



wwPDB EM Map/Model Validation Report ⓘ

Oct 24, 2016 – 07:56 PM EDT

PDB ID : 5L9T
EMDB ID: : EMD-3433
Title : Model of human Anaphase-promoting complex/Cyclosome (APC/C-CDH1) with E2 UBE2S poised for polyubiquitination where UBE2S, APC2, and APC11 are modeled into low resolution density
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>

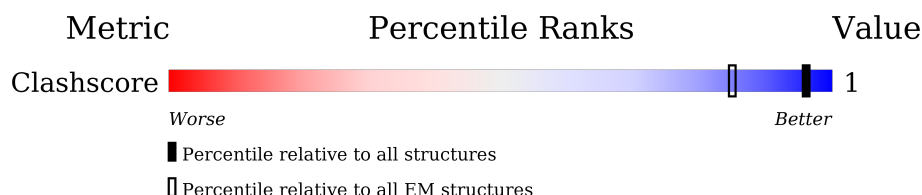
MolProbity : 4.02b-467
Mogul : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027939

1 Overall quality at a glance

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







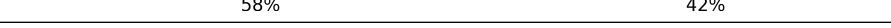
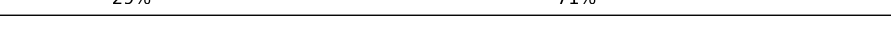

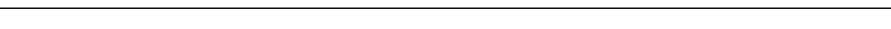

The reported resolution of this entry is 6.40 Å.

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		71% 29%
2	B	84		81% 19%
3	C	597		79% 20%
3	P	597		74% 26%
4	D	121		45% 55%
5	E	110		51% 49%
6	F	824		58% 42%
6	H	824		59% 41%
7	G	85		29% 71%
7	W	85		29% 71%
8	I	818		89% 11%
9	J	620		81% 19%

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Mol	Chain	Length	Quality of chain
9	K	620	 80% 20%
10	L	185	 91% 8%
11	M	74	 57% 43%
12	N	822	 66% 34%
13	O	755	 90% 9%
14	R	493	 77% 22%
15	S	108	 78% 22%
16	T	185	 52% 48%
17	X	565	 70% 30%
17	Y	565	 74% 26%

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 8038 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	1380	Total	C	0	1380
			1380	1380		

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

Mol	Chain	Residues	Atoms		AltConf	Trace
2	B	68	Total	C	0	68
			68	68		

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

Mol	Chain	Residues	Atoms		AltConf	Trace
3	C	475	Total	C	0	475
			475	475		
3	P	443	Total	C	0	443
			443	443		

- 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	727	Total C 727 727	0	727

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	504	Total C 504 504	0	504
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	170	Total	C	0	170
			170	170		

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

Mol	Chain	Residues	Atoms		AltConf	Trace
11	M	42	Total	C	0	42
			42	42		

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

Mol	Chain	Residues	Atoms		AltConf	Trace
12	N	546	Total	C	0	546
			546	546		

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

Mol	Chain	Residues	Atoms		AltConf	Trace
13	O	685	Total	C	0	685
			685	685		

- 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 Ubiquitin_variant-Hsl1(substrate) fusion.

Mol	Chain	Residues	Atoms		AltConf	Trace
15	S	84	Total	C	0	84
			84	84		

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S	-4	GLY	-	expression tag	UNP P0CG47
S	-3	SER	-	expression tag	UNP P0CG47
S	-2	GLY	-	expression tag	UNP P0CG47
S	-1	GLY	-	expression tag	UNP P0CG47
S	0	SER	-	expression tag	UNP P0CG47
S	4	LEU	PHE	engineered mutation	UNP P0CG47

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Chain	Residue	Modelled	Actual	Comment	Reference
S	8	PRO	LEU	engineered mutation	UNP P0CG47
S	9	ARG	THR	engineered mutation	UNP P0CG47
S	11	CYS	LYS	engineered mutation	UNP P0CG47
S	42	ILE	ARG	engineered mutation	UNP P0CG47
S	44	PHE	ILE	engineered mutation	UNP P0CG47
S	47	VAL	GLY	engineered mutation	UNP P0CG47
S	49	ARG	GLN	engineered mutation	UNP P0CG47
S	64	LYS	GLU	engineered mutation	UNP P0CG47
S	66	SER	THR	engineered mutation	UNP P0CG47
S	68	LEU	HIS	engineered mutation	UNP P0CG47
S	70	ALA	VAL	engineered mutation	UNP P0CG47
S	71	MET	LEU	engineered mutation	UNP P0CG47
S	73	VAL	LEU	engineered mutation	UNP P0CG47
S	74	PRO	ARG	engineered mutation	UNP P0CG47
S	815	LYS	GLY	engineered mutation	UNP P0CG47
S	817	LYS	-	linker	UNP P0CG47

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

Mol	Chain	Residues	Atoms	AltConf	Trace
16	T	97	Total C 97 97	0	97

There are 46 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
T	-3	GLY	-	expression tag	UNP Q16763
T	-2	PRO	-	expression tag	UNP Q16763
T	-1	GLY	-	expression tag	UNP Q16763
T	0	SER	-	expression tag	UNP Q16763
T	118	PHE	CYS	conflict	UNP Q16763
T	?	-	GLY	deletion	UNP Q16763
T	?	-	PRO	deletion	UNP Q16763
T	?	-	SER	deletion	UNP Q16763
T	?	-	GLY	deletion	UNP Q16763
T	?	-	ARG	deletion	UNP Q16763
T	?	-	ALA	deletion	UNP Q16763
T	?	-	GLU	deletion	UNP Q16763
T	?	-	ALA	deletion	UNP Q16763
T	?	-	GLY	deletion	UNP Q16763
T	?	-	ARG	deletion	UNP Q16763
T	?	-	ALA	deletion	UNP Q16763

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Chain	Residue	Modelled	Actual	Comment	Reference
T	?	-	LEU	deletion	UNP Q16763
T	?	-	ALA	deletion	UNP Q16763
T	?	-	SER	deletion	UNP Q16763
T	?	-	GLY	deletion	UNP Q16763
T	?	-	THR	deletion	UNP Q16763
T	?	-	GLU	deletion	UNP Q16763
T	?	-	ALA	deletion	UNP Q16763
T	?	-	SER	deletion	UNP Q16763
T	?	-	SER	deletion	UNP Q16763
T	?	-	THR	deletion	UNP Q16763
T	?	-	ASP	deletion	UNP Q16763
T	?	-	PRO	deletion	UNP Q16763
T	?	-	GLY	deletion	UNP Q16763
T	?	-	ALA	deletion	UNP Q16763
T	?	-	PRO	deletion	UNP Q16763
T	?	-	GLY	deletion	UNP Q16763
T	?	-	GLY	deletion	UNP Q16763
T	?	-	PRO	deletion	UNP Q16763
T	?	-	GLY	deletion	UNP Q16763
T	?	-	GLY	deletion	UNP Q16763
T	?	-	ALA	deletion	UNP Q16763
T	?	-	GLU	deletion	UNP Q16763
T	?	-	GLY	deletion	UNP Q16763
T	?	-	PRO	deletion	UNP Q16763
T	?	-	MET	deletion	UNP Q16763
T	?	-	ALA	deletion	UNP Q16763
T	?	-	LYS	deletion	UNP Q16763
T	?	-	LYS	deletion	UNP Q16763
T	?	-	HIS	deletion	UNP Q16763
T	?	-	ALA	deletion	UNP Q16763

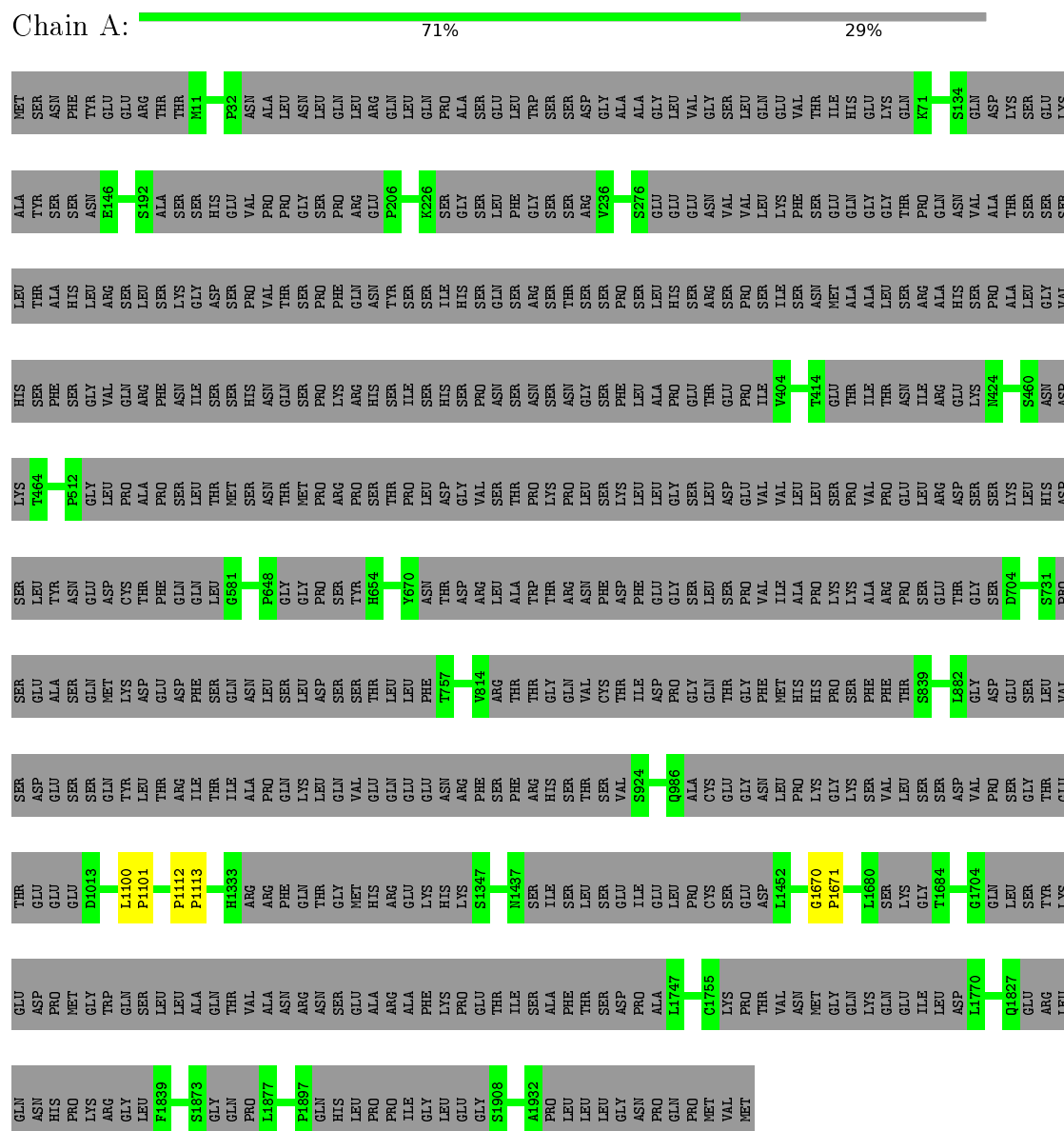
- Molecule 17 is a protein called Anaphase-promoting complex subunit 7.

Mol	Chain	Residues	Atoms	AltConf	Trace
17	X	397	Total C 397 397	0	397
17	Y	416	Total C 416 416	0	416

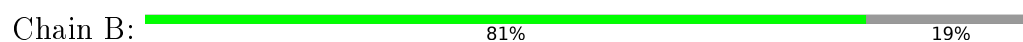
3 Residue-property plots

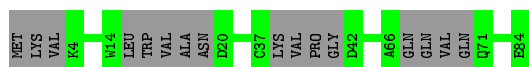
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric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



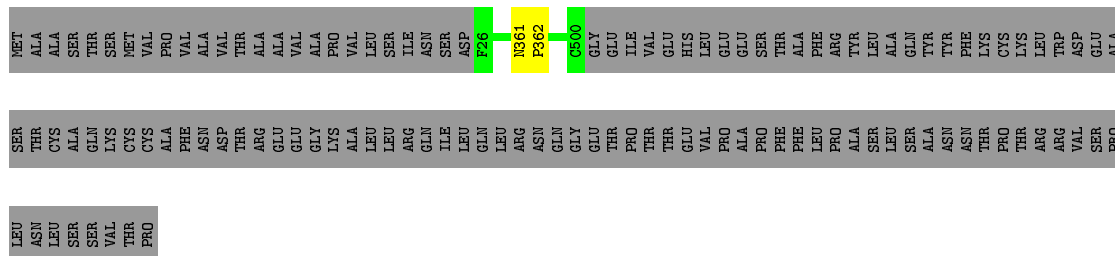
- Molecule 2: Anaphase-promoting complex subunit 11





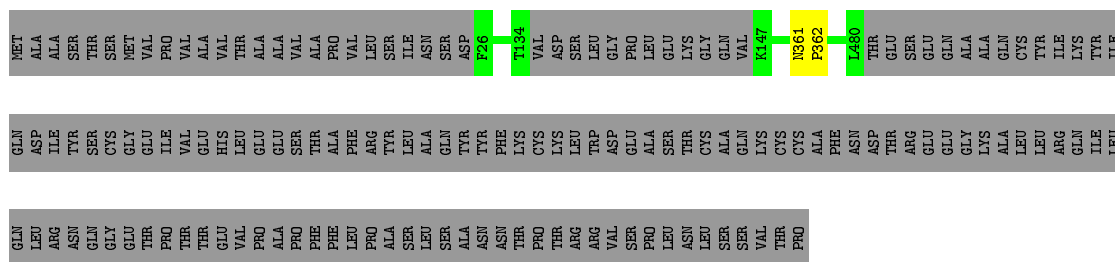
- Molecule 3: Cell division cycle protein 23 homolog

Chain C: 79% 20%



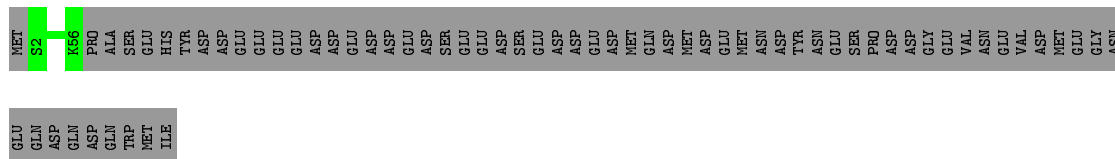
- Molecule 3: Cell division cycle protein 23 homolog

Chain P:  74% 26%



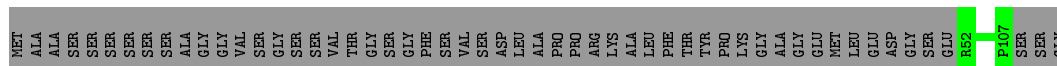
- Molecule 4: Anaphase-promoting complex subunit 15

Chain D:  45% 55%



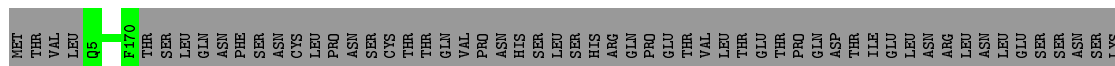
- Molecule 5: Anaphase-promoting complex subunit 16

Chain E: 51% 49%



- Molecule 6: Cell division cycle protein 27 homolog

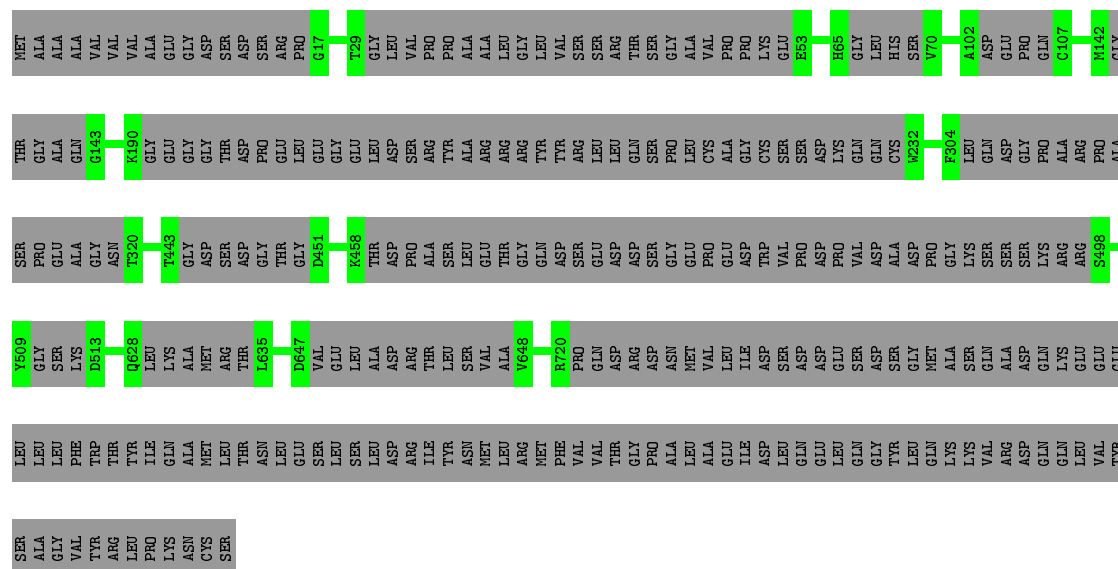
Chain F: 58% 42%



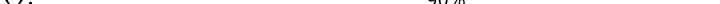


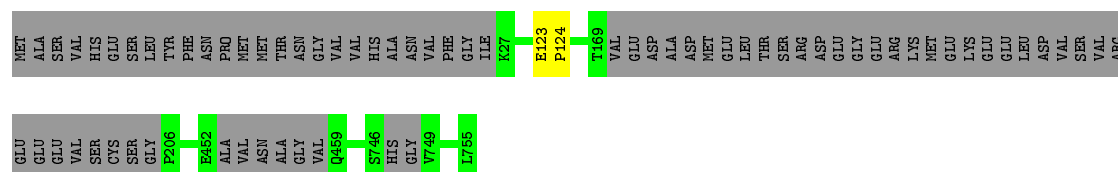

- Molecule 12: Anaphase-promoting complex subunit 2

Chain N:  66% 34%

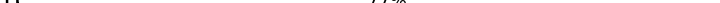


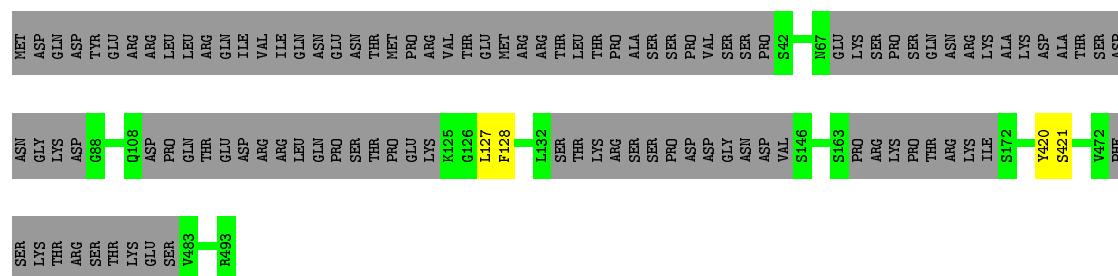
- Molecule 13: Anaphase-promoting complex subunit 5

Chain 0:  90% 9%

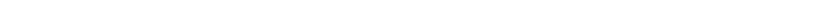


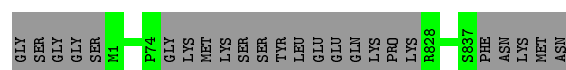
- Molecule 14: Fizzy-related protein homolog

Chain R:  77% • 22%



- Molecule 15: Ubiquitin_variant-Hsl1(substrate) fusion

Chain S:  78% 22%



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	1380	0	0	3	0
2	B	68	0	0	0	0
3	C	475	0	0	1	0
3	P	443	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	727	0	0	1	0
9	J	504	0	0	0	0
9	K	493	0	0	0	0
10	L	170	0	0	1	0
11	M	42	0	0	0	0
12	N	546	0	0	0	0
13	O	685	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	84	0	0	0	0
16	T	97	0	0	0	0
17	X	397	0	0	0	0
17	Y	416	0	0	0	0
All	All	8038	0	0	10	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 1.

All (10) 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	2.81	0.59
1:A:1670:GLY:CA	1:A:1671:PRO:CA	2.84	0.54
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
1:A:1100:LEU:CA	1:A:1101:PRO:CA	2.93	0.46
10:L:60:GLN:CA	10:L:61:PRO:CA	2.93	0.46
3:C:361:ASN:CA	3:C:362:PRO:CA	2.97	0.43
8:I:572:PHE:CA	8:I:573:PRO:CA	2.96	0.42
13:O:123:GLU:CA	13:O:124:PRO:CA	2.99	0.41
1:A:1112:PRO:CA	1:A:1113:PRO: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 [i](#)

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.