



wwPDB EM Validation Summary Report ⓘ

Sep 23, 2026 – 12:21 PM EDT

PDB ID : 11ST / pdb_000011st
EMDB ID : EMD-76021
Title : Structure of Yarrowia lipolytica ORC-Cdc6 bound to 54bp segment of OriC-061 DNA
Authors : Bauer, J.; Joshua-Tor, L.
Deposited on : 2026-03-11
Resolution : 2.73 Å(reported)
Based on initial model : .

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ 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.dev133
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) : 2.50

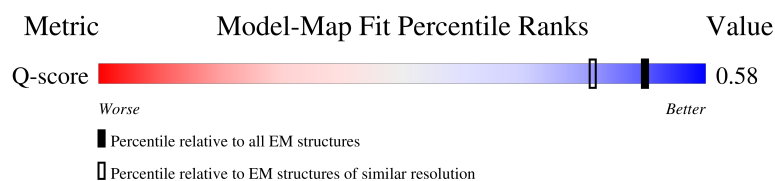
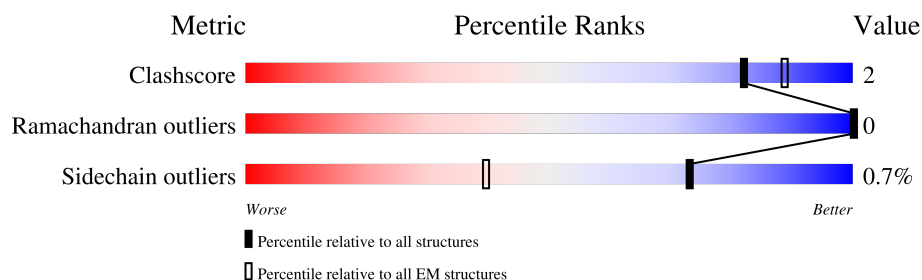
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.73 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	10432 (2.23 - 3.23)

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	A	861	
2	B	509	
3	C	685	
4	D	511	

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Mol	Chain	Length	Quality of chain
5	E	465	90%5%5%
6	F	365	41%56%
7	G	605	67%5%27%
7	K	605	98%
7	L	605	99%
8	X	54	43%24%33%
9	Y	54	57%7%35%

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 25039 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 Origin recognition complex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	416	Total	C	N	O	S	0	0
			3246	2044	570	620	12		

There are 143 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-142	MET	-	initiating methionine	UNP Q6C9L7
A	-141	SER	-	expression tag	UNP Q6C9L7
A	-140	ALA	-	expression tag	UNP Q6C9L7
A	-139	TRP	-	expression tag	UNP Q6C9L7
A	-138	SER	-	expression tag	UNP Q6C9L7
A	-137	HIS	-	expression tag	UNP Q6C9L7
A	-136	PRO	-	expression tag	UNP Q6C9L7
A	-135	GLN	-	expression tag	UNP Q6C9L7
A	-134	PHE	-	expression tag	UNP Q6C9L7
A	-133	GLU	-	expression tag	UNP Q6C9L7
A	-132	LYS	-	expression tag	UNP Q6C9L7
A	-131	GLY	-	expression tag	UNP Q6C9L7
A	-130	GLY	-	expression tag	UNP Q6C9L7
A	-129	GLY	-	expression tag	UNP Q6C9L7
A	-128	SER	-	expression tag	UNP Q6C9L7
A	-127	GLY	-	expression tag	UNP Q6C9L7
A	-126	GLY	-	expression tag	UNP Q6C9L7
A	-125	GLY	-	expression tag	UNP Q6C9L7
A	-124	SER	-	expression tag	UNP Q6C9L7
A	-123	GLY	-	expression tag	UNP Q6C9L7
A	-122	GLY	-	expression tag	UNP Q6C9L7
A	-121	SER	-	expression tag	UNP Q6C9L7
A	-120	ALA	-	expression tag	UNP Q6C9L7
A	-119	TRP	-	expression tag	UNP Q6C9L7
A	-118	SER	-	expression tag	UNP Q6C9L7
A	-117	HIS	-	expression tag	UNP Q6C9L7
A	-116	PRO	-	expression tag	UNP Q6C9L7
A	-115	GLN	-	expression tag	UNP Q6C9L7

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-114	PHE	-	expression tag	UNP Q6C9L7
A	-113	GLU	-	expression tag	UNP Q6C9L7
A	-112	LYS	-	expression tag	UNP Q6C9L7
A	-111	THR	-	expression tag	UNP Q6C9L7
A	-110	GLY	-	expression tag	UNP Q6C9L7
A	-109	SER	-	expression tag	UNP Q6C9L7
A	-108	LEU	-	expression tag	UNP Q6C9L7
A	-107	GLN	-	expression tag	UNP Q6C9L7
A	-106	ASP	-	expression tag	UNP Q6C9L7
A	-105	SER	-	expression tag	UNP Q6C9L7
A	-104	GLU	-	expression tag	UNP Q6C9L7
A	-103	VAL	-	expression tag	UNP Q6C9L7
A	-102	ASN	-	expression tag	UNP Q6C9L7
A	-101	GLN	-	expression tag	UNP Q6C9L7
A	-100	GLU	-	expression tag	UNP Q6C9L7
A	-99	ALA	-	expression tag	UNP Q6C9L7
A	-98	LYS	-	expression tag	UNP Q6C9L7
A	-97	PRO	-	expression tag	UNP Q6C9L7
A	-96	GLU	-	expression tag	UNP Q6C9L7
A	-95	VAL	-	expression tag	UNP Q6C9L7
A	-94	LYS	-	expression tag	UNP Q6C9L7
A	-93	PRO	-	expression tag	UNP Q6C9L7
A	-92	GLU	-	expression tag	UNP Q6C9L7
A	-91	VAL	-	expression tag	UNP Q6C9L7
A	-90	LYS	-	expression tag	UNP Q6C9L7
A	-89	PRO	-	expression tag	UNP Q6C9L7
A	-88	GLU	-	expression tag	UNP Q6C9L7
A	-87	THR	-	expression tag	UNP Q6C9L7
A	-86	HIS	-	expression tag	UNP Q6C9L7
A	-85	ILE	-	expression tag	UNP Q6C9L7
A	-84	ASN	-	expression tag	UNP Q6C9L7
A	-83	LEU	-	expression tag	UNP Q6C9L7
A	-82	LYS	-	expression tag	UNP Q6C9L7
A	-81	VAL	-	expression tag	UNP Q6C9L7
A	-80	SER	-	expression tag	UNP Q6C9L7
A	-79	ASP	-	expression tag	UNP Q6C9L7
A	-78	GLY	-	expression tag	UNP Q6C9L7
A	-77	SER	-	expression tag	UNP Q6C9L7
A	-76	SER	-	expression tag	UNP Q6C9L7
A	-75	GLU	-	expression tag	UNP Q6C9L7
A	-74	ILE	-	expression tag	UNP Q6C9L7
A	-73	PHE	-	expression tag	UNP Q6C9L7

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-72	PHE	-	expression tag	UNP Q6C9L7
A	-71	LYS	-	expression tag	UNP Q6C9L7
A	-70	ILE	-	expression tag	UNP Q6C9L7
A	-69	LYS	-	expression tag	UNP Q6C9L7
A	-68	LYS	-	expression tag	UNP Q6C9L7
A	-67	THR	-	expression tag	UNP Q6C9L7
A	-66	THR	-	expression tag	UNP Q6C9L7
A	-65	PRO	-	expression tag	UNP Q6C9L7
A	-64	LEU	-	expression tag	UNP Q6C9L7
A	-63	ARG	-	expression tag	UNP Q6C9L7
A	-62	ARG	-	expression tag	UNP Q6C9L7
A	-61	LEU	-	expression tag	UNP Q6C9L7
A	-60	MET	-	expression tag	UNP Q6C9L7
A	-59	GLU	-	expression tag	UNP Q6C9L7
A	-58	ALA	-	expression tag	UNP Q6C9L7
A	-57	PHE	-	expression tag	UNP Q6C9L7
A	-56	ALA	-	expression tag	UNP Q6C9L7
A	-55	LYS	-	expression tag	UNP Q6C9L7
A	-54	ARG	-	expression tag	UNP Q6C9L7
A	-53	GLN	-	expression tag	UNP Q6C9L7
A	-52	GLY	-	expression tag	UNP Q6C9L7
A	-51	LYS	-	expression tag	UNP Q6C9L7
A	-50	GLU	-	expression tag	UNP Q6C9L7
A	-49	MET	-	expression tag	UNP Q6C9L7
A	-48	ASP	-	expression tag	UNP Q6C9L7
A	-47	SER	-	expression tag	UNP Q6C9L7
A	-46	LEU	-	expression tag	UNP Q6C9L7
A	-45	THR	-	expression tag	UNP Q6C9L7
A	-44	PHE	-	expression tag	UNP Q6C9L7
A	-43	LEU	-	expression tag	UNP Q6C9L7
A	-42	TYR	-	expression tag	UNP Q6C9L7
A	-41	ASP	-	expression tag	UNP Q6C9L7
A	-40	GLY	-	expression tag	UNP Q6C9L7
A	-39	ILE	-	expression tag	UNP Q6C9L7
A	-38	GLU	-	expression tag	UNP Q6C9L7
A	-37	ILE	-	expression tag	UNP Q6C9L7
A	-36	GLN	-	expression tag	UNP Q6C9L7
A	-35	ALA	-	expression tag	UNP Q6C9L7
A	-34	ASP	-	expression tag	UNP Q6C9L7
A	-33	GLN	-	expression tag	UNP Q6C9L7
A	-32	THR	-	expression tag	UNP Q6C9L7
A	-31	PRO	-	expression tag	UNP Q6C9L7

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-30	GLU	-	expression tag	UNP Q6C9L7
A	-29	ASP	-	expression tag	UNP Q6C9L7
A	-28	LEU	-	expression tag	UNP Q6C9L7
A	-27	ASP	-	expression tag	UNP Q6C9L7
A	-26	MET	-	expression tag	UNP Q6C9L7
A	-25	GLU	-	expression tag	UNP Q6C9L7
A	-24	ASP	-	expression tag	UNP Q6C9L7
A	-23	ASN	-	expression tag	UNP Q6C9L7
A	-22	ASP	-	expression tag	UNP Q6C9L7
A	-21	ILE	-	expression tag	UNP Q6C9L7
A	-20	ILE	-	expression tag	UNP Q6C9L7
A	-19	GLU	-	expression tag	UNP Q6C9L7
A	-18	ALA	-	expression tag	UNP Q6C9L7
A	-17	HIS	-	expression tag	UNP Q6C9L7
A	-16	ARG	-	expression tag	UNP Q6C9L7
A	-15	GLU	-	expression tag	UNP Q6C9L7
A	-14	GLN	-	expression tag	UNP Q6C9L7
A	-13	ILE	-	expression tag	UNP Q6C9L7
A	-12	GLY	-	expression tag	UNP Q6C9L7
A	-11	GLY	-	expression tag	UNP Q6C9L7
A	-10	ILE	-	expression tag	UNP Q6C9L7
A	-9	PRO	-	expression tag	UNP Q6C9L7
A	-8	THR	-	expression tag	UNP Q6C9L7
A	-7	THR	-	expression tag	UNP Q6C9L7
A	-6	GLU	-	expression tag	UNP Q6C9L7
A	-5	ASN	-	expression tag	UNP Q6C9L7
A	-4	LEU	-	expression tag	UNP Q6C9L7
A	-3	TYR	-	expression tag	UNP Q6C9L7
A	-2	PHE	-	expression tag	UNP Q6C9L7
A	-1	GLN	-	expression tag	UNP Q6C9L7
A	0	GLY	-	expression tag	UNP Q6C9L7

- Molecule 2 is a protein called Origin recognition complex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	377	Total	C	N	O	S	0	0
			2997	1919	497	568	13		

- Molecule 3 is a protein called Origin recognition complex subunit 3 (Orc3).

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	630	Total	C	N	O	S	0	0
			5118	3267	857	976	18		

- Molecule 4 is a protein called Origin recognition complex subunit 4 (Orc4).

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	445	Total	C	N	O	S	0	0
			3584	2267	622	682	13		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	18	GLU	LYS	conflict	UNP Q6C5R0

- Molecule 5 is a protein called Origin recognition complex subunit 5 (Orc5).

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	441	Total	C	N	O	S	0	0
			3518	2234	614	656	14		

- Molecule 6 is a protein called Origin recognition complex subunit 6 (Orc6).

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	162	Total	C	N	O	S	0	0
			1353	869	243	235	6		

- Molecule 7 is a protein called Cell division control protein 6 (Cdc6).

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	441	Total	C	N	O	S	0	0
			3435	2176	608	629	22		
7	K	14	Total	C	N	O	S	0	0
			106	66	23	16	1		
7	L	9	Total	C	N	O		0	0
			82	50	21	11			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	0	GLY	-	expression tag	UNP Q6CDG7
K	0	GLY	-	expression tag	UNP Q6CDG7
L	0	GLY	-	expression tag	UNP Q6CDG7

- Molecule 8 is a DNA chain called DNA (54-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
8	X	36	Total	C	N	O	P	0	0
			733	350	136	211	36		

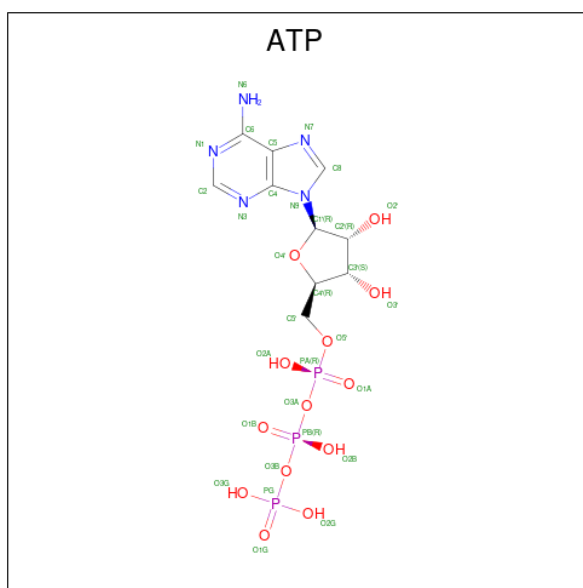
- Molecule 9 is a DNA chain called DNA (54-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
9	Y	35	Total	C	N	O	P	0	0
			722	345	126	216	35		

- Molecule 10 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
10	A	1	Total	Mg	0
			1	1	
10	D	1	Total	Mg	0
			1	1	
10	G	1	Total	Mg	0
			1	1	

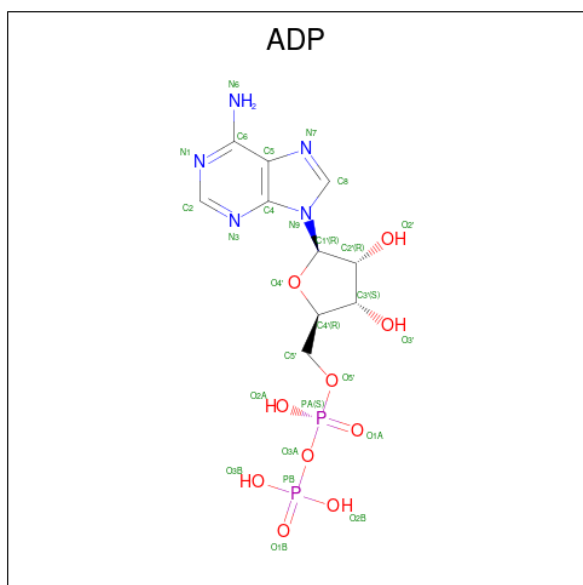
- Molecule 11 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).

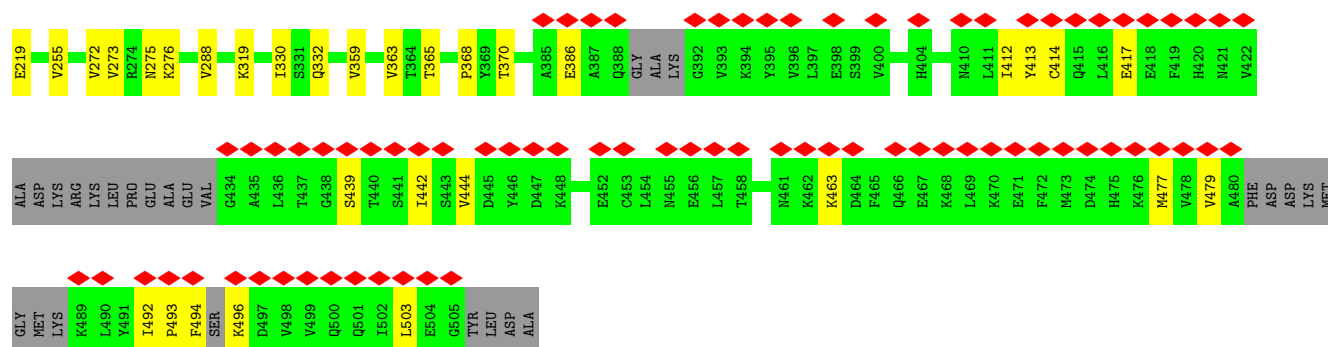


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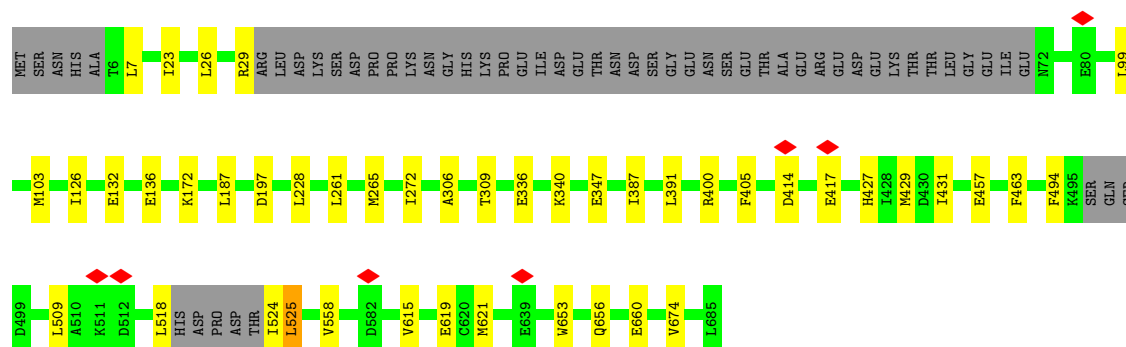
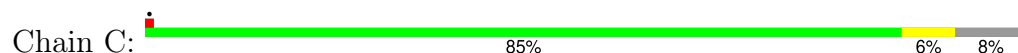
Mol	Chain	Residues	Atoms					AltConf
11	D	1	Total	C	N	O	P	0
			31	10	5	13	3	
11	G	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 12 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).

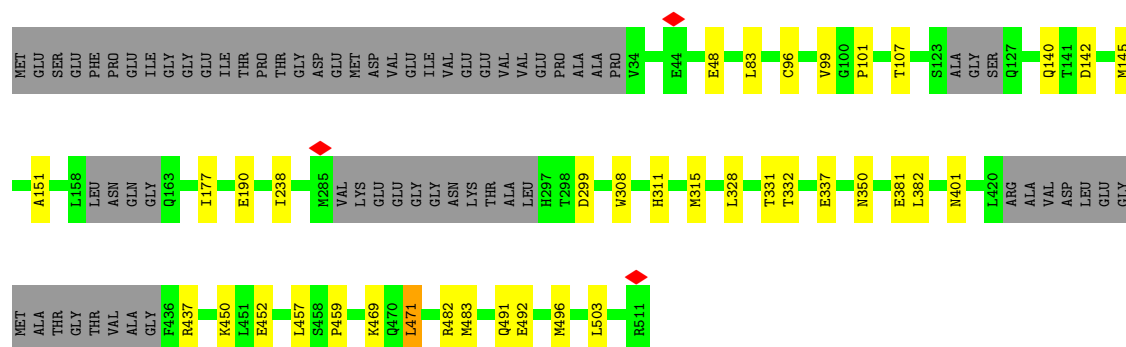




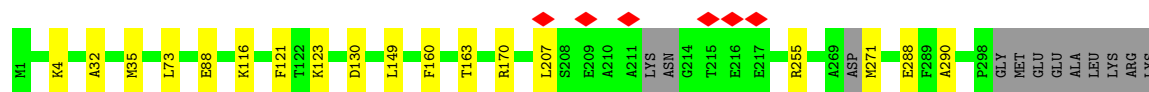
• Molecule 3: Origin recognition complex subunit 3 (Orc3)



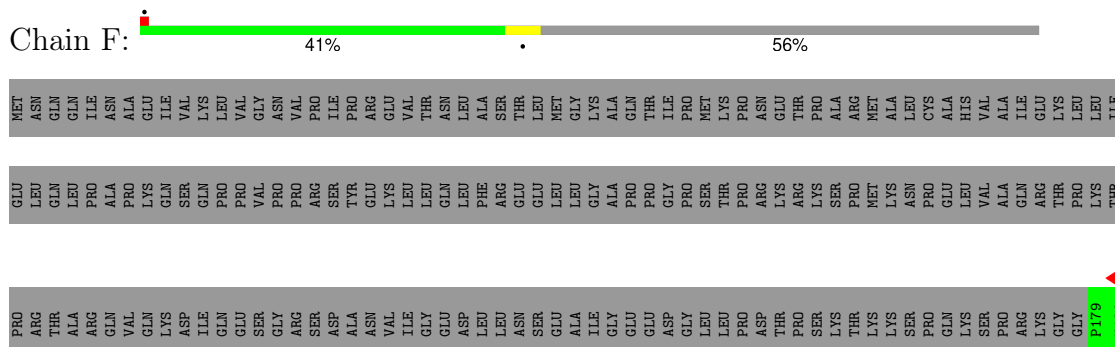
• Molecule 4: Origin recognition complex subunit 4 (Orc4)



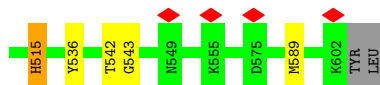
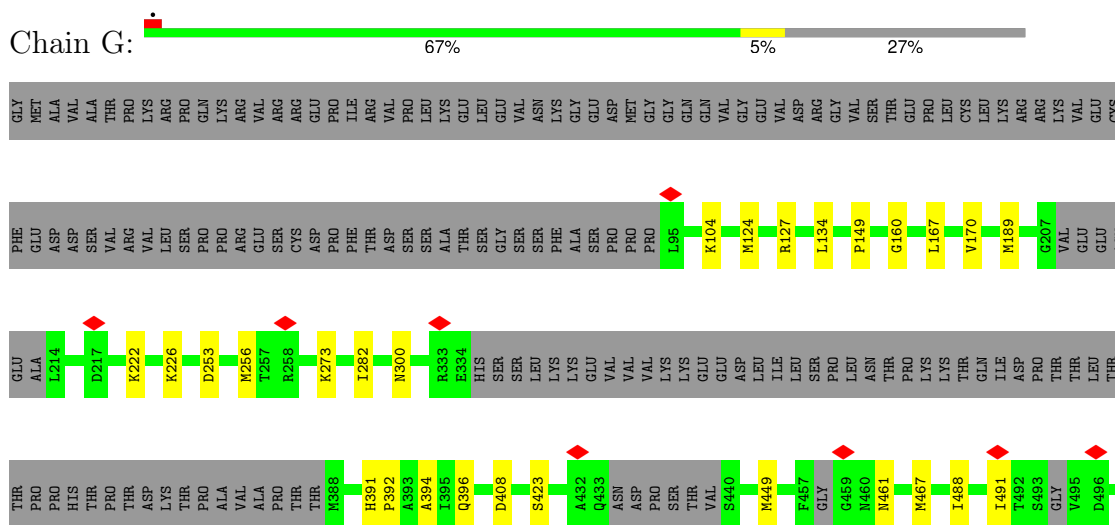
• Molecule 5: Origin recognition complex subunit 5 (Orc5)



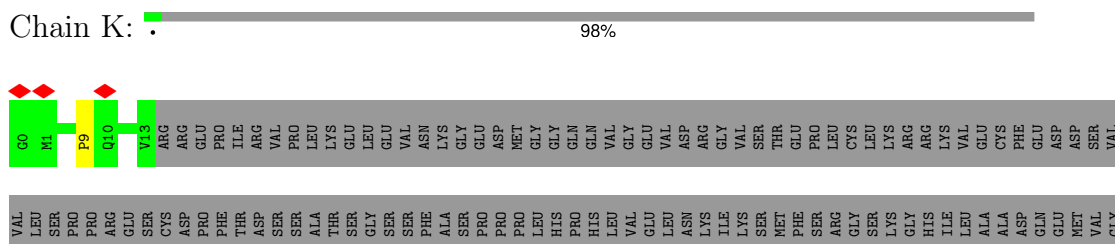
- Molecule 6: Origin recognition complex subunit 6 (Orc6)



- Molecule 7: Cell division control protein 6 (Cdc6)



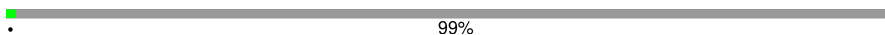
- Molecule 7: Cell division control protein 6 (Cdc6)



L	LYS	SER	PHE	THR	LYS	VAL	ASN	ARG
	LYS	ILE	ILE	THR	PHE	VAL	ASN	ARG
	ASN	GLU	GLN	THR	LYS	VAL	CYS	VAL
	LYS	ALA	LYS	THR	LYS	ASP	LEU	GLN
	ILE	ILE	LEU	THR	TYR	GLU	ALA	GLU
	ASN	SER	GLN	PRO	ASP	ILE	PRO	ALA
	GLY	GLY	ASN	HIS	ALA	ASP	SER	LEU
	LYS	VAL	ASP	THR	GLN	ILE	ALA	ARG
	GLY	VAL	PRO	THR	ILE	MET	ARG	LEU
	ARG	VAL	SER	THR	ALA	THR	ILE	TYR
I	ALA	PRO	THR	LYS	SER	ASP	MET	PHE
	SER	LEU	VAL	ILE	ILE	ASP	ASN	GLU
	LYS	THR	SER	THR	ILE	GLN	LEU	ARG
	GLY	GLY	LYS	ASP	LYS	PRO	ILE	ARG
	GLY	GLN	PRO	ALA	SER	ILE	TYR	LYS
	THR	ARG	VAL	VAL	ARG	LEU	LYS	GLN
	GLY	LEU	VAL	ALA	ILE	PHE	GLN	ALA
	ALA	PHE	SER	PRO	VAL	ARG	LEU	LYS
	SER	ASP	ILE	THR	LYS	ILE	SER	TYR
	LYS	THR	ALA	THR	ALA	PHE	GLY	SER
J	GLY	THR	ALA	THR	SER	GLY	VAL	GLN
	GLY	TYR	THR	MET	GLU	TRP	GLU	PRO
	VAL	SER	ALA	ILE	GLU	ALA	GLU	GLY
	TYR	SER	ARG	HIS	PHE	PHE	ASN	ALA
	GLY	CYS	VAL	PRO	SER	CYS	GLU	ALA
	ARG	LYS	CYS	ALA	ARG	LYS	ALA	LEU
	ASP	HIS	GLN	ILE	HIS	GLY	LEU	TYR
	ASP	ARG	VAL	GLN	SER	ARG	ALA	SER
	TYR	MET	PHE	CYS	SER	LEU	ASP	GLY
	GLN	LEU	GLY	ALA	LYS	ILE	PRO	PRO
K	ARG	PRO	ASN	ARG	LYS	VAL	PHE	GLY
	LYS	LEU	ASN	LYS	GLU	GLY	ASP	THR
	VAL	PHE	ILE	THR	LYS	LEU	LYS	GLY
	GLN	LEU	MET	GLY	GLU	ASP	LEU	LEU
	ARG	ASP	LEU	ASP	GLU	LEU	GLU	GLN
	MET	VAL	ASN	LEU	ASP	THR	GLU	ARG
	ASN	CYS	LEU	ARG	LEU	ASP	LEU	VAL
	ILE	SER	GLN	LYS	ILE	ARG	PHE	MET
	SER	LEU	LYS	PHE	SER	LEU	CYS	ASP
	ALA	GLU	ALA	ASP	PRO	PRO	GLN	VAL
M	ILE	SER	VAL	ILE	LEU	ARG	THR	PHE
	GLU	TYR	LEU	CYS	ASN	LEU	LYS	ARG
	VAL	SER	CYS	ARG	THR	LYS	GLY	GLY
	VAL	VAL	THR	LYS	PRO	ALA	GLU	LYS
	TRP	ILE	VAL	ALA	LYS	ASN	PHE	GLU
	LEU	ASN	ALA	LEU	LYS	ASN	ALA	GLY
	GLN	ILE	SER	GLU	THR	PHE	GLU	ILE
	LYS	THR	ALA	ILE	THR	GLU	ARG	LYS
	TYR	THR	ALA	ILE	ILE	TYR	GLU	VAL
	LEU	GLY	GLU	GLY	ILE	PRO	GLY	ALA
N	LYS	ILE	LYS	GLN	PRO	GLN	TYR	ILE
	ASN	GLU	GLN	THR	LYS	VAL	CYS	VAL
	LEU	ALA	LYS	THR	PRO	ASP	LEU	GLN
	ILE	ILE	LEU	THR	ASP	ILE	PRO	ALA
	ASN	SER	GLN	PRO	ALA	ASP	SER	LEU
	GLY	GLY	ASN	HIS	VAL	ASP	ALA	THR
	LYS	VAL	ASP	THR	GLN	ILE	ARG	LEU
	GLY	VAL	PRO	THR	ILE	GLN	ILE	ARG
	ARG	VAL	SER	THR	ALA	THR	GLY	VAL
	ALA	PRO	THR	LYS	ILE	ARG	GLU	GLY

- Molecule 7: Cell division control protein 6 (Cdc6)

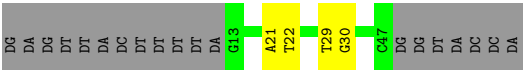
Chain L:

[illegible]

- Molecule 8: DNA (54-MER)



● Molecule 9: DNA (54-MER)



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	51599	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; CTF correction was done first in WARP during exposure/micrograph pre-processing, and re-corrected during the final refinements/reconstruction of the map in cryoSPARC	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	43.2	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.814	Depositor
Minimum map value	-0.280	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.019	Depositor
Recommended contour level	0.15	Depositor
Map size ($\text{\AA}$)	382.36002, 382.36002, 382.36002	wwPDB
Map dimensions	440, 440, 440	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.869, 0.869, 0.869	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: MG, ATP, ADP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.11	0/3296	0.24	0/4455
2	B	0.11	0/3057	0.25	0/4131
3	C	0.12	0/5224	0.25	0/7063
4	D	0.12	0/3645	0.26	0/4931
5	E	0.12	0/3584	0.25	0/4854
6	F	0.10	0/1387	0.24	0/1865
7	G	0.10	0/3482	0.25	0/4674
7	K	0.10	0/107	0.30	0/142
7	L	0.07	0/82	0.21	0/108
8	X	0.21	0/822	0.42	0/1264
9	Y	0.24	0/808	0.42	0/1247
All	All	0.13	0/25494	0.26	0/34734

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3246	0	3305	9	0
2	B	2997	0	2956	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	5118	0	5037	27	0
4	D	3584	0	3592	24	0
5	E	3518	0	3577	12	0
6	F	1353	0	1349	7	0
7	G	3435	0	3548	19	0
7	K	106	0	123	1	0
7	L	82	0	93	0	0
8	X	733	0	405	9	0
9	Y	722	0	399	2	0
10	A	1	0	0	0	0
10	D	1	0	0	0	0
10	G	1	0	0	0	0
11	A	31	0	12	1	0
11	D	31	0	12	1	0
11	G	31	0	12	0	0
12	E	27	0	12	0	0
13	A	1	0	0	0	0
13	B	1	0	0	0	0
13	C	3	0	0	0	0
13	G	1	0	0	0	0
13	X	8	0	0	0	0
13	Y	8	0	0	0	0
All	All	25039	0	24432	123	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 2.

The worst 5 of 123 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)
2:B:463:LYS:HZ1	7:G:461:ASN:H	1.31	0.78
2:B:414:CYS:HB3	2:B:444:VAL:HG21	1.66	0.77
3:C:309:THR:HG21	3:C:347:GLU:HG3	1.68	0.75
4:D:401:ASN:HD22	4:D:483:MET:HE1	1.52	0.74
3:C:414:ASP:HB3	3:C:417:GLU:HG3	1.74	0.69

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	412/861 (48%)	407 (99%)	5 (1%)	0	100	100
2	B	367/509 (72%)	360 (98%)	7 (2%)	0	100	100
3	C	622/685 (91%)	616 (99%)	6 (1%)	0	100	100
4	D	435/511 (85%)	428 (98%)	7 (2%)	0	100	100
5	E	433/465 (93%)	426 (98%)	7 (2%)	0	100	100
6	F	158/365 (43%)	157 (99%)	1 (1%)	0	100	100
7	G	429/605 (71%)	424 (99%)	5 (1%)	0	100	100
7	K	12/605 (2%)	11 (92%)	1 (8%)	0	100	100
7	L	7/605 (1%)	7 (100%)	0	0	100	100
All	All	2875/5211 (55%)	2836 (99%)	39 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	359/748 (48%)	359 (100%)	0	100	100
2	B	334/451 (74%)	330 (99%)	4 (1%)	63	77
3	C	564/614 (92%)	561 (100%)	3 (0%)	81	88
4	D	400/449 (89%)	397 (99%)	3 (1%)	73	83
5	E	395/417 (95%)	391 (99%)	4 (1%)	68	80

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	F	141/316 (45%)	140 (99%)	1 (1%)	76	85
7	G	374/522 (72%)	370 (99%)	4 (1%)	65	79
7	K	11/522 (2%)	11 (100%)	0	100	100
7	L	9/522 (2%)	9 (100%)	0	100	100
All	All	2587/4561 (57%)	2568 (99%)	19 (1%)	73	85

5 of 19 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	F	322	SER
7	G	423	SER
7	G	515	HIS
7	G	396	GLN
4	D	471	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
5	E	402	GLN
5	E	394	GLN
3	C	540	GLN
5	E	232	GLN
3	C	390	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 7 ligands modelled in this entry, 3 are monoatomic - leaving 4 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
12	ADP	E	501	-	28,29,29	1.39	4 (14%)	43,45,45	1.83	9 (20%)
11	ATP	D	601	10	32,33,33	0.46	0	48,52,52	0.33	0
11	ATP	G	702	10	32,33,33	0.35	0	48,52,52	0.34	0
11	ATP	A	802	10	32,33,33	0.43	0	48,52,52	0.34	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
12	ADP	E	501	-	-	3/16/32/32	0/3/3/3
11	ATP	D	601	10	-	4/22/38/38	0/3/3/3
11	ATP	G	702	10	-	4/22/38/38	0/3/3/3
11	ATP	A	802	10	-	2/22/38/38	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	E	501	ADP	C5-C4	4.55	1.47	1.39
12	E	501	ADP	C5-C6	2.65	1.48	1.41
12	E	501	ADP	C5-N7	-2.39	1.34	1.39
12	E	501	ADP	C8-N7	2.17	1.35	1.31

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	E	501	ADP	C5-C4-N3	-5.83	118.70	126.72
12	E	501	ADP	N3-C4-N9	4.62	135.02	127.17
12	E	501	ADP	C2-N3-C4	3.67	120.80	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	E	501	ADP	C4-C5-N7	-3.45	106.64	110.58
12	E	501	ADP	N3-C2-N1	-3.19	123.75	128.58

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

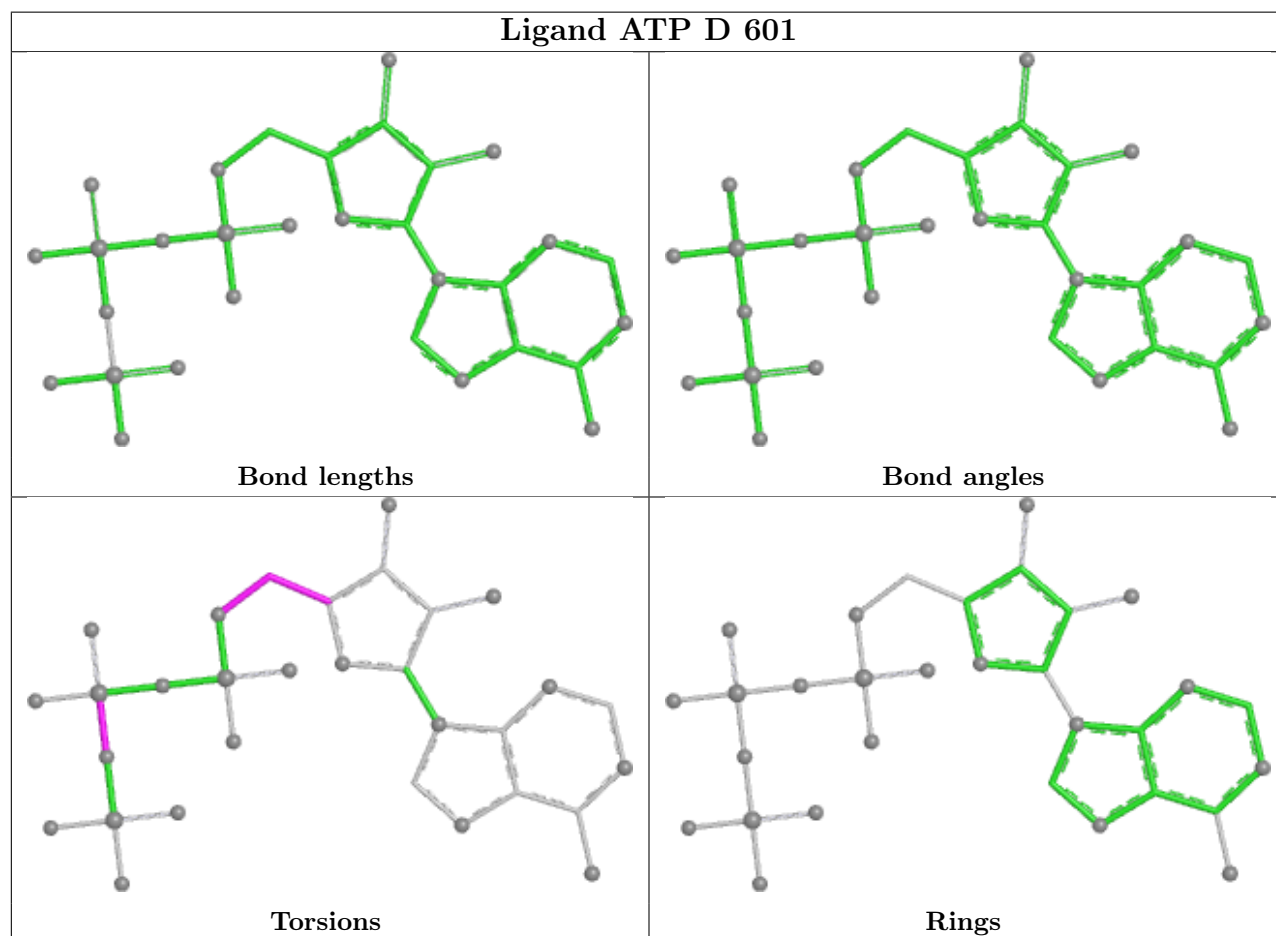
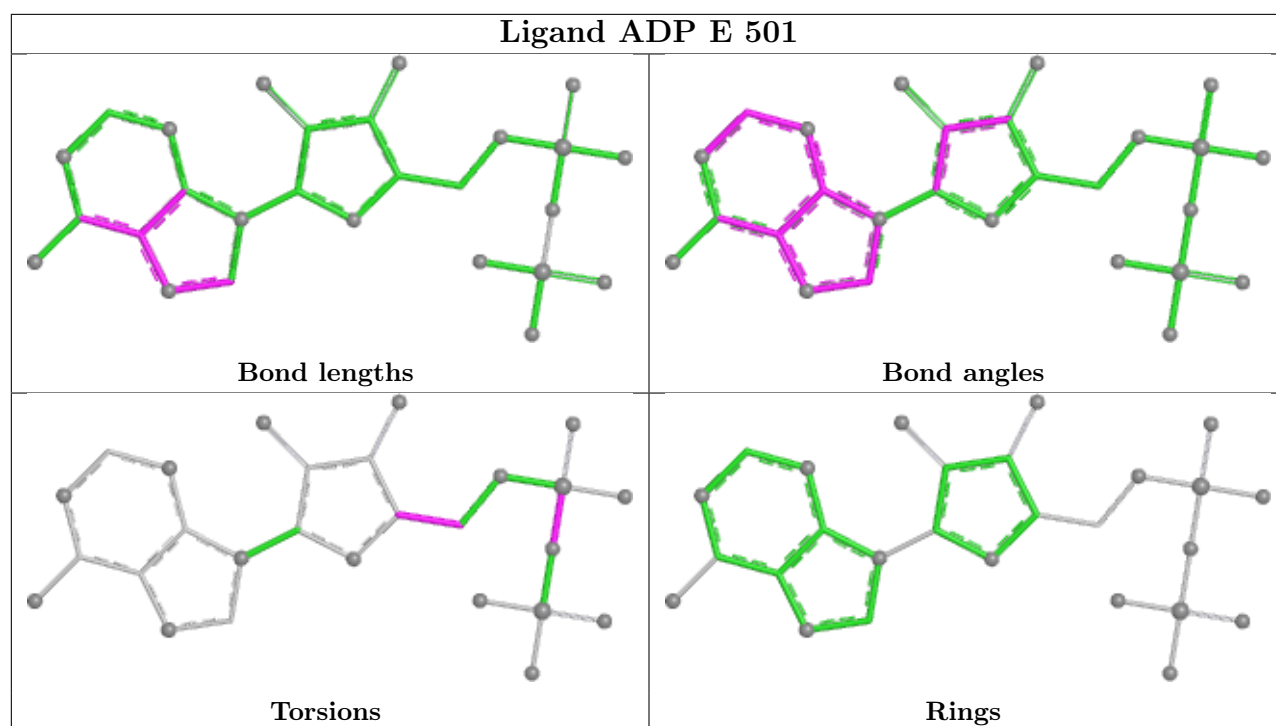
Mol	Chain	Res	Type	Atoms
11	G	702	ATP	O4'-C4'-C5'-O5'
11	G	702	ATP	C3'-C4'-C5'-O5'
12	E	501	ADP	O4'-C4'-C5'-O5'
11	D	601	ATP	O4'-C4'-C5'-O5'
11	D	601	ATP	PG-O3B-PB-O1B

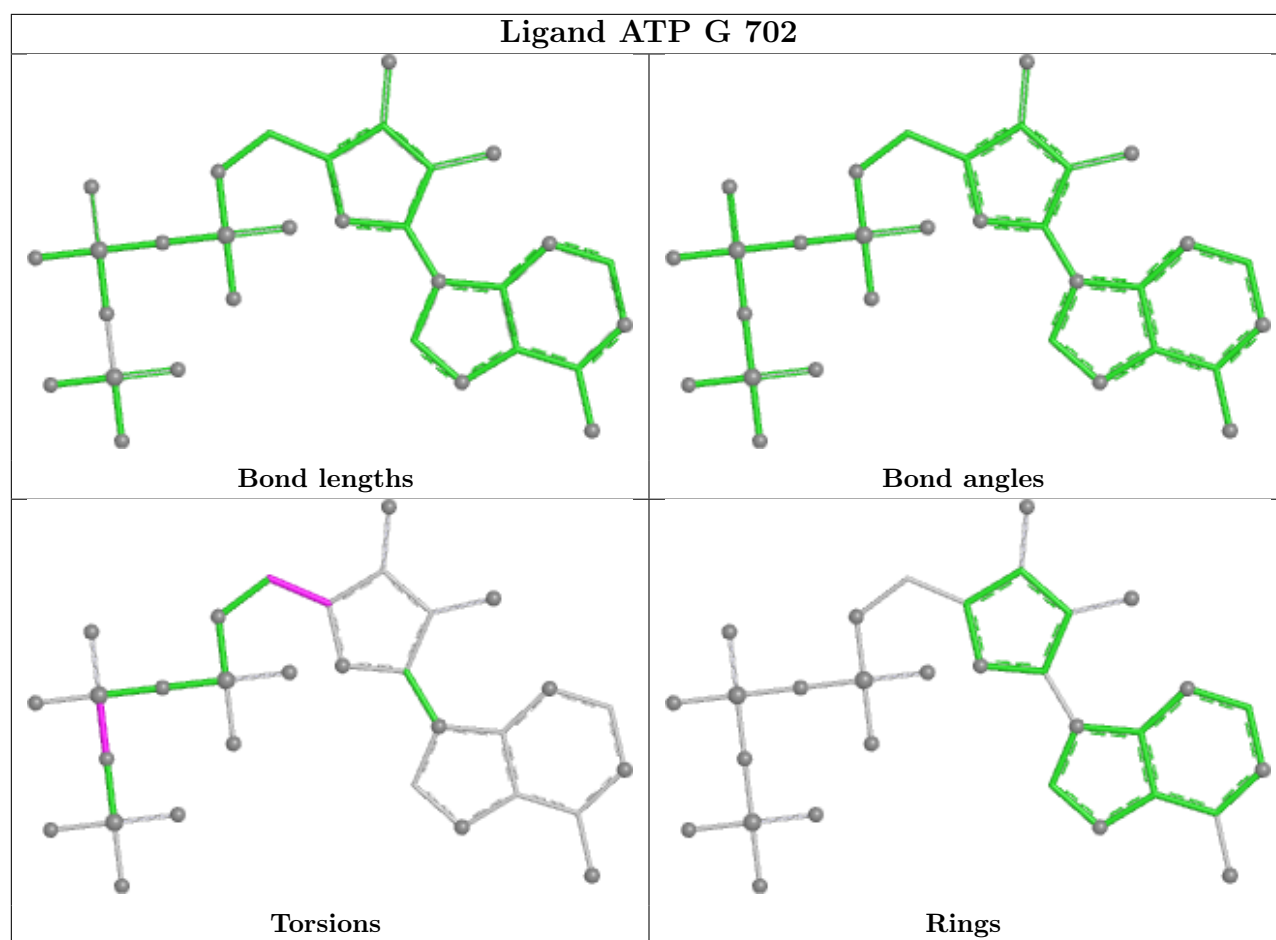
There are no ring outliers.

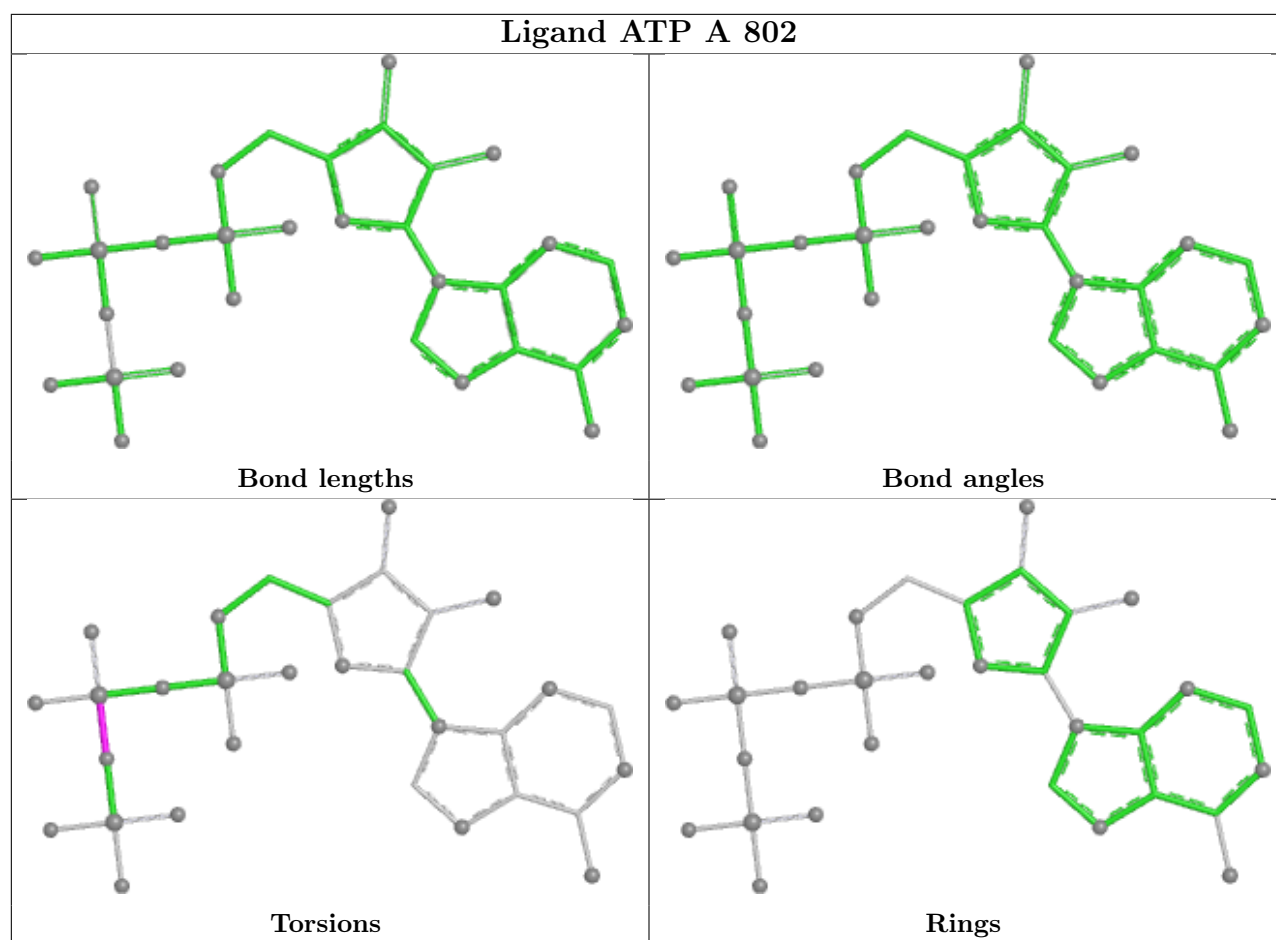
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	D	601	ATP	1	0
11	A	802	ATP	1	0

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







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

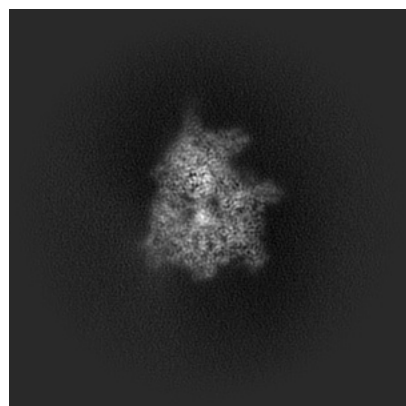
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-76021. These allow visual inspection of the internal detail of the map and identification of artifacts.

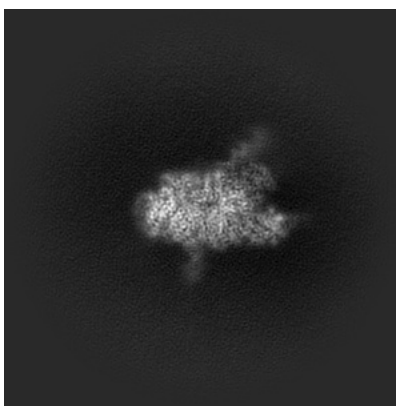
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

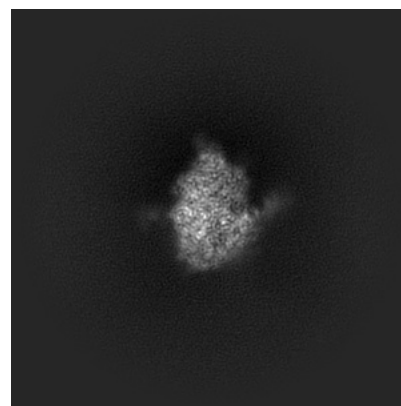
6.1.1 Primary map



X

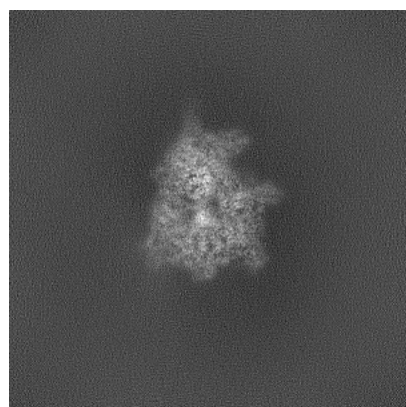


Y

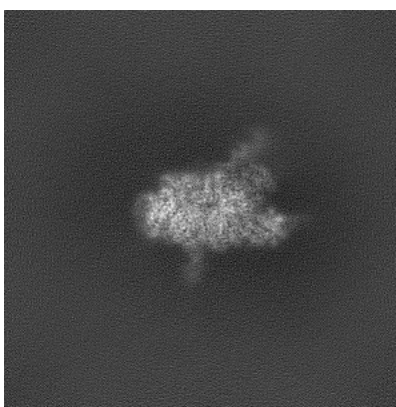


Z

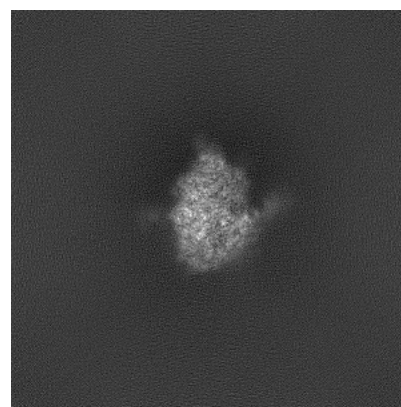
6.1.2 Raw map



X



Y

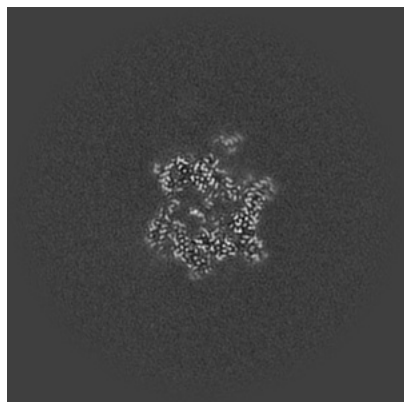


Z

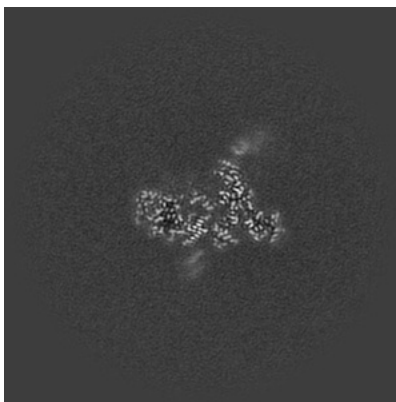
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

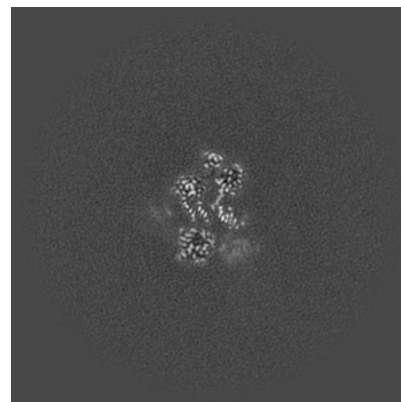
6.2.1 Primary map



X Index: 220

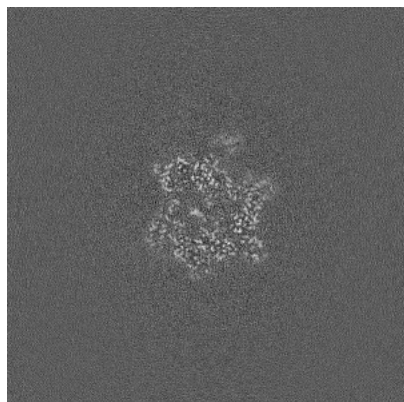


Y Index: 220

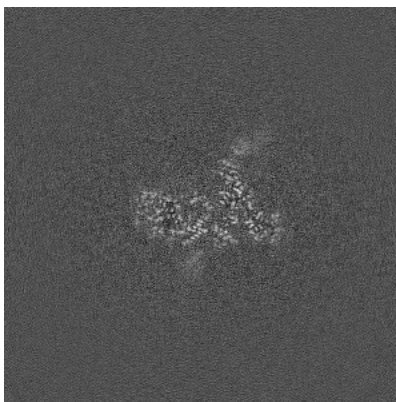


Z Index: 220

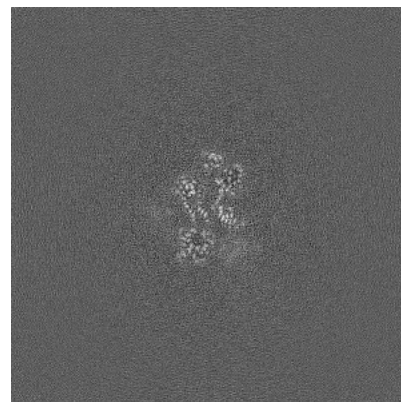
6.2.2 Raw map



X Index: 220



Y Index: 220

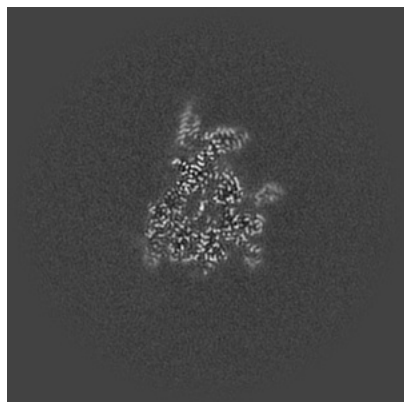


Z Index: 220

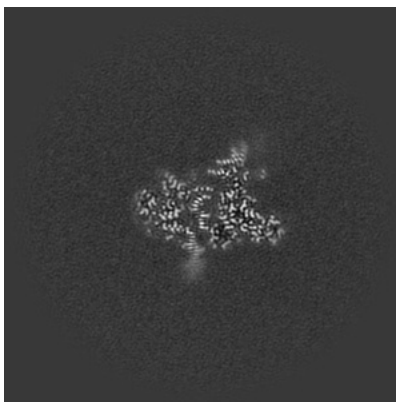
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

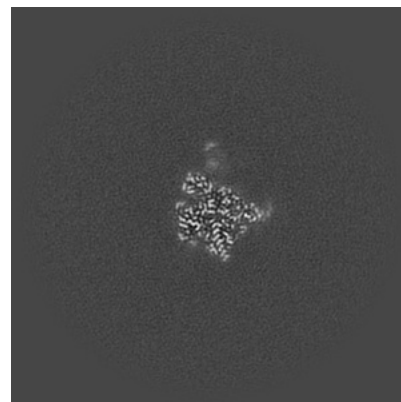
6.3.1 Primary map



X Index: 210

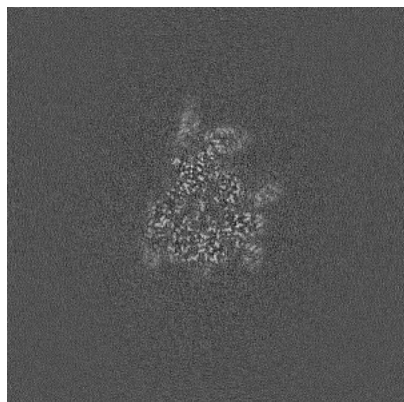


Y Index: 214

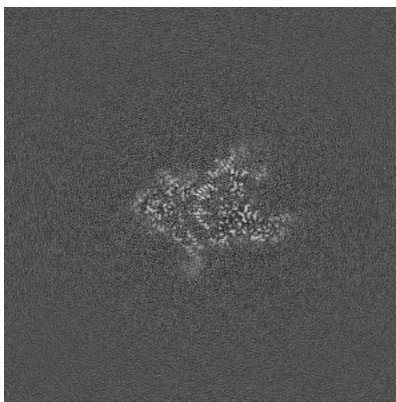


Z Index: 250

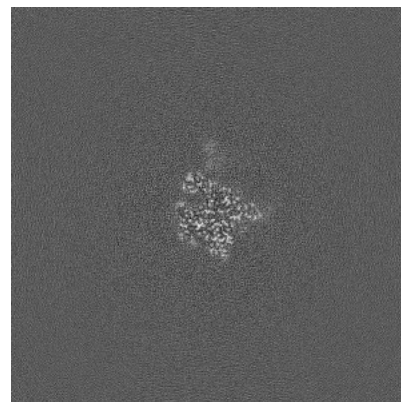
6.3.2 Raw map



X Index: 211



Y Index: 210

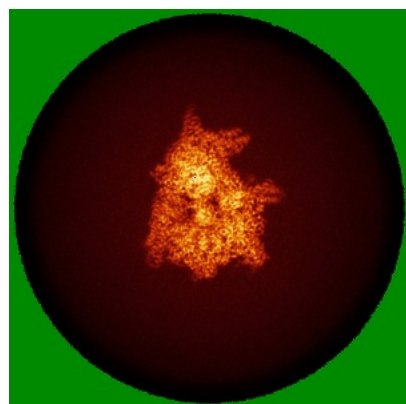


Z Index: 249

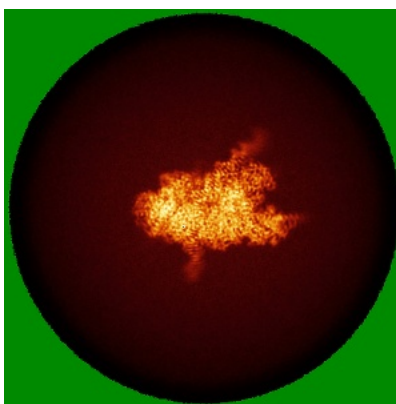
The images above show the largest variance slices of the map in three orthogonal directions.

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

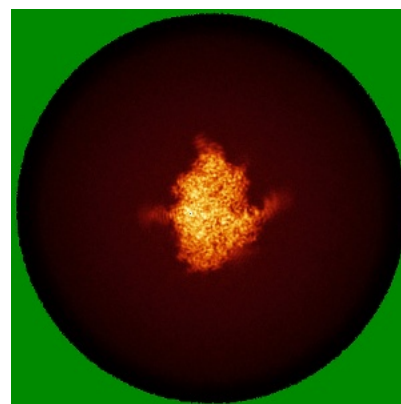
6.4.1 Primary map



X

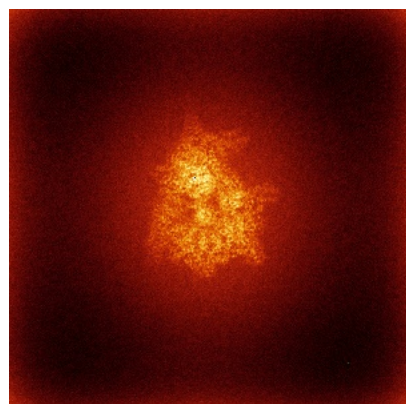


Y

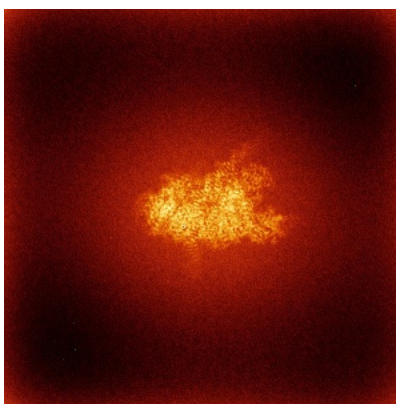


Z

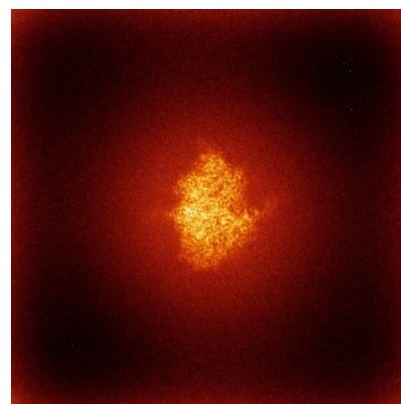
6.4.2 Raw map



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.

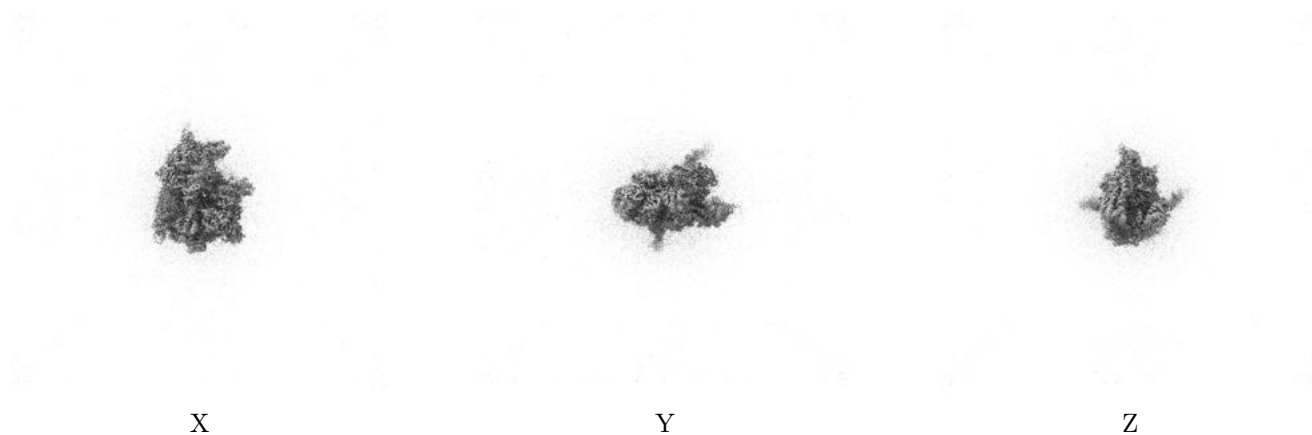
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.15. 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.

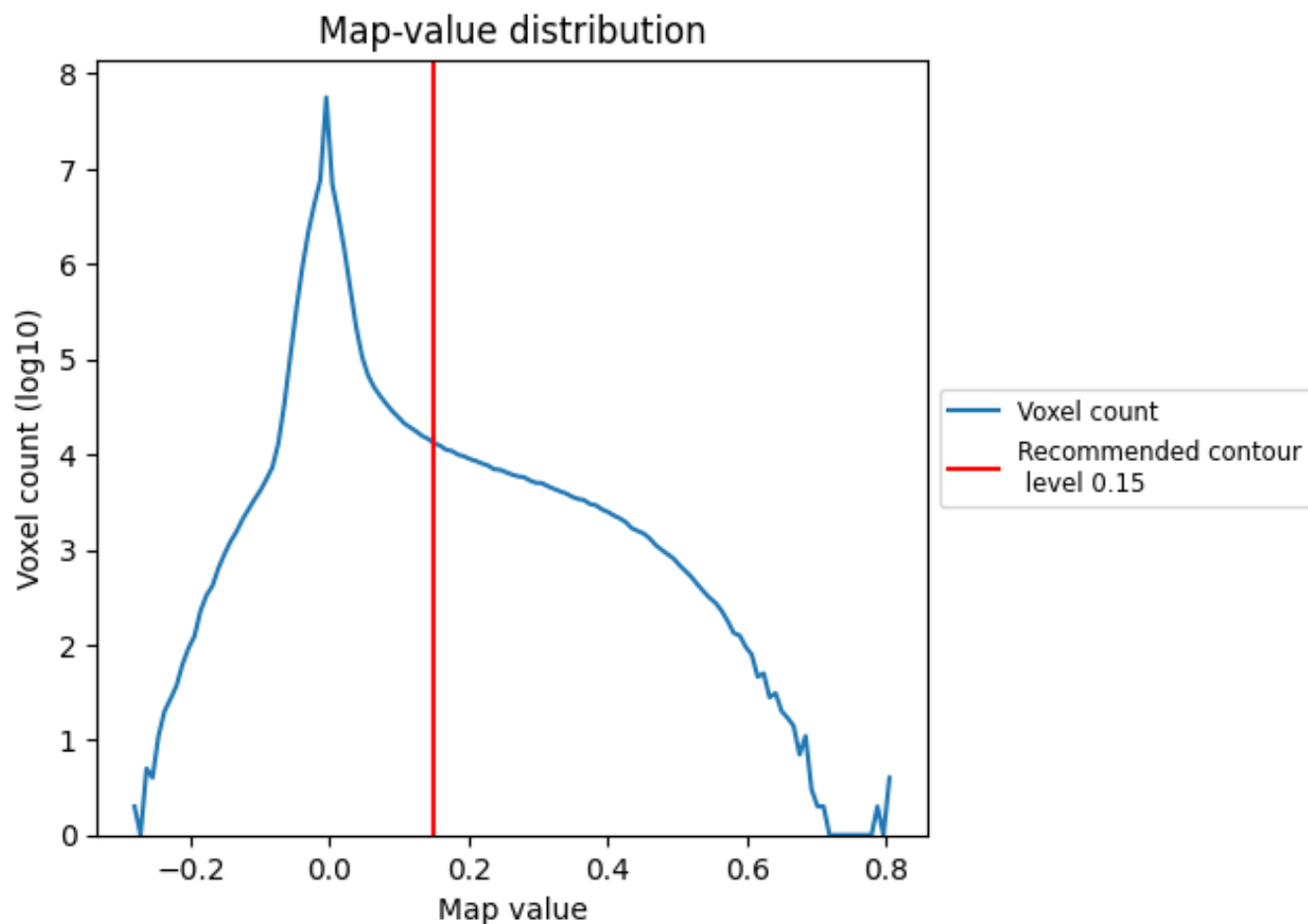
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

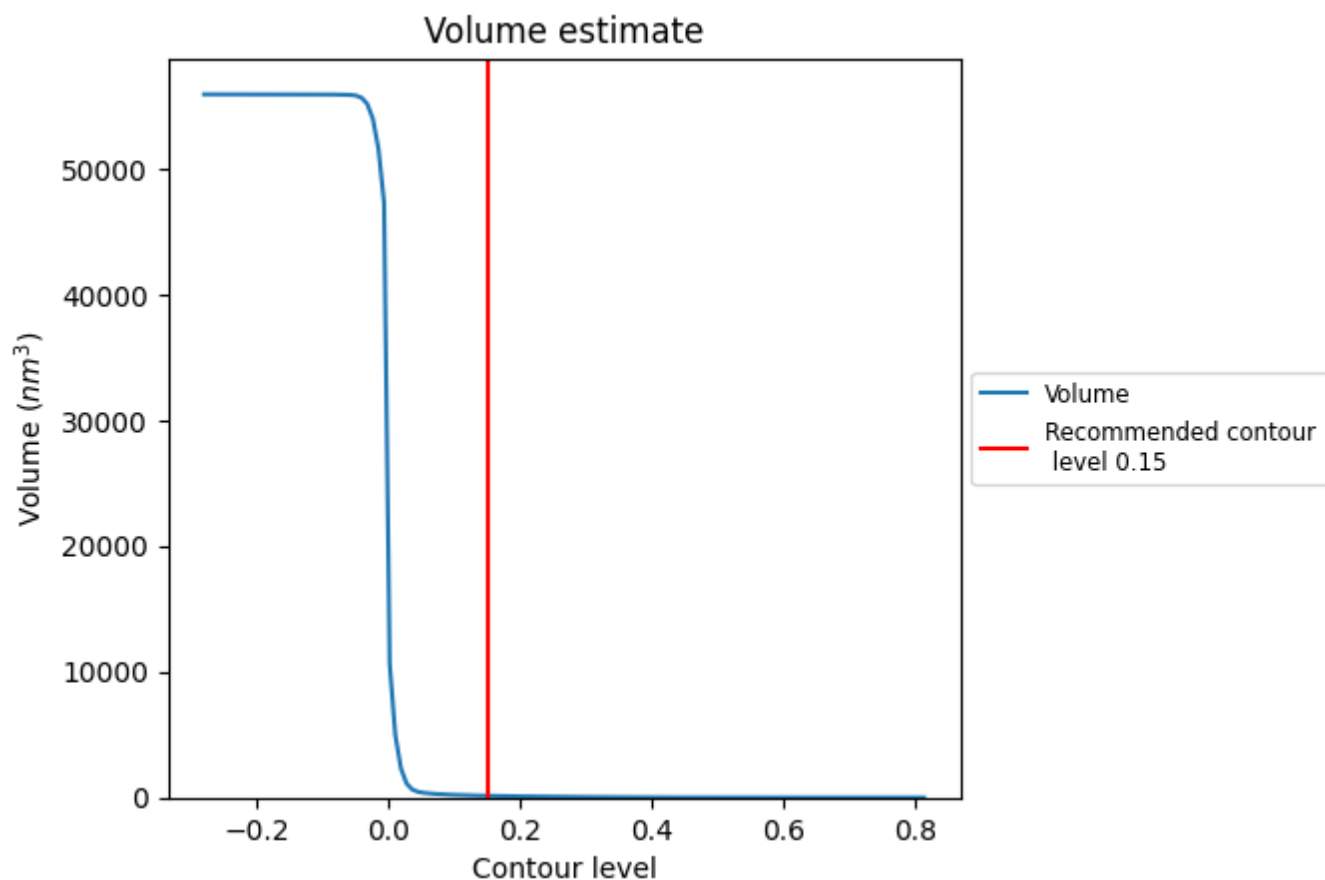
This section contains the results of statistical analysis of the map.

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.

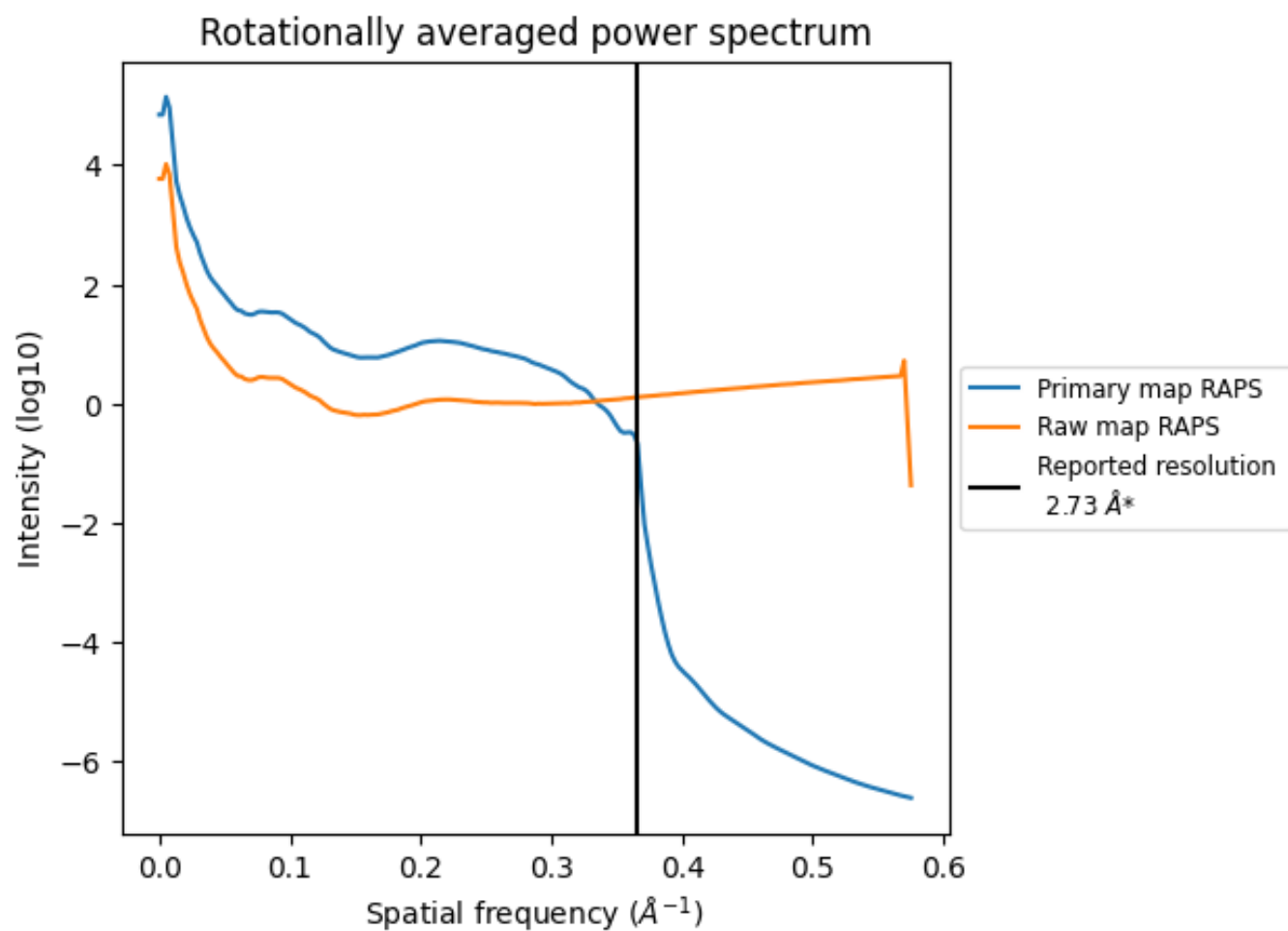
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 140 nm^3 ; this corresponds to an approximate mass of 126 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 ⓘ

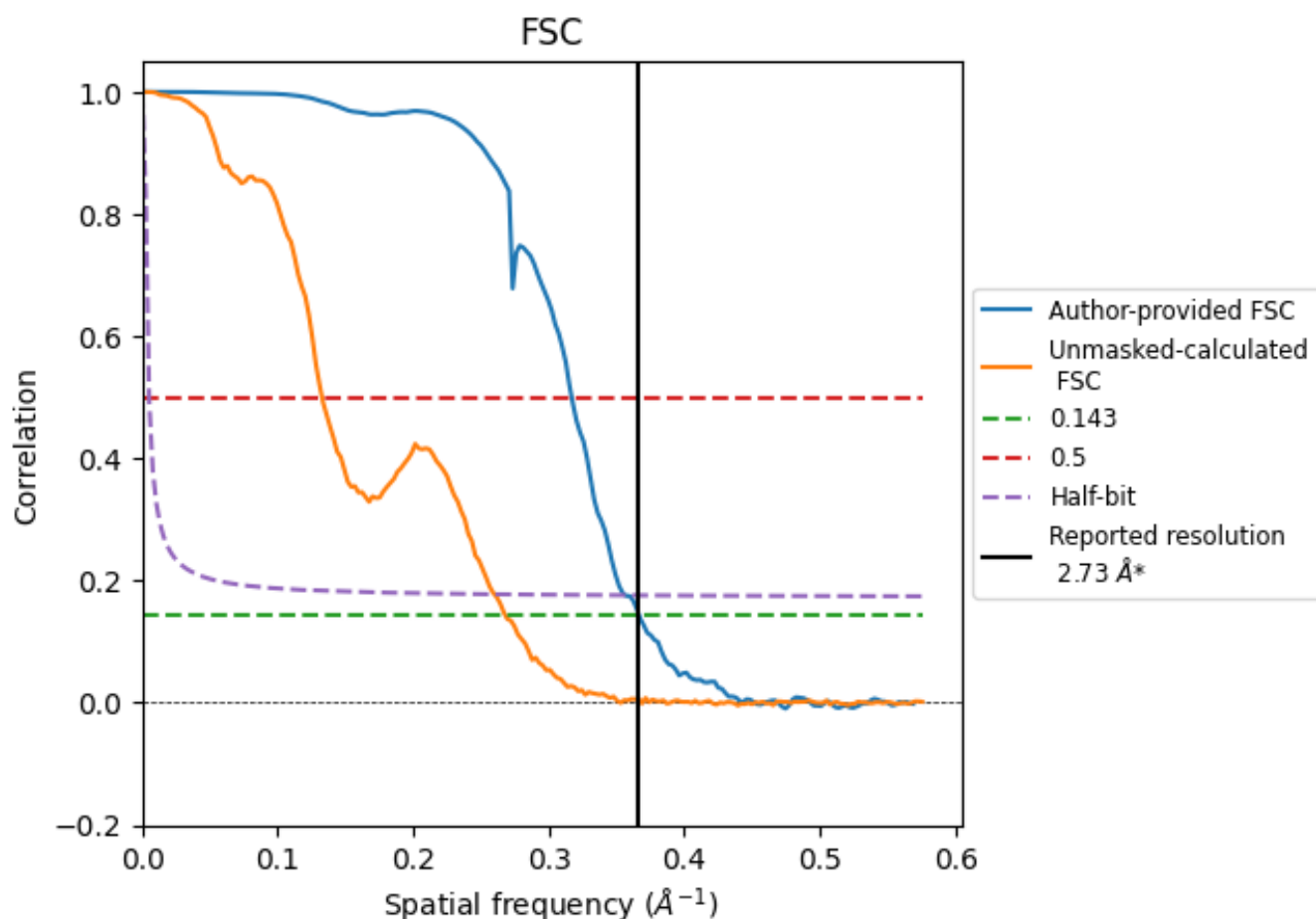


*Reported resolution corresponds to spatial frequency of 0.366 $\text{\AA}^{-1}$

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 0.366 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

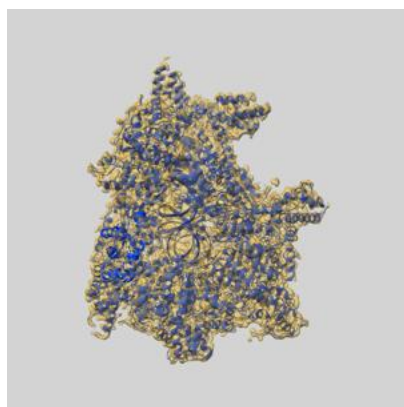
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.73	-	-
Author-provided FSC curve	2.73	3.16	2.81
Unmasked-calculated*	3.73	7.54	3.85

*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 3.73 differs from the reported value 2.73 by more than 10 %

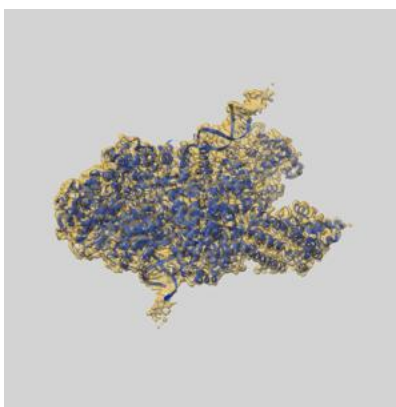
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-76021 and PDB model 11ST. Per-residue inclusion information can be found in section [3](#) on page [11](#).

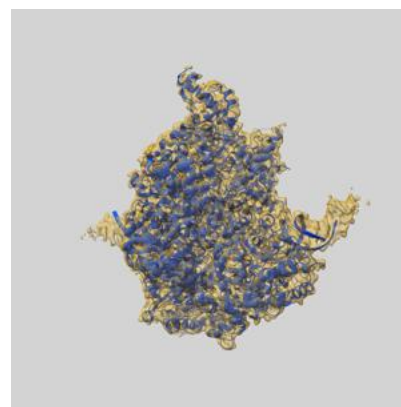
9.1 Map-model overlay [i](#)



X



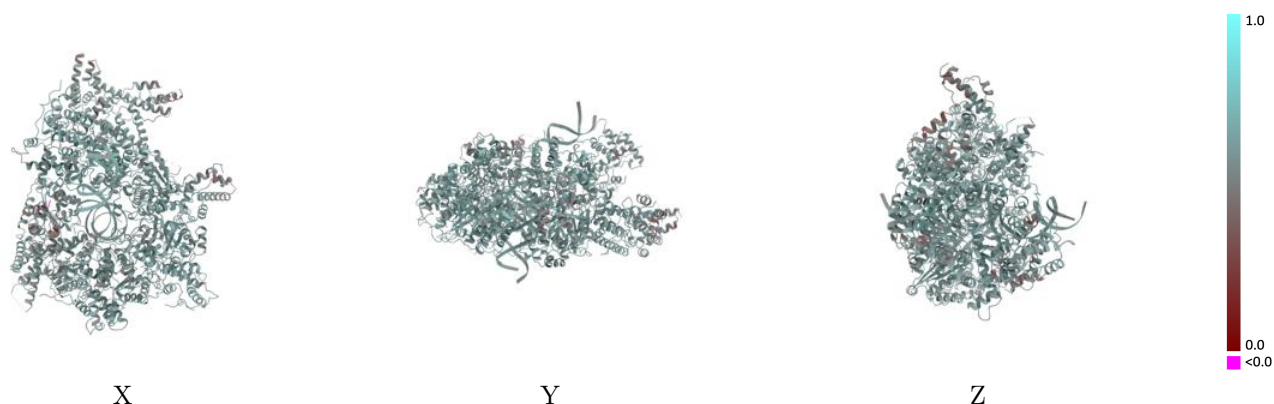
Y



Z

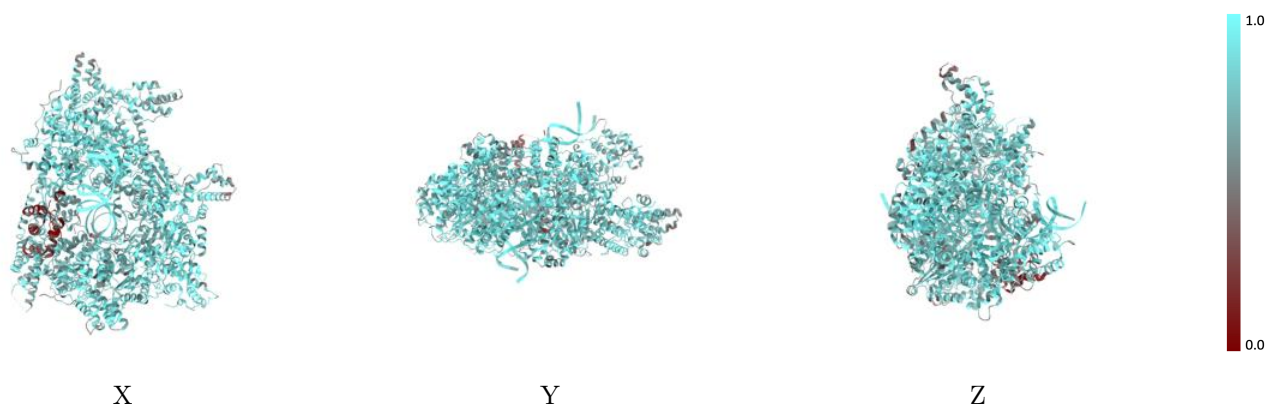
The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



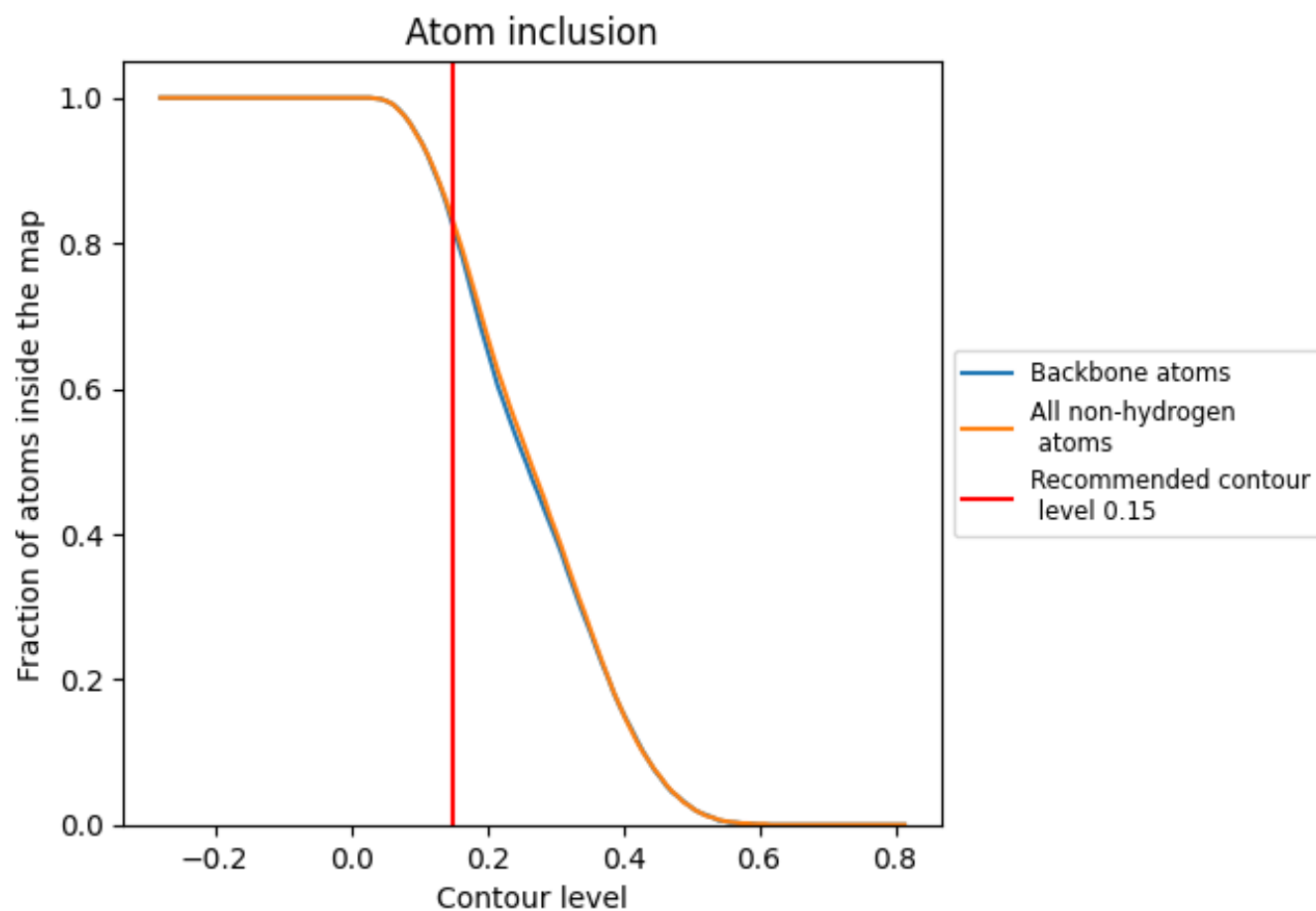
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.15).

9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 83% 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 (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8300	0.5800
A	0.8510	0.5860
B	0.7260	0.5640
C	0.8480	0.5780
D	0.8810	0.5930
E	0.8640	0.5840
F	0.8300	0.5620
G	0.7830	0.5750
K	0.6080	0.5770
L	0.5540	0.5500
X	0.9660	0.5940
Y	0.9740	0.6000

1.0

0.0

<0.0