



wwPDB EM Validation Summary Report ⓘ

Mar 26, 2026 – 06:34 PM UTC

PDB ID : 9OFG / pdb_00009ofg
EMDB ID : EMD-70431
Title : CI ring of daytime state KaiC
Authors : Dzimianski, J.V.; Sandate, C.R.; Balasco Serrao, V.H.; Lander, G.C.; Partch, C.L.
Deposited on : 2025-04-29
Resolution : 3.35 Å(reported)
Based on initial model : 7S66

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:

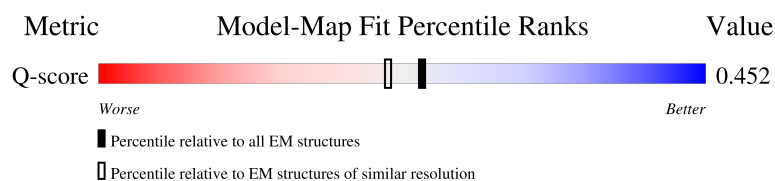
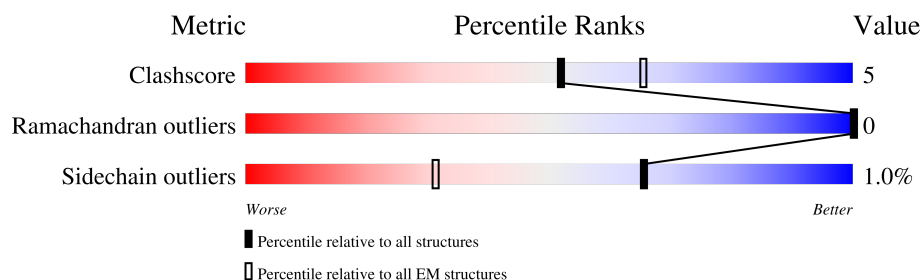
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 3.35 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	14390 (2.85 - 3.85)

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	519	
1	B	519	
1	C	519	
1	D	519	

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Mol	Chain	Length	Quality of chain
1	E	519	
1	F	519	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11004 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.

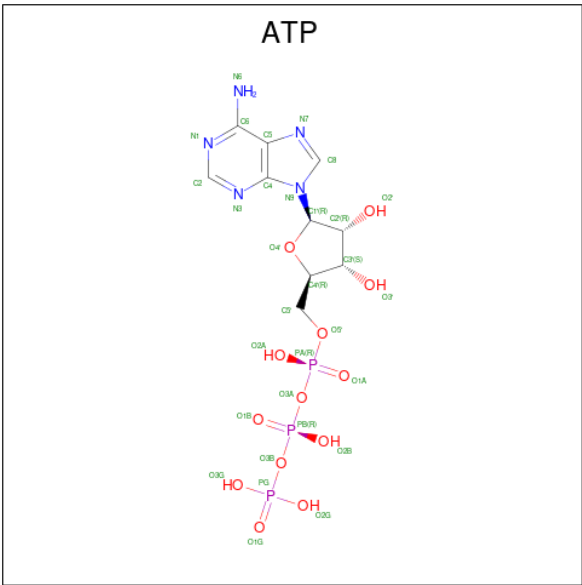
- Molecule 1 is a protein called Circadian clock protein kinase KaiC.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	226	Total	C	N	O	S	0	0
			1802	1145	314	339	4		
1	B	226	Total	C	N	O	S	0	0
			1802	1145	314	339	4		
1	C	226	Total	C	N	O	S	0	0
			1802	1145	314	339	4		
1	D	226	Total	C	N	O	S	0	0
			1802	1145	314	339	4		
1	E	226	Total	C	N	O	S	0	0
			1802	1145	314	339	4		
1	F	226	Total	C	N	O	S	0	0
			1802	1145	314	339	4		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	431	ALA	SER	engineered mutation	UNP Q79PF4
A	432	GLU	THR	engineered mutation	UNP Q79PF4
B	431	ALA	SER	engineered mutation	UNP Q79PF4
B	432	GLU	THR	engineered mutation	UNP Q79PF4
C	431	ALA	SER	engineered mutation	UNP Q79PF4
C	432	GLU	THR	engineered mutation	UNP Q79PF4
D	431	ALA	SER	engineered mutation	UNP Q79PF4
D	432	GLU	THR	engineered mutation	UNP Q79PF4
E	431	ALA	SER	engineered mutation	UNP Q79PF4
E	432	GLU	THR	engineered mutation	UNP Q79PF4
F	431	ALA	SER	engineered mutation	UNP Q79PF4
F	432	GLU	THR	engineered mutation	UNP Q79PF4

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).

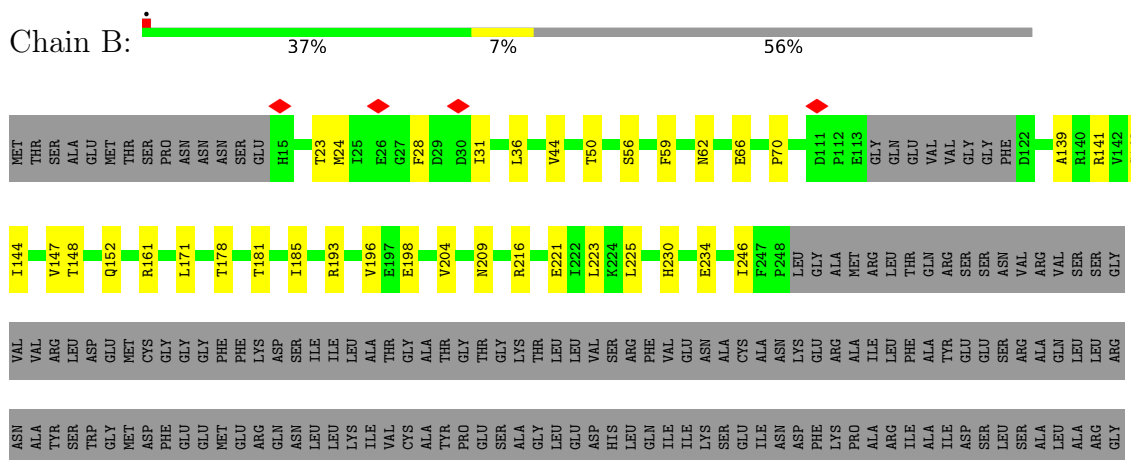
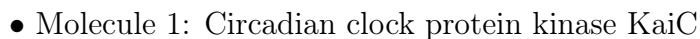


Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
2	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
2	C	1	Total	C	N	O	P	0
			31	10	5	13	3	
2	D	1	Total	C	N	O	P	0
			31	10	5	13	3	
2	E	1	Total	C	N	O	P	0
			31	10	5	13	3	
2	F	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
3	A	1	Total	Mg	0
			1	1	
3	B	1	Total	Mg	0
			1	1	
3	C	1	Total	Mg	0
			1	1	
3	D	1	Total	Mg	0
			1	1	
3	E	1	Total	Mg	0
			1	1	
3	F	1	Total	Mg	0
			1	1	

- Molecule 1: Circadian clock protein kinase KaiC



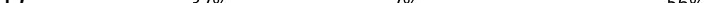
[illegible]

- Molecule 1: Circadian clock protein kinase KaiC

Chain C: 

ARG	SER	ASN	SER	LEU	S143
GLY	ARG	ALA	TRP	ASP	I144
VAL	ALA	PHE	GLY	GLU	
GLN	ILE	ARG	MET	MET	V147
GLU	ASN	GLN	ASP	CYS	T148
LYS	VAL	PHE	PHE	GLY	
GLY	PHE	VAL	GLU	GLY	Q152
PRO	LYS	ILE	GLU	GLY	
GLU	MET	GLY	MET	PHE	R161
SER	ARG	VAL	GLU	PHE	
	GLY	THR	ARG	LYS	L171
	SER	GLY	GLN	ASP	
	TRP	TTR	ASN	SER	T178
	HIS	ALA	LEU	ILE	
	ASP	LYS	LEU	ILE	T181
	LYS	GLN	LYS	LEU	
	ALA	GLU	ILE	ALA	I185
	ILE	GLU	VAL	THR	
	ARG	ILE	CYS	GLY	R193
	GLU	THR	ALA	ALA	
	PHE	GLY	TYR	THR	V196
	MET	LEU	PRO	GLY	E197
	ILE	PHE	GLU	THR	E198
	SER	THR	SER	GLY	
	ASP	ASN	ALA	LYS	V204
	LYS	THR	GLY	THR	
	GLY	SER	LEU	LEU	
	PRO	ASP	GLU	LEU	N209
	ASP	GLN	ASP	VAL	
	ILE	PHE	HIS	SER	E221
	LYS	MET	LEU	ARG	L222
	ASP	GLY	GLN	PHE	N224
	SER	ALA	ILE	VAL	L225
	PHE	HIS	ILE	GLU	
	ARG	SER	LYS	ASN	H230
	ASN	ILE	SER	ALA	
	PHE	THR	GLU	CYS	I246
	GLU	ASP	ILE	ALA	F247
	ARG	SER	ASN	ASN	P248
	ILE	HIS	ASP	LYS	
	ILE	ILE	PHE	GLU	LEU
	GLY	GLU	LYS	ARG	GLY
	GLY	GLU	PRO	ALA	ALA
	SER	ILE	ILE	ILE	MET
	PRO	THR	ARG	LEU	ARG
	THR	ASP	ILE	LEU	LEU
	ARG	THR	ILE	PHE	THR
	ILE	THR	ALA	ALA	GLN
	ILE	ILE	ILE	TYR	ARG
	THR	ILE	ASP	GLU	SER
	VAL	LEU	SER	GLU	GLY
	ASP	LEU	LEU	SER	ASN
	GLU	GLN	SER	ARG	VAL
	LYS	TTR	ALA	ALA	ARG
	SER	VAL	LEU	GLN	VAL
	GLU	ILE	ALA	LEU	VAL
	GLU	ILE	ARG	LEU	SER
	SER	ILE	GLY	ARG	GLY
	SER	ARG	VAL	VAL	ASN
	ILE	GLY	GLY	ALA	VAL
	VAL	MET	ASN	TYR	ARG

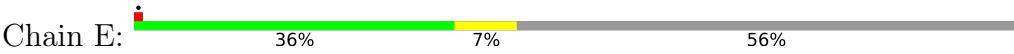
- Molecule 1: Circadian clock protein kinase KaiC

Chain D:  37% 7% 56%

[illegible]

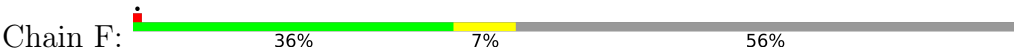
VAL
ARG
GLY
VAL
GLN
GLU
LYS
GLY
PRO
GLU
SER

● Molecule 1: Circadian clock protein kinase KaiC



MET	THR	ALA	GLU	MET	THR	SER	PRO	ASN	ASN	SER	GLU	H15	T23	M24	I25	E26	G27	F28	D29	D30	I31	L36	V44	T50	S56	F59	N62	E66	P70	D111	P112	E113	GLN	GLU	VAL	GLY	GLY	PHE	D122	T134	A139	R140	R141		
V142	S143	I144	V147	T148	Q152	R161	L171	T178	T181	I185	R193	V196	E197	E198	V204	N209	L210	L211	E214	R215	E221	I222	L223	K224	L225	H230	I246	F247	P248	LEU	GLY	ALA	MET	ARG	LEU	THR	GLN	ALA	TYR	ARG	SER	ASN	VAL	ARG	VAL
SER	SER	VAL	VAL	ARG	LEU	ASP	GLY	GLY	PHE	LYS	ASP	ILE	ILE	LEU	ALA	THR	GLY	THR	GLY	THR	LYS	THR	ALA	GLY	LEU	LEU	VAL	ARG	VAL	ASN	LYS	GLY	ARG	ALA	ILE	LEU	PHE	ALA	TYR	GLU	SER	ASN	ARG	ALA	GLN
LEU	ARG	ASN	ALA	TYR	SER	TRP	GLY	MET	GLU	GLN	ASN	LEU	LYS	LEU	ALA	PRO	GLY	THR	GLY	THR	ALA	GLY	LEU	LEU	ASP	HIS	LEU	GLN	ILE	LYS	ASN	ILE	ASP	ALA	PRO	ALA	ARG	ILE	ASP	ALA	THR	LEU	SER	ALA	LEU
ALA	ARG	GLY	SER	ASN	ASN	ALA	PHE	ARG	GLN	GLY	VAL	GLY	THR	TRP	ALA	LYS	GLN	GLY	GLU	ILE	THR	GLY	THR	ASN	THR	SER	GLY	ALA	HIS	THR	SER	ASP	SER	HIS	ILE	ALA	GLY	THR	ILE	THR	THR	LEU	TYR	VAL	
GLU	ILE	ARG	GLY	ILE	MET	ARG	VAL	ASN	VAL	LYS	PHE	MET	ARG	GLY	TRP	HIS	ASP	ALA	ILE	ARG	GLU	THR	PHE	ASP	LYS	GLY	THR	PHE	ARG	ASN	PHE	GLU	ARG	ILE	SER	GLY	PRO	THR	ILE	THR	VAL	ASP	GLY	LYS	SER
GLU	LEU	SER	VAL	VAL	ARG	GLY	VAL	GLN	GLU	LYS	SER	PRO	GLU	SER																															

● Molecule 1: Circadian clock protein kinase KaiC



SER	GLU	GLU	GLU	VAL	ARG	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY</
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C6	Depositor
Number of particles used	279379	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	36000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	3.938	Depositor
Minimum map value	-2.963	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.078	Depositor
Recommended contour level	0.2	Depositor
Map size (Å)	253.0, 253.0, 253.0	wwPDB
Map dimensions	220, 220, 220	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.15, 1.15, 1.15	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

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	0.12	0/1834	0.23	0/2475
1	B	0.12	0/1834	0.23	0/2475
1	C	0.12	0/1834	0.23	0/2475
1	D	0.12	0/1834	0.22	0/2475
1	E	0.12	0/1834	0.23	0/2475
1	F	0.12	0/1834	0.22	0/2475
All	All	0.12	0/11004	0.23	0/14850

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	1802	0	1808	20	0
1	B	1802	0	1808	21	0
1	C	1802	0	1808	20	0
1	D	1802	0	1808	19	0
1	E	1802	0	1808	23	0
1	F	1802	0	1808	23	0
2	A	31	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	31	0	12	0	0
2	C	31	0	12	0	0
2	D	31	0	12	0	0
2	E	31	0	12	0	0
2	F	31	0	12	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
All	All	11004	0	10920	119	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 5.

The worst 5 of 119 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)
1:B:44:VAL:HB	1:B:181:THR:HG22	1.72	0.71
1:A:44:VAL:HB	1:A:181:THR:HG22	1.72	0.70
1:C:44:VAL:HB	1:C:181:THR:HG22	1.72	0.70
1:D:44:VAL:HB	1:D:181:THR:HG22	1.72	0.70
1:E:44:VAL:HB	1:E:181:THR:HG22	1.72	0.70

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	A	222/519 (43%)	217 (98%)	5 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	222/519 (43%)	217 (98%)	5 (2%)	0	100	100
1	C	222/519 (43%)	217 (98%)	5 (2%)	0	100	100
1	D	222/519 (43%)	217 (98%)	5 (2%)	0	100	100
1	E	222/519 (43%)	217 (98%)	5 (2%)	0	100	100
1	F	222/519 (43%)	217 (98%)	5 (2%)	0	100	100
All	All	1332/3114 (43%)	1302 (98%)	30 (2%)	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	196/443 (44%)	194 (99%)	2 (1%)	68	74
1	B	196/443 (44%)	194 (99%)	2 (1%)	68	74
1	C	196/443 (44%)	194 (99%)	2 (1%)	68	74
1	D	196/443 (44%)	194 (99%)	2 (1%)	68	74
1	E	196/443 (44%)	194 (99%)	2 (1%)	68	74
1	F	196/443 (44%)	194 (99%)	2 (1%)	68	74
All	All	1176/2658 (44%)	1164 (99%)	12 (1%)	65	74

5 of 12 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	198	GLU
1	E	31	ILE
1	F	198	GLU
1	E	198	GLU
1	B	198	GLU

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

Mol	Chain	Res	Type
1	C	153	GLN
1	D	33	HIS
1	F	153	GLN
1	E	153	GLN
1	F	33	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 6 are monoatomic - leaving 6 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	ATP	B	1001	3	32,33,33	0.41	0	48,52,52	0.41	0
2	ATP	F	1001	3	32,33,33	0.41	0	48,52,52	0.41	0
2	ATP	C	1001	3	32,33,33	0.41	0	48,52,52	0.41	0
2	ATP	A	1001	3	32,33,33	0.41	0	48,52,52	0.41	0
2	ATP	D	1001	3	32,33,33	0.41	0	48,52,52	0.41	0
2	ATP	E	1001	3	32,33,33	0.41	0	48,52,52	0.41	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
2	ATP	B	1001	3	-	4/22/38/38	0/3/3/3
2	ATP	F	1001	3	-	4/22/38/38	0/3/3/3
2	ATP	C	1001	3	-	4/22/38/38	0/3/3/3
2	ATP	A	1001	3	-	4/22/38/38	0/3/3/3
2	ATP	D	1001	3	-	4/22/38/38	0/3/3/3
2	ATP	E	1001	3	-	4/22/38/38	0/3/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

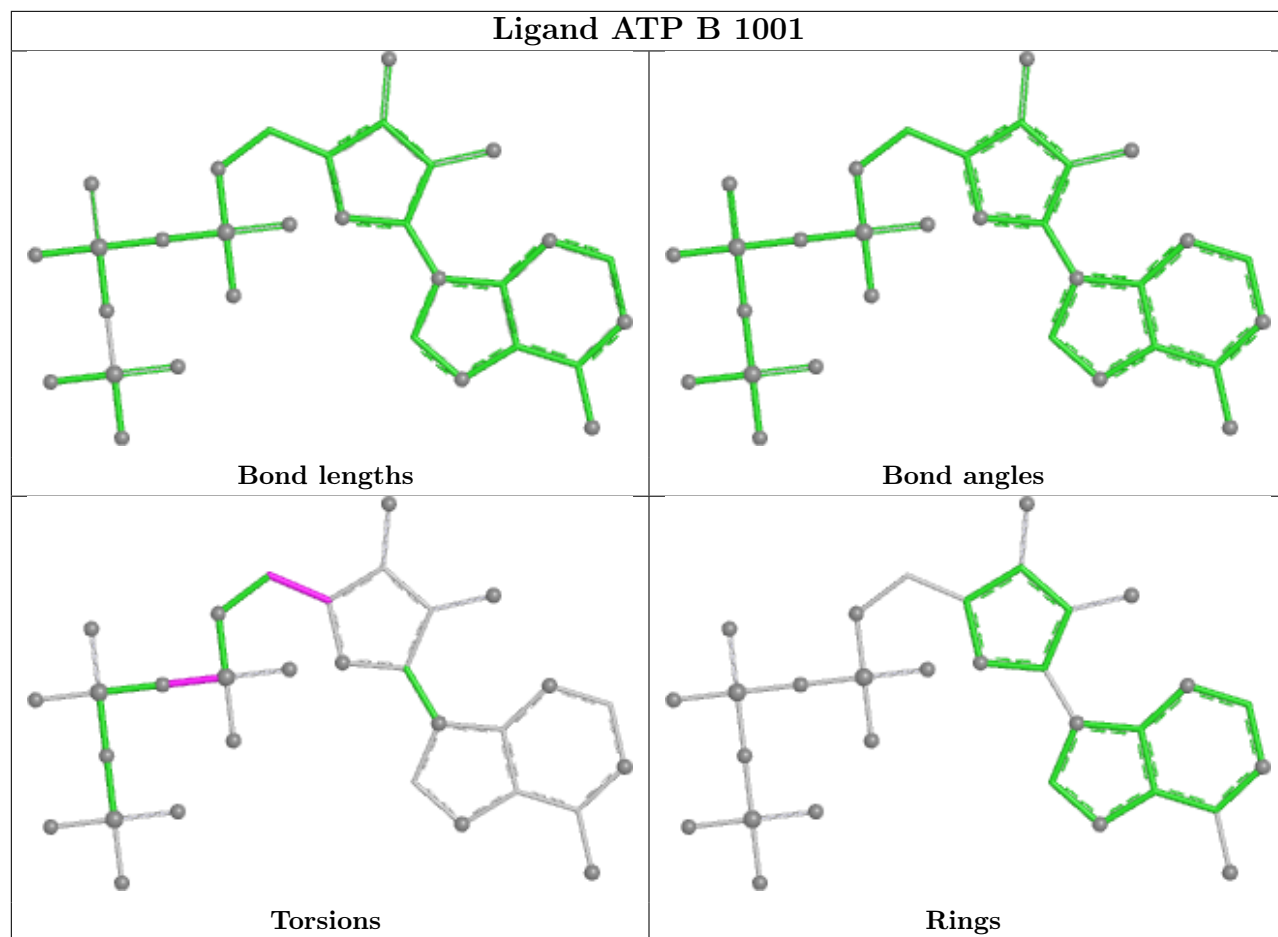
5 of 24 torsion outliers are listed below:

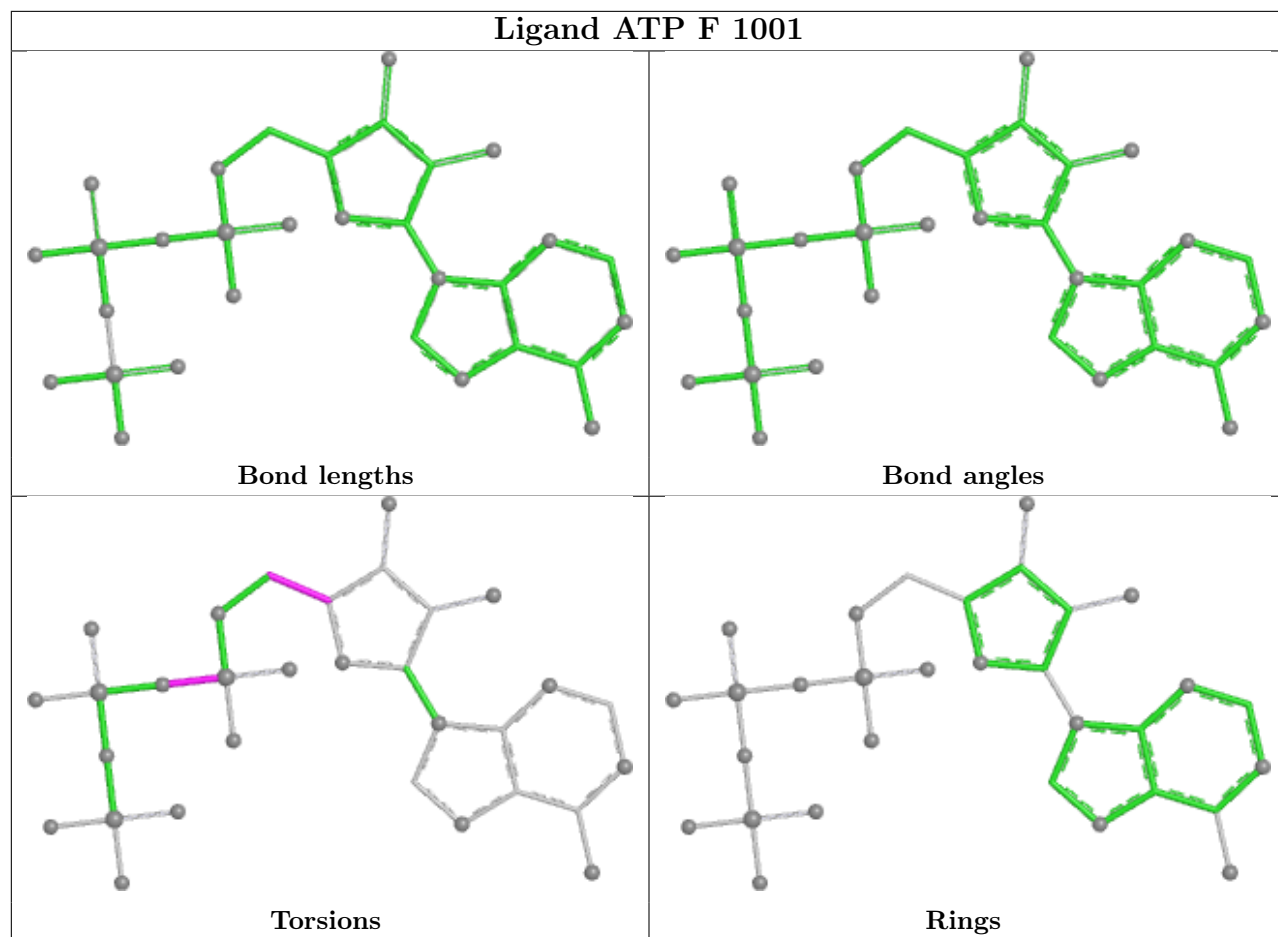
Mol	Chain	Res	Type	Atoms
2	A	1001	ATP	O4'-C4'-C5'-O5'
2	B	1001	ATP	O4'-C4'-C5'-O5'
2	C	1001	ATP	O4'-C4'-C5'-O5'
2	D	1001	ATP	O4'-C4'-C5'-O5'
2	E	1001	ATP	O4'-C4'-C5'-O5'

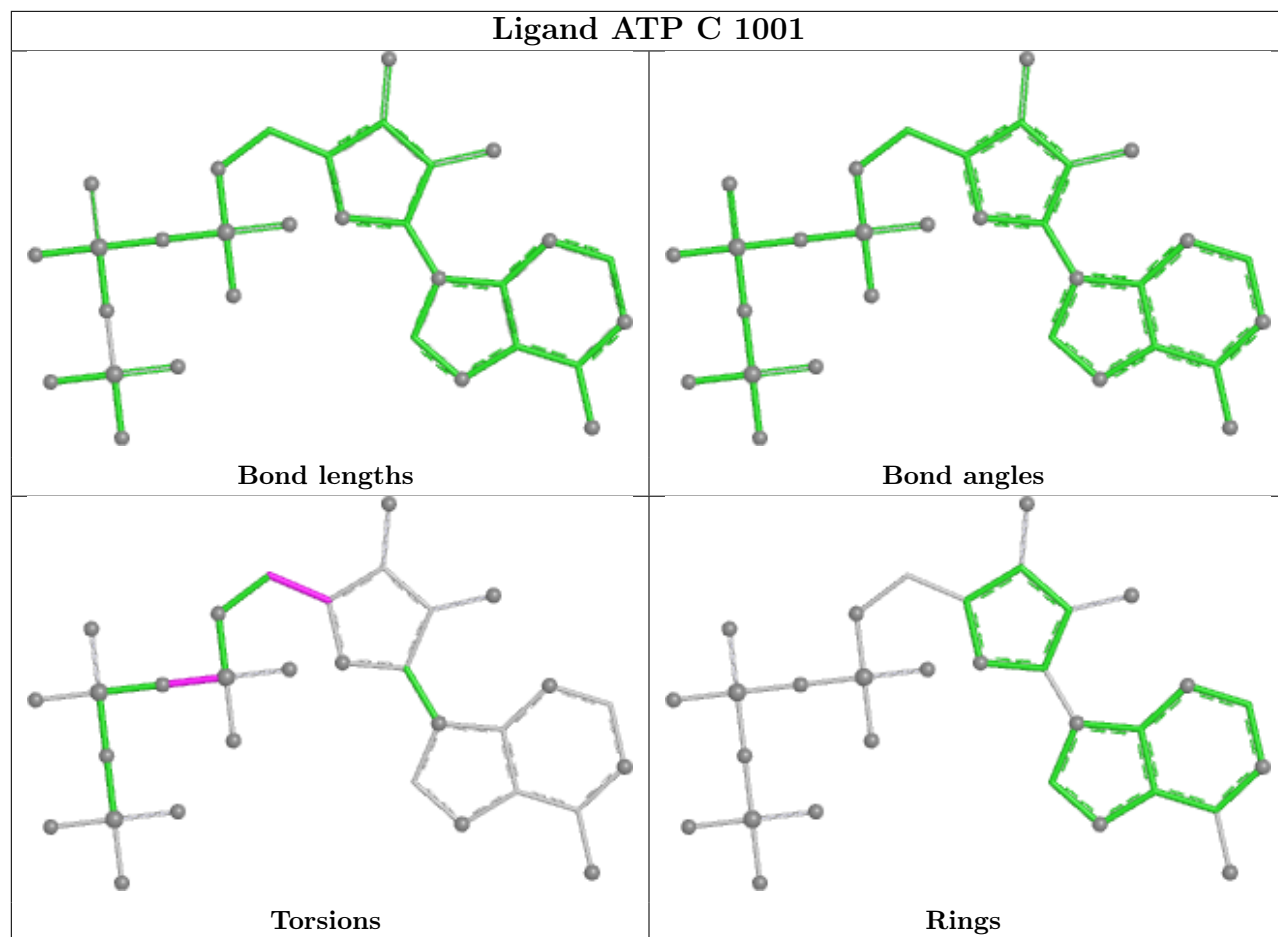
There are no ring outliers.

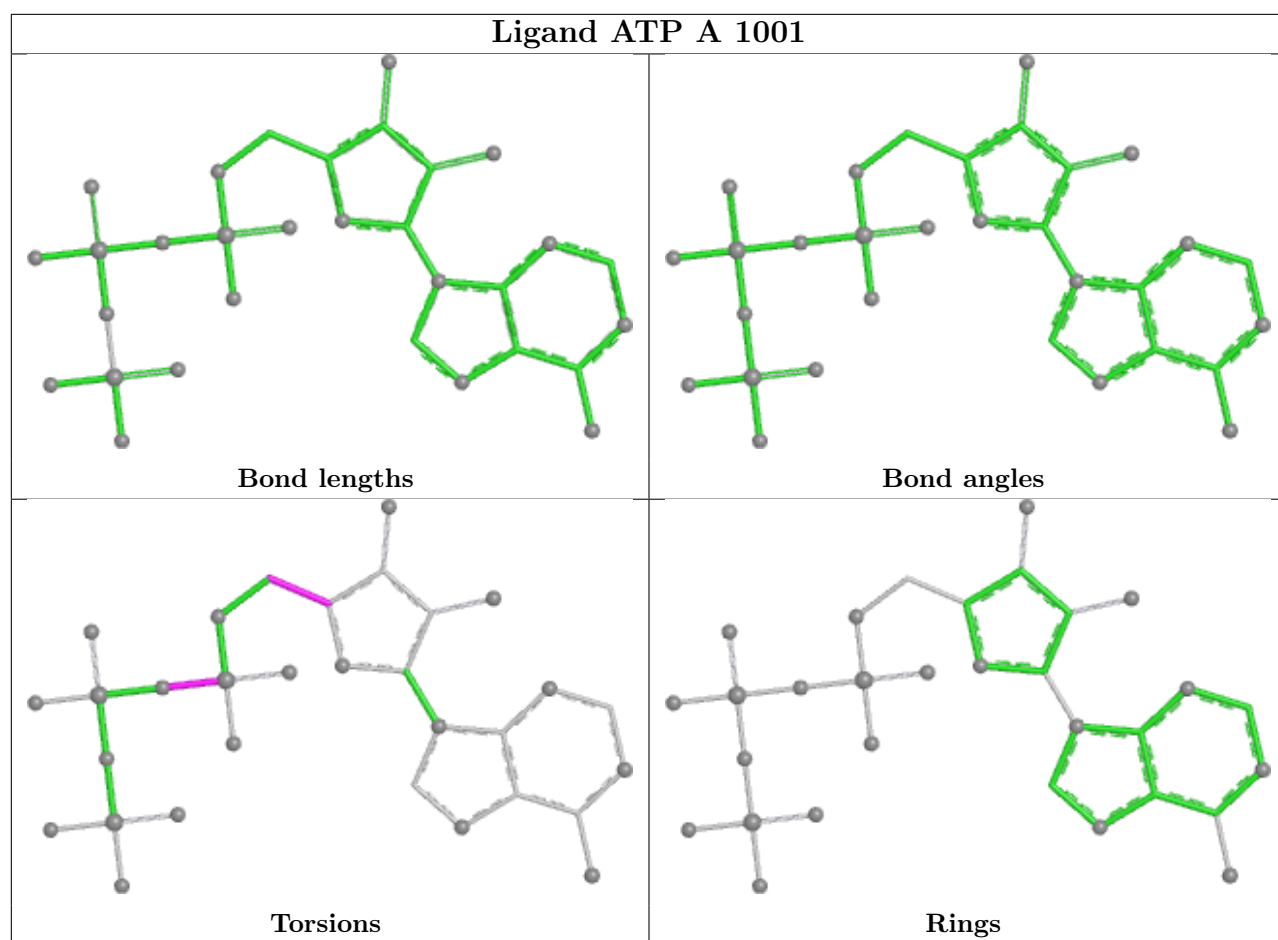
No monomer is involved in short contacts.

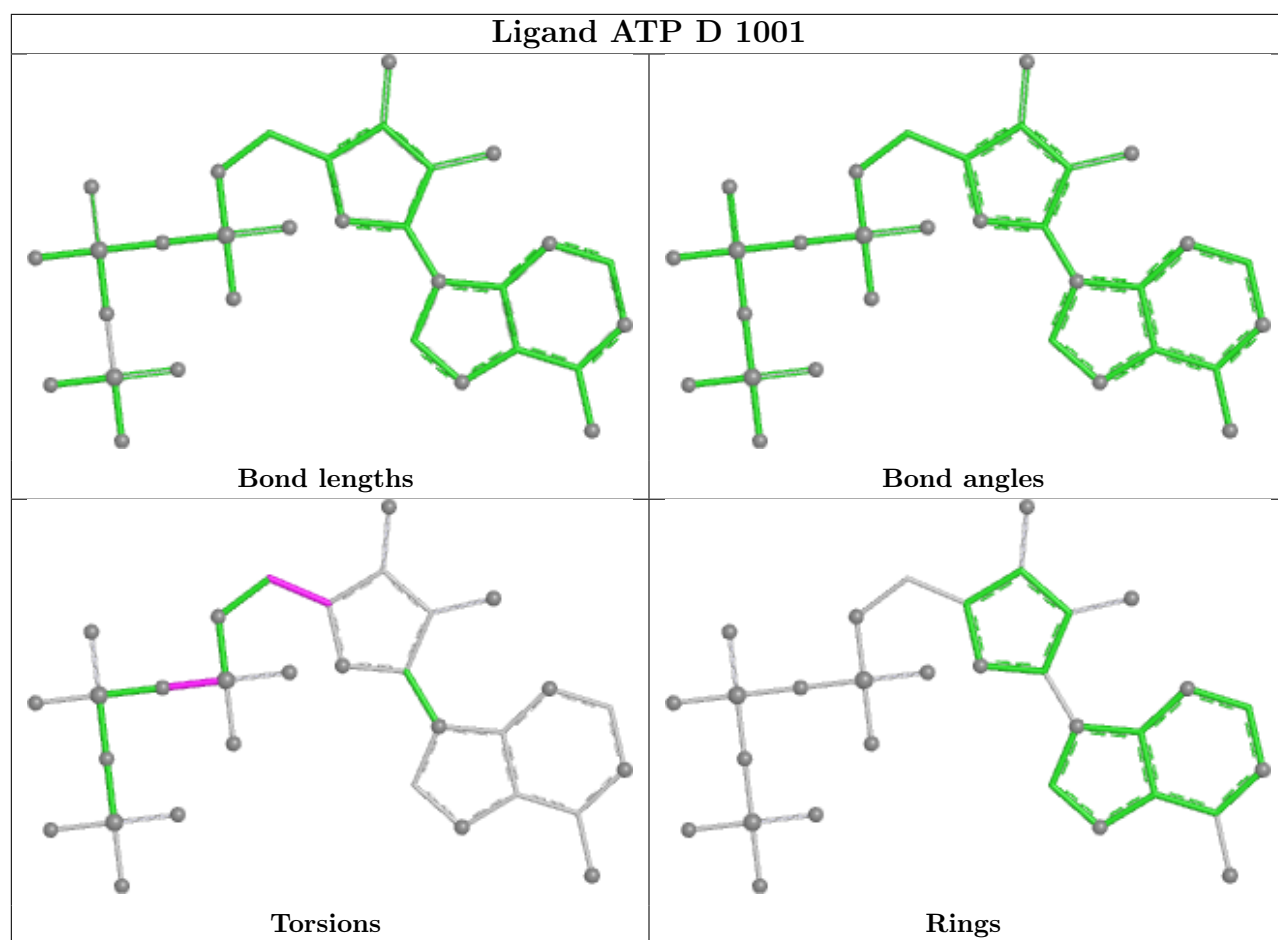
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

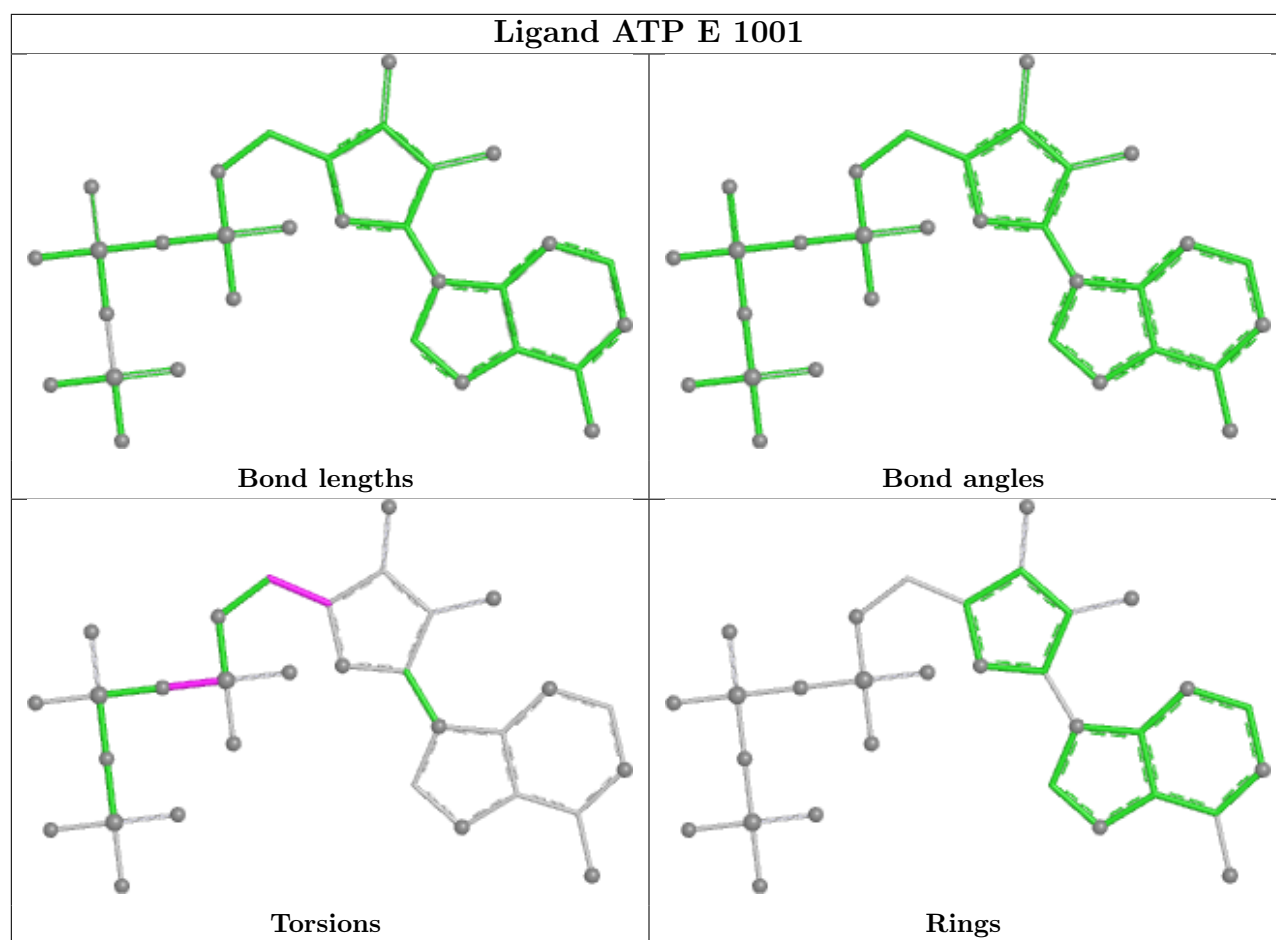












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

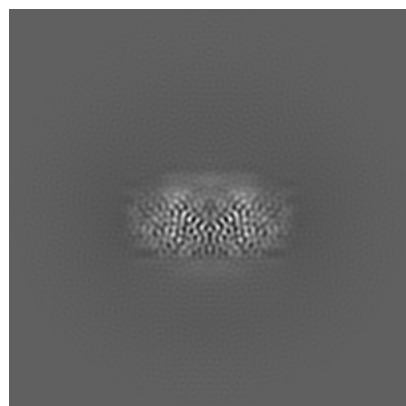
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-70431. 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](#)

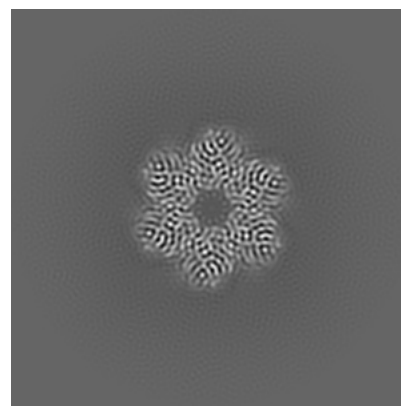
6.1.1 Primary map



X

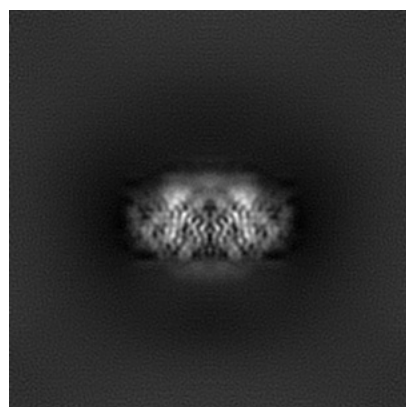


Y

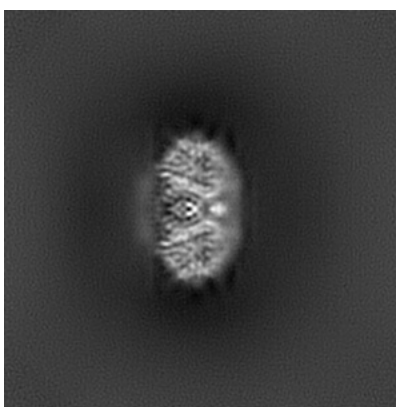


Z

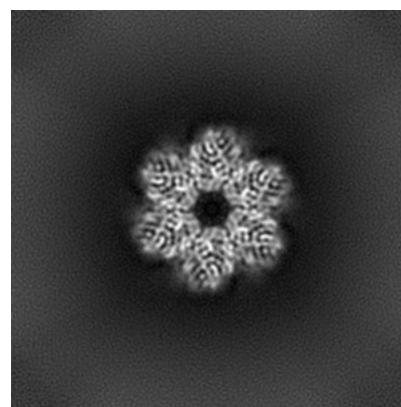
6.1.2 Raw map



X



Y

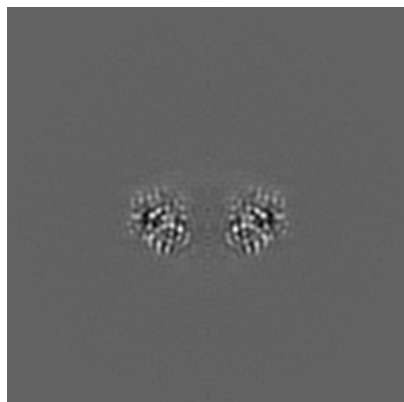


Z

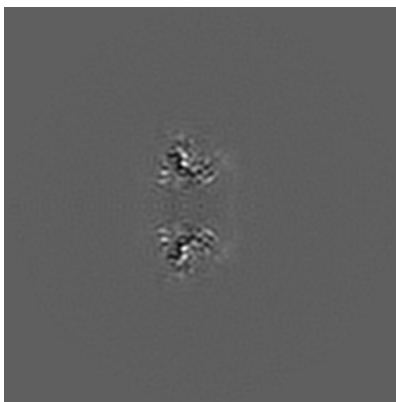
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

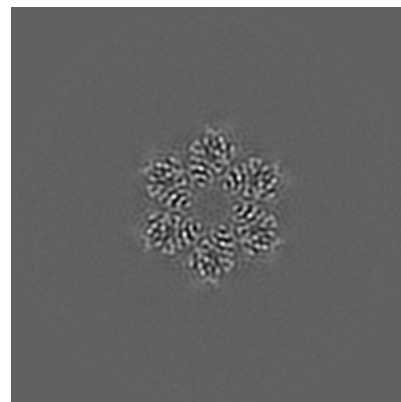
6.2.1 Primary map



X Index: 110

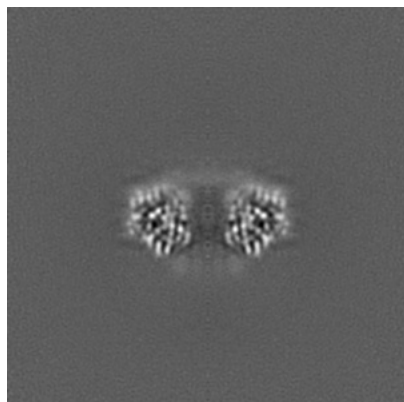


Y Index: 110

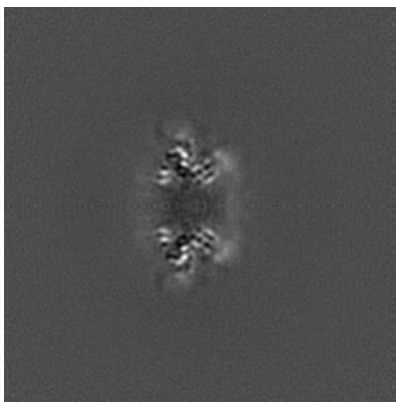


Z Index: 110

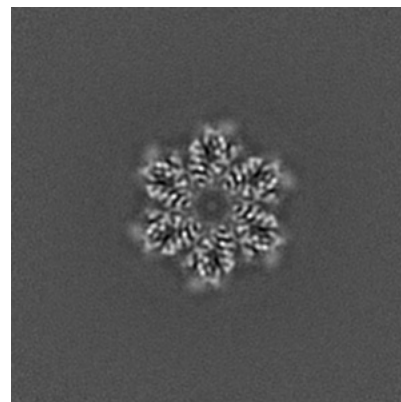
6.2.2 Raw map



X Index: 110



Y Index: 110

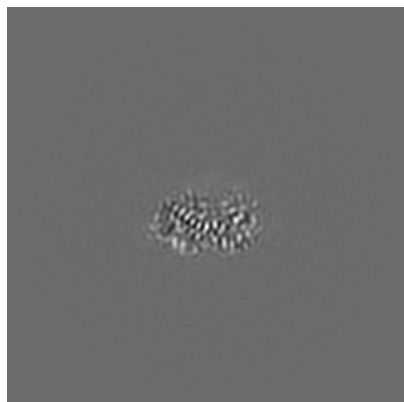


Z Index: 110

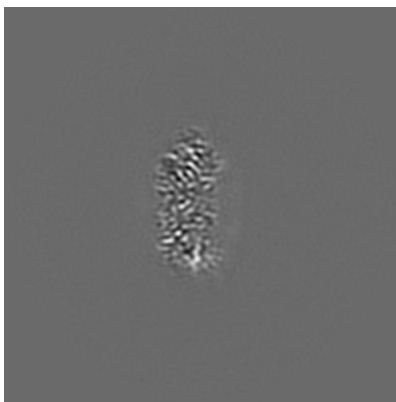
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

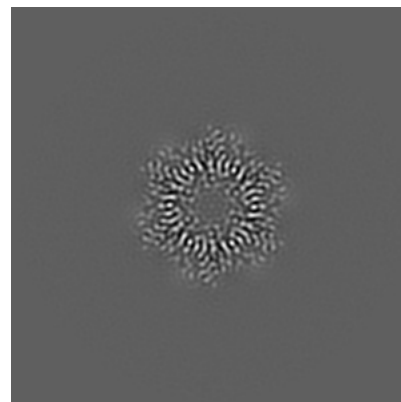
6.3.1 Primary map



X Index: 133

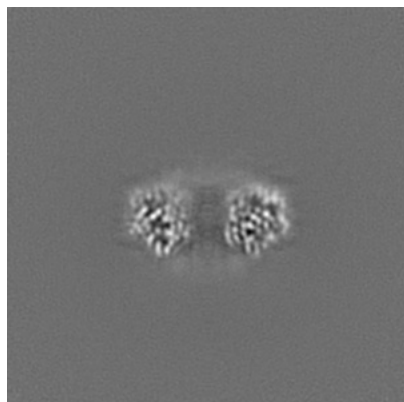


Y Index: 125

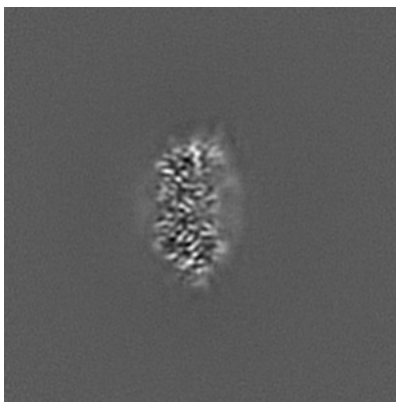


Z Index: 99

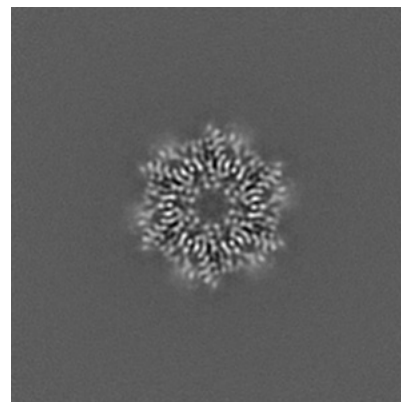
6.3.2 Raw map



X Index: 109



Y Index: 95

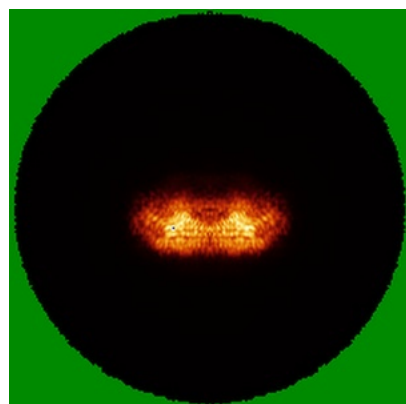


Z Index: 99

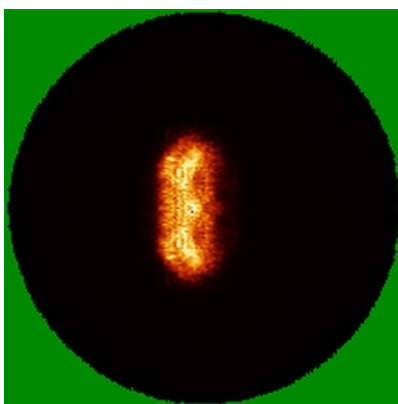
The images above show the largest variance slices of the map in three orthogonal directions.

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

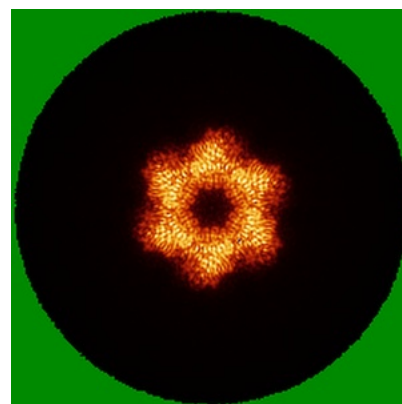
6.4.1 Primary map



X

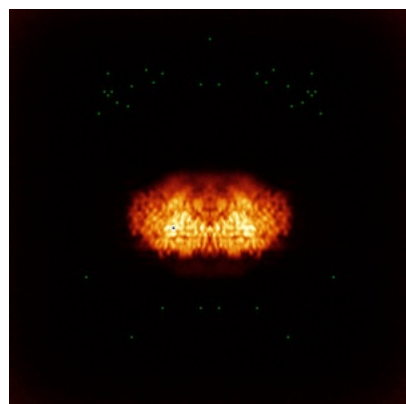


Y

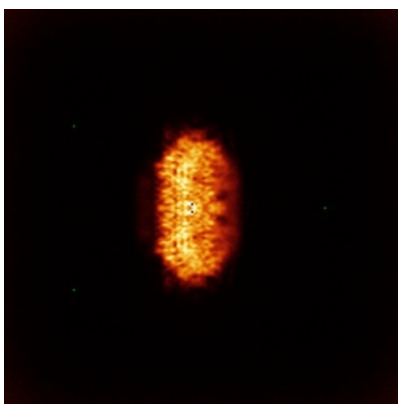


Z

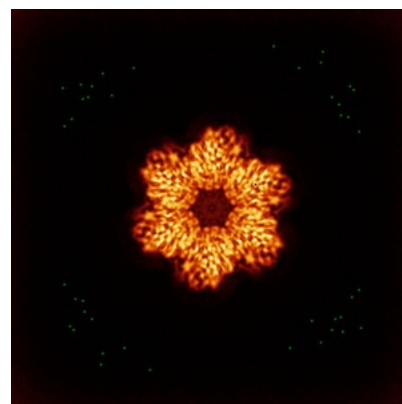
6.4.2 Raw map



X



Y

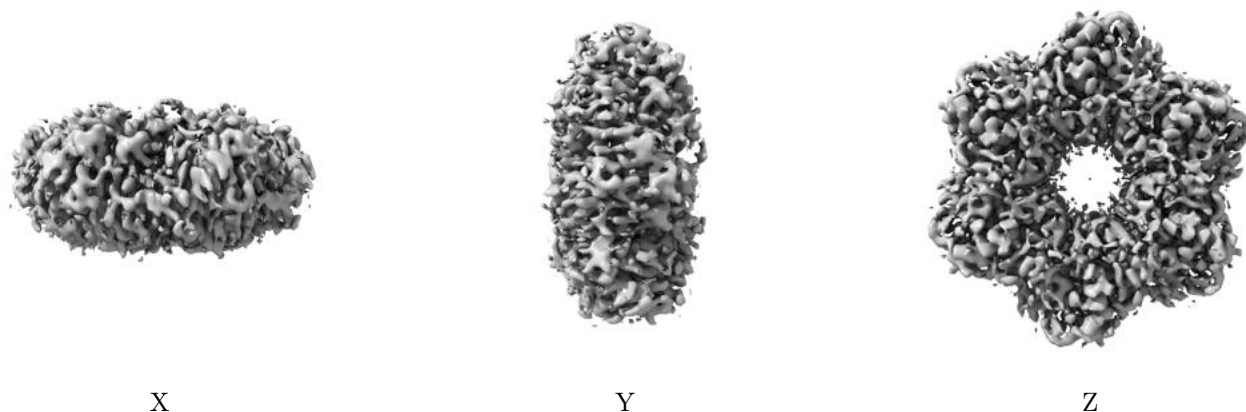


Z

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.

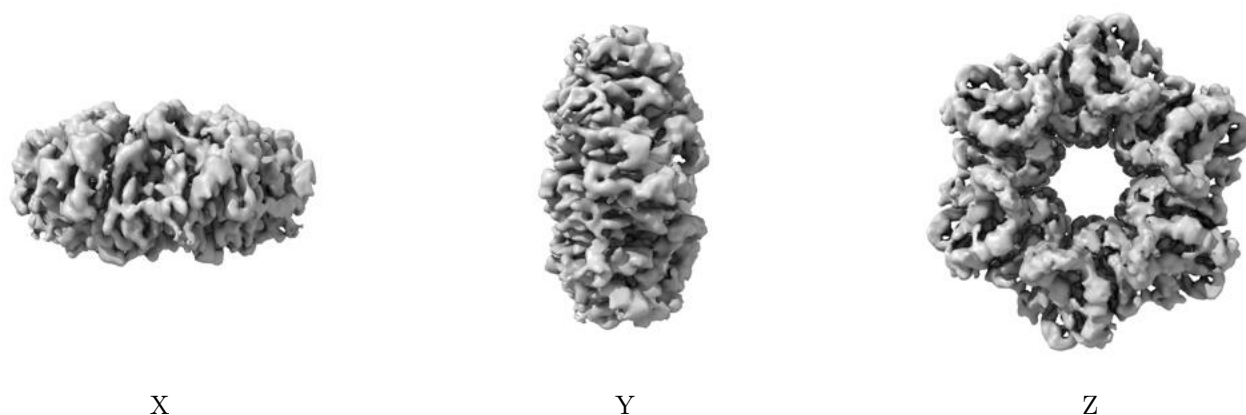
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.2. 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.

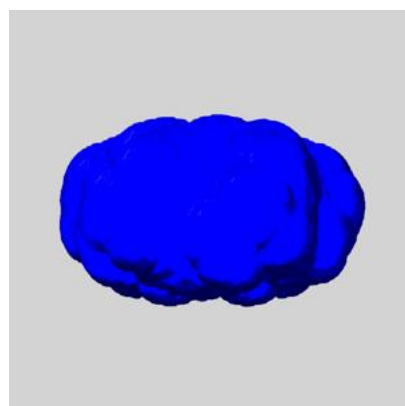
6.6 Mask visualisation [i](#)

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

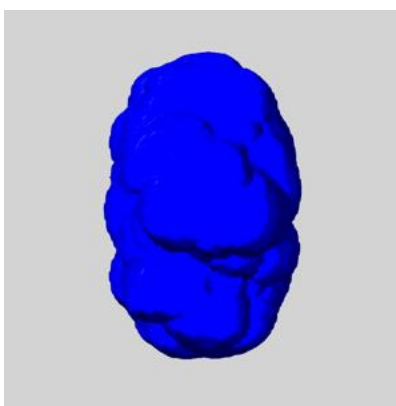
A mask typically either:

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

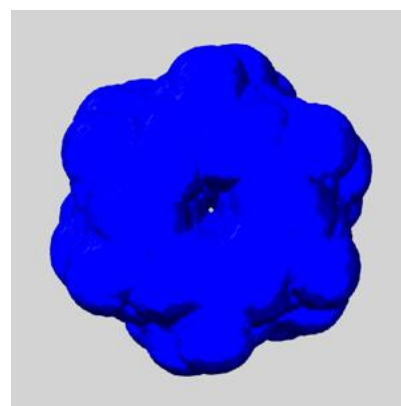
6.6.1 emd_70431_msk_1.map [i](#)



X



Y

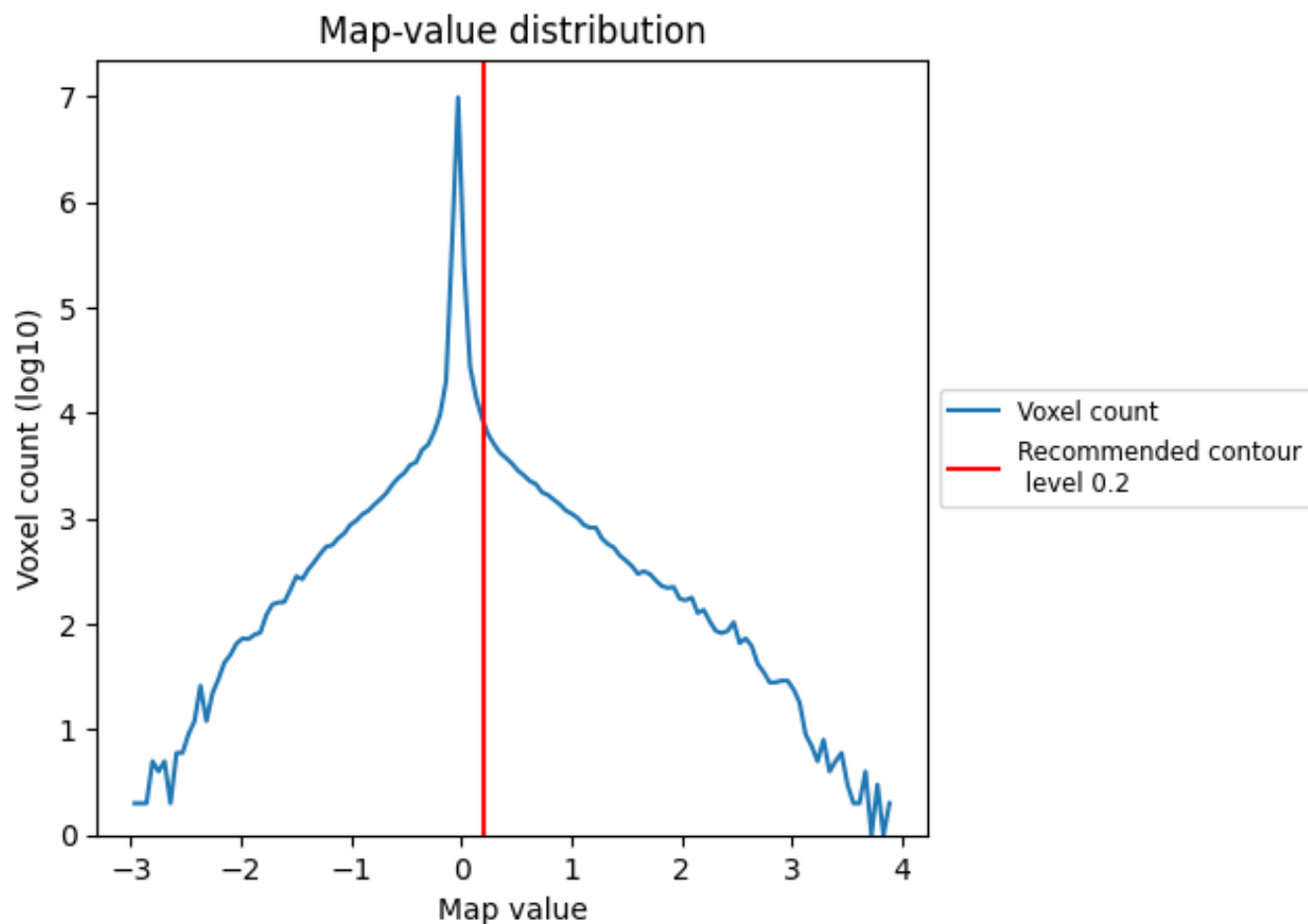


Z

7 Map analysis [i](#)

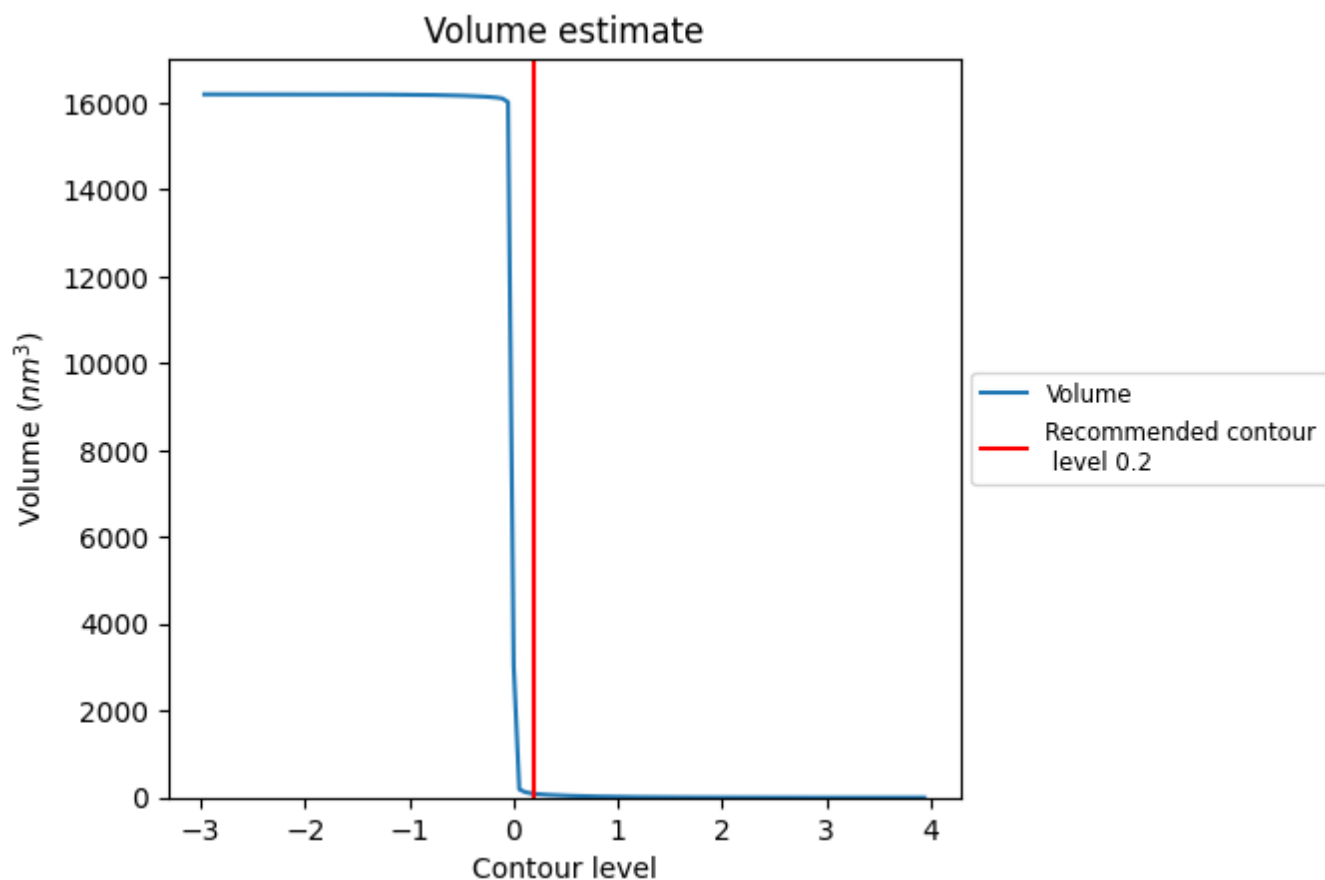
This section contains the results of statistical analysis of the map.

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.

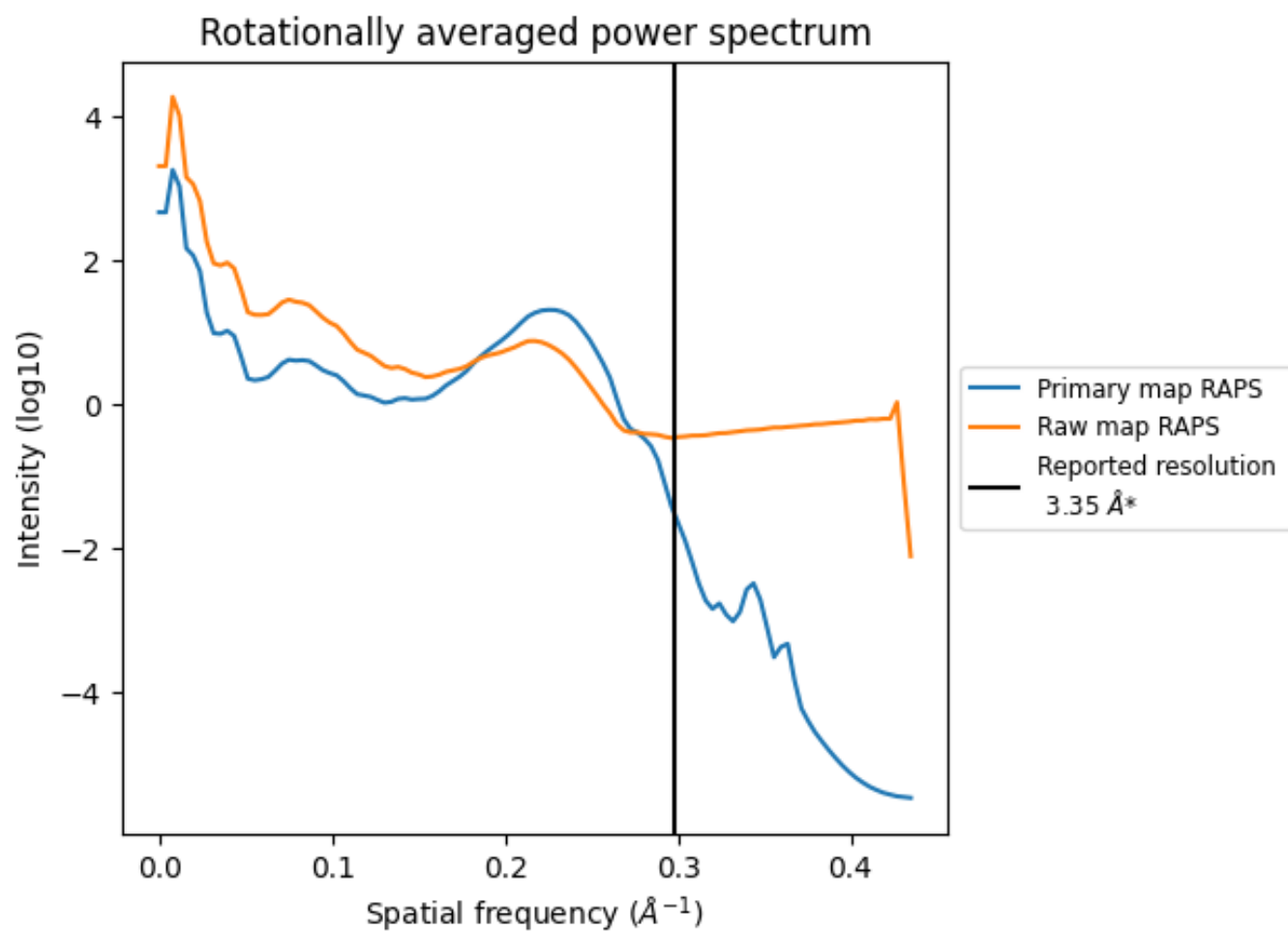
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 89 nm^3 ; this corresponds to an approximate mass of 80 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](#)

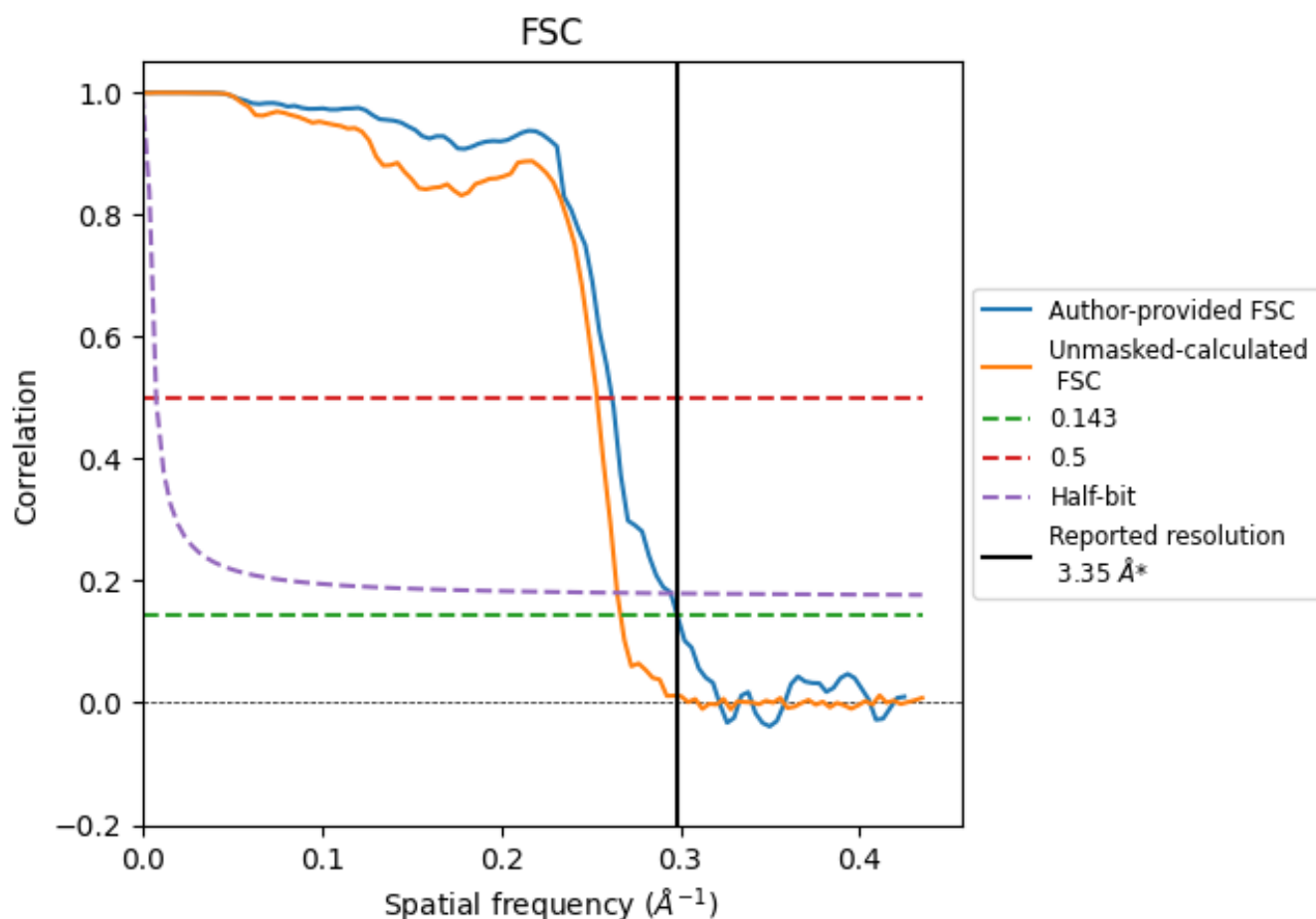


*Reported resolution corresponds to spatial frequency of 0.299 Å⁻¹

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 0.299 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

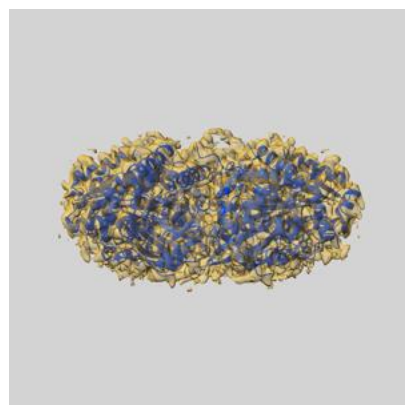
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.35	-	-
Author-provided FSC curve	3.35	3.82	3.39
Unmasked-calculated*	3.75	3.94	3.78

*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 3.75 differs from the reported value 3.35 by more than 10 %

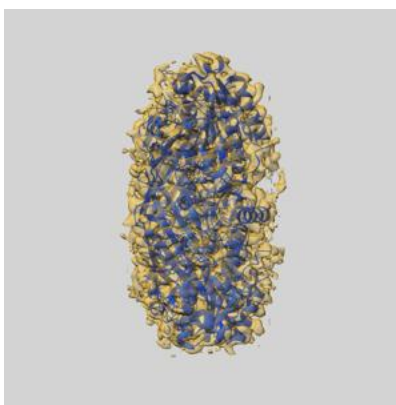
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-70431 and PDB model 9OFG. Per-residue inclusion information can be found in section [3](#) on page [6](#).

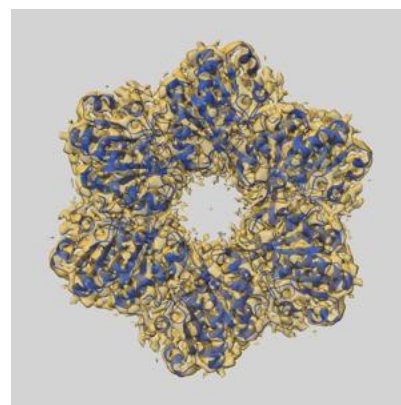
9.1 Map-model overlay [i](#)



X



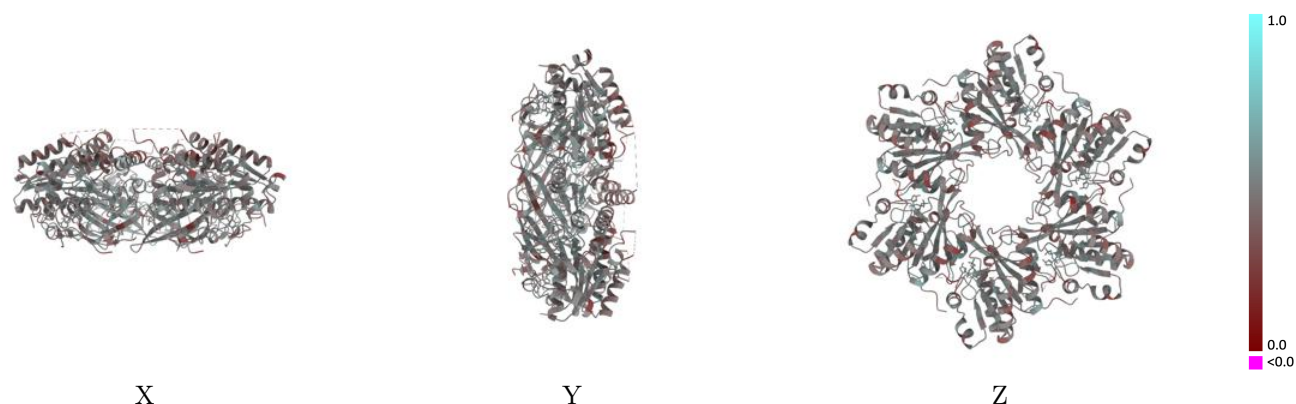
Y



Z

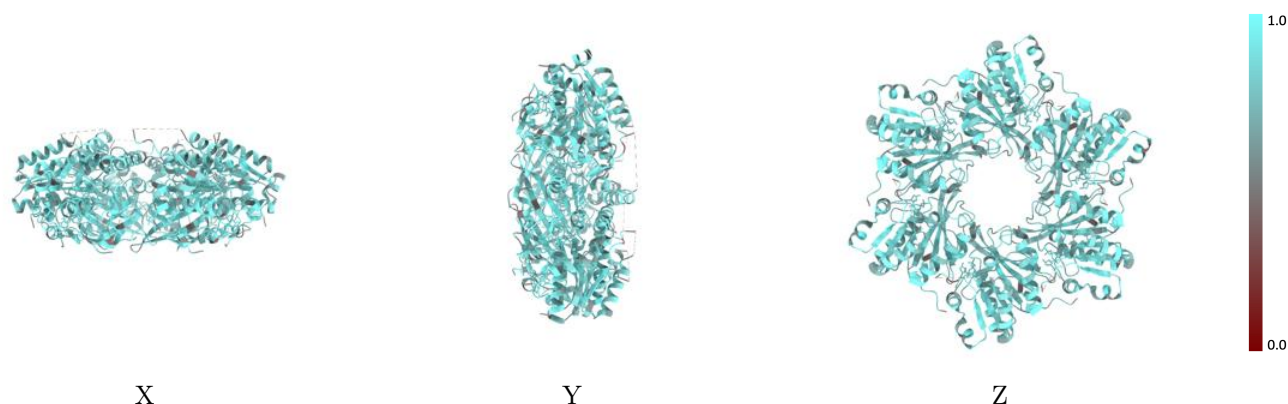
The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



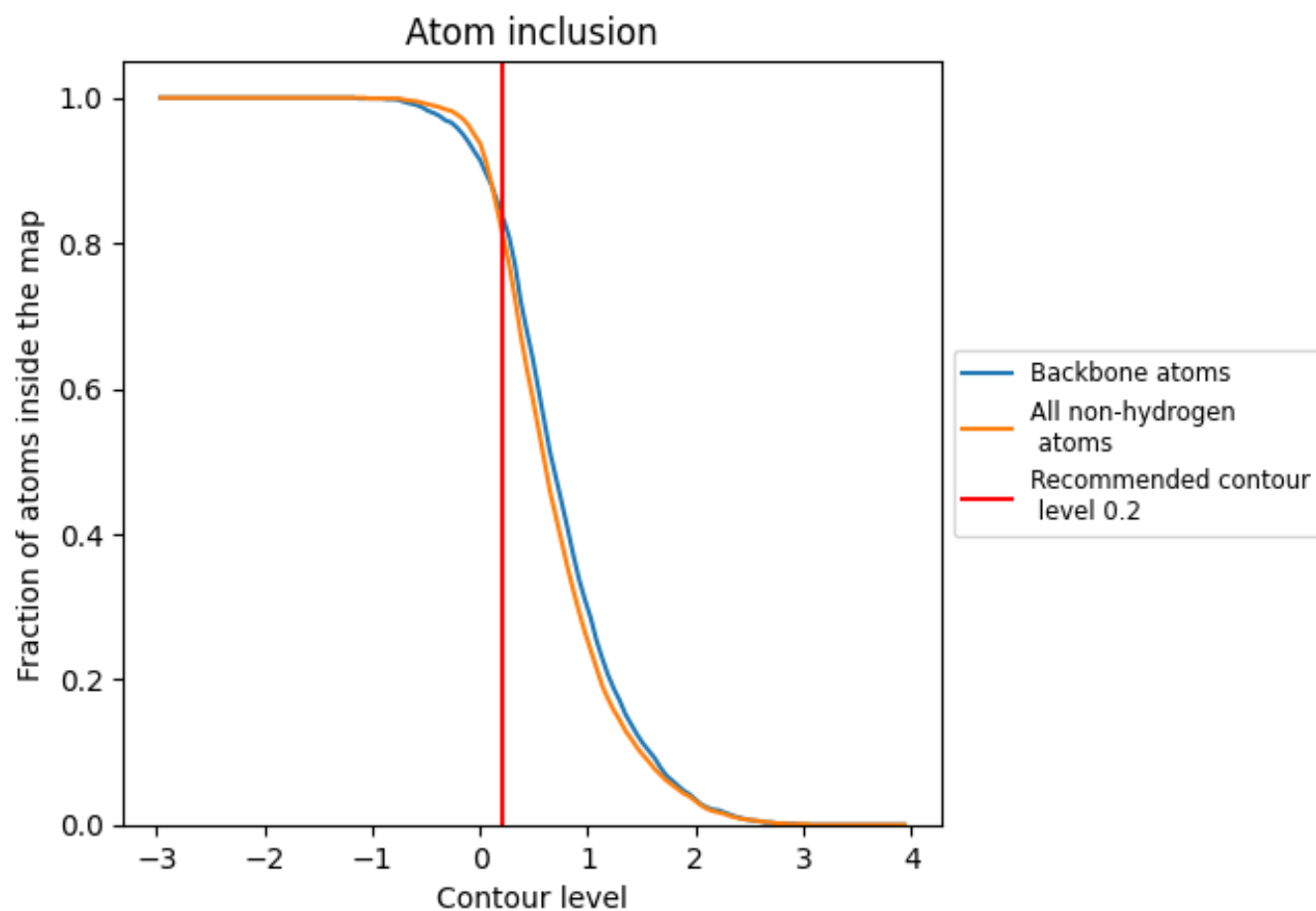
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.2).

9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 82% 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 (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8190	0.4520
A	0.8200	0.4530
B	0.8170	0.4540
C	0.8210	0.4520
D	0.8160	0.4520
E	0.8190	0.4520
F	0.8210	0.4500

1.0

0.0

<0.0