wwPDB/EMDataBank EM Map/Model Validation Summary Report (i)

Feb 7, 2017 – 01:01 PM EST

PDB ID	:	5H7I
EMDB ID:	:	EMD-6671
Title	:	Cryo-EM structure of the Cdt1-MCM2-7 complex in AMPPNP state
Authors	:	Zhai, Y.; Cheng, E.; Wu, H.; Li, N.; Yung, P.Y.; Gao, N.; Tye, B.K.
Deposited on	:	2016-11-18
Resolution	:	7.10 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*
A user guide is available at
http://wwpdb.org/validation/2016/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

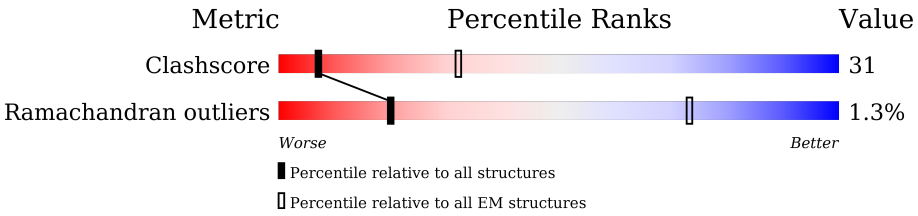
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20028442

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 7.10 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

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 <=5%

Mol	Chain	Length	Quality of chain
1	2	868	47% 20% • 32%
2	3	971	44% 18% • 38%
3	4	933	52% 24% • 23%
4	5	775	62% 19% 18%
5	6	1017	38% 23% • 36%
6	7	845	51% 22% 26%
7	C	604	51% 18% • 29%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 21016 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 DNA replication licensing factor MCM2.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
1	2	591	2924	1742	591	591	0	0

- Molecule 2 is a protein called DNA replication licensing factor MCM3.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	3	601	2974	1772	601	601	0	0

- Molecule 3 is a protein called DNA replication licensing factor MCM4.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	4	716	3551	2119	716	716	0	0

- Molecule 4 is a protein called Minichromosome maintenance protein 5.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	5	632	3130	1866	632	632	0	0

- Molecule 5 is a protein called DNA replication licensing factor MCM6.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
5	6	652	3230	1926	652	652	0	0

- Molecule 6 is a protein called DNA replication licensing factor MCM7.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
6	7	622	3076	1832	622	622	0	0

- Molecule 7 is a protein called Cell division cycle protein CDT1.

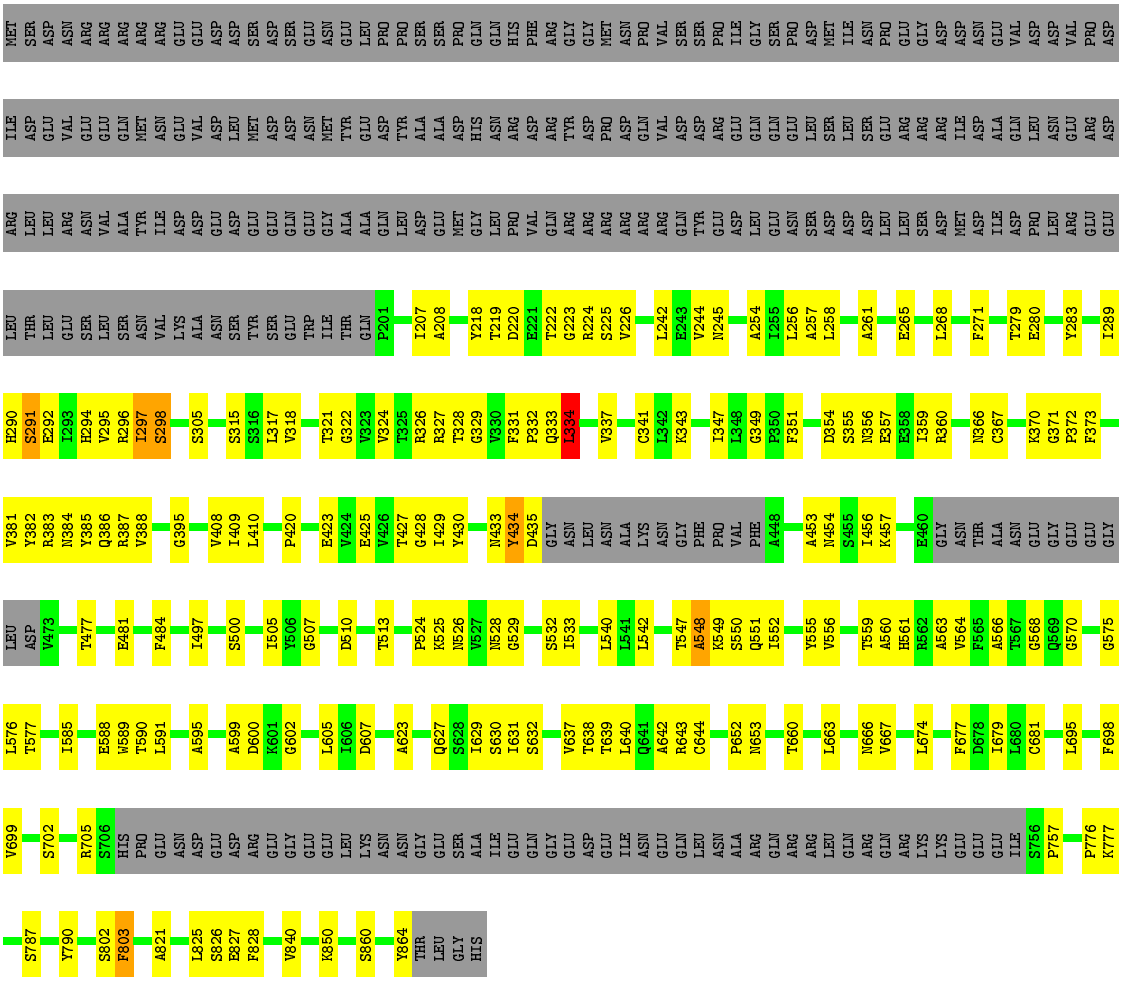
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
7	C	429	2131	1273	429	429	0	0

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.

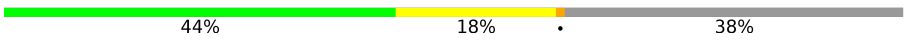
- Molecule 1: DNA replication licensing factor MCM2

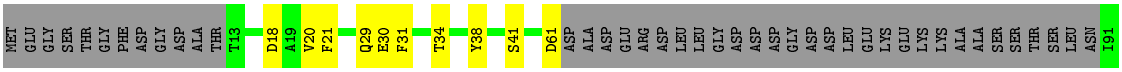
Chain 2:

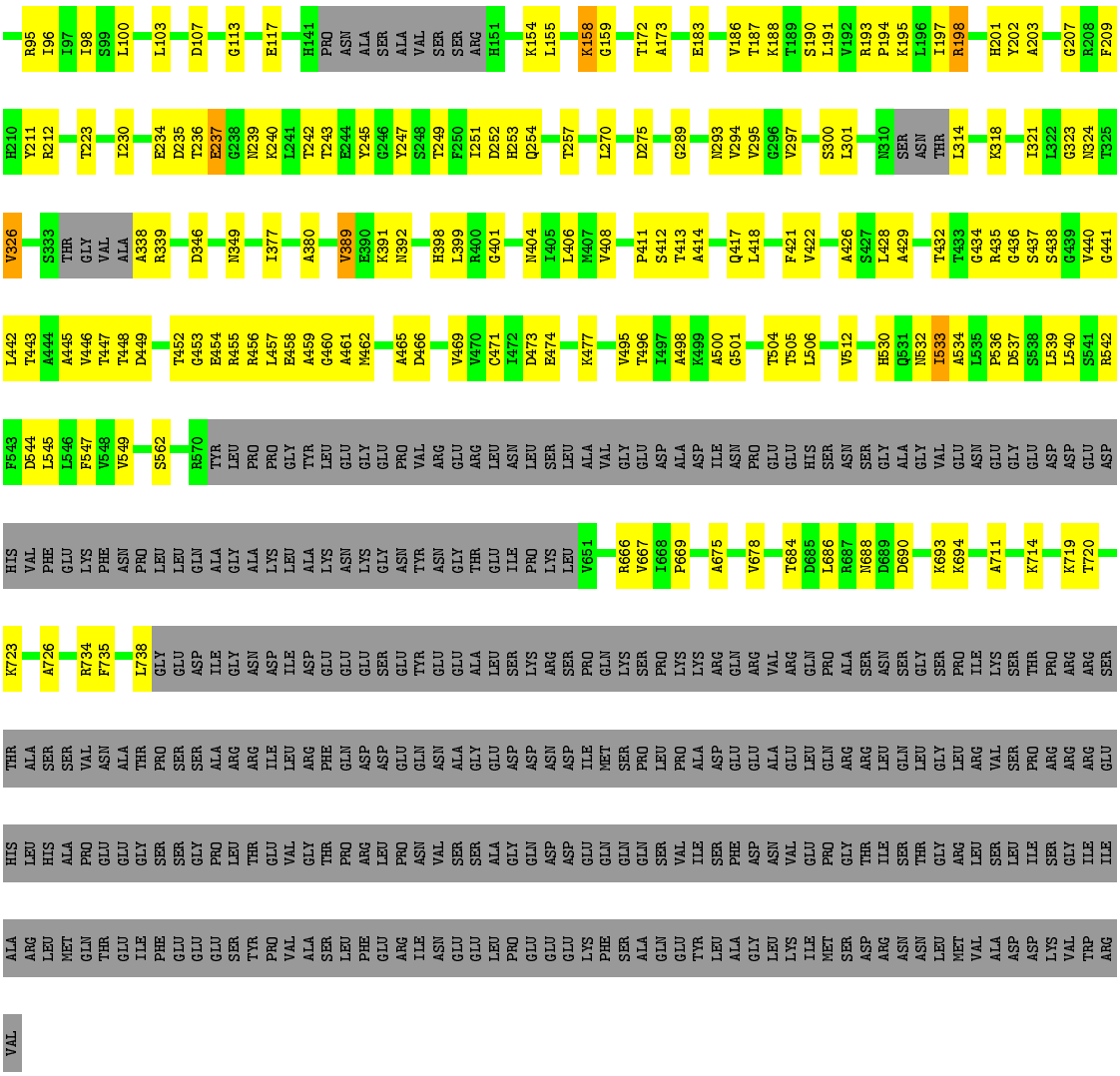


- Molecule 2: DNA replication licensing factor MCM3

Chain 3:

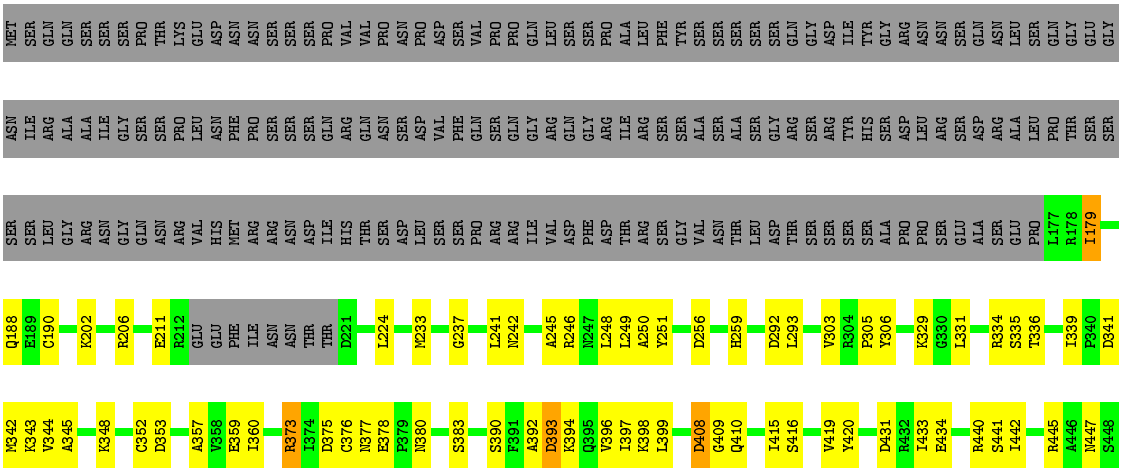


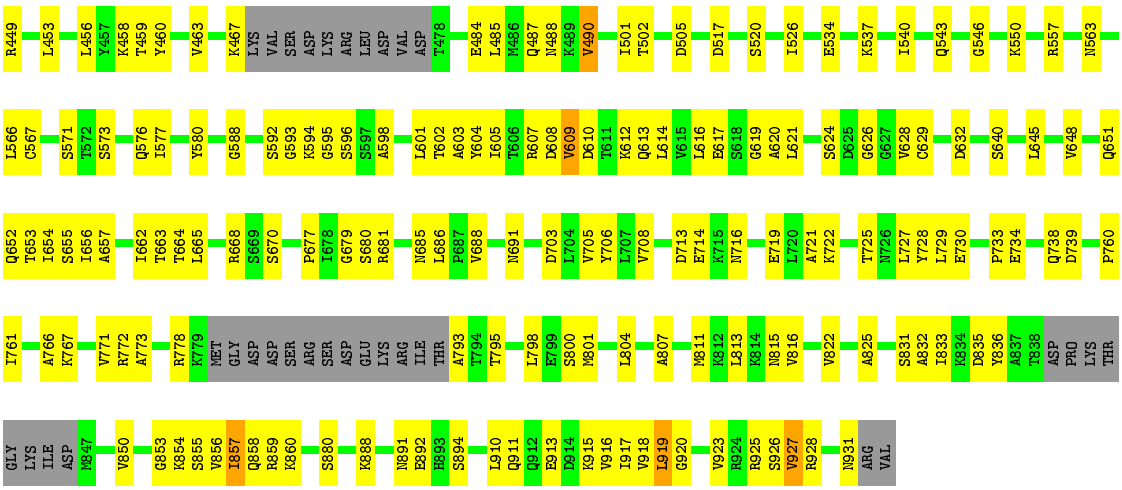




• Molecule 3: DNA replication licensing factor MCM4

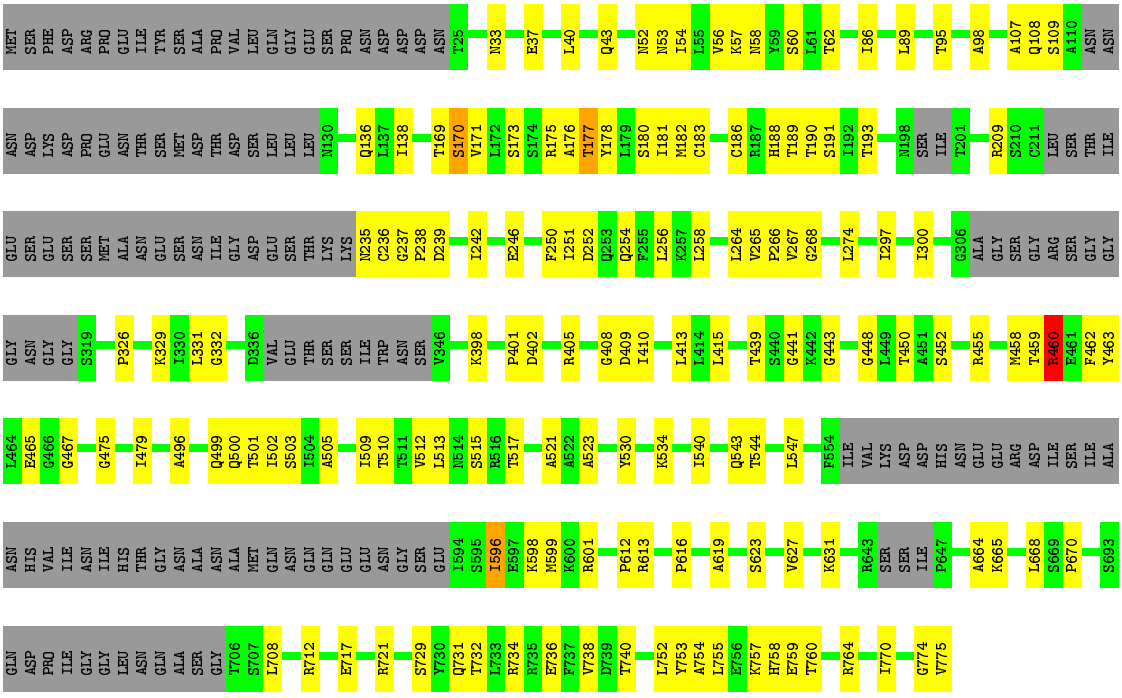
Chain 4:





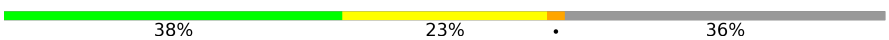
• Molecule 4: Minichromosome maintenance protein 5

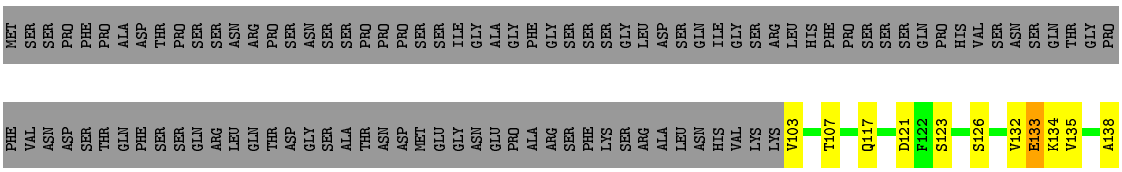
Chain 5:

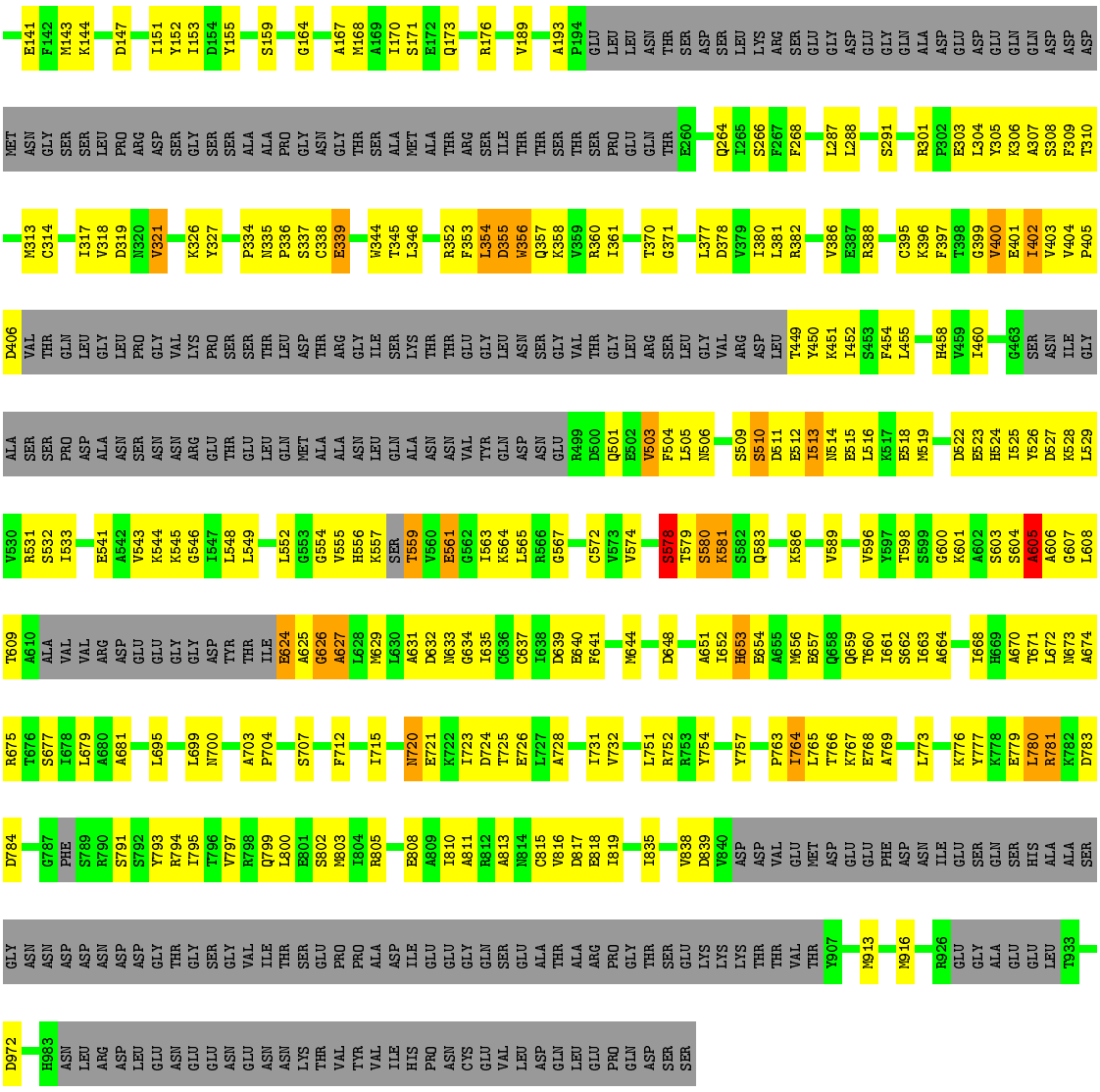


• Molecule 5: DNA replication licensing factor MCM6

Chain 6:

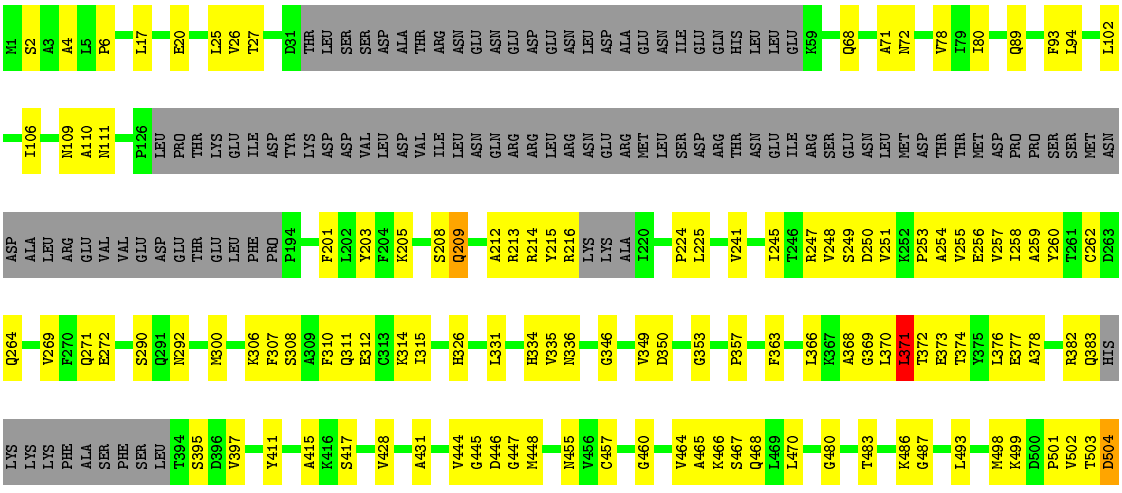


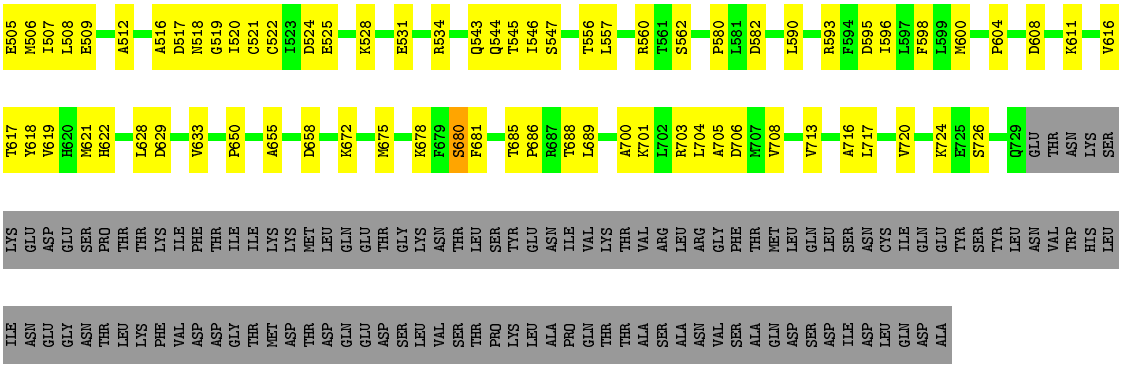




• Molecule 6: DNA replication licensing factor MCM7

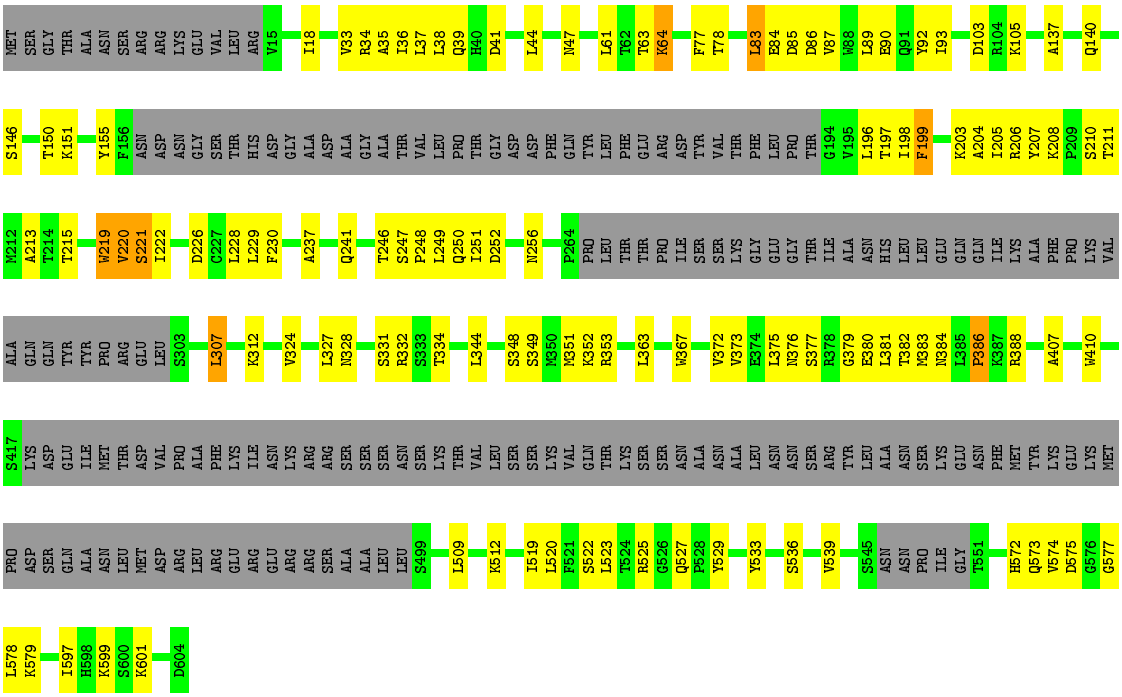
Chain 7:





- Molecule 7: Cell division cycle protein CDT1

Chain C:



4 Experimental information (i)

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	63000	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 ($e^-/Å^2$)	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

5.1 Standard geometry

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	2	0.52	0/2920	0.69	3/4063 (0.1%)
2	3	0.45	0/2968	0.62	0/4127
3	4	0.51	0/3546	0.69	4/4939 (0.1%)
4	5	0.39	0/3121	0.56	0/4337
5	6	0.54	0/3221	0.77	5/4477 (0.1%)
6	7	0.46	0/3071	0.64	0/4271
7	C	0.42	0/2126	0.71	2/2960 (0.1%)
All	All	0.48	0/20973	0.67	14/29174 (0.0%)

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	2	0	6
2	3	0	5
3	4	0	6
4	5	0	2
5	6	0	19
6	7	0	6
7	C	0	17
All	All	0	61

There are no bond length outliers.

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	6	626	GLY	N-CA-C	-6.63	96.52	113.10
5	6	561	GLU	N-CA-C	-6.51	93.41	111.00
1	2	334	LEU	N-CA-C	-6.49	93.48	111.00
1	2	570	GLY	N-CA-C	6.27	128.77	113.10
3	4	920	GLY	C-N-CA	-5.95	106.81	121.70

There are no chirality outliers.

5 of 61 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	2	218	TYR	Peptide
1	2	298	SER	Peptide
1	2	367	CYS	Peptide
1	2	434	TYR	Peptide
1	2	588	GLU	Peptide

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	2	2924	0	1308	149	0
2	3	2974	0	1349	134	0
3	4	3551	0	1537	162	0
4	5	3130	0	1369	97	0
5	6	3230	0	1449	202	0
6	7	3076	0	1381	157	0
7	C	2131	0	919	78	0
All	All	21016	0	9312	939	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 31.

The worst 5 of 939 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)
1:2:386:GLN:N	1:2:410:LEU:O	1.57	1.36
3:4:856:VAL:HA	3:4:860:LYS:CB	1.73	1.19
5:6:625:ALA:HB3	5:6:629:MET:H	1.04	1.13
2:3:190:SER:HA	2:3:456:ARG:HA	1.34	1.09
1:2:386:GLN:O	1:2:410:LEU:N	1.86	1.08

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	2	583/868 (67%)	503 (86%)	69 (12%)	11 (2%)	10 52
2	3	589/971 (61%)	516 (88%)	65 (11%)	8 (1%)	14 58
3	4	706/933 (76%)	603 (85%)	95 (14%)	8 (1%)	17 63
4	5	614/775 (79%)	564 (92%)	45 (7%)	5 (1%)	24 69
5	6	634/1017 (62%)	539 (85%)	80 (13%)	15 (2%)	7 47
6	7	612/845 (72%)	542 (89%)	62 (10%)	8 (1%)	15 60
7	C	419/604 (69%)	353 (84%)	65 (16%)	1 (0%)	52 86
All	All	4157/6013 (69%)	3620 (87%)	481 (12%)	56 (1%)	20 60

5 of 56 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	2	305	SER
1	2	334	LEU
2	3	198	ARG
3	4	179	ILE
3	4	490	VAL

5.3.2 Protein sidechains

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 (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.