



wwPDB EM Validation Summary Report ⓘ

Mar 30, 2026 – 04:22 PM UTC

PDB ID : 7Z13 / pdb_00007z13
EMDB ID : EMD-14439
Title : S. cerevisiae CMGE dimer nucleating origin DNA melting
Authors : Lewis, J.S.; Sousa, J.S.; Costa, A.
Deposited on : 2022-02-24
Resolution : 3.40 Å (reported)
Based on initial models : 7QHS, ?

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 ⓘ 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 ⓘ](#)) were used in the production of this report:

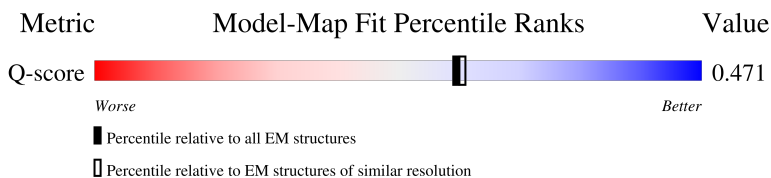
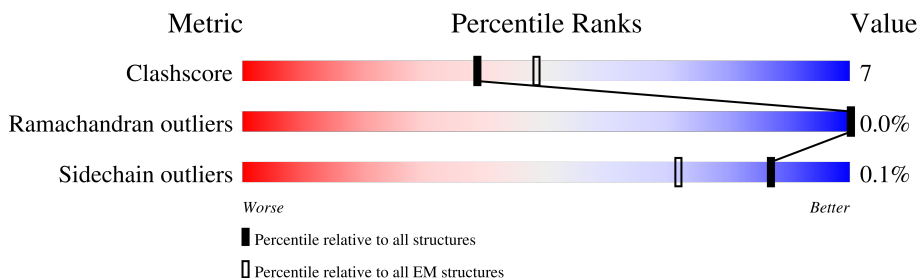
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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 3.40 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.



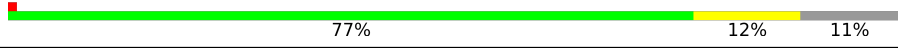
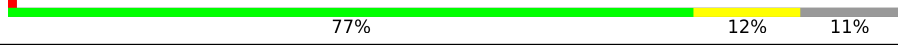
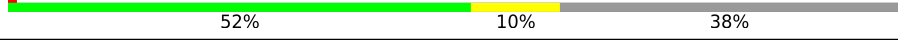
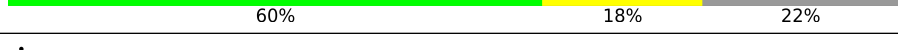
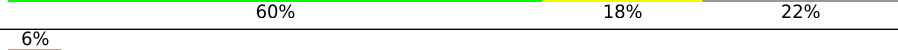
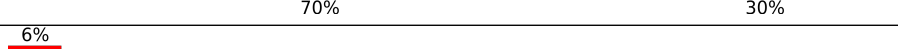
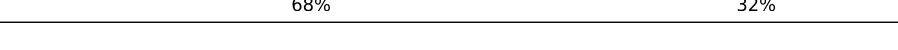
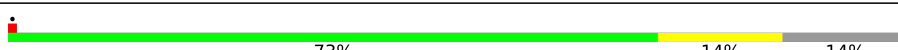
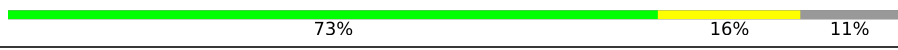
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14717 (2.90 - 3.90)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	2	868	 66% 10% 24%
1	a	868	 66% 10% 24%
2	3	1006	 56% 7% 37%
2	b	1006	 55% 8% 37%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	4	933	
3	c	933	
4	5	775	
4	d	775	
5	6	1017	
5	e	1017	
6	7	845	
6	f	845	
7	A	53	
8	B	53	
9	C	229	
9	J	229	
10	D	294	
10	K	294	
11	E	657	
11	L	657	
12	F	689	
12	M	689	
13	H	208	
13	O	208	
14	I	213	
14	P	213	
15	N	2222	
15	Q	2222	

2 Entry composition

There are 19 unique types of molecules in this entry. The entry contains 107381 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DNA replication licensing factor MCM2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	2	660	Total	C	N	O	S	0	0
			5231	3284	937	991	19		
1	a	660	Total	C	N	O	S	0	0
			5231	3284	937	991	19		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	3	633	Total	C	N	O	S	0	0
			4958	3119	882	944	13		
2	b	633	Total	C	N	O	S	0	0
			4958	3119	882	944	13		

There are 70 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
3	-34	MET	-	initiating methionine	UNP P24279
3	-33	LYS	-	expression tag	UNP P24279
3	-32	ARG	-	expression tag	UNP P24279
3	-31	ARG	-	expression tag	UNP P24279
3	-30	TRP	-	expression tag	UNP P24279
3	-29	LYS	-	expression tag	UNP P24279
3	-28	LYS	-	expression tag	UNP P24279
3	-27	ASN	-	expression tag	UNP P24279
3	-26	PHE	-	expression tag	UNP P24279
3	-25	ILE	-	expression tag	UNP P24279
3	-24	ALA	-	expression tag	UNP P24279
3	-23	VAL	-	expression tag	UNP P24279
3	-22	SER	-	expression tag	UNP P24279
3	-21	ALA	-	expression tag	UNP P24279
3	-20	ALA	-	expression tag	UNP P24279
3	-19	ASN	-	expression tag	UNP P24279
3	-18	ARG	-	expression tag	UNP P24279

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
3	-17	PHE	-	expression tag	UNP P24279
3	-16	LYS	-	expression tag	UNP P24279
3	-15	LYS	-	expression tag	UNP P24279
3	-14	ILE	-	expression tag	UNP P24279
3	-13	SER	-	expression tag	UNP P24279
3	-12	SER	-	expression tag	UNP P24279
3	-11	SER	-	expression tag	UNP P24279
3	-10	GLY	-	expression tag	UNP P24279
3	-9	ALA	-	expression tag	UNP P24279
3	-8	LEU	-	expression tag	UNP P24279
3	-7	GLU	-	expression tag	UNP P24279
3	-6	ASN	-	expression tag	UNP P24279
3	-5	LEU	-	expression tag	UNP P24279
3	-4	TYR	-	expression tag	UNP P24279
3	-3	PHE	-	expression tag	UNP P24279
3	-2	GLN	-	expression tag	UNP P24279
3	-1	GLY	-	expression tag	UNP P24279
3	0	GLU	-	expression tag	UNP P24279
b	-34	MET	-	initiating methionine	UNP P24279
b	-33	LYS	-	expression tag	UNP P24279
b	-32	ARG	-	expression tag	UNP P24279
b	-31	ARG	-	expression tag	UNP P24279
b	-30	TRP	-	expression tag	UNP P24279
b	-29	LYS	-	expression tag	UNP P24279
b	-28	LYS	-	expression tag	UNP P24279
b	-27	ASN	-	expression tag	UNP P24279
b	-26	PHE	-	expression tag	UNP P24279
b	-25	ILE	-	expression tag	UNP P24279
b	-24	ALA	-	expression tag	UNP P24279
b	-23	VAL	-	expression tag	UNP P24279
b	-22	SER	-	expression tag	UNP P24279
b	-21	ALA	-	expression tag	UNP P24279
b	-20	ALA	-	expression tag	UNP P24279
b	-19	ASN	-	expression tag	UNP P24279
b	-18	ARG	-	expression tag	UNP P24279
b	-17	PHE	-	expression tag	UNP P24279
b	-16	LYS	-	expression tag	UNP P24279
b	-15	LYS	-	expression tag	UNP P24279
b	-14	ILE	-	expression tag	UNP P24279
b	-13	SER	-	expression tag	UNP P24279
b	-12	SER	-	expression tag	UNP P24279
b	-11	SER	-	expression tag	UNP P24279

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
b	-10	GLY	-	expression tag	UNP P24279
b	-9	ALA	-	expression tag	UNP P24279
b	-8	LEU	-	expression tag	UNP P24279
b	-7	GLU	-	expression tag	UNP P24279
b	-6	ASN	-	expression tag	UNP P24279
b	-5	LEU	-	expression tag	UNP P24279
b	-4	TYR	-	expression tag	UNP P24279
b	-3	PHE	-	expression tag	UNP P24279
b	-2	GLN	-	expression tag	UNP P24279
b	-1	GLY	-	expression tag	UNP P24279
b	0	GLU	-	expression tag	UNP P24279

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	4	609	Total	C	N	O	S	0	0
			4850	3055	838	930	27		
3	c	609	Total	C	N	O	S	0	0
			4850	3055	838	930	27		

- Molecule 4 is a protein called DNA helicase.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	5	690	Total	C	N	O	S	0	0
			5450	3423	948	1055	24		
4	d	690	Total	C	N	O	S	0	0
			5450	3423	948	1055	24		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	6	629	Total	C	N	O	S	0	0
			4972	3134	867	946	25		
5	e	629	Total	C	N	O	S	0	0
			4972	3134	867	946	25		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	7	658	Total	C	N	O	S	0	0
			5181	3268	897	987	29		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
6	f	658	Total	C	N	O	S	0	0
			5181	3268	897	987	29		

- Molecule 7 is a DNA chain called DNA (53-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
7	A	53	Total	C	N	O	P	0	0
			1087	530	187	317	53		

- Molecule 8 is a DNA chain called DNA (53-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
8	B	53	Total	C	N	O	P	0	0
			1086	530	184	319	53		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	C	173	Total	C	N	O	S	0	0
			1398	911	224	256	7		
9	J	173	Total	C	N	O	S	0	0
			1398	911	224	256	7		

There are 70 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-34	TRP	-	expression tag	UNP Q12146
C	-33	SER	-	expression tag	UNP Q12146
C	-32	HIS	-	expression tag	UNP Q12146
C	-31	PRO	-	expression tag	UNP Q12146
C	-30	GLN	-	expression tag	UNP Q12146
C	-29	PHE	-	expression tag	UNP Q12146
C	-28	GLU	-	expression tag	UNP Q12146
C	-27	LYS	-	expression tag	UNP Q12146
C	-26	GLY	-	expression tag	UNP Q12146
C	-25	GLY	-	expression tag	UNP Q12146
C	-24	GLY	-	expression tag	UNP Q12146
C	-23	SER	-	expression tag	UNP Q12146
C	-22	GLY	-	expression tag	UNP Q12146
C	-21	GLY	-	expression tag	UNP Q12146
C	-20	GLY	-	expression tag	UNP Q12146
C	-19	SER	-	expression tag	UNP Q12146

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	-18	GLY	-	expression tag	UNP Q12146
C	-17	GLY	-	expression tag	UNP Q12146
C	-16	GLY	-	expression tag	UNP Q12146
C	-15	SER	-	expression tag	UNP Q12146
C	-14	TRP	-	expression tag	UNP Q12146
C	-13	SER	-	expression tag	UNP Q12146
C	-12	HIS	-	expression tag	UNP Q12146
C	-11	PRO	-	expression tag	UNP Q12146
C	-10	GLN	-	expression tag	UNP Q12146
C	-9	PHE	-	expression tag	UNP Q12146
C	-8	GLU	-	expression tag	UNP Q12146
C	-7	LYS	-	expression tag	UNP Q12146
C	-6	GLU	-	expression tag	UNP Q12146
C	-5	ASN	-	expression tag	UNP Q12146
C	-4	LEU	-	expression tag	UNP Q12146
C	-3	TYR	-	expression tag	UNP Q12146
C	-2	PHE	-	expression tag	UNP Q12146
C	-1	GLN	-	expression tag	UNP Q12146
C	0	SER	-	expression tag	UNP Q12146
J	-34	TRP	-	expression tag	UNP Q12146
J	-33	SER	-	expression tag	UNP Q12146
J	-32	HIS	-	expression tag	UNP Q12146
J	-31	PRO	-	expression tag	UNP Q12146
J	-30	GLN	-	expression tag	UNP Q12146
J	-29	PHE	-	expression tag	UNP Q12146
J	-28	GLU	-	expression tag	UNP Q12146
J	-27	LYS	-	expression tag	UNP Q12146
J	-26	GLY	-	expression tag	UNP Q12146
J	-25	GLY	-	expression tag	UNP Q12146
J	-24	GLY	-	expression tag	UNP Q12146
J	-23	SER	-	expression tag	UNP Q12146
J	-22	GLY	-	expression tag	UNP Q12146
J	-21	GLY	-	expression tag	UNP Q12146
J	-20	GLY	-	expression tag	UNP Q12146
J	-19	SER	-	expression tag	UNP Q12146
J	-18	GLY	-	expression tag	UNP Q12146
J	-17	GLY	-	expression tag	UNP Q12146
J	-16	GLY	-	expression tag	UNP Q12146
J	-15	SER	-	expression tag	UNP Q12146
J	-14	TRP	-	expression tag	UNP Q12146
J	-13	SER	-	expression tag	UNP Q12146
J	-12	HIS	-	expression tag	UNP Q12146

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
J	-11	PRO	-	expression tag	UNP Q12146
J	-10	GLN	-	expression tag	UNP Q12146
J	-9	PHE	-	expression tag	UNP Q12146
J	-8	GLU	-	expression tag	UNP Q12146
J	-7	LYS	-	expression tag	UNP Q12146
J	-6	GLU	-	expression tag	UNP Q12146
J	-5	ASN	-	expression tag	UNP Q12146
J	-4	LEU	-	expression tag	UNP Q12146
J	-3	TYR	-	expression tag	UNP Q12146
J	-2	PHE	-	expression tag	UNP Q12146
J	-1	GLN	-	expression tag	UNP Q12146
J	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	242	Total	C	N	O	S	0	0
			1990	1267	328	381	14		
10	K	242	Total	C	N	O	S	0	0
			1990	1267	328	381	14		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	E	566	Total	C	N	O	S	0	0
			4599	2937	778	870	14		
11	L	566	Total	C	N	O	S	0	0
			4599	2937	778	870	14		

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	167G	TYR	-	linker	UNP Q08032
E	167H	LYS	-	linker	UNP Q08032
E	167I	ASP	-	linker	UNP Q08032
E	167J	ASP	-	linker	UNP Q08032
E	167K	ASP	-	linker	UNP Q08032
E	167L	GLY	-	linker	UNP Q08032
E	167M	ASP	-	linker	UNP Q08032
E	167N	TYR	-	linker	UNP Q08032
E	167O	LYS	-	linker	UNP Q08032
E	167P	ASP	-	linker	UNP Q08032

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	167Q	ASP	-	linker	UNP Q08032
L	167G	TYR	-	linker	UNP Q08032
L	167H	LYS	-	linker	UNP Q08032
L	167I	ASP	-	linker	UNP Q08032
L	167J	ASP	-	linker	UNP Q08032
L	167K	ASP	-	linker	UNP Q08032
L	167L	GLY	-	linker	UNP Q08032
L	167M	ASP	-	linker	UNP Q08032
L	167N	TYR	-	linker	UNP Q08032
L	167O	LYS	-	linker	UNP Q08032
L	167P	ASP	-	linker	UNP Q08032
L	167Q	ASP	-	linker	UNP Q08032

- Molecule 12 is a protein called DNA polymerase epsilon subunit B.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	F	551	Total	C	N	O	S	0	0
			4396	2819	755	804	18		
12	M	551	Total	C	N	O	S	0	0
			4396	2819	755	804	18		

- Molecule 13 is a protein called DNA replication complex GINS protein PSF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	H	208	Total	C	N	O	S	0	0
			1697	1065	290	332	10		
13	O	208	Total	C	N	O	S	0	0
			1697	1065	290	332	10		

- Molecule 14 is a protein called DNA replication complex GINS protein PSF2.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	I	189	Total	C	N	O	S	0	0
			1581	1018	277	282	4		
14	P	189	Total	C	N	O	S	0	0
			1581	1018	277	282	4		

- Molecule 15 is a protein called DNA polymerase epsilon catalytic subunit A.

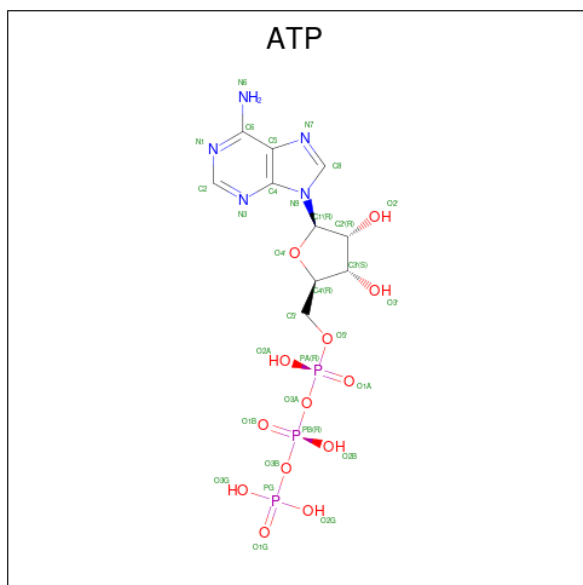
Mol	Chain	Residues	Atoms					AltConf	Trace
15	N	756	Total	C	N	O	S	0	0
			6113	3956	1006	1114	37		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	Q	756	6113	3956	1006	1114	37	0	0

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



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
16	2	1	Total 31	10	5	13	3	0
16	3	1	Total 31	10	5	13	3	0
16	5	1	Total 31	10	5	13	3	0
16	7	1	Total 31	10	5	13	3	0
16	a	1	Total 31	10	5	13	3	0
16	b	1	Total 31	10	5	13	3	0
16	d	1	Total 31	10	5	13	3	0
16	f	1	Total 31	10	5	13	3	0

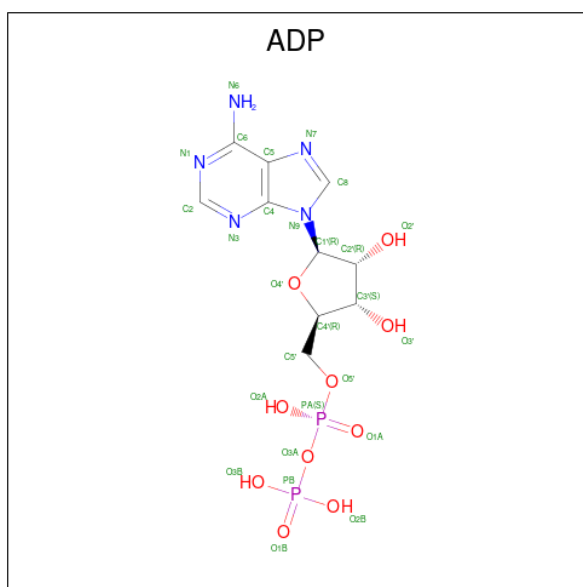
- Molecule 17 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
17	2	1	Total 1	Zn 1	0
17	4	1	Total 1	Zn 1	0
17	5	1	Total 1	Zn 1	0
17	6	1	Total 1	Zn 1	0
17	7	1	Total 1	Zn 1	0
17	N	2	Total 2	Zn 2	0
17	Q	2	Total 2	Zn 2	0
17	a	1	Total 1	Zn 1	0
17	c	1	Total 1	Zn 1	0
17	d	1	Total 1	Zn 1	0
17	e	1	Total 1	Zn 1	0
17	f	1	Total 1	Zn 1	0

- Molecule 18 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
18	3	1	Total 1	Mg 1	0
18	5	1	Total 1	Mg 1	0
18	7	1	Total 1	Mg 1	0
18	b	1	Total 1	Mg 1	0
18	d	1	Total 1	Mg 1	0
18	f	1	Total 1	Mg 1	0

- Molecule 19 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂) (labeled as "Ligand of Interest" by depositor).

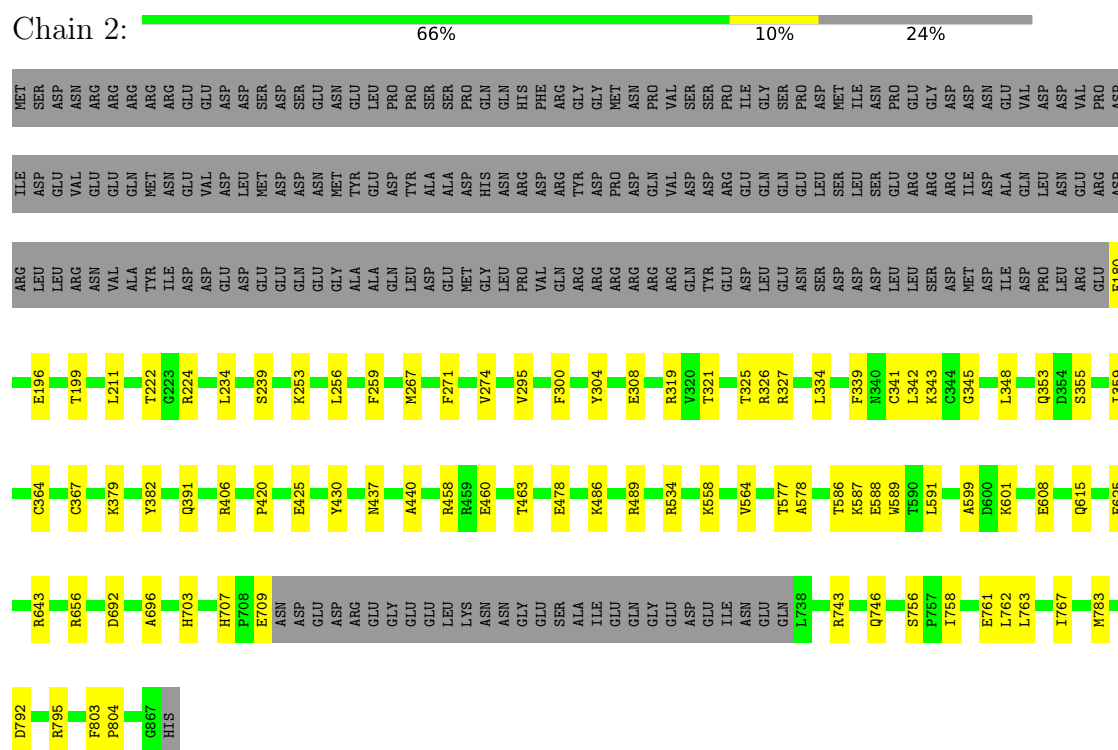


Mol	Chain	Residues	Atoms					AltConf
19	4	1	Total 27	C 10	N 5	O 10	P 2	0
19	6	1	Total 27	C 10	N 5	O 10	P 2	0
19	c	1	Total 27	C 10	N 5	O 10	P 2	0
19	e	1	Total 27	C 10	N 5	O 10	P 2	0

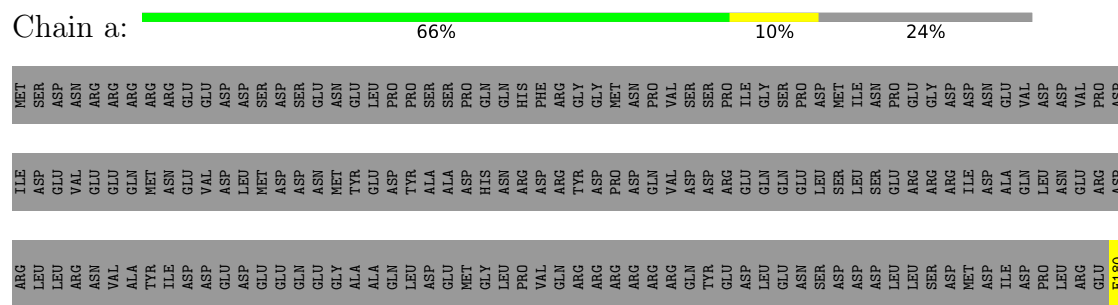
3 Residue-property plots

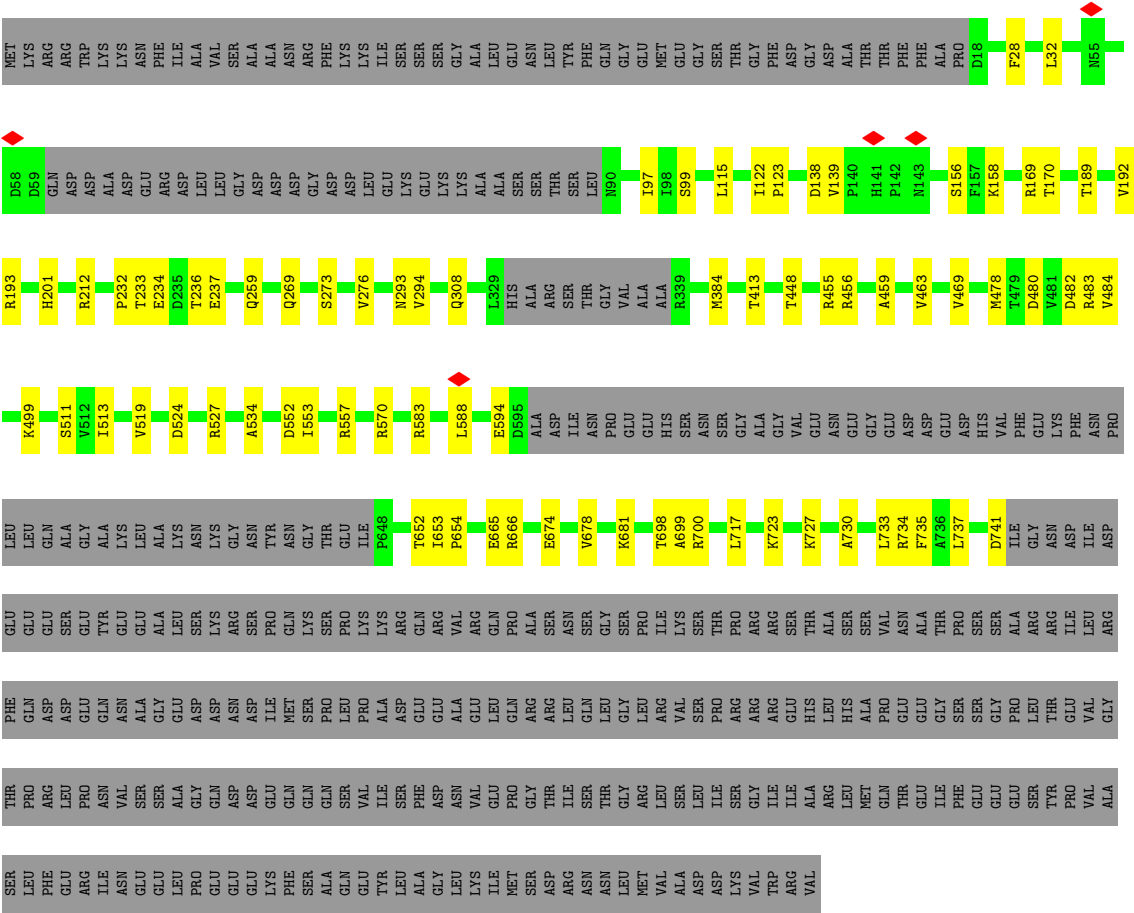
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. 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. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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

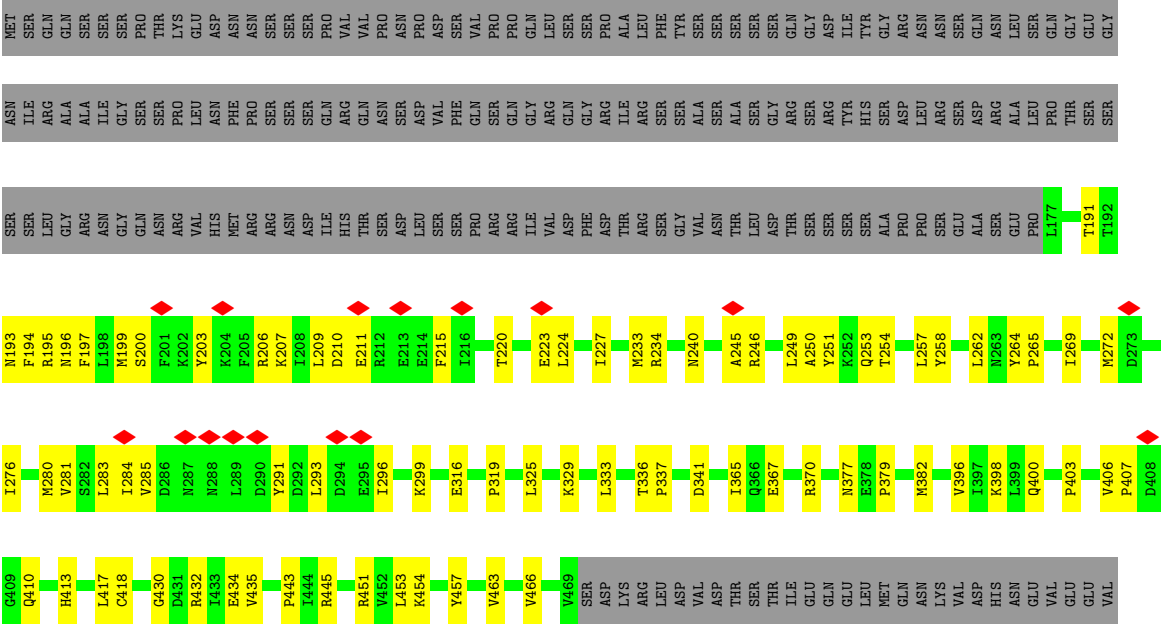


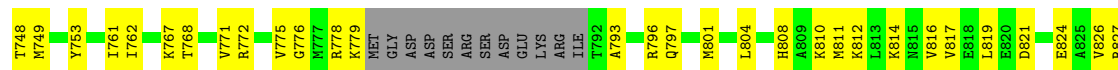
- Molecule 1: DNA replication licensing factor MCM2

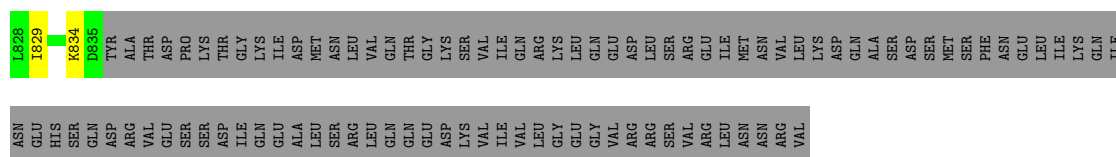




● Molecule 3: DNA replication licensing factor MCM4

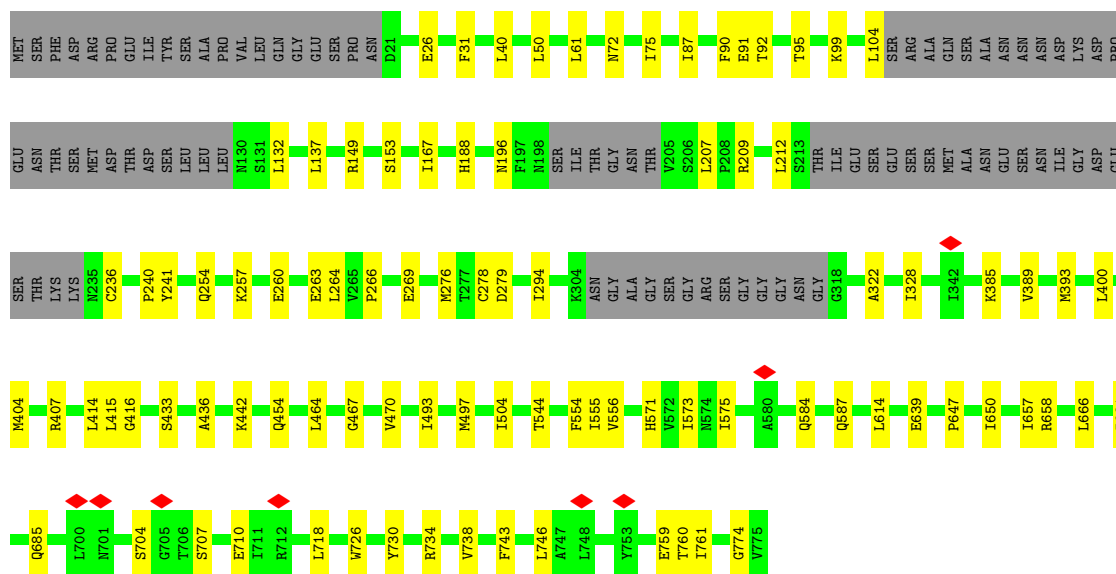






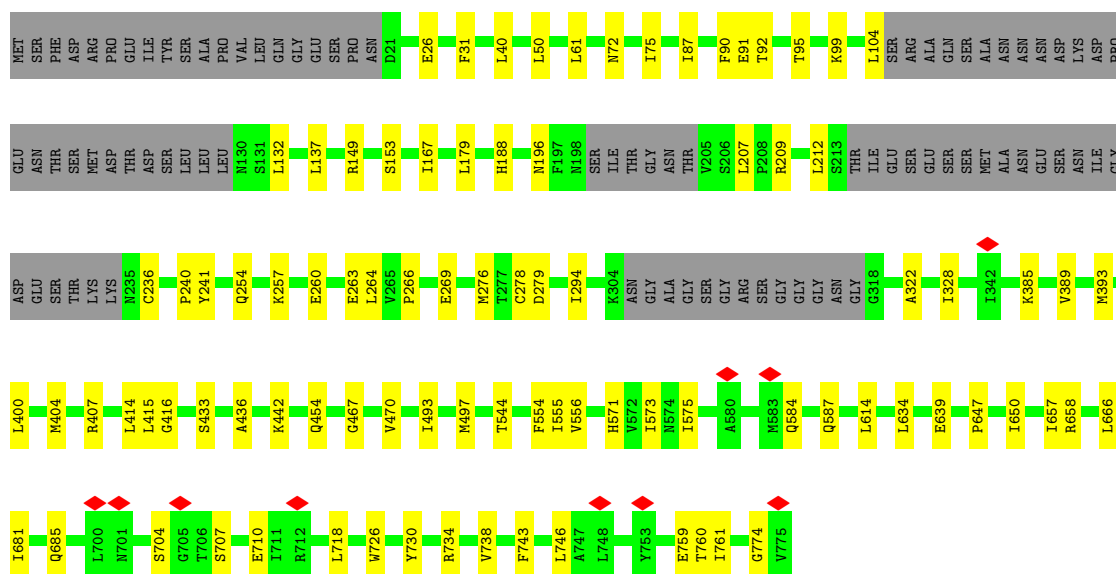
- Molecule 4: DNA helicase

Chain 5: 77% 12% 11%

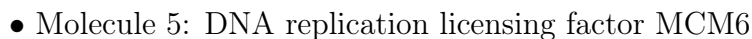


- Molecule 4: DNA helicase

Chain d: 77% 12% 11%



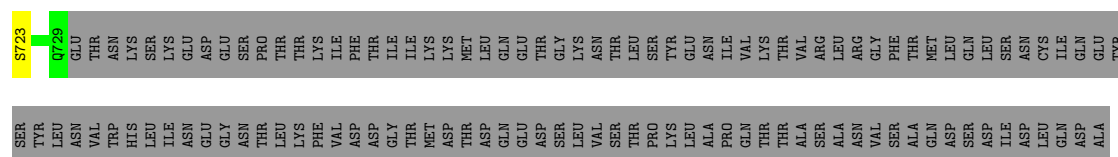
- Molecule 5: DNA replication licensing factor MCM6



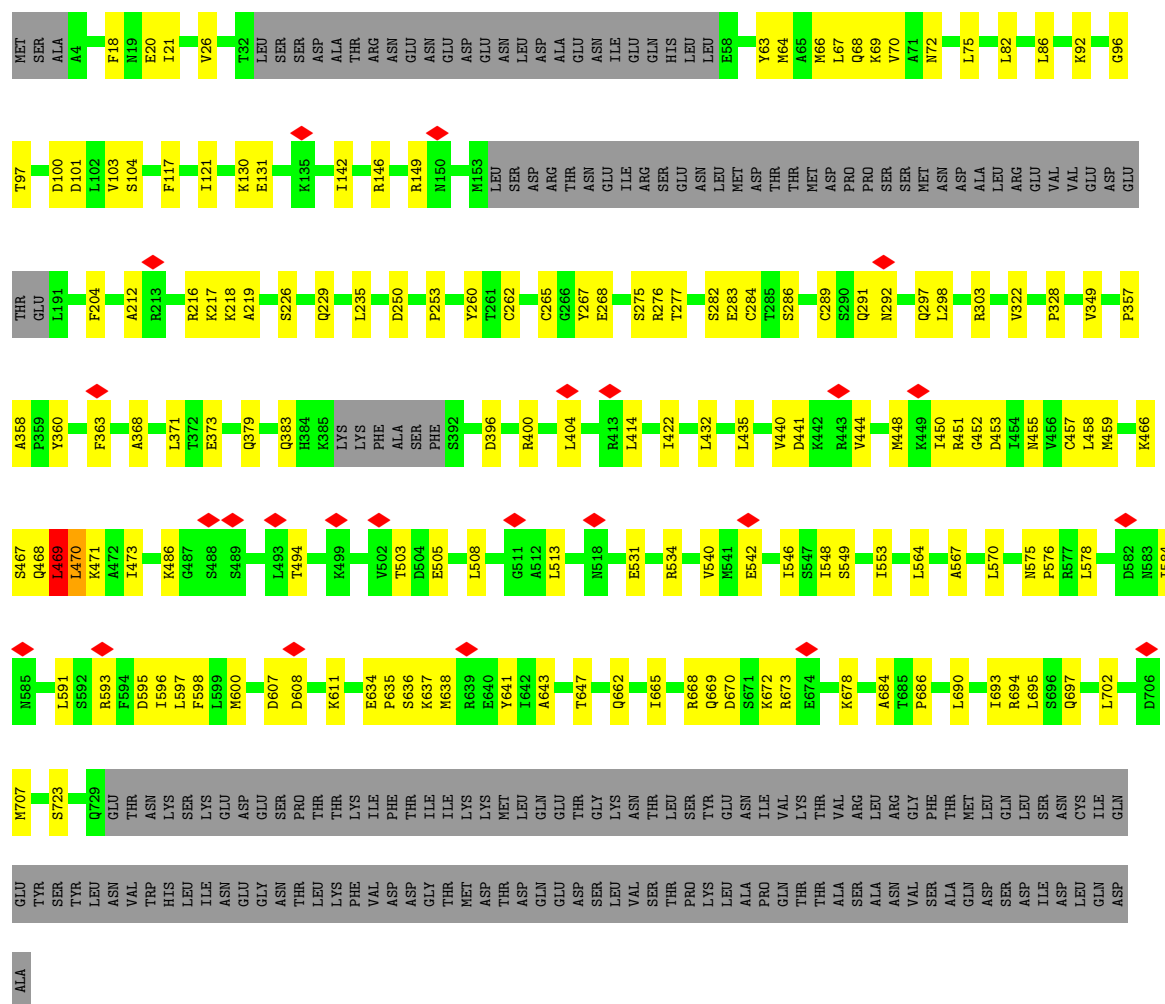


Frequency	Percentage
Daily	60%
Weekly	18%
Monthly	22%

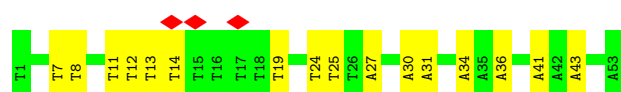




• Molecule 6: DNA replication licensing factor MCM7

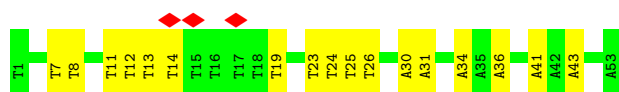


• Molecule 7: DNA (53-MER)



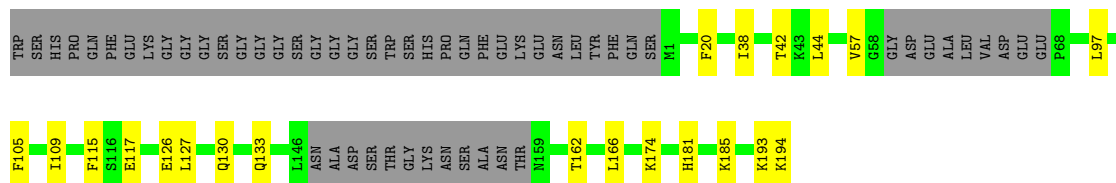
• Molecule 8: DNA (53-MER)





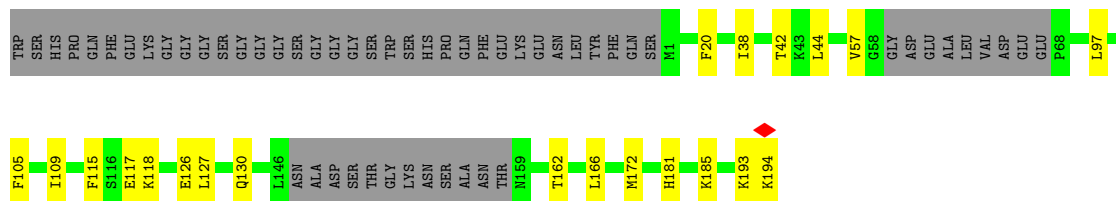
- Molecule 9: DNA replication complex GINS protein PSF3

Chain C: 66% 9% 24%



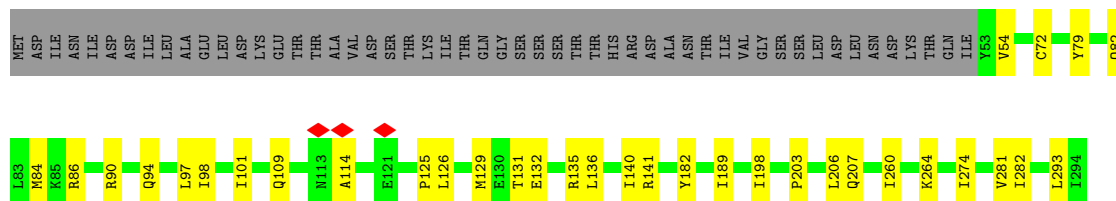
- Molecule 9: DNA replication complex GINS protein PSF3

Chain J: 66% 9% 24%



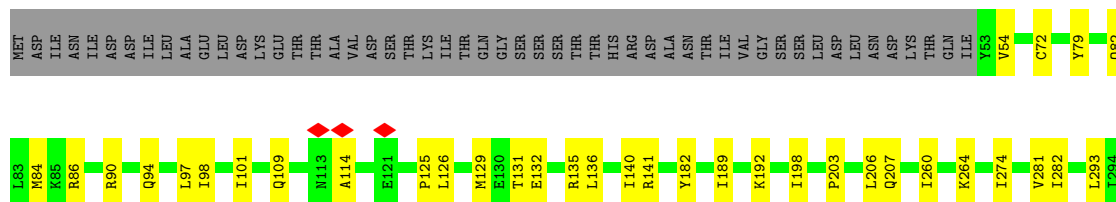
- Molecule 10: DNA replication complex GINS protein SLD5

Chain D: 71% 12% 18%



- Molecule 10: DNA replication complex GINS protein SLD5

Chain K: 70% 12% 18%

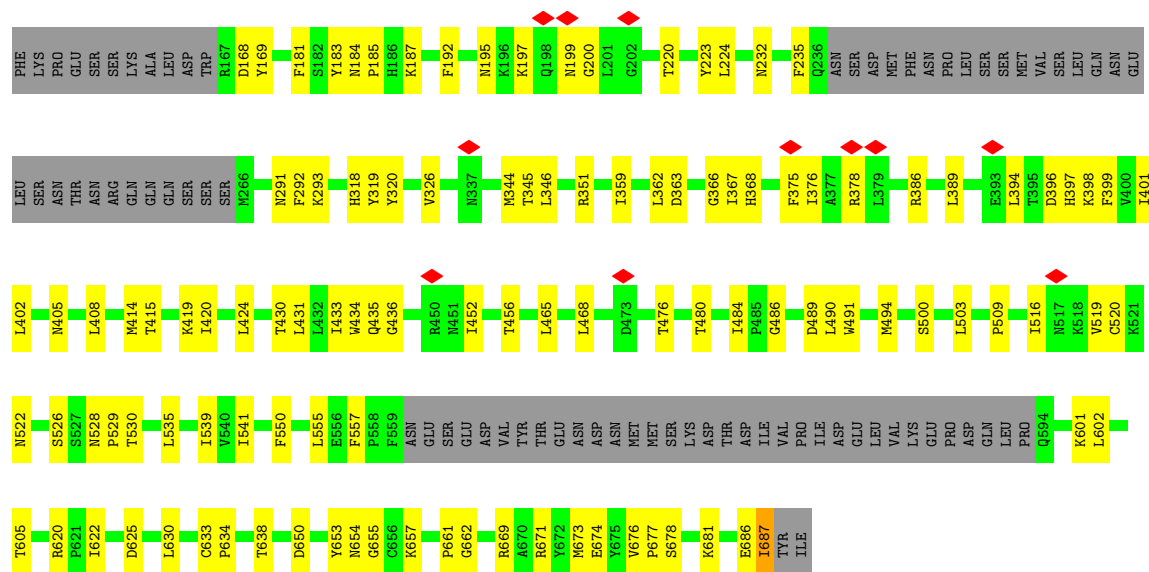


- Molecule 11: Cell division control protein 45

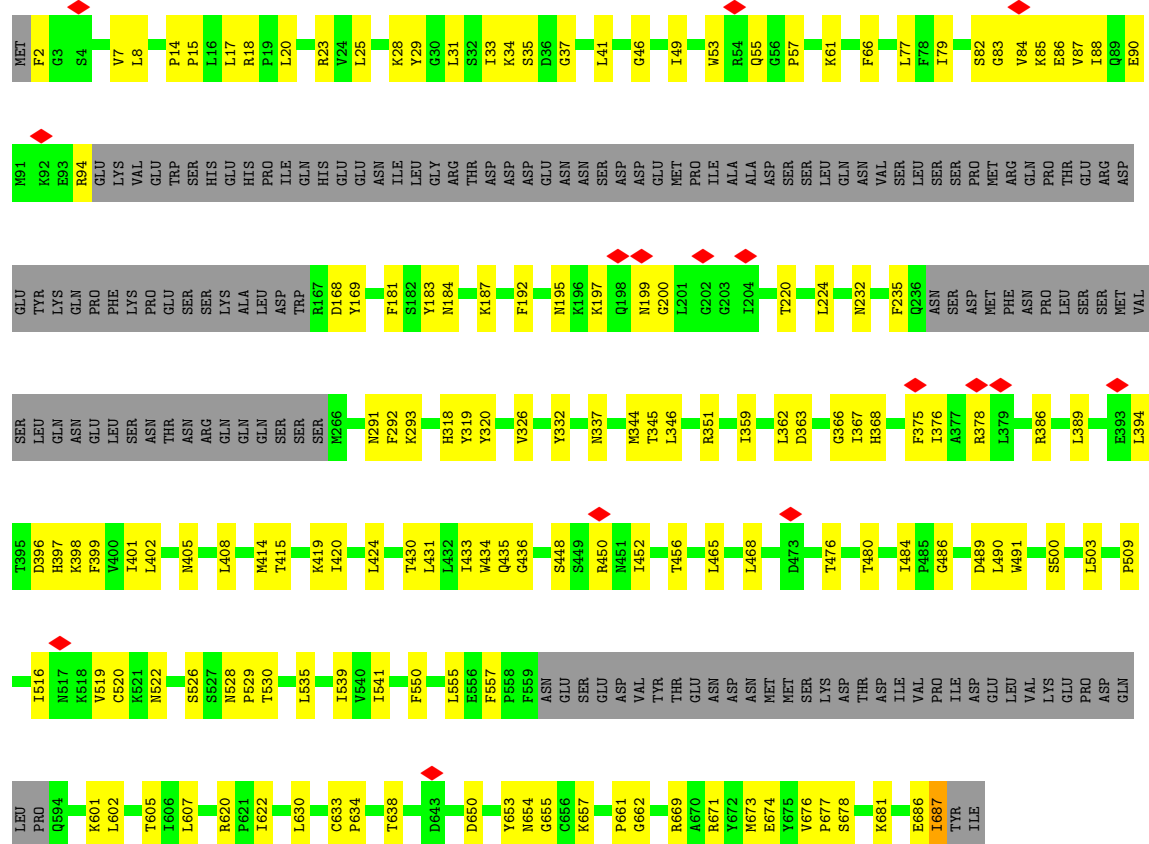
Chain E: 72% 14% 14%



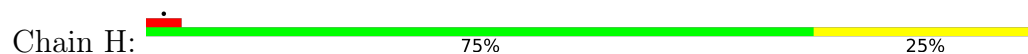


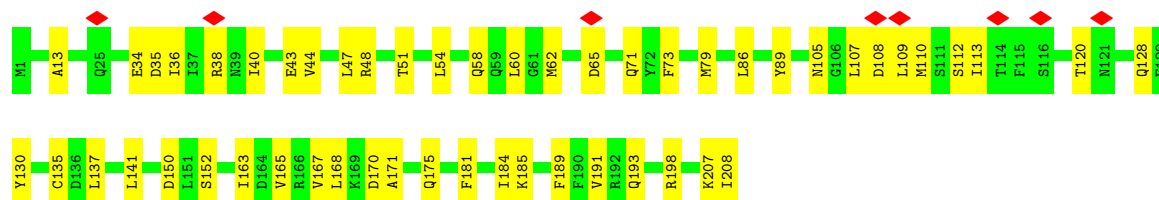


• Molecule 12: DNA polymerase epsilon subunit B

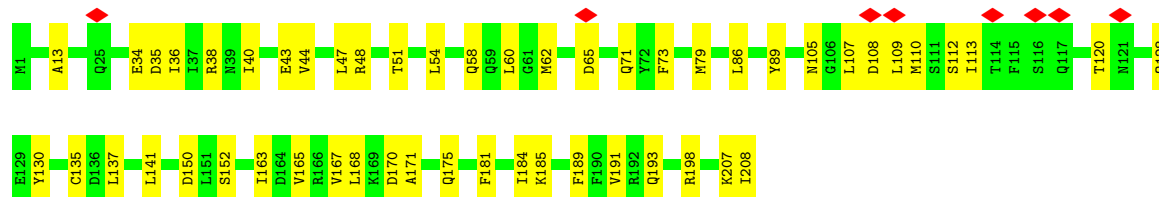
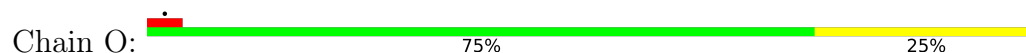


• Molecule 13: DNA replication complex GINS protein PSF1

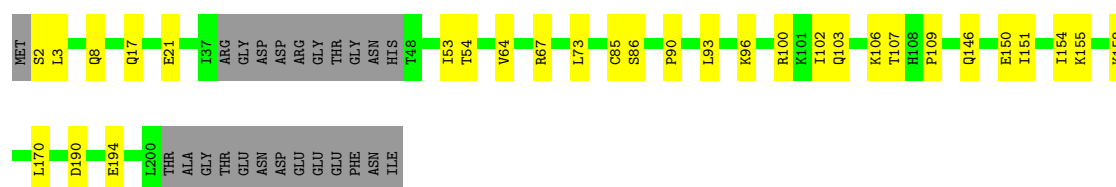




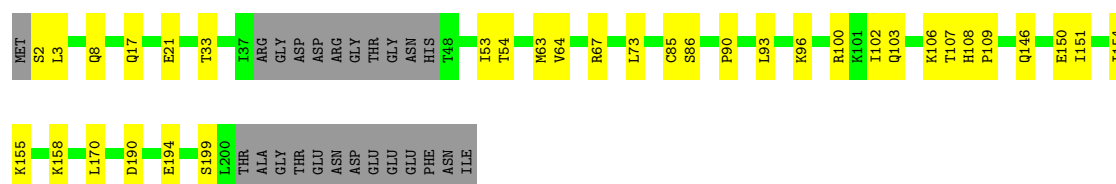
• Molecule 13: DNA replication complex GINS protein PSF1



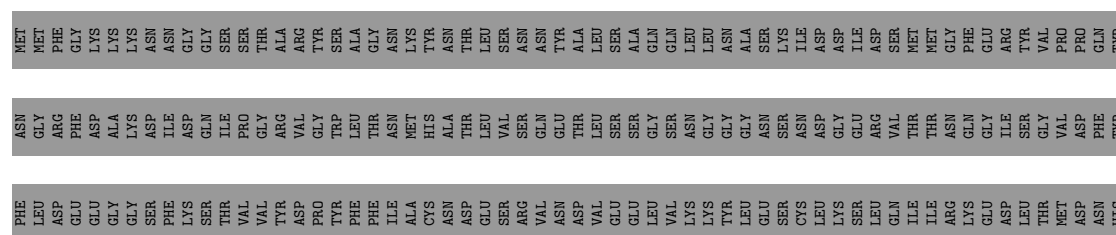
• Molecule 14: DNA replication complex GINS protein PSF2



• Molecule 14: DNA replication complex GINS protein PSF2



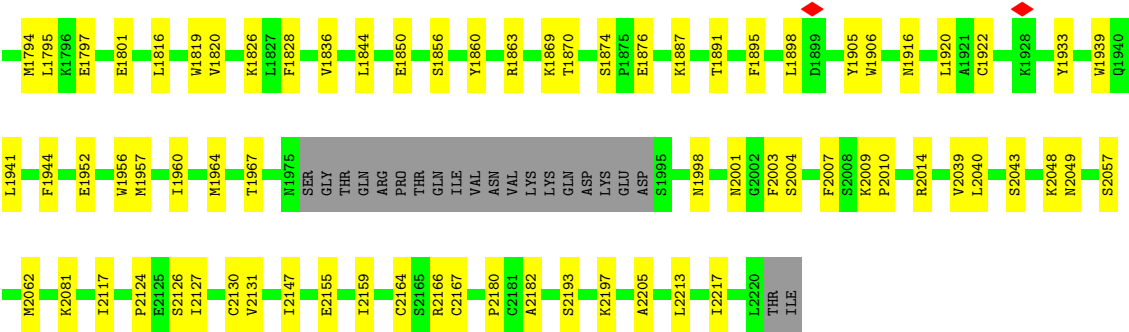
• Molecule 15: DNA polymerase epsilon catalytic subunit A











4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	71348	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.60	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	4400	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	1.913	Depositor
Minimum map value	-0.926	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.081	Depositor
Recommended contour level	0.055	Depositor
Map size (Å)	277.56, 387.72, 184.68001	wwPDB
Map dimensions	257, 359, 171	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.08, 1.08, 1.08	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ADP, ZN, MG, ATP

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	0.14	0/5319	0.37	0/7182
1	a	0.14	0/5319	0.37	0/7182
2	3	0.14	0/5044	0.35	0/6842
2	b	0.13	0/5044	0.35	0/6842
3	4	0.15	0/4921	0.40	0/6651
3	c	0.15	0/4921	0.40	0/6651
4	5	0.15	0/5530	0.37	0/7471
4	d	0.14	0/5530	0.37	0/7471
5	6	0.18	0/5051	0.41	2/6813 (0.0%)
5	e	0.18	0/5051	0.42	2/6813 (0.0%)
6	7	0.20	1/5261 (0.0%)	0.43	2/7110 (0.0%)
6	f	0.20	1/5261 (0.0%)	0.43	2/7110 (0.0%)
7	A	0.27	0/1219	0.50	1/1879 (0.1%)
8	B	0.25	0/1217	0.52	0/1876
9	C	0.13	0/1431	0.32	0/1933
9	J	0.13	0/1431	0.32	0/1933
10	D	0.17	0/2032	0.38	0/2750
10	K	0.17	0/2032	0.38	0/2750
11	E	0.14	0/4685	0.34	0/6341
11	L	0.14	0/4685	0.34	0/6341
12	F	0.19	0/4492	0.46	0/6078
12	M	0.18	0/4492	0.45	0/6078
13	H	0.16	0/1719	0.41	0/2314
13	O	0.16	0/1719	0.41	0/2314
14	I	0.14	0/1613	0.38	0/2182
14	P	0.14	0/1613	0.37	0/2182
15	N	0.16	0/6250	0.41	0/8458
15	Q	0.15	0/6250	0.41	0/8458
All	All	0.16	2/109132 (0.0%)	0.40	9/148005 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	7	467	SER	CA-CB	-5.77	1.45	1.53
6	f	467	SER	CA-CB	-5.70	1.45	1.53

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	f	468	GLN	N-CA-C	-10.62	100.82	113.88
6	7	468	GLN	N-CA-C	-10.61	100.83	113.88
5	e	333	CYS	CA-C-N	8.11	128.06	119.05
5	e	333	CYS	C-N-CA	8.11	128.06	119.05
5	6	334	PRO	N-CA-C	5.58	123.97	112.47

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	2	5231	0	5280	60	0
1	a	5231	0	5280	62	0
2	3	4958	0	5005	43	0
2	b	4958	0	5005	47	0
3	4	4850	0	4926	120	0
3	c	4850	0	4926	118	0
4	5	5450	0	5510	61	0
4	d	5450	0	5510	61	0
5	6	4972	0	5007	83	0
5	e	4972	0	5007	79	0
6	7	5181	0	5258	107	0
6	f	5181	0	5258	107	0
7	A	1087	0	610	12	0
8	B	1086	0	611	14	0
9	C	1398	0	1418	13	0
9	J	1398	0	1418	14	0
10	D	1990	0	1985	27	0
10	K	1990	0	1985	27	0
11	E	4599	0	4603	54	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	L	4599	0	4603	52	0
12	F	4396	0	4442	106	0
12	M	4396	0	4442	103	0
13	H	1697	0	1698	39	0
13	O	1697	0	1698	40	0
14	I	1581	0	1635	21	0
14	P	1581	0	1635	23	0
15	N	6113	0	6177	98	0
15	Q	6113	0	6177	101	0
16	2	31	0	12	0	0
16	3	31	0	12	0	0
16	5	31	0	12	0	0
16	7	31	0	12	1	0
16	a	31	0	12	0	0
16	b	31	0	12	0	0
16	d	31	0	12	0	0
16	f	31	0	12	1	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
17	N	2	0	0	0	0
17	Q	2	0	0	0	0
17	a	1	0	0	0	0
17	c	1	0	0	0	0
17	d	1	0	0	0	0
17	e	1	0	0	0	0
17	f	1	0	0	0	0
18	3	1	0	0	0	0
18	5	1	0	0	0	0
18	7	1	0	0	0	0
18	b	1	0	0	0	0
18	d	1	0	0	0	0
18	f	1	0	0	0	0
19	4	27	0	12	0	0
19	6	27	0	12	4	0
19	c	27	0	12	0	0
19	e	27	0	12	3	0
All	All	107381	0	107253	1559	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 1559 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)
5:6:333:CYS:SG	5:6:334:PRO:HD2	1.73	1.28
5:6:333:CYS:SG	5:6:334:PRO:CD	2.30	1.17
5:e:333:CYS:SG	5:e:334:PRO:HD2	2.09	0.92
12:M:526:SER:HB2	12:M:530:THR:HG21	1.48	0.92
12:F:526:SER:HB2	12:F:530:THR:HG21	1.48	0.91

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	656/868 (76%)	642 (98%)	14 (2%)	0	100	100
1	a	656/868 (76%)	641 (98%)	15 (2%)	0	100	100
2	3	625/1006 (62%)	609 (97%)	16 (3%)	0	100	100
2	b	625/1006 (62%)	609 (97%)	16 (3%)	0	100	100
3	4	601/933 (64%)	579 (96%)	22 (4%)	0	100	100
3	c	601/933 (64%)	579 (96%)	22 (4%)	0	100	100
4	5	680/775 (88%)	653 (96%)	27 (4%)	0	100	100
4	d	680/775 (88%)	653 (96%)	27 (4%)	0	100	100
5	6	619/1017 (61%)	594 (96%)	22 (4%)	3 (0%)	24	54
5	e	619/1017 (61%)	596 (96%)	22 (4%)	1 (0%)	43	71
6	7	650/845 (77%)	614 (94%)	36 (6%)	0	100	100
6	f	650/845 (77%)	614 (94%)	36 (6%)	0	100	100
9	C	167/229 (73%)	164 (98%)	3 (2%)	0	100	100
9	J	167/229 (73%)	164 (98%)	3 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	D	240/294 (82%)	231 (96%)	9 (4%)	0	100	100
10	K	240/294 (82%)	231 (96%)	9 (4%)	0	100	100
11	E	558/657 (85%)	546 (98%)	12 (2%)	0	100	100
11	L	558/657 (85%)	546 (98%)	12 (2%)	0	100	100
12	F	543/689 (79%)	510 (94%)	33 (6%)	0	100	100
12	M	543/689 (79%)	510 (94%)	33 (6%)	0	100	100
13	H	206/208 (99%)	195 (95%)	11 (5%)	0	100	100
13	O	206/208 (99%)	195 (95%)	11 (5%)	0	100	100
14	I	185/213 (87%)	174 (94%)	11 (6%)	0	100	100
14	P	185/213 (87%)	174 (94%)	11 (6%)	0	100	100
15	N	748/2222 (34%)	716 (96%)	32 (4%)	0	100	100
15	Q	748/2222 (34%)	715 (96%)	33 (4%)	0	100	100
All	All	12956/19912 (65%)	12454 (96%)	498 (4%)	4 (0%)	100	100

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	6	334	PRO
5	6	336	PRO
5	e	337	SER
5	6	335	ASN

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	2	578/770 (75%)	578 (100%)	0	100	100
1	a	578/770 (75%)	578 (100%)	0	100	100
2	3	549/864 (64%)	549 (100%)	0	100	100
2	b	549/864 (64%)	549 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	4	551/848 (65%)	551 (100%)	0	100	100
3	c	551/848 (65%)	551 (100%)	0	100	100
4	5	618/688 (90%)	618 (100%)	0	100	100
4	d	618/688 (90%)	618 (100%)	0	100	100
5	6	549/886 (62%)	546 (100%)	3 (0%)	81	81
5	e	549/886 (62%)	545 (99%)	4 (1%)	76	78
6	7	580/753 (77%)	577 (100%)	3 (0%)	81	81
6	f	580/753 (77%)	577 (100%)	3 (0%)	81	81
9	C	157/199 (79%)	157 (100%)	0	100	100
9	J	157/199 (79%)	157 (100%)	0	100	100
10	D	232/279 (83%)	232 (100%)	0	100	100
10	K	232/279 (83%)	232 (100%)	0	100	100
11	E	512/592 (86%)	512 (100%)	0	100	100
11	L	512/592 (86%)	512 (100%)	0	100	100
12	F	494/629 (78%)	493 (100%)	1 (0%)	87	85
12	M	494/629 (78%)	493 (100%)	1 (0%)	87	85
13	H	193/193 (100%)	193 (100%)	0	100	100
13	O	193/193 (100%)	193 (100%)	0	100	100
14	I	179/198 (90%)	179 (100%)	0	100	100
14	P	179/198 (90%)	179 (100%)	0	100	100
15	N	694/2014 (34%)	694 (100%)	0	100	100
15	Q	694/2014 (34%)	694 (100%)	0	100	100
All	All	11772/17826 (66%)	11757 (100%)	15 (0%)	87	89

5 of 15 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
12	M	687	ILE
6	f	469	LEU
5	e	269	ASN
6	f	470	LEU
5	e	339	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 127 such sidechains are listed below:

Mol	Chain	Res	Type
10	K	69	ASN
4	d	155	HIS
15	N	1391	ASN
3	c	646	HIS
5	e	434	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 32 ligands modelled in this entry, 20 are monoatomic - leaving 12 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	ATP	3	1101	18	32,33,33	0.34	0	48,52,52	0.31	0
16	ATP	5	1701	18	32,33,33	0.37	0	48,52,52	0.32	0
19	ADP	c	1001	-	28,29,29	1.42	4 (14%)	43,45,45	1.87	8 (18%)
16	ATP	7	901	18	32,33,33	0.30	0	48,52,52	0.38	0
19	ADP	e	1201	-	28,29,29	1.39	4 (14%)	43,45,45	1.79	9 (20%)
19	ADP	4	1001	-	28,29,29	1.41	4 (14%)	43,45,45	1.86	8 (18%)
16	ATP	f	901	18	32,33,33	0.30	0	48,52,52	0.38	0
16	ATP	a	901	-	32,33,33	0.29	0	48,52,52	0.33	0
19	ADP	6	1201	-	28,29,29	1.40	4 (14%)	43,45,45	1.80	10 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	ATP	2	901	-	32,33,33	0.29	0	48,52,52	0.33	0
16	ATP	d	1701	18	32,33,33	0.37	0	48,52,52	0.31	0
16	ATP	b	1101	18	32,33,33	0.34	0	48,52,52	0.31	0

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	ATP	3	1101	18	-	1/22/38/38	0/3/3/3
16	ATP	5	1701	18	-	0/22/38/38	0/3/3/3
19	ADP	c	1001	-	-	4/16/32/32	0/3/3/3
16	ATP	7	901	18	-	8/22/38/38	0/3/3/3
19	ADP	e	1201	-	-	6/16/32/32	0/3/3/3
19	ADP	4	1001	-	-	4/16/32/32	0/3/3/3
16	ATP	f	901	18	-	8/22/38/38	0/3/3/3
16	ATP	a	901	-	-	5/22/38/38	0/3/3/3
19	ADP	6	1201	-	-	6/16/32/32	0/3/3/3
16	ATP	2	901	-	-	5/22/38/38	0/3/3/3
16	ATP	d	1701	18	-	0/22/38/38	0/3/3/3
16	ATP	b	1101	18	-	1/22/38/38	0/3/3/3

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	c	1001	ADP	C5-C4	4.74	1.47	1.39
19	4	1001	ADP	C5-C4	4.73	1.47	1.39
19	6	1201	ADP	C5-C4	4.65	1.47	1.39
19	e	1201	ADP	C5-C4	4.64	1.47	1.39
19	c	1001	ADP	C5-C6	2.71	1.48	1.41

The worst 5 of 35 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	4	1001	ADP	C5-C4-N3	-6.22	118.16	126.72
19	c	1001	ADP	C5-C4-N3	-6.22	118.16	126.72
19	6	1201	ADP	C5-C4-N3	-5.68	118.90	126.72
19	e	1201	ADP	C5-C4-N3	-5.61	118.99	126.72
19	4	1001	ADP	N3-C4-N9	4.92	135.54	127.17

There are no chirality outliers.

5 of 48 torsion outliers are listed below:

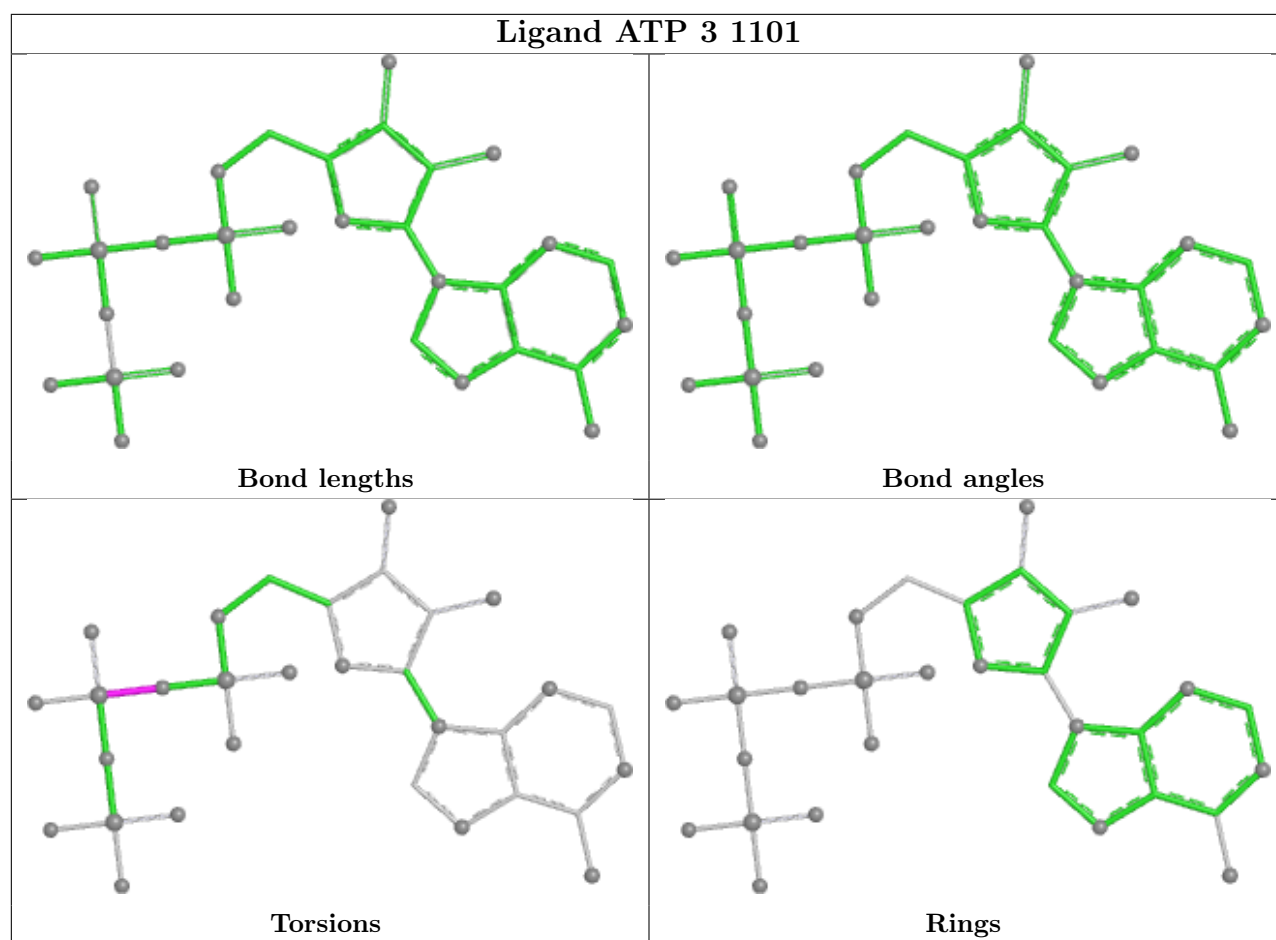
Mol	Chain	Res	Type	Atoms
16	7	901	ATP	PB-O3B-PG-O2G
16	7	901	ATP	C5'-O5'-PA-O3A
16	7	901	ATP	C4'-C5'-O5'-PA
16	f	901	ATP	PB-O3B-PG-O2G
16	f	901	ATP	C5'-O5'-PA-O3A

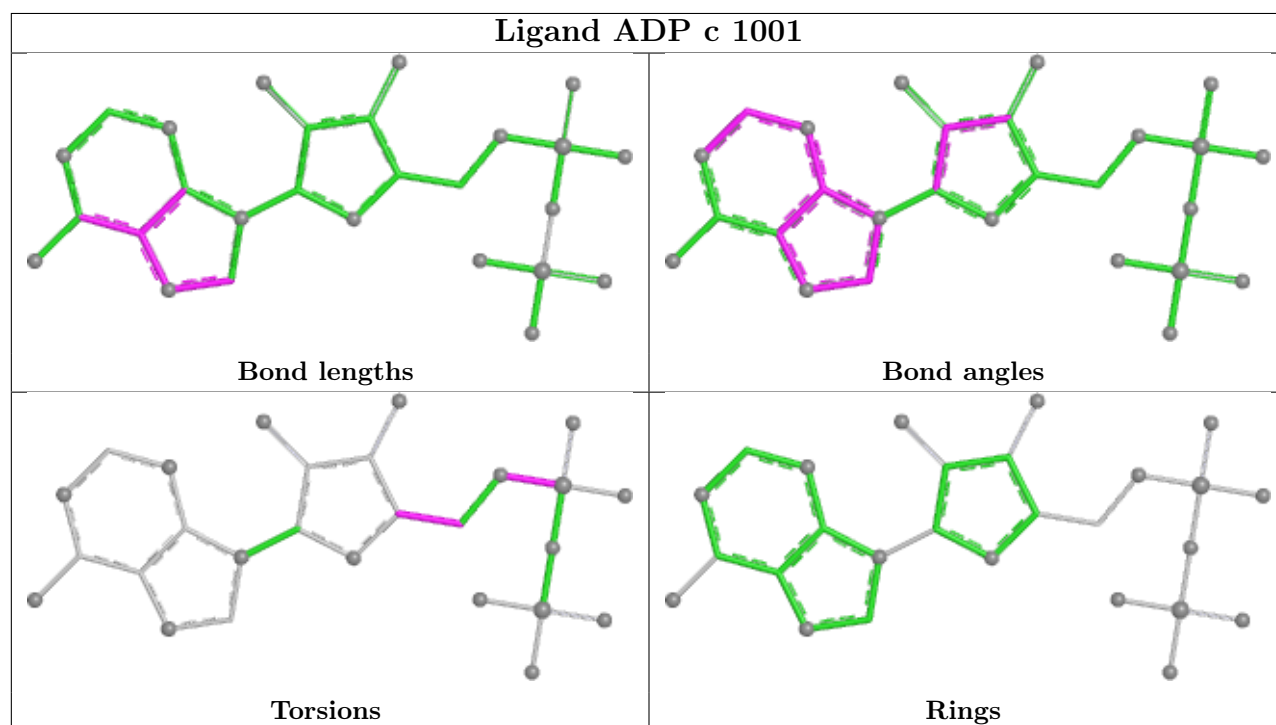
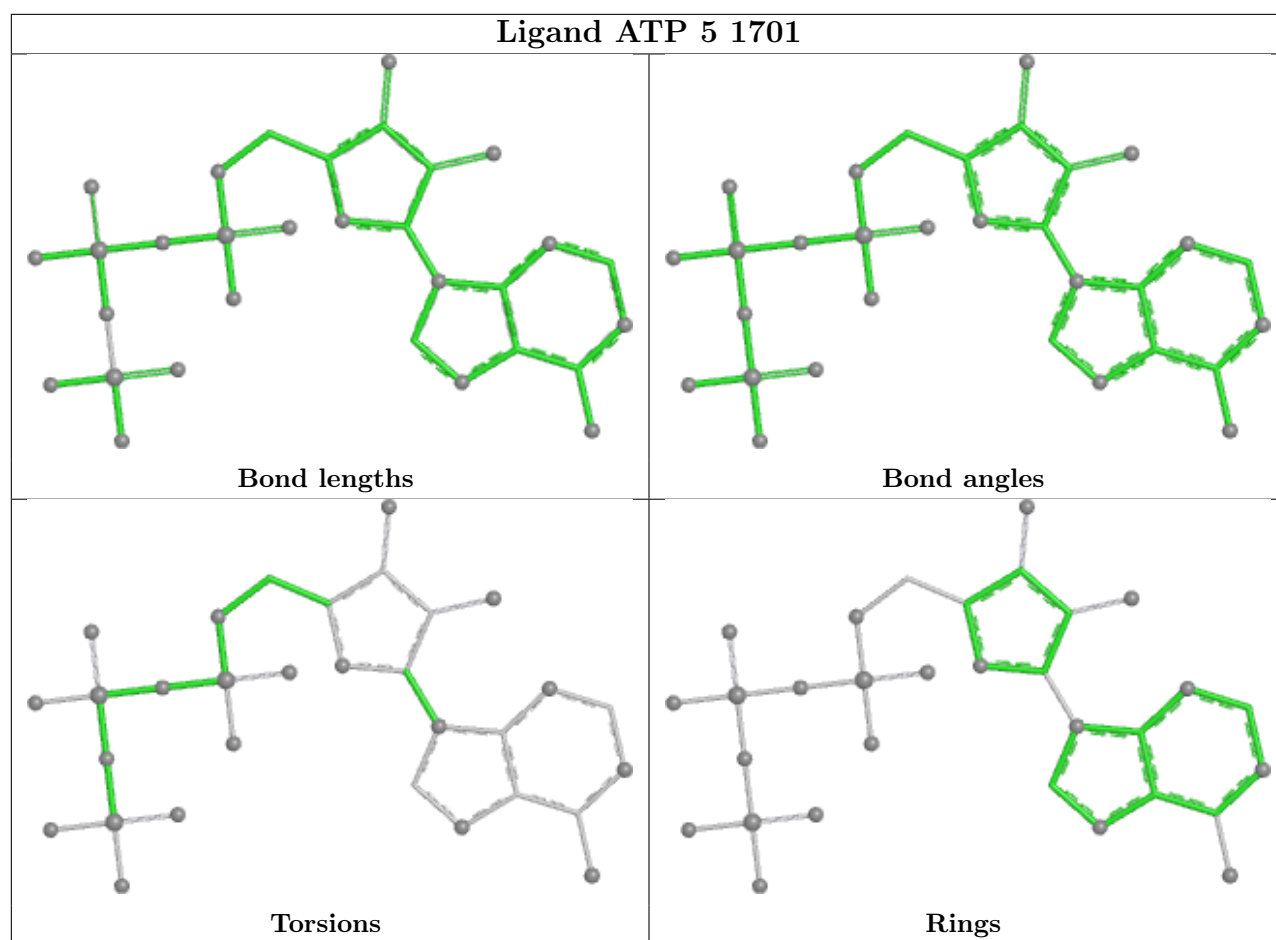
There are no ring outliers.

4 monomers are involved in 9 short contacts:

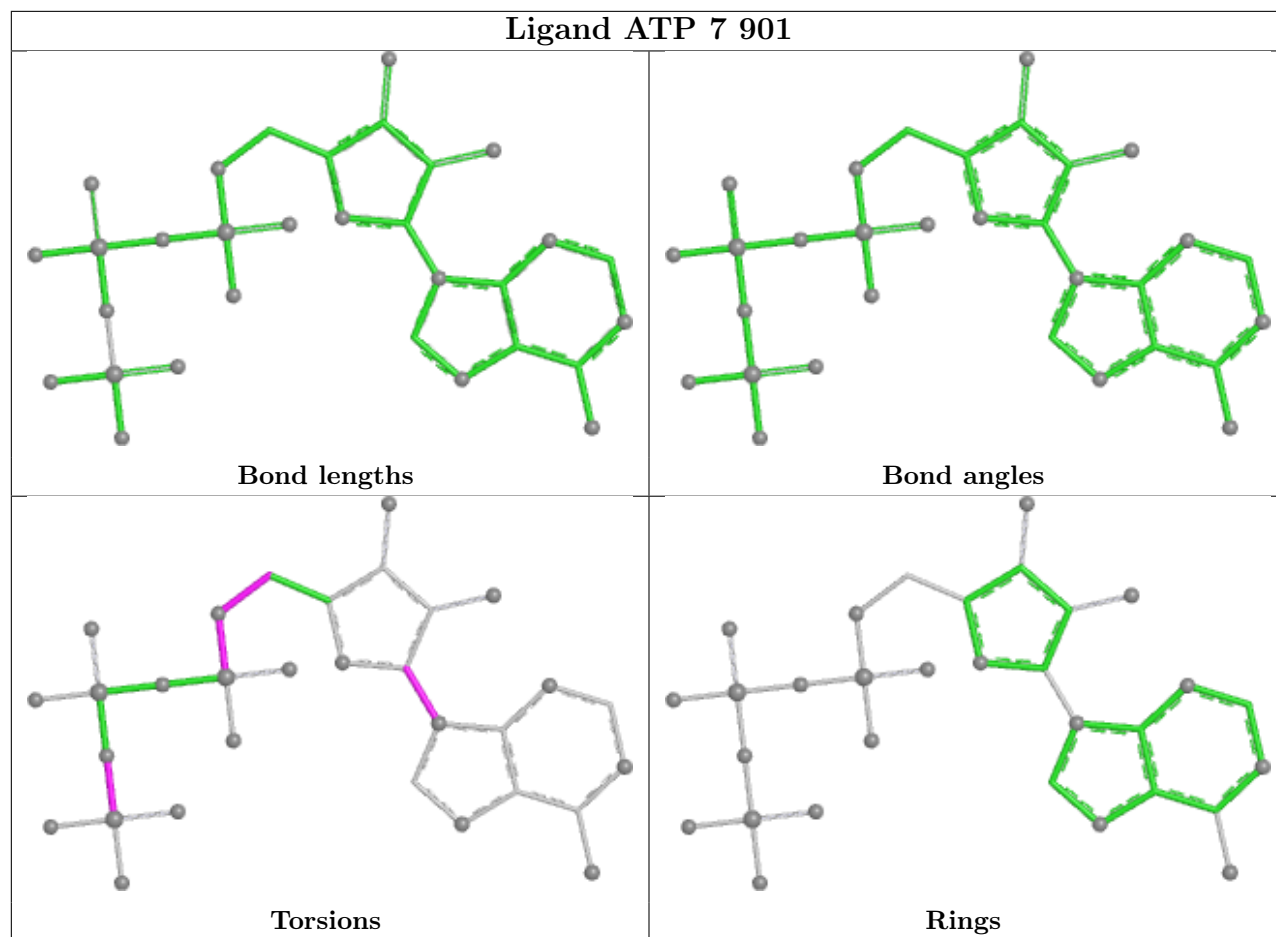
Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	7	901	ATP	1	0
19	e	1201	ADP	3	0
16	f	901	ATP	1	0
19	6	1201	ADP	4	0

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.

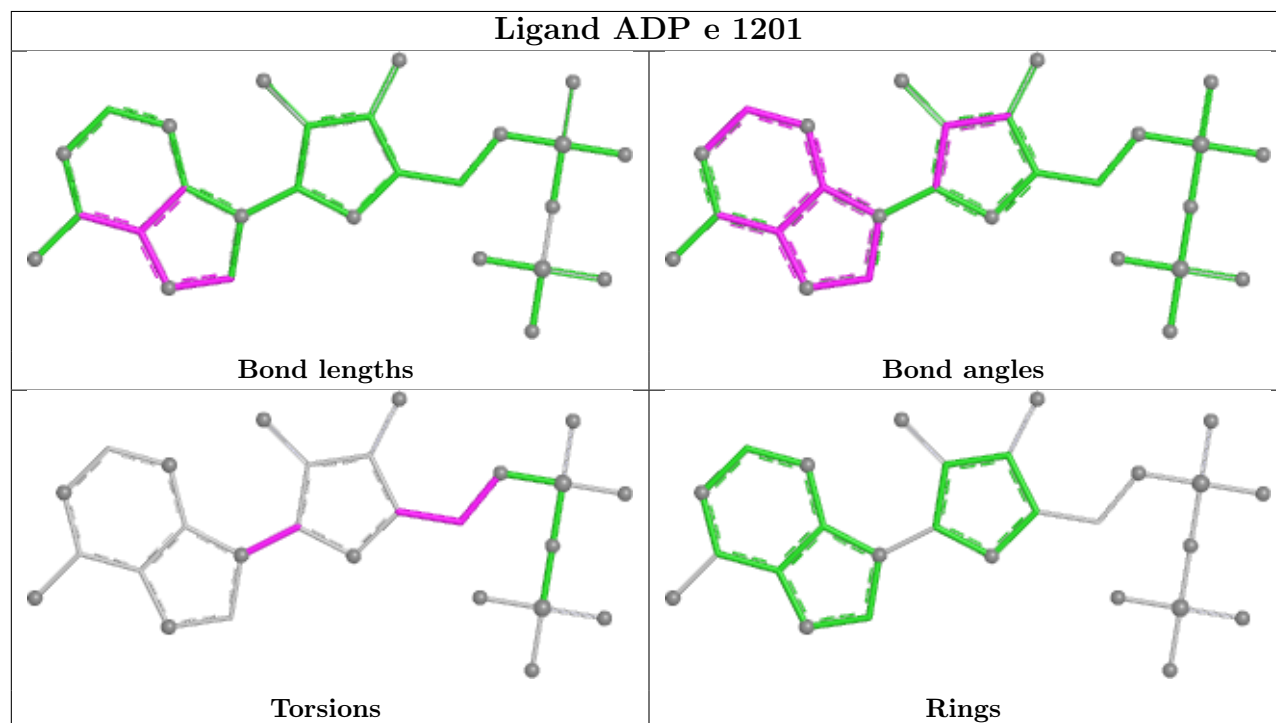


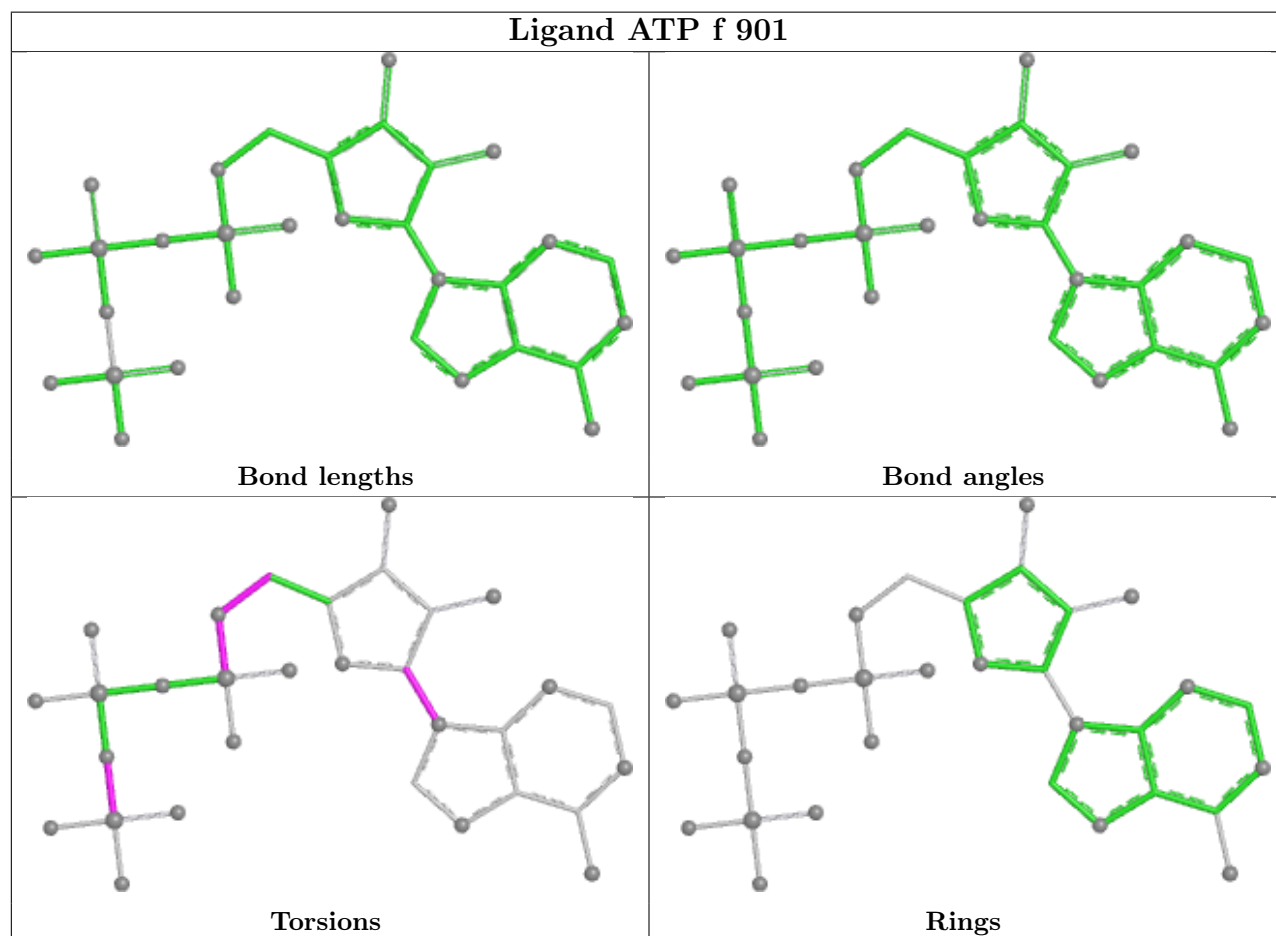
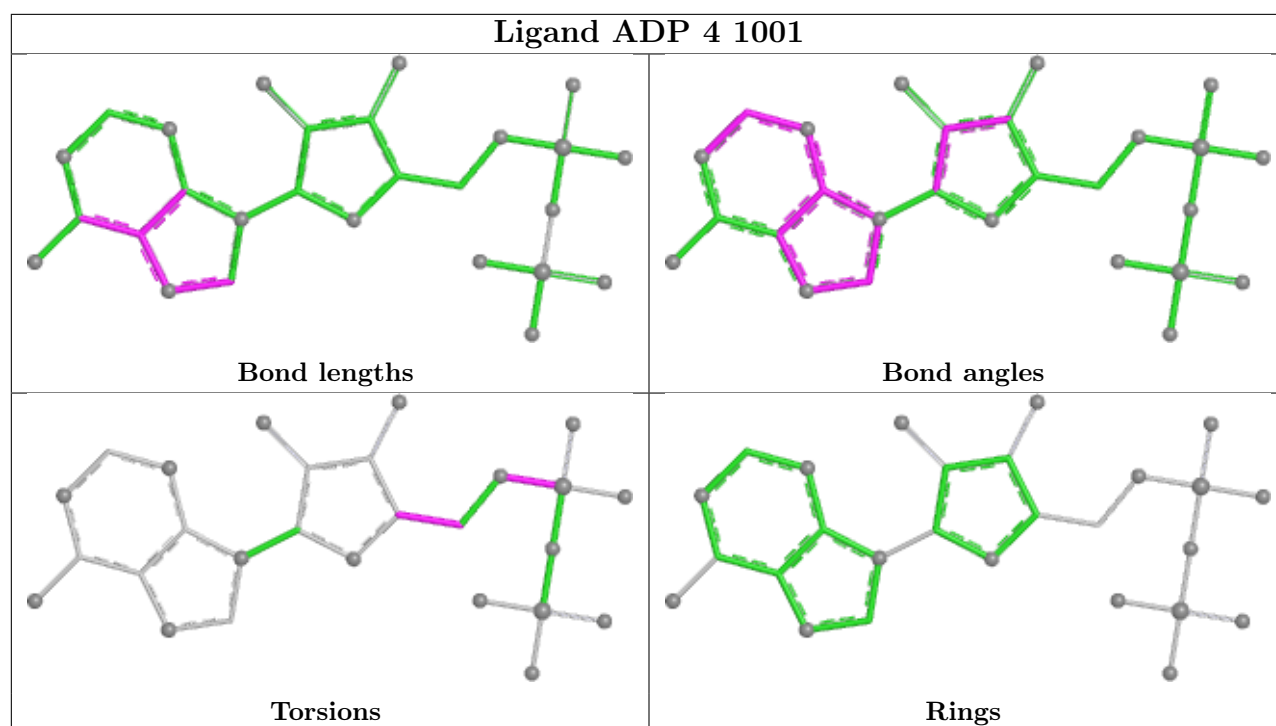


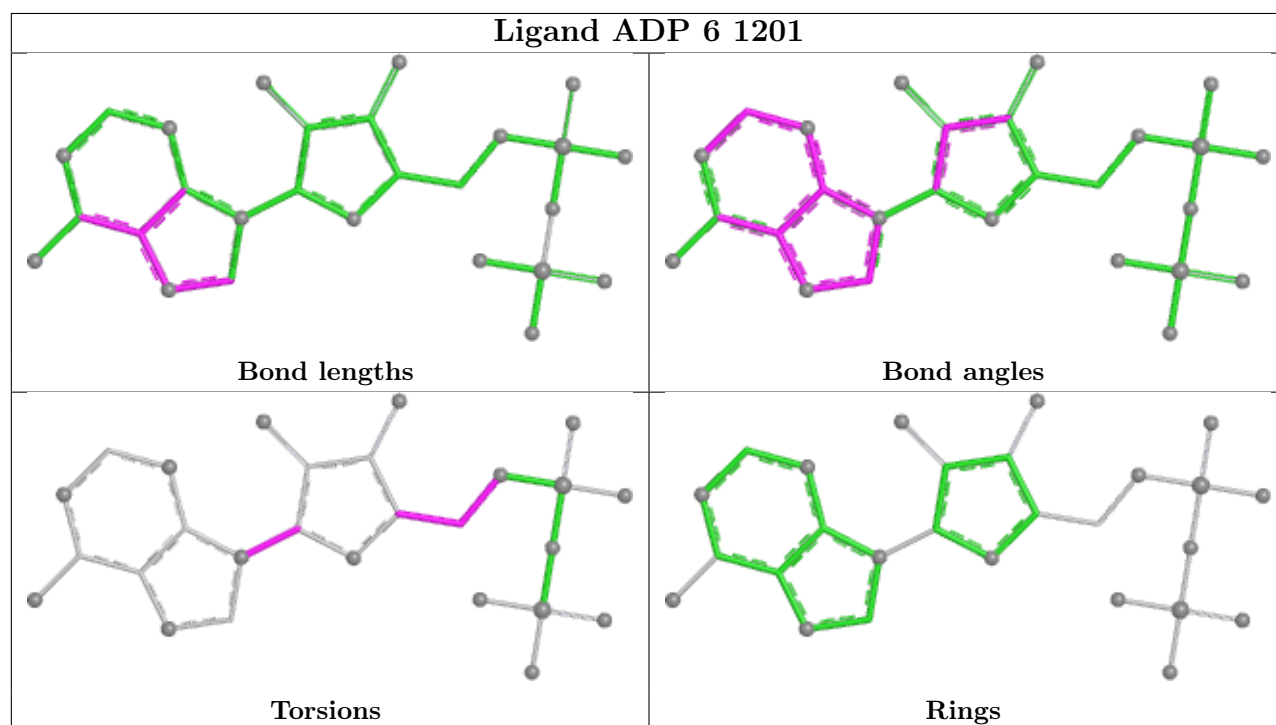
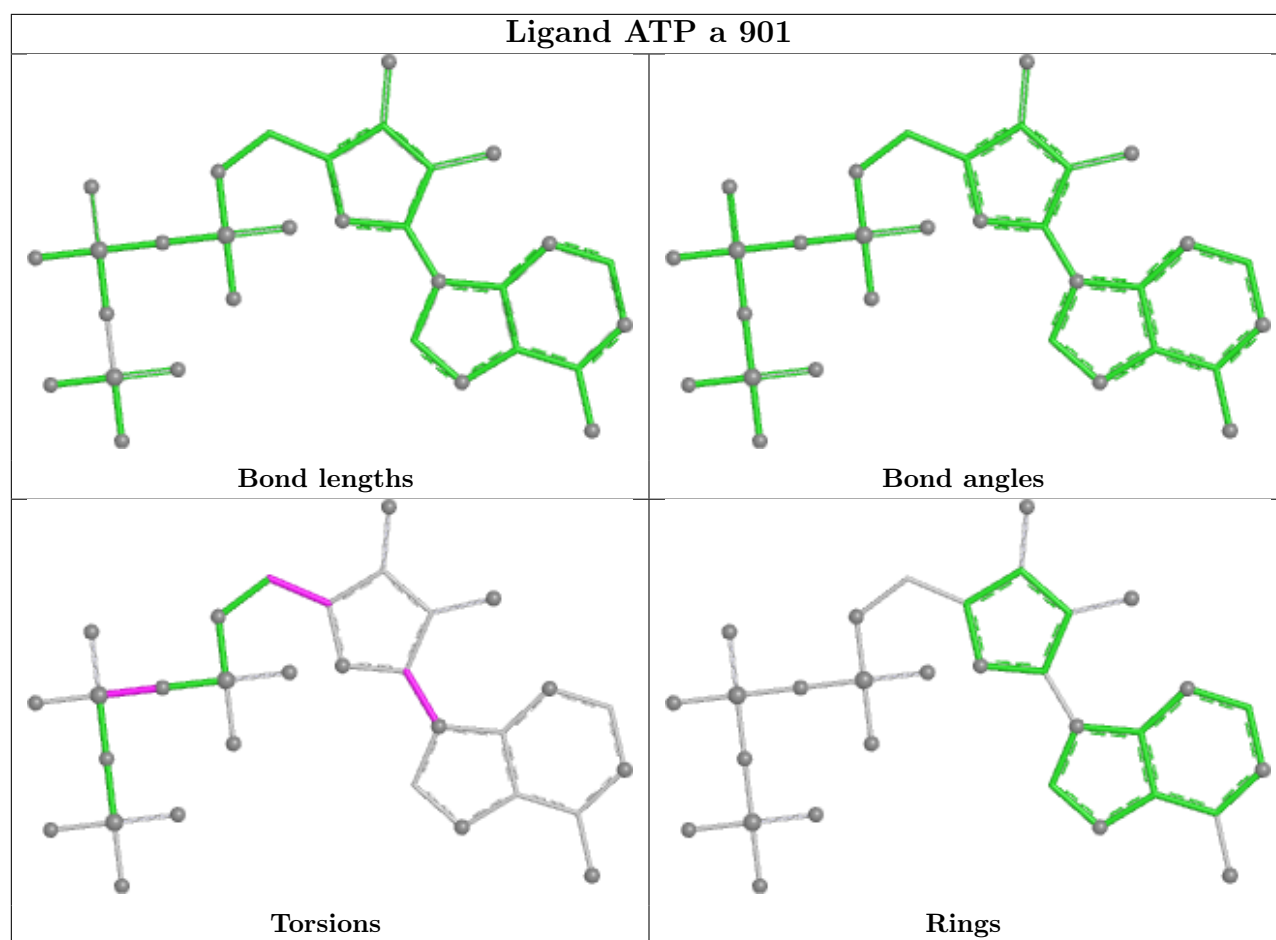
Ligand ATP 7 901

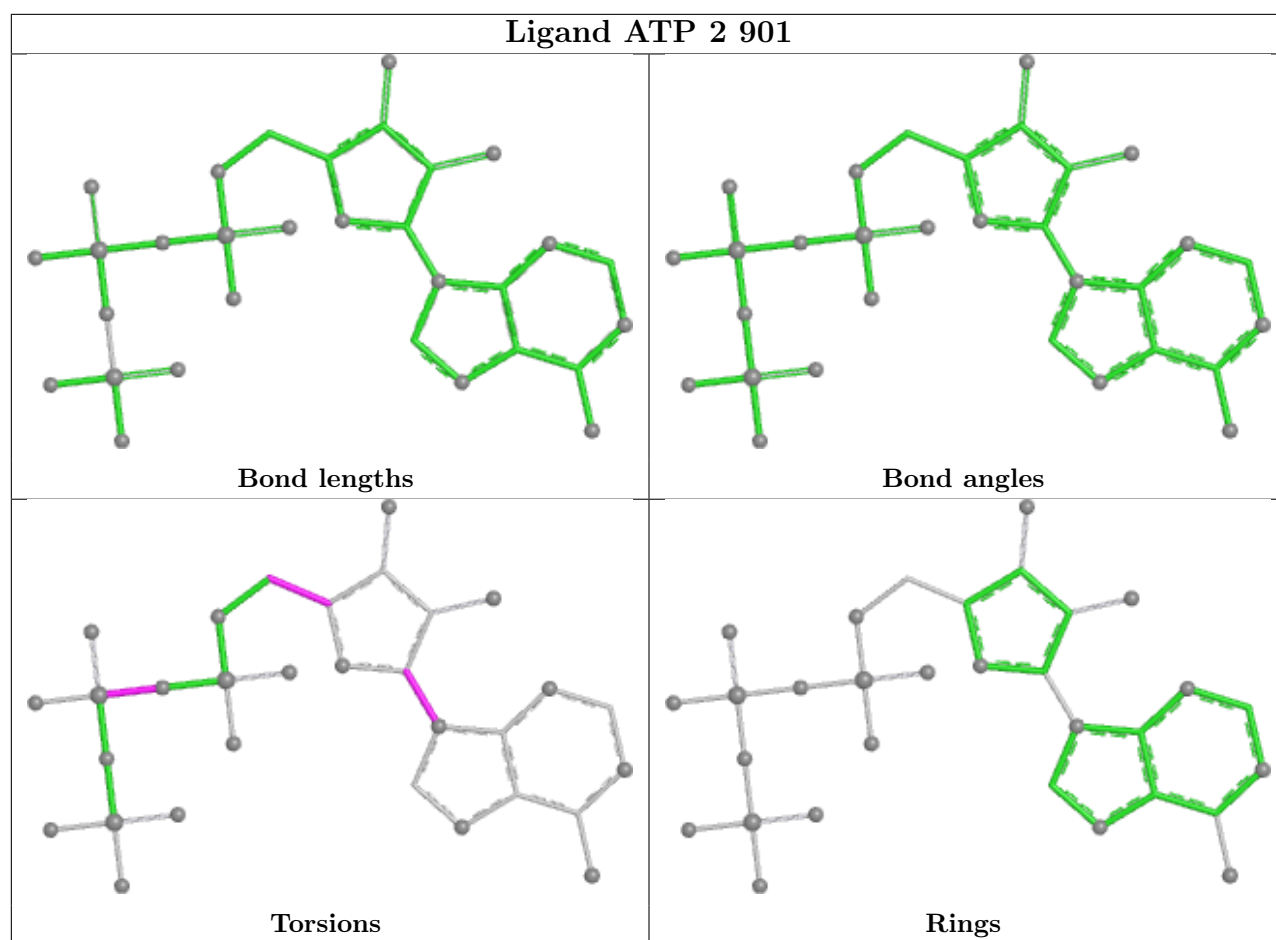


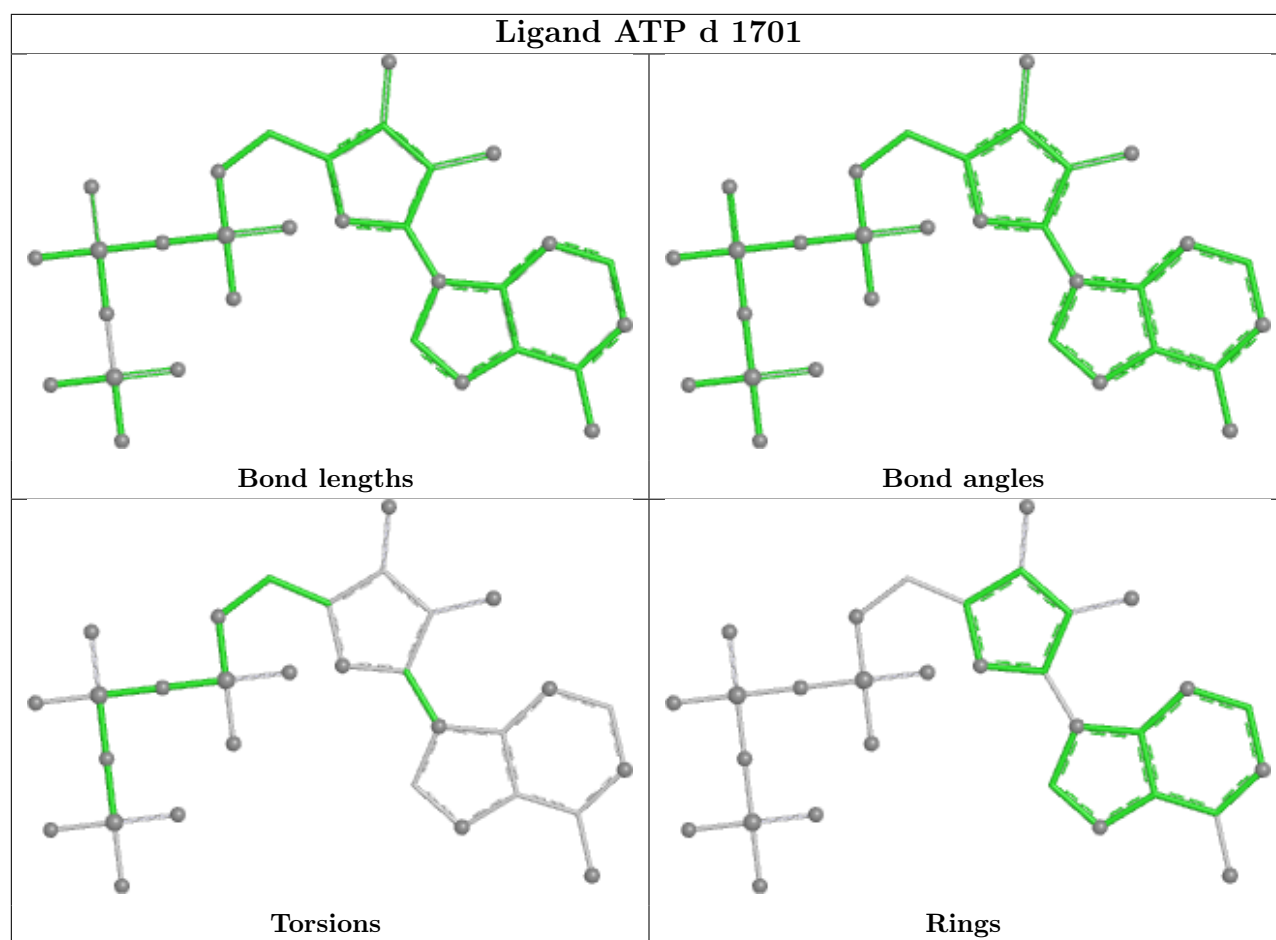
Ligand ADP e 1201

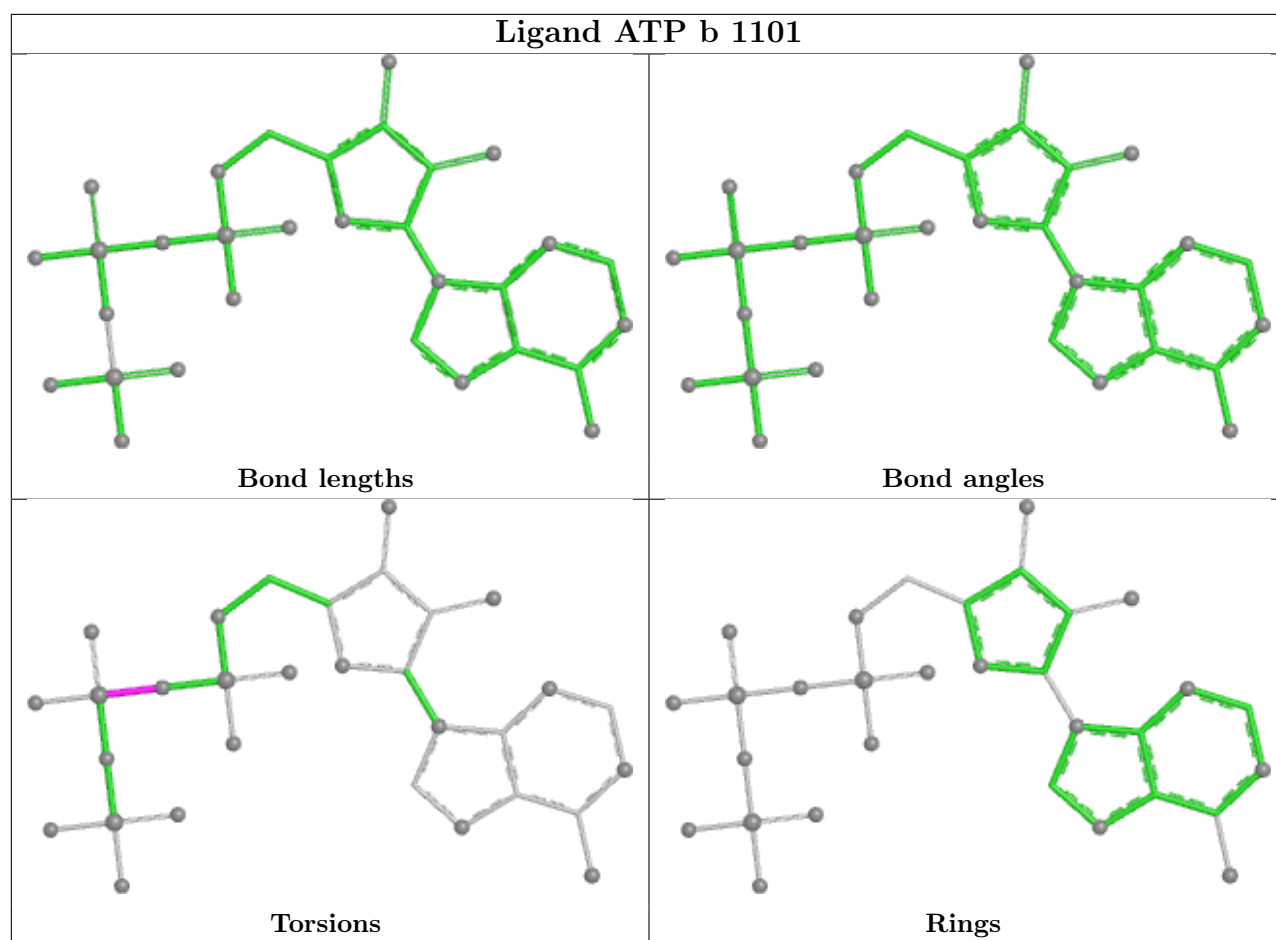












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

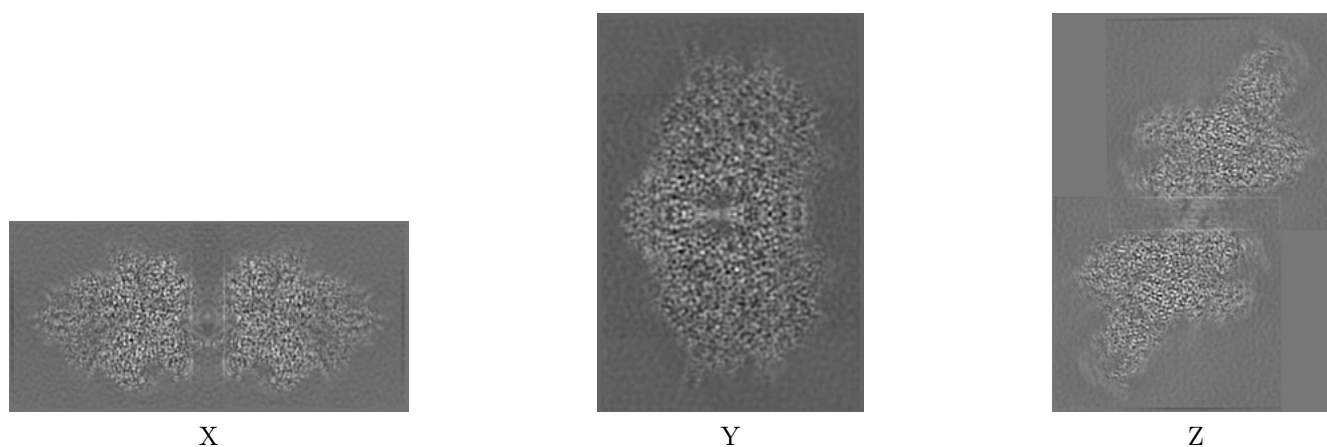
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-14439. 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 [i](#)

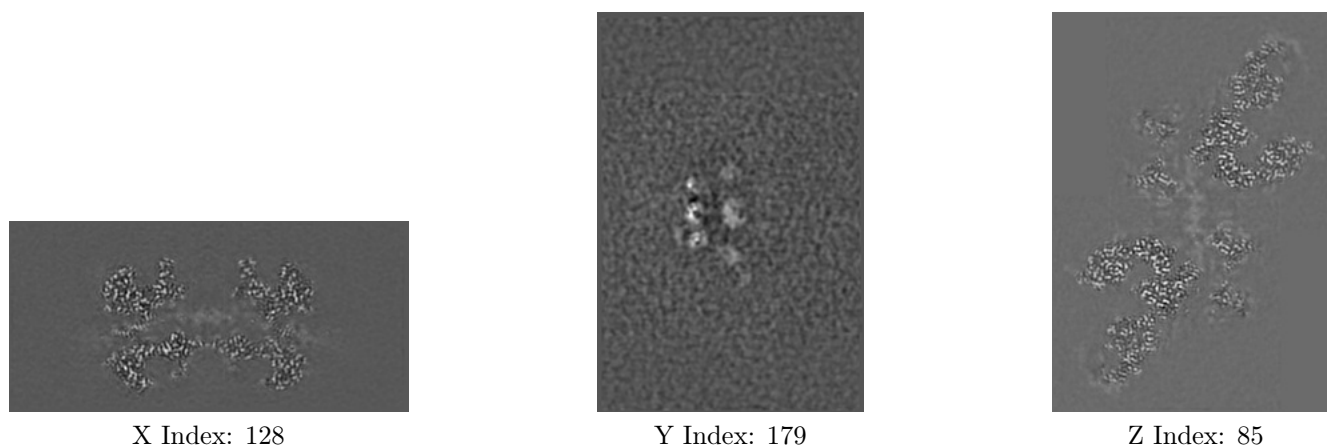
6.1.1 Primary map



The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

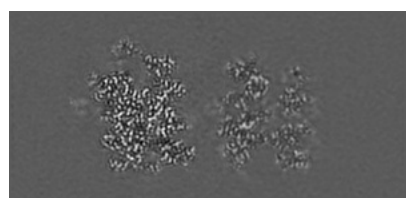
6.2.1 Primary map



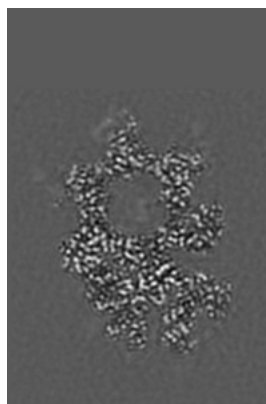
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

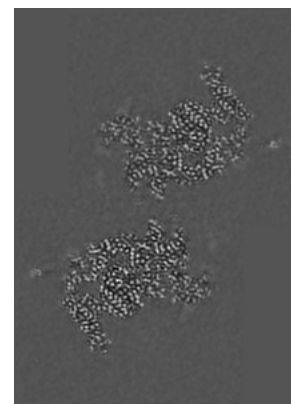
6.3.1 Primary map



X Index: 103



Y Index: 142

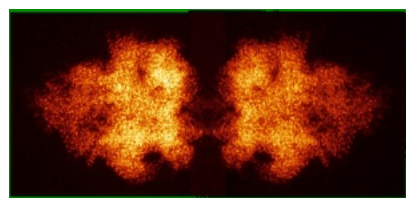


Z Index: 54

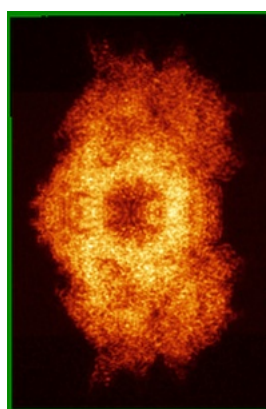
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

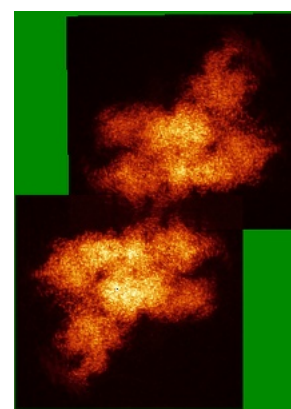
6.4.1 Primary map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.055. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

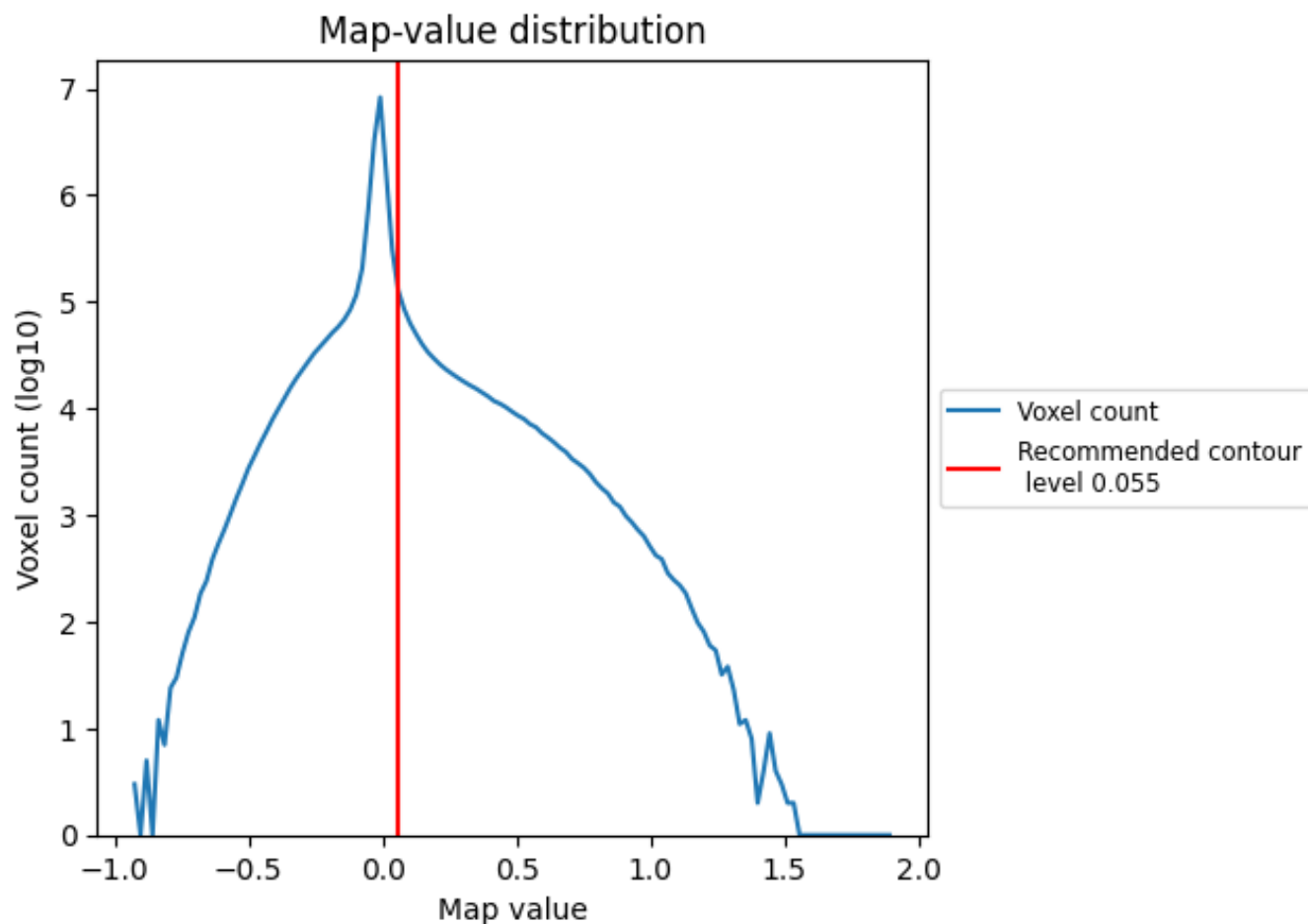
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

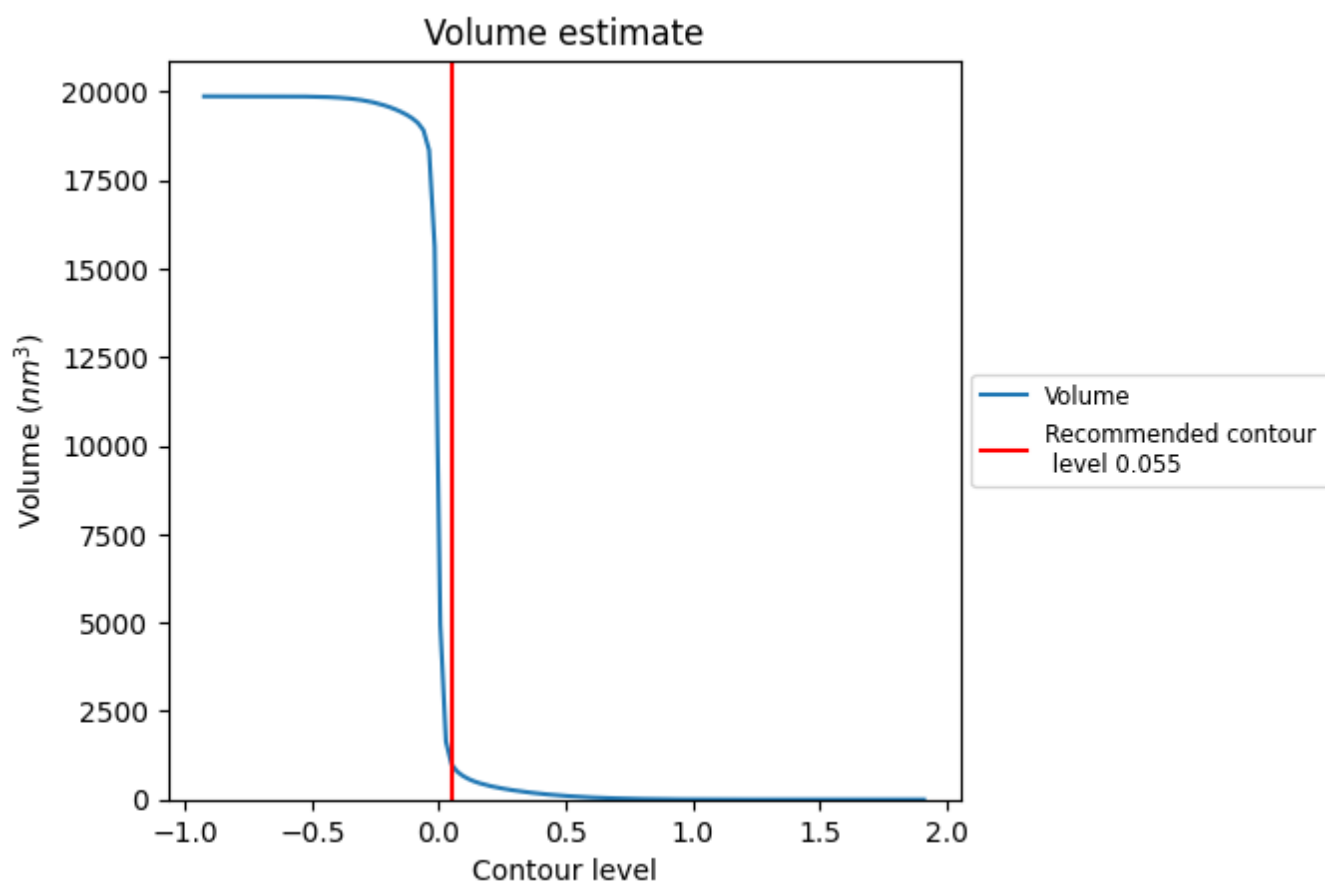
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

7.2 Volume estimate [i](#)



The volume at the recommended contour level is 945 nm³; this corresponds to an approximate mass of 853 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum [i](#)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

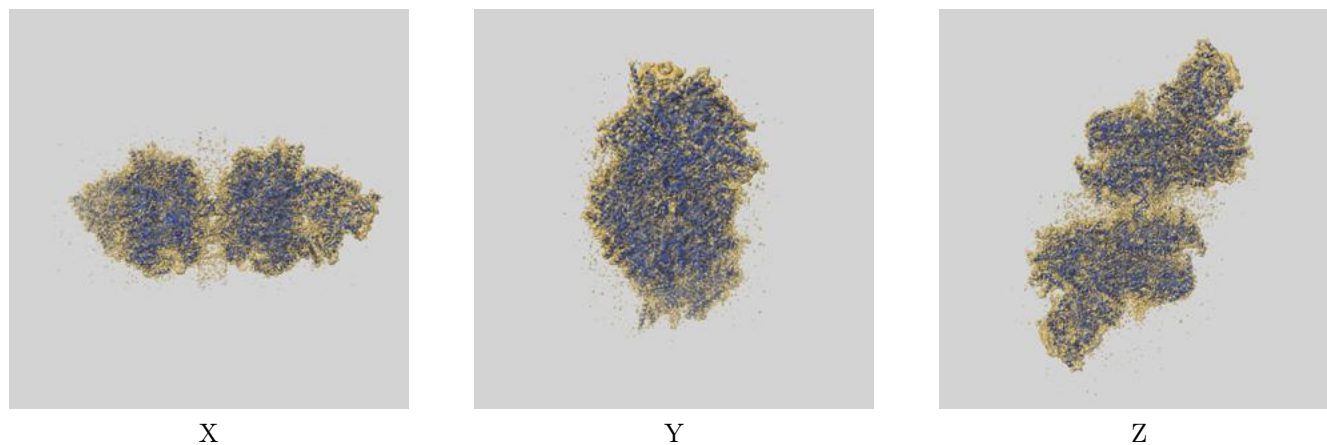
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

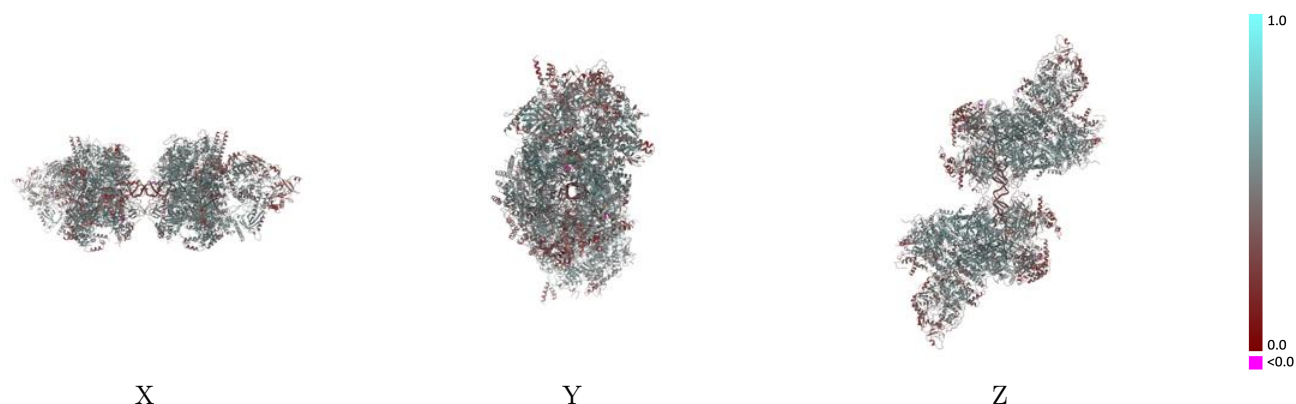
This section contains information regarding the fit between EMDB map EMD-14439 and PDB model 7Z13. Per-residue inclusion information can be found in [section 3](#) on [page 14](#).

9.1 Map-model overlay [i](#)



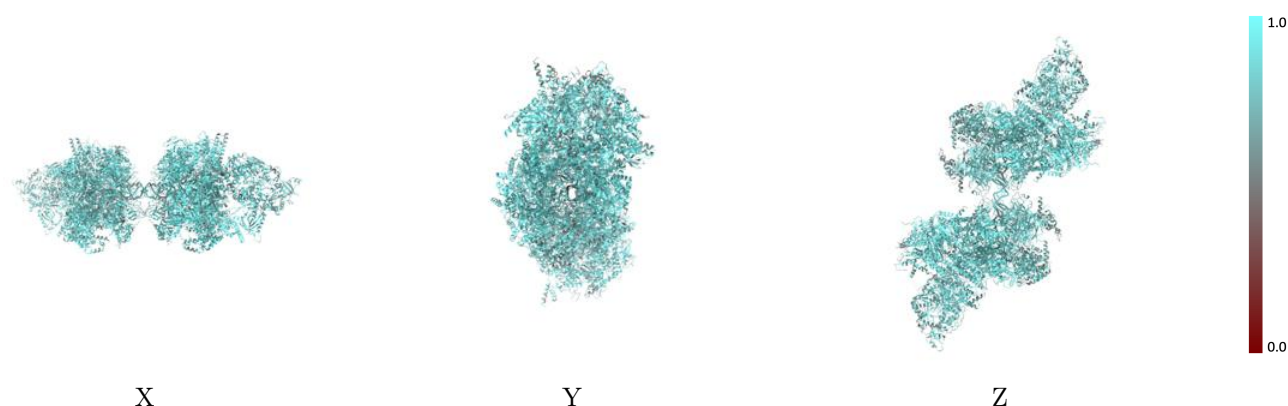
The images above show the 3D surface view of the map at the recommended contour level 0.055 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



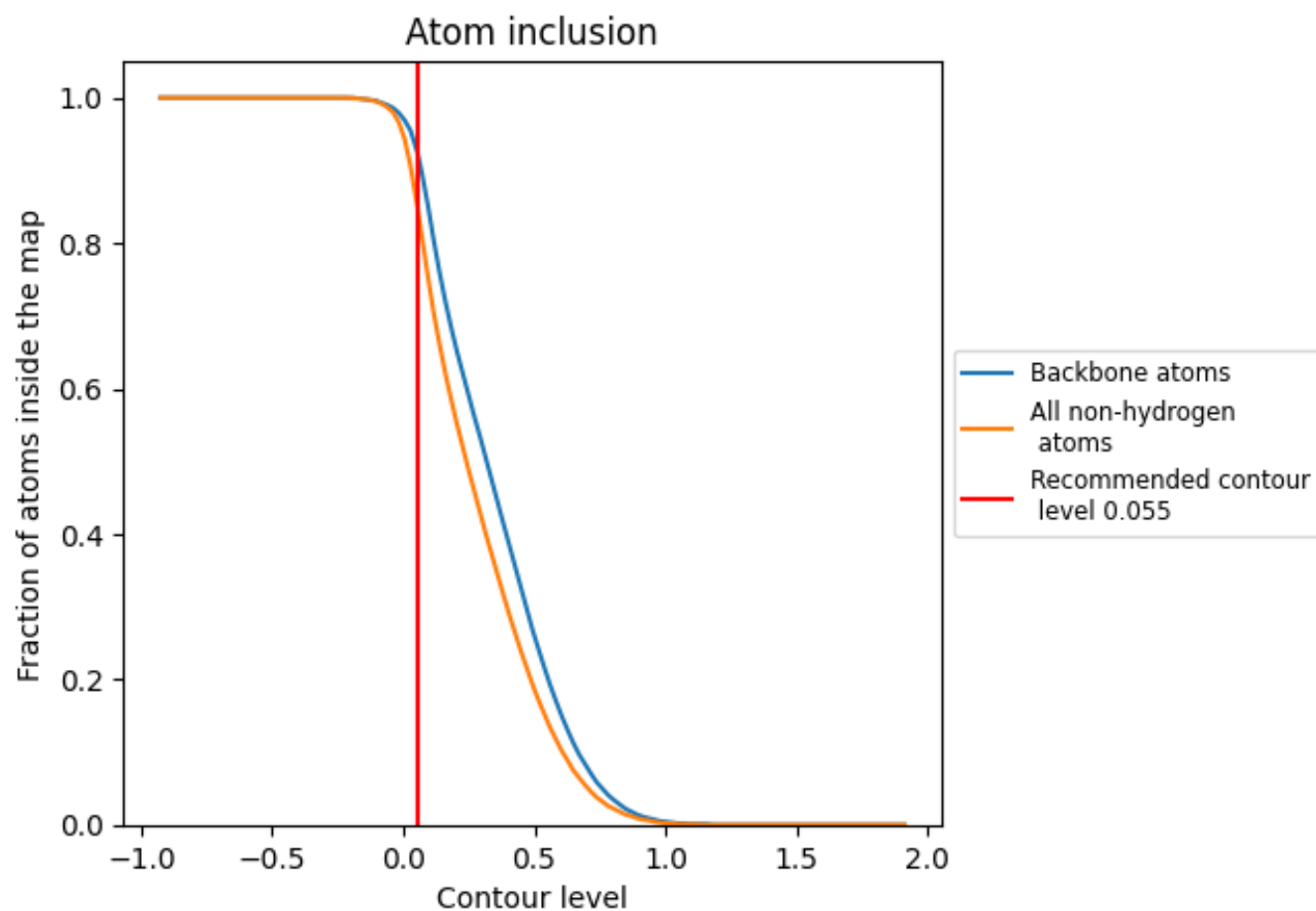
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.055).

9.4 Atom inclusion ⓘ



At the recommended contour level, 92% of all backbone atoms, 85% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.055) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8480	 0.4710
2	 0.9160	 0.5340
3	 0.9050	 0.5200
4	 0.7900	 0.4010
5	 0.8990	 0.5260
6	 0.8640	 0.4810
7	 0.7860	 0.4010
A	 0.8030	 0.3500
B	 0.8000	 0.3430
C	 0.8880	 0.5100
D	 0.8560	 0.4750
E	 0.8880	 0.5040
F	 0.8140	 0.4380
H	 0.8300	 0.4550
I	 0.9100	 0.5240
J	 0.8750	 0.5070
K	 0.8460	 0.4770
L	 0.8810	 0.5010
M	 0.7960	 0.4380
N	 0.8030	 0.4450
O	 0.8180	 0.4560
P	 0.8920	 0.5160
Q	 0.8170	 0.4480
a	 0.9070	 0.5270
b	 0.8930	 0.5170
c	 0.7770	 0.4000
d	 0.8910	 0.5200
e	 0.8510	 0.4760
f	 0.7670	 0.4010

