



wwPDB EM Validation Summary Report ⓘ

Jul 7, 2024 – 03:40 pm BST

PDB ID : 7P5Z
EMDB ID : EMD-13211
Title : Structure of a DNA-loaded MCM double hexamer engaged with the Dbf4-dependent kinase
Authors : Greiwe, J.F.; Miller, T.C.R.; Martino, F.; Costa, A.
Deposited on : 2021-07-15
Resolution : 3.30 Å (reported)
Based on initial models : 6EYC, 3QBZ, 6F0L, 5BK4, 6YA7

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.dev92
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.37.1

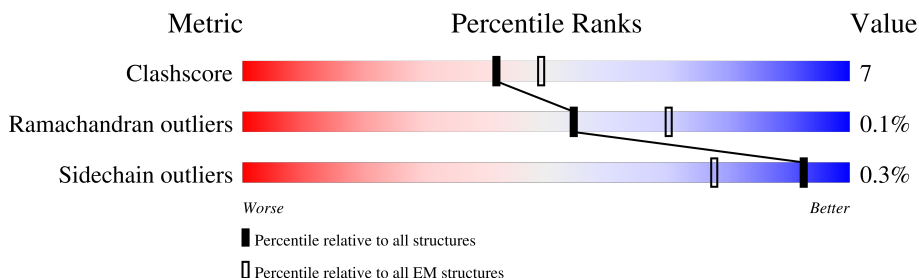
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 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.





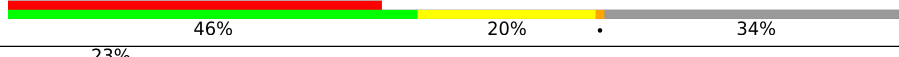

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	
1	A	868	
2	3	1006	
2	B	1006	
3	4	933	
3	C	933	
4	5	775	
4	D	775	

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Mol	Chain	Length	Quality of chain
5	6	1017	 50% 10% 40%
5	E	1017	 49% 11% 40%
6	7	845	 68% 13% 18%
6	F	845	 68% 14% 18%
7	1	507	 42% 46% 20% 34%
8	G	738	 23% 22% 7% 71%
9	X	53	 92% 8%
10	Y	53	 87% 13%

2 Entry composition [i](#)

There are 14 unique types of molecules in this entry. The entry contains 134297 atoms, of which 66896 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	623	9918	3109	4986	877	927	19	0	0
1	A	623	9915	3109	4983	877	927	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	595	9381	2930	4726	833	879	13	0	0
2	B	595	9381	2930	4726	833	879	13	0	0

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

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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

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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
			Total	C	H	N	O	S		
3	4	676	Total	C	H	N	O	S	0	0
			10697	3339	5364	918	1046	30		
3	C	654	Total	C	H	N	O	S	0	0
			10452	3259	5256	896	1011	30		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
4	5	652	Total	C	H	N	O	S	0	0
			10253	3198	5150	873	1007	25		
4	D	652	Total	C	H	N	O	S	0	0
			10251	3198	5148	873	1007	25		

- 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	609	Total	C	H	N	O	S	0	0
			9681	3041	4862	840	913	25		
5	E	609	Total	C	H	N	O	S	0	0
			9681	3041	4862	840	913	25		

- 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	689	Total	C	H	N	O	S	0	0
			10935	3421	5502	942	1041	29		

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Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
6	F	689	10935	3421	5502	942	1041	29	0	0

- Molecule 7 is a protein called Cell division control protein 7.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
7	1	336	5459	1749	2745	467	485	13	0	0

- Molecule 8 is a protein called DDK kinase regulatory subunit DBF4.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
8	G	213	3585	1162	1783	300	333	7	1	0

There are 38 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	-33	LYS	-	expression tag	UNP P32325
G	-32	ARG	-	expression tag	UNP P32325
G	-31	ARG	-	expression tag	UNP P32325
G	-30	TRP	-	expression tag	UNP P32325
G	-29	LYS	-	expression tag	UNP P32325
G	-28	LYS	-	expression tag	UNP P32325
G	-27	ASN	-	expression tag	UNP P32325
G	-26	PHE	-	expression tag	UNP P32325
G	-25	ILE	-	expression tag	UNP P32325
G	-24	ALA	-	expression tag	UNP P32325
G	-23	VAL	-	expression tag	UNP P32325
G	-22	SER	-	expression tag	UNP P32325
G	-21	ALA	-	expression tag	UNP P32325
G	-20	ALA	-	expression tag	UNP P32325
G	-19	ASN	-	expression tag	UNP P32325
G	-18	ARG	-	expression tag	UNP P32325
G	-17	PHE	-	expression tag	UNP P32325
G	-16	LYS	-	expression tag	UNP P32325
G	-15	LYS	-	expression tag	UNP P32325
G	-14	ILE	-	expression tag	UNP P32325
G	-13	SER	-	expression tag	UNP P32325
G	-12	SER	-	expression tag	UNP P32325
G	-11	SER	-	expression tag	UNP P32325
G	-10	GLY	-	expression tag	UNP P32325

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-9	ALA	-	expression tag	UNP P32325
G	-8	LEU	-	expression tag	UNP P32325
G	-7	GLU	-	expression tag	UNP P32325
G	-6	ASN	-	expression tag	UNP P32325
G	-5	LEU	-	expression tag	UNP P32325
G	-4	TYR	-	expression tag	UNP P32325
G	-3	PHE	-	expression tag	UNP P32325
G	-2	GLN	-	expression tag	UNP P32325
G	-1	GLY	-	expression tag	UNP P32325
G	0	GLU	-	expression tag	UNP P32325
G	10	ALA	ARG	conflict	UNP P32325
G	13	ALA	LEU	conflict	UNP P32325
G	62	ALA	ARG	conflict	UNP P32325
G	65	ALA	LEU	conflict	UNP P32325

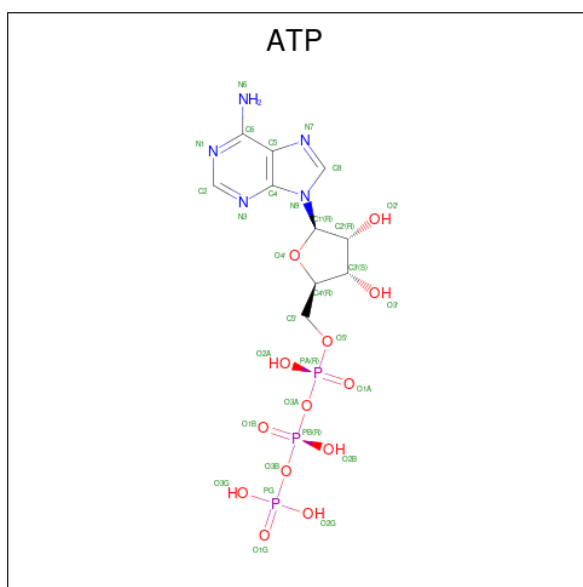
- Molecule 9 is a DNA chain called DNA (53-MER).

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
9	X	53	1682	515	596	199	319	53	0	0

- Molecule 10 is a DNA chain called DNA (53-MER).

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
10	Y	53	1682	515	595	202	317	53	0	0

- Molecule 11 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					AltConf	
			Total	C	H	N	O		P
11	2	1	42	10	11	5	13	3	0
11	A	1	42	10	11	5	13	3	0

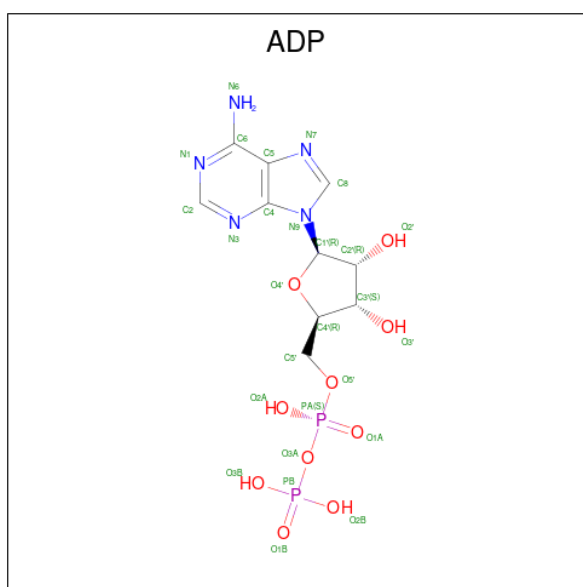
- Molecule 12 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
12	2	1	1	1	0
12	3	1	1	1	0
12	5	1	1	1	0
12	7	2	2	2	0
12	A	1	1	1	0
12	B	1	1	1	0
12	D	1	1	1	0
12	F	2	2	2	0

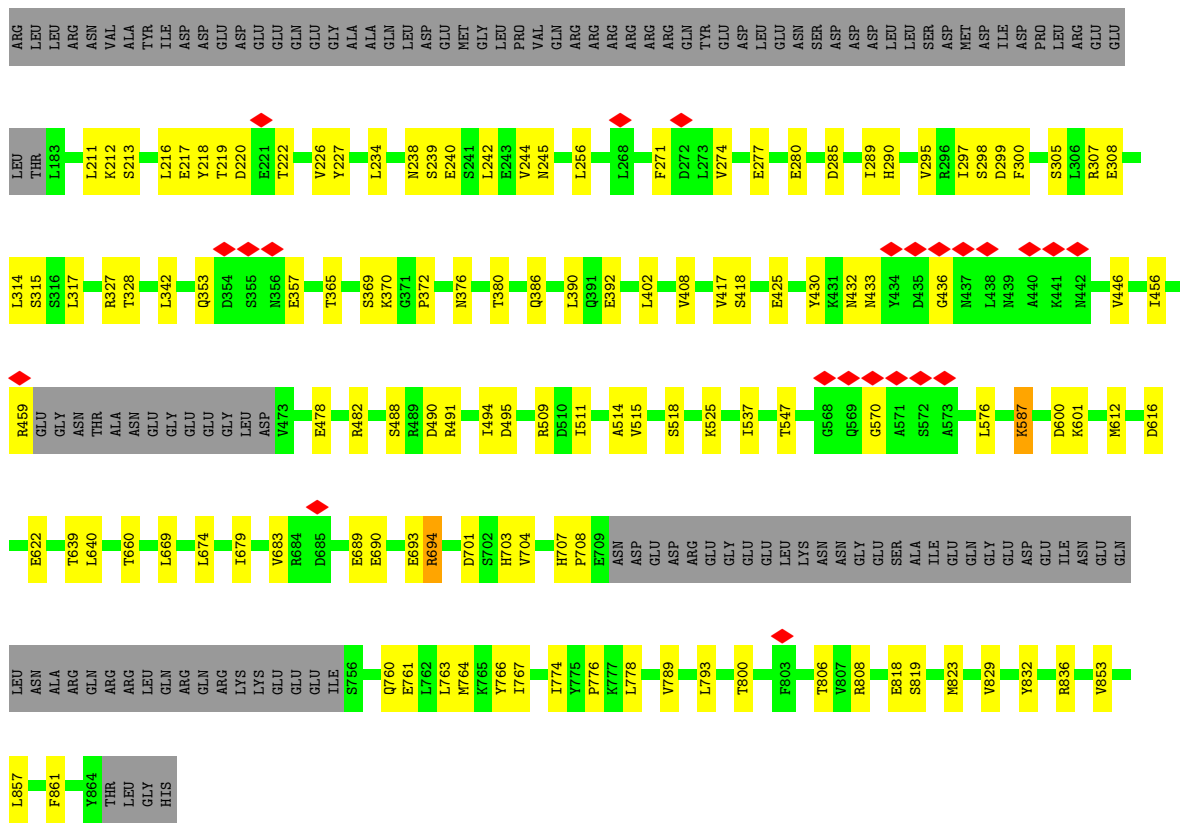
- Molecule 13 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
13	2	1	Total Zn 1 1	0
13	4	1	Total Zn 1 1	0
13	5	1	Total Zn 1 1	0
13	6	1	Total Zn 1 1	0
13	7	1	Total Zn 1 1	0
13	A	1	Total Zn 1 1	0
13	C	1	Total Zn 1 1	0
13	D	1	Total Zn 1 1	0
13	E	1	Total Zn 1 1	0
13	F	1	Total Zn 1 1	0
13	G	1	Total Zn 1 1	0

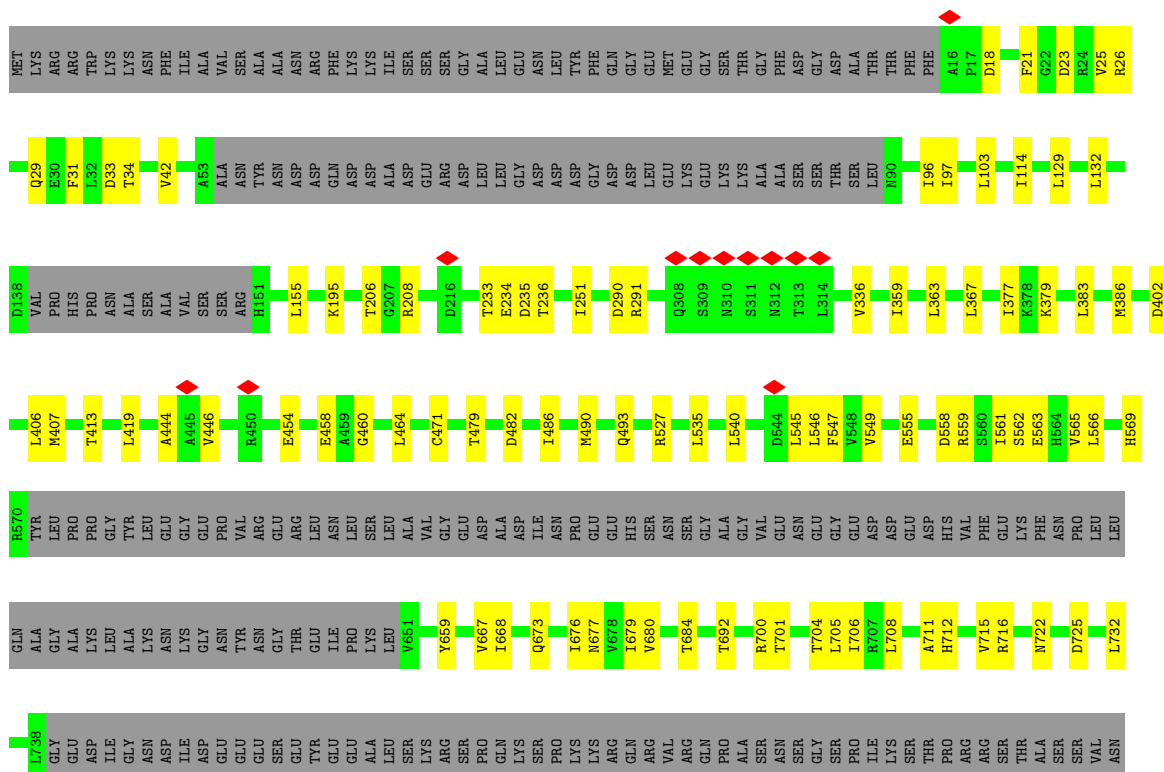
- Molecule 14 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).

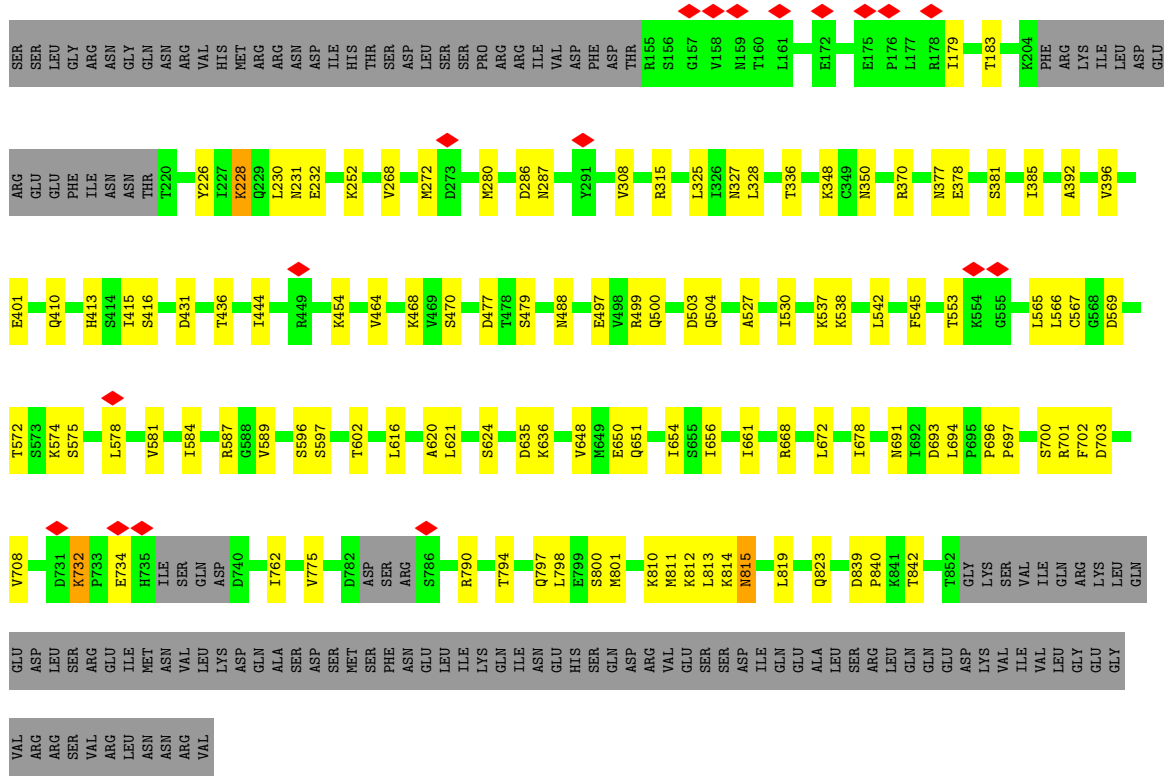


Mol	Chain	Residues	Atoms					AltConf	
14	3	1	Total 38	C 10	H 11	N 5	O 10	P 2	0
14	4	1	Total 38	C 10	H 11	N 5	O 10	P 2	0
14	5	1	Total 38	C 10	H 11	N 5	O 10	P 2	0
14	7	1	Total 38	C 10	H 11	N 5	O 10	P 2	0
14	B	1	Total 38	C 10	H 11	N 5	O 10	P 2	0
14	C	1	Total 38	C 10	H 11	N 5	O 10	P 2	0
14	D	1	Total 38	C 10	H 11	N 5	O 10	P 2	0
14	F	1	Total 38	C 10	H 11	N 5	O 10	P 2	0

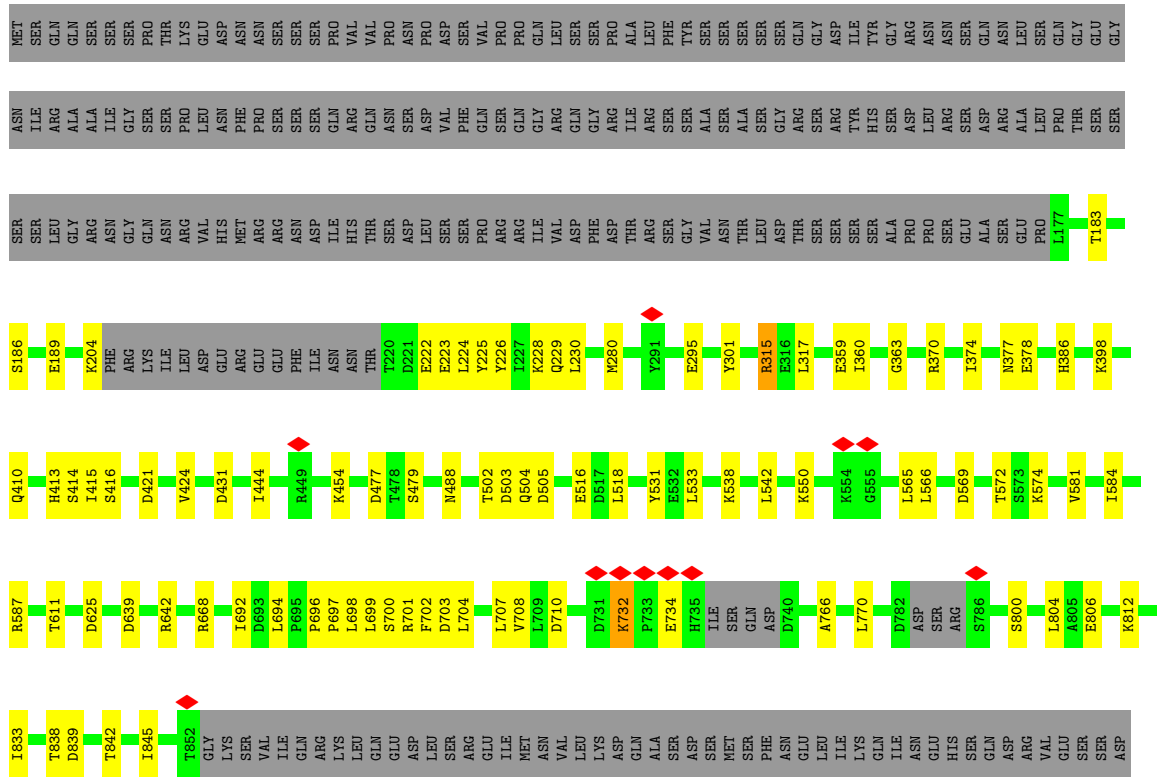


- Molecule 2: DNA replication licensing factor MCM3

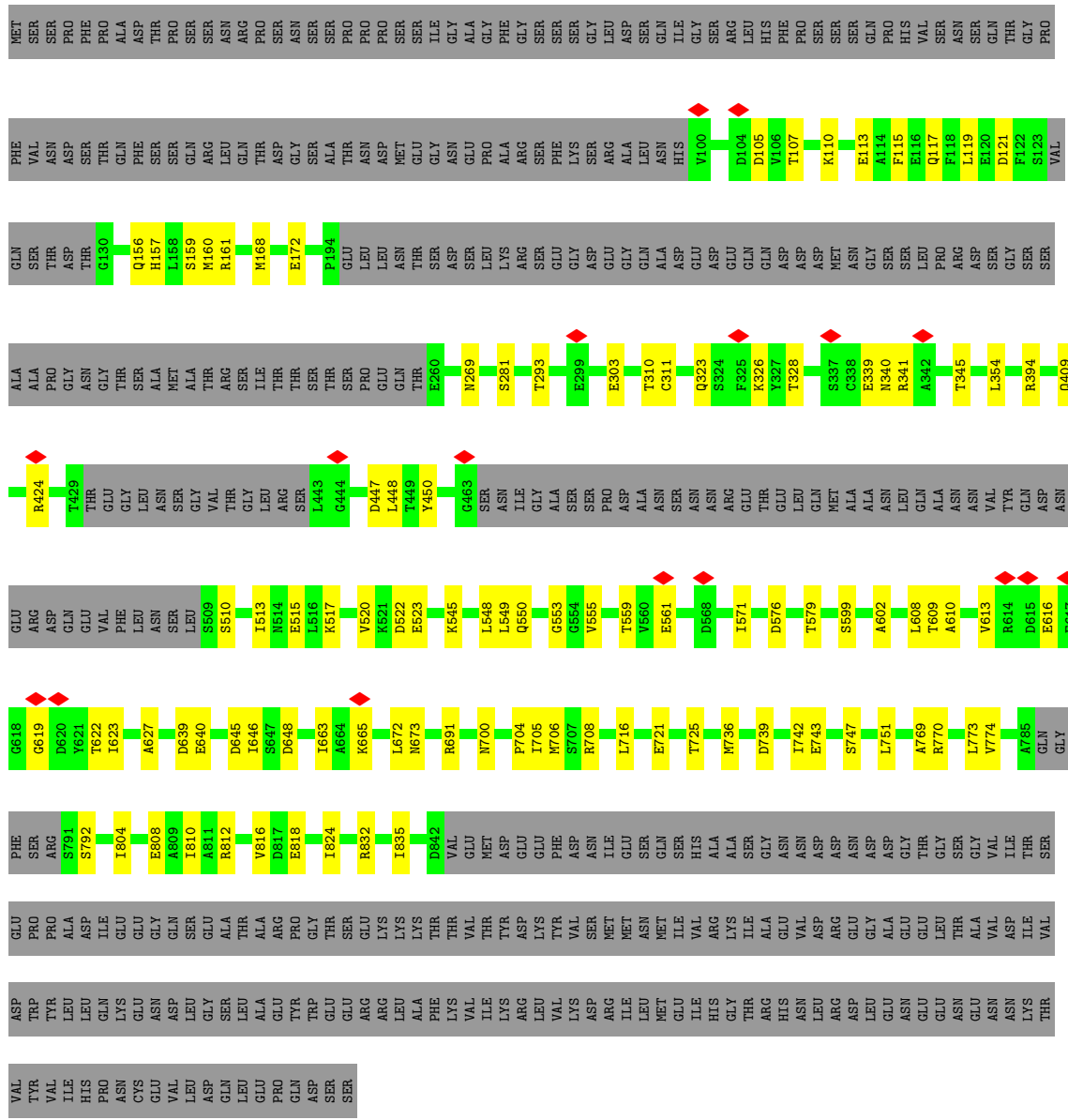




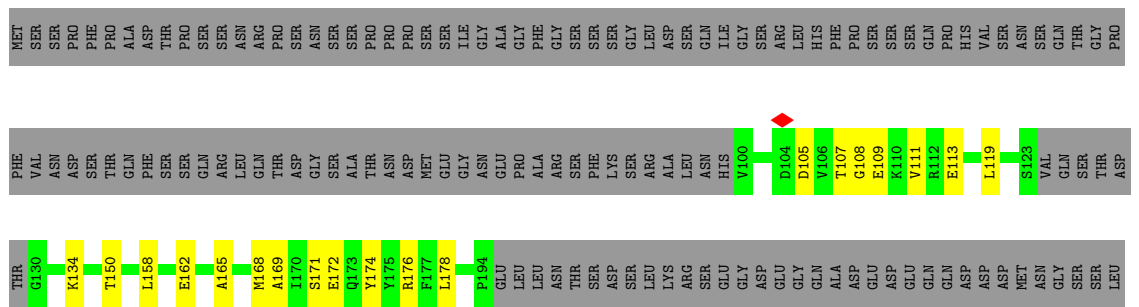
• Molecule 3: DNA replication licensing factor MCM4

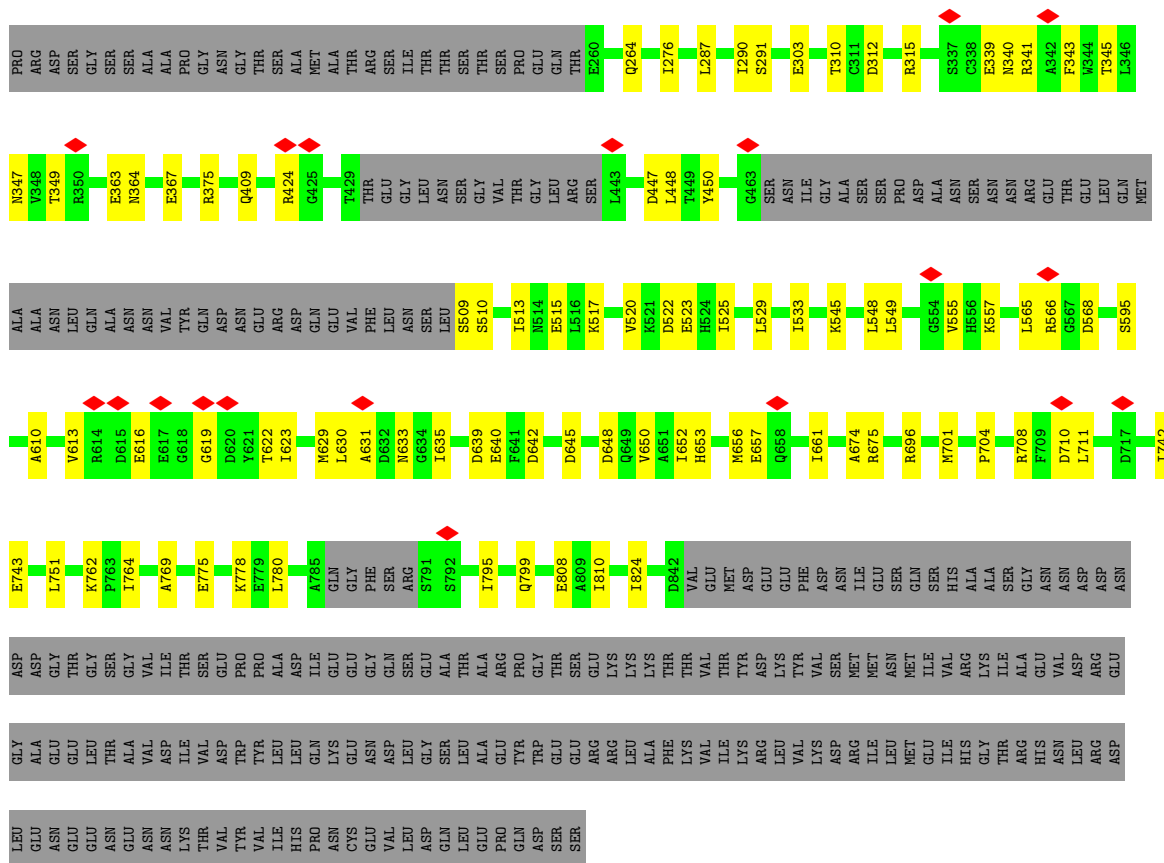


• Molecule 5: DNA replication licensing factor MCM6

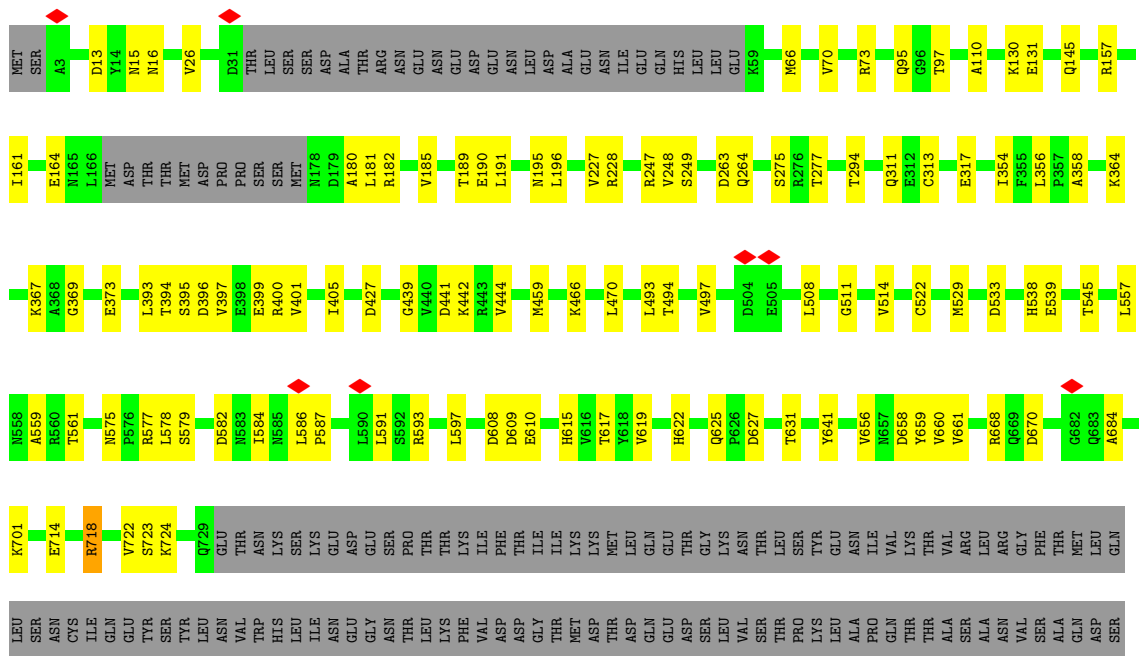


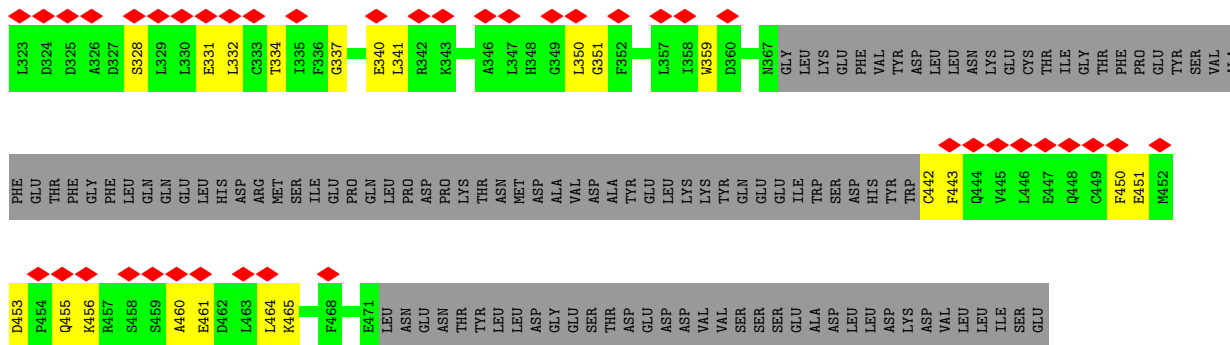
• Molecule 5: DNA replication licensing factor MCM6



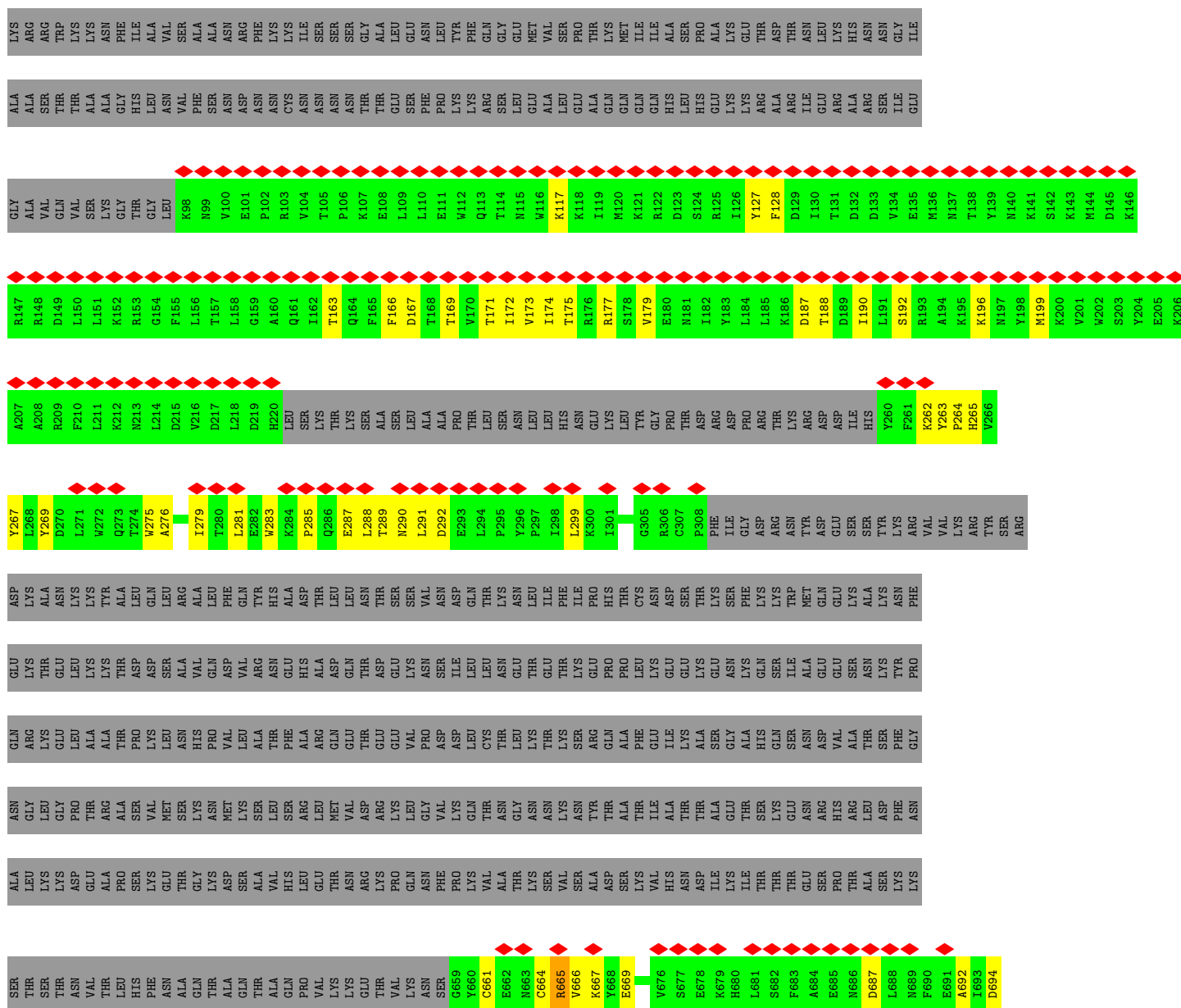


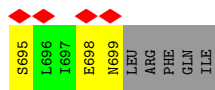
● Molecule 6: DNA replication licensing factor MCM7



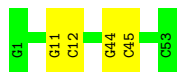


• Molecule 8: DDK kinase regulatory subunit DBF4

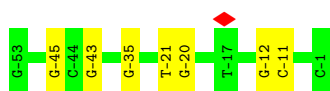
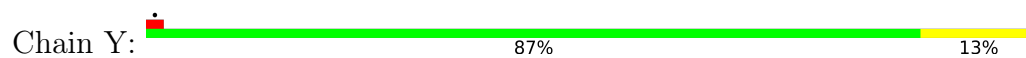




- Molecule 9: DNA (53-MER)



- Molecule 10: DNA (53-MER)



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	149876	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 ($e^-/\text{\AA}^2$)	51.3	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	4100	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.031	Depositor
Minimum map value	-0.018	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.0043	Depositor
Map size (\AA)	518.4, 518.4, 518.4	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.08, 1.08, 1.08	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: ATP, MG, ZN, ADP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	2	0.25	0/5019	0.51	0/6781
1	A	0.25	0/5019	0.54	1/6781 (0.0%)
2	3	0.24	0/4733	0.52	0/6417
2	B	0.24	0/4733	0.52	0/6417
3	4	0.25	0/5410	0.51	0/7317
3	C	0.24	0/5270	0.50	0/7123
4	5	0.25	0/5176	0.50	0/7000
4	D	0.25	0/5176	0.50	0/7000
5	6	0.25	0/4896	0.53	0/6601
5	E	0.25	0/4896	0.52	0/6601
6	7	0.25	0/5516	0.51	0/7454
6	F	0.25	0/5516	0.51	0/7454
7	1	0.26	0/2774	0.52	0/3735
8	G	0.25	0/1847	0.49	0/2498
9	X	0.49	0/1217	0.90	0/1876
10	Y	0.50	0/1219	0.87	0/1879
All	All	0.26	0/68417	0.53	1/92934 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	587	LYS	CD-CE-NZ	10.86	136.67	111.70

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	4932	4986	4984	64	0
1	A	4932	4983	4984	81	0
2	3	4655	4726	4723	67	0
2	B	4655	4726	4723	51	0
3	4	5333	5364	5362	73	0
3	C	5196	5256	5254	60	0
4	5	5103	5150	5147	78	0
4	D	5103	5148	5147	77	0
5	6	4819	4862	4856	71	0
5	E	4819	4862	4856	79	0
6	7	5433	5502	5500	79	0
6	F	5433	5502	5500	81	0
7	1	2714	2745	2745	87	0
8	G	1802	1783	1783	51	0
9	X	1086	596	596	4	0
10	Y	1087	595	595	6	0
11	2	31	11	12	0	0
11	A	31	11	12	0	0
12	2	1	0	0	0	0
12	3	1	0	0	0	0
12	5	1	0	0	0	0
12	7	2	0	0	0	0
12	A	1	0	0	0	0
12	B	1	0	0	0	0
12	D	1	0	0	0	0
12	F	2	0	0	0	0
13	2	1	0	0	0	0
13	4	1	0	0	0	0
13	5	1	0	0	0	0
13	6	1	0	0	0	0
13	7	1	0	0	0	0
13	A	1	0	0	0	0
13	C	1	0	0	0	0
13	D	1	0	0	0	0
13	E	1	0	0	0	0
13	F	1	0	0	0	0
13	G	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	3	27	11	12	0	0
14	4	27	11	12	1	0
14	5	27	11	12	4	0
14	7	27	11	12	1	0
14	B	27	11	12	0	0
14	C	27	11	12	0	0
14	D	27	11	12	3	0
14	F	27	11	12	1	0
All	All	67401	66896	66875	952	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 952 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)
6:7:591:LEU:HD12	6:7:597:LEU:HD11	1.50	0.91
1:2:193:SER:OG	1:2:196:GLU:OE1	1.90	0.88
1:A:495:ASP:OD1	1:A:509:ARG:NH2	2.08	0.86
8:G:279:ILE:HG23	8:G:281:LEU:HD23	1.60	0.84
6:F:591:LEU:HD12	6:F:597:LEU:HD11	1.57	0.84

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	617/868 (71%)	602 (98%)	15 (2%)	0	100	100
1	A	617/868 (71%)	599 (97%)	18 (3%)	0	100	100
2	3	587/1006 (58%)	566 (96%)	21 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	587/1006 (58%)	566 (96%)	21 (4%)	0	100	100
3	4	668/933 (72%)	647 (97%)	21 (3%)	0	100	100
3	C	646/933 (69%)	630 (98%)	16 (2%)	0	100	100
4	5	644/775 (83%)	615 (96%)	27 (4%)	2 (0%)	41	71
4	D	644/775 (83%)	615 (96%)	27 (4%)	2 (0%)	41	71
5	6	597/1017 (59%)	572 (96%)	25 (4%)	0	100	100
5	E	597/1017 (59%)	569 (95%)	28 (5%)	0	100	100
6	7	683/845 (81%)	662 (97%)	21 (3%)	0	100	100
6	F	683/845 (81%)	664 (97%)	19 (3%)	0	100	100
7	1	330/507 (65%)	300 (91%)	28 (8%)	2 (1%)	25	57
8	G	208/738 (28%)	193 (93%)	15 (7%)	0	100	100
All	All	8108/12133 (67%)	7800 (96%)	302 (4%)	6 (0%)	54	81

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	1	268	ASN
7	1	276	ALA
4	5	584	GLN
4	D	584	GLN
4	5	337	VAL

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	547/770 (71%)	546 (100%)	1 (0%)	93	97
1	A	547/770 (71%)	546 (100%)	1 (0%)	93	97
2	3	514/864 (60%)	513 (100%)	1 (0%)	93	97
2	B	514/864 (60%)	514 (100%)	0	100	100
3	4	607/848 (72%)	600 (99%)	7 (1%)	71	83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	593/848 (70%)	590 (100%)	3 (0%)	88	93
4	5	584/688 (85%)	583 (100%)	1 (0%)	93	97
4	D	584/688 (85%)	583 (100%)	1 (0%)	93	97
5	6	531/886 (60%)	530 (100%)	1 (0%)	93	97
5	E	531/886 (60%)	531 (100%)	0	100	100
6	7	608/753 (81%)	607 (100%)	1 (0%)	93	97
6	F	608/753 (81%)	607 (100%)	1 (0%)	93	97
7	1	294/454 (65%)	293 (100%)	1 (0%)	92	96
8	G	201/663 (30%)	199 (99%)	2 (1%)	76	86
All	All	7263/10735 (68%)	7242 (100%)	21 (0%)	92	96

5 of 21 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	488	ASN
6	F	95	GLN
8	G	665	ARG
7	1	195	MET
4	D	516	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
6	7	615	HIS
1	A	531	HIS
7	1	257	ASN
7	1	21	GLN
7	1	155	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 31 ligands modelled in this entry, 21 are monoatomic - leaving 10 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
14	ADP	3	1001	12	24,29,29	0.94	1 (4%)	29,45,45	1.50	4 (13%)
14	ADP	C	1001	12	24,29,29	0.96	1 (4%)	29,45,45	1.43	4 (13%)
14	ADP	F	902	12	24,29,29	0.95	1 (4%)	29,45,45	1.55	4 (13%)
11	ATP	2	901	12	26,33,33	0.62	0	31,52,52	1.06	1 (3%)
14	ADP	5	801	12	24,29,29	0.94	1 (4%)	29,45,45	1.52	4 (13%)
14	ADP	7	902	12	24,29,29	0.96	1 (4%)	29,45,45	1.53	4 (13%)
14	ADP	D	801	12	24,29,29	0.94	1 (4%)	29,45,45	1.52	4 (13%)
14	ADP	B	1001	12	24,29,29	0.94	1 (4%)	29,45,45	1.49	4 (13%)
11	ATP	A	901	12	26,33,33	0.62	0	31,52,52	1.05	1 (3%)
14	ADP	4	1001	12	24,29,29	0.94	1 (4%)	29,45,45	1.45	4 (13%)

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
14	ADP	3	1001	12	-	3/12/32/32	0/3/3/3
14	ADP	C	1001	12	-	7/12/32/32	0/3/3/3
14	ADP	F	902	12	-	3/12/32/32	0/3/3/3
11	ATP	2	901	12	-	4/18/38/38	0/3/3/3
14	ADP	5	801	12	-	3/12/32/32	0/3/3/3
14	ADP	7	902	12	-	2/12/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	ADP	D	801	12	-	4/12/32/32	0/3/3/3
14	ADP	B	1001	12	-	3/12/32/32	0/3/3/3
11	ATP	A	901	12	-	3/18/38/38	0/3/3/3
14	ADP	4	1001	12	-	7/12/32/32	0/3/3/3

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	F	902	ADP	C5-C4	2.38	1.47	1.40
14	7	902	ADP	C5-C4	2.37	1.47	1.40
14	4	1001	ADP	C5-C4	2.36	1.47	1.40
14	C	1001	ADP	C5-C4	2.35	1.47	1.40
14	5	801	ADP	C5-C4	2.33	1.47	1.40

The worst 5 of 34 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	D	801	ADP	PA-O3A-PB	-4.00	119.10	132.83
14	5	801	ADP	PA-O3A-PB	-3.94	119.31	132.83
14	F	902	ADP	PA-O3A-PB	-3.87	119.55	132.83
14	7	902	ADP	PA-O3A-PB	-3.65	120.32	132.83
14	5	801	ADP	N3-C2-N1	-3.61	123.03	128.68

There are no chirality outliers.

5 of 39 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	A	901	ATP	PB-O3B-PG-O3G
14	3	1001	ADP	C5'-O5'-PA-O1A
14	4	1001	ADP	PA-O3A-PB-O2B
14	4	1001	ADP	PA-O3A-PB-O3B
14	4	1001	ADP	C5'-O5'-PA-O1A

There are no ring outliers.

5 monomers are involved in 10 short contacts:

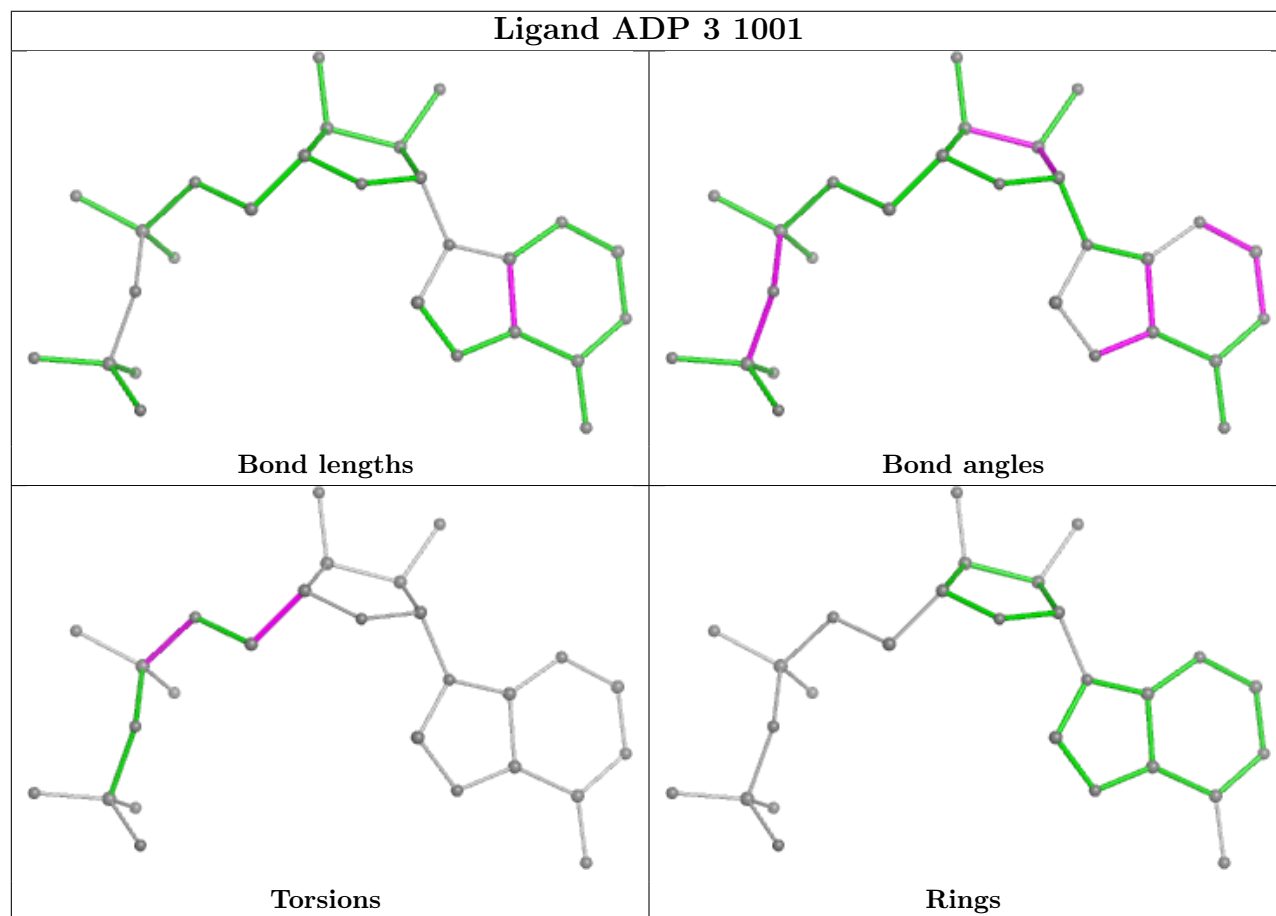
Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	F	902	ADP	1	0
14	5	801	ADP	4	0
14	7	902	ADP	1	0

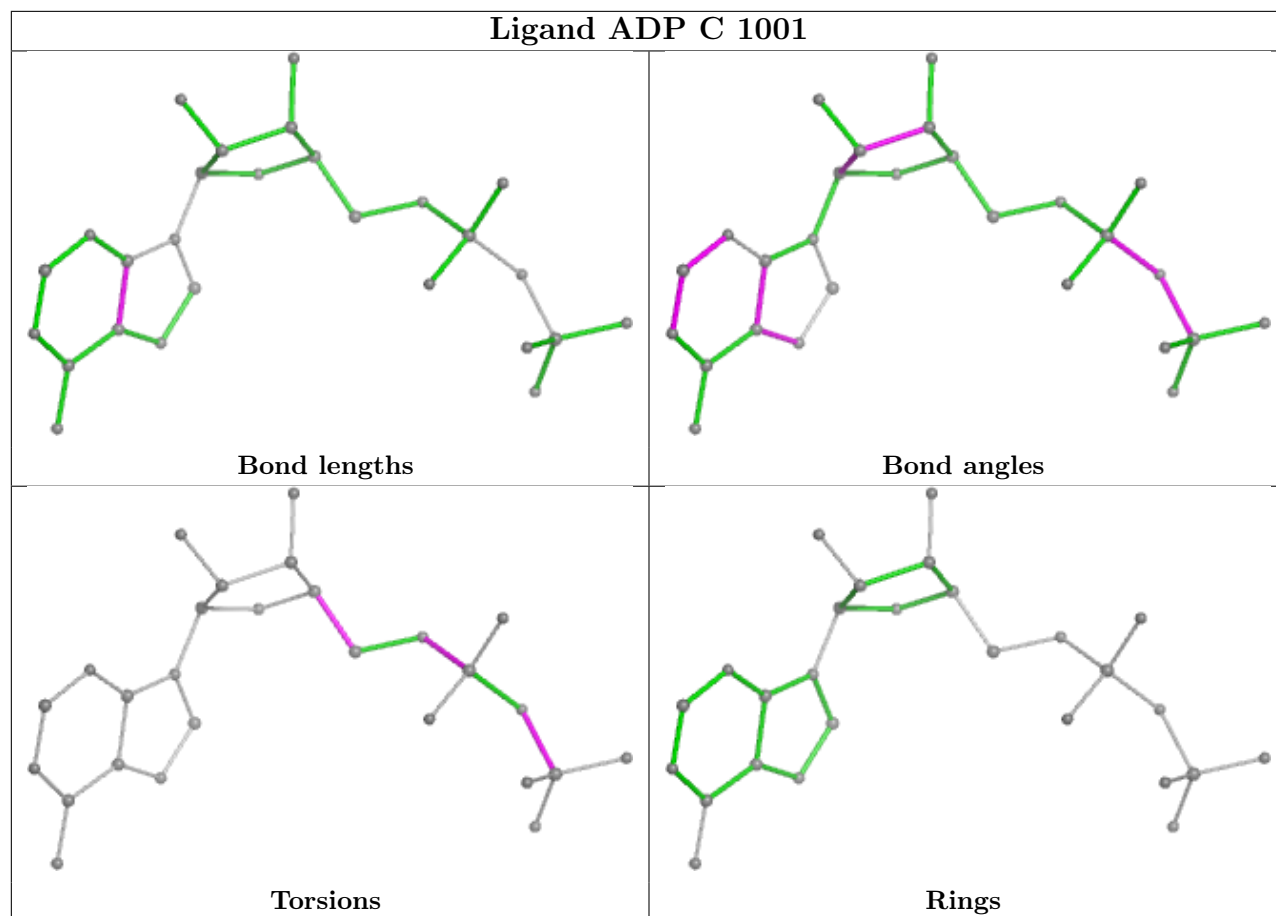
Continued on next page...

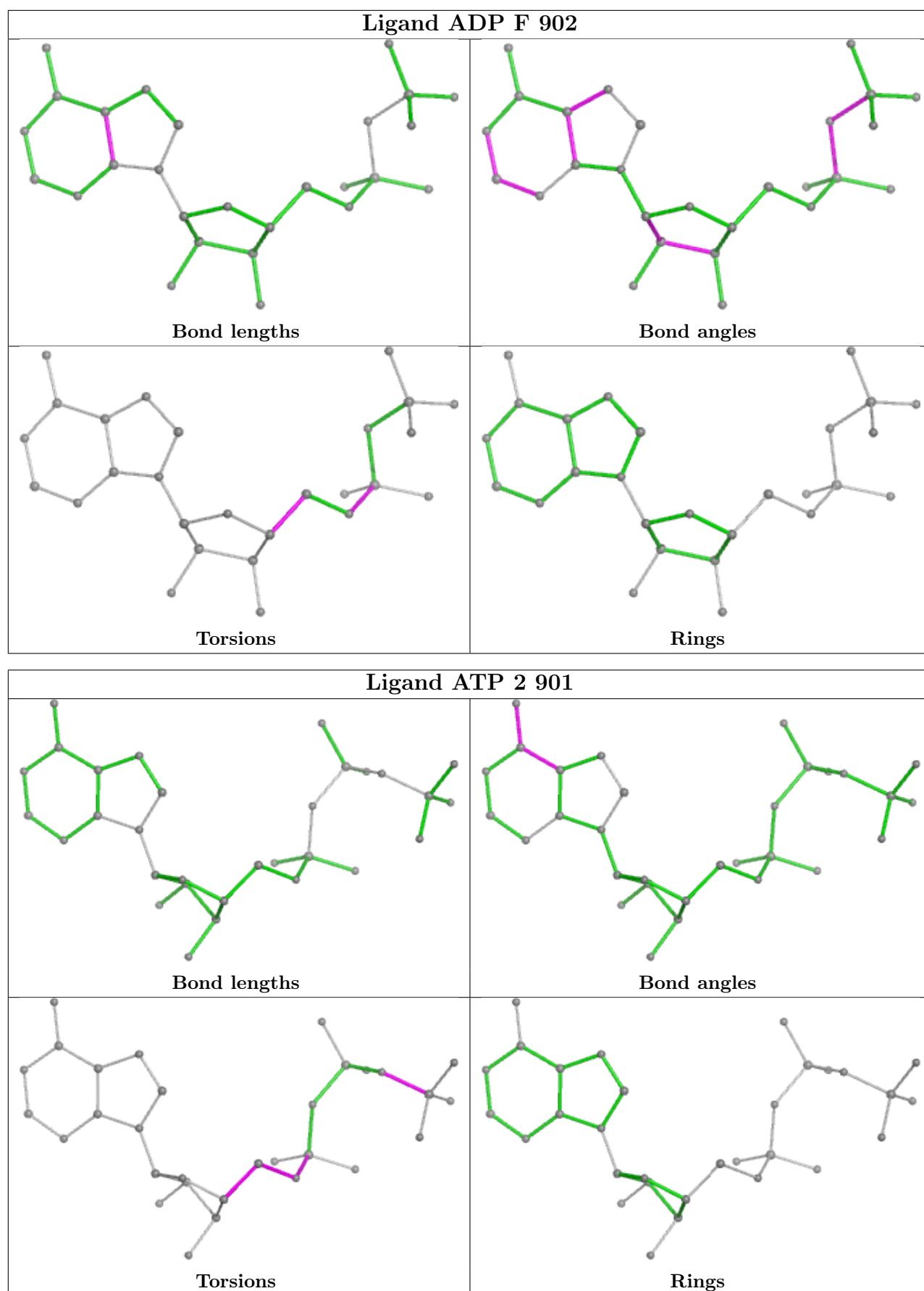
Continued from previous page...

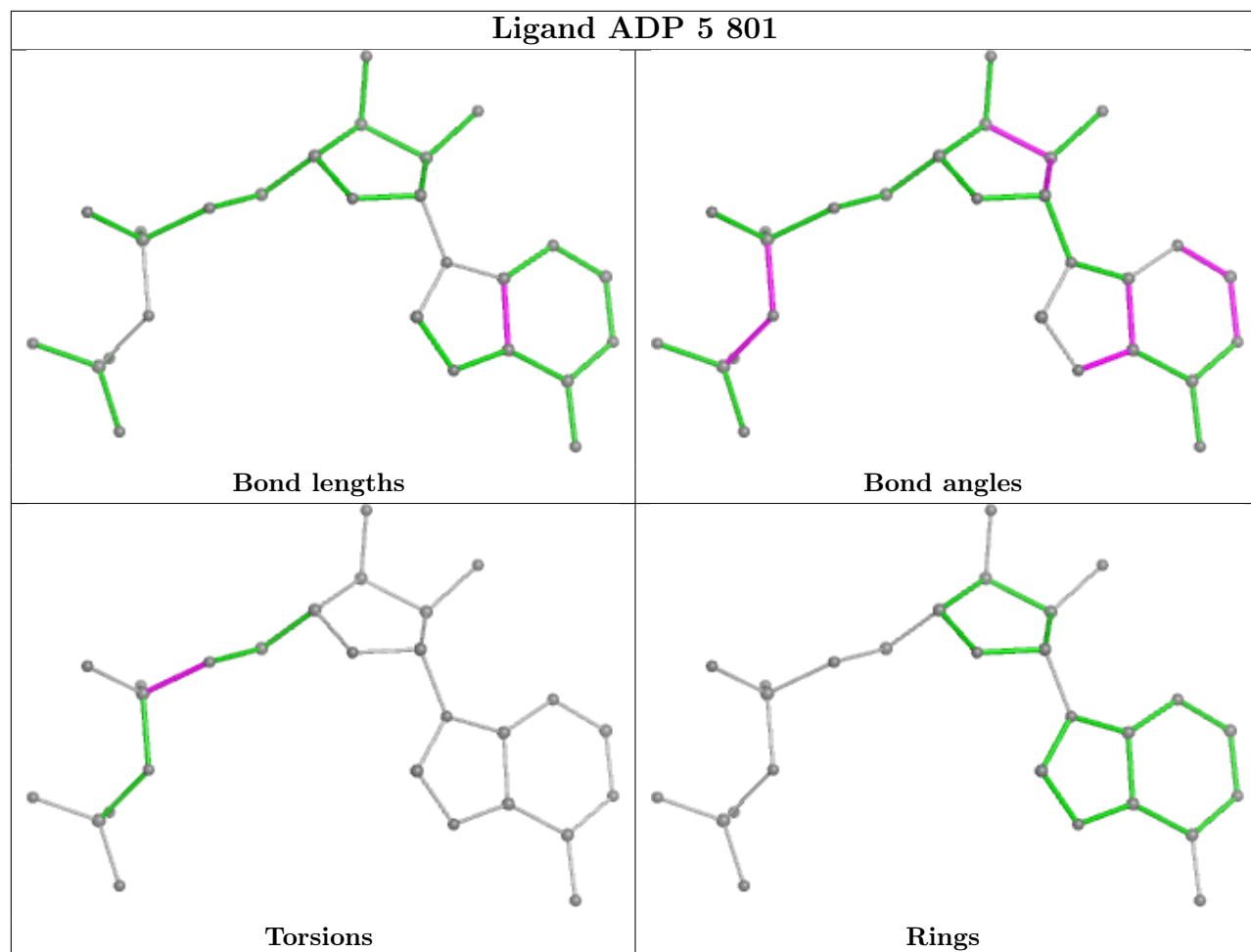
Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	D	801	ADP	3	0
14	4	1001	ADP	1	0

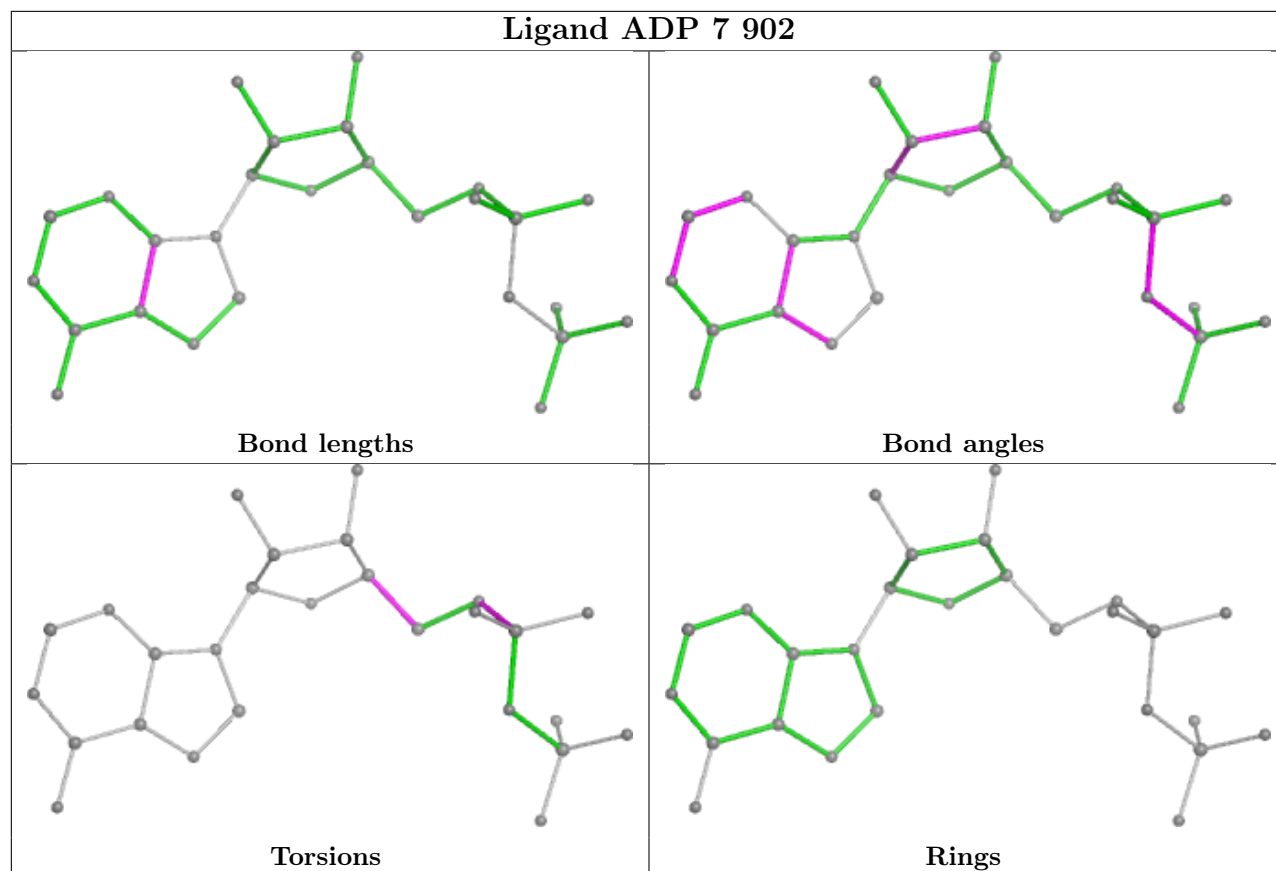
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

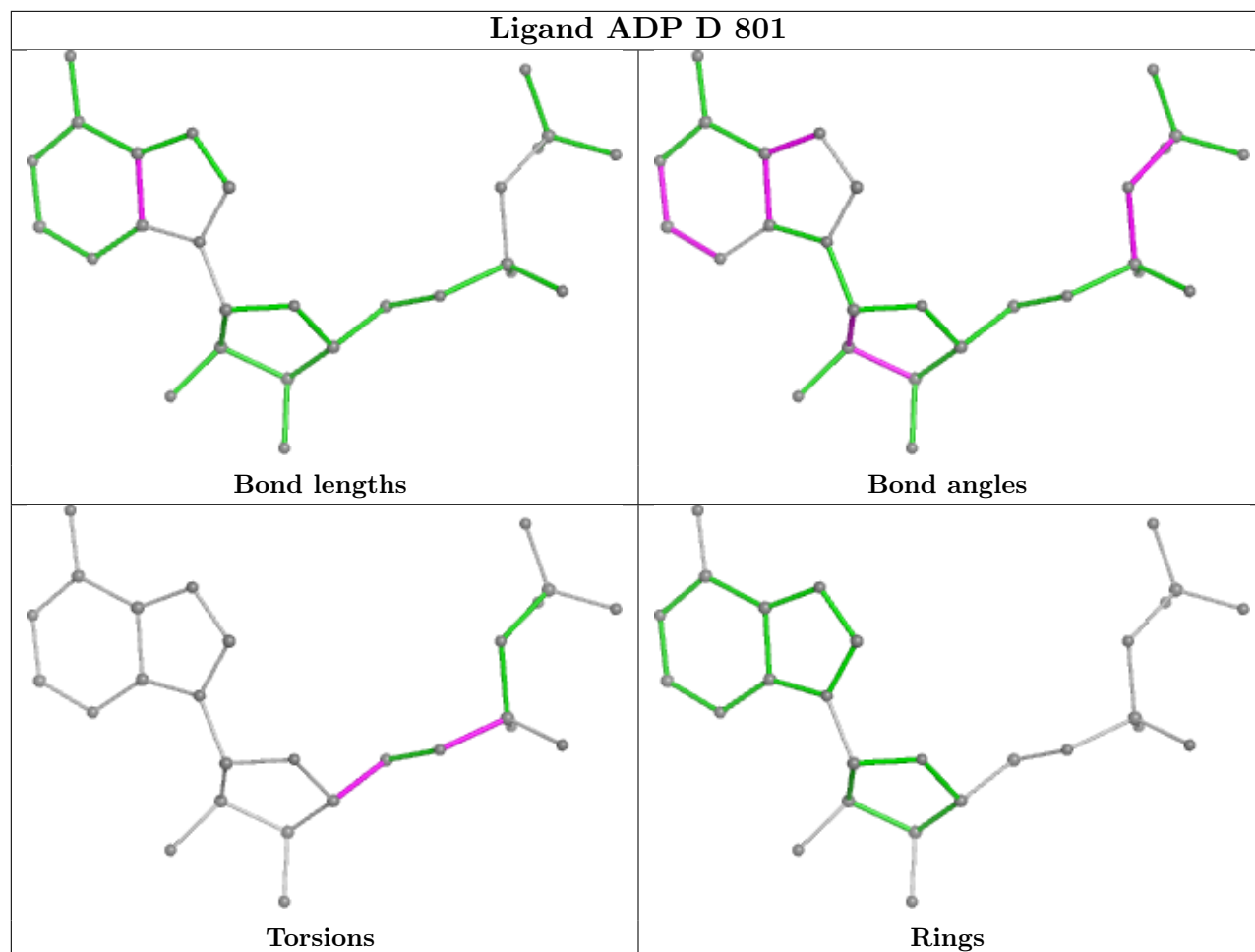


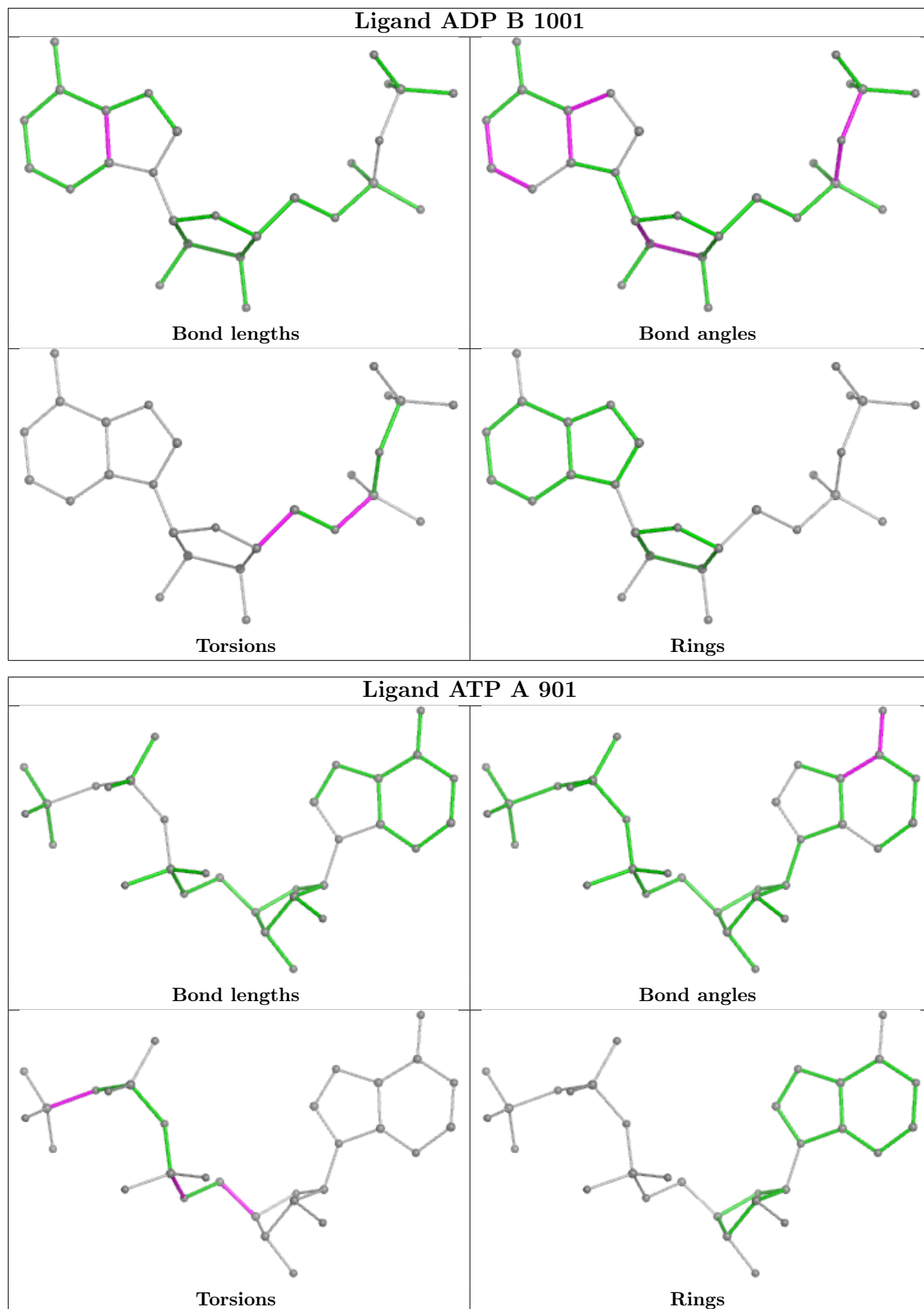


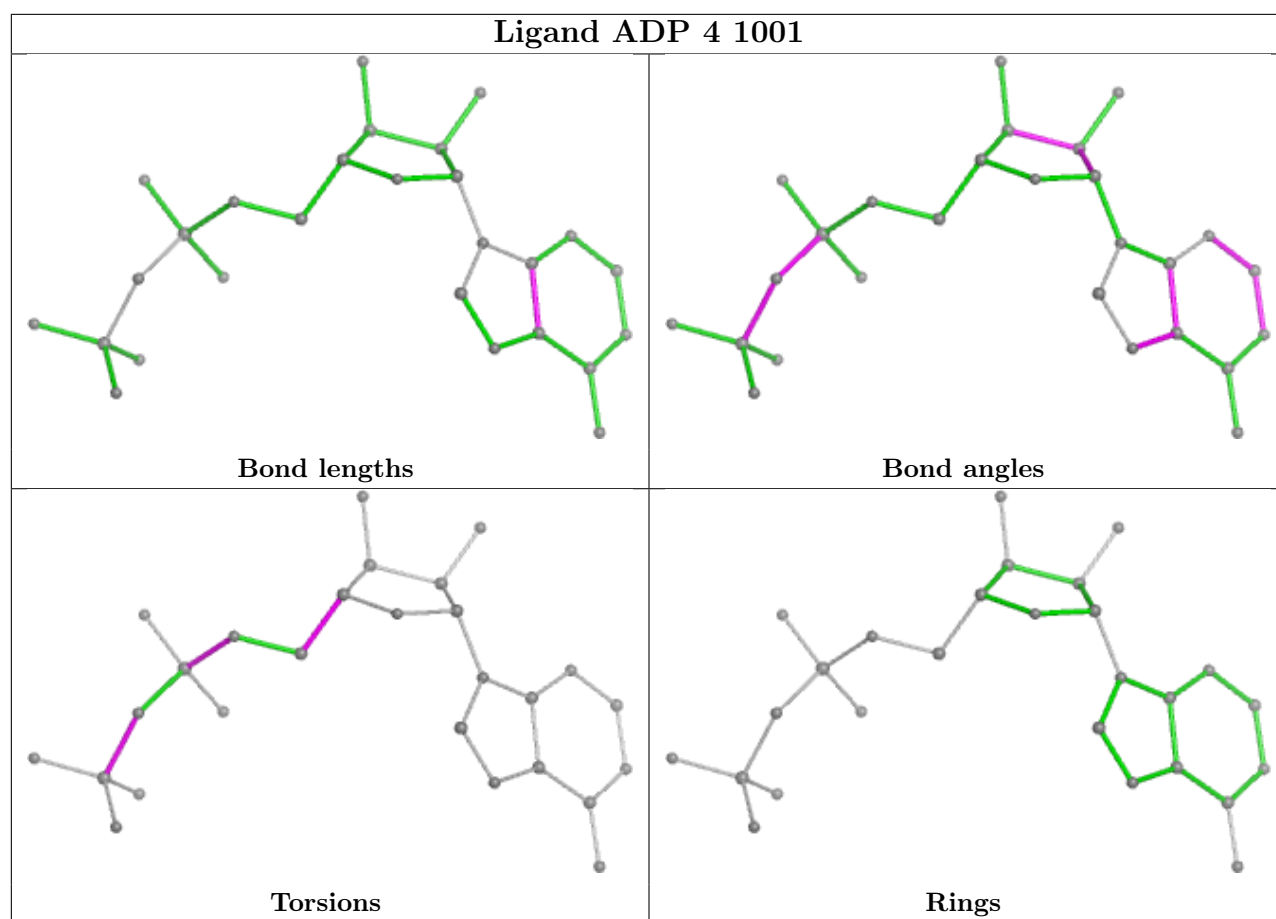












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

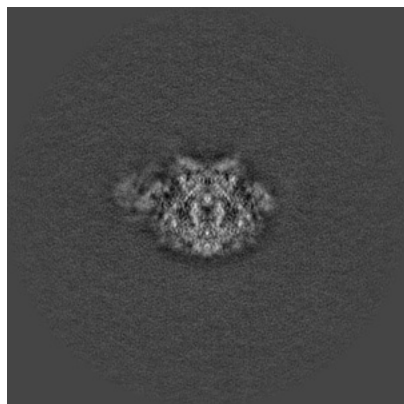
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-13211. These allow visual inspection of the internal detail of the map and identification of artifacts.

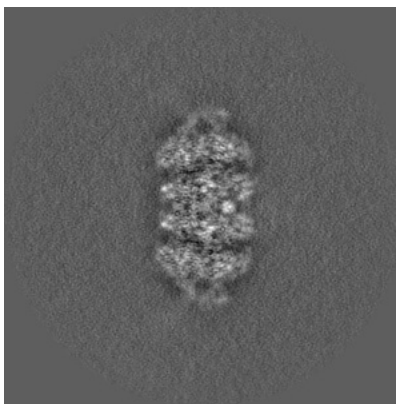
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

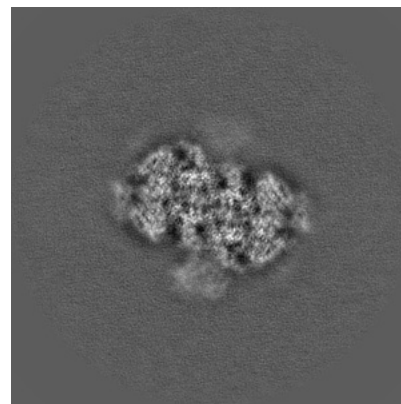
6.1.1 Primary map



X

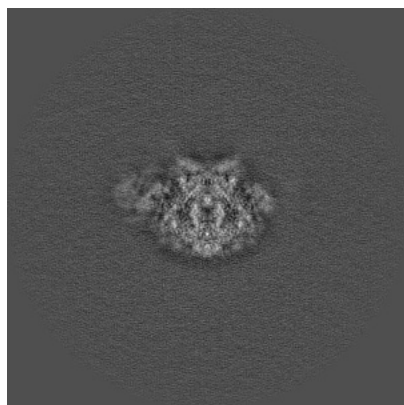


Y

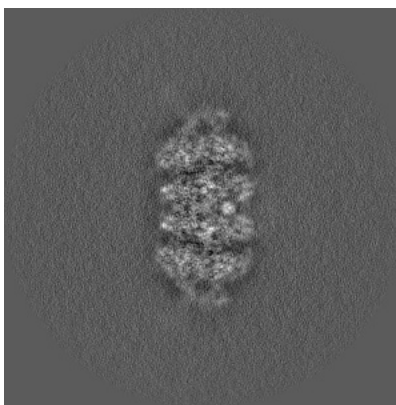


Z

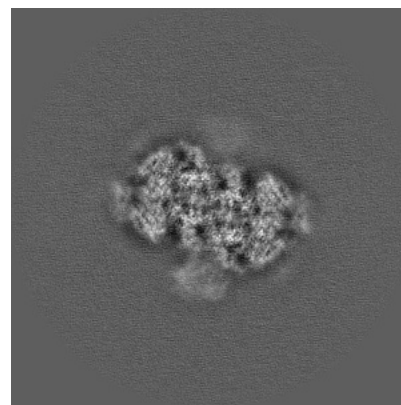
6.1.2 Raw map



X



Y

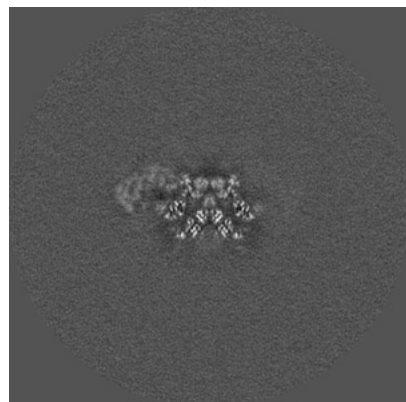


Z

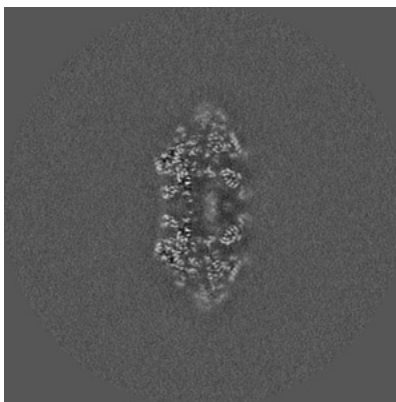
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

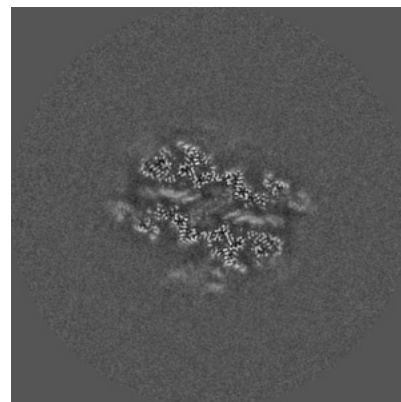
6.2.1 Primary map



X Index: 240

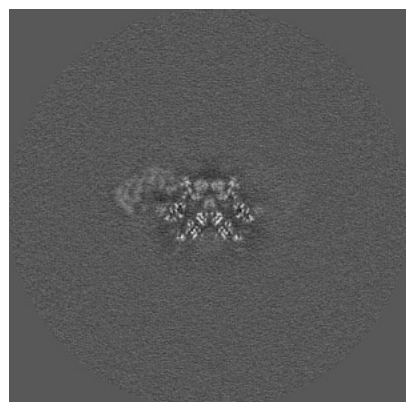


Y Index: 240

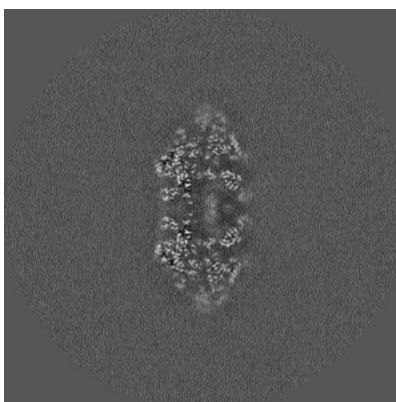


Z Index: 240

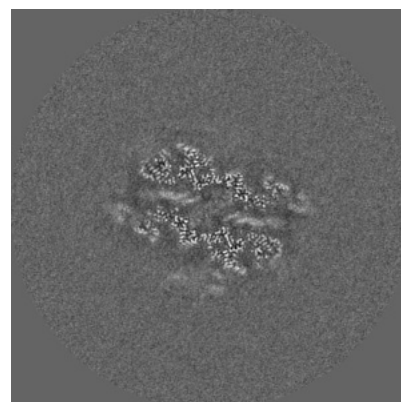
6.2.2 Raw map



X Index: 240



Y Index: 240

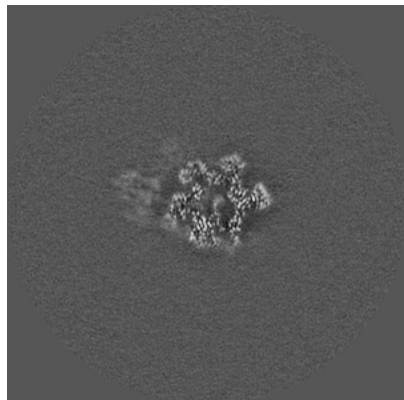


Z Index: 240

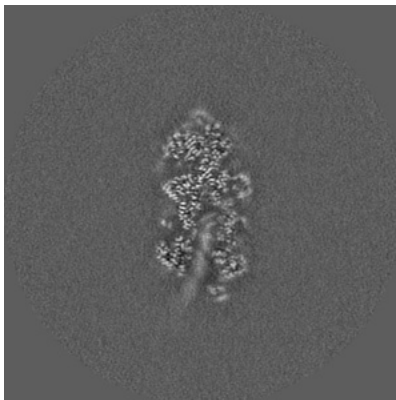
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

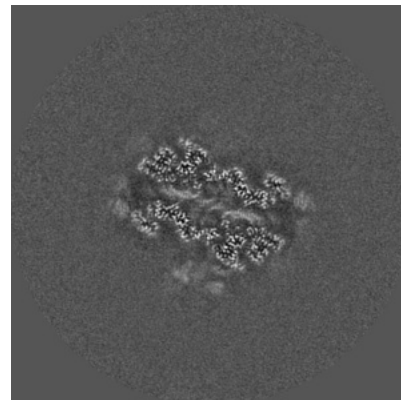
6.3.1 Primary map



X Index: 215

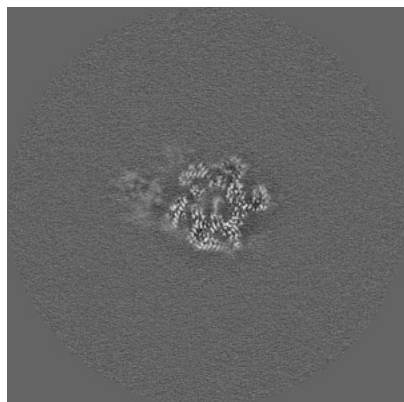


Y Index: 253

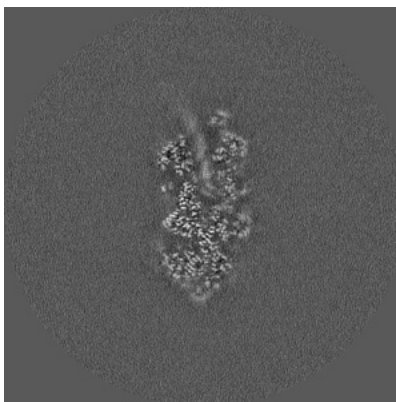


Z Index: 243

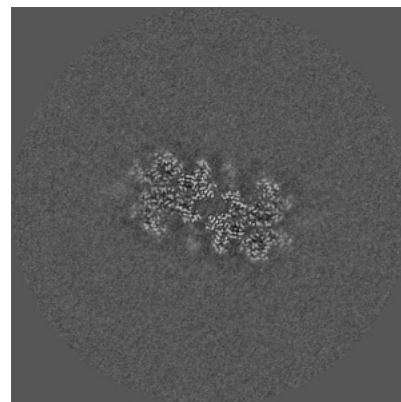
6.3.2 Raw map



X Index: 217



Y Index: 227

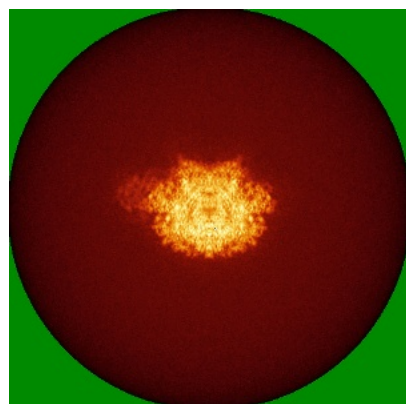


Z Index: 213

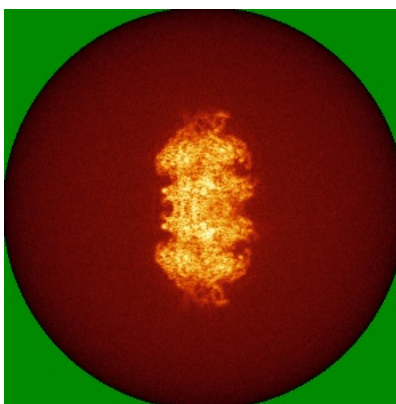
The images above show the largest variance slices of the map in three orthogonal directions.

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

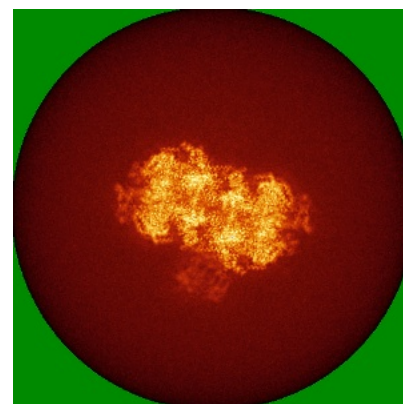
6.4.1 Primary map



X

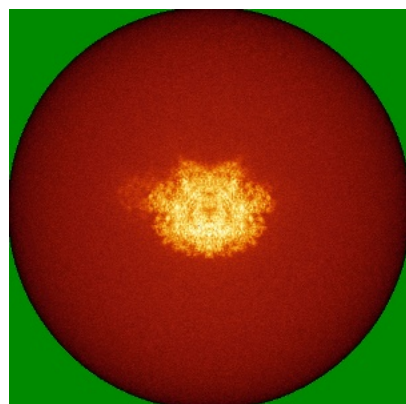


Y

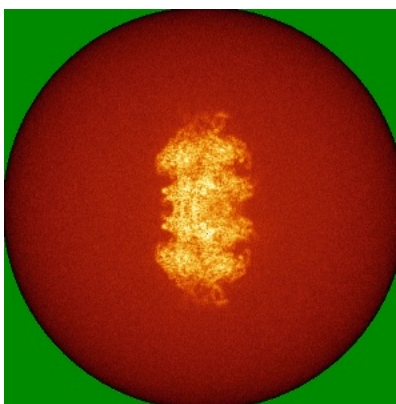


Z

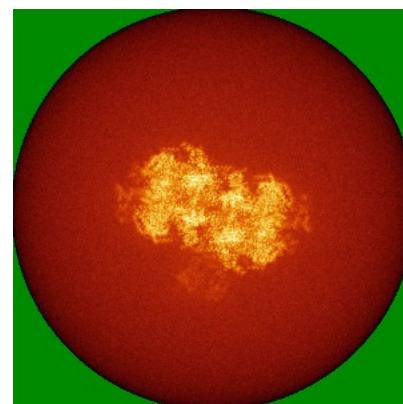
6.4.2 Raw map



X



Y

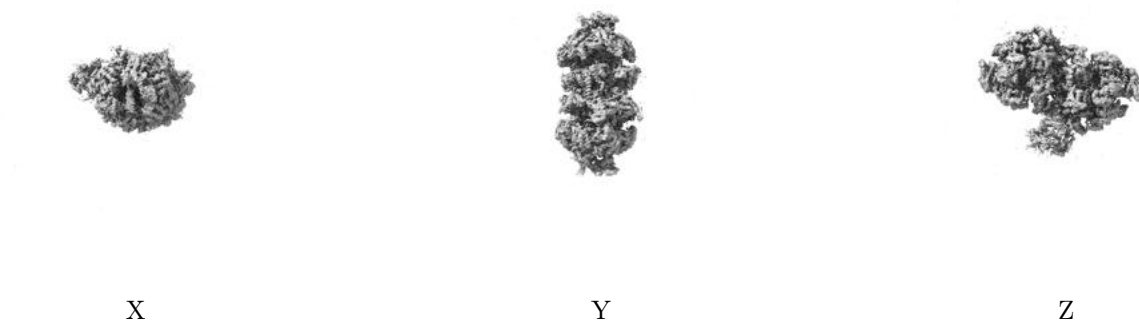


Z

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.

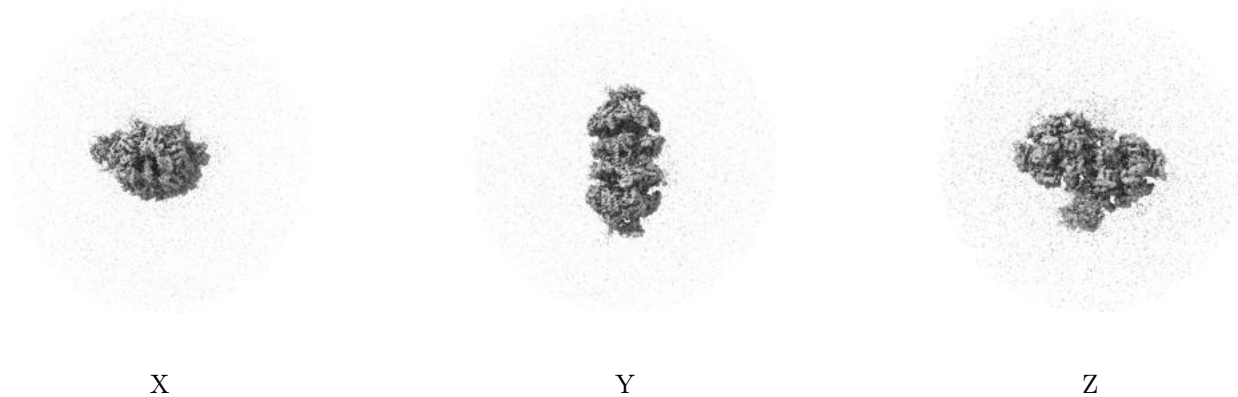
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0043. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

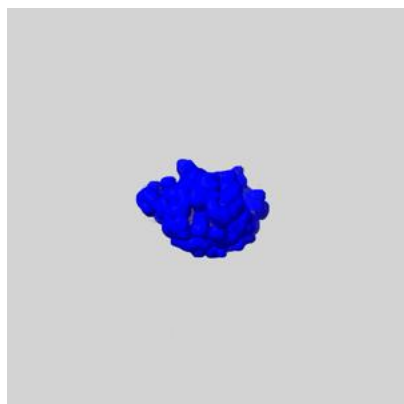
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

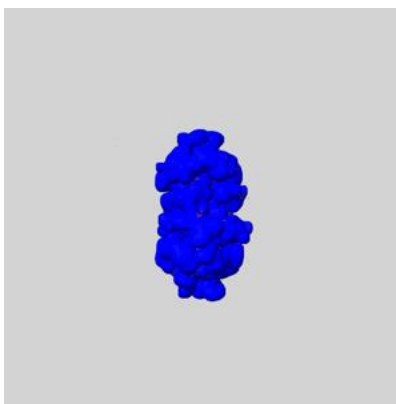
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

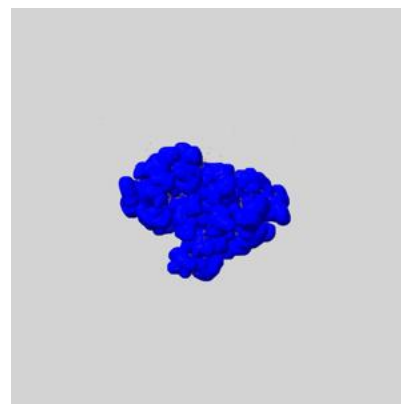
6.6.1 emd_13211_msk_1.map [i](#)



X



Y

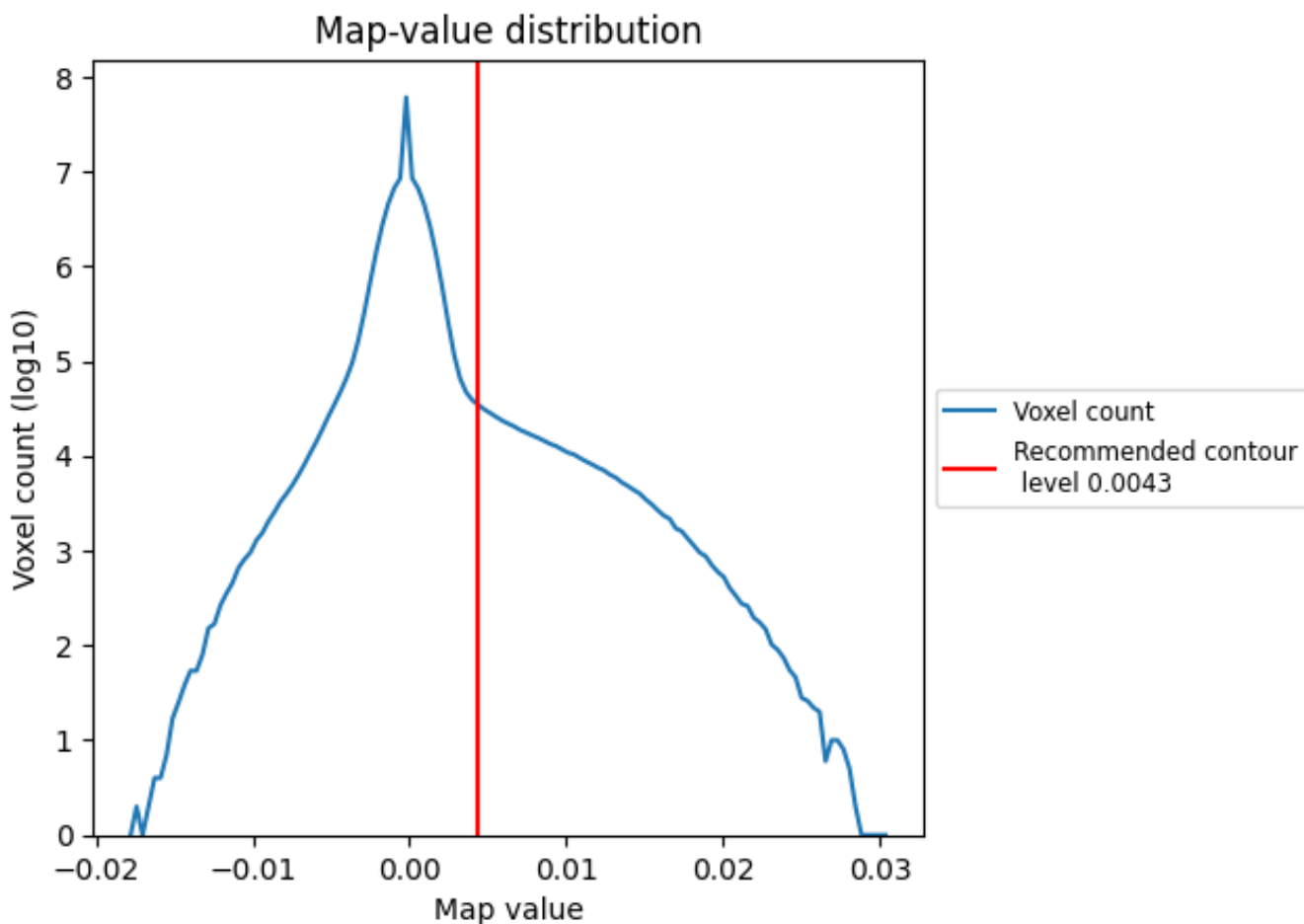


Z

7 Map analysis [i](#)

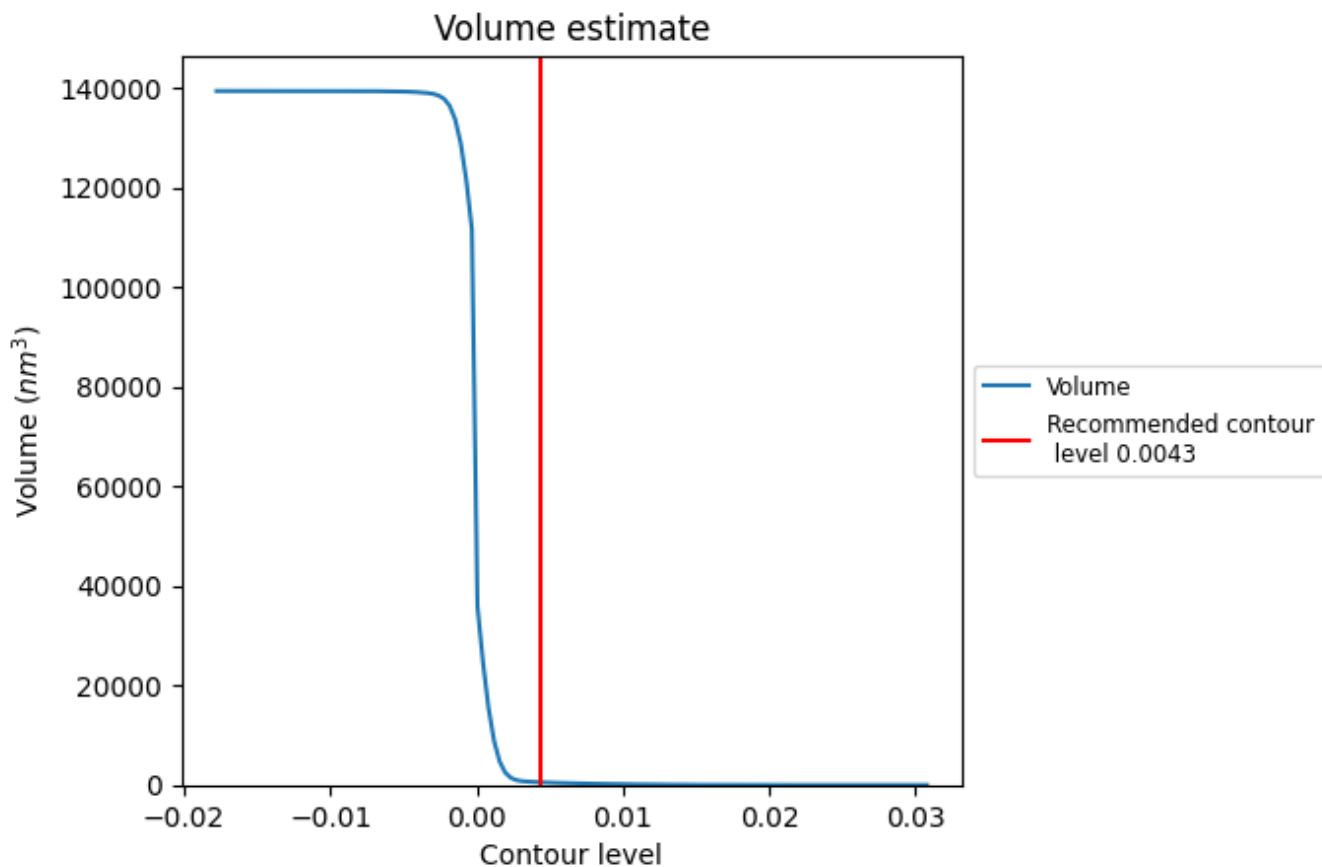
This section contains the results of statistical analysis of the map.

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.

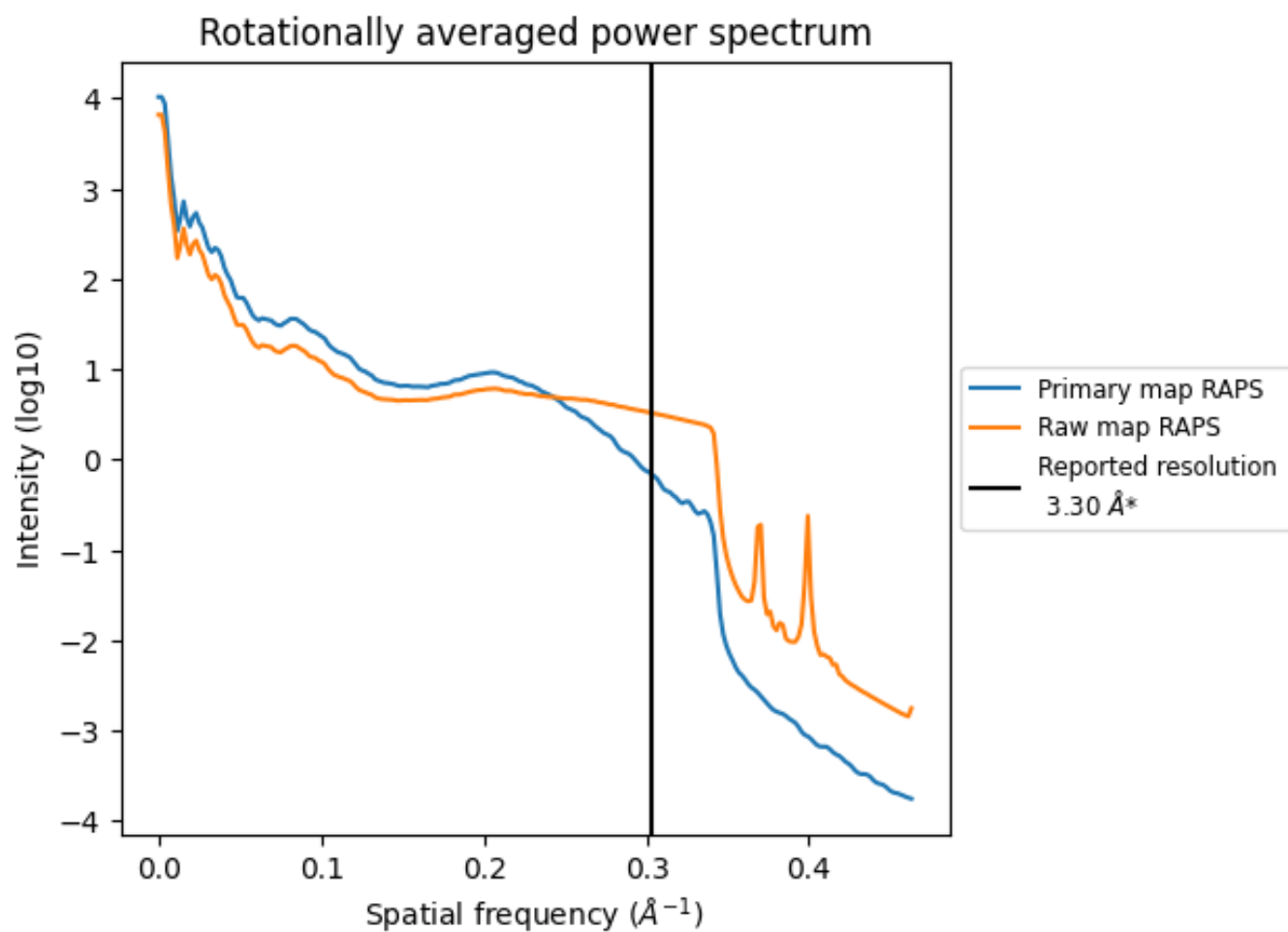
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 545 nm³; this corresponds to an approximate mass of 492 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

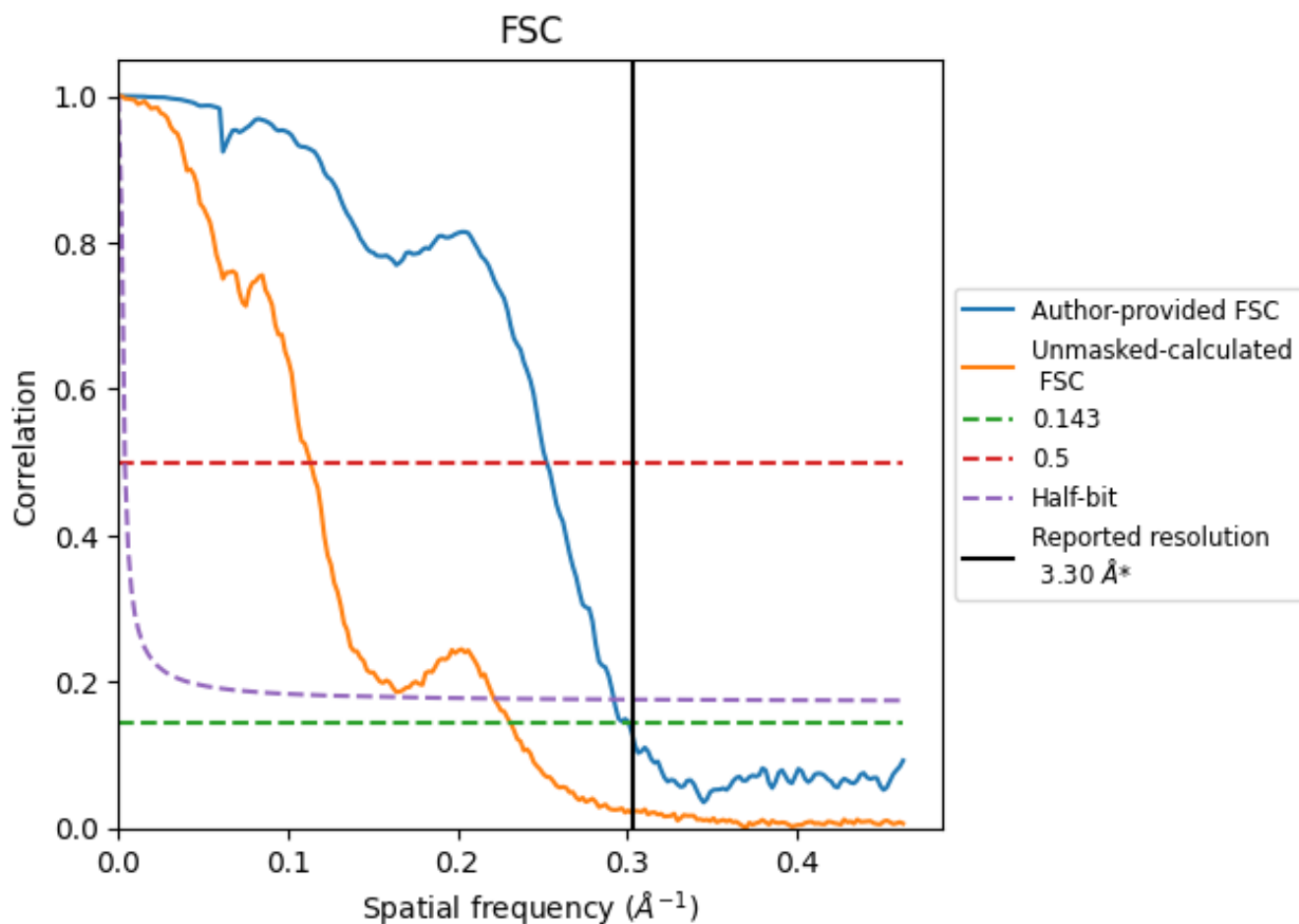


*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

8.2 Resolution estimates [i](#)

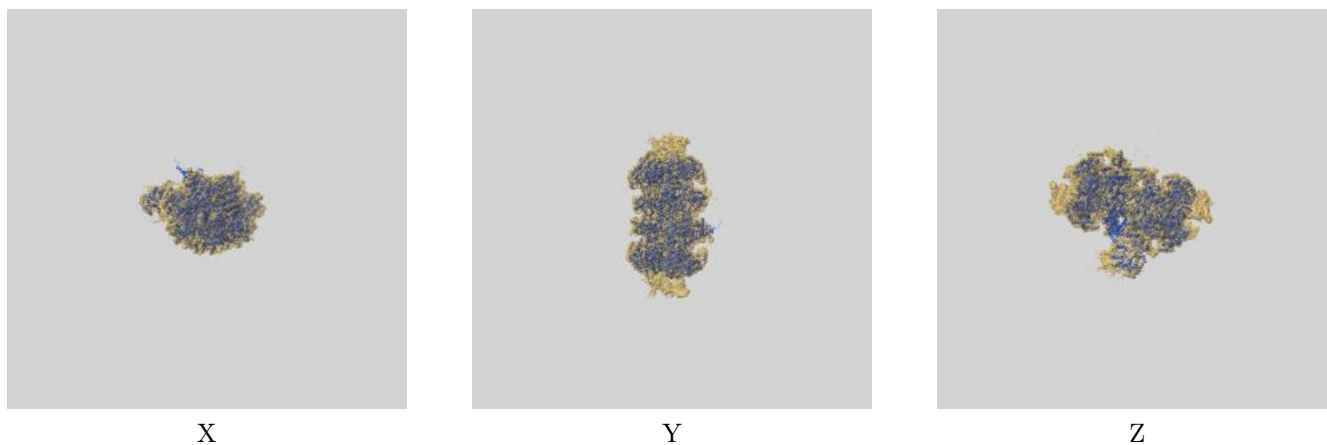
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.32	3.96	3.42
Unmasked-calculated*	4.32	8.83	4.51

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.32 differs from the reported value 3.3 by more than 10 %

9 Map-model fit [i](#)

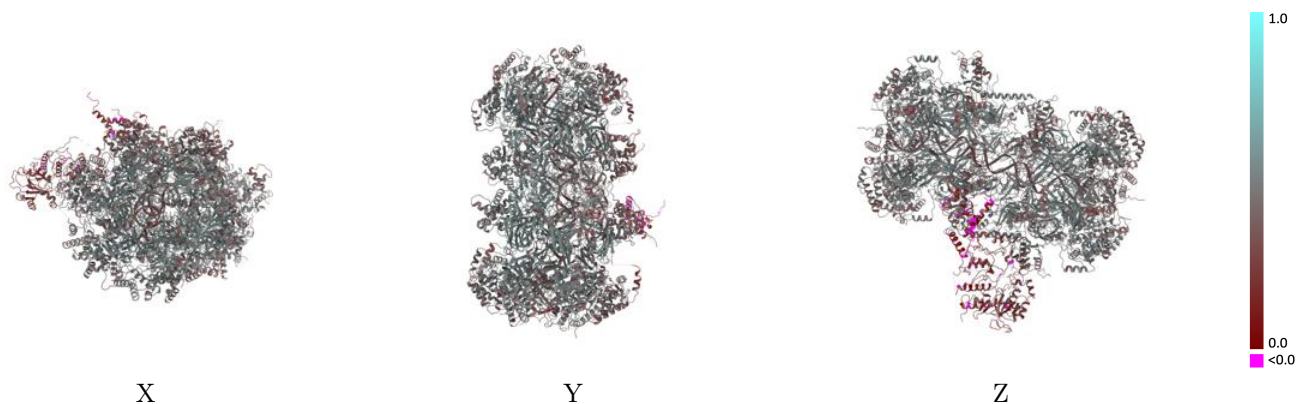
This section contains information regarding the fit between EMDB map EMD-13211 and PDB model 7P5Z. Per-residue inclusion information can be found in section [3](#) on page [12](#).

9.1 Map-model overlay [i](#)



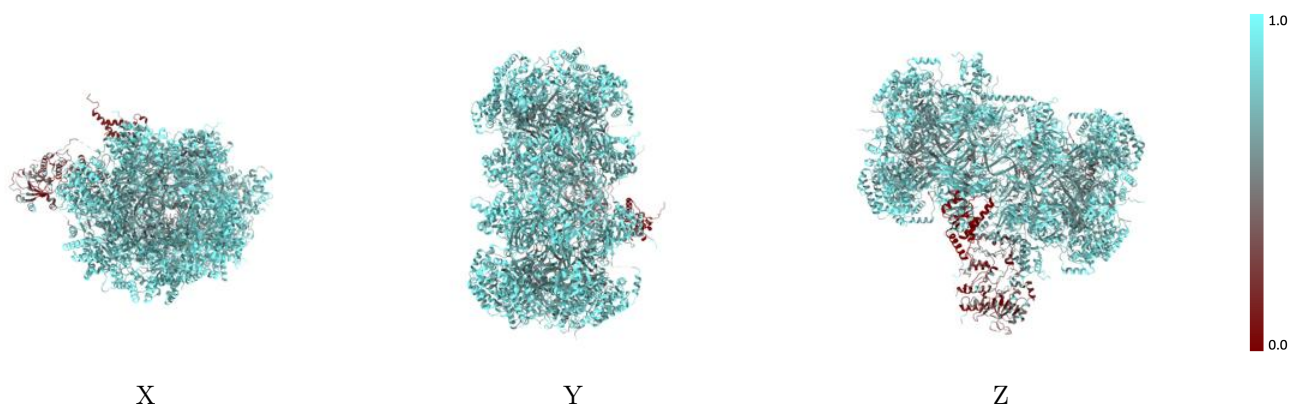
The images above show the 3D surface view of the map at the recommended contour level 0.0043 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



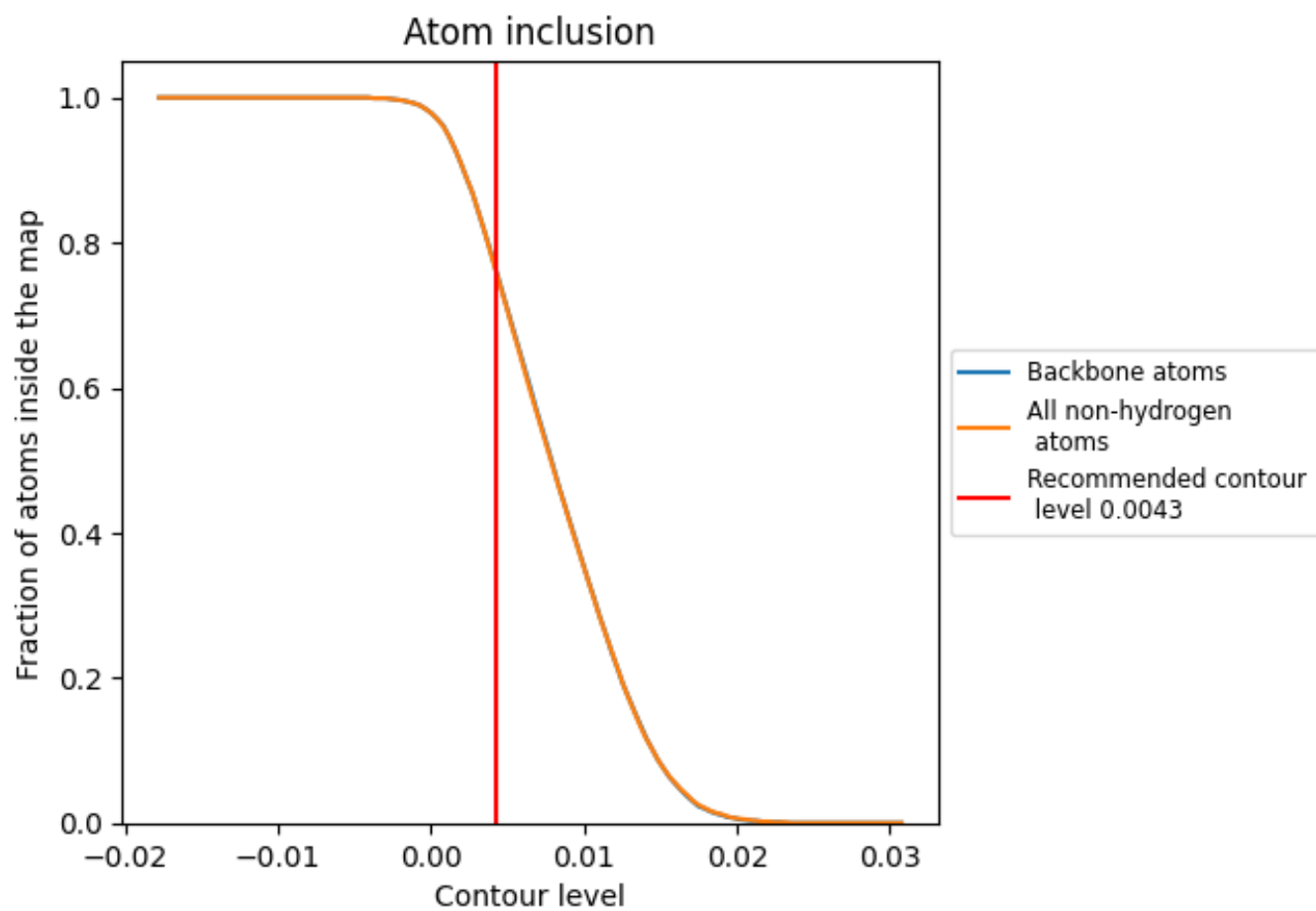
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0043).



































9.4 Atom inclusion [i](#)



At the recommended contour level, 76% of all backbone atoms, 76% 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 (0.0043) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7570	 0.4510
1	 0.3290	 0.2270
2	 0.7940	 0.4530
3	 0.8260	 0.4970
4	 0.7860	 0.4730
5	 0.8120	 0.4790
6	 0.7710	 0.4450
7	 0.8300	 0.4900
A	 0.7940	 0.4540
B	 0.8200	 0.4880
C	 0.8020	 0.4760
D	 0.8150	 0.4800
E	 0.7720	 0.4480
F	 0.8280	 0.4880
G	 0.1740	 0.1680
X	 0.6550	 0.3530
Y	 0.6620	 0.3540

