



## wwPDB EM Map/Model Validation Report ⓘ

Jun 2, 2016 – 07:35 PM EDT

PDB ID : 5G05  
EMDB ID: : EMD-3388  
Title : Cryo-EM structure of combined apo phosphorylated APC  
Authors : Zhang, S.; Chang, L.; Alfieri, C.; Zhang, Z.; Yang, J.; Maslen, S.; Skehel, M.; Barford, D.  
Deposited on : 2016-03-16  
Resolution : 3.50 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/EMValidationReportHelp>

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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-20027674

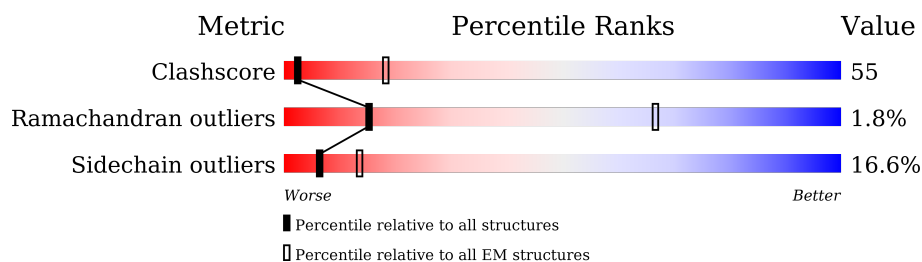
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.50 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.



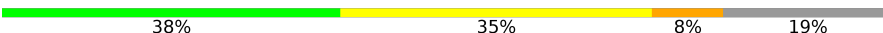
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

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	T	15	
15	X	599	
15	Y	599	

## 2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 63181 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	1569	Total	C	N	O	S	0	0
			11890	7656	2014	2140	80		

- Molecule 2 is a protein called ANAPHASE-PROMOTING COMPLEX SUBUNIT 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	84	Total	C	N	O	S	1	0
			649	416	117	99	17		

- 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	492	Total	C	N	O	S	0	0
			4046	2613	679	730	24		

- Molecule 4 is a protein called ANAPHASE-PROMOTING COMPLEX SUBUNIT 15.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	D	55	Total	C	N	O	0	0
			436	277	73	86		

- 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	460	Total	C	N	O	S	0	0
			3618	2320	608	666	24		
6	H	488	Total	C	N	O	S	0	0
			3879	2489	655	709	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
			220	137	41	41	1		
7	W	26	Total	C	N	O	S	0	0
			218	136	41	40	1		

- Molecule 8 is a protein called ANAPHASE-PROMOTING COMPLEX SUBUNIT 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	723	Total	C	N	O	S	0	0
			5634	3619	940	1041	34		

- 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
			4053	2604	687	737	25		
9	K	493	Total	C	N	O	S	0	0
			3988	2564	672	728	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
			481	304	79	96	2		

- Molecule 12 is a protein called ANAPHASE-PROMOTING COMPLEX SUBUNIT 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	N	604	Total	C	N	O	S	0	0
			4767	3053	851	841	22		

- Molecule 13 is a protein called ANAPHASE-PROMOTING COMPLEX SUBUNIT 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	O	688	Total	C	N	O	S	0	0
			5400	3443	940	989	28		

- Molecule 14 is a protein called UNIDENTIFIED PEPTIDE.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	T	15	Total	C	N	O	0	0
			79	47	16	16		

- Molecule 15 is a protein called ANAPHASE-PROMOTING COMPLEX SUBUNIT 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	X	484	Total	C	N	O	S	0	0
			3767	2390	649	704	24		
15	Y	496	Total	C	N	O	S	0	0
			3862	2446	666	724	26		

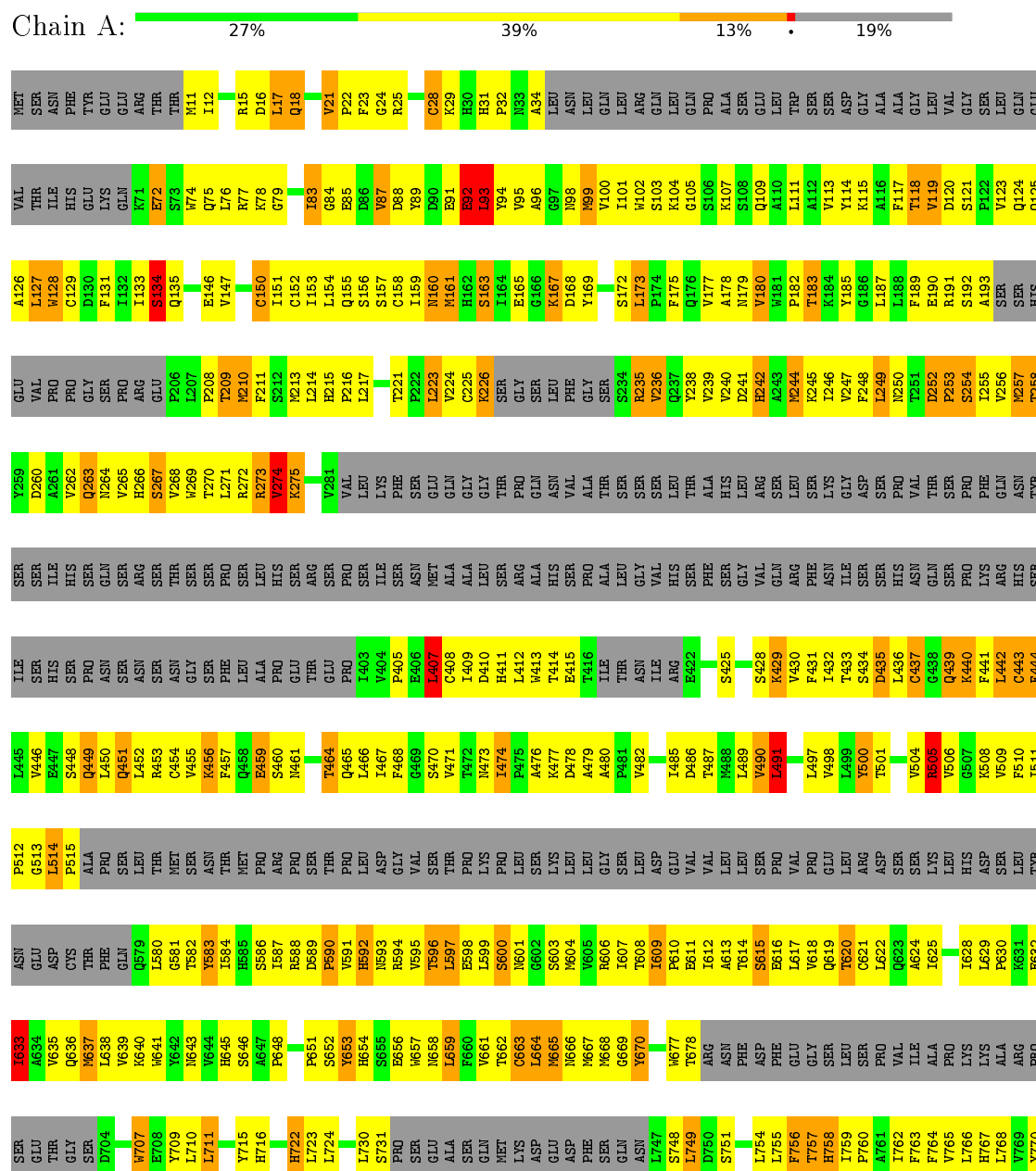
- Molecule 16 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
16	B	3	Total	Zn	0
			3	3	

### 3 Residue-property plots [i](#)

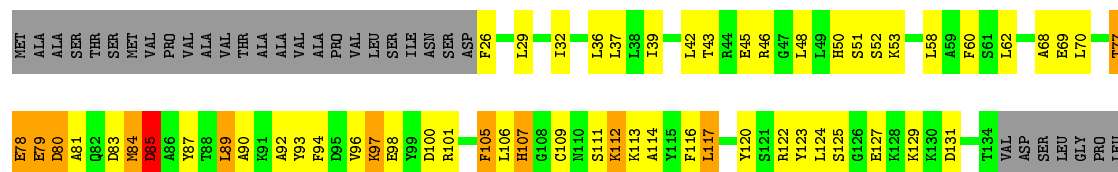
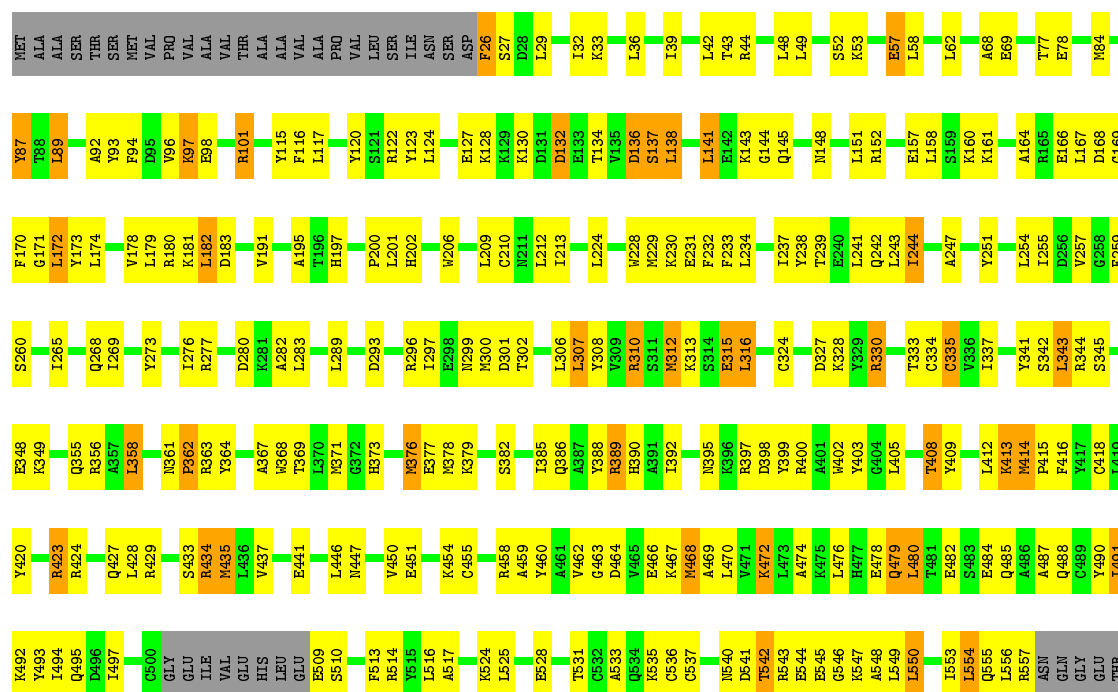
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric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

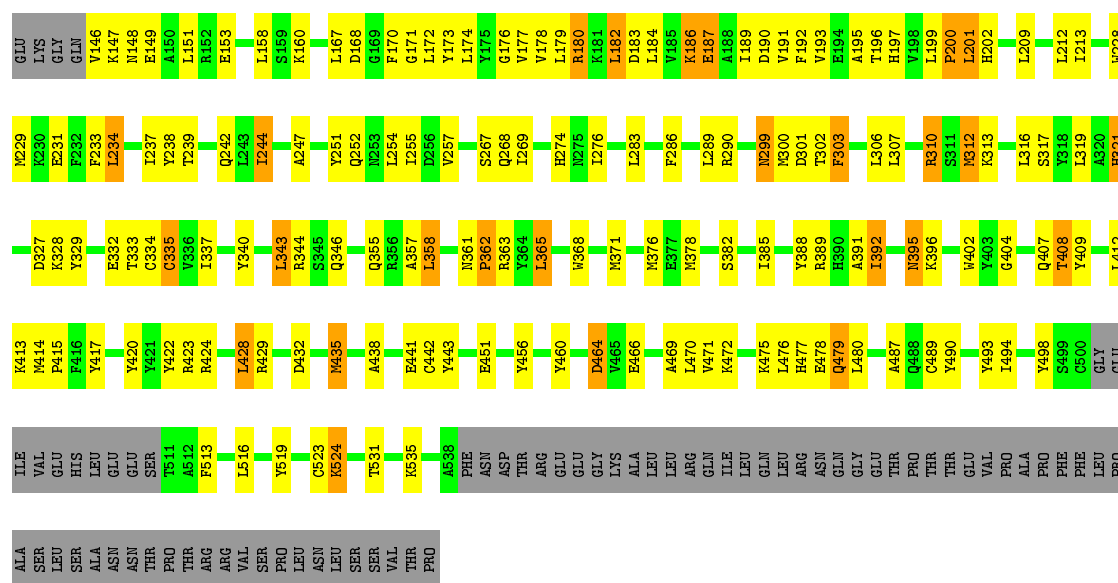
#### • Molecule 1: ANAPHASE-PROMOTING COMPLEX SUBUNIT 1





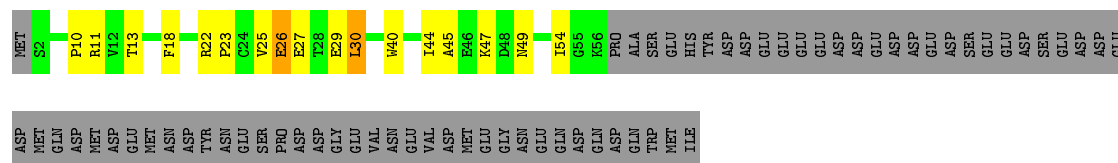




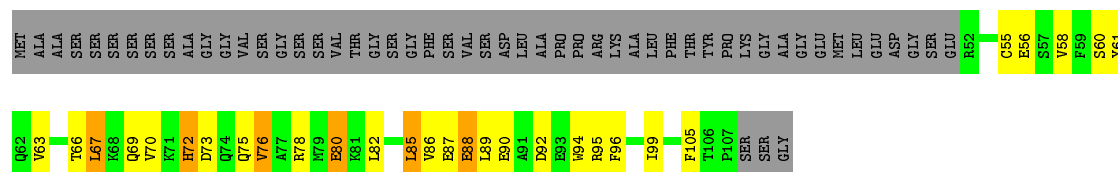
• Molecule 4: ANAPHASE-PROMOTING COMPLEX SUBUNIT 15

Chain D: 31% 12% 55%



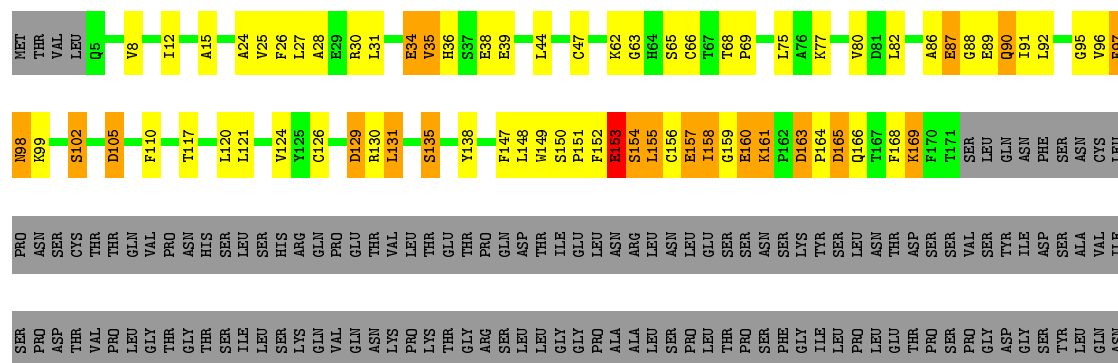
• Molecule 5: ANAPHASE-PROMOTING COMPLEX SUBUNIT 16

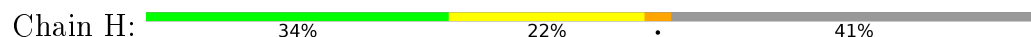
Chain E: 25% 21% 5% 49%

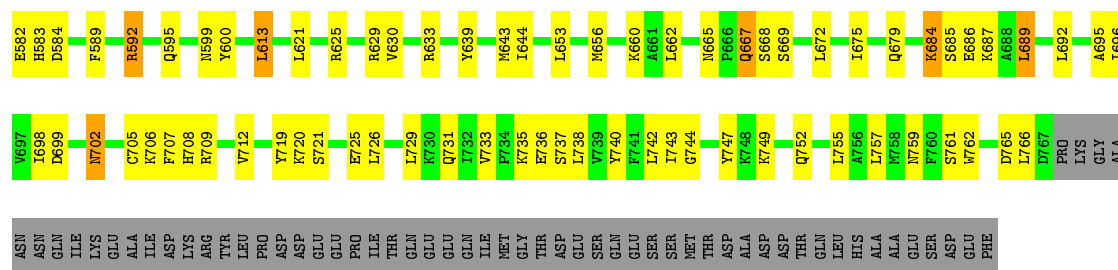


• Molecule 6: CELL DIVISION CYCLE PROTEIN 27 HOMOLOG

Chain F: 30% 21% 5% 44%

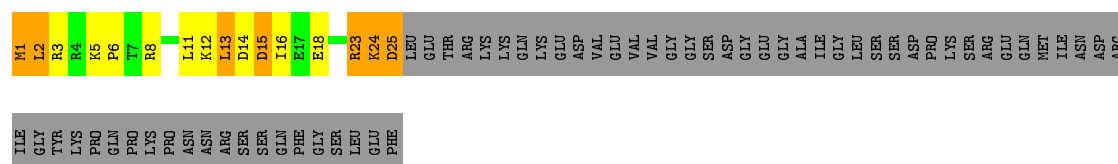






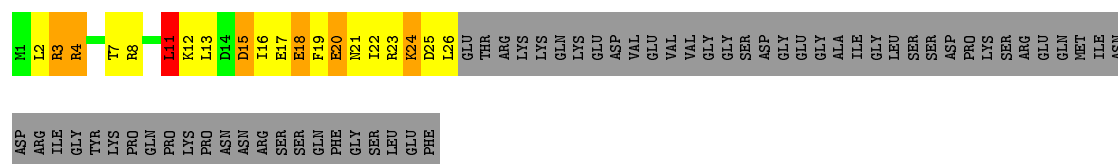
• Molecule 7: ANAPHASE-PROMOTING COMPLEX SUBUNIT CDC26

Chain G: 11% 11% 8% 71%



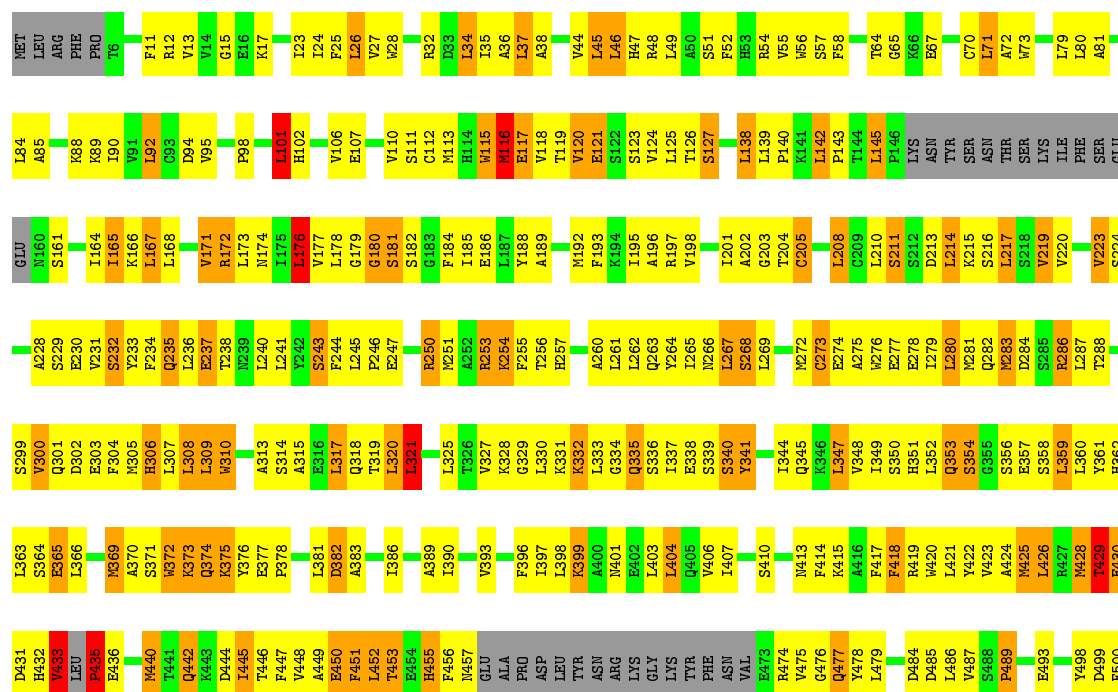
• Molecule 7: ANAPHASE-PROMOTING COMPLEX SUBUNIT CDC26

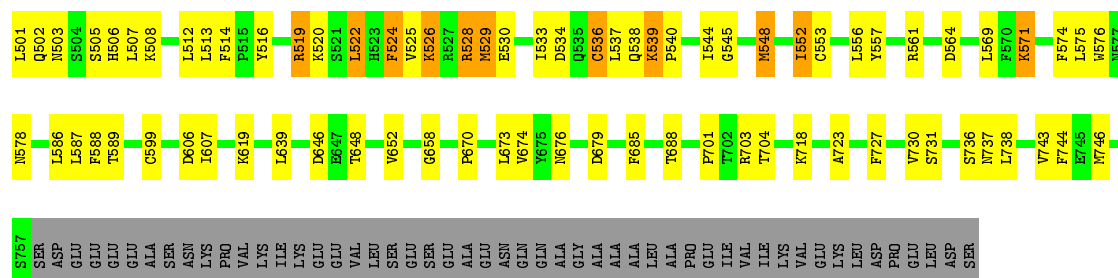
Chain W: 7% 15% 7% 69%



• Molecule 8: ANAPHASE-PROMOTING COMPLEX SUBUNIT 4

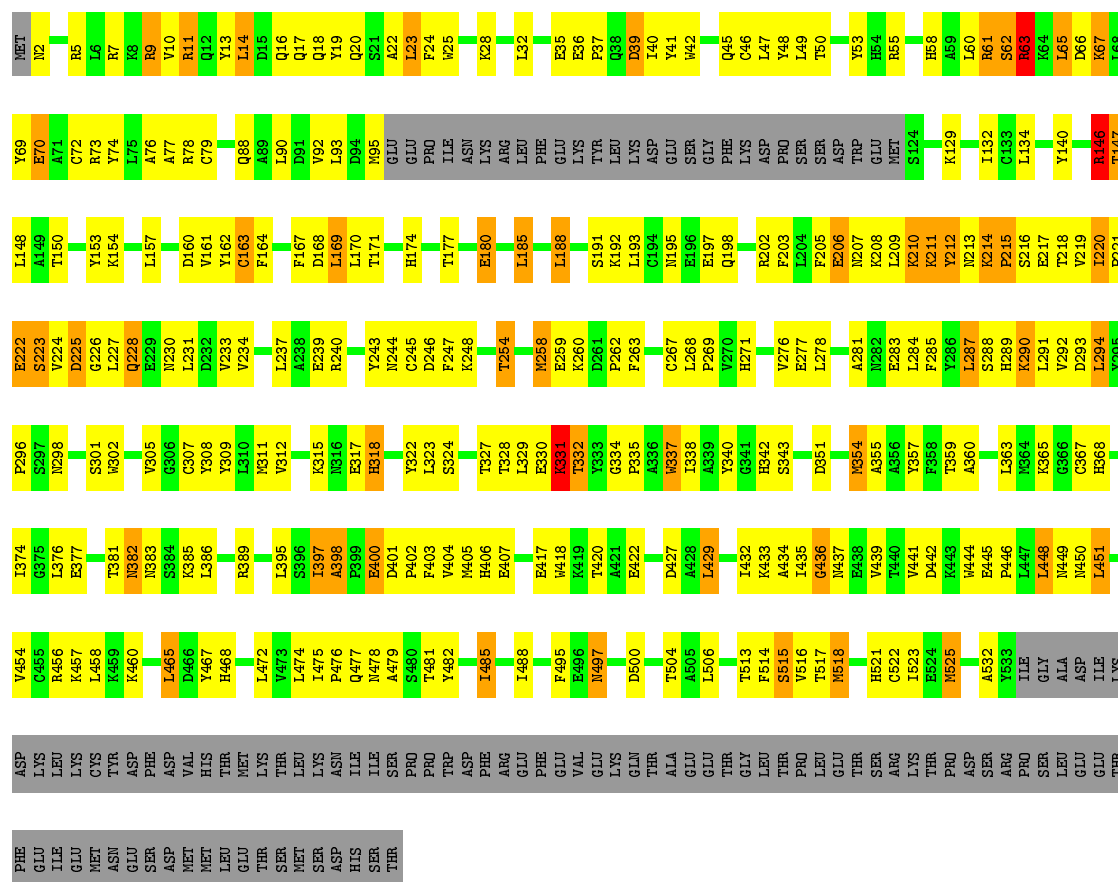
Chain I: 42% 35% 11% 11%





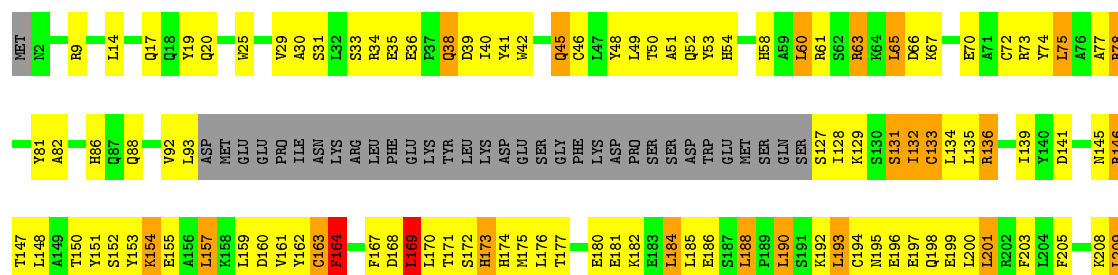
• Molecule 9: CELL DIVISION CYCLE PROTEIN 16 HOMOLOG

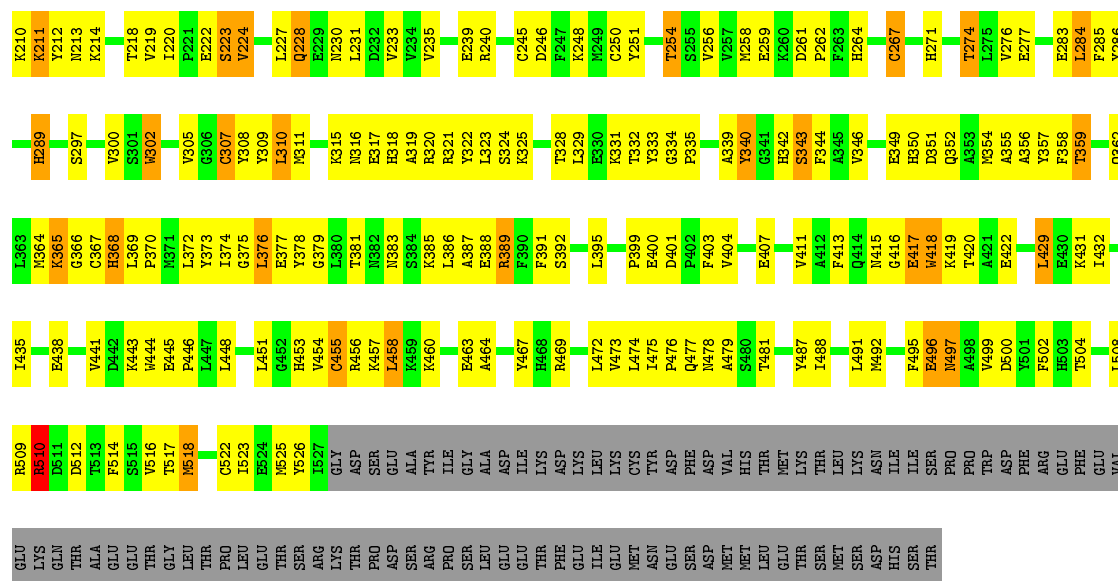
Chain J: 38% 35% 8% 19%



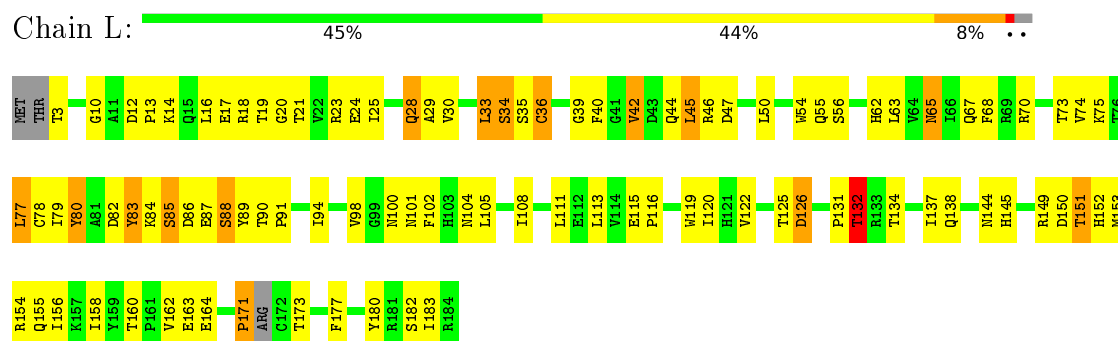
• Molecule 9: CELL DIVISION CYCLE PROTEIN 16 HOMOLOG

Chain K: 33% 38% 8% 20%

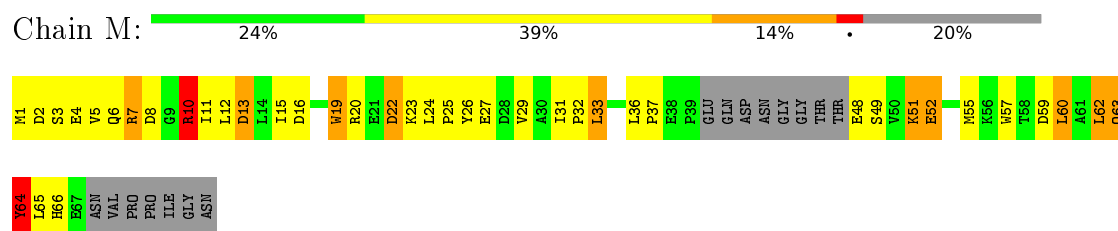




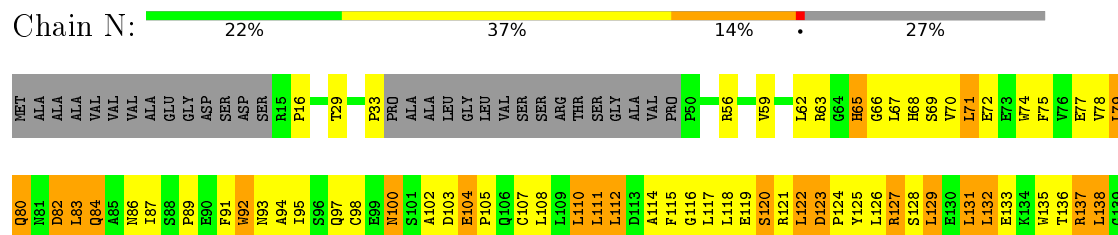
### • Molecule 10: ANAPHASE-PROMOTING COMPLEX SUBUNIT 10



### • Molecule 11: ANAPHASE-PROMOTING COMPLEX SUBUNIT 13



### • Molecule 12: ANAPHASE-PROMOTING COMPLEX SUBUNIT 2





Frequency	Percentage
Daily	41%
Weekly	37%
Monthly	12%
Other	9%







Chain Y:  41% 35% 6% 17%

MET	ASP	PRO	GLY	ASP	ALA	ALA	ILE	LEU	GLU	SER	SER	LEU	ARG	ILE	LEU	TYR	ARG	LEU	PHE	GLU	SER	VAL	LEU	PRO	PRO	LEU	GLN	SER	ARG	MET	N36	V37	N38	D39	H40	V41	R42	D43	N44	A45	A46	A47	G48	L49	H50	S51	N52	V53	R54	V55	L56	S57	S58	L59	PRO				
L61	T62	M63	S64	N65	N66		L70	F71	S72	P73		Y77	Q78	L79		Y82	H83	A84	D85	S86		L87		D90	K91	E92	Y93	R94	N95	A96	V97	S98	K99	Y100	T101	M102	A103	L104	Q105	K106	L107		L110	SER	LVS	THR	SER	LVS	VAL	ARG	PRO	SER	THR	GLY	ASN	SER	ALA	THR	PRO
GLN	SER	GLN	CYS	L132	P133	S134	E137	V138	K139	M142	C145	Y146	T147	M148	L149	D152	K153	D154	A155	I156	A157	I158	L159		I162	P163	S164	R167	T168	P169	K170	I171	L175	N170	A176		Y179	R186	P187	S188	V189	T190	S191	Y192	K193	E194	V195	L196	R197	Q198	C199	P200	L201						
A202	L203		I206		L209		L212	S213	V214	K215		V219		N225	V226	T229	V230		W235	L236		W239	I240	K241	A242	Y243	A244	F245	V246	H247	T248	R253	A254	I255	D269	N270	V271	D272	L273	A278		Y281		D286	N289	S290	V291	L292	K293	F294	E295	Q296		W299					
L300	D301	P302	Y303	L304	I305	K306	G307	M308	D309	V310	Y311	G312	Y313	A316	D323	V324	E325		I334	S335	D336		Q337	H338	A339	E340	P341	W342	V343		G346	C347	H348	S349	F350	Y351	S352	R353	Y355	R356	A357	L359	Y360	L361	G362	K363	K364	A365	L366		N371	S372	V373		L376	L377			
L378	K379		A382	L383	R384	N385	P386		E391	T394	H395		E398		R401	L402	A403		R406	L407	D408	C409		Y410	E411	G412	L413	I414	E415	C416	Y417	L418	A419		I423	A426		M429	N432	V433	Y434	K435	T436	L437		T443	L444	T445	L446	L447	A448	T449	V450	C451	L452	E453	D454		
P455	V456	T457	Q458	E459	K460	A461	K462	L465	D466	L469	D474	Y475	K477	L478	V479	V480	L481	K482		L485	L486	R487	R488	E489	Q490	K491	D494	G495	L496	L497	L498	L499	A502	L503	A504	N505	Q506	S507	D508	C509	V510		L515	E516	D517	F518	L519	V520	A521	V522		Q526	E527						
Y532	S533	I534	L546	E547	G548	M549	Q550	K551	M552	GLU	LYS	GLU	GLU	SER	PRO	THR	ASP	ALA	GLN	GLU	ASP	VAL	ASP	ASP	MET	GLU	GLY	SER	GLY	GLU	GLU	GLY	ASP	SER	GLU	ALA	GLN	TRP	ALA	ASP	GLN	GLU	GLN	GLN	TRP	PHE	GLY	MET	GLN										

## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	Not provided	Depositor
Microscope	OTHER	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	27	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	78000	Depositor
Image detector	FEI FALCON II (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	$\# Z  > 2$	RMSZ	$\# Z  > 2$
1	A	0.73	11/12168 (0.1%)	0.93	35/16587 (0.2%)
10	L	0.74	1/1468 (0.1%)	0.93	3/1993 (0.2%)
11	M	0.65	1/490 (0.2%)	0.98	5/665 (0.8%)
12	N	0.75	7/4860 (0.1%)	0.98	16/6584 (0.2%)
13	O	0.87	3/5499 (0.1%)	0.95	12/7432 (0.2%)
14	T	0.70	0/78	1.02	0/107
15	X	0.64	2/3827 (0.1%)	0.87	6/5180 (0.1%)
15	Y	0.56	0/3922	0.83	9/5304 (0.2%)
2	B	0.63	0/674	0.95	2/913 (0.2%)
3	C	0.73	1/4403 (0.0%)	0.93	10/5942 (0.2%)
3	P	0.66	1/4141 (0.0%)	0.89	6/5593 (0.1%)
4	D	0.62	0/446	0.83	1/610 (0.2%)
5	E	0.56	0/459	0.68	0/619
6	F	0.68	1/3704 (0.0%)	0.82	4/5019 (0.1%)
6	H	0.71	1/3969 (0.0%)	0.85	2/5366 (0.0%)
7	G	0.56	0/221	0.93	1/292 (0.3%)
7	W	0.57	0/219	0.93	1/291 (0.3%)
8	I	0.72	3/5754 (0.1%)	0.96	20/7806 (0.3%)
9	J	0.72	3/4152 (0.1%)	0.97	10/5623 (0.2%)
9	K	0.71	2/4085 (0.0%)	0.90	6/5530 (0.1%)
All	All	0.71	37/64539 (0.1%)	0.91	149/87456 (0.2%)

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	1
14	T	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
8	I	0	5
All	All	0	8

The worst 5 of 37 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	O	116	SER	C-N	24.88	1.91	1.34
13	O	135	PHE	C-N	13.64	1.65	1.34
12	N	427	TYR	CG-CD2	-9.69	1.26	1.39
12	N	600	PHE	CG-CD1	-9.42	1.24	1.38
1	A	236	VAL	N-CA	8.96	1.64	1.46

The worst 5 of 149 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	I	433	VAL	O-C-N	-16.78	89.22	121.10
1	A	505	ARG	NE-CZ-NH1	11.43	126.01	120.30
9	J	61	ARG	NE-CZ-NH2	-11.40	114.60	120.30
13	O	388	ARG	NE-CZ-NH2	-10.83	114.89	120.30
9	J	61	ARG	NE-CZ-NH1	10.42	125.51	120.30

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1652	MET	Peptide
8	I	429	THR	Mainchain
8	I	433	VAL	Mainchain,Peptide
8	I	658	GLY	Peptide
8	I	727	PHE	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	11890	0	11555	1834	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	649	0	595	33	0
3	C	4306	0	4273	274	0
3	P	4046	0	3998	248	0
4	D	436	0	396	25	0
5	E	450	0	435	31	0
6	F	3618	0	3452	380	0
6	H	3879	0	3805	267	0
7	G	220	0	233	30	0
7	W	218	0	222	26	0
8	I	5634	0	5522	590	0
9	J	4053	0	3960	371	0
9	K	3988	0	3911	440	0
10	L	1435	0	1381	165	0
11	M	481	0	457	72	0
12	N	4767	0	4685	1269	0
13	O	5400	0	5416	464	0
14	T	79	0	77	8	0
15	X	3767	0	3820	438	0
15	Y	3862	0	3914	412	0
16	B	3	0	0	0	0
All	All	63181	0	62107	6915	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 55.

The worst 5 of 6915 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)
3:P:89:LEU:HD11	3:P:105:PHE:CE2	1.34	1.62
12:N:184:TYR:CZ	12:N:302:LYS:HE2	1.22	1.62
15:Y:104:LEU:HD11	15:Y:142:MET:CE	1.20	1.59
3:P:89:LEU:HD11	3:P:105:PHE:CD2	1.37	1.58
1:A:948:PRO:CB	1:A:1813:GLN:HE22	1.12	1.57

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	1539/1944 (79%)	1372 (89%)	112 (7%)	55 (4%)	4	37
2	B	83/84 (99%)	72 (87%)	7 (8%)	4 (5%)	3	28
3	C	518/597 (87%)	490 (95%)	23 (4%)	5 (1%)	19	66
3	P	486/597 (81%)	466 (96%)	16 (3%)	4 (1%)	24	70
4	D	53/121 (44%)	47 (89%)	5 (9%)	1 (2%)	10	51
5	E	54/110 (49%)	54 (100%)	0	0	100	100
6	F	454/824 (55%)	433 (95%)	19 (4%)	2 (0%)	39	81
6	H	484/824 (59%)	469 (97%)	10 (2%)	5 (1%)	19	66
7	G	23/85 (27%)	23 (100%)	0	0	100	100
7	W	24/85 (28%)	23 (96%)	0	1 (4%)	3	32
8	I	717/808 (89%)	682 (95%)	20 (3%)	15 (2%)	9	50
9	J	500/620 (81%)	468 (94%)	25 (5%)	7 (1%)	14	58
9	K	487/620 (78%)	456 (94%)	27 (6%)	4 (1%)	24	70
10	L	180/185 (97%)	169 (94%)	9 (5%)	2 (1%)	17	63
11	M	55/74 (74%)	49 (89%)	5 (9%)	1 (2%)	11	53
12	N	590/822 (72%)	547 (93%)	26 (4%)	17 (3%)	6	42
13	O	682/755 (90%)	643 (94%)	27 (4%)	12 (2%)	11	53
14	T	13/15 (87%)	11 (85%)	1 (8%)	1 (8%)	1	14
15	X	480/599 (80%)	463 (96%)	12 (2%)	5 (1%)	19	66
15	Y	492/599 (82%)	473 (96%)	15 (3%)	4 (1%)	24	70
All	All	7914/10368 (76%)	7410 (94%)	359 (4%)	145 (2%)	15	53

5 of 145 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	274	VAL

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Mol	Chain	Res	Type
1	A	514	LEU
1	A	723	LEU
1	A	813	LEU
1	A	823	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	1243/1720 (72%)	967 (78%)	276 (22%)	1	6
2	B	65/75 (87%)	54 (83%)	11 (17%)	2	15
3	C	452/520 (87%)	384 (85%)	68 (15%)	3	21
3	P	422/520 (81%)	368 (87%)	54 (13%)	5	28
4	D	46/115 (40%)	41 (89%)	5 (11%)	8	37
5	E	47/89 (53%)	35 (74%)	12 (26%)	1	4
6	F	371/727 (51%)	310 (84%)	61 (16%)	3	17
6	H	408/727 (56%)	368 (90%)	40 (10%)	10	42
7	G	25/77 (32%)	16 (64%)	9 (36%)	0	1
7	W	23/77 (30%)	15 (65%)	8 (35%)	0	2
8	I	607/730 (83%)	508 (84%)	99 (16%)	3	17
9	J	425/548 (78%)	363 (85%)	62 (15%)	4	22
9	K	423/548 (77%)	356 (84%)	67 (16%)	3	19
10	L	155/170 (91%)	139 (90%)	16 (10%)	9	40
11	M	52/67 (78%)	38 (73%)	14 (27%)	0	4
12	N	489/724 (68%)	371 (76%)	118 (24%)	1	5
13	O	573/650 (88%)	469 (82%)	104 (18%)	2	12
14	T	1/2 (50%)	1 (100%)	0	100	100
15	X	406/513 (79%)	370 (91%)	36 (9%)	12	47
15	Y	417/513 (81%)	373 (89%)	44 (11%)	8	38

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	6650/9112 (73%)	5546 (83%)	1104 (17%)	<b>6</b> <b>16</b>

5 of 1104 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	I	165	ILE
9	J	294	LEU
7	W	15	ASP
8	I	254	LYS
8	I	450	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 190 such sidechains are listed below:

Mol	Chain	Res	Type
8	I	477	GLN
9	K	318	HIS
15	X	371	ASN
9	J	38	GLN
9	J	406	HIS

### 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](#)

Of 3 ligands modelled in this entry, 3 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

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.