



wwPDB EM Validation Summary Report ⓘ

Mar 5, 2026 – 10:38 AM UTC

PDB ID : 9Q57 / pdb_00009q57
EMDB ID : EMD-72222
Title : XZ440 integrase inhibitor bound to Wild-type HIV-1 intasome
Authors : Jing, T.; Li, M.; Lyumkis, D.
Deposited on : 2025-08-20
Resolution : 2.28 Å(reported)

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:

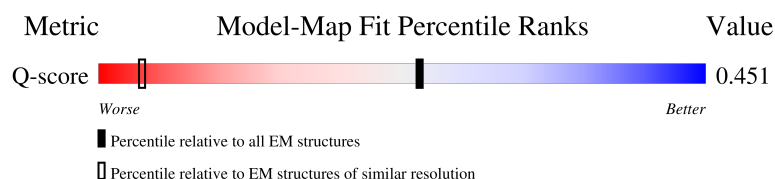
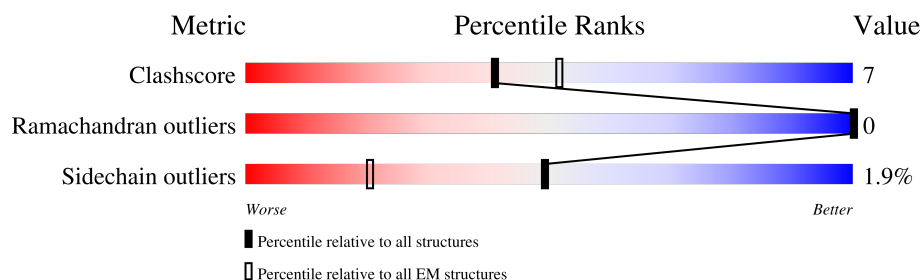
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 2.28 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	3643 (1.78 - 2.78)

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	363	
1	B	363	
1	C	363	
1	D	363	

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Mol	Chain	Length	Quality of chain
2	F	19	 26% 58% 16%
3	E	17	 29% 53% 18%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 5336 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 Integrase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	220	Total	C	N	O	S	0	0
			1713	1088	296	320	9		
1	C	69	Total	C	N	O	S	0	0
			565	358	105	100	2		
1	D	47	Total	C	N	O		0	0
			388	251	73	64			
1	B	242	Total	C	N	O	S	0	0
			1916	1226	337	346	7		

There are 300 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-74	MET	-	initiating methionine	UNP P12497
A	-73	ALA	-	expression tag	UNP P12497
A	-72	THR	-	expression tag	UNP P12497
A	-71	VAL	-	expression tag	UNP P12497
A	-70	LYS	-	expression tag	UNP P12497
A	-69	PHE	-	expression tag	UNP P12497
A	-68	LYS	-	expression tag	UNP P12497
A	-67	TYR	-	expression tag	UNP P12497
A	-66	LYS	-	expression tag	UNP P12497
A	-65	GLY	-	expression tag	UNP P12497
A	-64	GLU	-	expression tag	UNP P12497
A	-63	GLU	-	expression tag	UNP P12497
A	-62	LYS	-	expression tag	UNP P12497
A	-61	GLU	-	expression tag	UNP P12497
A	-60	VAL	-	expression tag	UNP P12497
A	-59	ASP	-	expression tag	UNP P12497
A	-58	ILE	-	expression tag	UNP P12497
A	-57	SER	-	expression tag	UNP P12497
A	-56	LYS	-	expression tag	UNP P12497
A	-55	ILE	-	expression tag	UNP P12497
A	-54	LYS	-	expression tag	UNP P12497
A	-53	LYS	-	expression tag	UNP P12497

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-52	VAL	-	expression tag	UNP P12497
A	-51	TRP	-	expression tag	UNP P12497
A	-50	ARG	-	expression tag	UNP P12497
A	-49	VAL	-	expression tag	UNP P12497
A	-48	GLY	-	expression tag	UNP P12497
A	-47	LYS	-	expression tag	UNP P12497
A	-46	MET	-	expression tag	UNP P12497
A	-45	ILE	-	expression tag	UNP P12497
A	-44	SER	-	expression tag	UNP P12497
A	-43	PHE	-	expression tag	UNP P12497
A	-42	THR	-	expression tag	UNP P12497
A	-41	TYR	-	expression tag	UNP P12497
A	-40	ASP	-	expression tag	UNP P12497
A	-39	GLU	-	expression tag	UNP P12497
A	-38	GLY	-	expression tag	UNP P12497
A	-37	GLY	-	expression tag	UNP P12497
A	-36	GLY	-	expression tag	UNP P12497
A	-35	LYS	-	expression tag	UNP P12497
A	-34	THR	-	expression tag	UNP P12497
A	-33	GLY	-	expression tag	UNP P12497
A	-32	ARG	-	expression tag	UNP P12497
A	-31	GLY	-	expression tag	UNP P12497
A	-30	ALA	-	expression tag	UNP P12497
A	-29	VAL	-	expression tag	UNP P12497
A	-28	SER	-	expression tag	UNP P12497
A	-27	GLU	-	expression tag	UNP P12497
A	-26	LYS	-	expression tag	UNP P12497
A	-25	ASP	-	expression tag	UNP P12497
A	-24	ALA	-	expression tag	UNP P12497
A	-23	PRO	-	expression tag	UNP P12497
A	-22	LYS	-	expression tag	UNP P12497
A	-21	GLU	-	expression tag	UNP P12497
A	-20	LEU	-	expression tag	UNP P12497
A	-19	LEU	-	expression tag	UNP P12497
A	-18	GLN	-	expression tag	UNP P12497
A	-17	MET	-	expression tag	UNP P12497
A	-16	LEU	-	expression tag	UNP P12497
A	-15	GLU	-	expression tag	UNP P12497
A	-14	LYS	-	expression tag	UNP P12497
A	-13	GLN	-	expression tag	UNP P12497
A	-12	LYS	-	expression tag	UNP P12497
A	-11	LYS	-	expression tag	UNP P12497

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-10	GLY	-	expression tag	UNP P12497
A	-9	GLY	-	expression tag	UNP P12497
A	-8	GLY	-	expression tag	UNP P12497
A	-7	GLY	-	expression tag	UNP P12497
A	-6	GLY	-	expression tag	UNP P12497
A	-5	GLY	-	expression tag	UNP P12497
A	-4	GLY	-	expression tag	UNP P12497
A	-3	GLY	-	expression tag	UNP P12497
A	-2	GLY	-	expression tag	UNP P12497
A	-1	GLY	-	expression tag	UNP P12497
A	0	GLY	-	expression tag	UNP P12497
C	-74	MET	-	initiating methionine	UNP P12497
C	-73	ALA	-	expression tag	UNP P12497
C	-72	THR	-	expression tag	UNP P12497
C	-71	VAL	-	expression tag	UNP P12497
C	-70	LYS	-	expression tag	UNP P12497
C	-69	PHE	-	expression tag	UNP P12497
C	-68	LYS	-	expression tag	UNP P12497
C	-67	TYR	-	expression tag	UNP P12497
C	-66	LYS	-	expression tag	UNP P12497
C	-65	GLY	-	expression tag	UNP P12497
C	-64	GLU	-	expression tag	UNP P12497
C	-63	GLU	-	expression tag	UNP P12497
C	-62	LYS	-	expression tag	UNP P12497
C	-61	GLU	-	expression tag	UNP P12497
C	-60	VAL	-	expression tag	UNP P12497
C	-59	ASP	-	expression tag	UNP P12497
C	-58	ILE	-	expression tag	UNP P12497
C	-57	SER	-	expression tag	UNP P12497
C	-56	LYS	-	expression tag	UNP P12497
C	-55	ILE	-	expression tag	UNP P12497
C	-54	LYS	-	expression tag	UNP P12497
C	-53	LYS	-	expression tag	UNP P12497
C	-52	VAL	-	expression tag	UNP P12497
C	-51	TRP	-	expression tag	UNP P12497
C	-50	ARG	-	expression tag	UNP P12497
C	-49	VAL	-	expression tag	UNP P12497
C	-48	GLY	-	expression tag	UNP P12497
C	-47	LYS	-	expression tag	UNP P12497
C	-46	MET	-	expression tag	UNP P12497
C	-45	ILE	-	expression tag	UNP P12497
C	-44	SER	-	expression tag	UNP P12497

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-43	PHE	-	expression tag	UNP P12497
C	-42	THR	-	expression tag	UNP P12497
C	-41	TYR	-	expression tag	UNP P12497
C	-40	ASP	-	expression tag	UNP P12497
C	-39	GLU	-	expression tag	UNP P12497
C	-38	GLY	-	expression tag	UNP P12497
C	-37	GLY	-	expression tag	UNP P12497
C	-36	GLY	-	expression tag	UNP P12497
C	-35	LYS	-	expression tag	UNP P12497
C	-34	THR	-	expression tag	UNP P12497
C	-33	GLY	-	expression tag	UNP P12497
C	-32	ARG	-	expression tag	UNP P12497
C	-31	GLY	-	expression tag	UNP P12497
C	-30	ALA	-	expression tag	UNP P12497
C	-29	VAL	-	expression tag	UNP P12497
C	-28	SER	-	expression tag	UNP P12497
C	-27	GLU	-	expression tag	UNP P12497
C	-26	LYS	-	expression tag	UNP P12497
C	-25	ASP	-	expression tag	UNP P12497
C	-24	ALA	-	expression tag	UNP P12497
C	-23	PRO	-	expression tag	UNP P12497
C	-22	LYS	-	expression tag	UNP P12497
C	-21	GLU	-	expression tag	UNP P12497
C	-20	LEU	-	expression tag	UNP P12497
C	-19	LEU	-	expression tag	UNP P12497
C	-18	GLN	-	expression tag	UNP P12497
C	-17	MET	-	expression tag	UNP P12497
C	-16	LEU	-	expression tag	UNP P12497
C	-15	GLU	-	expression tag	UNP P12497
C	-14	LYS	-	expression tag	UNP P12497
C	-13	GLN	-	expression tag	UNP P12497
C	-12	LYS	-	expression tag	UNP P12497
C	-11	LYS	-	expression tag	UNP P12497
C	-10	GLY	-	expression tag	UNP P12497
C	-9	GLY	-	expression tag	UNP P12497
C	-8	GLY	-	expression tag	UNP P12497
C	-7	GLY	-	expression tag	UNP P12497
C	-6	GLY	-	expression tag	UNP P12497
C	-5	GLY	-	expression tag	UNP P12497
C	-4	GLY	-	expression tag	UNP P12497
C	-3	GLY	-	expression tag	UNP P12497
C	-2	GLY	-	expression tag	UNP P12497

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	GLY	-	expression tag	UNP P12497
C	0	GLY	-	expression tag	UNP P12497
D	-74	MET	-	initiating methionine	UNP P12497
D	-73	ALA	-	expression tag	UNP P12497
D	-72	THR	-	expression tag	UNP P12497
D	-71	VAL	-	expression tag	UNP P12497
D	-70	LYS	-	expression tag	UNP P12497
D	-69	PHE	-	expression tag	UNP P12497
D	-68	LYS	-	expression tag	UNP P12497
D	-67	TYR	-	expression tag	UNP P12497
D	-66	LYS	-	expression tag	UNP P12497
D	-65	GLY	-	expression tag	UNP P12497
D	-64	GLU	-	expression tag	UNP P12497
D	-63	GLU	-	expression tag	UNP P12497
D	-62	LYS	-	expression tag	UNP P12497
D	-61	GLU	-	expression tag	UNP P12497
D	-60	VAL	-	expression tag	UNP P12497
D	-59	ASP	-	expression tag	UNP P12497
D	-58	ILE	-	expression tag	UNP P12497
D	-57	SER	-	expression tag	UNP P12497
D	-56	LYS	-	expression tag	UNP P12497
D	-55	ILE	-	expression tag	UNP P12497
D	-54	LYS	-	expression tag	UNP P12497
D	-53	LYS	-	expression tag	UNP P12497
D	-52	VAL	-	expression tag	UNP P12497
D	-51	TRP	-	expression tag	UNP P12497
D	-50	ARG	-	expression tag	UNP P12497
D	-49	VAL	-	expression tag	UNP P12497
D	-48	GLY	-	expression tag	UNP P12497
D	-47	LYS	-	expression tag	UNP P12497
D	-46	MET	-	expression tag	UNP P12497
D	-45	ILE	-	expression tag	UNP P12497
D	-44	SER	-	expression tag	UNP P12497
D	-43	PHE	-	expression tag	UNP P12497
D	-42	THR	-	expression tag	UNP P12497
D	-41	TYR	-	expression tag	UNP P12497
D	-40	ASP	-	expression tag	UNP P12497
D	-39	GLU	-	expression tag	UNP P12497
D	-38	GLY	-	expression tag	UNP P12497
D	-37	GLY	-	expression tag	UNP P12497
D	-36	GLY	-	expression tag	UNP P12497
D	-35	LYS	-	expression tag	UNP P12497

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-34	THR	-	expression tag	UNP P12497
D	-33	GLY	-	expression tag	UNP P12497
D	-32	ARG	-	expression tag	UNP P12497
D	-31	GLY	-	expression tag	UNP P12497
D	-30	ALA	-	expression tag	UNP P12497
D	-29	VAL	-	expression tag	UNP P12497
D	-28	SER	-	expression tag	UNP P12497
D	-27	GLU	-	expression tag	UNP P12497
D	-26	LYS	-	expression tag	UNP P12497
D	-25	ASP	-	expression tag	UNP P12497
D	-24	ALA	-	expression tag	UNP P12497
D	-23	PRO	-	expression tag	UNP P12497
D	-22	LYS	-	expression tag	UNP P12497
D	-21	GLU	-	expression tag	UNP P12497
D	-20	LEU	-	expression tag	UNP P12497
D	-19	LEU	-	expression tag	UNP P12497
D	-18	GLN	-	expression tag	UNP P12497
D	-17	MET	-	expression tag	UNP P12497
D	-16	LEU	-	expression tag	UNP P12497
D	-15	GLU	-	expression tag	UNP P12497
D	-14	LYS	-	expression tag	UNP P12497
D	-13	GLN	-	expression tag	UNP P12497
D	-12	LYS	-	expression tag	UNP P12497
D	-11	LYS	-	expression tag	UNP P12497
D	-10	GLY	-	expression tag	UNP P12497
D	-9	GLY	-	expression tag	UNP P12497
D	-8	GLY	-	expression tag	UNP P12497
D	-7	GLY	-	expression tag	UNP P12497
D	-6	GLY	-	expression tag	UNP P12497
D	-5	GLY	-	expression tag	UNP P12497
D	-4	GLY	-	expression tag	UNP P12497
D	-3	GLY	-	expression tag	UNP P12497
D	-2	GLY	-	expression tag	UNP P12497
D	-1	GLY	-	expression tag	UNP P12497
D	0	GLY	-	expression tag	UNP P12497
B	-74	MET	-	initiating methionine	UNP P12497
B	-73	ALA	-	expression tag	UNP P12497
B	-72	THR	-	expression tag	UNP P12497
B	-71	VAL	-	expression tag	UNP P12497
B	-70	LYS	-	expression tag	UNP P12497
B	-69	PHE	-	expression tag	UNP P12497
B	-68	LYS	-	expression tag	UNP P12497

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-67	TYR	-	expression tag	UNP P12497
B	-66	LYS	-	expression tag	UNP P12497
B	-65	GLY	-	expression tag	UNP P12497
B	-64	GLU	-	expression tag	UNP P12497
B	-63	GLU	-	expression tag	UNP P12497
B	-62	LYS	-	expression tag	UNP P12497
B	-61	GLU	-	expression tag	UNP P12497
B	-60	VAL	-	expression tag	UNP P12497
B	-59	ASP	-	expression tag	UNP P12497
B	-58	ILE	-	expression tag	UNP P12497
B	-57	SER	-	expression tag	UNP P12497
B	-56	LYS	-	expression tag	UNP P12497
B	-55	ILE	-	expression tag	UNP P12497
B	-54	LYS	-	expression tag	UNP P12497
B	-53	LYS	-	expression tag	UNP P12497
B	-52	VAL	-	expression tag	UNP P12497
B	-51	TRP	-	expression tag	UNP P12497
B	-50	ARG	-	expression tag	UNP P12497
B	-49	VAL	-	expression tag	UNP P12497
B	-48	GLY	-	expression tag	UNP P12497
B	-47	LYS	-	expression tag	UNP P12497
B	-46	MET	-	expression tag	UNP P12497
B	-45	ILE	-	expression tag	UNP P12497
B	-44	SER	-	expression tag	UNP P12497
B	-43	PHE	-	expression tag	UNP P12497
B	-42	THR	-	expression tag	UNP P12497
B	-41	TYR	-	expression tag	UNP P12497
B	-40	ASP	-	expression tag	UNP P12497
B	-39	GLU	-	expression tag	UNP P12497
B	-38	GLY	-	expression tag	UNP P12497
B	-37	GLY	-	expression tag	UNP P12497
B	-36	GLY	-	expression tag	UNP P12497
B	-35	LYS	-	expression tag	UNP P12497
B	-34	THR	-	expression tag	UNP P12497
B	-33	GLY	-	expression tag	UNP P12497
B	-32	ARG	-	expression tag	UNP P12497
B	-31	GLY	-	expression tag	UNP P12497
B	-30	ALA	-	expression tag	UNP P12497
B	-29	VAL	-	expression tag	UNP P12497
B	-28	SER	-	expression tag	UNP P12497
B	-27	GLU	-	expression tag	UNP P12497
B	-26	LYS	-	expression tag	UNP P12497

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-25	ASP	-	expression tag	UNP P12497
B	-24	ALA	-	expression tag	UNP P12497
B	-23	PRO	-	expression tag	UNP P12497
B	-22	LYS	-	expression tag	UNP P12497
B	-21	GLU	-	expression tag	UNP P12497
B	-20	LEU	-	expression tag	UNP P12497
B	-19	LEU	-	expression tag	UNP P12497
B	-18	GLN	-	expression tag	UNP P12497
B	-17	MET	-	expression tag	UNP P12497
B	-16	LEU	-	expression tag	UNP P12497
B	-15	GLU	-	expression tag	UNP P12497
B	-14	LYS	-	expression tag	UNP P12497
B	-13	GLN	-	expression tag	UNP P12497
B	-12	LYS	-	expression tag	UNP P12497
B	-11	LYS	-	expression tag	UNP P12497
B	-10	GLY	-	expression tag	UNP P12497
B	-9	GLY	-	expression tag	UNP P12497
B	-8	GLY	-	expression tag	UNP P12497
B	-7	GLY	-	expression tag	UNP P12497
B	-6	GLY	-	expression tag	UNP P12497
B	-5	GLY	-	expression tag	UNP P12497
B	-4	GLY	-	expression tag	UNP P12497
B	-3	GLY	-	expression tag	UNP P12497
B	-2	GLY	-	expression tag	UNP P12497
B	-1	GLY	-	expression tag	UNP P12497
B	0	GLY	-	expression tag	UNP P12497

- Molecule 2 is a DNA chain called DNA (5'-D(*AP*CP*TP*GP*CP*TP*AP*GP*AP*GP*AP*TP*TP*TP*TP*C)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
2	F	16	Total	C	N	O	P	0	0
			324	157	56	96	15		

- Molecule 3 is a DNA chain called DNA (5'-D(P*GP*AP*AP*AP*AP*TP*CP*TP*CP*TP*AP*GP*CP*A)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	14	Total	C	N	O	P	1	0
			308	147	60	86	15		

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of

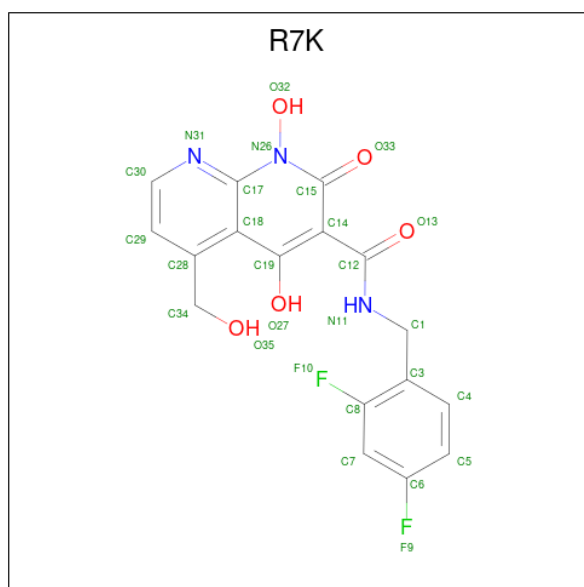
Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
4	A	2	Total	Mg	0
			2	2	

- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
5	A	1	Total	Zn	0
			1	1	
5	B	1	Total	Zn	0
			1	1	

- Molecule 6 is {N}-[[2,4-bis(fluoranyl)phenyl]methyl]-5-(hydroxymethyl)-1,4-bis(oxidanyl)-2-oxidanylidene-1,8-naphthyridine-3-carboxamide (CCD ID: R7K) (formula: C₁₇H₁₃F₂N₃O₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
6	E	1	Total	C	F	N	O	0
			27	17	2	3	5	

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		AltConf
7	A	23	Total	O	0
			23	23	
7	C	3	Total	O	0
			3	3	

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Mol	Chain	Residues	Atoms		AltConf
7	D	1	Total 1	O 1	0
7	F	30	Total 30	O 30	0
7	E	34	Total 34	O 34	0

[illegible]

Chain B:

44% 55% 11% 33%

MET THR VAL LYS PHE TYR LYS GLY GLU GLU LYS VAL THR ARG ASP GLY GLY GLY LYS THR TYR ASP GLU GLY GLY GLY LYS THR ARG ASP ALA PRO LYS GLU LEU LEU GLN MET LEU GLU

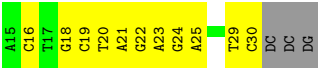
LYS GLN LYS LYS GLY GLY GLY GLY GLY GLY GLY GLY GLY GLY F1 L2 D3 G4 I5 D6 K7 A8 Q9 E10 E11 H12 E13 K14 Y15 H16 S17 N18 W19 R20 A21 W22 A23 S24 D25 F26 M27 P30 V31 V32 A33 K34 E35 I36 V37 A38 S39 C40 D41 K42 C43 G44 L45 LYS

GLY GLU ALA MET HIS GLN VAL ASP CYS S57 S58 G59 Q62 L63 D64 C65 T66 H67 L68 E69 G70 K71 W72 I73 L74 V75 A76 A86 E87 P90 A91 G94 Q95 E96 T97 A98 Y99 L102 K103 L104 R107 V110 K111 T112 V113 H114 T115 D116 N117 G118 S119 N120

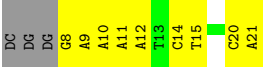
F121 T122 S123 T124 V125 V126 K127 A128 A129 C130 G134 I135 K136 Q137 E138 F139 G149 V150 I151 E152 S153 M154 W155 K156 E157 L158 K159 L160 I161 I162 G163 Q164 V165 L166 D167 Q168 A169 E170 H171 L172 K173 M178 H183 R187 K188 G189 G190

I191 G192 G193 Y194 G197 I200 V201 I204 T210 Q214 K215 Q216 A217 T218 K219 I220 Q221 N222 F223 R224 R225 V226 Y227 R228 ASP SER ARG ASP PRO VAL W235 K236 G237 P238 A239 K240 L241 L242 W243 K244 G245 E246 G247 A248 V249 V250 I251 Q252 D253 N254 S255 D256 I257 K258

Chain F: 26% 58% 16%



● Molecule 3: DNA (5'-D(P*GP*AP*AP*AP*AP*TP*CP*TP*CP*TP*AP*GP*CP*A)-3')



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	261868	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	58	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.035	Depositor
Minimum map value	-0.013	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.0055	Depositor
Map size (Å)	298.8, 298.8, 298.8	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83, 0.83, 0.83	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, ZN, R7K

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	0.27	1/1749 (0.1%)	0.44	2/2365 (0.1%)
1	B	0.39	0/1954	0.62	3/2635 (0.1%)
1	C	0.22	0/575	0.40	0/771
1	D	0.27	0/397	0.50	0/535
2	F	0.27	0/362	0.60	0/557
3	E	0.26	0/345	0.46	0/527
All	All	0.31	1/5382 (0.0%)	0.52	5/7390 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	151	ILE	C-O	-5.02	1.17	1.24

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	150	VAL	CA-C-O	-6.21	114.59	121.17
1	B	204	ILE	CA-C-O	-6.07	113.92	120.47
1	B	66	THR	CA-CB-OG1	-5.69	101.07	109.60
1	B	86	ALA	CA-C-O	-5.64	114.98	121.47
1	A	151	ILE	CA-C-O	-5.11	114.95	120.47

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	1713	0	1708	20	0
1	B	1916	0	1940	32	0
1	C	565	0	582	5	0
1	D	388	0	406	2	0
2	F	324	0	184	12	0
3	E	308	0	170	10	0
4	A	2	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	E	27	0	0	1	0
7	A	23	0	0	0	0
7	C	3	0	0	0	0
7	D	1	0	0	0	0
7	E	34	0	0	4	0
7	F	30	0	0	2	0
All	All	5336	0	4990	71	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 71 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)
3:E:21[B]:DA:N3	7:E:201:HOH:O	2.18	0.76
1:B:16:HIS:CE1	1:B:42:LYS:HE3	2.24	0.73
1:B:16:HIS:CE1	1:B:42:LYS:CE	2.73	0.71
3:E:8:DG:H1'	3:E:9:DA:H5'	1.71	0.70
1:B:12:HIS:CE1	1:B:43:CYS:SG	2.86	0.69

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	218/363 (60%)	213 (98%)	5 (2%)	0	100	100
1	B	234/363 (64%)	227 (97%)	7 (3%)	0	100	100
1	C	67/363 (18%)	65 (97%)	2 (3%)	0	100	100
1	D	45/363 (12%)	42 (93%)	3 (7%)	0	100	100
All	All	564/1452 (39%)	547 (97%)	17 (3%)	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	182/294 (62%)	179 (98%)	3 (2%)	55	71
1	B	202/294 (69%)	198 (98%)	4 (2%)	48	65
1	C	60/294 (20%)	59 (98%)	1 (2%)	53	70
1	D	41/294 (14%)	40 (98%)	1 (2%)	43	59
All	All	485/1176 (41%)	476 (98%)	9 (2%)	49	66

5 of 9 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	68	LEU
1	B	87	GLU
1	C	244	LYS
1	D	262	ARG
1	B	32	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	114	HIS
1	C	221	GLN
1	B	114	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 5 ligands modelled in this entry, 4 are monoatomic - leaving 1 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	$\# Z > 2$
6	R7K	E	101	4	29,29,29	2.53	8 (27%)	36,42,42	2.06	12 (33%)

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
6	R7K	E	101	4	-	4/11/11/11	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)
6	E	101	R7K	O33-C15	8.47	1.40	1.23
6	E	101	R7K	C12-N11	7.07	1.45	1.33
6	E	101	R7K	C15-N26	-3.89	1.32	1.38
6	E	101	R7K	C18-C17	-3.26	1.36	1.41
6	E	101	R7K	O27-C19	2.71	1.40	1.33

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	E	101	R7K	C17-N26-C15	-6.70	121.41	126.72
6	E	101	R7K	C30-N31-C17	2.97	121.77	115.05
6	E	101	R7K	C8-C7-C6	2.92	119.78	116.67
6	E	101	R7K	C29-C30-N31	-2.87	120.46	123.97
6	E	101	R7K	C14-C15-N26	2.85	120.91	113.58

There are no chirality outliers.

All (4) torsion outliers are listed below:

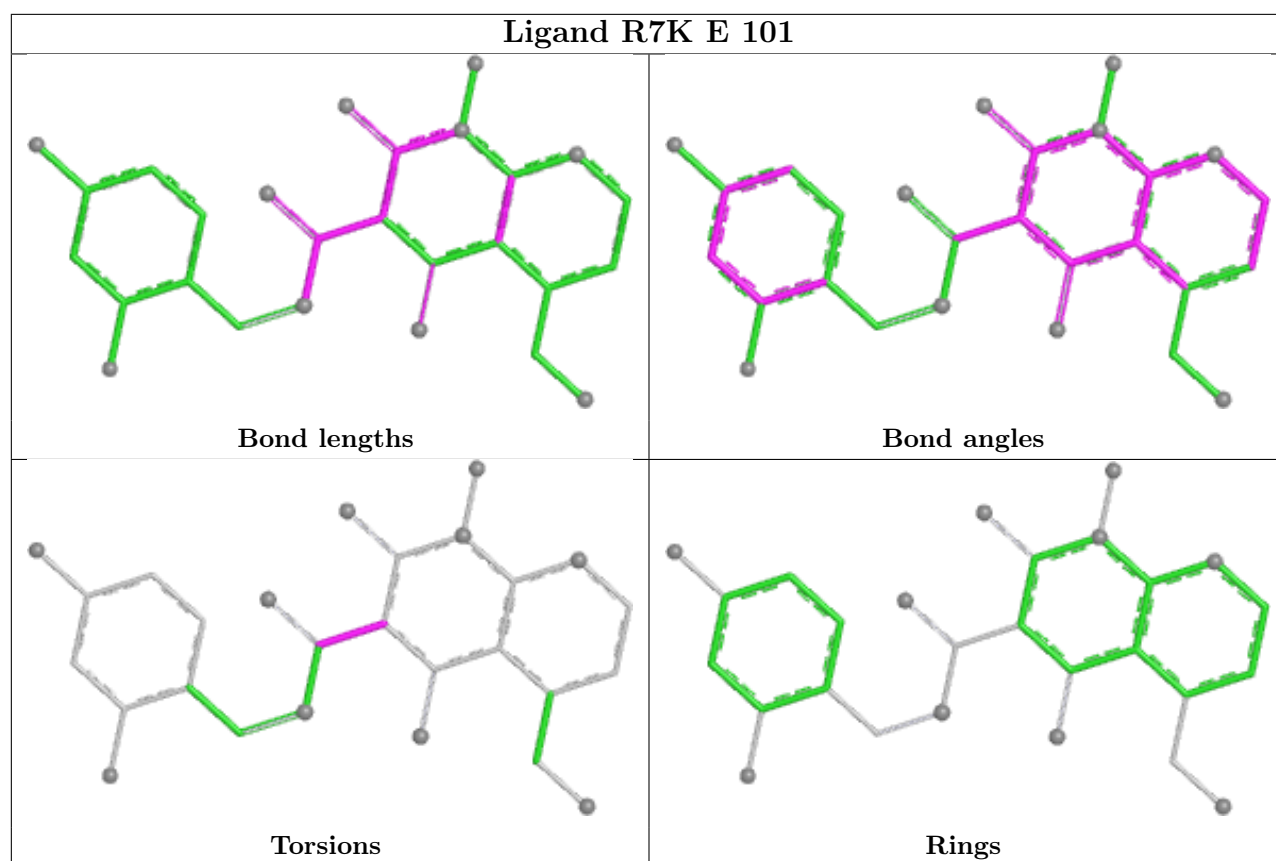
Mol	Chain	Res	Type	Atoms
6	E	101	R7K	O13-C12-C14-C15
6	E	101	R7K	O13-C12-C14-C19
6	E	101	R7K	N11-C12-C14-C15
6	E	101	R7K	N11-C12-C14-C19

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	E	101	R7K	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.

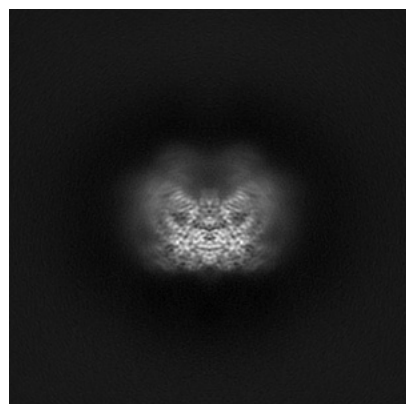
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-72222. These allow visual inspection of the internal detail of the map and identification of artifacts.

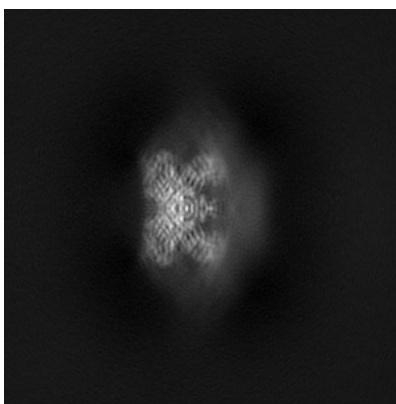
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

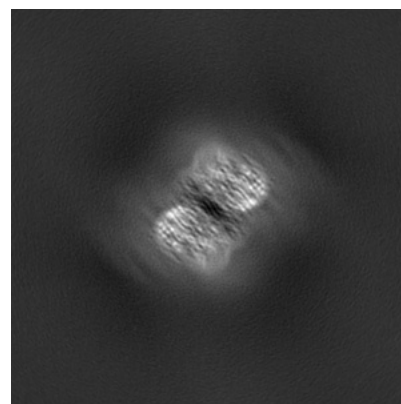
6.1.1 Primary map



X

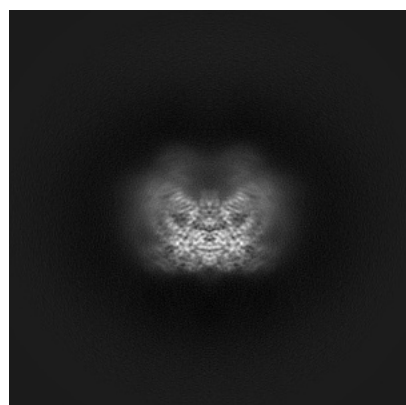


Y

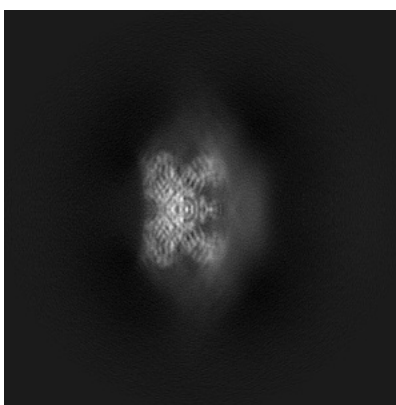


Z

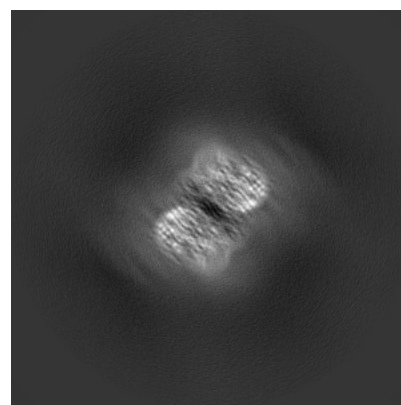
6.1.2 Raw map



X



Y

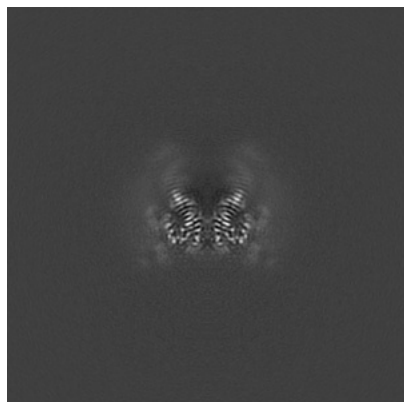


Z

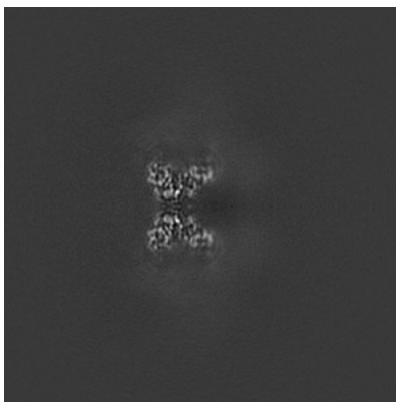
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

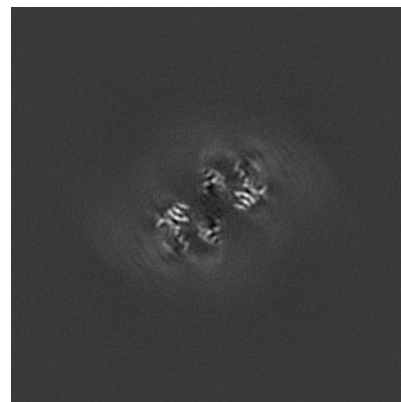
6.2.1 Primary map



X Index: 180

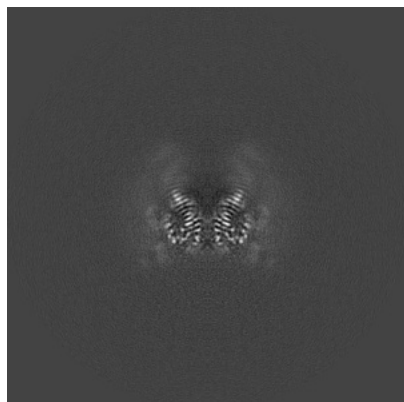


Y Index: 180

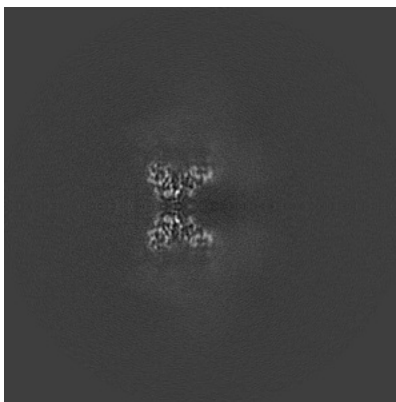


Z Index: 180

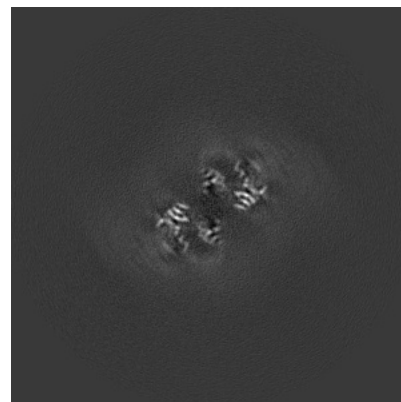
6.2.2 Raw map



X Index: 180



Y Index: 180

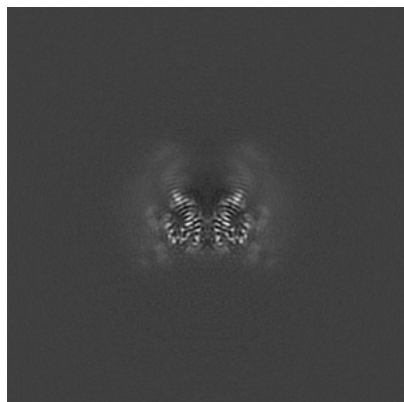


Z Index: 180

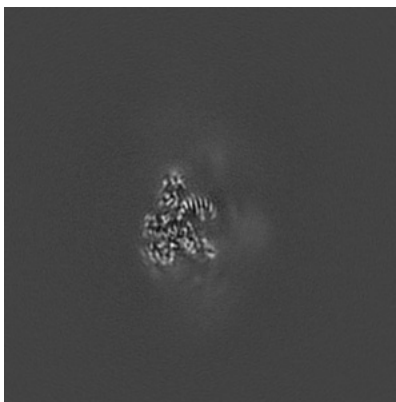
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

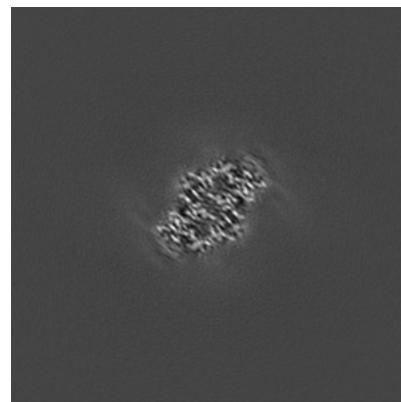
6.3.1 Primary map



X Index: 180

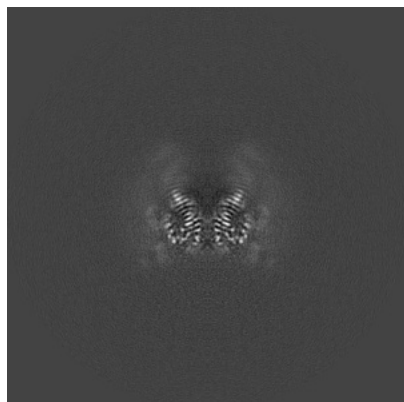


Y Index: 161

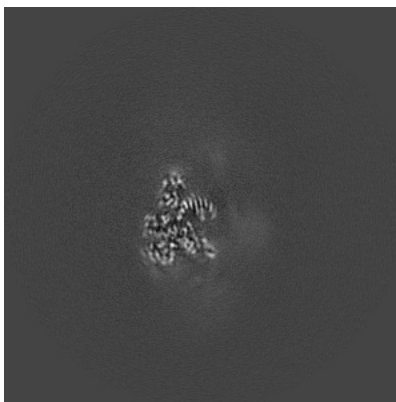


Z Index: 151

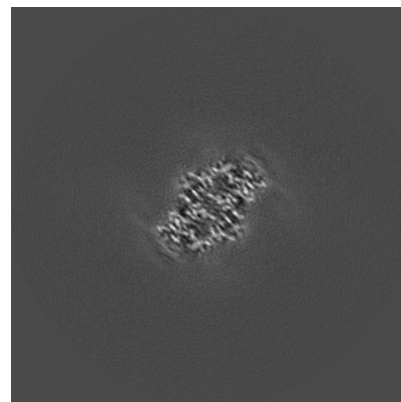
6.3.2 Raw map



X Index: 180



Y Index: 161

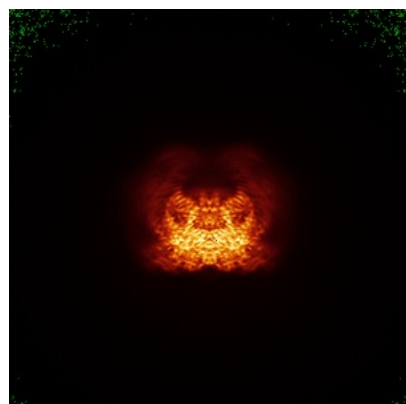


Z Index: 151

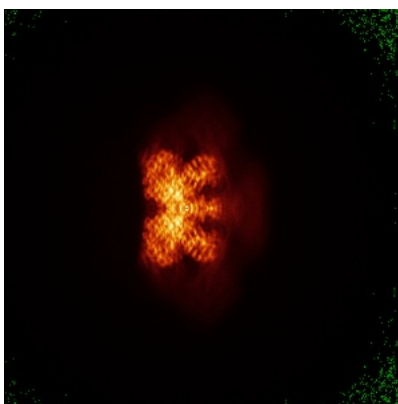
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) ⓘ

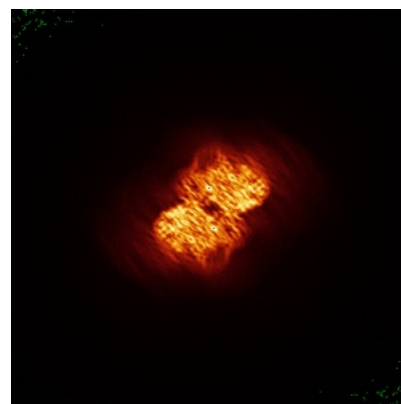
6.4.1 Primary map



X

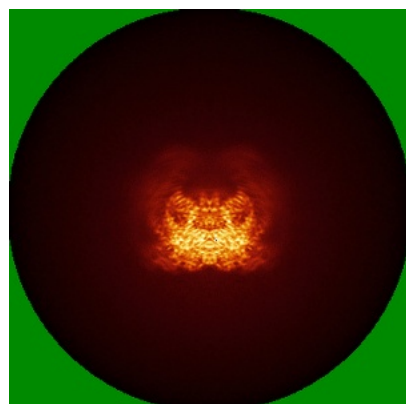


Y

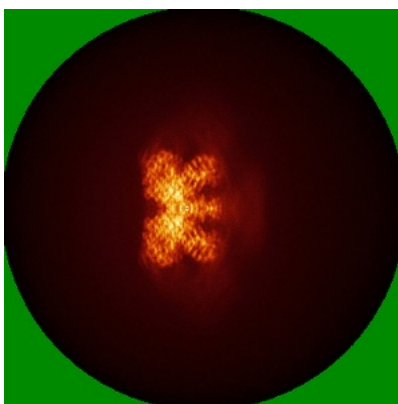


Z

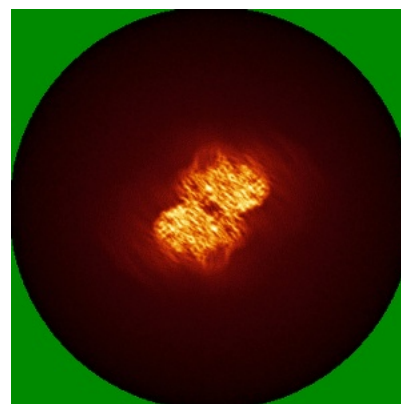
6.4.2 Raw map



X



Y

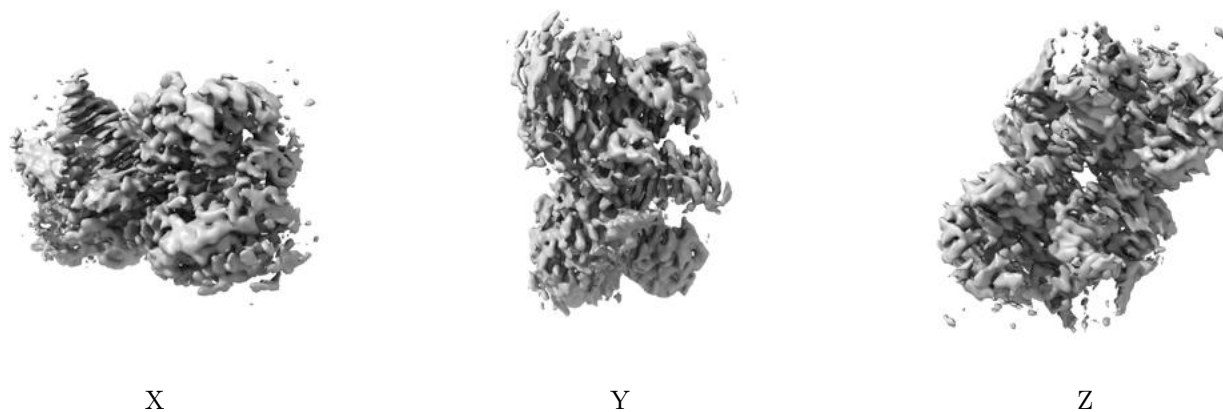


Z

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.

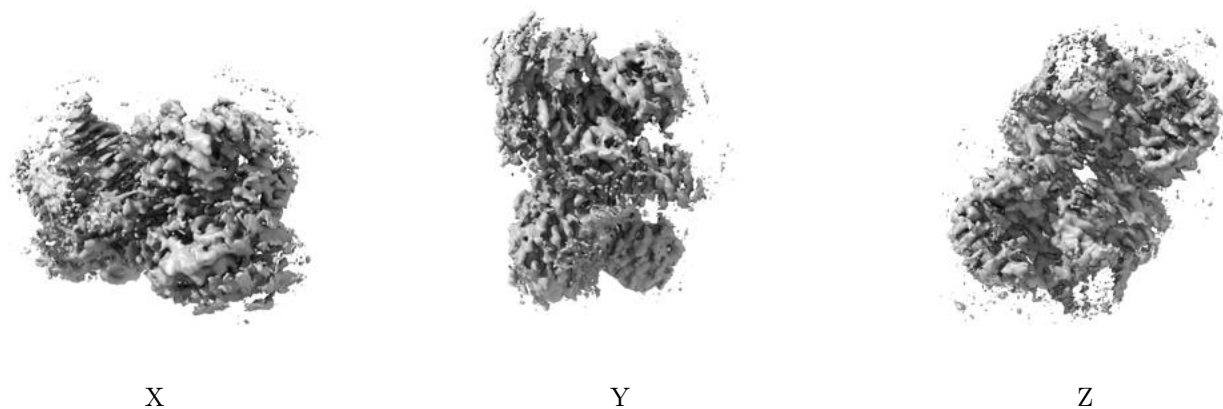
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0055. 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.

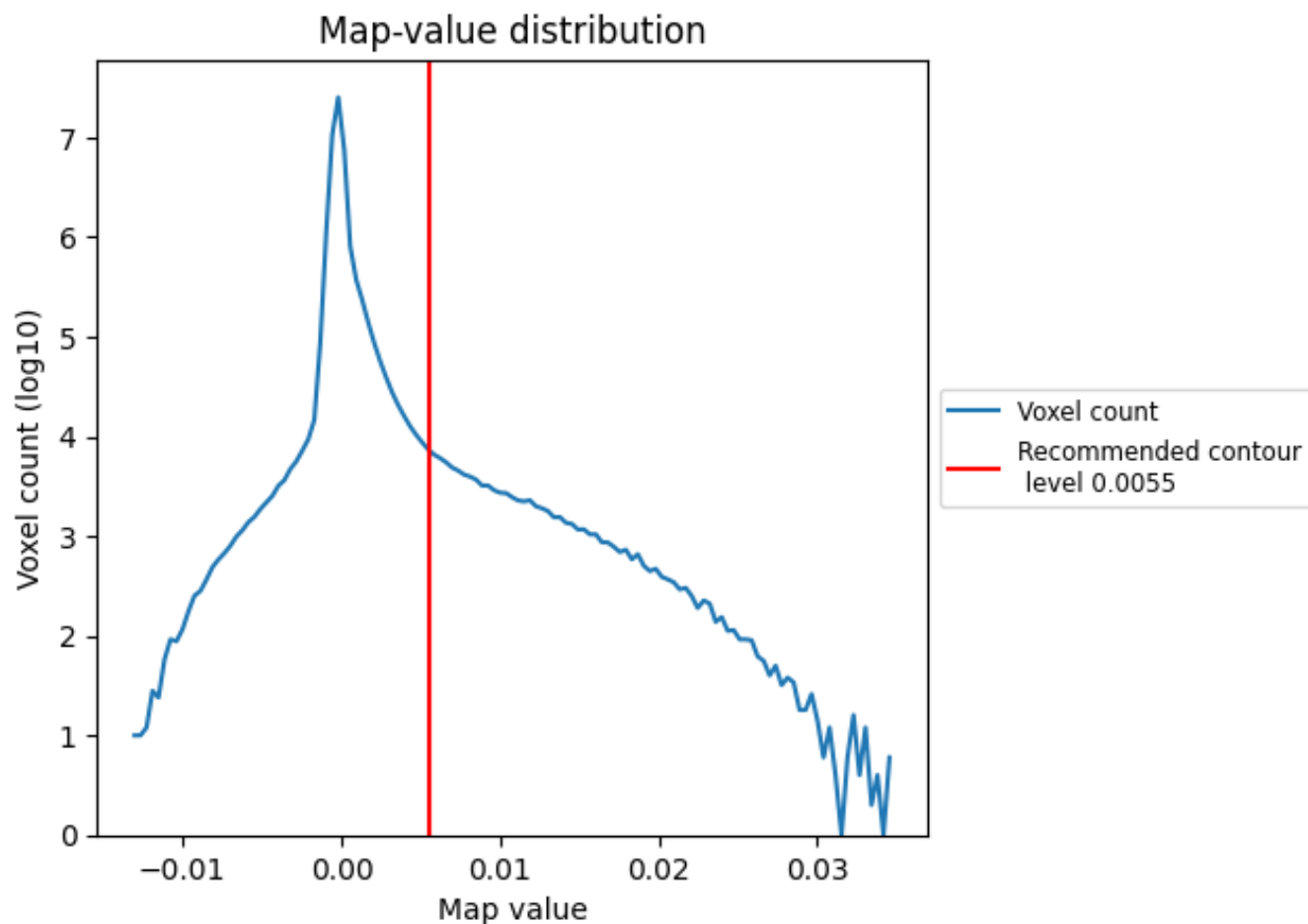
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

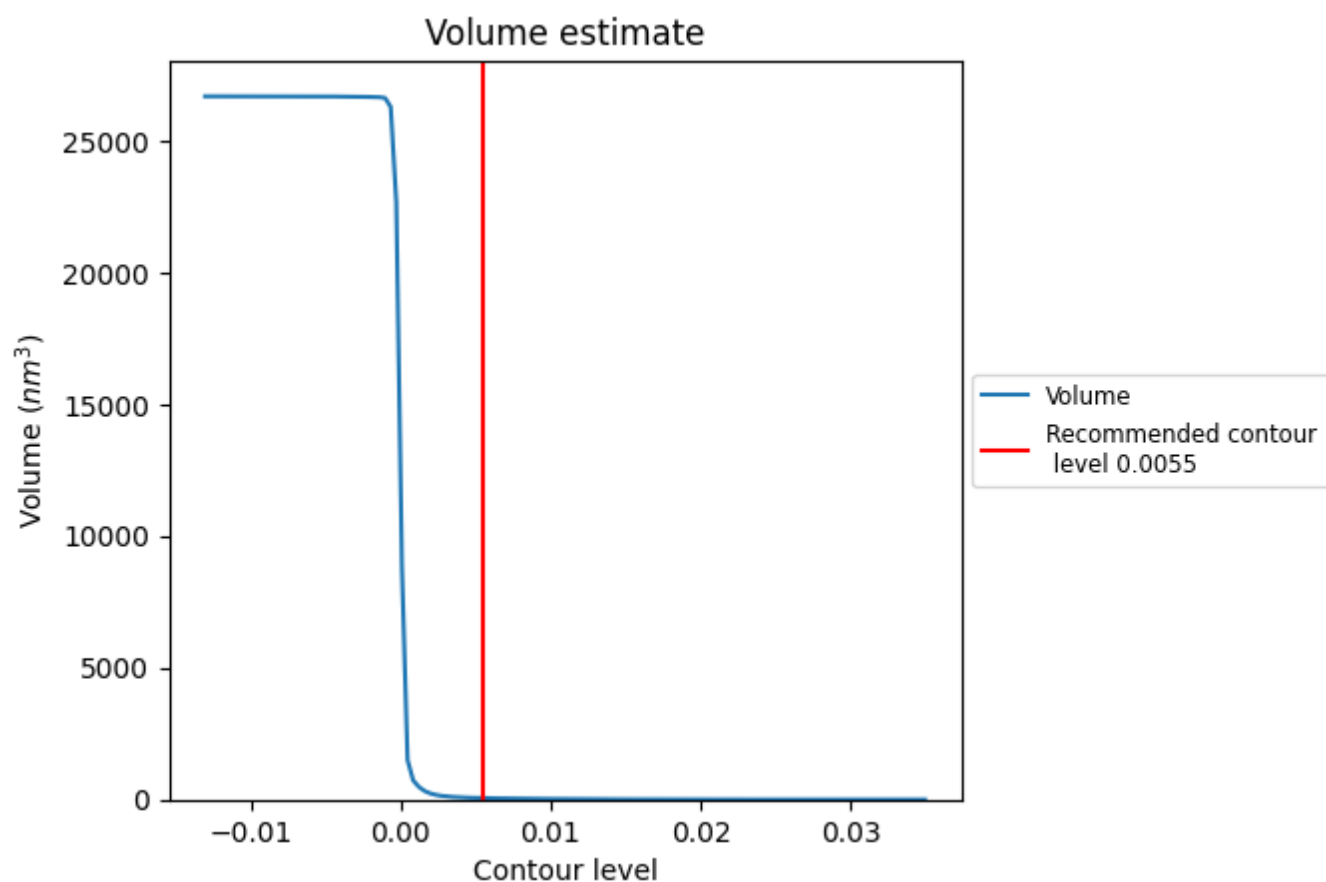
This section contains the results of statistical analysis of the map.

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.

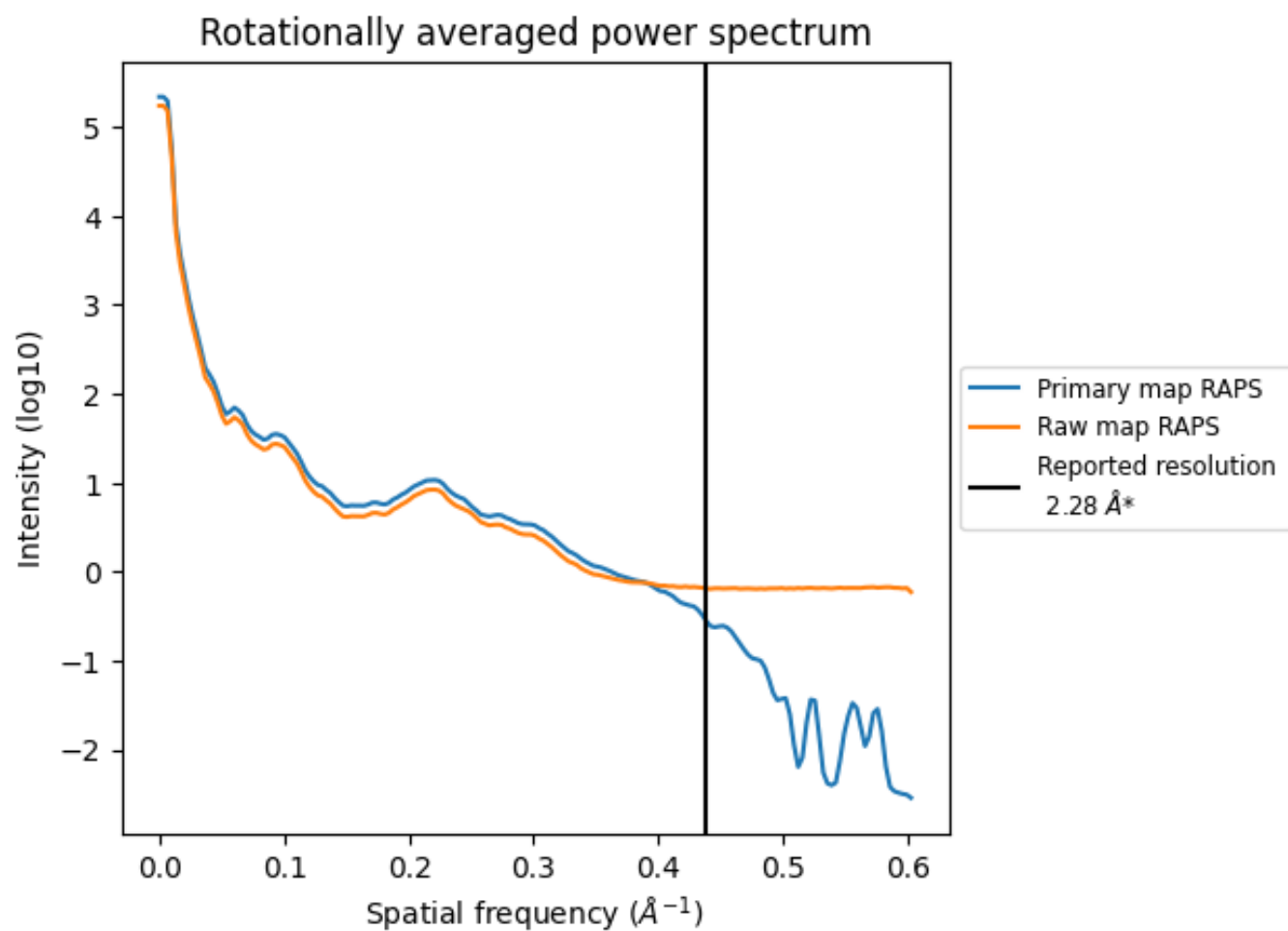
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 55 nm^3 ; this corresponds to an approximate mass of 50 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 ⓘ

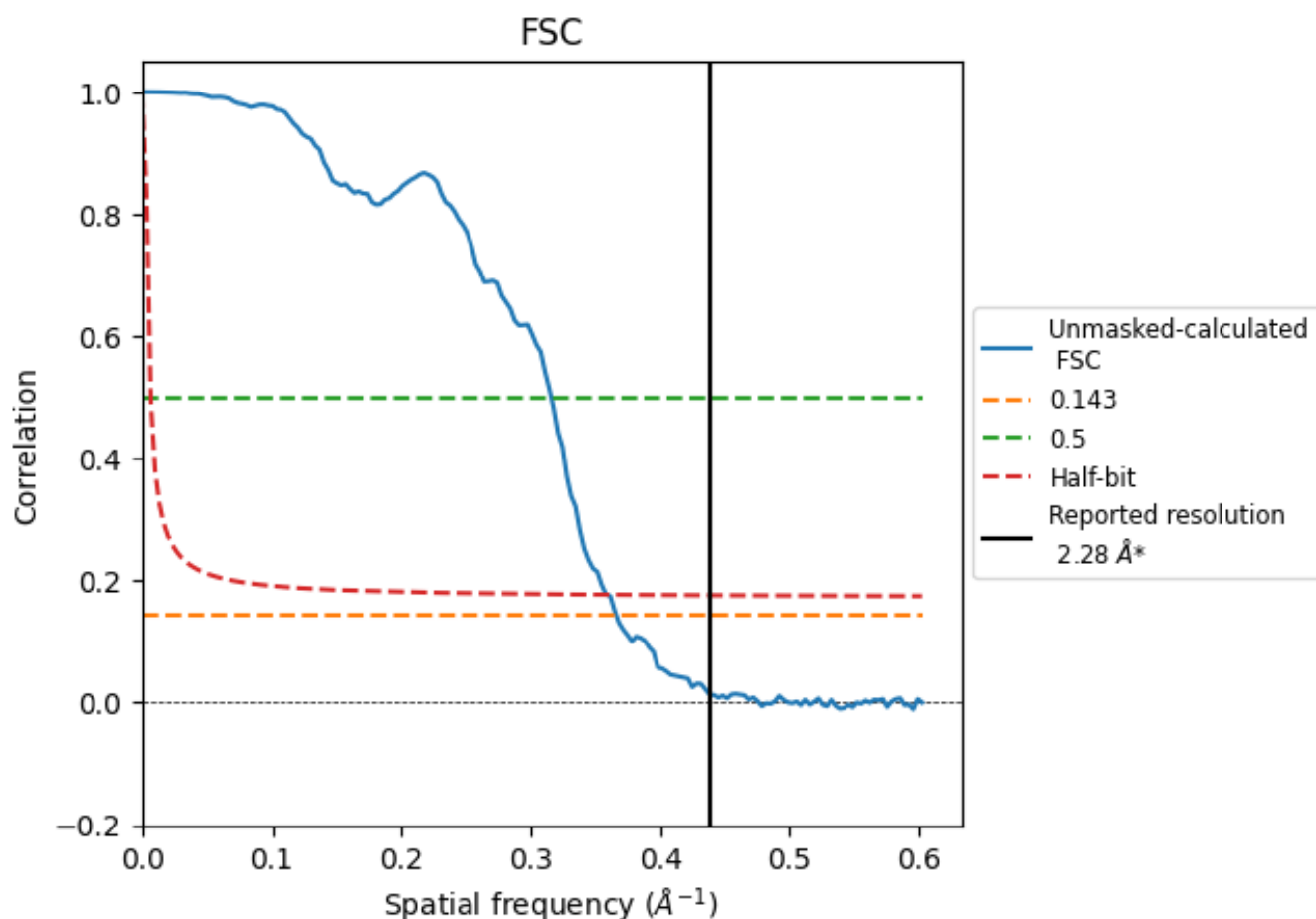


*Reported resolution corresponds to spatial frequency of 0.439 Å⁻¹

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 0.439 Å⁻¹

8.2 Resolution estimates [i](#)

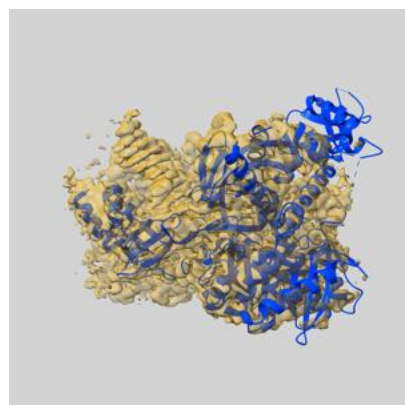
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.28	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	2.73	3.16	2.79

*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 2.73 differs from the reported value 2.28 by more than 10 %

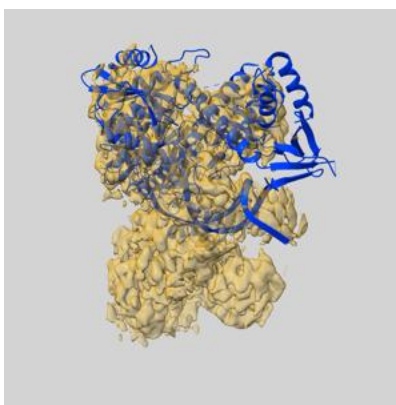
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-72222 and PDB model 9Q57. Per-residue inclusion information can be found in [section 3](#) on [page 14](#).

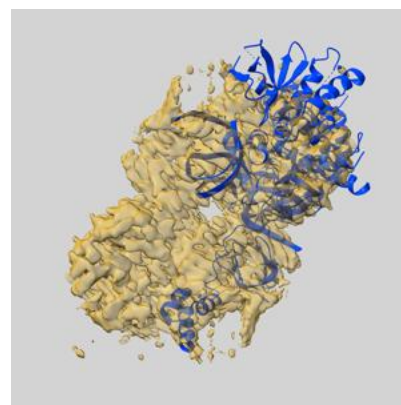
9.1 Map-model overlay [i](#)



X



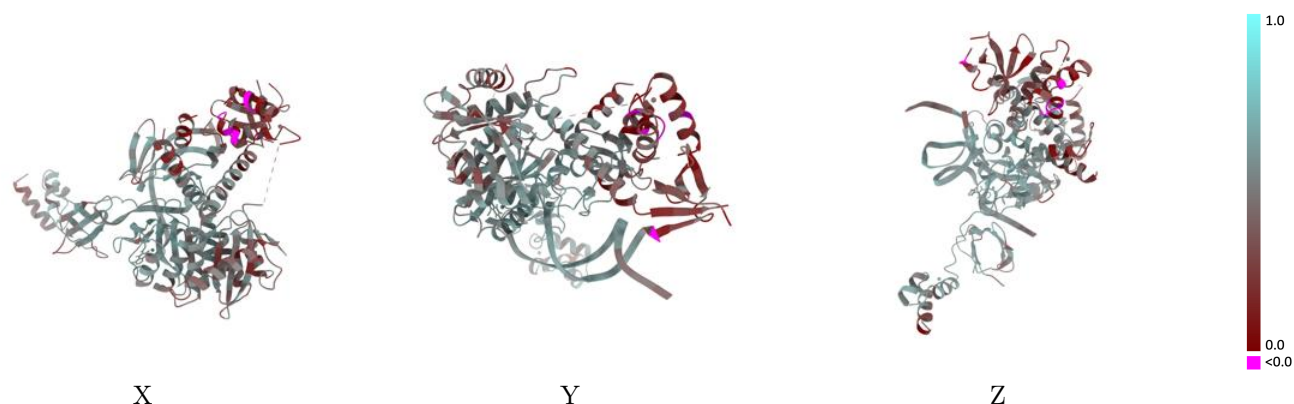
Y



Z

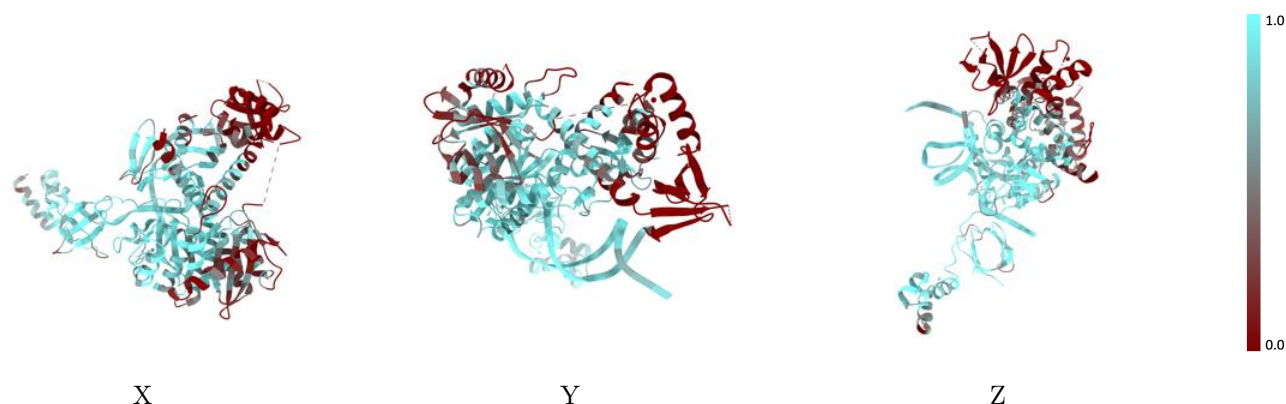
The images above show the 3D surface view of the map at the recommended contour level 0.0055 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



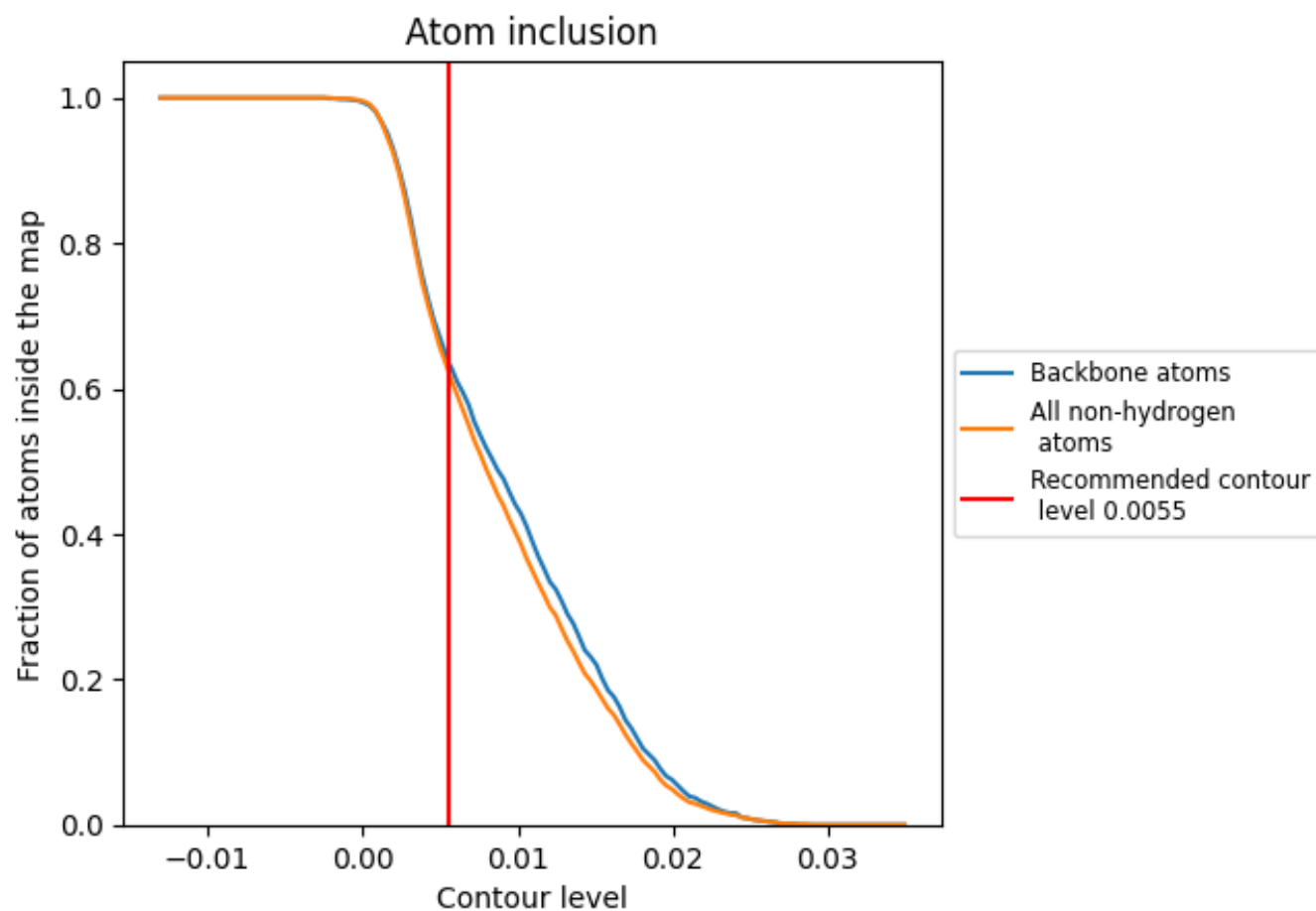
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0055).

9.4 Atom inclusion [i](#)



At the recommended contour level, 64% of all backbone atoms, 63% 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 (0.0055) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6260	0.4510
A	0.8200	0.5260
B	0.3010	0.3400
C	0.7350	0.4740
D	0.8260	0.4990
E	0.8690	0.5260
F	0.8580	0.5350

1.0

0.0

<0.0