	0.56	0/931
8	K	0.33	0/4431	0.41	0/5998
8	Q	0.33	0/4205	0.42	0/5691
9	G	0.26	0/234	0.38	0/310
9	W	0.27	0/226	0.41	0/299
10	M	0.30	0/563	0.45	0/765
11	H	0.29	0/484	0.39	0/651
12	J	0.32	0/4196	0.42	0/5672
12	P	0.33	0/4090	0.41	0/5527
13	Y	0.26	0/3982	0.44	0/5380
13	Z	0.26	0/3893	0.49	0/5262
14	U	0.32	0/4544	0.43	0/6133
14	V	0.36	0/4483	0.43	0/6056
15	R	0.27	0/3446	0.49	0/4670
16	C	0.24	0/639	0.44	0/874
All	All	0.31	0/72750	0.44	0/98460

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	L	1479	0	1462	33	0
2	D	470	0	458	3	0
3	A	12968	0	12918	247	0
4	N	5505	0	5487	154	0
5	I	5925	0	5902	115	0
6	O	5593	0	5659	100	0
7	S	692	0	698	32	0
8	K	4323	0	4229	62	0
8	Q	4103	0	4026	70	0
9	G	233	0	246	5	0
9	W	225	0	242	10	0
10	M	553	0	516	15	0
11	H	475	0	469	12	0
12	J	4097	0	4058	71	0
12	P	3994	0	3955	68	0
13	Y	3922	0	3989	93	0
13	Z	3830	0	3909	133	0
14	U	4442	0	4409	83	0
14	V	4380	0	4326	69	0
15	R	3375	0	3341	114	0
16	C	618	0	542	19	0
17	C	3	0	0	0	0
17	N	1	0	0	0	0
17	S	2	0	0	0	0
All	All	71208	0	70841	1374	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 10.

The worst 5 of 1374 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)
13:Z:451:CYS:HB2	13:Z:457:THR:HG21	1.24	1.11
4:N:666:ILE:HD11	4:N:685:VAL:HG11	1.53	0.87
15:R:195:TRP:HE1	15:R:453:PRO:HD3	1.40	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:Z:267:LEU:HD21	13:Z:273:LEU:HD22	1.58	0.86
13:Z:451:CYS:HB2	13:Z:457:THR:CG2	2.06	0.86

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains (i)

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	L	168/170 (99%)	168 (100%)	0	100	100
2	D	54/115 (47%)	54 (100%)	0	100	100
3	A	1450/1720 (84%)	1450 (100%)	0	100	100
4	N	600/724 (83%)	594 (99%)	6 (1%)	76	92
5	I	663/736 (90%)	661 (100%)	2 (0%)	92	98
6	O	604/650 (93%)	603 (100%)	1 (0%)	93	98
7	S	76/403 (19%)	74 (97%)	2 (3%)	46	77
8	K	463/548 (84%)	463 (100%)	0	100	100
8	Q	437/548 (80%)	437 (100%)	0	100	100
9	G	26/77 (34%)	26 (100%)	0	100	100
9	W	25/77 (32%)	25 (100%)	0	100	100
10	M	61/67 (91%)	61 (100%)	0	100	100
11	H	52/89 (58%)	52 (100%)	0	100	100
12	J	439/727 (60%)	439 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
12	P	429/727 (59%)	429 (100%)	0	100 100
13	Y	425/513 (83%)	423 (100%)	2 (0%)	88 96
13	Z	417/513 (81%)	416 (100%)	1 (0%)	93 98
14	U	471/520 (91%)	471 (100%)	0	100 100
14	V	463/520 (89%)	463 (100%)	0	100 100
15	R	370/431 (86%)	369 (100%)	1 (0%)	92 98
16	C	62/75 (83%)	62 (100%)	0	100 100
All	All	7755/9950 (78%)	7740 (100%)	15 (0%)	93 98

5 of 15 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	I	615	LEU
13	Z	264	LYS
6	O	167	LYS
15	R	86	LYS
13	Y	88	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 35 such sidechains are listed below:

Mol	Chain	Res	Type
14	V	71	GLN
14	V	242	GLN
15	R	310	GLN
5	I	720	GLN
5	I	668	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Map visualisation

This section contains visualisations of the EMDB entry EMD-13931. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1 Orthogonal projections

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

6.5 Orthogonal surface views

This section was not generated.

6.6 Mask visualisation

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

7 Map analysis

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

7.1 Map-value distribution

This section was not generated.

7.2 Volume estimate versus contour level

This section was not generated.

7.3 Rotationally averaged power spectrum

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit

This section was not generated.