



Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Mar 2, 2017 – 12:44 pm GMT

PDB ID : 5KHU
EMDB ID: : EMD-4021
Title : Model of human Anaphase-promoting complex/Cyclosome (APC15 deletion mutant), in complex with the Mitotic checkpoint complex (APC/C-CDC20-MCC) based on cryo EM data at 4.8 Angstrom resolution
Authors : Yamaguchi, M.; VanderLinden, R.; Dube, P.; Stark, H.; Schulman, B.
Deposited on : 2016-06-15
Resolution : 4.80 Å (reported)

This is a Full wwPDB/EMDatabank EM Map/Model Validation 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) : recalc29047

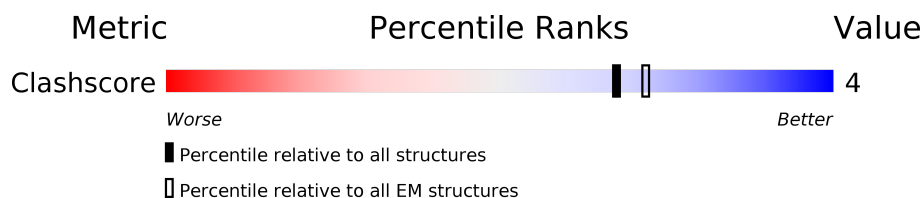
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY













The reported resolution of this entry is 4.80 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.




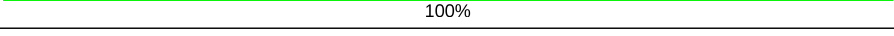
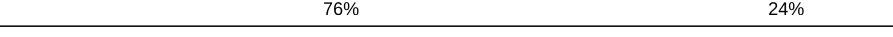
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	125131	1336

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	 70% 29%
2	B	84	 17% 81%
3	C	597	 77% 22%
3	P	597	 74% 26%
4	E	110	 51% 49%
5	F	824	 57% 43%
5	H	824	 58% 42%
6	G	85	 29% 71%
6	W	85	 29% 71%
7	I	808	 87% 13%
8	J	620	 81% 19%
8	K	620	 80% 20%

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Mol	Chain	Length	Quality of chain
9	L	185	
10	M	74	
11	N	822	
12	O	755	
13	Q	1050	
14	R	499	
14	S	499	
15	T	205	
16	U	9	
17	X	565	
17	Y	565	

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 8453 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	1374	Total C 1374 1374	0	1374

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	202	GLU	SER	engineered mutation	UNP Q9H1A4
A	286	GLU	SER	engineered mutation	UNP Q9H1A4
A	291	GLU	THR	engineered mutation	UNP Q9H1A4
A	313	GLU	SER	engineered mutation	UNP Q9H1A4
A	316	GLU	THR	engineered mutation	UNP Q9H1A4
A	317	GLU	SER	engineered mutation	UNP Q9H1A4
A	334	GLU	SER	engineered mutation	UNP Q9H1A4
A	341	GLU	SER	engineered mutation	UNP Q9H1A4
A	343	GLU	SER	engineered mutation	UNP Q9H1A4
A	355	GLU	SER	engineered mutation	UNP Q9H1A4
A	362	GLU	SER	engineered mutation	UNP Q9H1A4
A	372	GLU	SER	engineered mutation	UNP Q9H1A4
A	377	GLU	SER	engineered mutation	UNP Q9H1A4
A	?	GLU	THR	engineered mutation	UNP Q9H1A4
A	?	GLU	SER	engineered mutation	UNP Q9H1A4
A	?	GLU	SER	engineered mutation	UNP Q9H1A4
A	?	GLU	SER	engineered mutation	UNP Q9H1A4
A	671	GLN	ASN	conflict	UNP Q9H1A4
A	?	GLU	SER	engineered mutation	UNP Q9H1A4
A	?	GLU	SER	engineered mutation	UNP Q9H1A4
A	916	GLU	SER	engineered mutation	UNP Q9H1A4
A	1347	GLU	SER	engineered mutation	UNP Q9H1A4

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

Mol	Chain	Residues	Atoms	AltConf	Trace
2	B	16	Total C 16 16	0	16

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

Mol	Chain	Residues	Atoms	AltConf	Trace
3	C	463	Total C 463 463	0	463
3	P	442	Total C 442 442	0	442

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	542	GLU	THR	engineered mutation	UNP Q9UJX2
C	562	GLU	THR	engineered mutation	UNP Q9UJX2
C	582	GLU	THR	engineered mutation	UNP Q9UJX2
C	588	GLU	SER	engineered mutation	UNP Q9UJX2
C	596	GLU	THR	engineered mutation	UNP Q9UJX2
P	542	GLU	THR	engineered mutation	UNP Q9UJX2
P	562	GLU	THR	engineered mutation	UNP Q9UJX2
P	582	GLU	THR	engineered mutation	UNP Q9UJX2
P	588	GLU	SER	engineered mutation	UNP Q9UJX2
P	596	GLU	THR	engineered mutation	UNP Q9UJX2

- Molecule 4 is a protein called Anaphase-promoting complex subunit 16.

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

- Molecule 5 is a protein called Cell division cycle protein 27 homolog.

Mol	Chain	Residues	Atoms	AltConf	Trace
5	F	473	Total C 473 473	0	473
5	H	479	Total C 479 479	0	479

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	200	GLU	THR	engineered mutation	UNP P30260
F	205	GLU	THR	engineered mutation	UNP P30260
F	220	GLU	SER	engineered mutation	UNP P30260
F	241	GLU	SER	engineered mutation	UNP P30260
F	276	GLU	SER	engineered mutation	UNP P30260
F	320	GLU	SER	engineered mutation	UNP P30260
F	336	GLU	SER	engineered mutation	UNP P30260
F	339	GLU	SER	engineered mutation	UNP P30260
F	386	GLU	SER	engineered mutation	UNP P30260
F	387	GLU	SER	engineered mutation	UNP P30260
F	393	GLU	SER	engineered mutation	UNP P30260
F	426	GLU	SER	engineered mutation	UNP P30260
F	435	GLU	SER	engineered mutation	UNP P30260
F	446	GLU	THR	engineered mutation	UNP P30260
H	200	GLU	THR	engineered mutation	UNP P30260
H	205	GLU	THR	engineered mutation	UNP P30260
H	220	GLU	SER	engineered mutation	UNP P30260
H	241	GLU	SER	engineered mutation	UNP P30260
H	276	GLU	SER	engineered mutation	UNP P30260
H	320	GLU	SER	engineered mutation	UNP P30260
H	336	GLU	SER	engineered mutation	UNP P30260
H	339	GLU	SER	engineered mutation	UNP P30260
H	386	GLU	SER	engineered mutation	UNP P30260
H	387	GLU	SER	engineered mutation	UNP P30260
H	393	GLU	SER	engineered mutation	UNP P30260
H	426	GLU	SER	engineered mutation	UNP P30260
H	435	GLU	SER	engineered mutation	UNP P30260
H	446	GLU	THR	engineered mutation	UNP P30260

- Molecule 6 is a protein called Anaphase-promoting complex subunit CDC26.

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

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	51	GLU	SER	engineered mutation	UNP Q8NHZ8
G	52	GLU	SER	engineered mutation	UNP Q8NHZ8
G	82	GLU	SER	engineered mutation	UNP Q8NHZ8

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Chain	Residue	Modelled	Actual	Comment	Reference
W	51	GLU	SER	engineered mutation	UNP Q8NHZ8
W	52	GLU	SER	engineered mutation	UNP Q8NHZ8
W	82	GLU	SER	engineered mutation	UNP Q8NHZ8

- Molecule 7 is a protein called Anaphase-promoting complex subunit 4.

Mol	Chain	Residues	Atoms	AltConf	Trace
7	I	706	Total C 706 706	0	706

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	777	GLU	SER	engineered mutation	UNP Q9UJX5
I	779	GLU	SER	engineered mutation	UNP Q9UJX5

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

Mol	Chain	Residues	Atoms	AltConf	Trace
8	J	504	Total C 504 504	0	504
8	K	493	Total C 493 493	0	493

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	112	GLU	SER	engineered mutation	UNP Q13042
J	560	GLU	SER	engineered mutation	UNP Q13042
J	581	GLU	THR	engineered mutation	UNP Q13042
J	585	GLU	THR	engineered mutation	UNP Q13042
J	586	GLU	SER	engineered mutation	UNP Q13042
K	112	GLU	SER	engineered mutation	UNP Q13042
K	560	GLU	SER	engineered mutation	UNP Q13042
K	581	GLU	THR	engineered mutation	UNP Q13042
K	585	GLU	THR	engineered mutation	UNP Q13042
K	586	GLU	SER	engineered mutation	UNP Q13042

- Molecule 9 is a protein called Anaphase-promoting complex subunit 10.

Mol	Chain	Residues	Atoms		AltConf	Trace
9	L	169	Total	C	0	169
			169	169		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	3	GLU	THR	engineered mutation	UNP Q9UM13

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

Mol	Chain	Residues	Atoms		AltConf	Trace
10	M	43	Total	C	0	43
			43	43		

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

Mol	Chain	Residues	Atoms		AltConf	Trace
11	N	627	Total	C	0	627
			627	627		

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
N	218	GLU	SER	engineered mutation	UNP Q9UJX6
N	314	GLU	SER	engineered mutation	UNP Q9UJX6
N	470	GLU	SER	engineered mutation	UNP Q9UJX6
N	534	GLU	SER	engineered mutation	UNP Q9UJX6
N	811	GLU	SER	engineered mutation	UNP Q9UJX6

- Molecule 12 is a protein called Anaphase-promoting complex subunit 5.

Mol	Chain	Residues	Atoms		AltConf	Trace
12	O	608	Total	C	0	608
			608	608		

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	178	GLU	THR	engineered mutation	UNP Q9UJX4
O	179	GLU	SER	engineered mutation	UNP Q9UJX4
O	195	GLU	SER	engineered mutation	UNP Q9UJX4
O	202	GLU	SER	engineered mutation	UNP Q9UJX4

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Chain	Residue	Modelled	Actual	Comment	Reference
O	221	GLU	SER	engineered mutation	UNP Q9UJX4
O	232	GLU	THR	engineered mutation	UNP Q9UJX4
O	364	GLU	SER	engineered mutation	UNP Q9UJX4

- Molecule 13 is a protein called Mitotic checkpoint serine/threonine-protein kinase BUB1 beta.

Mol	Chain	Residues	Atoms	AltConf	Trace
13	Q	219	Total C 219 219	0	219

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	367	GLU	SER	engineered mutation	UNP O60566
Q	435	GLU	SER	engineered mutation	UNP O60566
Q	543	GLU	SER	engineered mutation	UNP O60566
Q	600	GLU	THR	engineered mutation	UNP O60566
Q	665	GLU	SER	engineered mutation	UNP O60566
Q	670	GLU	SER	engineered mutation	UNP O60566
Q	720	GLU	SER	engineered mutation	UNP O60566
Q	1043	GLU	SER	engineered mutation	UNP O60566

- Molecule 14 is a protein called Cell division cycle protein 20 homolog.

Mol	Chain	Residues	Atoms	AltConf	Trace
14	R	378	Total C 378 378	0	378
14	S	333	Total C 333 333	0	333

- Molecule 15 is a protein called Mitotic spindle assembly checkpoint protein MAD2A.

Mol	Chain	Residues	Atoms	AltConf	Trace
15	T	183	Total C 183 183	0	183

- Molecule 16 is a protein called unknown.

Mol	Chain	Residues	Atoms	AltConf	Trace
16	U	9	Total C 9 9	0	9

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

Mol	Chain	Residues	Atoms	AltConf	Trace
17	X	396	Total C 396 396	0	396
17	Y	432	Total C 432 432	0	432

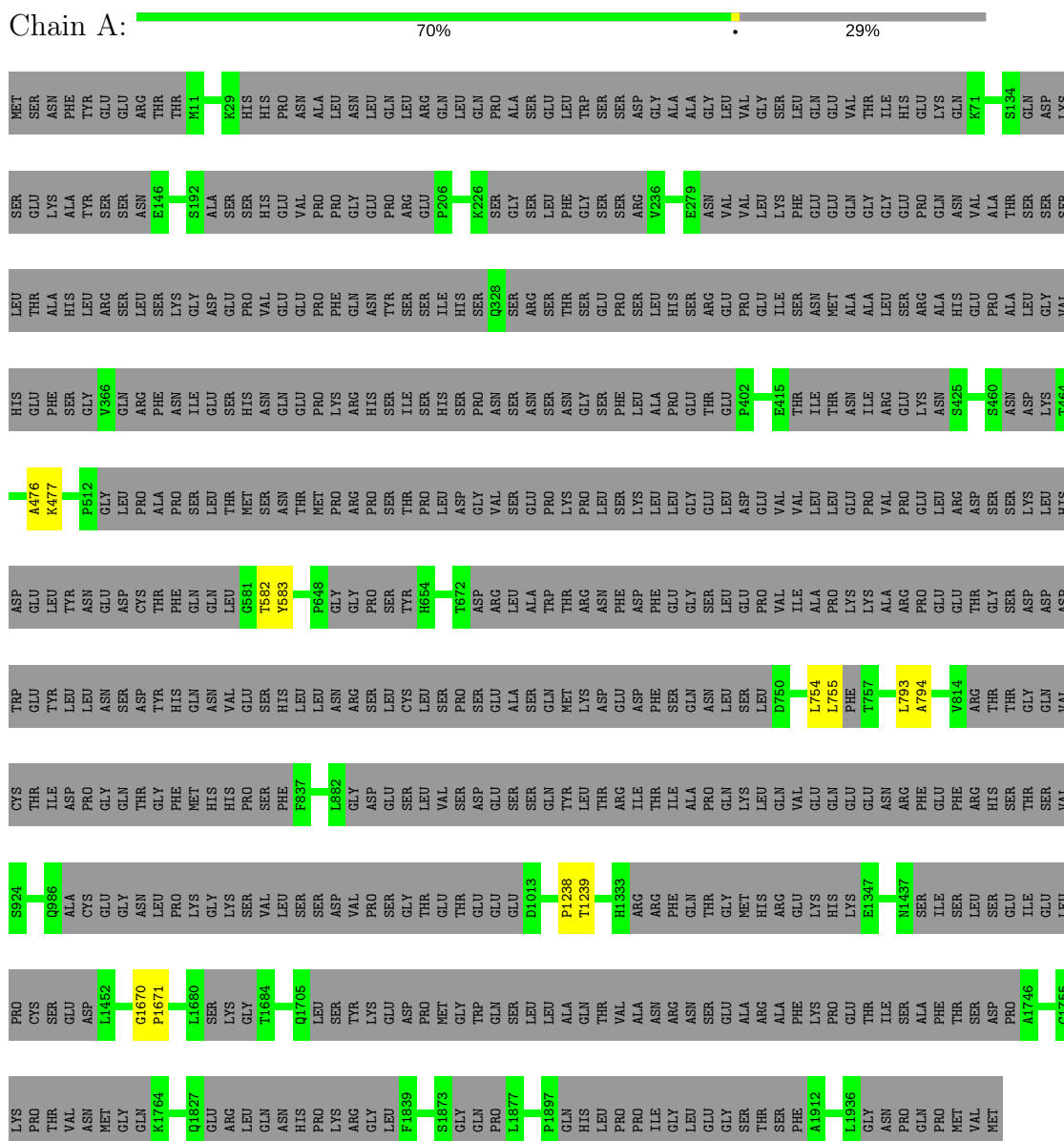
There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	119	GLU	SER	engineered mutation	UNP Q9UJX3
X	120	GLU	THR	engineered mutation	UNP Q9UJX3
X	123	GLU	SER	engineered mutation	UNP Q9UJX3
X	125	GLU	SER	engineered mutation	UNP Q9UJX3
X	126	GLU	THR	engineered mutation	UNP Q9UJX3
Y	119	GLU	SER	engineered mutation	UNP Q9UJX3
Y	120	GLU	THR	engineered mutation	UNP Q9UJX3
Y	123	GLU	SER	engineered mutation	UNP Q9UJX3
Y	125	GLU	SER	engineered mutation	UNP Q9UJX3
Y	126	GLU	THR	engineered mutation	UNP Q9UJX3

3 Residue-property plots

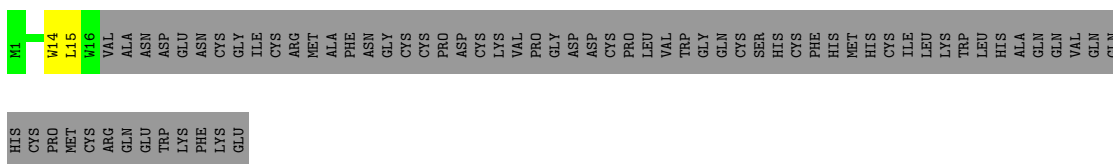
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according 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 1

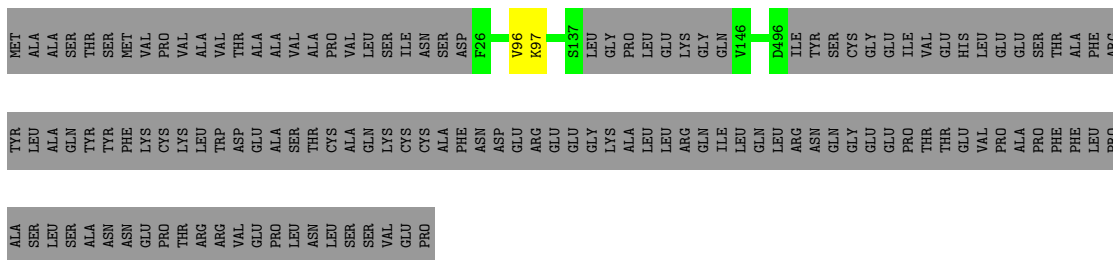


- Molecule 2: Anaphase-promoting complex subunit 11

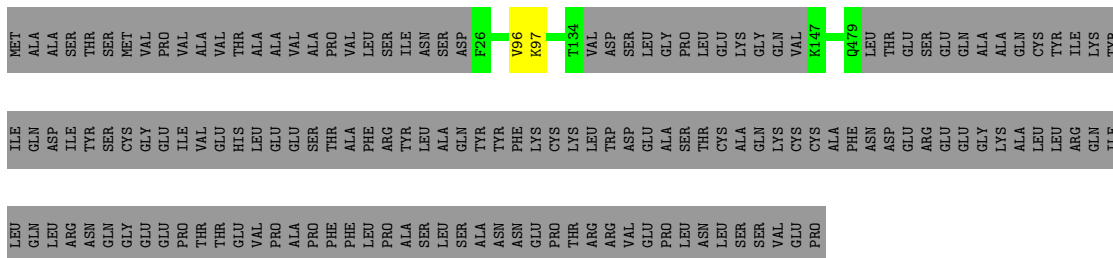




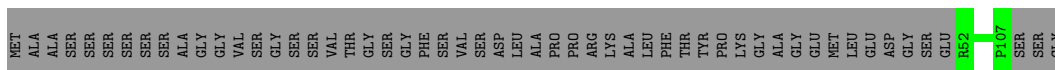
- Molecule 3: Cell division cycle protein 23 homolog



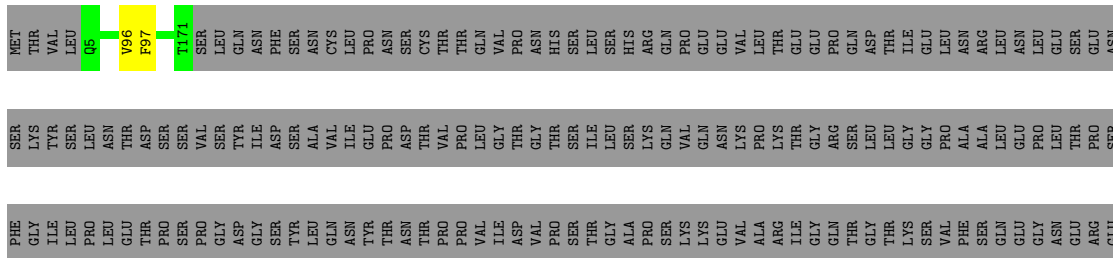
- Molecule 3: Cell division cycle protein 23 homolog

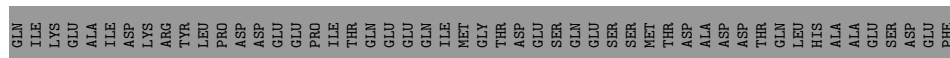
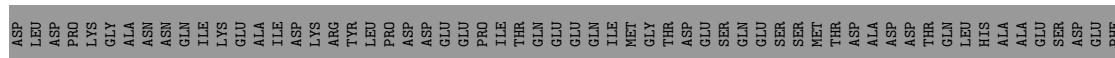


- Molecule 4: Anaphase-promoting complex subunit 16

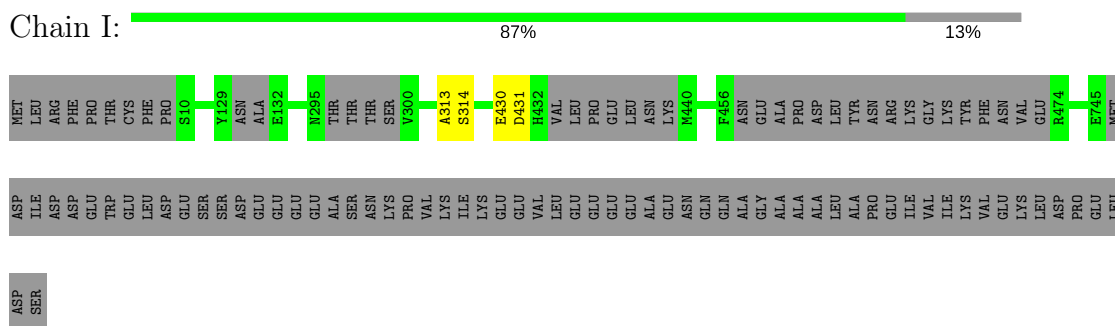


- Molecule 5: Cell division cycle protein 27 homolog



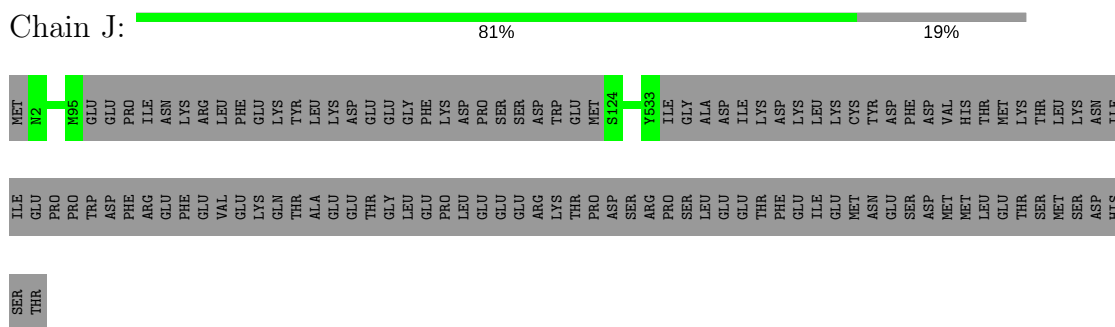


Chain I:



- Molecule 8: Cell division cycle protein 16 homolog

Chain J:



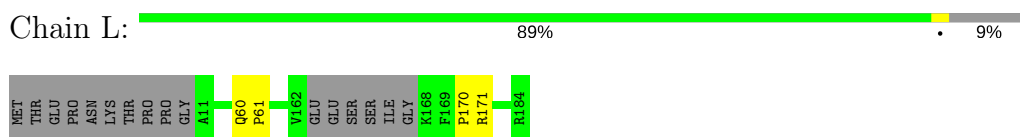
- Molecule 8: Cell division cycle protein 16 homolog

Chain K:



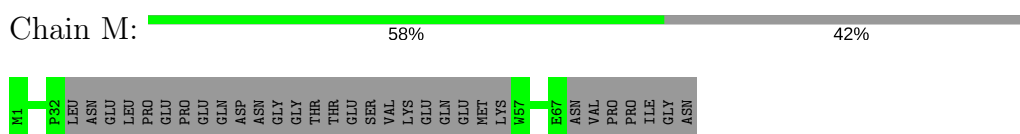
- Molecule 9: Anaphase-promoting complex subunit 10

Chain L:



- Molecule 10: Anaphase-promoting complex subunit 13

Chain M:



- Molecule 11: Anaphase-promoting complex subunit 2

[illegible]

GLU	GLU	GLU	VAL	GLU	CYS	SER	GLY	P206	L283	THR	GLY	ALA	GLU	SER	LYS	ASN	ASN	VAL	GLY	ALA	GLU	GLY	THR	GLY	R298	L350	GLN	LYS	ARG	SER	ASP	SER	THR	VAL	LEU	GLU	GLU	HIS	GLU	GLU	VAL	LYS	ALA	VAL	HIS	PHE	GLY	LEU	THR	LEU	ALA	LEU	GLY	ILE	ASP			
SER	LEU	VAL	GLN	GLN	ARG	ALA	PHE	ALA	LYS	ALA	ALA	LYS	ASN	LEU	MET	ASP	ALA	LEU	LEU	LYS	HIS	LYS	HIS	TRP	L350	GLN	LYS	ARG	SER	ASP	VAL	ASN	ALA	GLY	VAL	GLY	GLU	Q459	L785	GLU	GLU	ARG	ASP	GLY	GLU	ARG	LYS	MET	GLU	LYS	GLU	GLU	ASP	VAL	GLY	ILE	VAL	ASP
MET	ALA	SER	VAL	HIS	GLU	SER	LEU	PHE	ASN	PRO	MET	THR	ASN	THR	ASN	GLY	VAL	HIS	ALA	ASN	VAL	GLY	ILE	LYS	D228	K167	LYS	THR	GLU	VAL	ASP	ALA	ASP	MET	GLU	LEU	GLU	GLU	ARG	ASP	GLY	GLU	ARG	LYS	MET	GLU	LYS	GLU	GLU	ASP	VAL	VAL	ASP					

SER	ALA	GLY	GLY	ARG	ARG	MET
SER	GLU	ASP	GLY	VAL	VAL	ALA
VAL	LYS	PRO	SER	GLY	GLY	ALA
GLN	ARG	LEU	LEU	ALA	ALA	LYS
VAL	ALA	GLN	GLU	ALA	LEU	LYS
ASN	MET	VAL	ARG	HIS	ARG	GLU
CYS	GLN	VAL	ARG	HIS	ARG	GLY
CYS	GLN	GLN	PRO	PRO	PRO	ALA
CYS	LYS	SER	ARG	GLY	SER	ALA
ALA	GLN	HIS	GLY	GLY	SER	ALA
ARG	ILE	GLN	ASN	GLN	GLN	LEU
GLU	GLU	GLN	THR	THR	ASN	SER
THR	GLU	ALA	ALA	ALA	ARG	GLU
SER	MET	SER	SER	GLY	GLY	ALA
LEU	GLU	GLU	LEU	LEU	GLN	MET
ALA	LYS	GLU	ILE	GLN	GLN	SER
GLU	LYS	LYS	ALA	ASN	LEU	LEU
ASN	LEU	LYS	VAL	PRO	PHE	E18
ILE	LYS	GLU	PRO	PHE		
TRP	GLU	LYS	ALA	ALA	PRO	E184
GLN	ILE	MET	VAL	GLN	GLN	P185
GLU	GLN	MET	LEU	GLN		
GLN	THR	TYR	PRO	MET		L205
PRO	THR	CYS	SER	GLN	LEU	LEU
HIS	GLN	LYS	PHE	ASN	ALA	ALA
SER	GLN	GLU	THR	ASN	GLU	LEU
LYS	GLN	LYS	PRO	ASN	GLY	LYS
GLY	ARG	ILE	TYR	VAL		
PRO	THR	TYR	VAL	GLU	I272	GLU
SER	GLY	ALA	GLU	THR		GLU
VAL	ASP	GLY	THR	THR	E277	GLU
PRO	GLN	VAL	GLU	ASN	ALA	GLU
PHE	GLN	GLY	ALA	ALA	VAL	VAL
ILE	GLU	GLU	ARG	ASP	GLU	PHE
THR	GLU	PHE	GLN	GLU	ALA	GLU
ASP	MET	SER	PRO	ALA	SER	SER
GLU	PRO	PHE	VAL	THR	SER	SER
PHE	THR	GLU	THR	ALA	ALA	VAL
LEU	LYS	ILE	PRO	GLU	PRO	PRO
LEU	GLU	ARG	CYS	LEU	GLN	GLN
SER	THR	ALA	LYS	SER		R224
GLU	THR	GLU	ILE	LYS	LYS	L227
LYS	LYS	VAL	GLU	PRO	T291	A228
ASN	GLN	ARG	SER	SER	V292	A229
ILE	ILE	LYS	ILE	ASN	Q293	L230
GLU	ALA	LYS	ASN	P294		LYS
PRO	SER	LEU	HIS			SER
PRO	GLU	LYS	ILE	M300		LYS
ALA	SER	GLU	LEU			GLY
ASP	GLN	GLN	THR	GLU		LYS
PRO	LYS	ARG	THR	THR	L308	LYS
PRO	ILE	GLU	ARG	GLN		THR
ARG	PRO	ALA	LYS	ALA	GLY	ALA
VAL	GLY	GLU	PRO	GLY	GLY	ARG
LEU	MET	LEU	GLY	THR	PRO	ALA
ALA	THR	LEU	LYS	TRP	PRO	PRO
GLN	LEU	THR	GLU	ASN	ILE	ILE
	SER	GLU	THR	THR		ILE

[illegible]

- Molecule 14: Cell division cycle protein 20 homolog

Chain R:  74% . 24%

F420	GLY	LYS	GLN	NET
A421	SER	GLN	ALA	
Y430	SER	PHE	ALA	
P431	SER	ALA		
	LYS	PHE		
D476	VAL	GLU		
PRO	GLN	SER		
ALA	THR	ASP		
ARG	THR	LEU		
ARG	PRO	HIS		
ARG	SER	SER		
GLU	K73	LEU		
ARG	P74	LEU		
GLU	G75	GLN		
LYS		LEU		
ALA	K97	ASP		
SER	E98	ALA		
ALA	N99	PRO		
ALA	Q100	ILE		
LYS	P101	PRO		
SER	GLU	ASN		
S492	ASN	ALA		
	SER	PRO		
R499	GLN	PRO		
	THR	ALA		
	P107	ARG		
	G135	TRP		
	LYS	GLN		
	PRO	ARG		
	GLN	LYS		
	ASN	LYS		
	ALA	GLY		
	PRO	ALA		
	GLU	ALA		
	GLY	GLY		
	TYR	PRO		
	GLN	PRO		
	ASN	SER		
	ARG	SER		
	LEU	PRO		
	LYS	NET		
	VAL	ARG		
	LEU	ALA		
	TYR	ALA		
	SER	ASN		
	GLN	ARG		
	LYS	SER		
	ALA	HIS		
	THR	SER		
	PRO	ALA		
	GLY	GLY		
	SER	ARG		
	SER	THR		
	ARG	PRO		
	LYS	GLY		
	THR	ARG		
	G165	THR		
		PRO		

- Molecule 14: Cell division cycle protein 20 homolog

Chain S:  65% . 33%

[illegible]

4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	268851	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	1374	0	0	6	0
2	B	16	0	0	1	0
3	C	463	0	0	1	0
3	P	442	0	0	1	0
4	E	56	0	0	0	0
5	F	473	0	0	1	0
5	H	479	0	0	0	0
6	G	25	0	0	0	0
6	W	25	0	0	0	0
7	I	706	0	0	2	0
8	J	504	0	0	0	0
8	K	493	0	0	0	0
9	L	169	0	0	2	0
10	M	43	0	0	0	0
11	N	627	0	0	10	0
12	O	608	0	0	0	0
13	Q	219	0	0	4	0
14	R	378	0	0	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	S	333	0	0	4	0
15	T	183	0	0	0	0
16	U	9	0	0	0	0
17	X	396	0	0	0	0
17	Y	432	0	0	0	0
All	All	8453	0	0	38	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 4.

All (38) 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:97:LYS:CA	14:R:98:GLU:CA	2.65	0.74
14:R:420:PHE:CA	14:R:421:ALA:CA	2.75	0.65
14:R:99:ASN:CA	14:R:100:GLN:CA	2.77	0.62
11:N:164:SER:CA	11:N:165:THR:CA	2.78	0.60
11:N:280:GLU:CA	11:N:281:TYR:CA	2.82	0.57
14:S:145:GLN:CA	14:S:146:ASN:CA	2.81	0.57
13:Q:184:GLU:CA	13:Q:185:PRO:CA	2.82	0.57
11:N:550:GLY:CA	11:N:551:GLU:CA	2.84	0.56
14:S:146:ASN:CA	14:S:147:ARG:CA	2.85	0.55
11:N:162:PHE:CA	11:N:163:PHE:CA	2.85	0.55
7:I:313:ALA:CA	7:I:314:SER:CA	2.85	0.55
11:N:165:THR:CA	11:N:166:PRO:CA	2.85	0.55
14:S:420:PHE:CA	14:S:421:ALA:CA	2.84	0.55
9:L:170:PRO:CA	9:L:171:ARG:CA	2.84	0.55
1:A:754:LEU:CA	1:A:755:LEU:CA	2.86	0.54
1:A:793:LEU:CA	1:A:794:ALA:CA	2.85	0.54
14:R:100:GLN:CA	14:R:101:PRO:CA	2.87	0.53
9:L:60:GLN:CA	9:L:61:PRO:CA	2.87	0.52
13:Q:293:GLN:CA	13:Q:294:PRO:CA	2.88	0.52
3:P:96:VAL:CA	3:P:97:LYS:CA	2.88	0.51
2:B:14:TRP:CA	2:B:15:LEU:CA	2.88	0.51
11:N:368:THR:CA	11:N:369:ASP:CA	2.88	0.51
13:Q:227:LEU:CA	13:Q:228:ALA:CA	2.88	0.51
14:S:430:TYR:CA	14:S:431:PRO:CA	2.90	0.49
5:F:96:VAL:CA	5:F:97:PHE:CA	2.91	0.49
1:A:1238:PRO:CA	1:A:1239:THR:CA	2.91	0.49
13:Q:299:PRO:CA	13:Q:300:MET:CA	2.91	0.49
11:N:532:SER:CA	11:N:533:PHE:CA	2.92	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:476:ALA:CA	1:A:477:LYS:CA	2.92	0.48
11:N:511:SER:CA	11:N:512:LYS:CA	2.91	0.48
11:N:483:ASP:CA	11:N:484:PRO:CA	2.92	0.47
1:A:1670:GLY:CA	1:A:1671:PRO:CA	2.92	0.47
14:R:430:TYR:CA	14:R:431:PRO:CA	2.97	0.43
1:A:582:THR:CA	1:A:583:TYR:CA	2.97	0.42
11:N:493:SER:CA	11:N:494:SER:CA	2.97	0.42
3:C:96:VAL:CA	3:C:97:LYS:CA	2.99	0.41
7:I:430:GLU:CA	7:I:431:ASP:CA	2.99	0.41
14:R:74:PRO:CA	14:R:75:GLY:CA	3.00	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 [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](#)

There are no ligands in this entry.

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.