



wwPDB EM Map/Model Validation Report ⓘ

Sep 12, 2016 – 12:09 PM EDT

PDB ID : 5L9U
EMDB ID: : unknown
Title : Model of human Anaphase-promoting complex/Cyclosome (APC/C-CDH1) with a cross linked Ubiquitin variant-substrate-UBE2C (UBCH10) complex representing key features of multiubiquitination
Authors : Brown, N.G.; VanderLinden, R.; Dube, P.; Haselbach, D.; Peters, J.M.; Stark, H.; Schulman, B.A.
Deposited on : 2016-06-11
Resolution : 6.40 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>

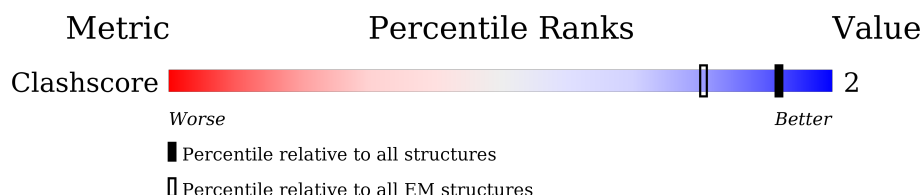
MolProbity : 4.02b-467
Mogul : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027939

1 Overall quality at a glance

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






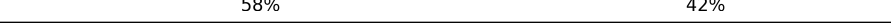
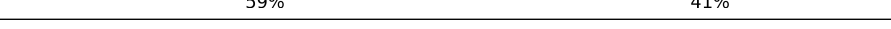
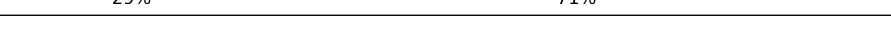

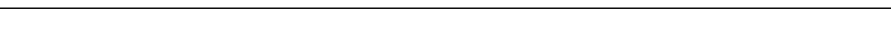

The reported resolution of this entry is 6.40 Å.

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.




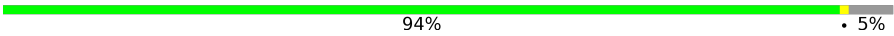








Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924

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		
7	W	85		
8	I	818		
9	J	620		

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Mol	Chain	Length	Quality of chain
9	K	620	 80% 20%
10	L	185	 94% • 5%
11	M	74	 66% 34%
12	N	822	 73% • 26%
13	O	755	 89% 10%
14	R	493	 77% • 22%
15	S	157	 55% 45%
16	U	188	 77% 23%
17	X	565	 67% 33%
17	Y	565	 70% 29%

2 Entry composition [i](#)

There are 17 unique types of molecules in this entry. The entry contains 8055 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	1342	Total	C	0	1342
			1342	1342		

- Molecule 2 is a protein called Anaphase-promoting complex subunit 11.

Mol	Chain	Residues	Atoms		AltConf	Trace
2	B	71	Total	C	0	71
			71	71		

- Molecule 3 is a protein called Cell division cycle protein 23 homolog.

Mol	Chain	Residues	Atoms		AltConf	Trace
3	C	474	Total	C	0	474
			474	474		
3	P	425	Total	C	0	425
			425	425		

- Molecule 4 is a protein called Anaphase-promoting complex subunit 15.

Mol	Chain	Residues	Atoms		AltConf	Trace
4	D	55	Total	C	0	55
			55	55		

- Molecule 5 is a protein called Anaphase-promoting complex subunit 16.

Mol	Chain	Residues	Atoms		AltConf	Trace
5	E	56	Total	C	0	56
			56	56		

- Molecule 6 is a protein called Cell division cycle protein 27 homolog.

Mol	Chain	Residues	Atoms	AltConf	Trace
6	F	482	Total C 482 482	0	482
6	H	483	Total C 483 483	0	483

- Molecule 7 is a protein called Anaphase-promoting complex subunit CDC26.

Mol	Chain	Residues	Atoms	AltConf	Trace
7	G	25	Total C 25 25	0	25
7	W	25	Total C 25 25	0	25

- Molecule 8 is a protein called Anaphase-promoting complex subunit 4.

Mol	Chain	Residues	Atoms	AltConf	Trace
8	I	719	Total C 719 719	0	719

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	809	GLY	-	expression tag	UNP Q9UJX5
I	810	GLY	-	expression tag	UNP Q9UJX5
I	811	SER	-	expression tag	UNP Q9UJX5
I	812	LEU	-	expression tag	UNP Q9UJX5
I	813	GLU	-	expression tag	UNP Q9UJX5
I	814	VAL	-	expression tag	UNP Q9UJX5
I	815	LEU	-	expression tag	UNP Q9UJX5
I	816	PHE	-	expression tag	UNP Q9UJX5
I	817	GLN	-	expression tag	UNP Q9UJX5
I	818	GLY	-	expression tag	UNP Q9UJX5

- Molecule 9 is a protein called Cell division cycle protein 16 homolog.

Mol	Chain	Residues	Atoms	AltConf	Trace
9	J	499	Total C 499 499	0	499
9	K	493	Total C 493 493	0	493

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

Mol	Chain	Residues	Atoms		AltConf	Trace
10	L	176	Total	C	0	176
			176	176		

- Molecule 11 is a protein called Anaphase-promoting complex subunit 13.

Mol	Chain	Residues	Atoms		AltConf	Trace
11	M	49	Total	C	0	49
			49	49		

- Molecule 12 is a protein called Anaphase-promoting complex subunit 2.

Mol	Chain	Residues	Atoms		AltConf	Trace
12	N	610	Total	C	0	610
			610	610		

- Molecule 13 is a protein called Anaphase-promoting complex subunit 5.

Mol	Chain	Residues	Atoms		AltConf	Trace
13	O	676	Total	C	0	676
			676	676		

- Molecule 14 is a protein called Fizzy-related protein homolog.

Mol	Chain	Residues	Atoms		AltConf	Trace
14	R	385	Total	C	0	385
			385	385		

- Molecule 15 is a protein called Hsl1(substrate)_peptide-Ubiquitin_variant fusion.

Mol	Chain	Residues	Atoms		AltConf	Trace
15	S	86	Total	C	0	86
			86	86		

There are 66 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S	760	GLY	-	linker	PDB ?
S	761	SER	-	linker	PDB ?
S	762	GLY	-	linker	PDB ?
S	763	SER	-	linker	PDB ?
S	764	GLY	-	linker	PDB ?
S	765	SER	-	linker	PDB ?

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Chain	Residue	Modelled	Actual	Comment	Reference
S	766	GLY	-	linker	PDB ?
S	767	SER	-	linker	PDB ?
S	?	-	LYS	deletion	UNP P34244
S	?	-	ASN	deletion	UNP P34244
S	?	-	GLN	deletion	UNP P34244
S	?	-	PHE	deletion	UNP P34244
S	?	-	ASN	deletion	UNP P34244
S	?	-	MET	deletion	UNP P34244
S	?	-	SER	deletion	UNP P34244
S	?	-	TYR	deletion	UNP P34244
S	?	-	LYS	deletion	UNP P34244
S	?	-	PRO	deletion	UNP P34244
S	?	-	SER	deletion	UNP P34244
S	?	-	GLU	deletion	UNP P34244
S	?	-	ASN	deletion	UNP P34244
S	?	-	MET	deletion	UNP P34244
S	?	-	SER	deletion	UNP P34244
S	?	-	GLY	deletion	UNP P34244
S	?	-	LEU	deletion	UNP P34244
S	?	-	SER	deletion	UNP P34244
S	?	-	SER	deletion	UNP P34244
S	?	-	PHE	deletion	UNP P34244
S	?	-	PRO	deletion	UNP P34244
S	?	-	ILE	deletion	UNP P34244
S	?	-	PHE	deletion	UNP P34244
S	?	-	GLU	deletion	UNP P34244
S	?	-	LYS	deletion	UNP P34244
S	?	-	GLU	deletion	UNP P34244
S	?	-	ASN	deletion	UNP P34244
S	?	-	THR	deletion	UNP P34244
S	?	-	LEU	deletion	UNP P34244
S	?	-	SER	deletion	UNP P34244
S	?	-	SER	deletion	UNP P34244
S	819	CYS	SER	engineered mutation	UNP P34244
S	843	SER	-	linker	UNP P34244
S	844	GLY	-	linker	UNP P34244
S	845	SER	-	linker	UNP P34244
S	846	SER	-	linker	UNP P34244
S	847	GLY	-	linker	UNP P34244
S	848	SER	-	linker	UNP P34244
S	849	GLY	-	linker	UNP P34244
S	850	SER	-	linker	UNP P34244

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Chain	Residue	Modelled	Actual	Comment	Reference
S	851	SER	-	linker	UNP P34244
S	852	GLY	-	linker	UNP P34244
S	856	LEU	PHE	engineered mutation	UNP Q63429
S	860	PRO	LEU	engineered mutation	UNP Q63429
S	861	ARG	THR	engineered mutation	UNP Q63429
S	894	ILE	ARG	engineered mutation	UNP Q63429
S	896	PHE	ILE	engineered mutation	UNP Q63429
S	899	VAL	GLY	engineered mutation	UNP Q63429
S	901	ARG	GLN	engineered mutation	UNP Q63429
S	916	LYS	GLU	engineered mutation	UNP Q63429
S	918	SER	THR	engineered mutation	UNP Q63429
S	920	LEU	HIS	engineered mutation	UNP Q63429
S	922	ALA	VAL	engineered mutation	UNP Q63429
S	923	MET	LEU	engineered mutation	UNP Q63429
S	925	VAL	LEU	engineered mutation	UNP Q63429
S	926	PRO	ARG	engineered mutation	UNP Q63429
S	928	LYS	GLY	engineered mutation	UNP Q63429
S	930	LYS	GLN	engineered mutation	UNP Q63429

- Molecule 16 is a protein called Ubiquitin-conjugating enzyme E2 C.

Mol	Chain	Residues	Atoms	AltConf	Trace
16	U	145	Total C 145 145	0	145

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
U	-1	SEC	-	expression tag	UNP O00762
U	0	ASX	-	expression tag	UNP O00762
U	102	ALA	CYS	engineered mutation	UNP O00762
U	180	TRP	-	expression tag	UNP O00762
U	181	SER	-	expression tag	UNP O00762
U	182	HIS	-	expression tag	UNP O00762
U	183	PRO	-	expression tag	UNP O00762
U	184	GLN	-	expression tag	UNP O00762
U	185	GLU	-	expression tag	UNP O00762
U	186	LYS	-	expression tag	UNP O00762

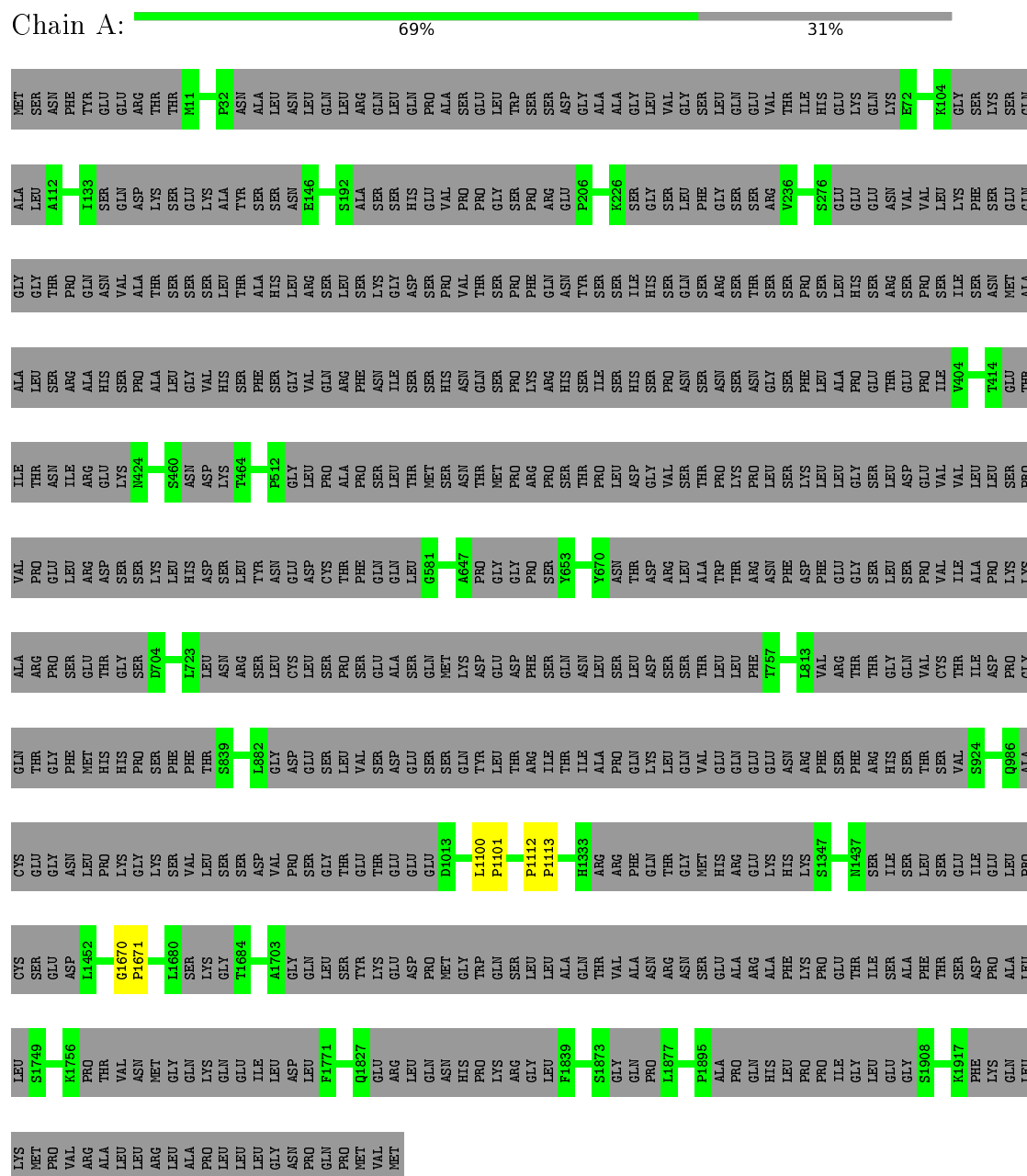
- Molecule 17 is a protein called Anaphase-promoting complex subunit 7.

Mol	Chain	Residues	Atoms		AltConf	Trace
17	X	380	Total 380	C 380	0	380
17	Y	399	Total 399	C 399	0	399


3 Residue-property plots

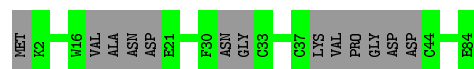
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric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

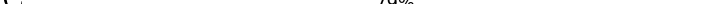


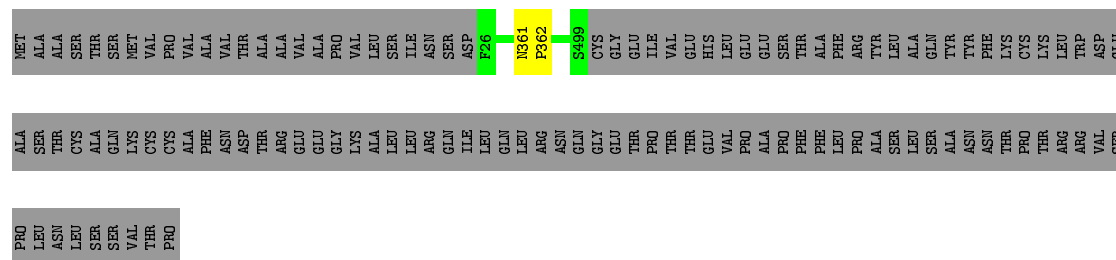
- Molecule 2: Anaphase-promoting complex subunit 11

Chain B:  85% 15%



- Molecule 3: Cell division cycle protein 23 homolog

Chain C:  79% 21%



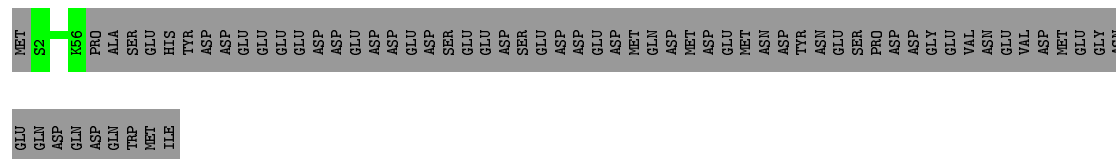
- Molecule 3: Cell division cycle protein 23 homolog

Chain P:  71% 29%



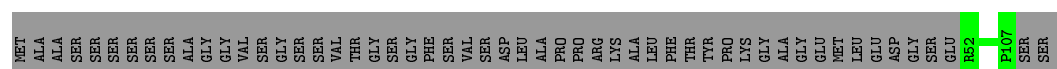
- Molecule 4: Anaphase-promoting complex subunit 15

Chain D:  45% 55%

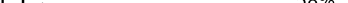


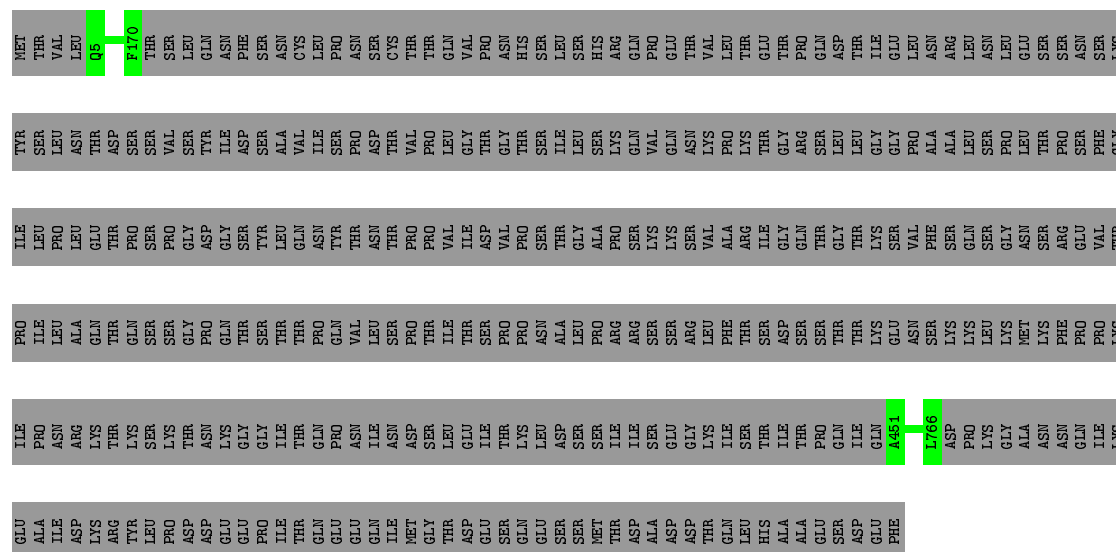
- Molecule 5: Anaphase-promoting complex subunit 16

Chain E: 51% 49%



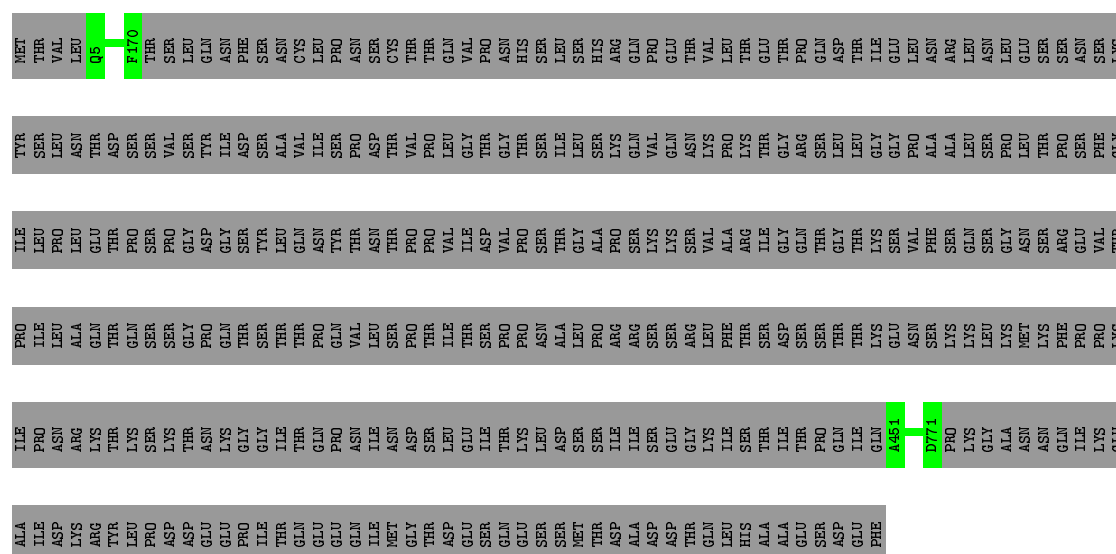
- Molecule 6: Cell division cycle protein 27 homolog

Chain F:  58% 42%



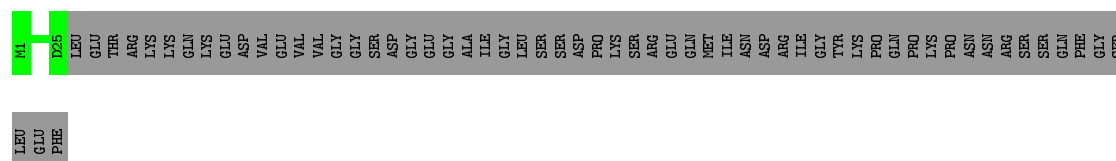
- Molecule 6: Cell division cycle protein 27 homolog

Chain H: 59% 41%



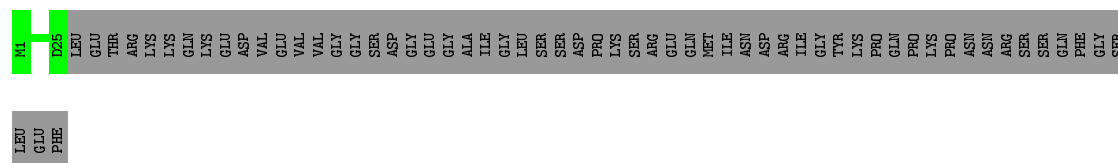
- Molecule 7: Anaphase-promoting complex subunit CDC26

Chain G:  29% 71%




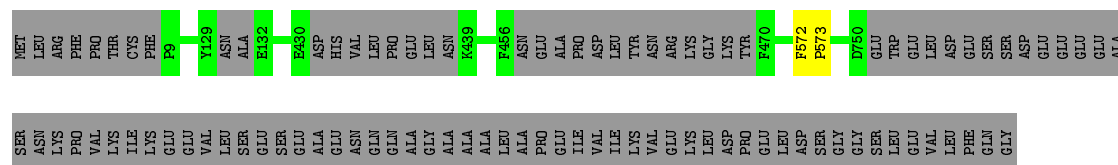
- Molecule 7: Anaphase-promoting complex subunit CDC26

Chain W:  29% 71%




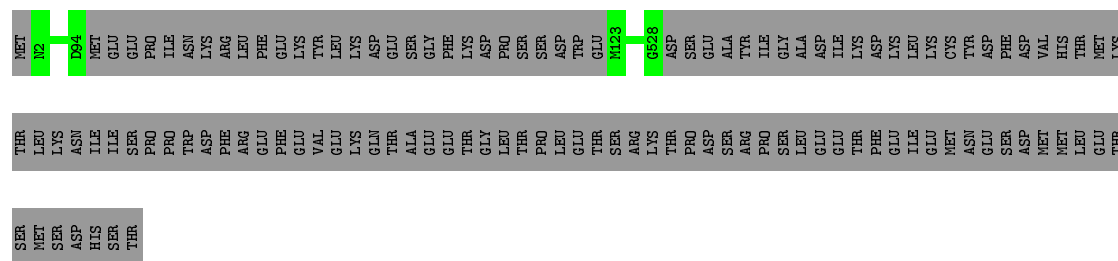
- Molecule 8: Anaphase-promoting complex subunit 4

Chain I:  88% 12%




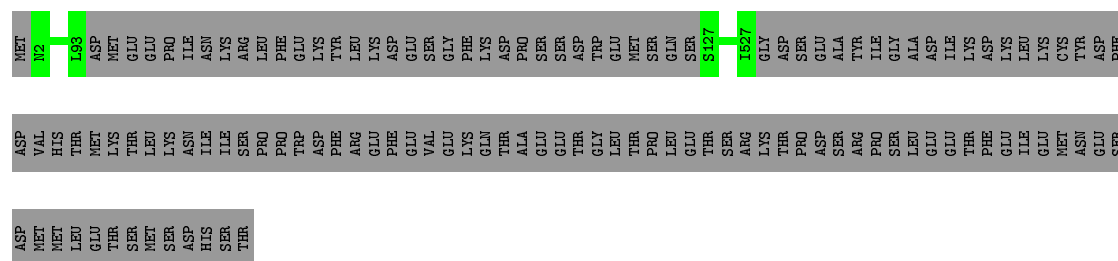
- Molecule 9: Cell division cycle protein 16 homolog

Chain J:  80% 20%



- Molecule 9: Cell division cycle protein 16 homolog

Chain K:  80% 20%



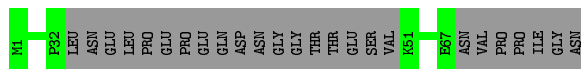
- Molecule 10: Anaphase-promoting complex subunit 10

Chain L:  94% 5%



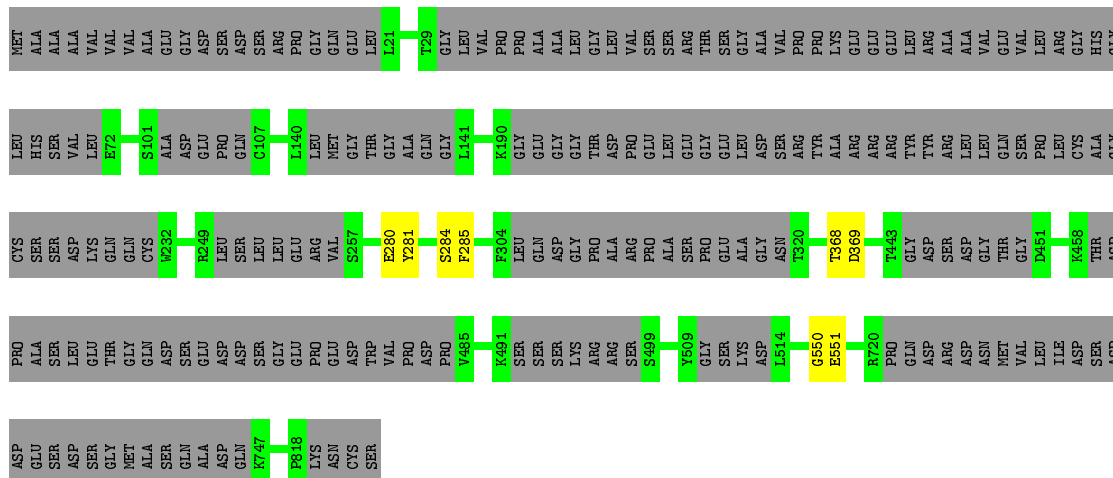
- Molecule 11: Anaphase-promoting complex subunit 13

Chain M:  66% 34%



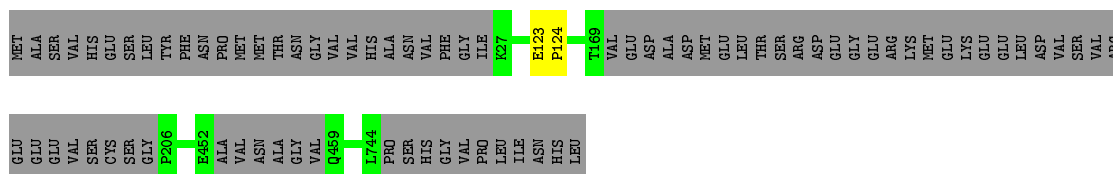
- Molecule 12: Anaphase-promoting complex subunit 2

Chain N: 73% . 26%



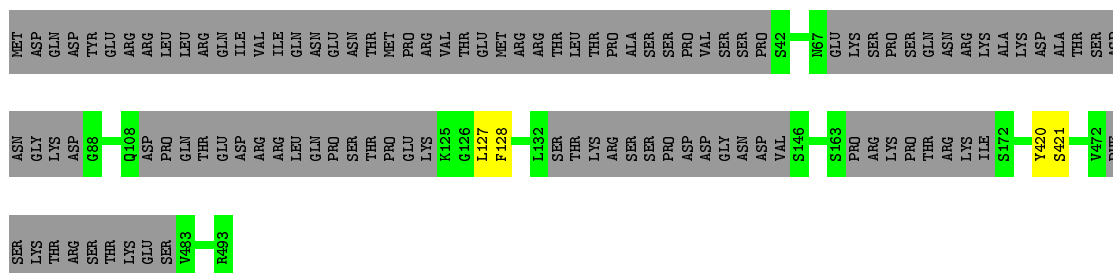
- Molecule 13: Anaphase-promoting complex subunit 5

Chain 0: 89% 10%



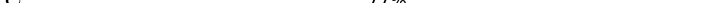
- Molecule 14: Fizzy-related protein homolog

Chain R: 77% . 22%



- Molecule 15: Hsl1(substrate)_peptide-Ubiquitin_variant fusion

[illegible]

- Chain U:  77% 23%

SEC	ASX	MET	SER	GLN	ASN	ARG	ASP	PRO	ALA	THR	SER	VAL	ALA	ALA	ALA	ARG	LYS	GLY	ALA	GLU	PRO	SER	GLY	GLY	ALA	ARG	629	6173	VAL	THR	SER	SER	GLN	GLU	PRO	TRP	SER	HIS	PRO	GLN	GLU	LYS
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

- Chain X:  67% 33%

[illegible]

- Chain Y:  70% 29%

[illegible]

4 Experimental information ⓘ

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	135578	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	Not provided	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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).

There are no protein, RNA or DNA chains available to summarize Z scores of covalent bonds and angles.

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	A	1342	0	0	3	0
2	B	71	0	0	0	0
3	C	474	0	0	1	0
3	P	425	0	0	1	0
4	D	55	0	0	0	0
5	E	56	0	0	0	0
6	F	482	0	0	0	0
6	H	483	0	0	0	0
7	G	25	0	0	0	0
7	W	25	0	0	0	0
8	I	719	0	0	1	0
9	J	499	0	0	0	0
9	K	493	0	0	0	0
10	L	176	0	0	1	0
11	M	49	0	0	0	0
12	N	610	0	0	4	0
13	O	676	0	0	1	0
14	R	385	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	S	86	0	0	0	0
16	U	145	0	0	0	0
17	X	380	0	0	0	0
17	Y	399	0	0	1	0
All	All	8055	0	0	15	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 2.

All (15) 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)
14:R:420:TYR:CA	14:R:421:SER:CA	2.80	0.59
12:N:280:GLU:CA	12:N:281:TYR:CA	2.82	0.57
1:A:1670:GLY:CA	1:A:1671:PRO:CA	2.84	0.55
17:Y:199:CYS:CA	17:Y:200:PRO:CA	2.85	0.55
13:O:123:GLU:CA	13:O:124:PRO:CA	2.85	0.54
12:N:368:THR:CA	12:N:369:ASP:CA	2.85	0.54
12:N:550:GLY:CA	12:N:551:GLU:CA	2.89	0.50
14:R:127:LEU:CA	14:R:128:PHE:CA	2.92	0.48
3:P:361:ASN:CA	3:P:362:PRO:CA	2.92	0.47
10:L:60:GLN:CA	10:L:61:PRO:CA	2.93	0.47
1:A:1100:LEU:CA	1:A:1101:PRO:CA	2.93	0.46
3:C:361:ASN:CA	3:C:362:PRO:CA	2.96	0.43
8:I:572:PHE:CA	8:I:573:PRO:CA	2.96	0.43
1:A:1112:PRO:CA	1:A:1113:PRO:CA	2.99	0.41
12:N:284:SER:CA	12:N:285:PHE:CA	2.99	0.40

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](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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 ⓘ

There are no ligands in this entry.

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.