



## wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Mar 2, 2017 – 12:53 pm GMT

PDB ID : 5LCW  
EMDB ID: : EMD-4037  
Title : Cryo-EM structure of the Anaphase-promoting complex/Cyclosome, in complex with the Mitotic checkpoint complex (APC/C-MCC) at 4.2 angstrom resolution  
Authors : Alfieri, C.; Chang, L.; Zhang, Z.; Yang, J.; Maslen, S.; Skehel, M.; Barford, D.  
Deposited on : 2016-06-22  
Resolution : 4.00 Å(reported)

This is a wwPDB/EMDataBank EM Map/Model Validation Summary Report for a publicly released PDB/EMDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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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

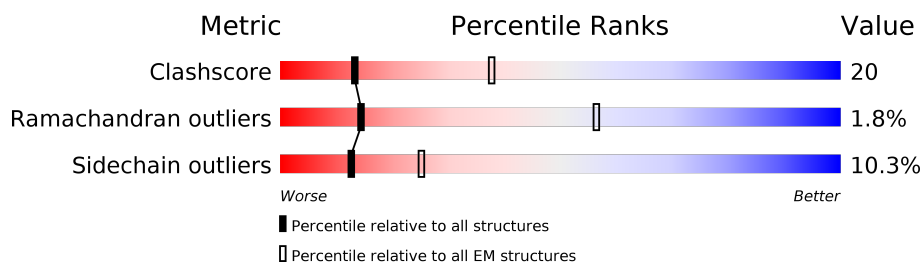
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.00 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	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

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  $\geq 3$ , 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	

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Mol	Chain	Length	Quality of chain
7	W	85	
8	I	808	
9	J	620	
9	K	620	
10	L	185	
11	M	74	
12	N	822	
13	O	755	
14	Q	374	
15	R	499	
16	S	342	
17	X	599	
17	Y	599	
18	Z	205	

## 2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 72075 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	1441	Total	C	N	O	S	0	0
			10949	7039	1853	1983	74		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	356	PHE	PRO	conflict	UNP Q9H1A4

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	79	Total	C	N	O	S	0	0
			643	411	116	100	16		

- 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
			4043	2611	679	729	24		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
4	D	18	Total	C	N	O	0	0
			153	104	23	26		

- 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	483	Total	C	N	O	S	0	0
			3849	2470	649	704	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	733	Total	C	N	O	S	0	0
			5716	3665	951	1067	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		

- 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	703	Total	C	N	O	S	0	0
			5403	3436	971	971	25		

- 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
			5402	3446	940	988	28		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	Q	354	Total	C	N	O	S	0	0
			2671	1676	488	496	11		

- Molecule 15 is a protein called Cell division cycle protein 20 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	R	383	Total	C	N	O	S	0	0
			2953	1855	538	548	12		

- Molecule 16 is a protein called Mitotic checkpoint serine/threonine-protein kinase BUB1 beta,Mitotic checkpoint serine/threonine-protein kinase BUB1 beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	S	277	Total	C	N	O	S	0	0
			2077	1292	380	400	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
17	X	484	Total	C	N	O	S	0	0
			3773	2393	652	704	24		
17	Y	496	Total	C	N	O	S	0	0
			3868	2449	669	724	26		

- Molecule 18 is a protein called Mitotic spindle assembly checkpoint protein MAD2A.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	Z	195	Total	C	N	O	S	0	0
			1577	1012	256	305	4		

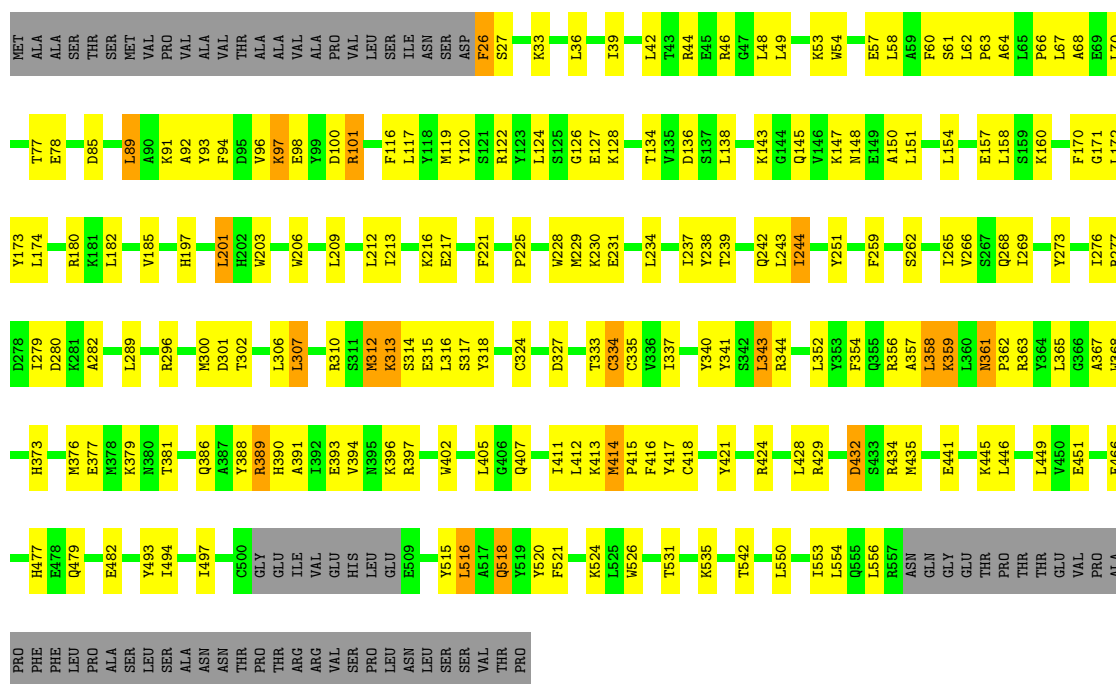


- Molecule 1: Anaphase-promoting complex subunit 1

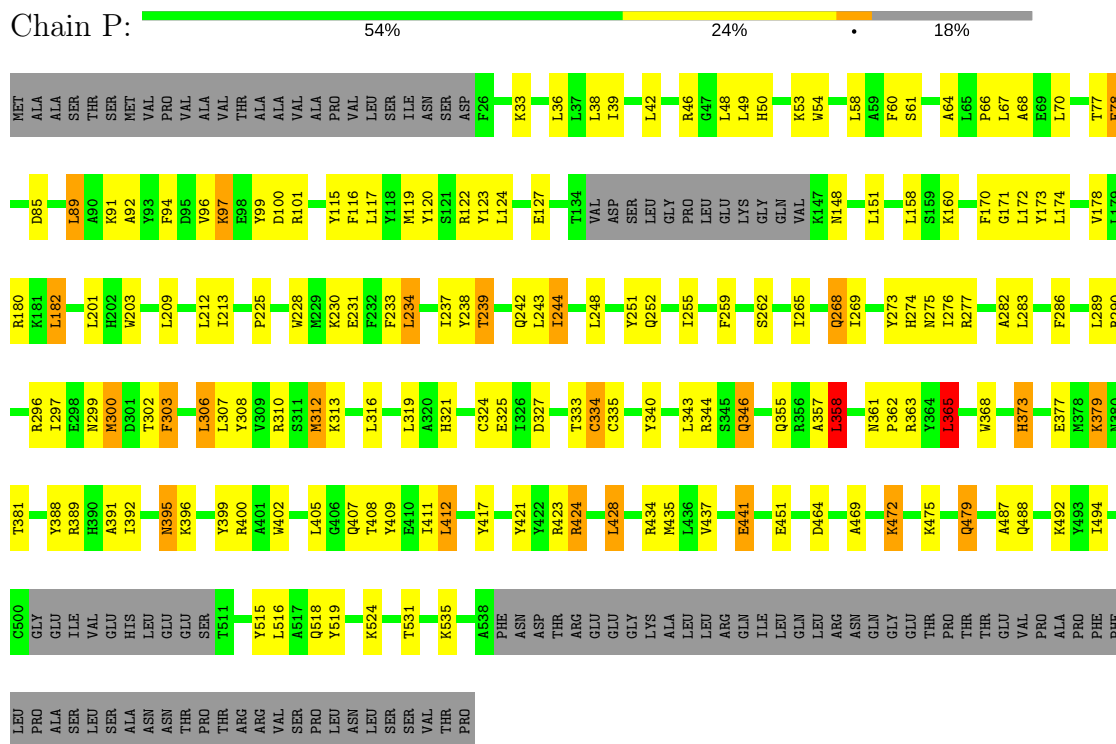








### • Molecule 3: Cell division cycle protein 23 homolog



### • Molecule 4: Anaphase-promoting complex subunit 15



[illegible]

- Molecule 5: Anaphase-promoting complex subunit 16

Chain E:  34% 15% 1% 49%

Met	Ala	Ala	Ala	Ser	Ser	Ser	Ser	Ser	Ser	Ala	Gly	Gly	Val	Ser	Gly	Gly	Gly	Gly	Phe	Ser	Val	Ser	Asp	Leu	Ala	Ala	Pro	Pro	Arg	Lys	Ala	Ala	Leu	Phe	Thr	Thr	Tyr	Pro	Pro	Lys	Gly	Gly	Ala	Gly	Gly	Met	Leu	Met	Glu	Asp	Gly	Ser	Ser	Glu	R52	C85	E56	S57	F58	F59	S60	S61	S62	S63	S64	S65	S66	S67	S68	S69	S70	S71	S72	S73	S74	S75	S76	S77	S78	S79	S80	S81	S82	S83	S84	S85	S86	S87	S88	S89	S90	S91	S92	S93	S94	S95	S96	S97	S98	S99	S100
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- Molecule 6: Cell division cycle protein 27 homolog

Chain F:  40% 17% 41%

Met	Thr	Val	Leu	Q5	E6	P7		A15		Y19		R22		F26	L27		R30	L31	Y32		L41	F42	L43	L44	A45		R50		Y88	R89	L60	L61	K62		T67		Q70	C71	K72	Y73	L74	L75			C78		E89	Q90	I91		V96	F97	N98		H103	D104		T117	L118
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C137  
  
S141  
I142  
A143  
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N145  
P146  
F147  
  
F152  
  
E160  
K161  
P162  
D163  
P164  
D165  
Q166  
T167  
F168  
K169  
F170  
THR  
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	GLN	PRO	PRO	GLU	THR	VAL	LEU	THR	GLU	GLY	THR	PRO	PRO	ASP	ASN	ARG	LEU	ASN	LEU	GLU	SER	SER	ASN	SER	LYS	Tyr	LEU	ASN	ASP	SER	SER	VAL	SER	TYR	ILE	ASP	ALA	VAL	ILE	SER	PRO	ASP	THR	VAL	PRO	LEU	GLY	THR	GLY	THR	SER	ILE	SER	LYS
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GLN	VAL	GLN	ASN	ASN	PRO	LYS	THR	THR	GLY	ARG	GLY	SER	LEU	LEU	GLY	GLY	ALA	ALA	LEU	SER	SER	PHE	GLY	LEU	LEU	PRO	PRO	GLU	GLU	THR	PRO	SER	SER	TYR	LEU	GLN	ASN	TYR	THR	ASN	THR	PRO	PRO	VAL	VAL	ILE	ASP	VAL	PRO	SER	THR	GLY	ALA	PRO
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SER	LYS	SER	VAL	ALA	ARG	ILE	GLY	GLN	THR	GLY	THR	LYS	SER	VAL	PHE	SER	GLN	SER	SER	GLY	ASN	ARG	SER	ARG	GLU	VAL	THR	PRO	ILE	LEU	ALA	GLN	THR	GLN	SER	SER	GLY	PRO	GLN	THR	SER	SER	THR	THR	PRO	PRO	GLN	VAL	GLN	LEU	SER	SER	PRO	PRO	ASN	ALA	LEU	ALA	PRO	PRO	ARG
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ARG	SER	SER	LEU	PHE	THR	SER	ASP	SER	SER	THR	LYS	GLU	ASN	LYS	LYS	MET	PHE	PRO	PRO	LYS	ILE	PRO	ASN	ARG	LYS	THR	LYS	SER	LYS	THR	ASN	GLN	PRO	ASN	ILE	GLY	ILE	THR	GLN	PRO	ASN	ILE	GLY	GLY	ILE	THR	LYS	LEU	ASP	SER	THR	ILE
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I1E	SE1	GL1	GLY	LVS	I1E	SE1	THR	THR	PRO	GLM	I1E	GLN	A451	A457	A458	A459	A460	A461	A462	L465	L466	R467		K471	C477	C481	K482	E483		L487	S493	H494	H495	W500	F501	F502	C503	Q504	I505	G506	R507		L512		R520	I521	F522		V525	R526	R527	F528	F529
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E529	N530	V533	M536	E537	E538	V539	S540	T541	M544	D549	V550	A551	V554	L555	S556	L559	M562	D563	K564	G574	N575	C576	F577	S578	K588	R592	A593	I594	A601	G601	Y602	A603	Y604	T605	L606	T614	E615	E616	L617	D618
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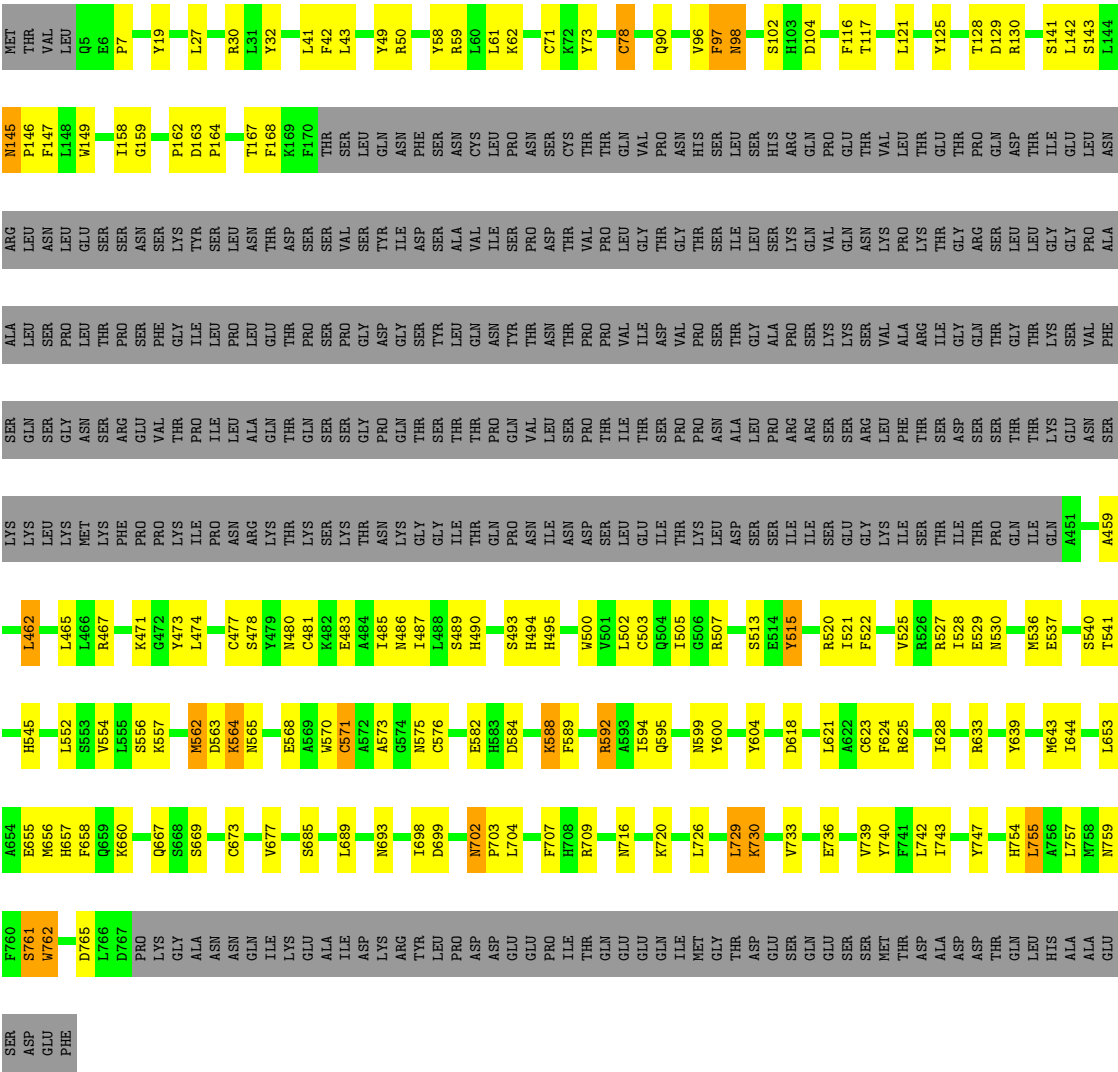
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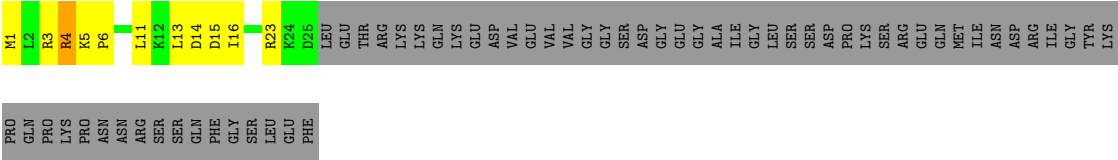
- Molecule 6: Cell division cycle protein 27 homolog

Chain H:  40% 17% 0% 41%



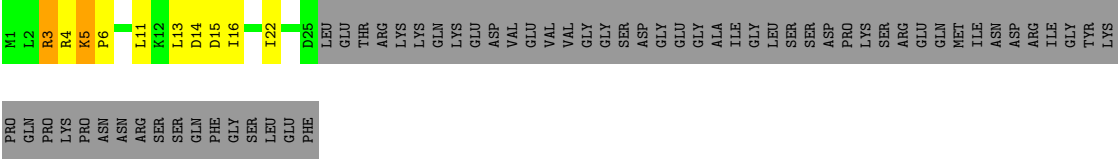
● Molecule 7: Anaphase-promoting complex subunit CDC26

Chain G: 16% 12% 71%

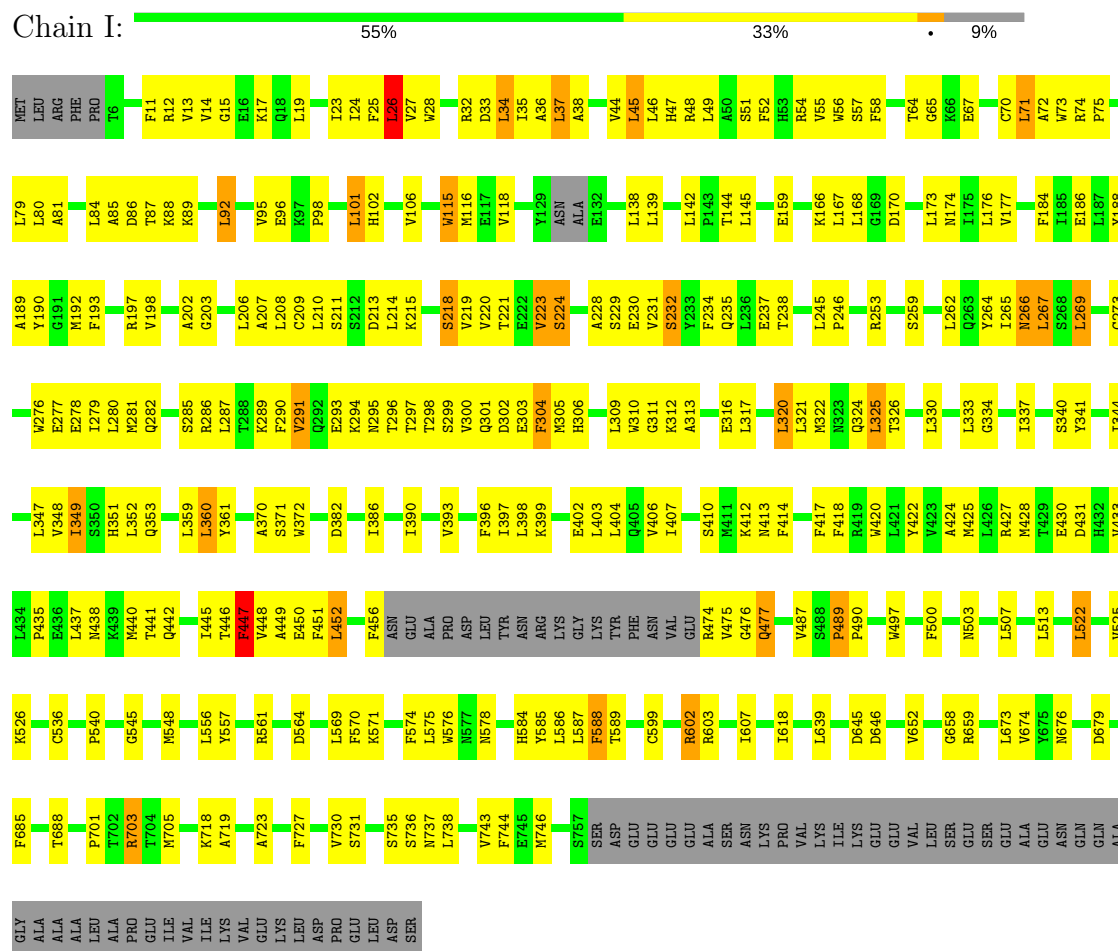


● Molecule 7: Anaphase-promoting complex subunit CDC26

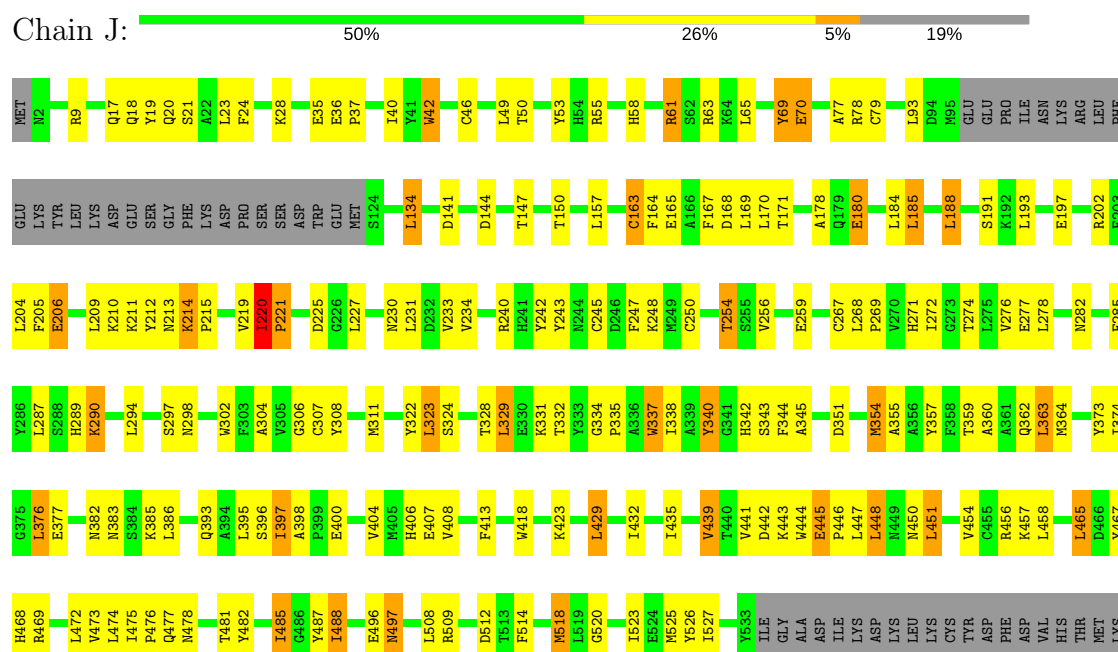
Chain W: 18% 9% 71%

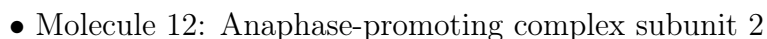


• Molecule 8: Anaphase-promoting complex subunit 4

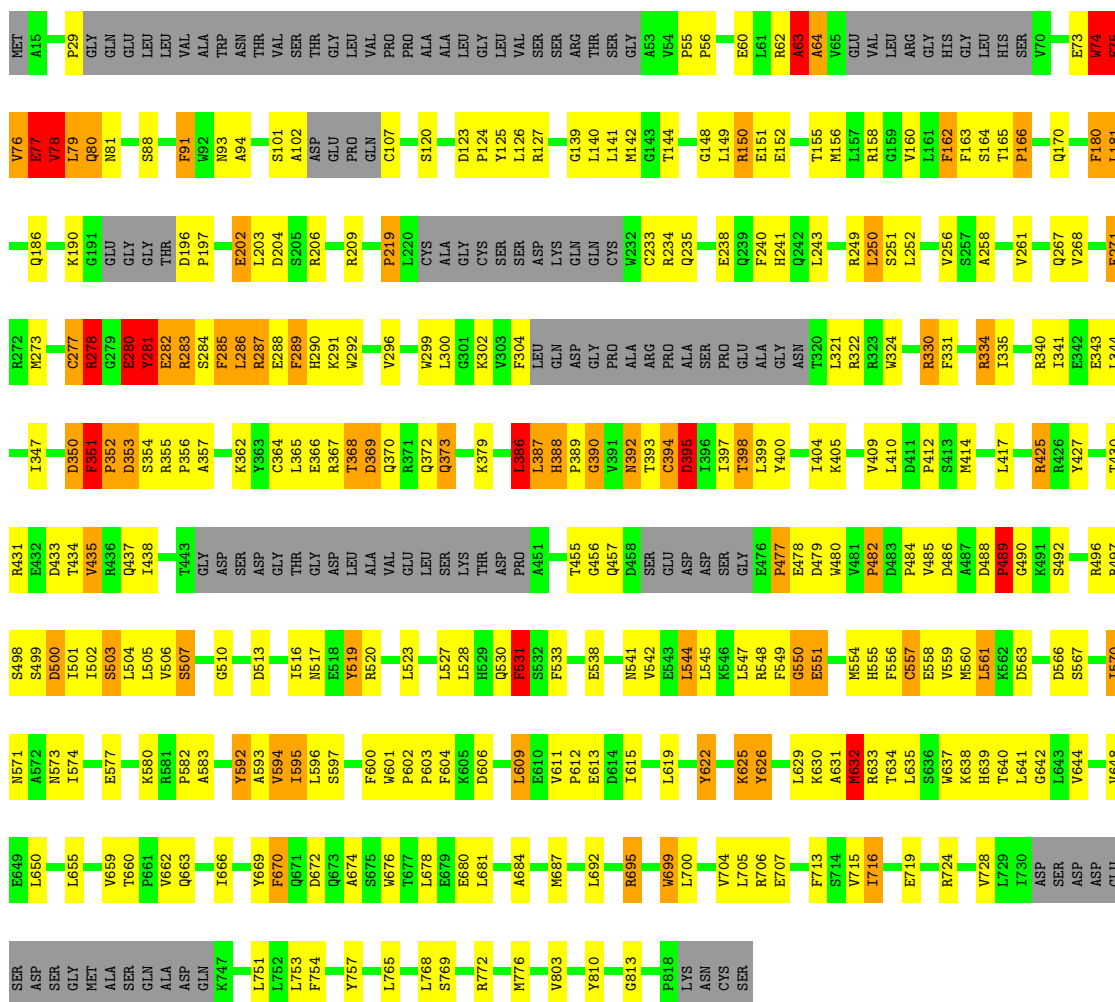


• Molecule 9: Cell division cycle protein 16 homolog



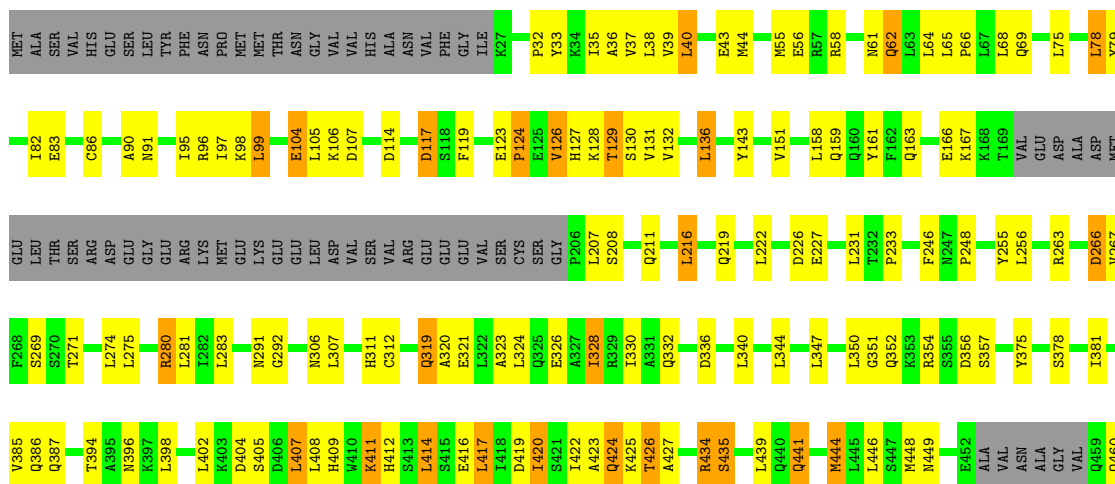


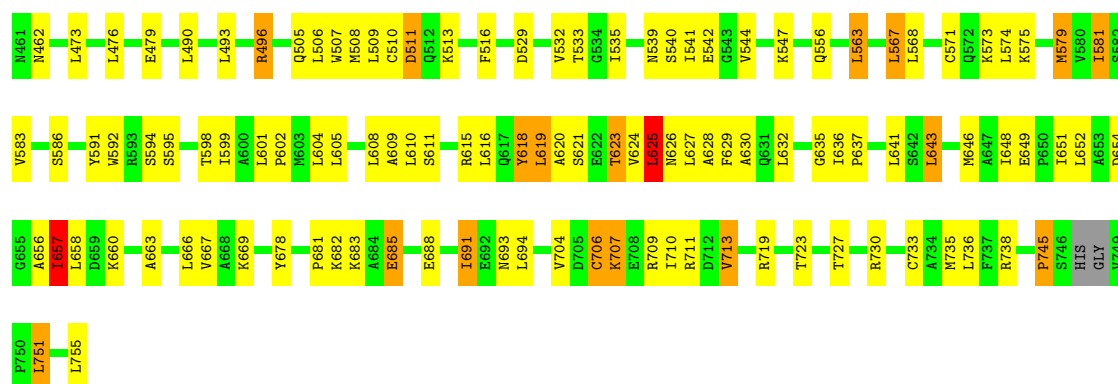
Chain N:



- Molecule 13: Anaphase-promoting complex subunit 5

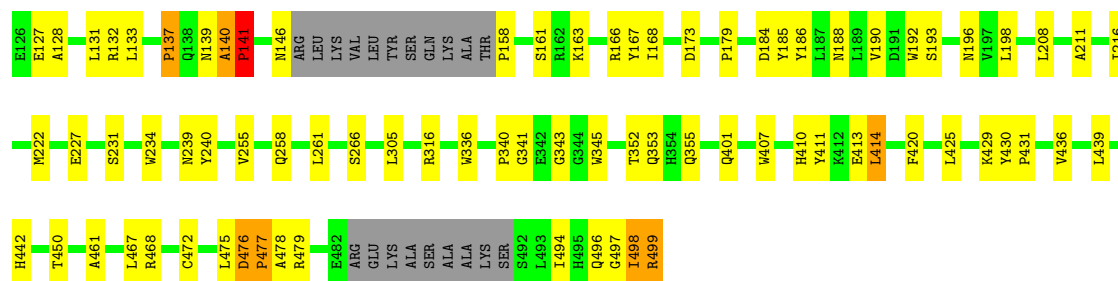
Chain 0:





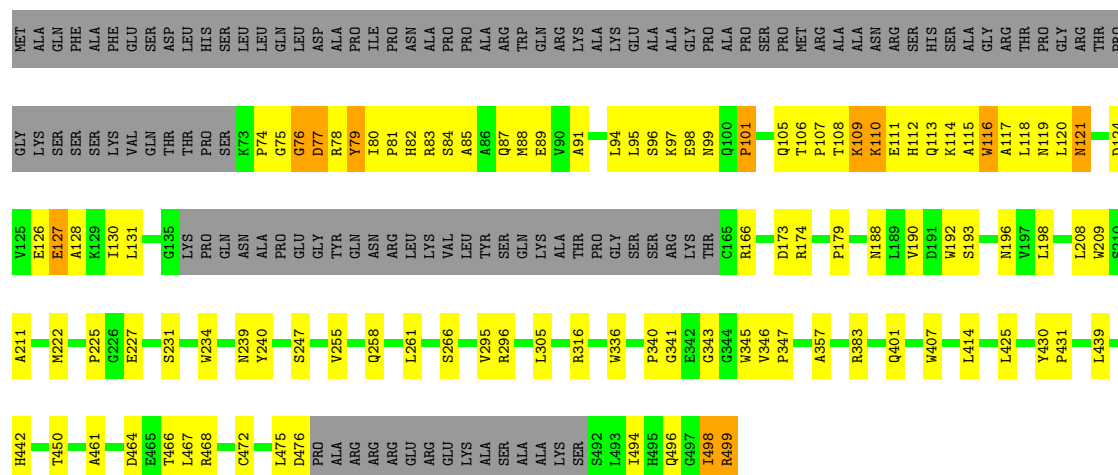
• Molecule 14: Cell division cycle protein 20 homolog

Chain Q: 74% 19% 5%



• Molecule 15: Cell division cycle protein 20 homolog

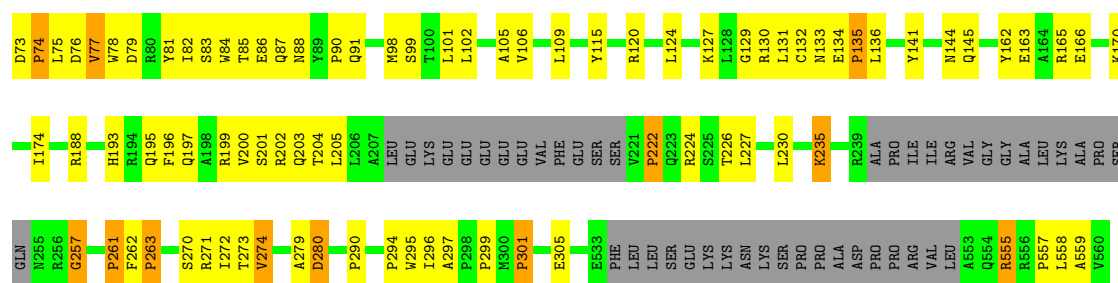
Chain R: 56% 19% 23%



• Molecule 16: Mitotic checkpoint serine/threonine-protein kinase BUB1 beta, Mitotic checkpoint serine/threonine-protein kinase BUB1 beta

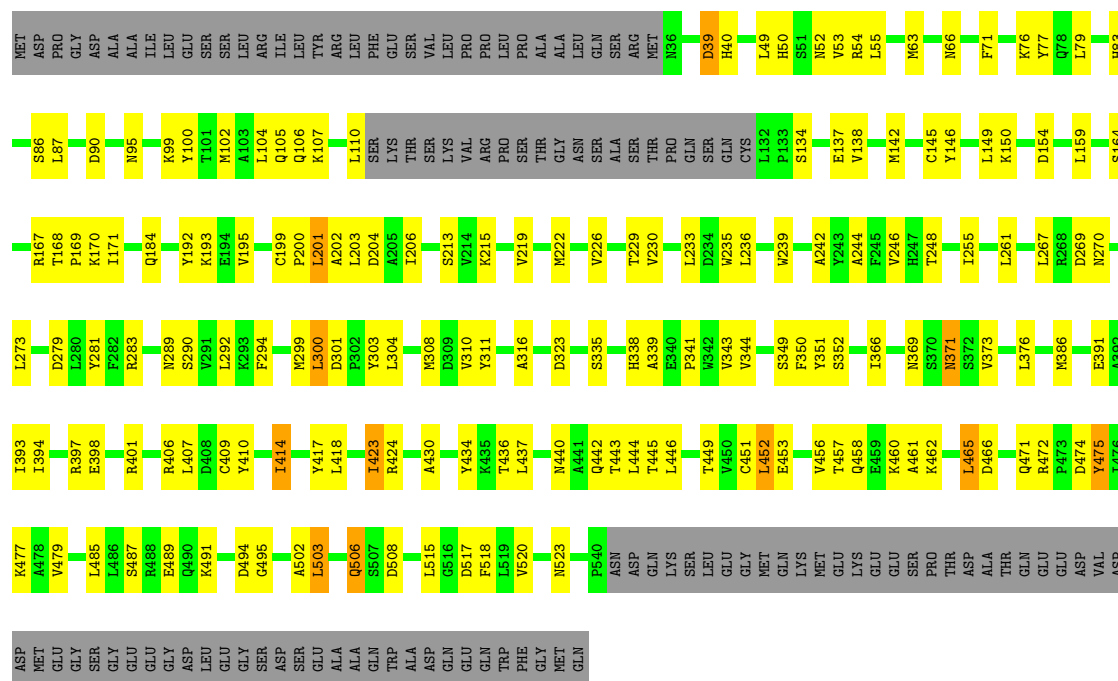
Chain S: 47% 29% 5% 19%





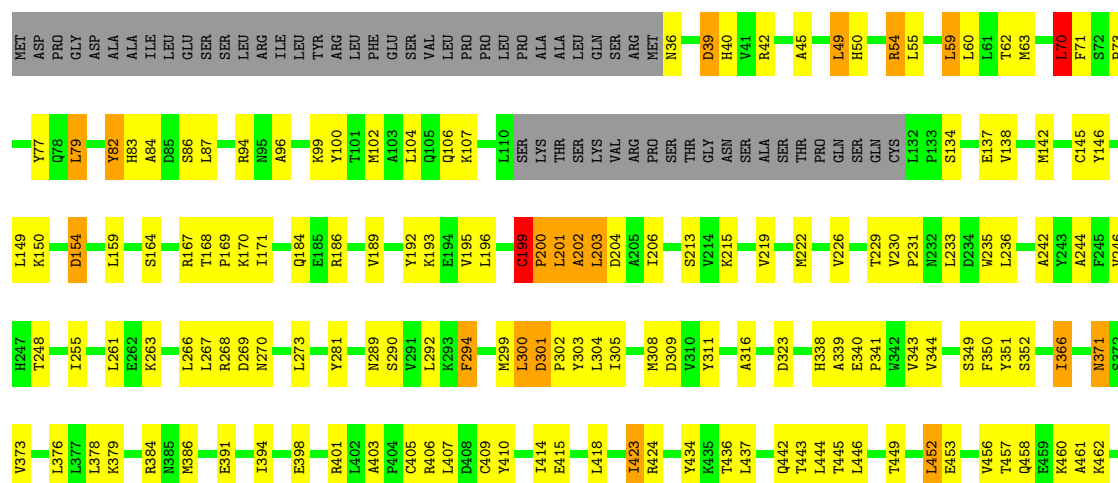
• Molecule 17: Anaphase-promoting complex subunit 7

Chain X: 53% 26% 19%

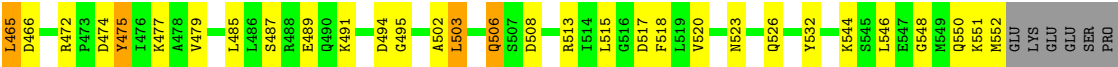


• Molecule 17: Anaphase-promoting complex subunit 7

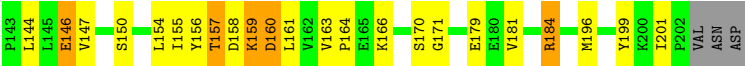
Chain Y: 52% 27% 17%







• Molecule 18: Mitotic spindle assembly checkpoint protein MAD2A



## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	155263	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI POLARA 300	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).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 2$	RMSZ	# $ Z  > 2$
1	A	0.67	6/11190 (0.1%)	0.89	23/15236 (0.2%)
10	L	0.54	0/1468	0.83	0/1993
11	M	0.66	0/502	0.95	0/680
12	N	0.63	3/5495 (0.1%)	0.94	18/7441 (0.2%)
13	O	0.58	0/5501	0.85	8/7432 (0.1%)
14	Q	0.72	0/2737	0.86	4/3732 (0.1%)
15	R	0.73	0/3029	0.86	2/4124 (0.0%)
16	S	0.66	0/2112	0.88	12/2863 (0.4%)
17	X	0.57	0/3833	0.82	3/5187 (0.1%)
17	Y	0.58	0/3928	0.84	9/5311 (0.2%)
18	Z	0.64	0/1605	0.79	2/2176 (0.1%)
2	B	0.81	2/665 (0.3%)	0.98	2/896 (0.2%)
3	C	0.57	0/4404	0.83	4/5945 (0.1%)
3	P	0.60	0/4138	0.86	5/5587 (0.1%)
4	D	0.69	0/159	0.89	0/218
5	E	0.60	0/459	0.80	0/619
6	F	0.58	0/3939	0.82	3/5325 (0.1%)
6	H	0.61	2/3943 (0.1%)	0.82	2/5329 (0.0%)
7	G	0.63	0/214	1.02	1/284 (0.4%)
7	W	0.66	0/214	0.97	1/284 (0.4%)
8	I	0.66	1/5834 (0.0%)	0.92	11/7909 (0.1%)
9	J	0.71	2/4146 (0.0%)	0.95	5/5616 (0.1%)
9	K	0.73	1/4086 (0.0%)	0.93	7/5534 (0.1%)
All	All	0.64	17/73601 (0.0%)	0.88	122/99721 (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
12	N	0	16

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Mol	Chain	#Chirality outliers	#Planarity outliers
16	S	0	1
8	I	0	2
9	J	0	1
All	All	0	21

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1030	GLU	CD-OE1	21.93	1.49	1.25
1	A	1030	GLU	CD-OE2	15.62	1.42	1.25
1	A	1199	LYS	CE-NZ	9.92	1.73	1.49
12	N	209	ARG	NE-CZ	9.66	1.45	1.33
1	A	1030	GLU	CG-CD	8.25	1.64	1.51

The worst 5 of 122 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	N	330	ARG	NE-CZ-NH2	-13.57	113.52	120.30
16	S	60	ARG	NE-CZ-NH1	9.25	124.92	120.30
9	K	351	ASP	CB-CG-OD1	8.97	126.37	118.30
1	A	1235	LEU	CB-CG-CD2	-8.77	96.09	111.00
3	P	358	LEU	CB-CG-CD1	-8.46	96.62	111.00

There are no chirality outliers.

5 of 21 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1191	LEU	Peptide
8	I	658	GLY	Peptide
8	I	727	PHE	Peptide
9	J	220	ILE	Peptide
12	N	62	ARG	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	10949	0	10690	418	0
2	B	643	0	617	80	0
3	C	4306	0	4272	161	0
3	P	4043	0	4000	137	0
4	D	153	0	148	8	0
5	E	450	0	435	10	0
6	F	3849	0	3783	108	0
6	H	3853	0	3794	128	0
7	G	213	0	220	11	0
7	W	213	0	220	12	0
8	I	5716	0	5587	345	0
9	J	4047	0	3949	185	0
9	K	3988	0	3908	174	0
10	L	1435	0	1382	55	0
11	M	493	0	469	24	0
12	N	5403	0	5103	276	0
13	O	5402	0	5436	221	0
14	Q	2671	0	2516	103	0
15	R	2953	0	2839	111	0
16	S	2077	0	1827	327	0
17	X	3773	0	3831	163	0
17	Y	3868	0	3925	169	0
18	Z	1577	0	1592	89	0
All	All	72075	0	70543	2914	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 20.

The worst 5 of 2914 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)
16:S:38:MET:CE	18:Z:181:VAL:HG23	1.22	1.65
16:S:22:TRP:CZ3	16:S:41:LEU:HB2	1.31	1.64
16:S:19:GLY:CA	18:Z:134:GLN:HE21	1.16	1.54
8:I:413:ASN:HA	8:I:447:PHE:CZ	1.38	1.53
1:A:1199:LYS:CE	1:A:1199:LYS:NZ	1.73	1.45

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	1397/1944 (72%)	1267 (91%)	106 (8%)	24 (2%)	11	52
2	B	75/84 (89%)	62 (83%)	8 (11%)	5 (7%)	1	22
3	C	520/597 (87%)	498 (96%)	20 (4%)	2 (0%)	38	77
3	P	485/597 (81%)	465 (96%)	20 (4%)	0	100	100
4	D	16/121 (13%)	14 (88%)	2 (12%)	0	100	100
5	E	54/110 (49%)	53 (98%)	1 (2%)	0	100	100
6	F	479/824 (58%)	458 (96%)	13 (3%)	8 (2%)	11	52
6	H	479/824 (58%)	459 (96%)	14 (3%)	6 (1%)	14	57
7	G	23/85 (27%)	23 (100%)	0	0	100	100
7	W	23/85 (27%)	23 (100%)	0	0	100	100
8	I	725/808 (90%)	683 (94%)	35 (5%)	7 (1%)	18	61
9	J	500/620 (81%)	467 (93%)	29 (6%)	4 (1%)	22	66
9	K	489/620 (79%)	456 (93%)	27 (6%)	6 (1%)	15	58
10	L	180/185 (97%)	165 (92%)	14 (8%)	1 (1%)	28	70
11	M	55/74 (74%)	46 (84%)	9 (16%)	0	100	100
12	N	679/822 (83%)	557 (82%)	68 (10%)	54 (8%)	1	17
13	O	677/755 (90%)	640 (94%)	29 (4%)	8 (1%)	15	58
14	Q	348/374 (93%)	317 (91%)	21 (6%)	10 (3%)	5	41
15	R	377/499 (76%)	344 (91%)	26 (7%)	7 (2%)	9	50
16	S	267/342 (78%)	237 (89%)	18 (7%)	12 (4%)	3	31
17	X	480/599 (80%)	464 (97%)	13 (3%)	3 (1%)	28	70
17	Y	492/599 (82%)	474 (96%)	13 (3%)	5 (1%)	18	61
18	Z	193/205 (94%)	186 (96%)	6 (3%)	1 (0%)	32	73
All	All	9013/11773 (77%)	8358 (93%)	492 (6%)	163 (2%)	14	51

5 of 163 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	274	VAL
1	A	630	PRO
1	A	857	MET
1	A	1125	ILE
1	A	1358	ILE

### 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	1151/1720 (67%)	1011 (88%)	140 (12%)	6	30
2	B	71/75 (95%)	59 (83%)	12 (17%)	2	18
3	C	452/520 (87%)	390 (86%)	62 (14%)	4	27
3	P	422/520 (81%)	374 (89%)	48 (11%)	7	33
4	D	18/115 (16%)	15 (83%)	3 (17%)	2	19
5	E	47/89 (53%)	37 (79%)	10 (21%)	1	9
6	F	407/727 (56%)	361 (89%)	46 (11%)	7	34
6	H	408/727 (56%)	368 (90%)	40 (10%)	9	39
7	G	23/77 (30%)	20 (87%)	3 (13%)	5	28
7	W	23/77 (30%)	21 (91%)	2 (9%)	12	45
8	I	617/730 (84%)	579 (94%)	38 (6%)	21	58
9	J	424/548 (77%)	373 (88%)	51 (12%)	6	31
9	K	423/548 (77%)	383 (90%)	40 (10%)	10	41
10	L	155/170 (91%)	137 (88%)	18 (12%)	6	33
11	M	55/67 (82%)	45 (82%)	10 (18%)	2	14
12	N	518/724 (72%)	448 (86%)	70 (14%)	4	27
13	O	577/650 (89%)	503 (87%)	74 (13%)	5	29
14	Q	271/310 (87%)	264 (97%)	7 (3%)	51	78
15	R	311/411 (76%)	293 (94%)	18 (6%)	23	60

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	S	186/293 (64%)	181 (97%)	5 (3%)	50	77
17	X	407/513 (79%)	376 (92%)	31 (8%)	15	51
17	Y	418/513 (82%)	381 (91%)	37 (9%)	11	44
18	Z	181/190 (95%)	170 (94%)	11 (6%)	22	58
All	All	7565/10314 (73%)	6789 (90%)	776 (10%)	13	37

5 of 776 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	I	688	THR
9	K	376	LEU
17	X	423	ILE
9	J	157	LEU
9	J	445	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 162 such sidechains are listed below:

Mol	Chain	Res	Type
9	J	17	GLN
9	K	316	ASN
17	X	338	HIS
9	J	58	HIS
9	J	393	GLN

### 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 [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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
12	N	2
8	I	1
16	S	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	S	310:ALA	C	529:SER	N	39.42
1	N	92:TRP	C	93:ASN	N	3.29
1	N	563:ASP	C	564:MET	N	2.78
1	I	302:ASP	C	303:GLU	N	2.26