wwPDB EM Validation Summary Report (i)

Mar 19, 2025 – 04:21 PM EDT

PDB ID	:	9E2W
EMDB ID	:	EMD-47470
Title	:	Cryo-EM structure of yeast CMG helicase stalled at G4-containing DNA template, state 1
Authors	:	Allwein, B.; Batra, S.; Remus, D.; Hite, R.
Deposited on	:	2024-10-23
Resolution	:	3.30 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:

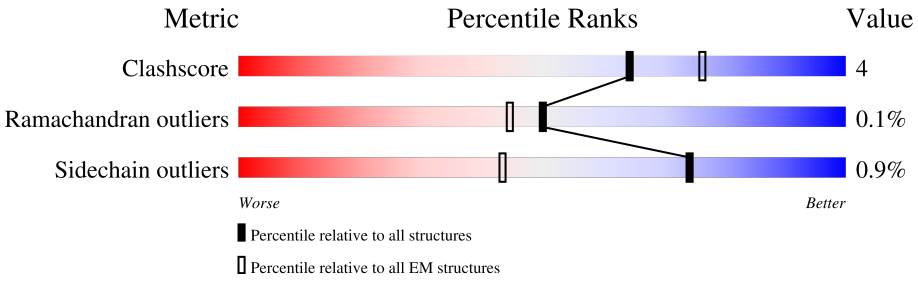
EMDB validation analysis	:	0.0.1.dev117
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 3.30 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	2	868	65% 11% 24%
2	3	971	56% 7% 36%
3	4	933	56% 9% · 34%
4	5	775	67% 9% 23%
5	6	1017	53% 9% · 38%
6	7	845	62% 11% 27%
7	A	208	81% 13% 6%
8	B	213	77% 11% 11%
9	C	217	73% 6% 20%

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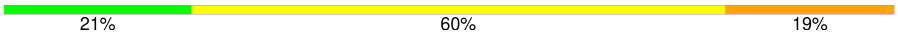
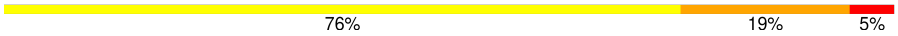
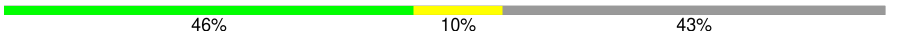
Mol	Chain	Length	Quality of chain
10	D	294	
11	E	650	
12	F	48	
13	G	21	
14	X	1238	
15	Y	92	

2 Entry composition (i)

There are 19 unique types of molecules in this entry. The entry contains 96909 atoms, of which 48318 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	H	N	O	S		
1	2	664	10576	3305	5309	944	999	19	0	0

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

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
2	3	618	9718	3044	4893	860	908	13	0	0

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

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
3	4	614	9812	3077	4933	840	934	28	0	0

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

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
4	5	594	9417	2945	4746	798	905	23	0	0

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

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
5	6	634	10040	3159	5035	873	948	25	0	0

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

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
6	7	615	9786	3075	4921	847	917	26	0	0

- Molecule 7 is a protein called DNA replication complex GINS protein PSF1.

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

- Molecule 8 is a protein called DNA replication complex GINS protein PSF2.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	B	189	Total	C	H	N	O	S	0	0
			3195	1014	1618	276	282	5		

- Molecule 9 is a protein called DNA replication complex GINS protein PSF3.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	C	173	Total	C	H	N	O	S	0	0
			2805	910	1409	224	256	6		

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
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 10 is a protein called DNA replication complex GINS protein SLD5.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	D	222	Total	C	H	N	O	S	0	0
			3671	1170	1843	299	347	12		

- Molecule 11 is a protein called Cell division control protein 45.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	E	566	Total	C	H	N	O	S	0	0
			9129	2922	4560	770	863	14		

- Molecule 12 is a DNA chain called Leading strand DNA template.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	F	48	Total	C	H	N	O	P	0	0
			1547	475	544	182	298	48		

- Molecule 13 is a DNA chain called Lagging strand DNA template.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	G	21	Total	C	H	N	O	P	0	0
			664	204	234	84	121	21		

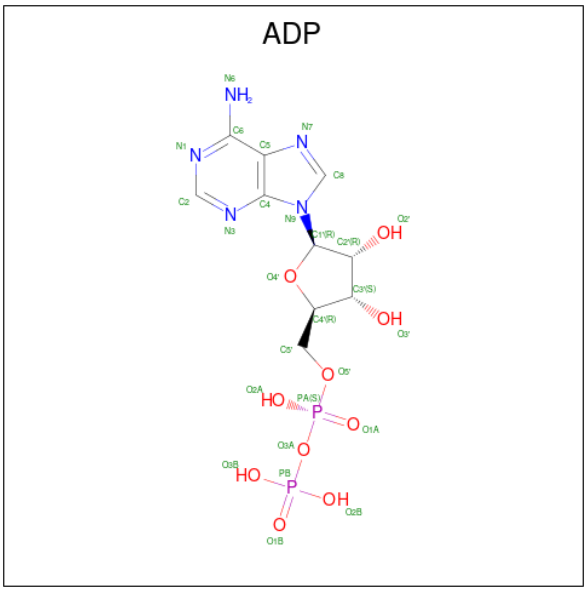
- Molecule 14 is a protein called Topoisomerase 1-associated factor 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
14	X	705	Total	C	H	N	O	S	0	0
			11543	3691	5828	962	1043	19		

- Molecule 15 is a protein called Chromosome segregation in meiosis protein 3.

Mol	Chain	Residues	Atoms						AltConf	Trace
15	Y	92	Total	C	H	N	O	S	0	0
			1539	495	771	138	131	4		

- Molecule 16 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms						AltConf
16	2	1	Total	C	H	N	O	P	0
			39	10	12	5	10	2	

- Molecule 17 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
17	2	1	Total	Mg	0
			1	1	
17	3	1	Total	Mg	0
			1	1	
17	4	1	Total	Mg	0
			1	1	
17	5	1	Total	Mg	0
			1	1	
17	6	1	Total	Mg	0
			1	1	
17	7	1	Total	Mg	0
			1	1	

- Molecule 18 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
18	2	1	Total	Zn	0
			1	1	
18	4	1	Total	Zn	0
			1	1	

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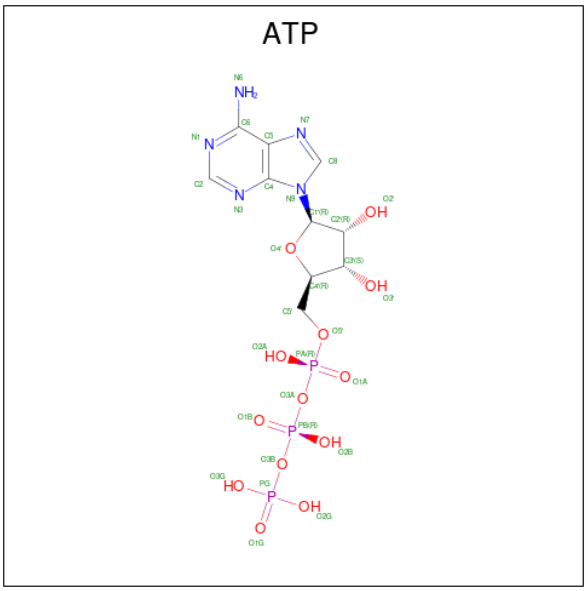
Mol	Chain	Residues	Atoms	AltConf
18	5	1	Total Zn 1 1	0
18	6	1	Total Zn 1 1	0
18	7	1	Total Zn 1 1	0

- Molecule 19 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



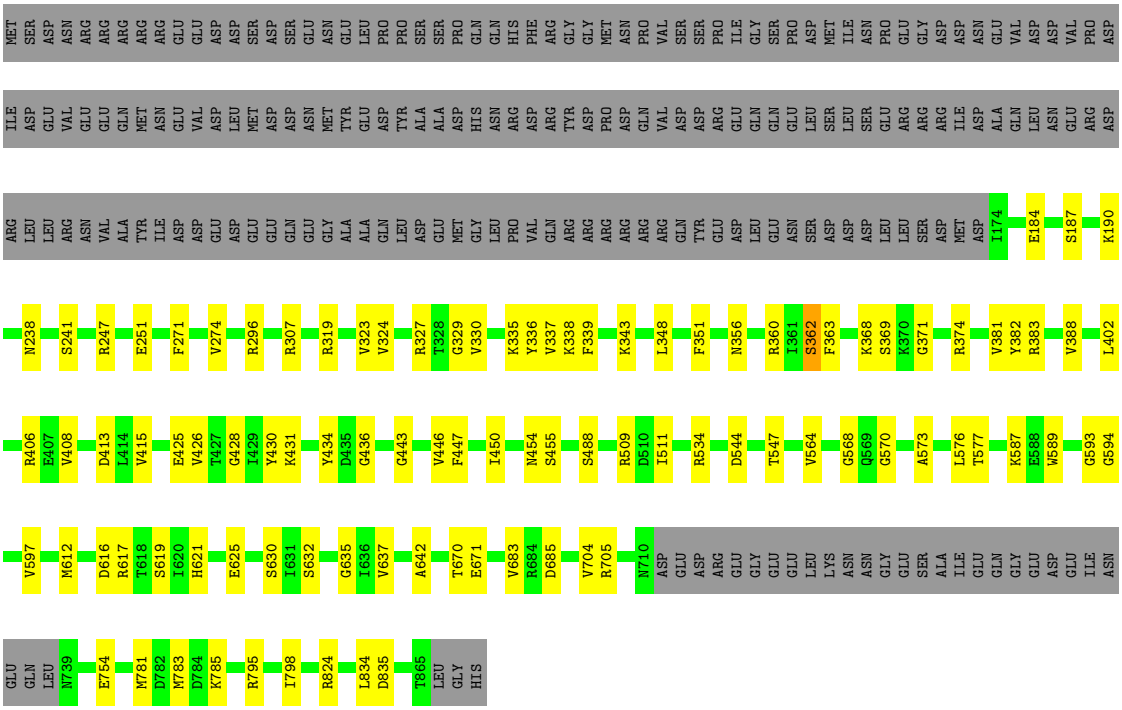
Mol	Chain	Residues	Atoms	AltConf
19	3	1	Total C H N O P 43 10 12 5 13 3	0
19	4	1	Total C H N O P 43 10 12 5 13 3	0
19	5	1	Total C H N O P 43 10 12 5 13 3	0
19	6	1	Total C H N O P 43 10 12 5 13 3	0
19	7	1	Total C H N O P 43 10 12 5 13 3	0

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.

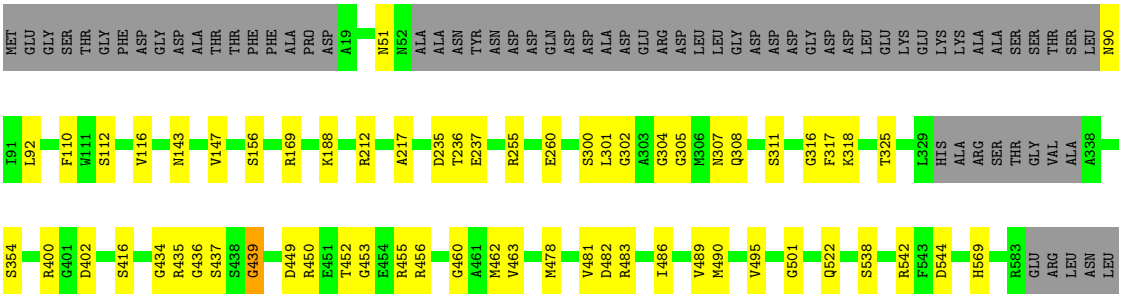
- Molecule 1: DNA replication licensing factor MCM2

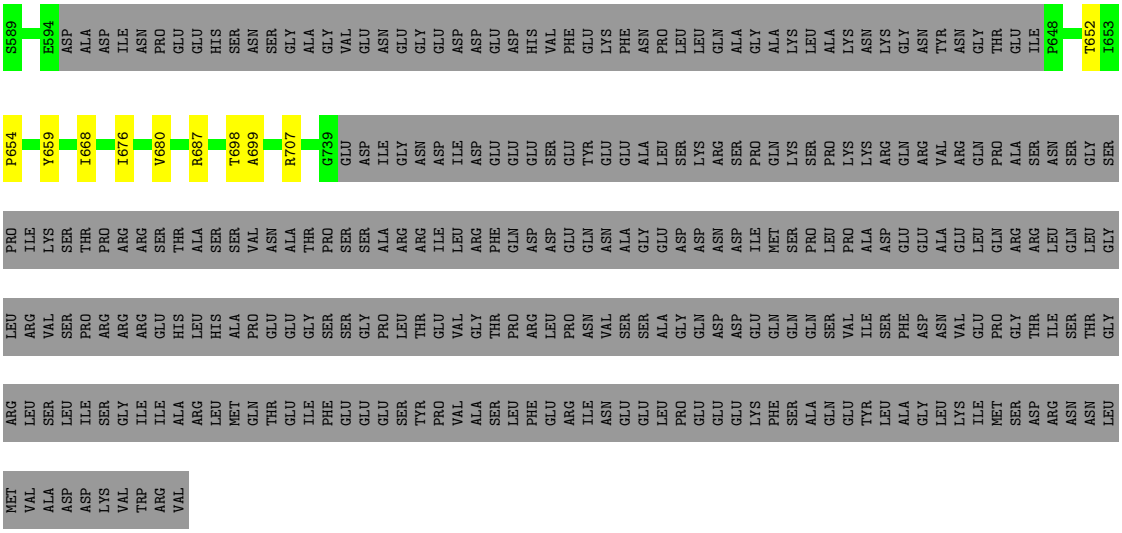
Chain 2:



- Molecule 2: DNA replication licensing factor MCM3

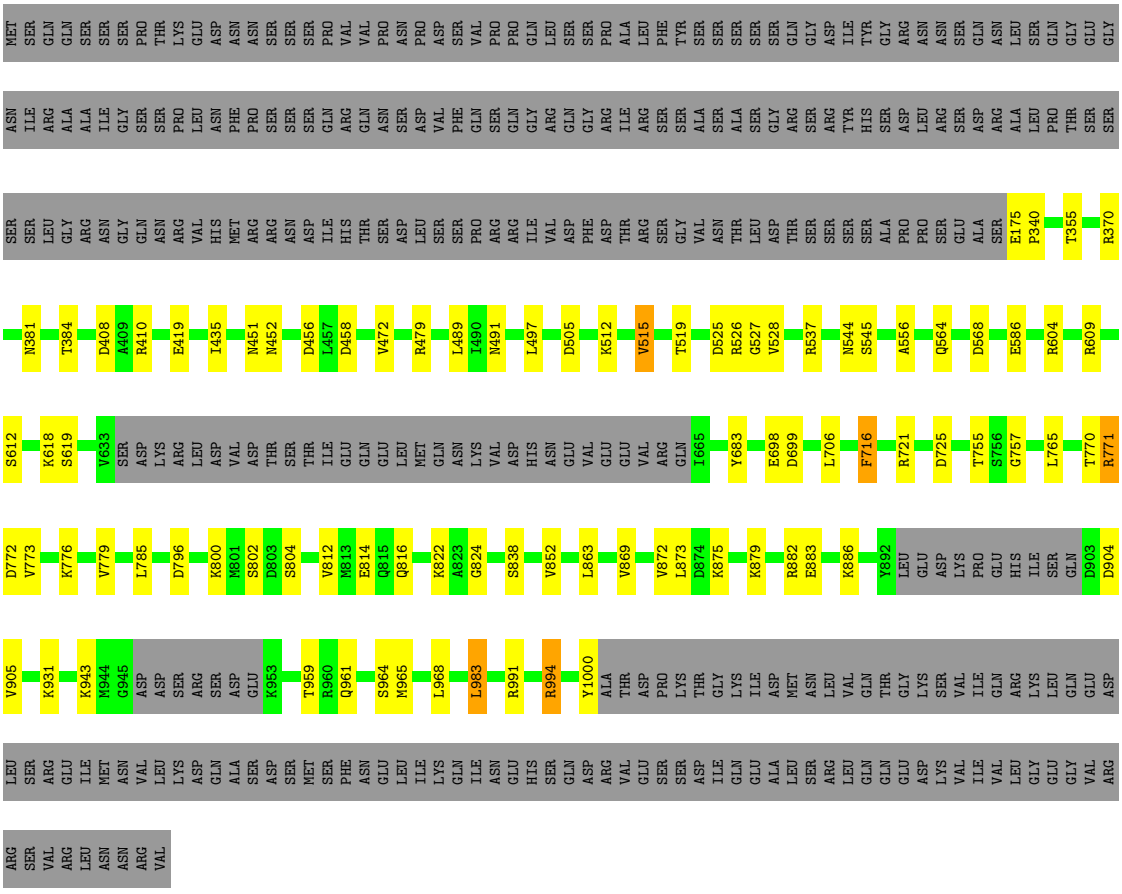
Chain 3:





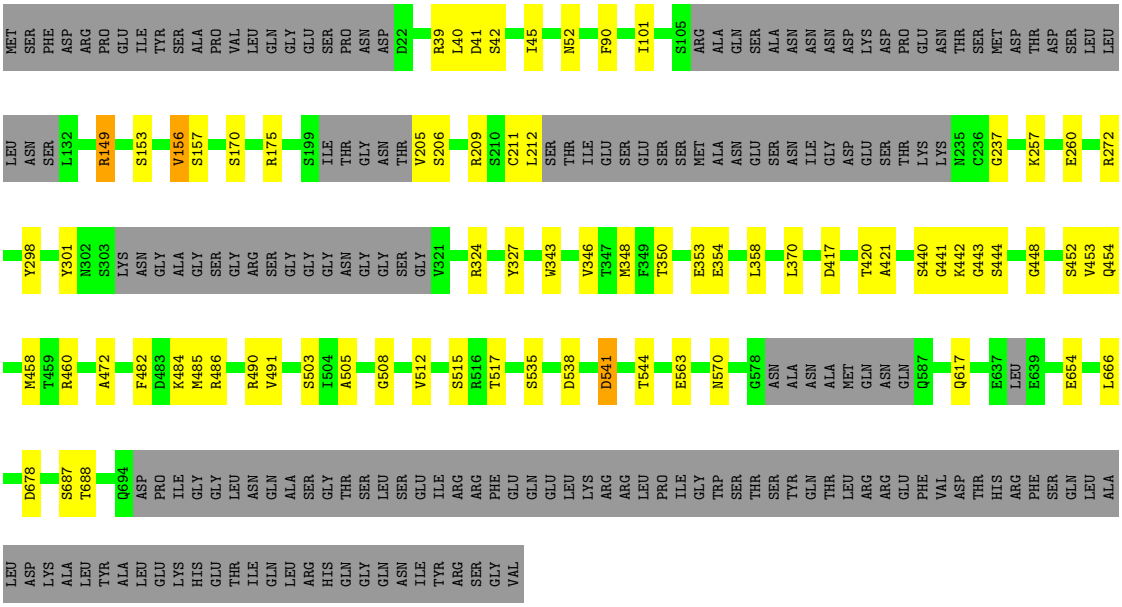
• Molecule 3: DNA replication licensing factor MCM4

Chain 4:



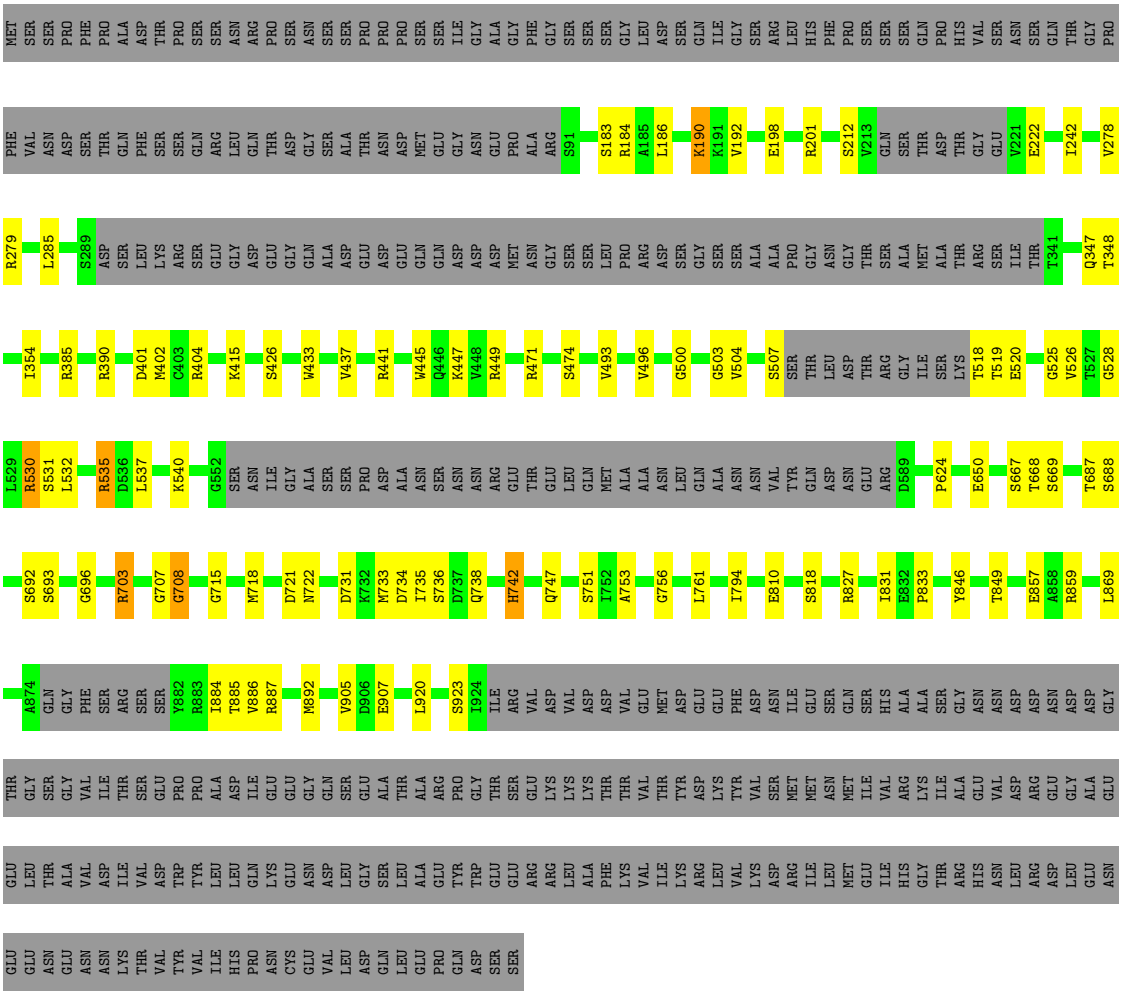
• Molecule 4: Minichromosome maintenance protein 5

Chain 5:



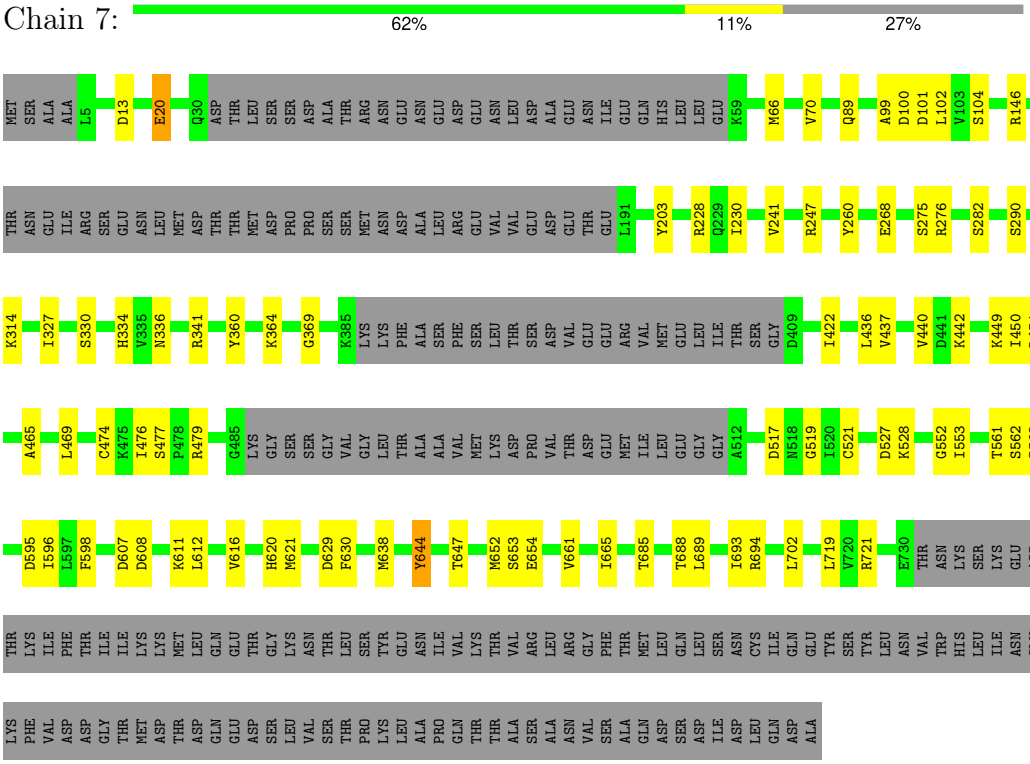
• Molecule 5: DNA replication licensing factor MCM6

Chain 6:



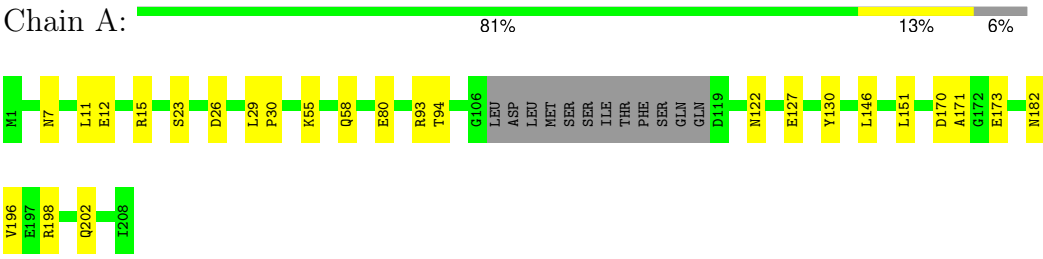
• Molecule 6: DNA replication licensing factor MCM7

Chain 7:



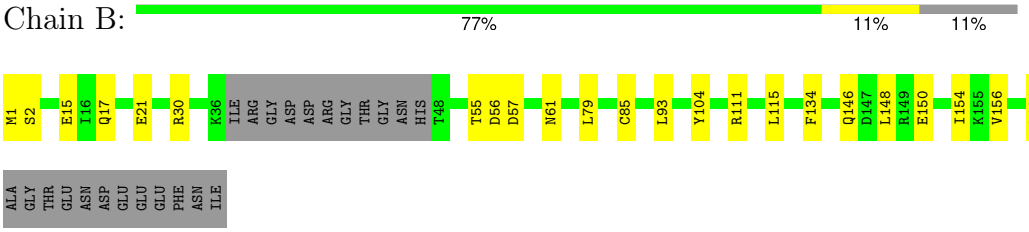
• Molecule 7: DNA replication complex GINS protein PSF1

Chain A:



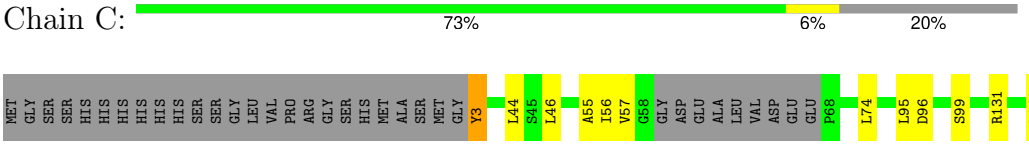
• Molecule 8: DNA replication complex GINS protein PSF2

Chain B:



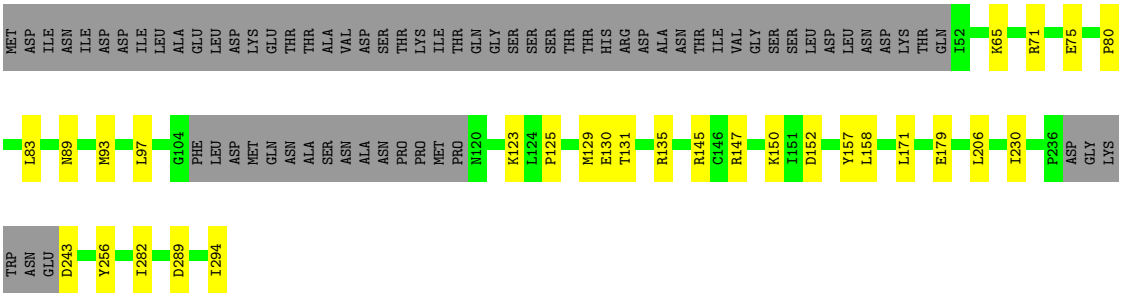
• Molecule 9: DNA replication complex GINS protein PSF3

Chain C:



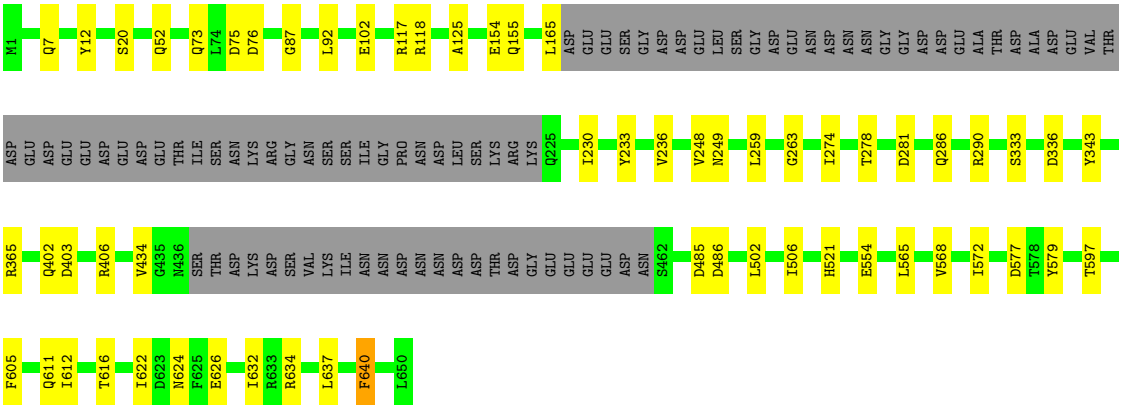
• Molecule 10: DNA replication complex GINS protein SLD5

Chain D:



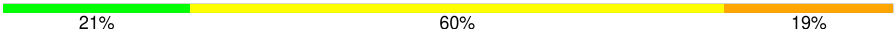
• Molecule 11: Cell division control protein 45

Chain E:



• Molecule 12: Leading strand DNA template

Chain F:

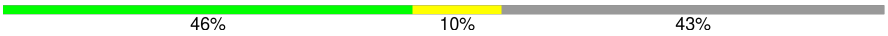


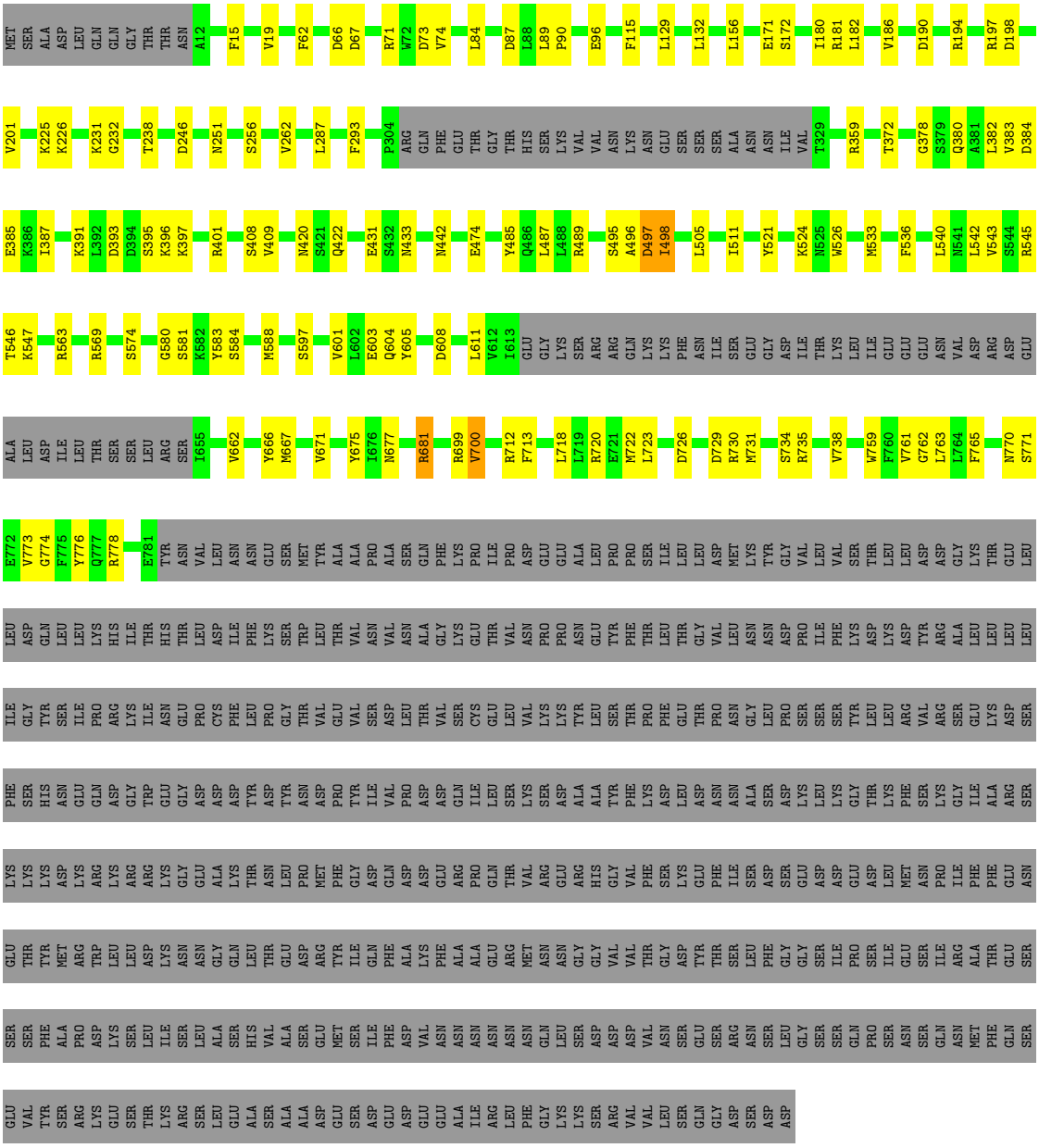
• Molecule 13: Lagging strand DNA template

Chain G:

• Molecule 14: Topoisomerase 1-associated factor 1

Chain X:





• Molecule 15: Chromosome segregation in meiosis protein 3

Chain Y:

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	66410	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: ATP, ADP, ZN, MG

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	2	1.16	67/5356 (1.3%)	1.03	12/7233 (0.2%)
2	3	0.93	34/4909 (0.7%)	0.84	7/6657 (0.1%)
3	4	0.74	23/4952 (0.5%)	0.72	3/6693 (0.0%)
4	5	1.00	43/4737 (0.9%)	0.89	11/6403 (0.2%)
5	6	1.02	44/5086 (0.9%)	0.89	8/6860 (0.1%)
6	7	0.73	17/4943 (0.3%)	0.72	3/6682 (0.0%)
7	A	0.25	0/1620	0.46	0/2179
8	B	0.24	0/1609	0.48	0/2177
9	C	0.33	0/1429	0.51	2/1932 (0.1%)
10	D	0.25	0/1861	0.45	0/2512
11	E	0.25	0/4656	0.48	0/6306
12	F	1.55	0/1125	2.37	73/1741 (4.2%)
13	G	1.52	0/483	2.44	44/742 (5.9%)
14	X	0.97	45/5828 (0.8%)	0.88	15/7868 (0.2%)
15	Y	1.71	18/784 (2.3%)	1.45	6/1049 (0.6%)
All	All	0.89	291/49378 (0.6%)	0.91	184/67034 (0.3%)

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	3
2	3	0	1
3	4	0	4
4	5	0	2
8	B	0	1
11	E	0	1
12	F	0	11
13	G	0	5

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Mol	Chain	#Chirality outliers	#Planarity outliers
15	Y	0	2
All	All	0	30

The worst 5 of 291 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	406	ARG	CZ-NH2	-8.04	1.22	1.33
1	2	383	ARG	CZ-NH2	-8.02	1.22	1.33
4	5	272	ARG	CZ-NH2	-8.02	1.22	1.33
3	4	609	ARG	CZ-NH2	-8.01	1.22	1.33
5	6	184	ARG	CZ-NH2	-7.99	1.22	1.33

The worst 5 of 184 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	F	45	DT	O4'-C1'-N1	12.83	116.98	108.00
12	F	53	DT	N3-C2-O2	-9.48	116.61	122.30
13	G	20	DA	N1-C6-N6	-9.35	112.99	118.60
12	F	60	DA	N1-C6-N6	-9.27	113.04	118.60
12	F	29	DA	N1-C6-N6	-9.18	113.09	118.60

There are no chirality outliers.

5 of 30 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	2	274	VAL	Mainchain
1	2	374	ARG	Sidechain
1	2	509	ARG	Sidechain
2	3	687	ARG	Sidechain
3	4	526	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	2	5267	5309	5311	28	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	3	4825	4893	4897	29	0
3	4	4879	4933	4949	57	0
4	5	4671	4746	4742	34	0
5	6	5005	5035	5035	47	0
6	7	4865	4921	4919	42	0
7	A	1600	1602	1602	16	0
8	B	1577	1618	1625	18	0
9	C	1396	1409	1410	14	0
10	D	1828	1843	1842	20	0
11	E	4569	4560	4562	38	0
12	F	1003	544	545	2	0
13	G	430	234	235	1	0
14	X	5715	5828	5833	69	0
15	Y	768	771	801	16	0
16	2	27	12	12	2	0
17	2	1	0	0	0	0
17	3	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	2	1	0	0	0	0
18	4	1	0	0	0	0
18	5	1	0	0	0	0
18	6	1	0	0	0	0
18	7	1	0	0	0	0
19	3	31	12	12	1	0
19	4	31	12	12	0	0
19	5	31	12	12	0	0
19	6	31	12	12	0	0
19	7	31	12	12	0	0
All	All	48591	48318	48380	375	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.

The worst 5 of 375 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:X:720:ARG:NH2	15:Y:92:ILE:HG21	1.32	1.41
14:X:720:ARG:HH22	15:Y:92:ILE:CG2	1.51	1.20

Continued on next page...

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:X:720:ARG:NH2	15:Y:92:ILE:CG2	2.06	1.19
14:X:66:ASP:OD1	14:X:74:VAL:HB	1.47	1.13
14:X:511:ILE:HG21	14:X:563:ARG:NH1	1.72	1.05

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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	660/868 (76%)	645 (98%)	15 (2%)	0	100	100
2	3	608/971 (63%)	594 (98%)	14 (2%)	0	100	100
3	4	606/933 (65%)	598 (99%)	8 (1%)	0	100	100
4	5	582/775 (75%)	562 (97%)	20 (3%)	0	100	100
5	6	622/1017 (61%)	609 (98%)	12 (2%)	1 (0%)	44	71
6	7	605/845 (72%)	594 (98%)	11 (2%)	0	100	100
7	A	192/208 (92%)	190 (99%)	2 (1%)	0	100	100
8	B	185/213 (87%)	183 (99%)	2 (1%)	0	100	100
9	C	167/217 (77%)	166 (99%)	1 (1%)	0	100	100
10	D	214/294 (73%)	210 (98%)	4 (2%)	0	100	100
11	E	560/650 (86%)	548 (98%)	12 (2%)	0	100	100
14	X	699/1238 (56%)	682 (98%)	15 (2%)	2 (0%)	37	66
15	Y	90/92 (98%)	86 (96%)	4 (4%)	0	100	100
All	All	5790/8321 (70%)	5667 (98%)	120 (2%)	3 (0%)	50	76

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	6	707	GLY
14	X	498	ILE
14	X	495	SER

5.3.2 Protein sidechains (i)

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	2	582/770 (76%)	577 (99%)	5 (1%)	75 85
2	3	533/835 (64%)	531 (100%)	2 (0%)	89 93
3	4	553/848 (65%)	546 (99%)	7 (1%)	65 79
4	5	534/688 (78%)	529 (99%)	5 (1%)	75 85
5	6	552/886 (62%)	548 (99%)	4 (1%)	81 88
6	7	542/753 (72%)	532 (98%)	10 (2%)	54 74
7	A	180/193 (93%)	180 (100%)	0	100 100
8	B	178/198 (90%)	178 (100%)	0	100 100
9	C	156/192 (81%)	156 (100%)	0	100 100
10	D	213/279 (76%)	211 (99%)	2 (1%)	75 85
11	E	505/586 (86%)	503 (100%)	2 (0%)	89 93
14	X	639/1125 (57%)	630 (99%)	9 (1%)	62 78
15	Y	85/85 (100%)	84 (99%)	1 (1%)	67 80
All	All	5252/7438 (71%)	5205 (99%)	47 (1%)	74 85

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

Mol	Chain	Res	Type
6	7	608	ASP
11	E	554	GLU
6	7	620	HIS
6	7	719	LEU
14	X	115	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such

sidechains are listed below:

Mol	Chain	Res	Type
11	E	521	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 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	$\#\|Z\| > 2$
16	ADP	2	1001	17	24,29,29	0.89	0	29,45,45	1.28	2 (6%)
19	ATP	6	1201	17	28,33,33	0.63	0	34,52,52	1.18	2 (5%)
19	ATP	3	1001	17	28,33,33	0.63	0	34,52,52	1.18	2 (5%)
19	ATP	7	1001	17	28,33,33	0.62	0	34,52,52	1.20	2 (5%)
19	ATP	4	1101	17	28,33,33	0.61	0	34,52,52	0.93	3 (8%)
19	ATP	5	1001	17	28,33,33	0.63	0	34,52,52	0.93	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
16	ADP	2	1001	17	-	3/12/32/32	0/3/3/3
19	ATP	6	1201	17	-	8/18/38/38	0/3/3/3
19	ATP	3	1001	17	-	8/18/38/38	0/3/3/3
19	ATP	7	1001	17	-	5/18/38/38	0/3/3/3
19	ATP	4	1101	17	-	1/18/38/38	0/3/3/3
19	ATP	5	1001	17	-	3/18/38/38	0/3/3/3

There are no bond length outliers.

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	7	1001	ATP	C4'-O4'-C1'	-4.51	105.79	109.92
19	3	1001	ATP	C4'-O4'-C1'	-4.37	105.92	109.92
19	6	1201	ATP	C4'-O4'-C1'	-4.30	105.98	109.92
16	2	1001	ADP	N3-C2-N1	-4.16	123.03	128.67
16	2	1001	ADP	C4-C5-N7	-2.52	106.67	109.34

There are no chirality outliers.

5 of 28 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
16	2	1001	ADP	C5'-O5'-PA-O1A
16	2	1001	ADP	C5'-O5'-PA-O3A
19	3	1001	ATP	PB-O3B-PG-O2G
19	3	1001	ATP	C5'-O5'-PA-O3A
19	3	1001	ATP	O4'-C4'-C5'-O5'

There are no ring outliers.

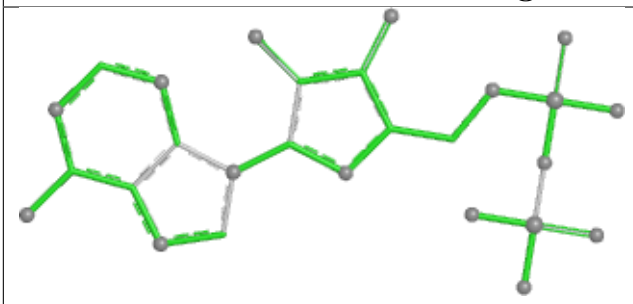
2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	2	1001	ADP	2	0
19	3	1001	ATP	1	0

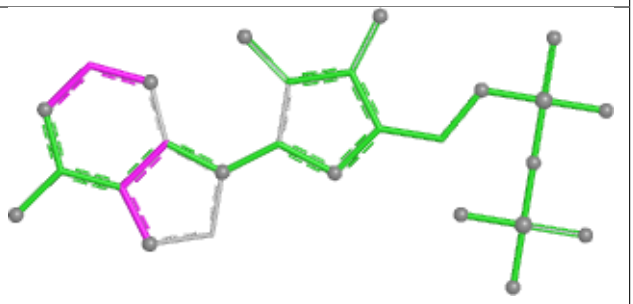
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

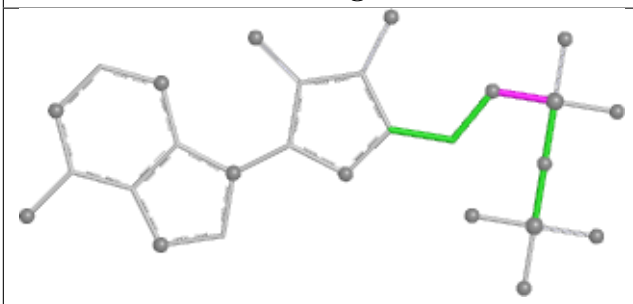
Ligand ADP 2 1001



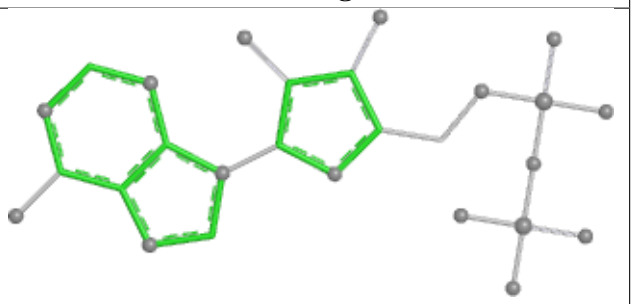
Bond lengths



Bond angles

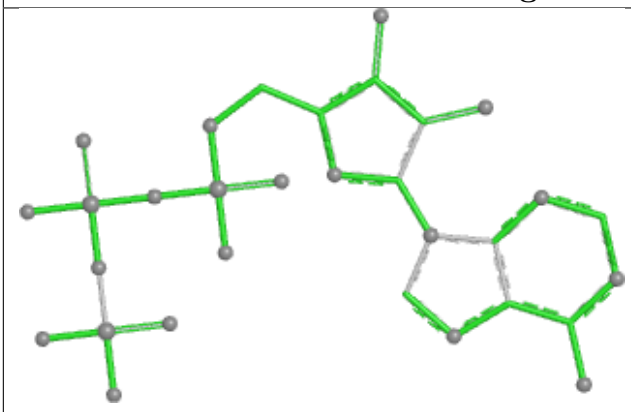


Torsions

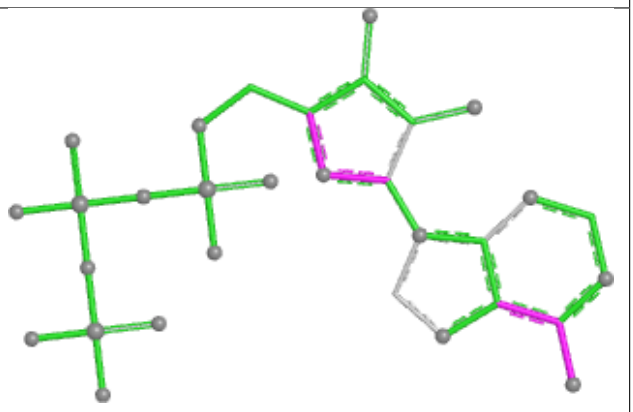


Rings

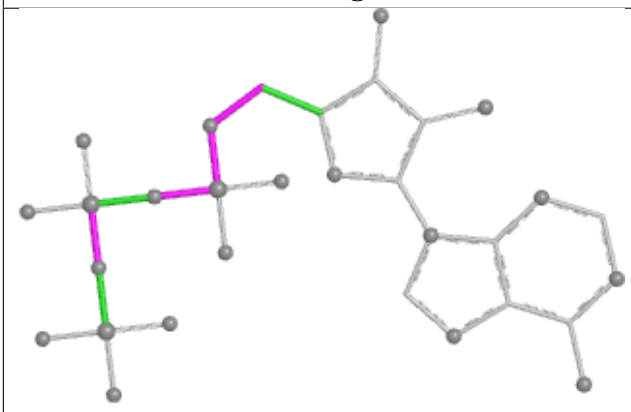
Ligand ATP 6 1201



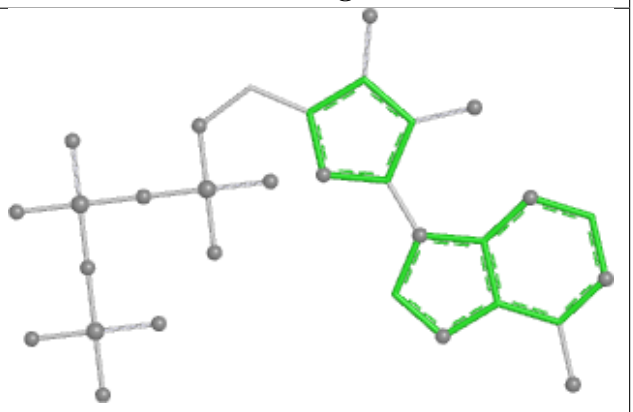
Bond lengths



Bond angles

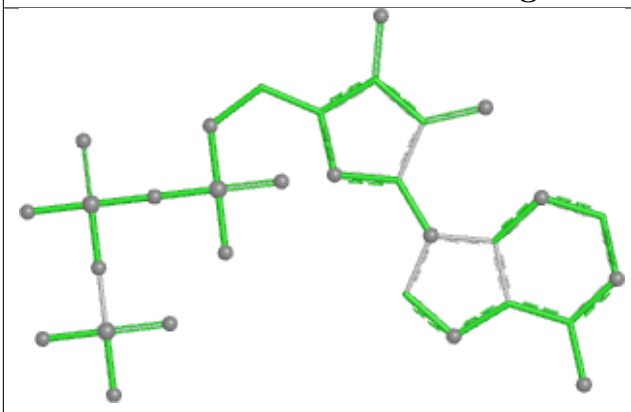


Torsions

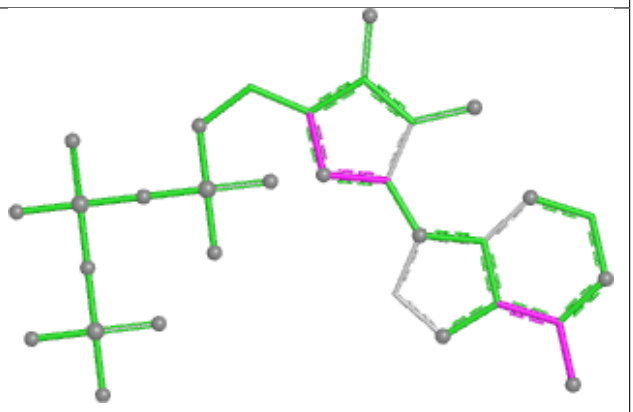


Rings

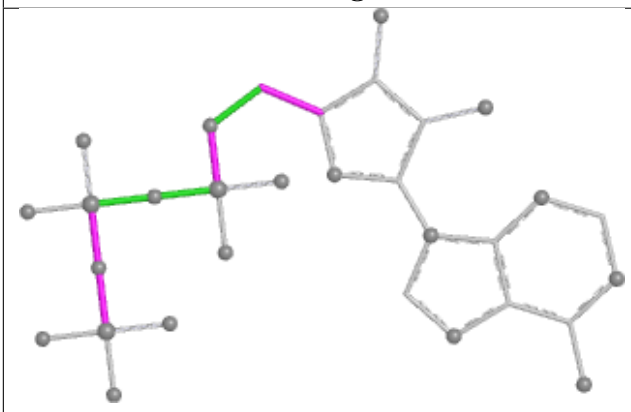
Ligand ATP 3 1001



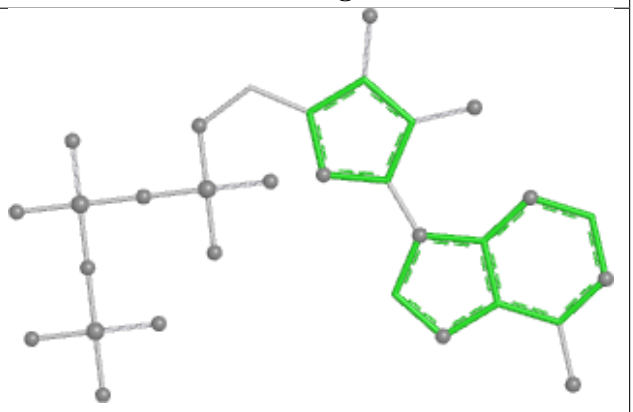
Bond lengths



Bond angles

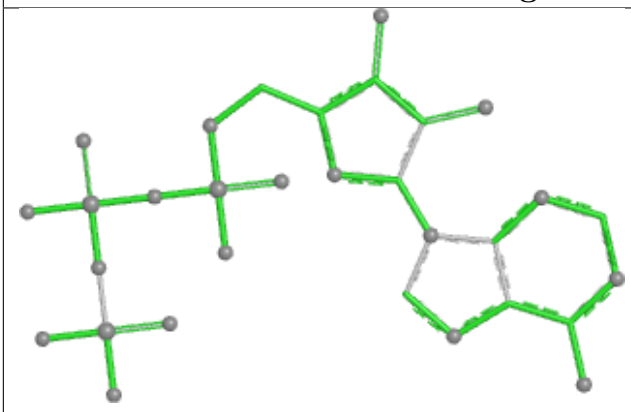


Torsions

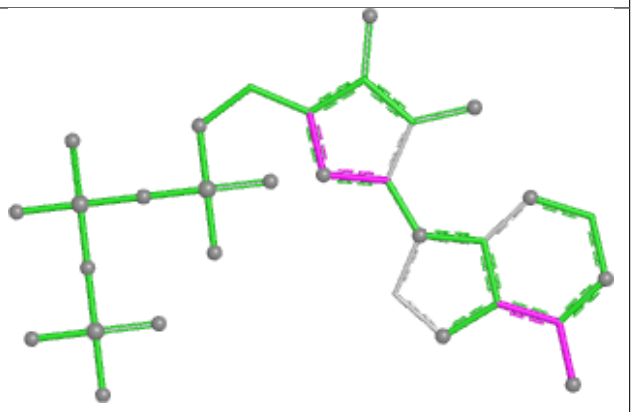


Rings

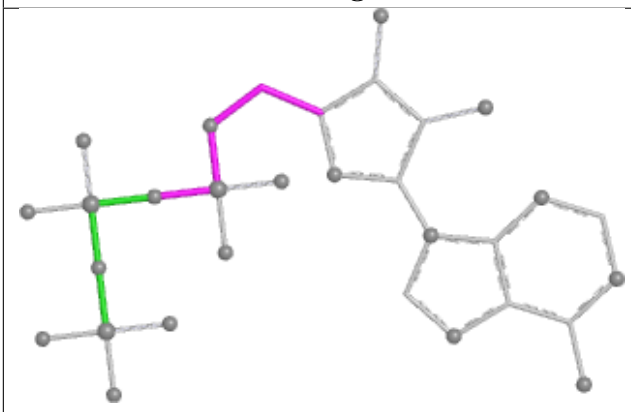
Ligand ATP 7 1001



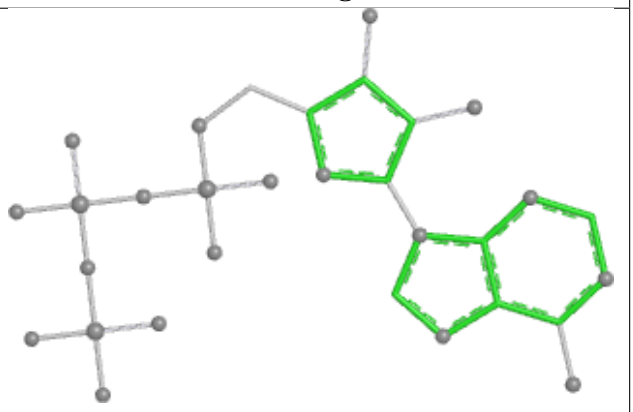
Bond lengths



Bond angles

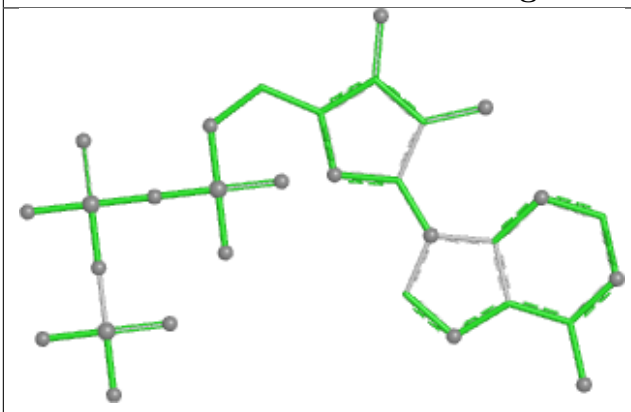


Torsions

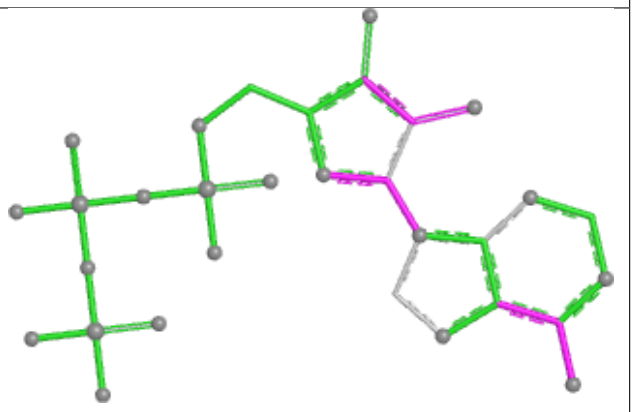


Rings

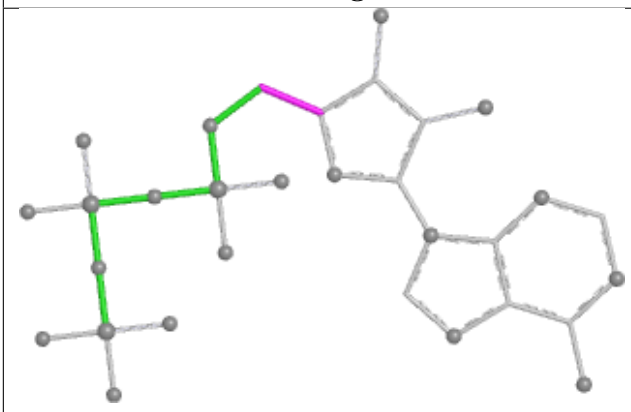
Ligand ATP 4 1101



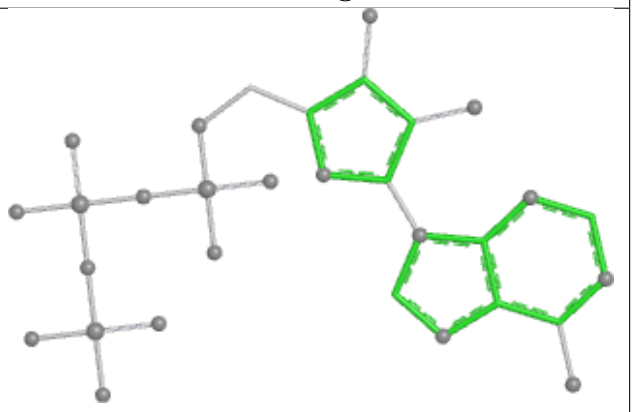
Bond lengths



Bond angles

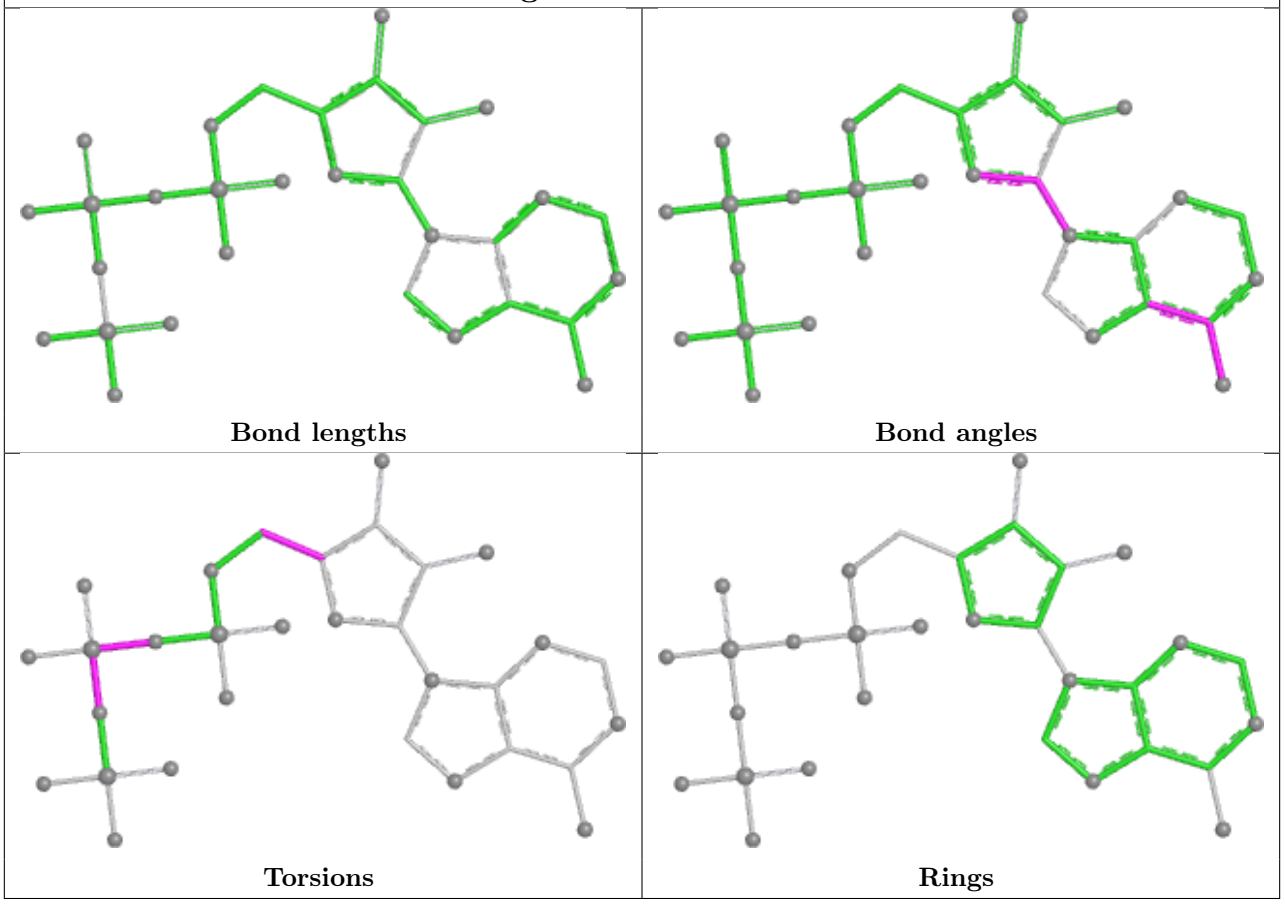


Torsions



Rings

Ligand ATP 5 1001



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-47470. 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 (i)

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

9 Map-model fit

This section was not generated.