wwPDB EM Validation Summary Report (i)

Mar 16, 2025 – 02:11 PM EDT

PDB ID	:	9E2Y
EMDB ID	:	EMD-47472
Title	:	Cryo-EM structure of yeast CMG helicase stalled at G4-containing DNA template, state 3
Authors	:	Allwein, B.; Batra, S.; Remus, D.; Hite, R.
Deposited on	:	2024-10-23
Resolution	:	3.20 Å(reported)
Based on initial model	:	.

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

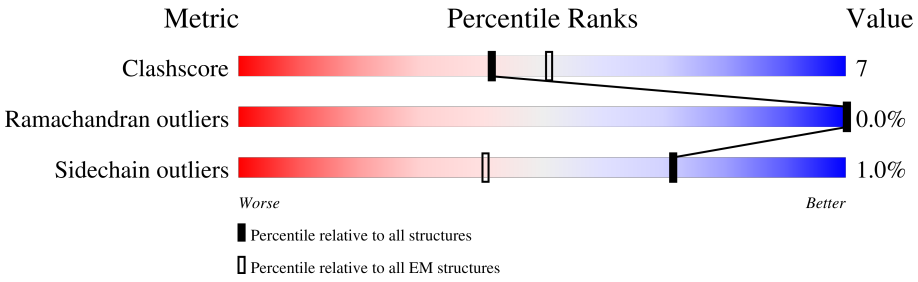
EMDB validation analysis	:	0.0.1.dev117
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.4

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.20 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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	A	208	83% 11% 6%
2	B	213	72% 16% 11%
3	C	217	71% 9% 20%
4	D	294	64% 12% 24%
5	E	650	76% 11% 13%
6	F	35	71% 29%
7	G	7	71% 29%
8	2	868	66% 9% • 24%
9	3	971	56% 7% 36%

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Mol	Chain	Length	Quality of chain
10	4	933	
11	5	775	
12	6	1017	
13	7	845	
14	X	43	

2 Entry composition (i)

There are 18 unique types of molecules in this entry. The entry contains 83461 atoms, of which 41584 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 complex GINS protein PSF1.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	A	196	3202	1005	1602	276	310	9	0	0

- Molecule 2 is a protein called DNA replication complex GINS protein PSF2.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
2	B	189	3193	1014	1616	276	282	5	0	0

- Molecule 3 is a protein called DNA replication complex GINS protein PSF3.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
3	C	174	2813	912	1413	225	257	6	0	0

There are 23 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-22	MET	-	expression tag	UNP Q12146
C	-21	GLY	-	expression tag	UNP Q12146
C	-20	SER	-	expression tag	UNP Q12146
C	-19	SER	-	expression tag	UNP Q12146
C	-18	HIS	-	expression tag	UNP Q12146
C	-17	HIS	-	expression tag	UNP Q12146
C	-16	HIS	-	expression tag	UNP Q12146
C	-15	HIS	-	expression tag	UNP Q12146
C	-14	HIS	-	expression tag	UNP Q12146
C	-13	HIS	-	expression tag	UNP Q12146
C	-12	SER	-	expression tag	UNP Q12146
C	-11	SER	-	expression tag	UNP Q12146
C	-10	GLY	-	expression tag	UNP Q12146
C	-9	LEU	-	expression tag	UNP Q12146
C	-8	VAL	-	expression tag	UNP Q12146

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-7	PRO	-	expression tag	UNP Q12146
C	-6	ARG	-	expression tag	UNP Q12146
C	-5	GLY	-	expression tag	UNP Q12146
C	-4	SER	-	expression tag	UNP Q12146
C	-3	HIS	-	expression tag	UNP Q12146
C	-2	MET	-	expression tag	UNP Q12146
C	-1	ALA	-	expression tag	UNP Q12146
C	0	SER	-	expression tag	UNP Q12146

- Molecule 4 is a protein called DNA replication complex GINS protein SLD5.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	D	222	Total	C	H	N	O	S	0	0
			3672	1170	1843	300	347	12		

- Molecule 5 is a protein called Cell division control protein 45.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	E	566	Total	C	H	N	O	S	0	0
			9124	2922	4555	770	863	14		

- Molecule 6 is a DNA chain called Leading strand DNA template.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	F	35	Total	C	H	N	O	P	0	0
			1047	347	314	133	218	35		

- Molecule 7 is a DNA chain called Lagging strand DNA template.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	G	7	Total	C	H	N	O	P	0	0
			178	69	32	30	40	7		

- Molecule 8 is a protein called DNA replication licensing factor MCM2.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	2	664	Total	C	H	N	O	S	0	0
			10572	3305	5305	944	999	19		

- Molecule 9 is a protein called DNA replication licensing factor MCM3.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	3	618	Total	C	H	N	O	S	0	0
			9718	3044	4893	860	908	13		

- Molecule 10 is a protein called DNA replication licensing factor MCM4.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	4	612	Total	C	H	N	O	S	0	0
			9785	3067	4921	838	931	28		

- Molecule 11 is a protein called Minichromosome maintenance protein 5.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	5	595	Total	C	H	N	O	S	0	0
			9407	2951	4730	799	904	23		

- Molecule 12 is a protein called DNA replication licensing factor MCM6.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	6	634	Total	C	H	N	O	S	0	0
			10036	3159	5031	873	948	25		

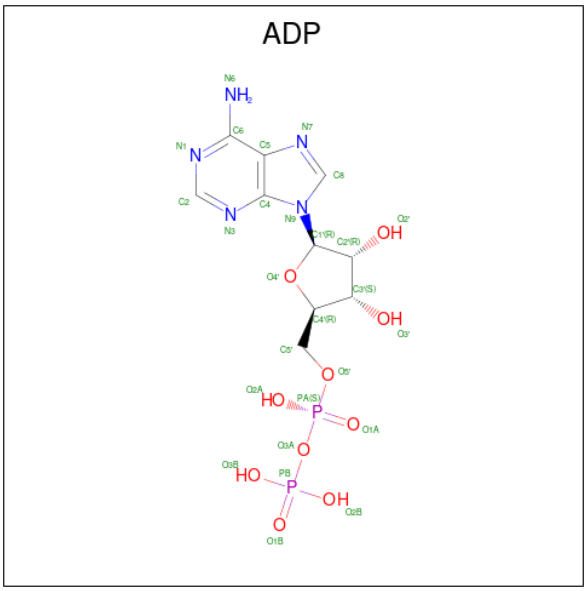
- Molecule 13 is a protein called DNA replication licensing factor MCM7.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	7	615	Total	C	H	N	O	S	0	0
			9784	3075	4919	847	917	26		

- Molecule 14 is a protein called Topoisomerase 1-associated factor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	X	43	Total	C	H	N	O	0	0
			665	201	338	61	65		

- Molecule 15 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
15	2	1	Total	C	H	N	O	P	0
			39	10	12	5	10	2	

- Molecule 16 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
16	2	1	Total	Mg	0
			1	1	
16	3	1	Total	Mg	0
			1	1	
16	4	1	Total	Mg	0
			1	1	
16	5	1	Total	Mg	0
			1	1	
16	6	1	Total	Mg	0
			1	1	
16	7	1	Total	Mg	0
			1	1	

- Molecule 17 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
17	2	1	Total	Zn	0
			1	1	
17	4	1	Total	Zn	0
			1	1	

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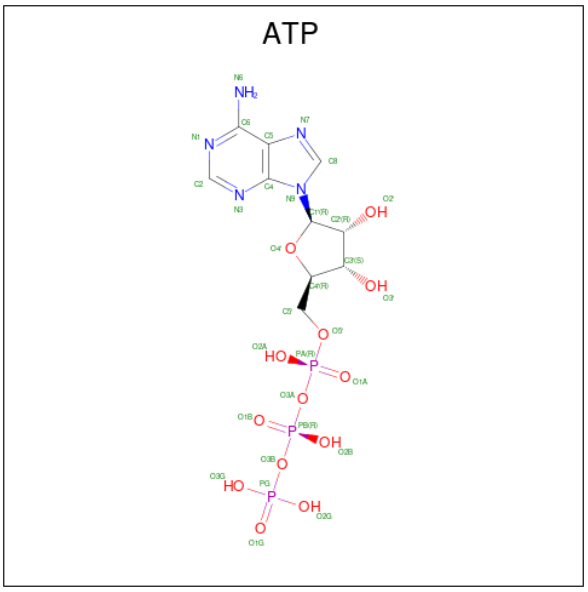
Mol	Chain	Residues	Atoms	AltConf
17	5	1	Total Zn 1 1	0
17	6	1	Total Zn 1 1	0
17	7	1	Total Zn 1 1	0

- Molecule 18 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



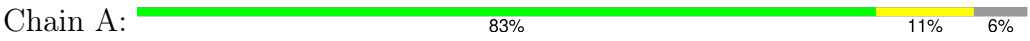
Mol	Chain	Residues	Atoms	AltConf
18	4	1	Total C H N O P 43 10 12 5 13 3	0
18	5	1	Total C H N O P 43 10 12 5 13 3	0
18	5	1	Total C H N O P 43 10 12 5 13 3	0
18	6	1	Total C H N O P 43 10 12 5 13 3	0
18	7	1	Total C H N O P 43 10 12 5 13 3	0

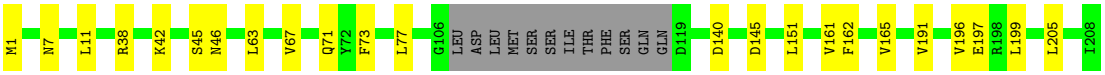
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: DNA replication complex GINS protein PSF1

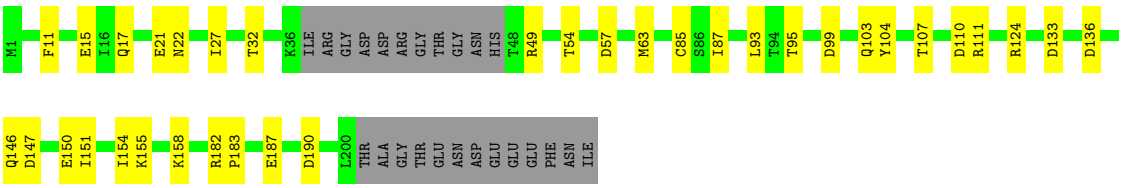
Chain A:





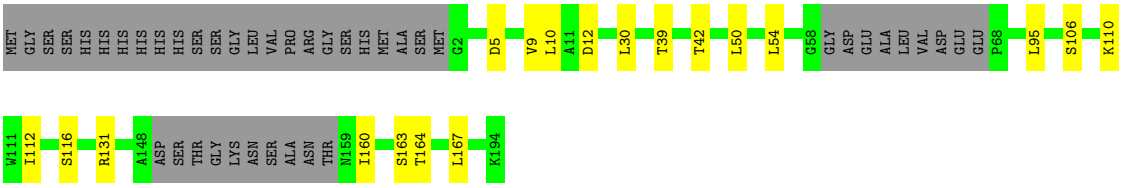
• Molecule 2: DNA replication complex GINS protein PSF2

Chain B:



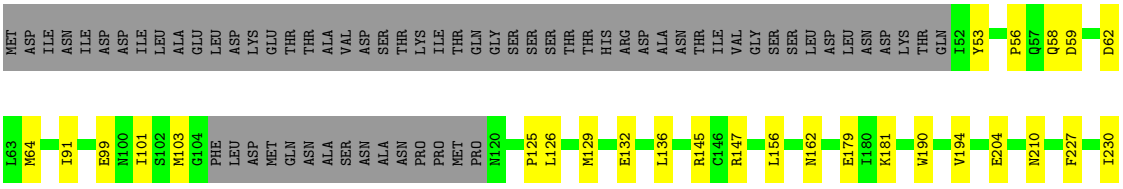
• Molecule 3: DNA replication complex GINS protein PSF3

Chain C:



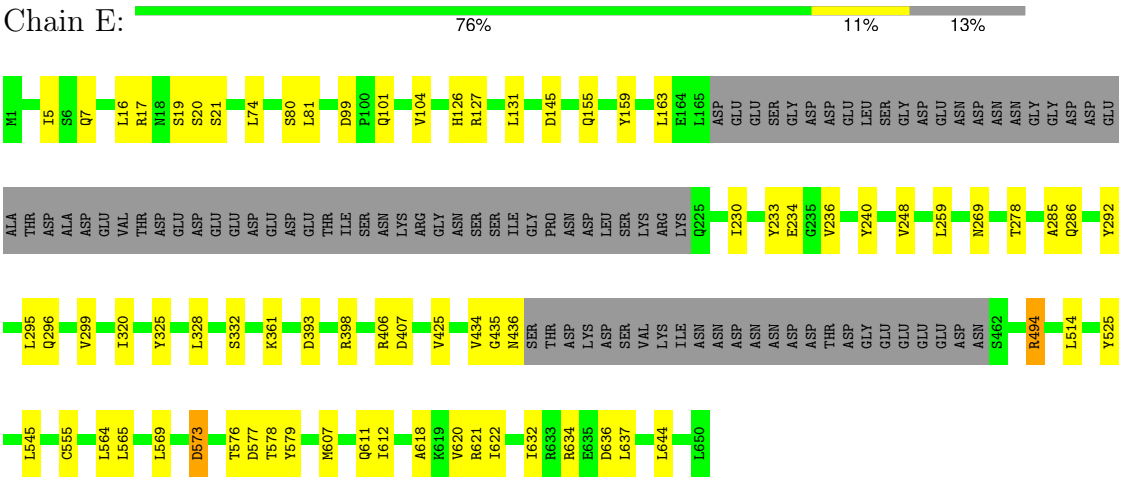
• Molecule 4: DNA replication complex GINS protein SLD5

Chain D:



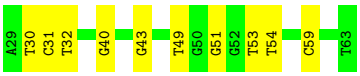
• Molecule 5: Cell division control protein 45

Chain E:



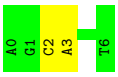
• Molecule 6: Leading strand DNA template

Chain F:



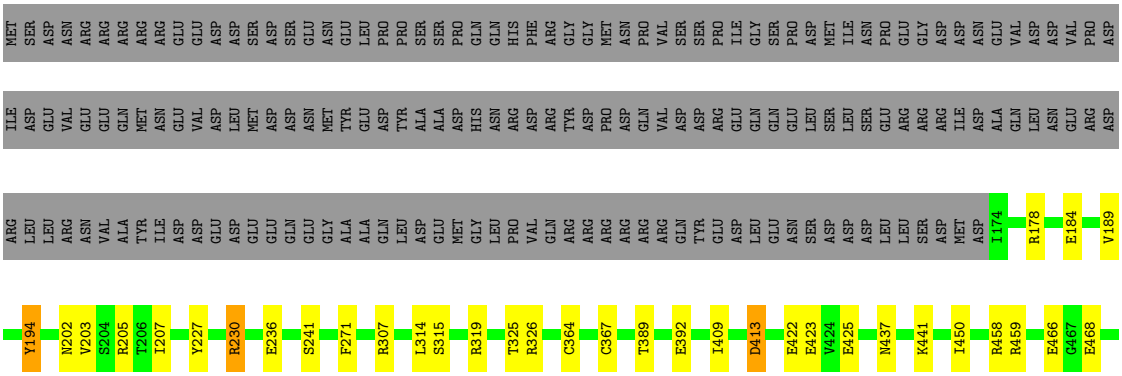
• Molecule 7: Lagging strand DNA template

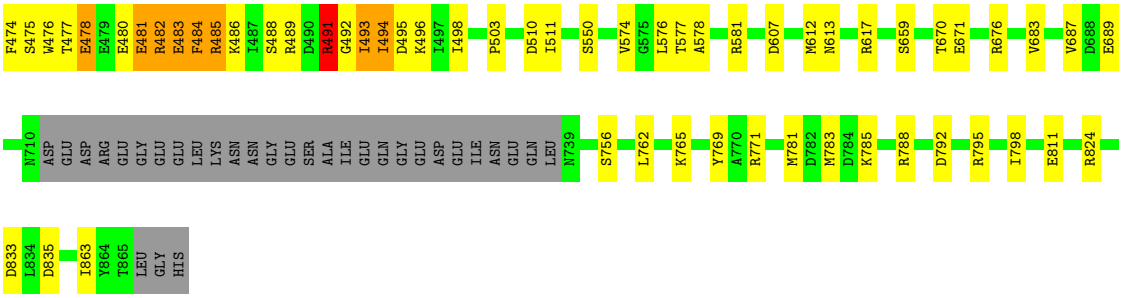
Chain G:



• Molecule 8: DNA replication licensing factor MCM2

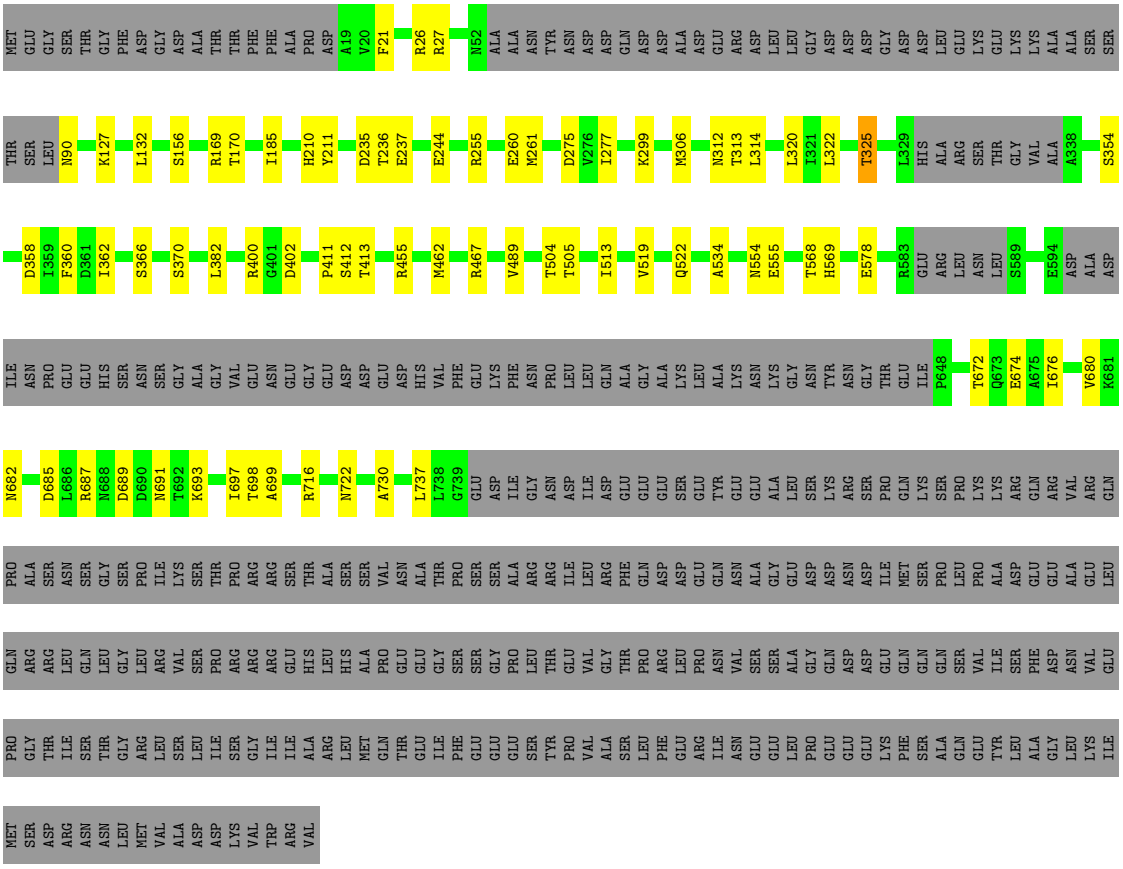
Chain 2:





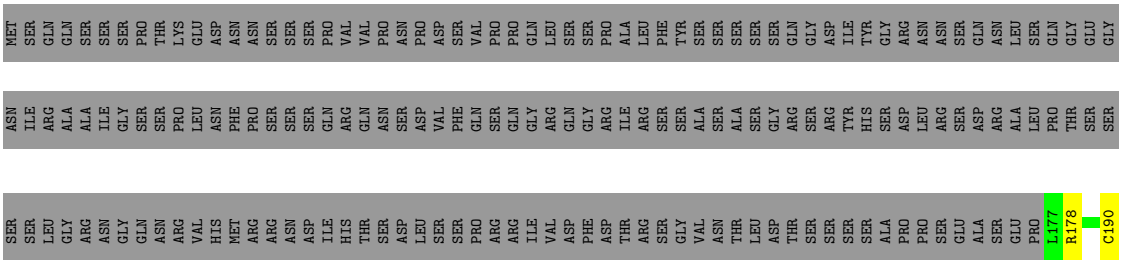
• Molecule 9: DNA replication licensing factor MCM3

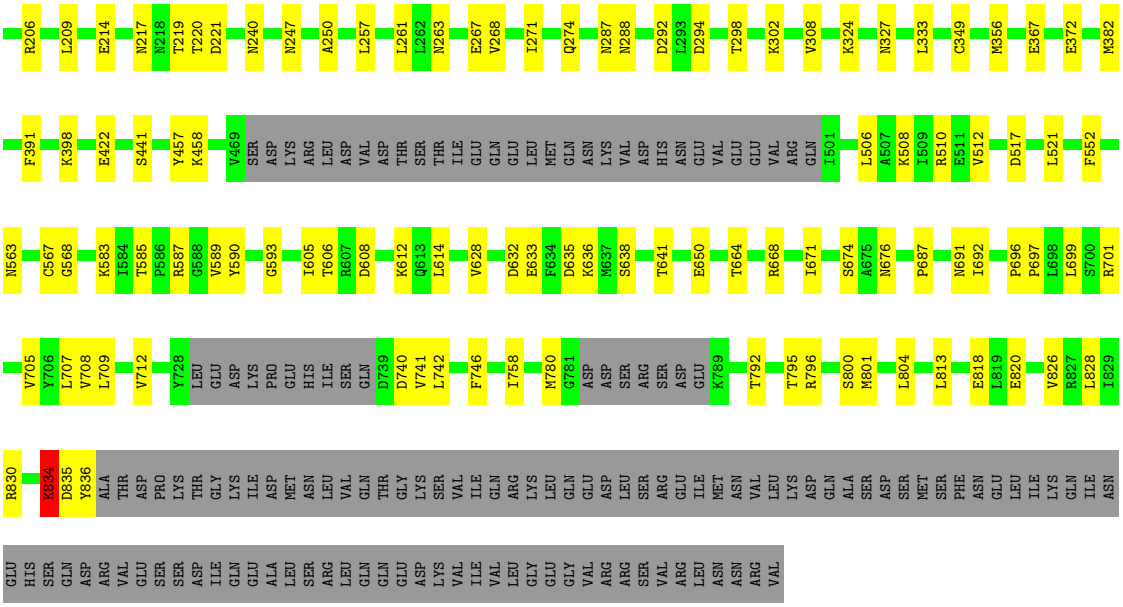
Chain 3:



• Molecule 10: DNA replication licensing factor MCM4

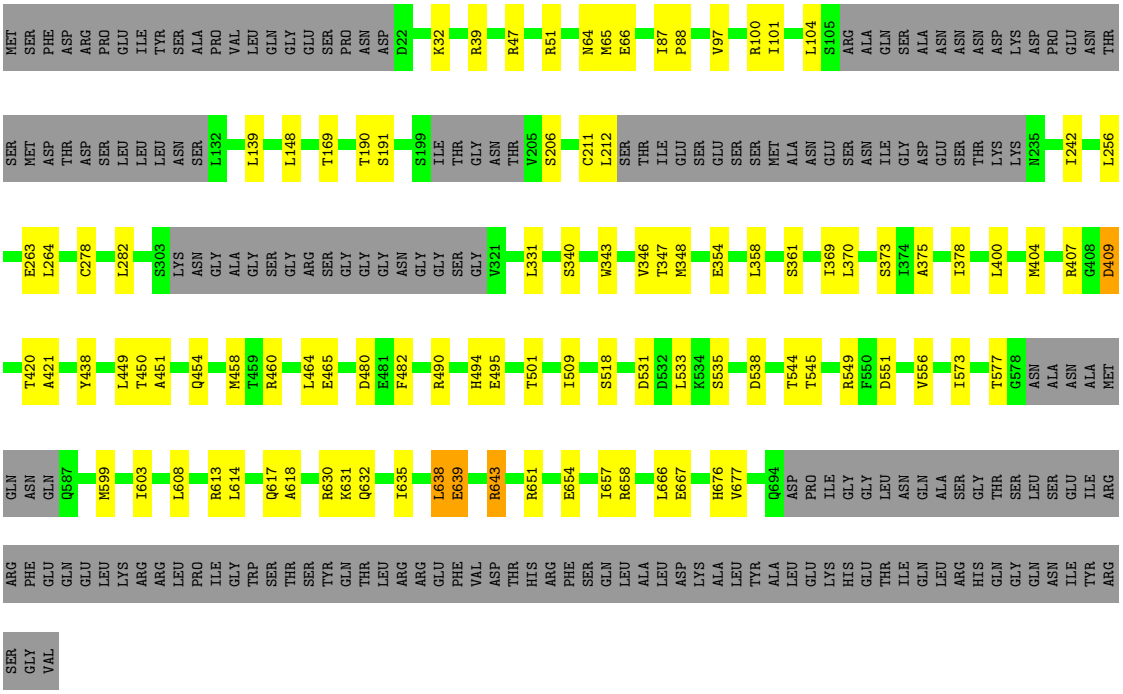
Chain 4:





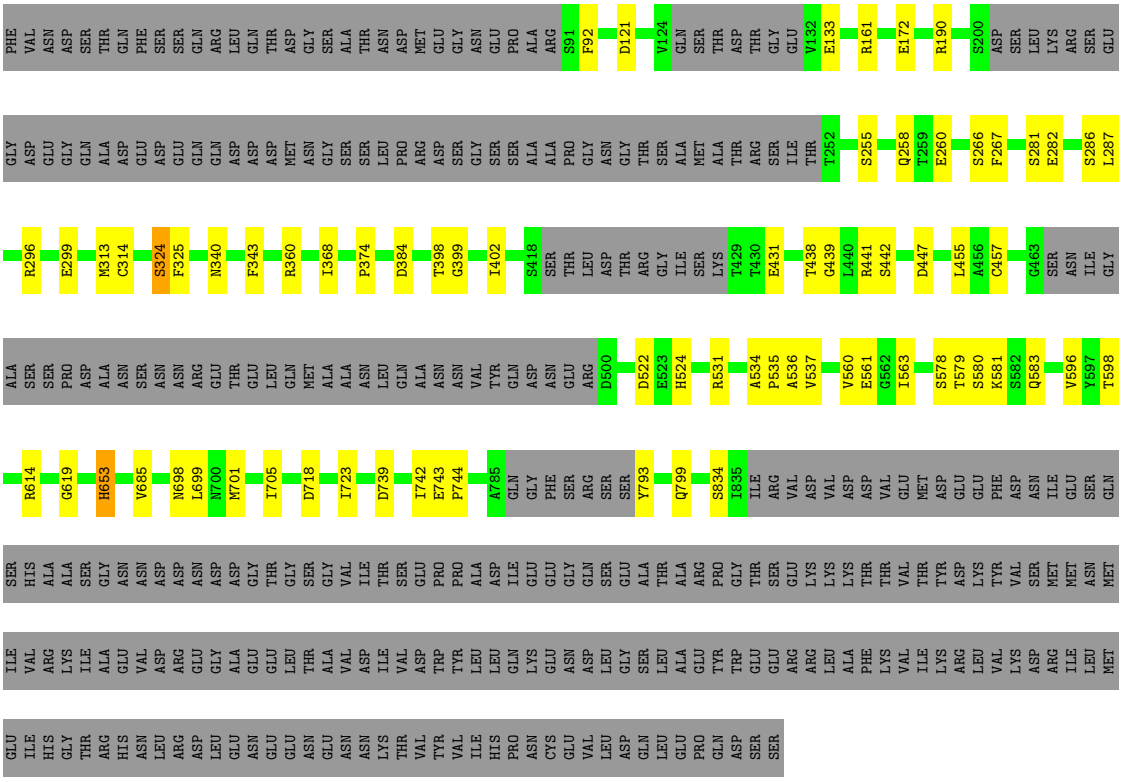
• Molecule 11: Minichromosome maintenance protein 5

Chain 5:



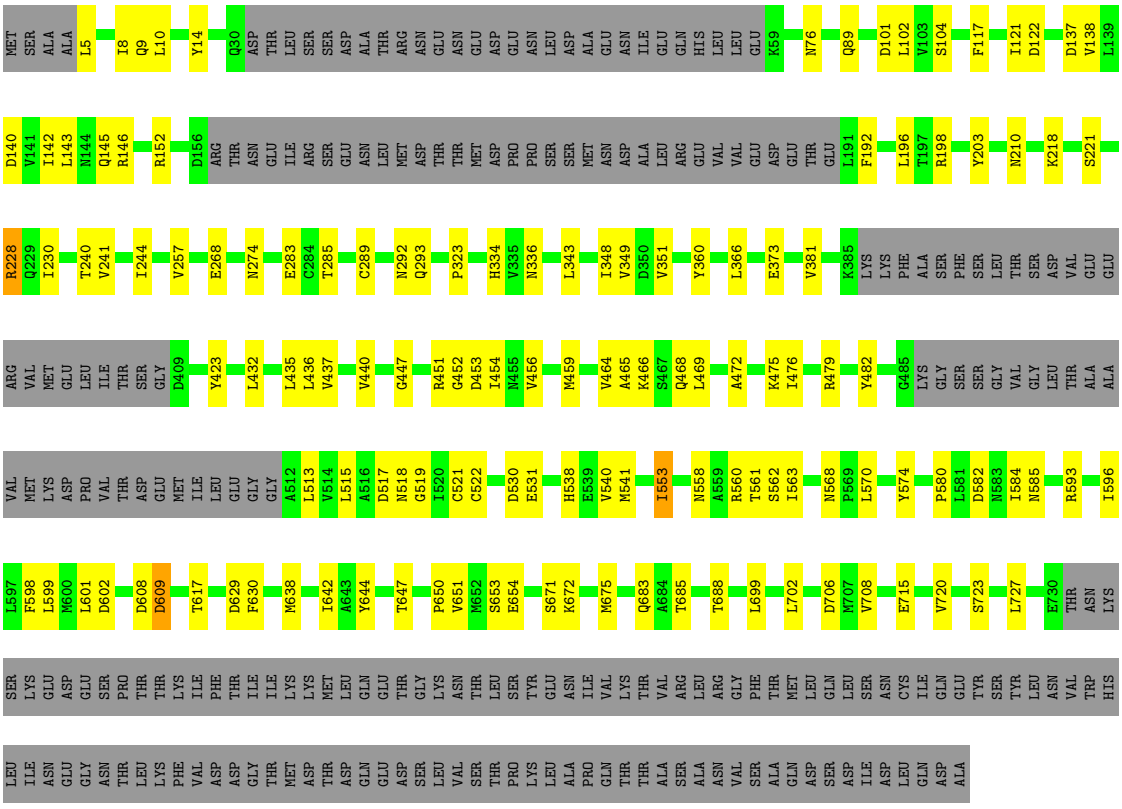
• Molecule 12: DNA replication licensing factor MCM6

Chain 6:



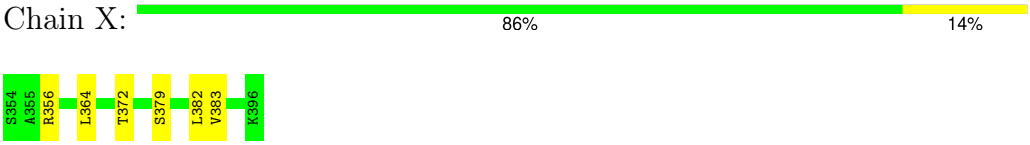
• Molecule 13: DNA replication licensing factor MCM7

Chain 7:



• Molecule 14: Topoisomerase 1-associated factor 1

Chain X:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	81996	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	66	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	29000	Depositor
Image detector	GATAN K3 (6k 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, MG, ATP, ADP

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	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.27	0/1620	0.49	0/2179
2	B	0.25	0/1609	0.50	0/2177
3	C	0.27	0/1433	0.45	0/1937
4	D	0.27	0/1863	0.48	0/2517
5	E	0.30	2/4656 (0.0%)	0.51	0/6306
6	F	0.51	0/822	0.93	0/1272
7	G	0.52	0/164	0.84	0/251
8	2	0.65	15/5356 (0.3%)	0.65	8/7233 (0.1%)
9	3	0.25	0/4909	0.51	0/6657
10	4	0.27	0/4936	0.54	1/6671 (0.0%)
11	5	0.35	0/4743	0.57	0/6410
12	6	0.26	0/5086	0.51	0/6861
13	7	0.26	0/4943	0.50	0/6682
14	X	0.24	0/329	0.54	0/440
All	All	0.36	17/42469 (0.0%)	0.55	9/57593 (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
2	B	0	2
5	E	0	3
8	2	0	7
9	3	0	3
10	4	0	3
11	5	0	7
12	6	0	2
13	7	0	1
All	All	0	28

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	2	475	SER	CA-CB	-15.56	1.29	1.52
8	2	488	SER	CA-CB	-12.56	1.34	1.52
8	2	474	PHE	C-O	-11.03	1.02	1.23
8	2	475	SER	C-O	-10.08	1.04	1.23
8	2	494	ILE	C-O	-9.90	1.04	1.23

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	4	834	LYS	C-N-CA	-8.42	100.65	121.70
8	2	495	ASP	CB-CA-C	-8.23	93.93	110.40
8	2	468	GLU	N-CA-CB	-6.79	98.38	110.60
8	2	491	ARG	CB-CA-C	-6.25	97.90	110.40
8	2	476	TRP	CA-CB-CG	6.00	125.11	113.70

There are no chirality outliers.

5 of 28 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	124	ARG	Sidechain
2	B	49	ARG	Sidechain
5	E	17	ARG	Sidechain
5	E	494	ARG	Sidechain
5	E	621	ARG	Sidechain

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	1600	1602	1602	16	0
2	B	1577	1616	1625	26	0
3	C	1400	1413	1413	10	0
4	D	1829	1843	1844	26	0
5	E	4569	4555	4562	44	0
6	F	733	314	398	12	0
7	G	146	32	79	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	2	5267	5305	5309	56	0
9	3	4825	4893	4897	63	0
10	4	4864	4921	4937	101	0
11	5	4677	4730	4751	70	0
12	6	5005	5031	5032	51	0
13	7	4865	4919	4919	130	0
14	X	327	338	340	16	0
15	2	27	12	12	0	0
16	2	1	0	0	0	0
16	3	1	0	0	0	0
16	4	1	0	0	0	0
16	5	1	0	0	0	0
16	6	1	0	0	0	0
16	7	1	0	0	0	0
17	2	1	0	0	0	0
17	4	1	0	0	0	0
17	5	1	0	0	0	0
17	6	1	0	0	0	0
17	7	1	0	0	0	0
18	4	31	12	12	0	0
18	5	62	24	24	5	0
18	6	31	12	12	2	0
18	7	31	12	12	1	0
All	All	41877	41584	41780	553	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 7.

The worst 5 of 553 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)
11:5:278:CYS:SG	11:5:282:LEU:HB2	1.51	1.48
11:5:278:CYS:SG	11:5:282:LEU:CB	2.04	1.46
10:4:458:LYS:HE2	12:6:431:GLU:O	1.16	1.33
13:7:459:MET:SD	13:7:584:ILE:HD12	1.67	1.32
13:7:538:HIS:CD2	13:7:593:ARG:NH1	2.01	1.28

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	192/208 (92%)	187 (97%)	5 (3%)	0	100	100
2	B	185/213 (87%)	179 (97%)	6 (3%)	0	100	100
3	C	168/217 (77%)	166 (99%)	2 (1%)	0	100	100
4	D	216/294 (74%)	206 (95%)	10 (5%)	0	100	100
5	E	560/650 (86%)	546 (98%)	14 (2%)	0	100	100
8	2	660/868 (76%)	641 (97%)	19 (3%)	0	100	100
9	3	608/971 (63%)	594 (98%)	14 (2%)	0	100	100
10	4	604/933 (65%)	591 (98%)	12 (2%)	1 (0%)	44	75
11	5	583/775 (75%)	555 (95%)	28 (5%)	0	100	100
12	6	622/1017 (61%)	599 (96%)	23 (4%)	0	100	100
13	7	605/845 (72%)	590 (98%)	15 (2%)	0	100	100
14	X	41/43 (95%)	40 (98%)	1 (2%)	0	100	100
All	All	5044/7034 (72%)	4894 (97%)	149 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	4	834	LYS

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	180/193 (93%)	177 (98%)	3 (2%)	56	78
2	B	178/198 (90%)	176 (99%)	2 (1%)	70	86
3	C	156/192 (81%)	155 (99%)	1 (1%)	84	92
4	D	214/279 (77%)	212 (99%)	2 (1%)	75	89
5	E	505/586 (86%)	500 (99%)	5 (1%)	73	87
8	2	582/770 (76%)	577 (99%)	5 (1%)	75	89
9	3	533/835 (64%)	531 (100%)	2 (0%)	89	94
10	4	551/848 (65%)	547 (99%)	4 (1%)	81	92
11	5	535/688 (78%)	528 (99%)	7 (1%)	65	83
12	6	551/886 (62%)	544 (99%)	7 (1%)	65	83
13	7	542/753 (72%)	533 (98%)	9 (2%)	56	78
14	X	37/37 (100%)	37 (100%)	0	100	100
All	All	4564/6265 (73%)	4517 (99%)	47 (1%)	71	87

5 of 47 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	5	638	LEU
12	6	447	ASP
11	5	639	GLU
12	6	324	SER
12	6	739	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
11	5	64	ASN
11	5	454	GLN
13	7	585	ASN
12	6	524	HIS
4	D	210	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 17 ligands modelled in this entry, 11 are monoatomic - leaving 6 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
15	ADP	2	1001	16	24,29,29	0.88	1 (4%)	29,45,45	1.31	2 (6%)
18	ATP	5	801	16	28,33,33	0.68	0	34,52,52	1.21	2 (5%)
18	ATP	4	1001	16	28,33,33	0.64	0	34,52,52	0.95	2 (5%)
18	ATP	6	1101	16	28,33,33	0.65	0	34,52,52	1.12	2 (5%)
18	ATP	7	1001	16	28,33,33	0.63	0	34,52,52	0.99	2 (5%)
18	ATP	5	802	16	28,33,33	0.69	0	34,52,52	1.10	2 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	ADP	2	1001	16	-	1/12/32/32	0/3/3/3
18	ATP	5	801	16	-	5/18/38/38	0/3/3/3
18	ATP	4	1001	16	-	6/18/38/38	0/3/3/3
18	ATP	6	1101	16	-	0/18/38/38	0/3/3/3
18	ATP	7	1001	16	-	6/18/38/38	0/3/3/3
18	ATP	5	802	16	-	6/18/38/38	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	2	1001	ADP	O4'-C1'	2.05	1.43	1.40

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	5	801	ATP	C4'-O4'-C1'	-4.63	105.69	109.92
15	2	1001	ADP	N3-C2-N1	-4.25	122.90	128.67
18	5	802	ATP	C4'-O4'-C1'	-3.88	106.38	109.92
18	6	1101	ATP	C4'-O4'-C1'	-3.70	106.54	109.92
15	2	1001	ADP	C4-C5-N7	-2.50	106.69	109.34

There are no chirality outliers.

5 of 24 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	4	1001	ATP	PB-O3B-PG-O2G
18	4	1001	ATP	C5'-O5'-PA-O2A
18	4	1001	ATP	C5'-O5'-PA-O3A
18	5	801	ATP	C5'-O5'-PA-O1A
18	5	801	ATP	C5'-O5'-PA-O3A

There are no ring outliers.

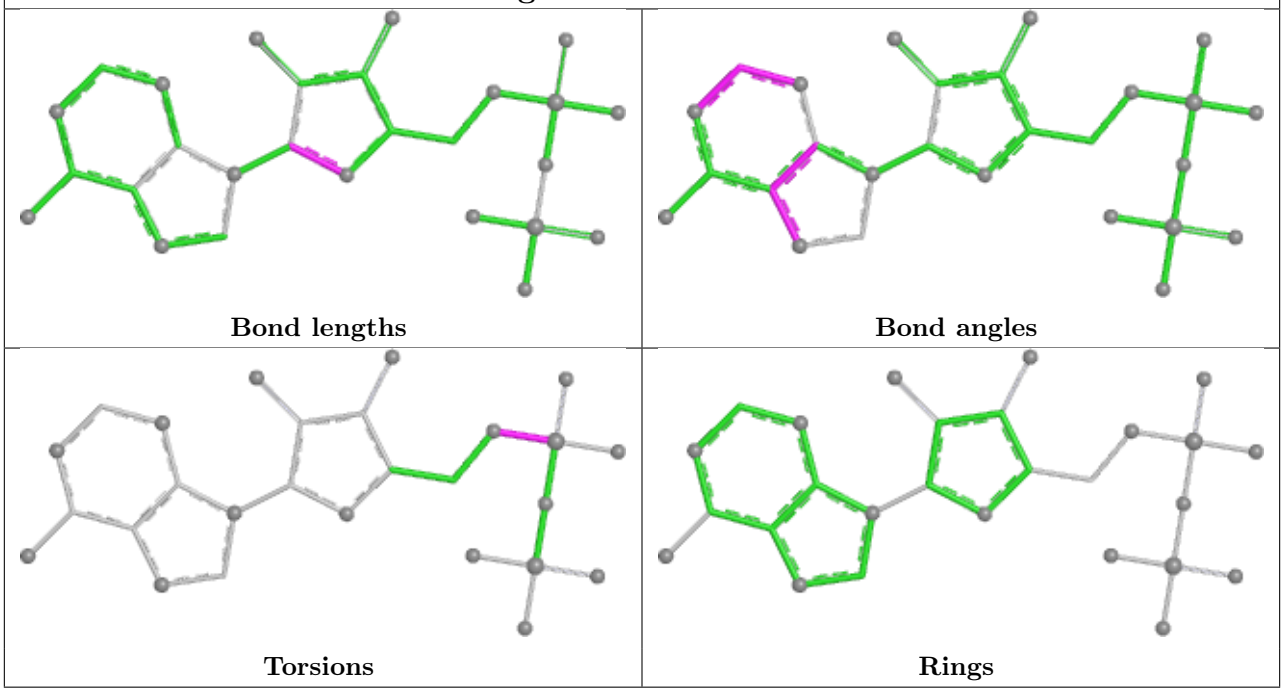
4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	5	801	ATP	2	0
18	6	1101	ATP	2	0
18	7	1001	ATP	1	0
18	5	802	ATP	3	0

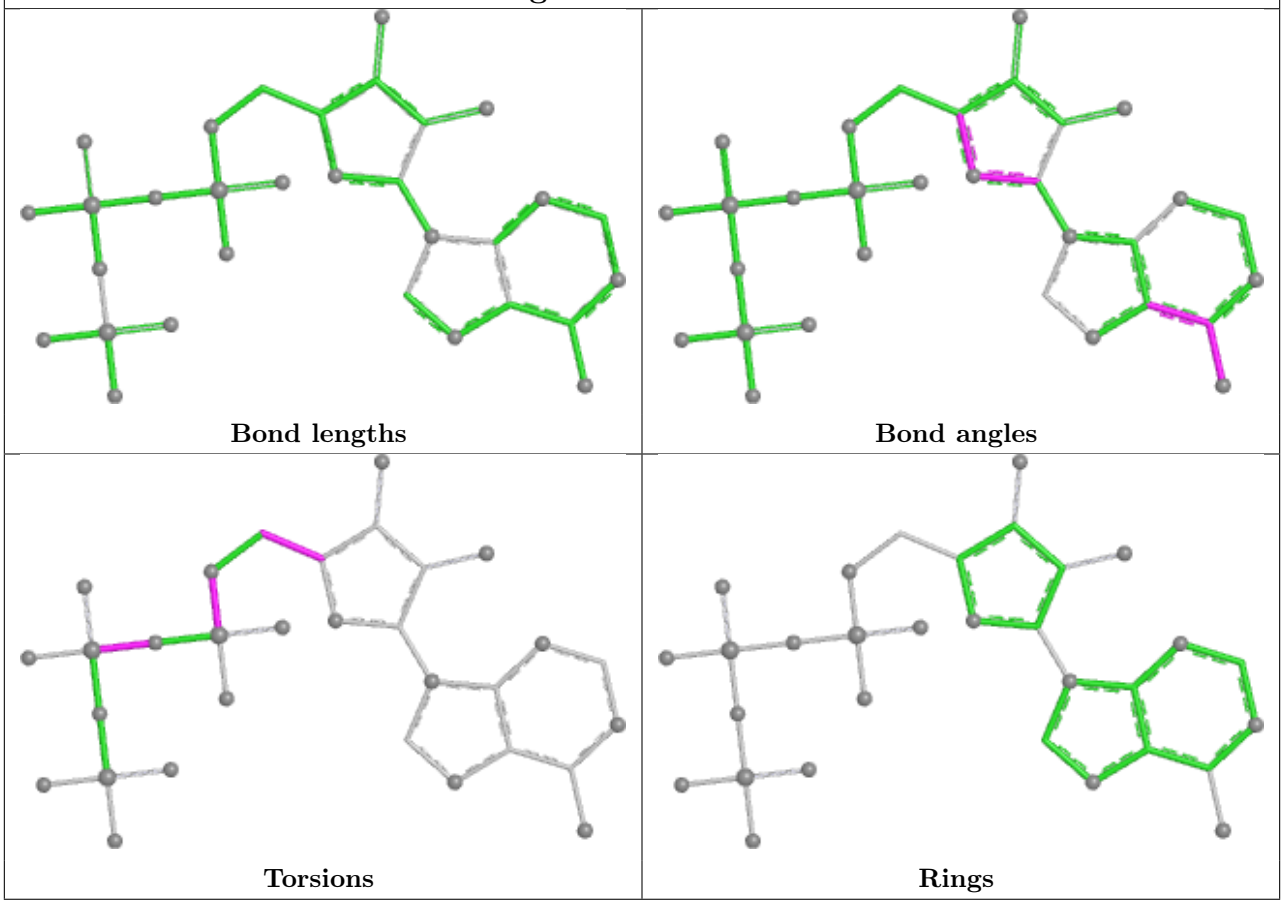
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient

equivalents in the CSD to analyse the geometry.

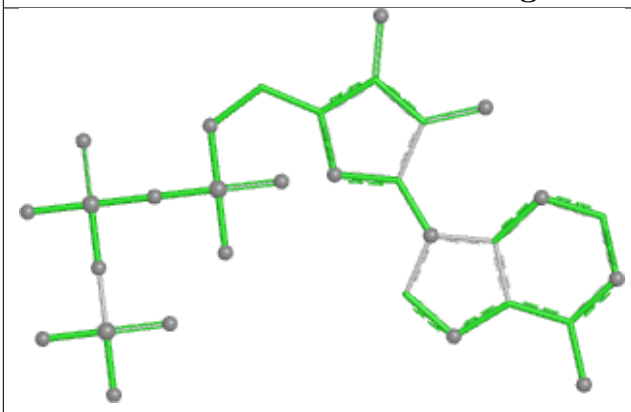
Ligand ADP 2 1001



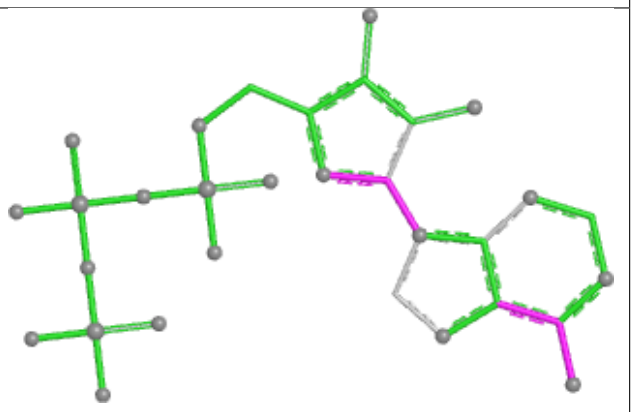
Ligand ATP 5 801



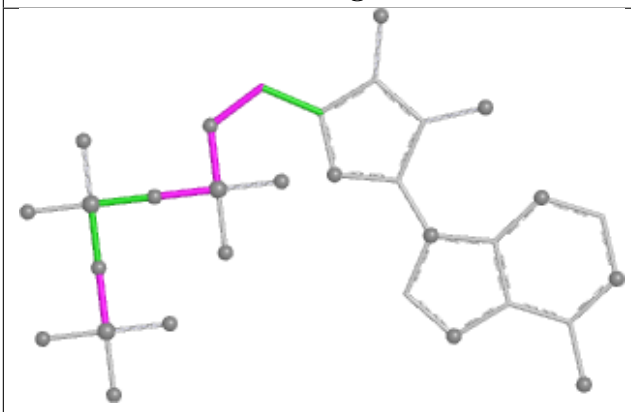
Ligand ATP 4 1001



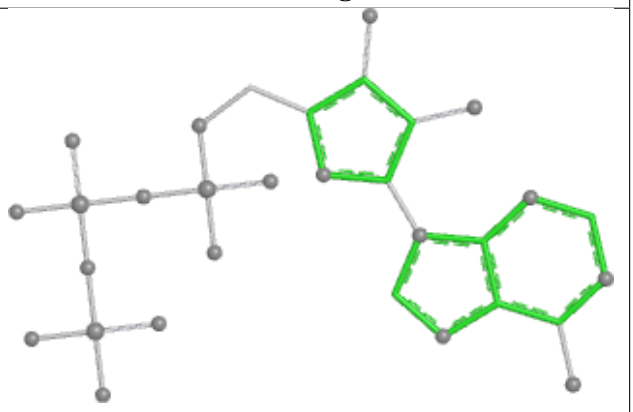
Bond lengths



Bond angles

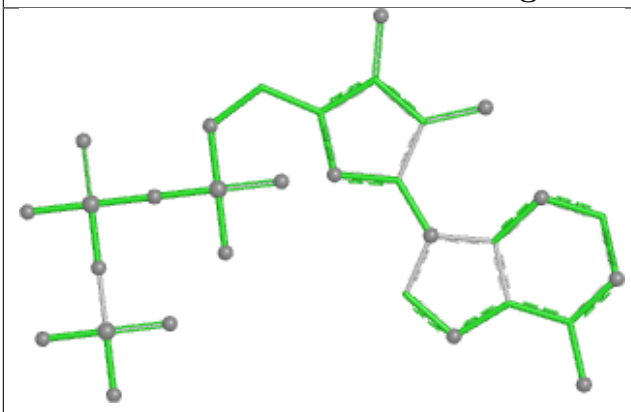


Torsions

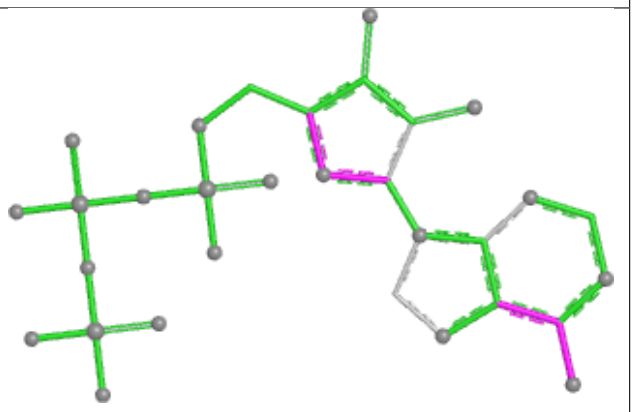


Rings

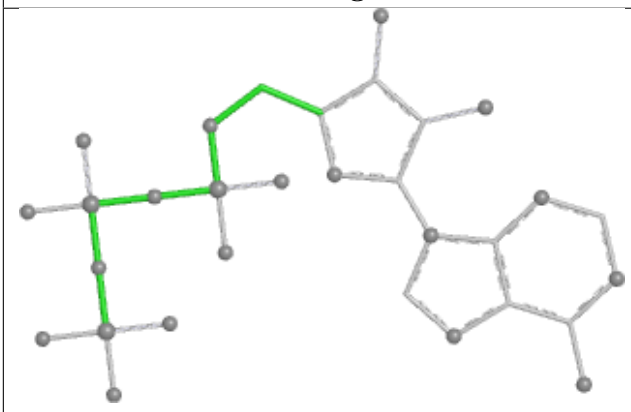
Ligand ATP 6 1101



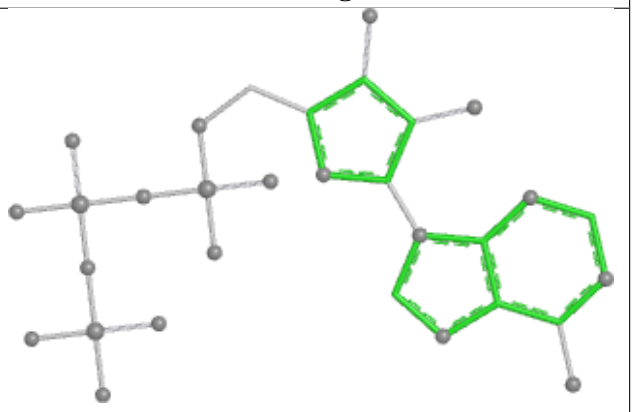
Bond lengths



Bond angles

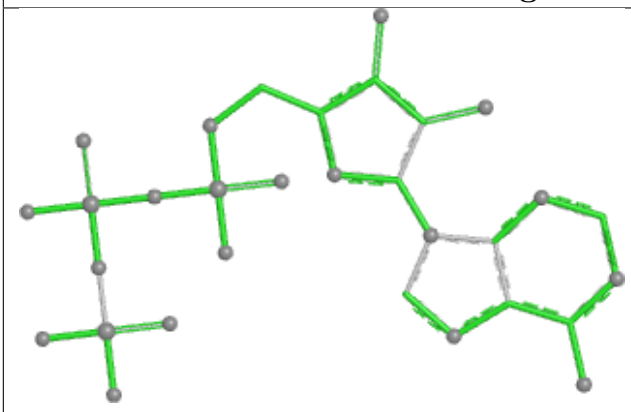


Torsions

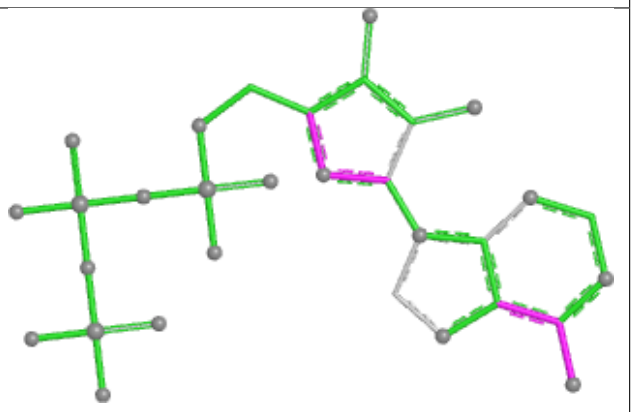


Rings

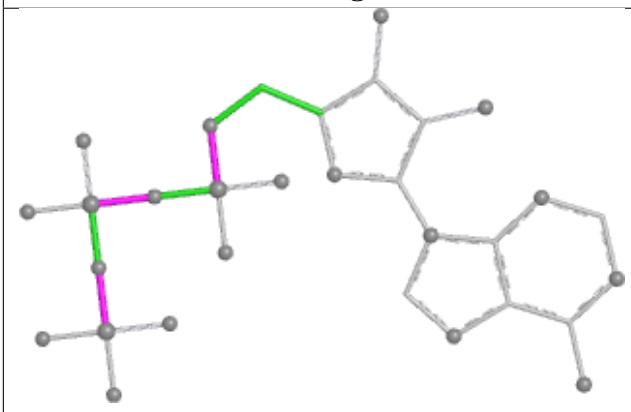
Ligand ATP 7 1001



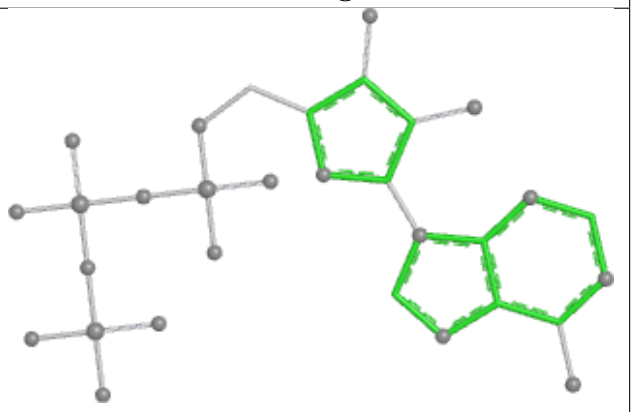
Bond lengths



Bond angles

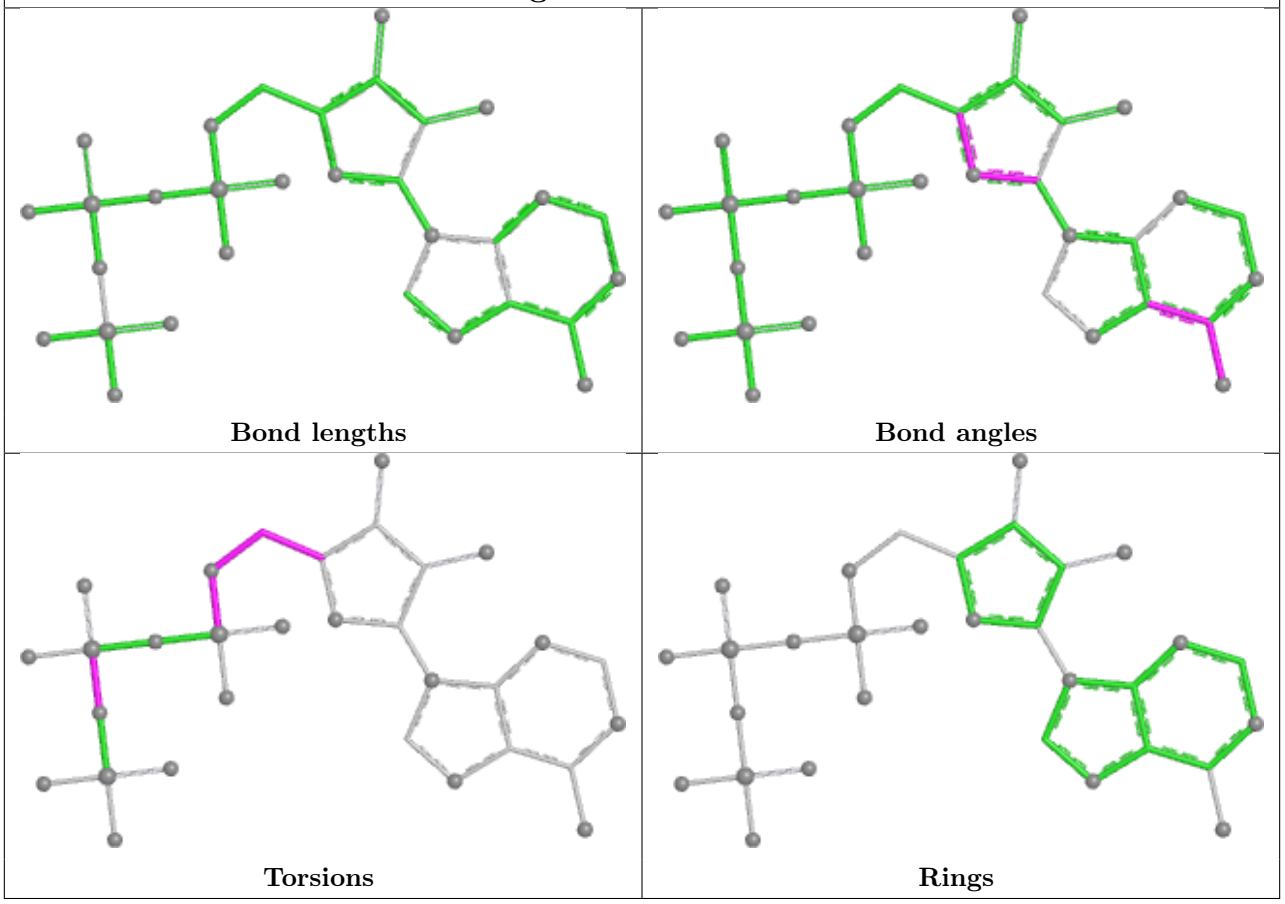


Torsions



Rings

Ligand ATP 5 802



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.

6 Map visualisation

This section contains visualisations of the EMDB entry EMD-47472. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

6.5 Orthogonal surface views

This section was not generated.

6.6 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

7 Map analysis

This section contains the results of statistical analysis of the map.

7.1 Map-value distribution

This section was not generated.

7.2 Volume estimate versus contour level

This section was not generated.

7.3 Rotationally averaged power spectrum

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit

This section was not generated.