



## wwPDB EM Validation Summary Report ⓘ

Mar 16, 2025 – 02:11 PM EDT

PDB ID : 9E2X  
EMDB ID : EMD-47471  
Title : Cryo-EM structure of yeast CMG helicase stalled at G4-containing DNA template, state 2  
Authors : Allwein, B.; Batra, S.; Remus, D.; Hite, R.  
Deposited on : 2024-10-23  
Resolution : 3.50 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](mailto: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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references ⓘ](#)) 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

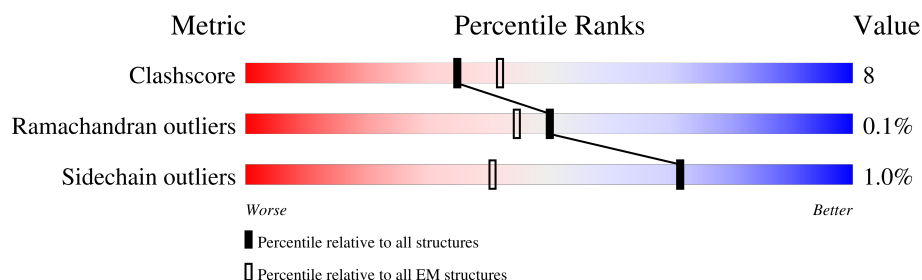
# 1 Overall quality at a glance

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	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  $\geq 3$ , 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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A	208	78% 15% 7%
2	B	213	74% 14% 11%
3	C	217	67% 12% 20%
4	D	294	63% 12% 24%
5	E	650	76% 11% 13%
6	F	48	73% 23% .
7	G	20	85% 15%
8	2	868	62% 13% 25%
9	3	971	54% 12% 34%

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Mol	Chain	Length	Quality of chain
10	4	933	
11	5	775	
12	6	1017	
13	7	845	
14	X	1238	
15	Y	92	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
18	ZN	2	1003	-	-	X	-

## 2 Entry composition

There are 19 unique types of molecules in this entry. The entry contains 98329 atoms, of which 49013 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
1	A	194	Total	C	H	N	O	S	0	0
			3180	999	1592	273	307	9		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
2	B	189	Total	C	H	N	O	S	0	0
			3191	1014	1614	276	282	5		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
3	C	174	Total	C	H	N	O	S	0	0
			2813	913	1412	225	257	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

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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
			3671	1170	1844	300	345	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
			9119	2920	4552	770	863	14		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
6	F	48	Total	C	H	N	O	P	0	0
			1548	475	545	182	298	48		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
7	G	20	Total	C	H	N	O	P	0	0
			633	194	224	79	116	20		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
8	2	655	Total	C	H	N	O	S	0	0
			10454	3271	5250	933	981	19		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
9	3	644	Total	C	H	N	O	S	0	0
			10097	3173	5073	894	944	13		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
10	4	611	Total	C	H	N	O	S	0	0
			9772	3062	4914	836	932	28		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
11	5	641	Total	C	H	N	O	S	0	0
			10249	3208	5164	882	973	22		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
12	6	642	Total	C	H	N	O	S	0	0
			10130	3189	5068	882	966	25		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
13	7	641	Total	C	H	N	O	S	0	0
			10141	3184	5101	875	953	28		

- 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
			11536	3691	5821	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
			1537	495	769	138	131	4		

- Molecule 16 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
16	2	1	Total 43	C 10	H 12	N 5	O 13	P 3	0
16	3	1	Total 43	C 10	H 12	N 5	O 13	P 3	0
16	5	1	Total 41	C 10	H 10	N 5	O 13	P 3	0
16	7	1	Total 43	C 10	H 12	N 5	O 13	P 3	0

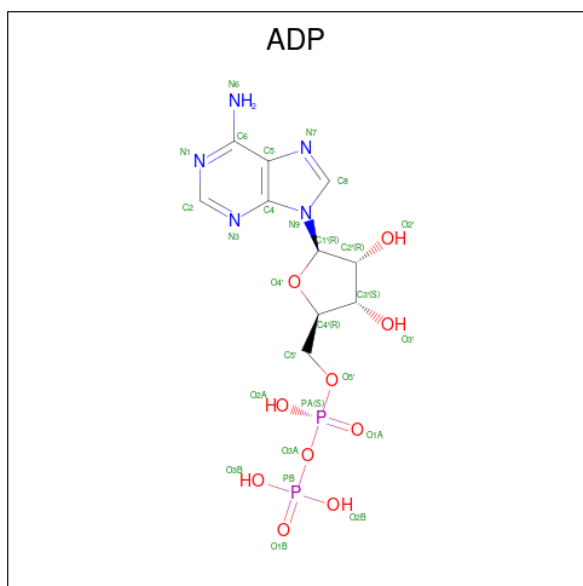
- Molecule 17 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- 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	
18	5	1	Total	Zn	0
			1	1	
18	6	1	Total	Zn	0
			1	1	
18	7	1	Total	Zn	0
			1	1	

- Molecule 19 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).

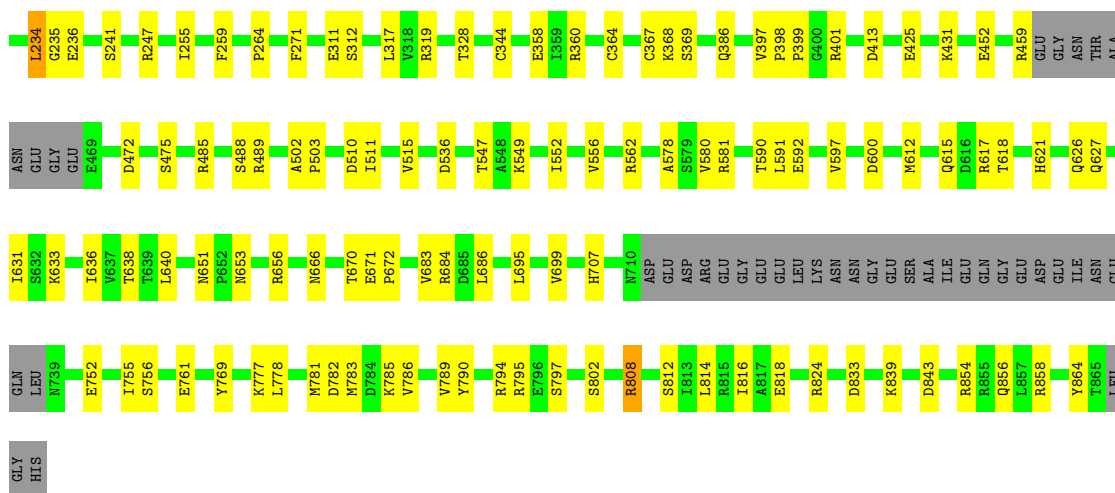


Mol	Chain	Residues	Atoms						AltConf
19	4	1	Total	C	H	N	O	P	0
			39	10	12	5	10	2	
19	4	1	Total	C	H	N	O	P	0
			39	10	12	5	10	2	

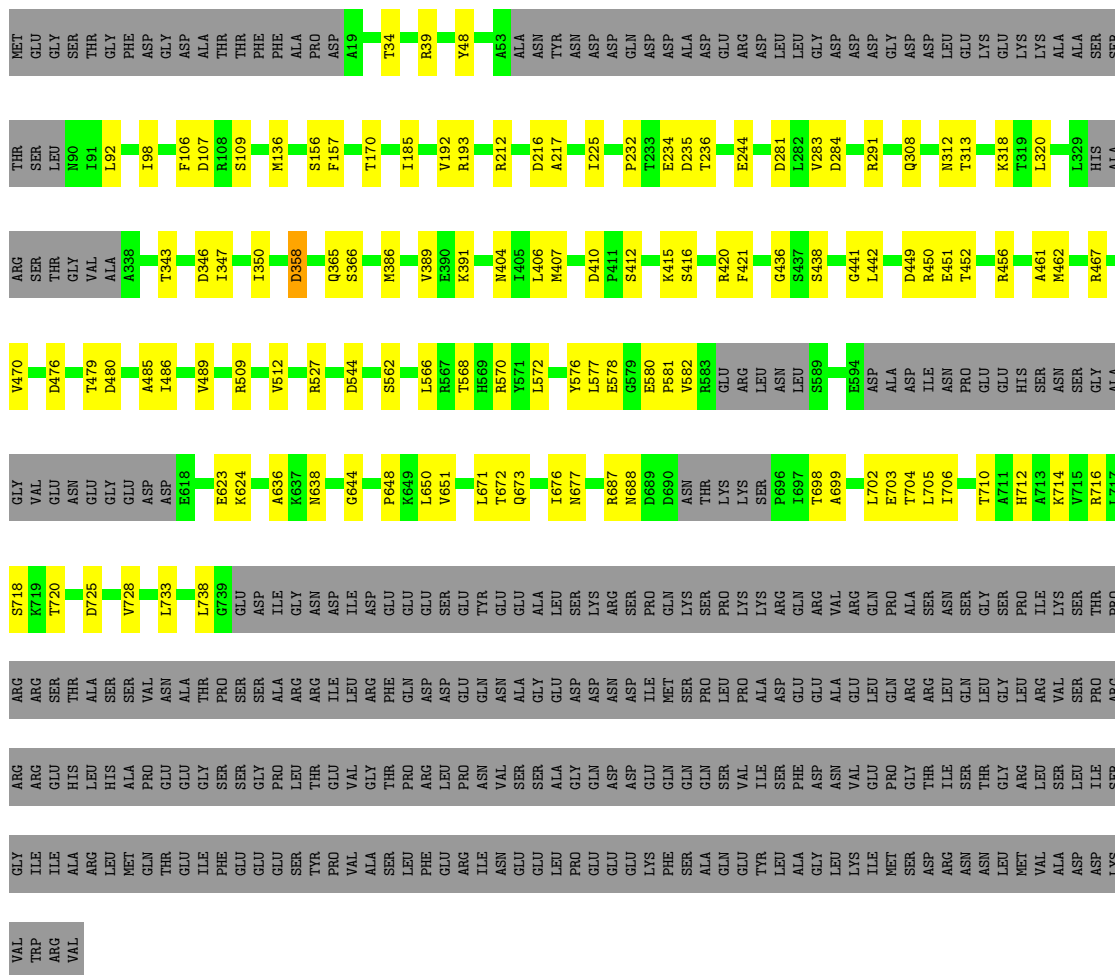








- Molecule 9: DNA replication licensing factor MCM3



- Molecule 10: DNA replication licensing factor MCM4

Device Type	Percentage
Smartphone	53%
Tablet	12%
Feature Phone	35%

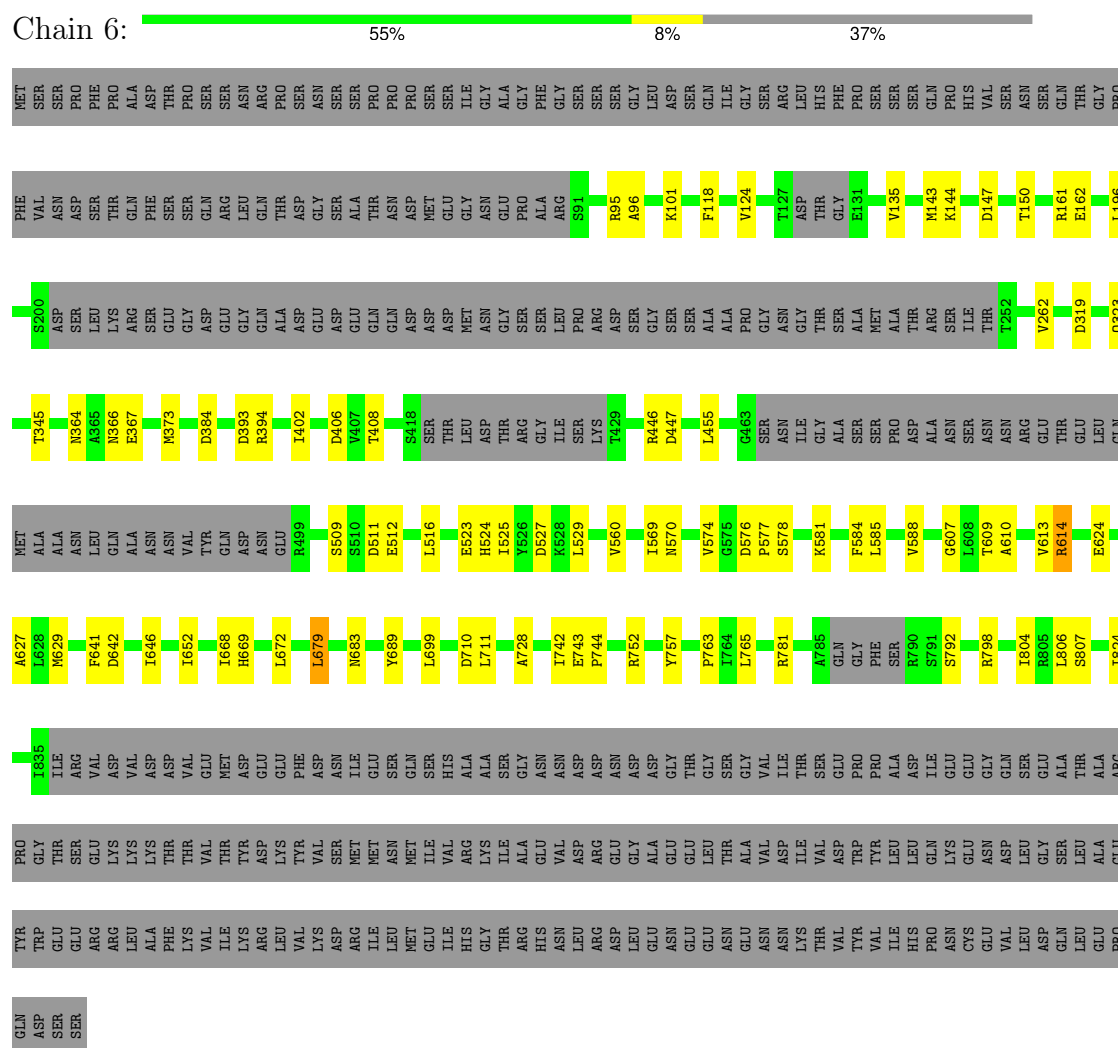


Response	Percentage
U.S. should take action to protect the environment	69%
U.S. should not take action to protect the environment	14%
U.S. should not take action to protect the environment (Unsure)	17%



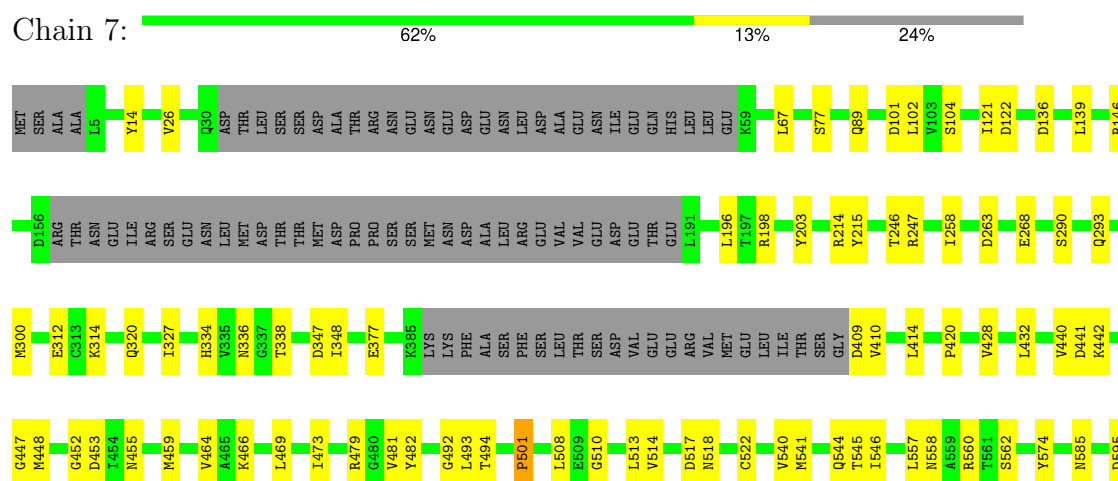
• Molecule 12: DNA replication licensing factor MCM6

Chain 6:



• Molecule 13: DNA replication licensing factor MCM7

Chain 7:




L596	L597	F598	L599	D602	S605	R606	D607	D608	L612	H615	T616	T617	H620	Q625	D629	F630	E634	M638	I665	S677	T685	T688	L695	D709	I710	D711	V712	V713	E714	E715	R718	R721	S722	S723	S726	L727	Y728	Q729	E730	THR								
LYS	SER	LYS	GLU	ASP	GLU	SER	PRO	THR	LYS	ILE	PHE	THR	LYS	MET	LEU	GLN	GLU	THR	GLY	LYS	ASN	VAL	LYS	THR	ALA	VAL	ARG	LEU	ASN	ARG	GLY	PHE	THR	THR	MET	LEU	GLN	SER	ASN	CYS	ILE	GLN	GLU	THR	THR	LEU	ASN	VAL
HIS	LEU	ILE	ASN	GLY	GLY	ASN	THR	THR	LYS	PHE	THR	VAL	ASP	ASP	THR	ASP	GLN	GLU	THR	LEU	ALA	PRO	GLN	THR	THR	THR	THR	GLN	ASP	GLN	ASP	ILE	ASP	GLN	ASP	ALA												

• Molecule 14: Topoisomerase 1-associated factor 1

Chain X:  48% 9% 43%

ASP	GLU	GLU	ASP	GLU	GLU	GLU	ASP	GLN	ASP	ILE	GLN	ASP	ILE	SER	GLN	ASP	GLN	ASP	PHE	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN
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• Molecule 15: Chromosome segregation in meiosis protein 3

Chain Y:  77% 22%

R48	R49	D62	K63	K70	N71	I78	I91	I92	Q93	F94	L97	K105	G119	L125	R126	E127	Y128	R129	V130	S131	L132	F133	R134	M137	G138	M139
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## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	40714	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 ( $e^-/\text{\AA}^2$ )	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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ADP, ZN, ATP, 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	A	0.26	0/1608	0.48	0/2163
2	B	0.27	0/1609	0.51	0/2177
3	C	0.55	1/1434 (0.1%)	0.42	0/1938
4	D	0.24	0/1861	0.45	0/2514
5	E	0.25	0/4654	0.47	0/6303
6	F	0.54	0/1125	1.08	5/1741 (0.3%)
7	G	0.57	0/459	0.96	0/705
8	2	0.25	0/5292	0.52	0/7145
9	3	0.25	0/5112	0.51	0/6930
10	4	0.26	0/4931	0.50	0/6666
11	5	0.24	0/5155	0.50	0/6956
12	6	0.25	0/5143	0.51	0/6938
13	7	0.39	1/5120 (0.0%)	0.52	0/6921
14	X	0.24	0/5828	0.45	0/7868
15	Y	0.34	0/784	0.55	1/1049 (0.1%)
All	All	0.30	2/50115 (0.0%)	0.53	6/68014 (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
5	E	0	1
8	2	0	3
10	4	0	3
12	6	0	3
13	7	0	3
14	X	0	1
15	Y	0	4
All	All	0	18

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	37	PRO	N-CD	18.57	1.73	1.47
13	7	501	PRO	N-CD	18.34	1.73	1.47

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	34	DC	O4'-C4'-C3'	-9.12	100.53	106.00
6	F	34	DC	O4'-C1'-N1	6.69	112.68	108.00
6	F	34	DC	C4'-C3'-C2'	-5.53	98.13	103.10
15	Y	128	TYR	N-CA-CB	-5.11	101.40	110.60
6	F	27	DA	O4'-C1'-N9	5.08	111.56	108.00

There are no chirality outliers.

5 of 18 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
8	2	581	ARG	Sidechain
8	2	795	ARG	Sidechain
8	2	808	ARG	Sidechain
10	4	246	ARG	Sidechain
5	E	398	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	1588	1592	1593	23	0
2	B	1577	1614	1625	36	0
3	C	1401	1412	1415	25	0
4	D	1827	1844	1844	34	0
5	E	4567	4552	4555	54	0
6	F	1003	545	545	11	0
7	G	409	224	224	2	0
8	2	5204	5250	5261	100	0
9	3	5024	5073	5087	111	0
10	4	4858	4914	4924	85	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	5	5085	5164	5177	112	0
12	6	5062	5068	5078	61	0
13	7	5040	5101	5101	115	0
14	X	5715	5821	5833	79	0
15	Y	768	769	801	14	0
16	2	31	12	12	2	0
16	3	31	12	12	1	0
16	5	31	10	11	1	0
16	7	31	12	12	1	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	7	1	0	0	0	0
18	2	1	0	0	2	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	4	54	24	24	2	0
All	All	49316	49013	49134	763	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 8.

The worst 5 of 763 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)
11:5:755:LEU:HD13	11:5:761:ILE:CD1	1.48	1.40
8:2:854:ARG:NH2	8:2:858:ARG:HH22	1.20	1.39
2:B:99:ASP:OD1	2:B:144:LYS:CE	1.75	1.33
3:C:37:PRO:N	3:C:37:PRO:CD	1.73	1.32
2:B:146:GLN:CG	11:5:47:ARG:HH11	1.41	1.32

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	190/208 (91%)	186 (98%)	4 (2%)	0	100	100
2	B	185/213 (87%)	176 (95%)	8 (4%)	1 (0%)	25	59
3	C	168/217 (77%)	163 (97%)	5 (3%)	0	100	100
4	D	216/294 (74%)	211 (98%)	5 (2%)	0	100	100
5	E	560/650 (86%)	548 (98%)	12 (2%)	0	100	100
8	2	649/868 (75%)	625 (96%)	24 (4%)	0	100	100
9	3	632/971 (65%)	613 (97%)	19 (3%)	0	100	100
10	4	603/933 (65%)	582 (96%)	19 (3%)	2 (0%)	37	68
11	5	623/775 (80%)	597 (96%)	26 (4%)	0	100	100
12	6	630/1017 (62%)	610 (97%)	20 (3%)	0	100	100
13	7	633/845 (75%)	603 (95%)	29 (5%)	1 (0%)	44	75
14	X	699/1238 (56%)	683 (98%)	16 (2%)	0	100	100
15	Y	90/92 (98%)	86 (96%)	4 (4%)	0	100	100
All	All	5878/8321 (71%)	5683 (97%)	191 (3%)	4 (0%)	50	79

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	4	834	LYS
2	B	94	THR
13	7	493	LEU
10	4	694	LEU

### 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	179/193 (93%)	179 (100%)	0	100	100
2	B	178/198 (90%)	176 (99%)	2 (1%)	70	83
3	C	156/192 (81%)	155 (99%)	1 (1%)	84	91
4	D	213/279 (76%)	211 (99%)	2 (1%)	75	86
5	E	504/586 (86%)	500 (99%)	4 (1%)	79	88
8	2	576/770 (75%)	571 (99%)	5 (1%)	75	86
9	3	551/835 (66%)	546 (99%)	5 (1%)	75	86
10	4	551/848 (65%)	545 (99%)	6 (1%)	70	83
11	5	577/688 (84%)	575 (100%)	2 (0%)	91	96
12	6	559/886 (63%)	553 (99%)	6 (1%)	70	83
13	7	560/753 (74%)	556 (99%)	4 (1%)	81	89
14	X	639/1125 (57%)	625 (98%)	14 (2%)	47	70
15	Y	85/85 (100%)	84 (99%)	1 (1%)	67	82
All	All	5328/7438 (72%)	5276 (99%)	52 (1%)	71	84

5 of 52 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
12	6	319	ASP
13	7	677	SER
14	X	559	PHE
12	6	614	ARG
12	6	679	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
13	7	615	HIS
13	7	585	ASN
10	4	683	ASN
10	4	274	GLN
13	7	332	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 16 ligands modelled in this entry, 10 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$
19	ADP	4	1004	-	24,29,29	0.91	0	29,45,45	1.19	2 (6%)
16	ATP	7	1001	17	28,33,33	0.64	0	34,52,52	0.97	1 (2%)
16	ATP	5	1001	17	28,33,33	0.73	0	34,52,52	1.25	3 (8%)
19	ADP	4	1001	17	24,29,29	0.90	0	29,45,45	1.30	2 (6%)
16	ATP	2	1001	17	28,33,33	0.65	0	34,52,52	0.94	2 (5%)
16	ATP	3	1001	17	28,33,33	0.64	0	34,52,52	1.19	3 (8%)

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
19	ADP	4	1004	-	-	5/12/32/32	0/3/3/3
16	ATP	7	1001	17	-	6/18/38/38	0/3/3/3

*Continued on next page...*

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	ATP	5	1001	17	-	5/18/38/38	0/3/3/3
19	ADP	4	1001	17	-	1/12/32/32	0/3/3/3
16	ATP	2	1001	17	-	7/18/38/38	0/3/3/3
16	ATP	3	1001	17	-	0/18/38/38	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(°)	Ideal(°)
16	3	1001	ATP	C4'-O4'-C1'	-4.47	105.83	109.92
16	5	1001	ATP	C4'-O4'-C1'	-4.28	106.00	109.92
19	4	1004	ADP	N3-C2-N1	-4.24	122.92	128.67
19	4	1001	ADP	N3-C2-N1	-4.15	123.04	128.67
16	5	1001	ATP	O2'-C2'-C3'	3.76	123.88	111.82

There are no chirality outliers.

5 of 24 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
16	2	1001	ATP	PB-O3B-PG-O2G
16	5	1001	ATP	PB-O3B-PG-O3G
16	5	1001	ATP	C4'-C5'-O5'-PA
16	7	1001	ATP	PB-O3B-PG-O2G
16	7	1001	ATP	PB-O3B-PG-O3G

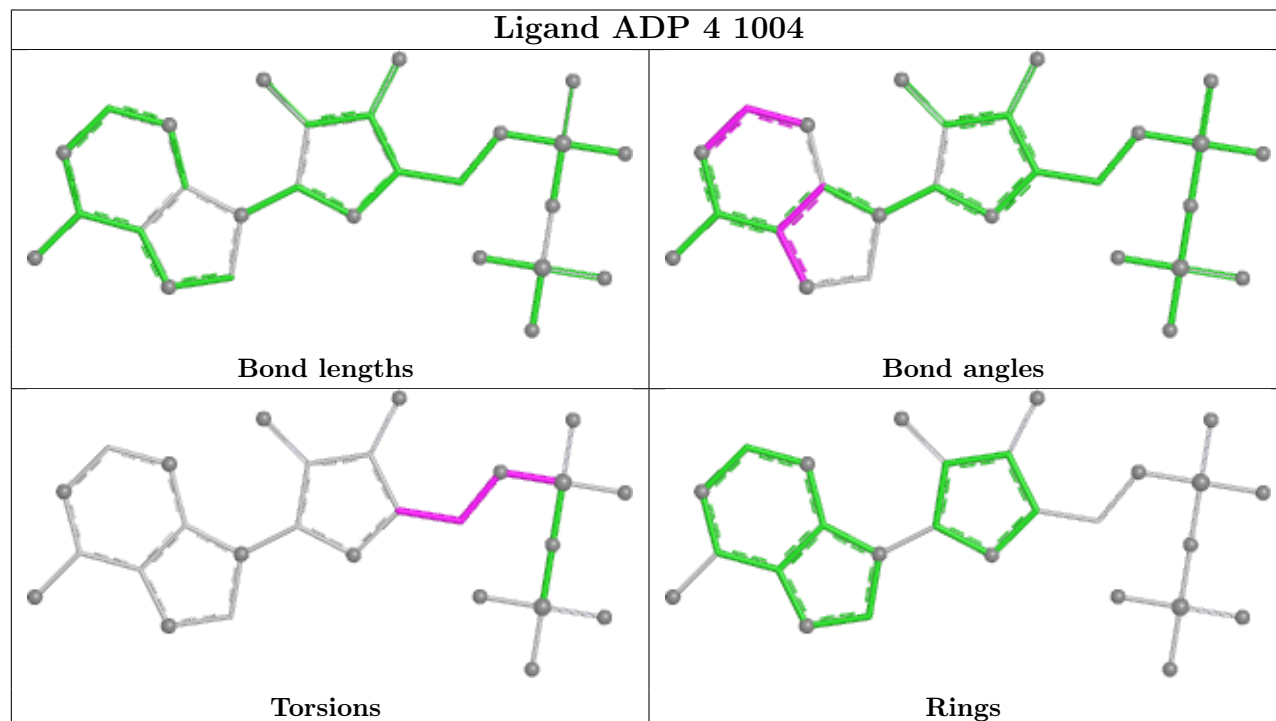
There are no ring outliers.

6 monomers are involved in 7 short contacts:

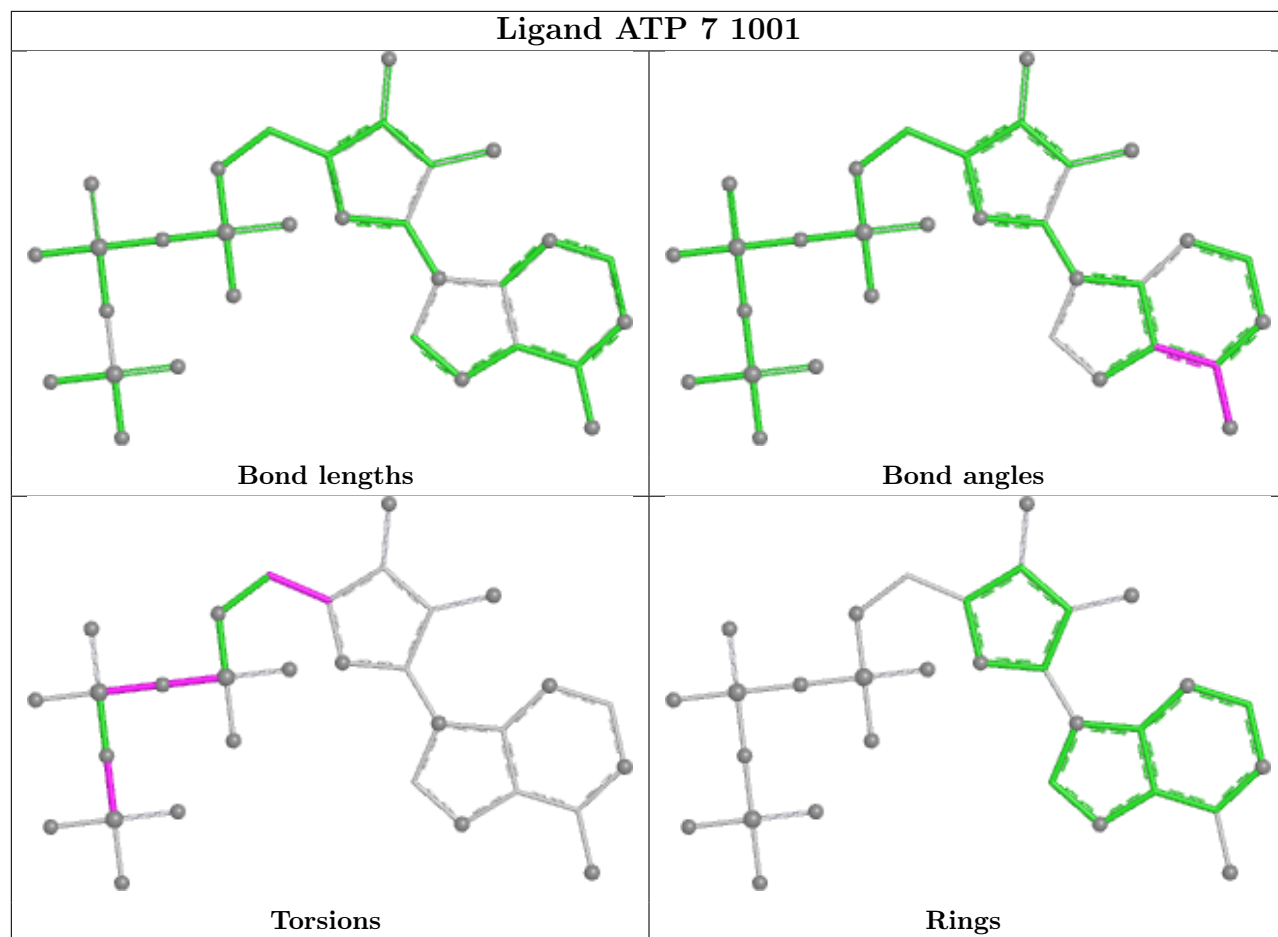
Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	4	1004	ADP	1	0
16	7	1001	ATP	1	0
16	5	1001	ATP	1	0
19	4	1001	ADP	1	0
16	2	1001	ATP	2	0
16	3	1001	ATP	1	0

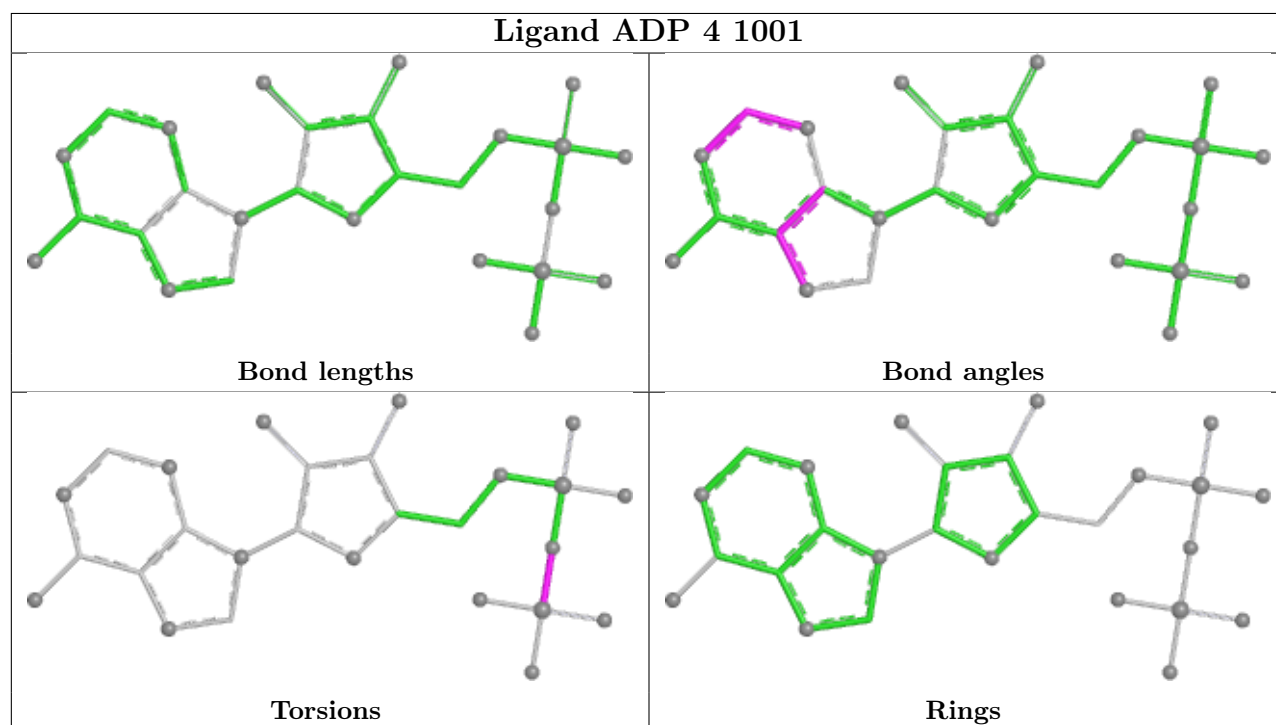
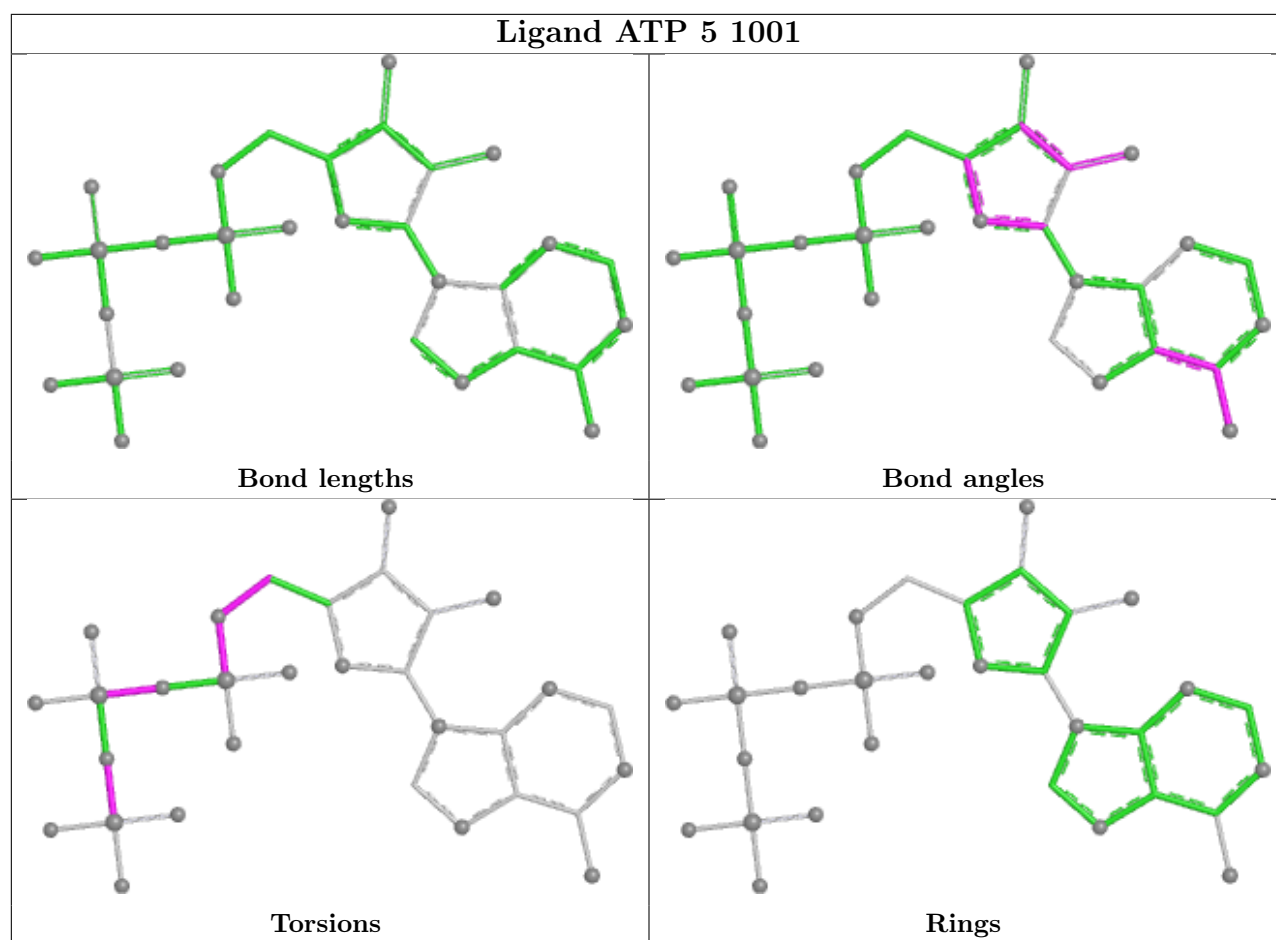
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is

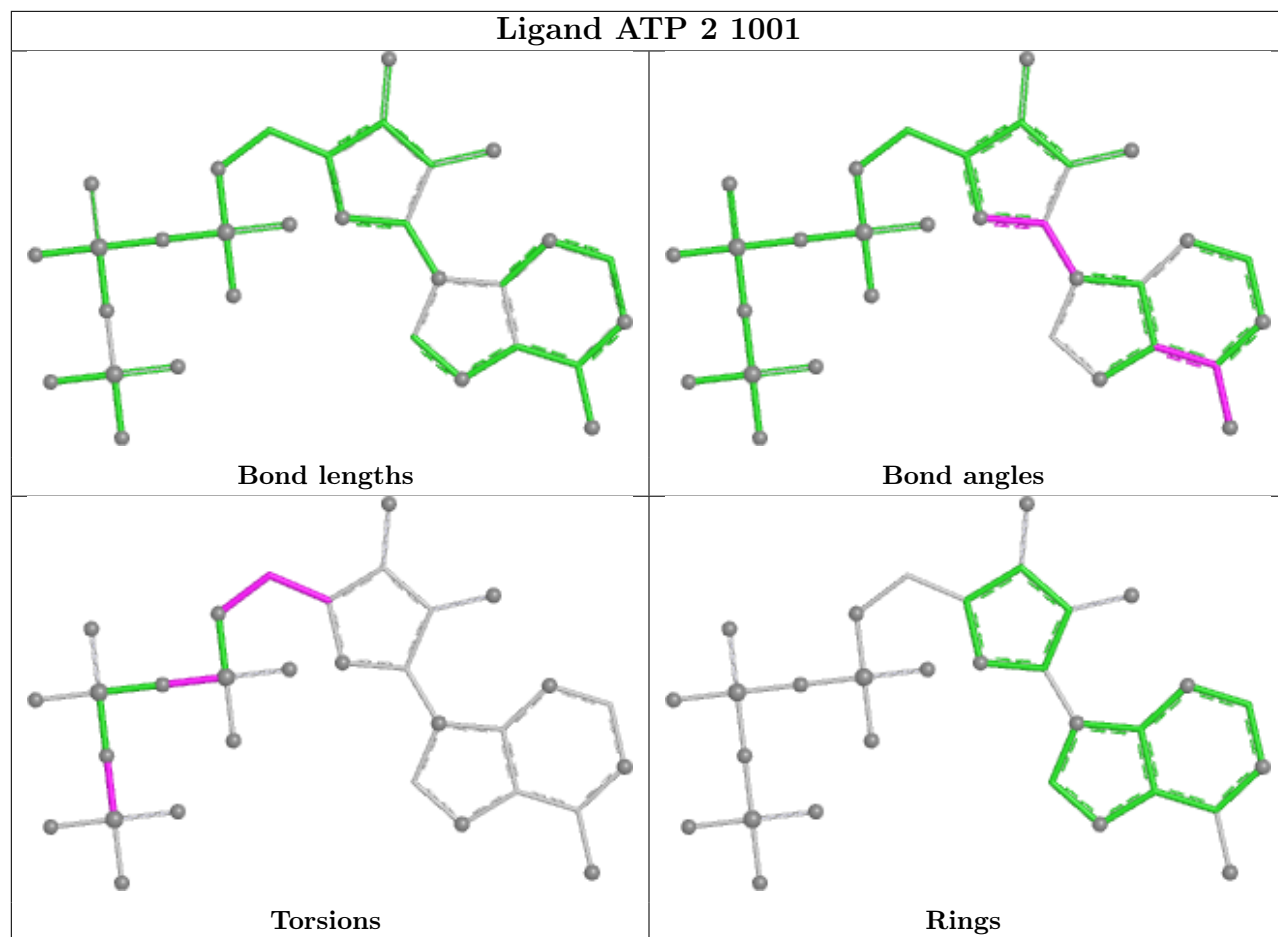
within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question 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.

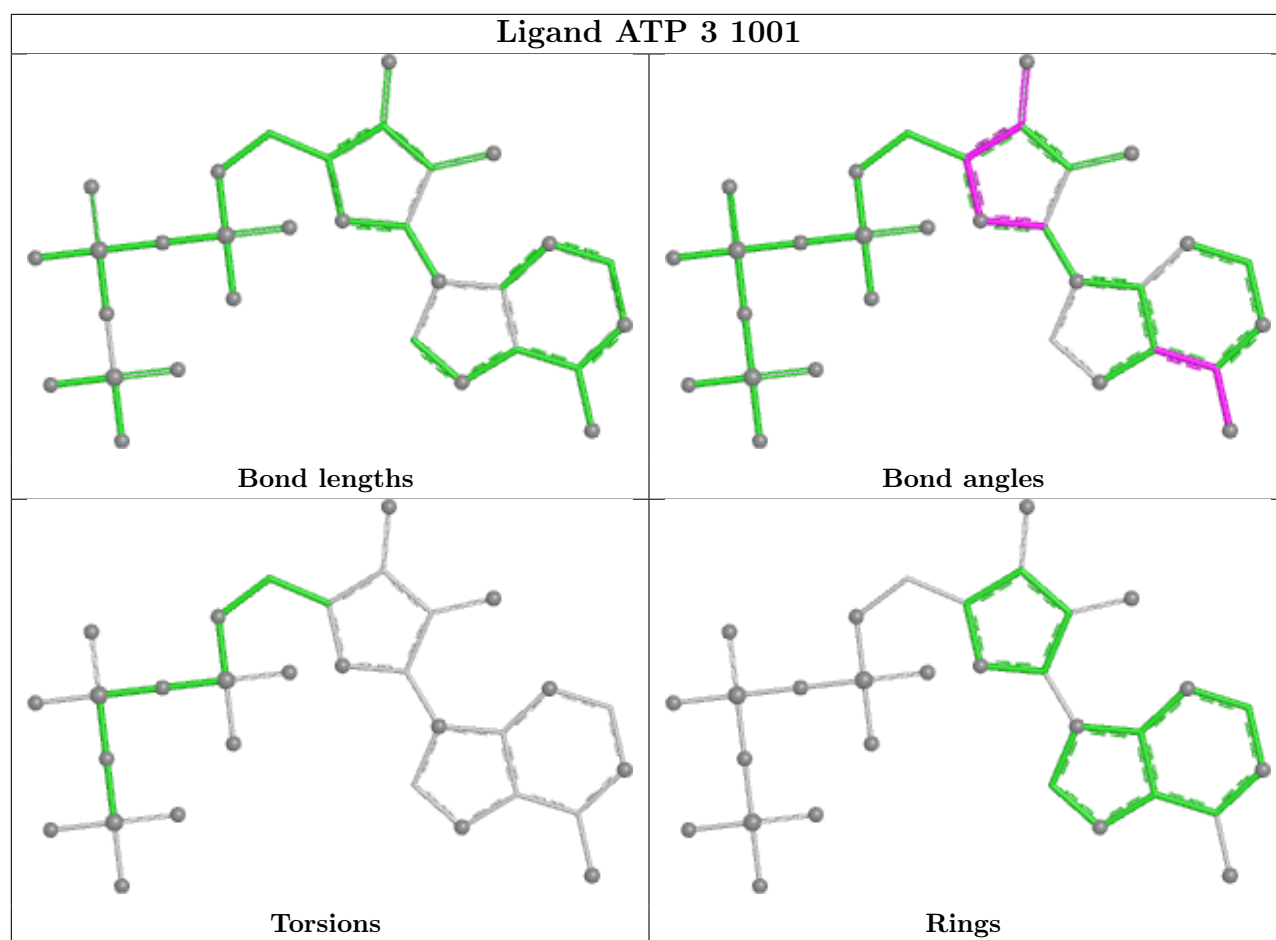












## 5.7 Other polymers [i](#)

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-47471. 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.