



## Full wwPDB EM Validation Report ⓘ

Apr 15, 2025 – 07:27 PM EDT

PDB ID : 9N81 / pdb\_00009n81  
EMDB ID : EMD-49108  
Title : A gap-filling complex with Pol mu engaged in the NHEJ Pathway  
Authors : Li, J.; Liu, L.; Gellert, M.; Yang, W.  
Deposited on : 2025-02-07  
Resolution : 2.80 Å(reported)  
Based on initial model : 9CQ3

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

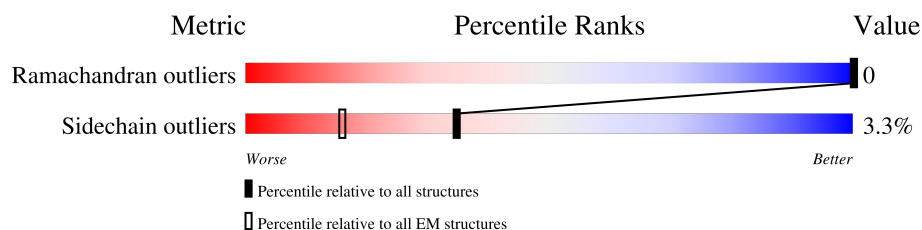
EMDB validation analysis : 0.0.1.dev117  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.42

# 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 2.80 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)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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  $\geq 3$ , 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	612	83% 16%
1	a	612	81% 17%
2	B	732	69% 30%
2	b	732	68% 30%
3	C	302	75% 21%
3	c	302	76% 22%
4	D	336	58% 40%
4	E	336	55% 5% 40%
4	d	336	58% 40%

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Mol	Chain	Length	Quality of chain
4	e	336	
5	F	914	
5	f	914	
6	G	218	
6	H	218	
7	I	68	
8	J	68	
9	K	51	
10	L	50	
11	M	512	
11	m	512	

## 2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 41888 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 X-ray repair cross-complementing protein 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	516	Total	C	N	O	S	0	0
			4169	2665	704	781	19		
1	a	507	Total	C	N	O	S	0	0
			4094	2617	693	766	18		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP P12956
A	-1	PRO	-	expression tag	UNP P12956
A	0	VAL	-	expression tag	UNP P12956
a	-2	GLY	-	expression tag	UNP P12956
a	-1	PRO	-	expression tag	UNP P12956
a	0	VAL	-	expression tag	UNP P12956

- Molecule 2 is a protein called X-ray repair cross-complementing protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	512	Total	C	N	O	S	1	0
			4115	2631	691	770	23		
2	b	511	Total	C	N	O	S	0	0
			4100	2623	686	768	23		

- Molecule 3 is a protein called Non-homologous end-joining factor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	238	Total	C	N	O	S	0	0
			1887	1207	317	348	15		
3	c	235	Total	C	N	O	S	0	0
			1869	1195	314	345	15		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	GLY	-	expression tag	UNP Q9H9Q4
C	-1	PRO	-	expression tag	UNP Q9H9Q4
C	0	VAL	-	expression tag	UNP Q9H9Q4
c	-2	GLY	-	expression tag	UNP Q9H9Q4
c	-1	PRO	-	expression tag	UNP Q9H9Q4
c	0	VAL	-	expression tag	UNP Q9H9Q4

- Molecule 4 is a protein called DNA repair protein XRCC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	202	Total	C	N	O	S	0	0
			1633	1034	279	313	7		
4	E	201	Total	C	N	O	S	0	0
			1628	1031	278	312	7		
4	d	200	Total	C	N	O	S	0	0
			1623	1028	277	311	7		
4	e	200	Total	C	N	O	S	0	0
			1623	1028	277	311	7		

- Molecule 5 is a protein called DNA ligase 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	679	Total	C	N	O	S	0	0
			5503	3504	945	1021	33		
5	f	255	Total	C	N	O	S	0	0
			2069	1315	349	392	13		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	-2	GLY	-	expression tag	UNP P49917
F	-1	PRO	-	expression tag	UNP P49917
F	0	VAL	-	expression tag	UNP P49917
f	-2	GLY	-	expression tag	UNP P49917
f	-1	PRO	-	expression tag	UNP P49917
f	0	VAL	-	expression tag	UNP P49917

- Molecule 6 is a protein called Protein PAXX.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	23	Total	C	N	O	S	0	0
			165	105	27	32	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
6	H	23	Total	C	N	O	S	0	0
			165	105	27	32	1		

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	-13	MET	-	expression tag	UNP Q9BUH6
G	-12	GLY	-	expression tag	UNP Q9BUH6
G	-11	SER	-	expression tag	UNP Q9BUH6
G	-10	SER	-	expression tag	UNP Q9BUH6
G	-9	HIS	-	expression tag	UNP Q9BUH6
G	-8	HIS	-	expression tag	UNP Q9BUH6
G	-7	HIS	-	expression tag	UNP Q9BUH6
G	-6	HIS	-	expression tag	UNP Q9BUH6
G	-5	HIS	-	expression tag	UNP Q9BUH6
G	-4	HIS	-	expression tag	UNP Q9BUH6
G	-3	SER	-	expression tag	UNP Q9BUH6
G	-2	GLN	-	expression tag	UNP Q9BUH6
G	-1	ASP	-	expression tag	UNP Q9BUH6
G	0	PRO	-	expression tag	UNP Q9BUH6
H	-13	MET	-	expression tag	UNP Q9BUH6
H	-12	GLY	-	expression tag	UNP Q9BUH6
H	-11	SER	-	expression tag	UNP Q9BUH6
H	-10	SER	-	expression tag	UNP Q9BUH6
H	-9	HIS	-	expression tag	UNP Q9BUH6
H	-8	HIS	-	expression tag	UNP Q9BUH6
H	-7	HIS	-	expression tag	UNP Q9BUH6
H	-6	HIS	-	expression tag	UNP Q9BUH6
H	-5	HIS	-	expression tag	UNP Q9BUH6
H	-4	HIS	-	expression tag	UNP Q9BUH6
H	-3	SER	-	expression tag	UNP Q9BUH6
H	-2	GLN	-	expression tag	UNP Q9BUH6
H	-1	ASP	-	expression tag	UNP Q9BUH6
H	0	PRO	-	expression tag	UNP Q9BUH6

- Molecule 7 is a DNA chain called DNA (38-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	38	Total	C	N	O	P	0	0
			771	370	131	232	38		

- Molecule 8 is a DNA chain called DNA (42-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
8	J	42	Total	C	N	O	P	0	0
			857	410	154	251	42		

- Molecule 9 is a DNA chain called DNA (34-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
9	K	34	Total	C	N	O	P	0	0
			702	335	136	198	33		

- Molecule 10 is a DNA chain called DNA (37-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
10	L	37	Total	C	N	O	P	0	0
			763	364	137	225	37		

- Molecule 11 is a protein called DNA-directed DNA/RNA polymerase mu.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	M	428	Total	C	N	O	S	0	0
			3389	2139	622	614	14		
11	m	96	Total	C	N	O	S	0	0
			732	457	135	134	6		

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	-17	HIS	-	expression tag	UNP Q9NP87
M	-16	HIS	-	expression tag	UNP Q9NP87
M	-15	HIS	-	expression tag	UNP Q9NP87
M	-14	HIS	-	expression tag	UNP Q9NP87
M	-13	HIS	-	expression tag	UNP Q9NP87
M	-12	HIS	-	expression tag	UNP Q9NP87
M	-11	SER	-	expression tag	UNP Q9NP87
M	-10	SER	-	expression tag	UNP Q9NP87
M	-9	GLY	-	expression tag	UNP Q9NP87
M	-8	LEU	-	expression tag	UNP Q9NP87
M	-7	GLU	-	expression tag	UNP Q9NP87
M	-6	VAL	-	expression tag	UNP Q9NP87
M	-5	LEU	-	expression tag	UNP Q9NP87
M	-4	PHE	-	expression tag	UNP Q9NP87
M	-3	GLN	-	expression tag	UNP Q9NP87
M	-2	GLY	-	expression tag	UNP Q9NP87
M	-1	PRO	-	expression tag	UNP Q9NP87

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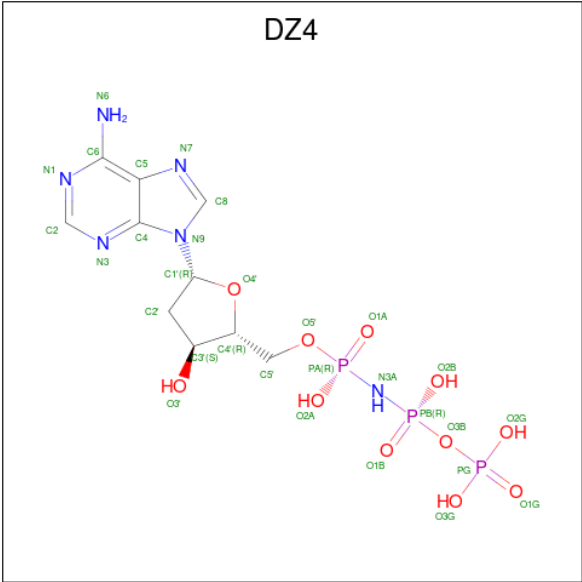
Chain	Residue	Modelled	Actual	Comment	Reference
M	0	HIS	-	expression tag	UNP Q9NP87
m	-17	HIS	-	expression tag	UNP Q9NP87
m	-16	HIS	-	expression tag	UNP Q9NP87
m	-15	HIS	-	expression tag	UNP Q9NP87
m	-14	HIS	-	expression tag	UNP Q9NP87
m	-13	HIS	-	expression tag	UNP Q9NP87
m	-12	HIS	-	expression tag	UNP Q9NP87
m	-11	SER	-	expression tag	UNP Q9NP87
m	-10	SER	-	expression tag	UNP Q9NP87
m	-9	GLY	-	expression tag	UNP Q9NP87
m	-8	LEU	-	expression tag	UNP Q9NP87
m	-7	GLU	-	expression tag	UNP Q9NP87
m	-6	VAL	-	expression tag	UNP Q9NP87
m	-5	LEU	-	expression tag	UNP Q9NP87
m	-4	PHE	-	expression tag	UNP Q9NP87
m	-3	GLN	-	expression tag	UNP Q9NP87
m	-2	GLY	-	expression tag	UNP Q9NP87
m	-1	PRO	-	expression tag	UNP Q9NP87
m	0	HIS	-	expression tag	UNP Q9NP87

- Molecule 12 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
12	M	1	Total Mg 1 1	0

- Molecule 13 is 2'-deoxy-5'-O-[(R)-hydroxy{[(R)-hydroxy(phosphonooxy)phosphoryl]amino}phosphoryl]adenosine (CCD ID: DZ4) (formula: C<sub>10</sub>H<sub>17</sub>N<sub>6</sub>O<sub>11</sub>P<sub>3</sub>).





Mol	Chain	Residues	Atoms					AltConf
13	M	1	Total	C	N	O	P	0
			30	10	6	11	3	

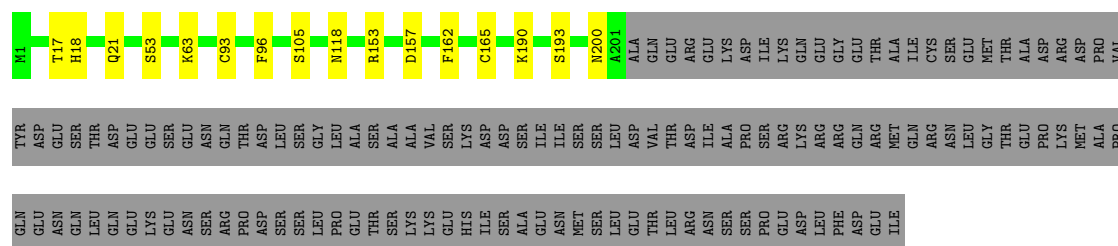


- Molecule 3: Non-homologous end-joining factor 1

- Molecule 3: Non-homologous end-joining factor 1

- Molecule 4: DNA repair protein XRCC4

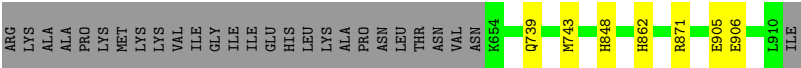
- Molecule 4: DNA repair protein XRCC4



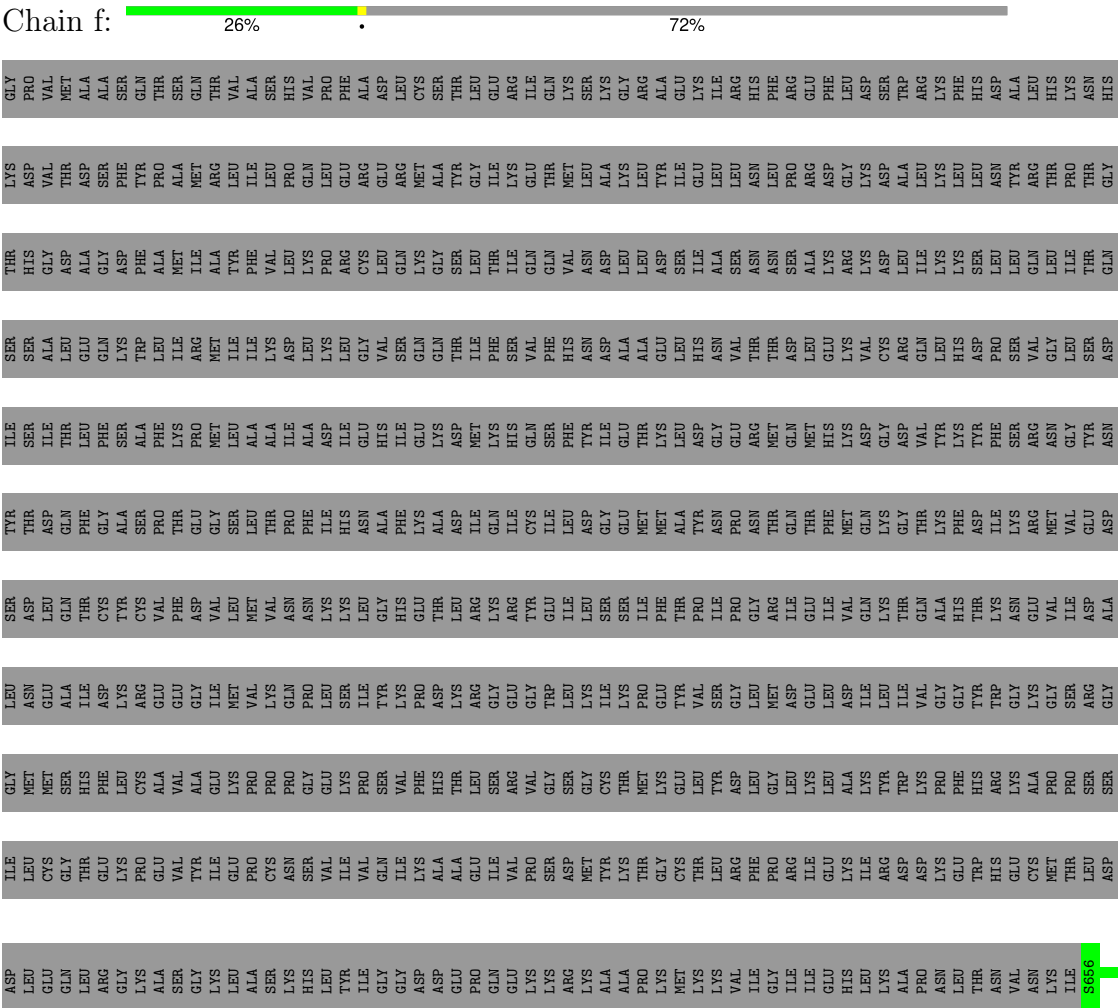
THR	SER
LYS	ALA
LYS	VAL
GLU	SER
HIS	LYS
ILE	ASP
SER	ASP
ALA	SER
GLU	ILE
ASN	ILE
MET	SER
SER	SER
LEU	LEU
GLU	VAL
THR	THR
ARG	ASP
ASN	ILE
SER	ALA
SER	PRO
PRO	SER
ASP	ARG
LYS	LYS
LEU	ARG
PHE	ARG
ASP	GLN
GLU	GLY
ILE	MET
	GLN
	ARG
	ASN
	LEU
	GLY
	THR
	GLU
	PRO
	LYS
	MET
	ALA
	PRO
	GLN
	GLU
	ASN
	GLN
	LEU
	GLN
	LYS
	GLU
	ASN
	SER
	ARG
	PRO
	THR
	ASP
	GLN
	THR
	LEU
	GLY
	SER
	SER
	LEU
	PRO
	GLU
	ALA

PRO	GLU	THR	LYS	LYS	GLU	HIS	ILE	SER	ALA	GLU	ASN	MET	SER	SER	LEU	GLU	THR	LEU	THR	ARG	ASN	LEU	ASP	PHE	GLU	ILE
LEU	ALA	SER	ALA	VAL	SER	LYS	ASP	SER	SER	ILE	LEU	ASP	THR	VAL	ASP	LEU	THR	GLN	GLU	THR	ASN	GLY	THR	ALA	ILE	
#1	R7	D38	E55	F106	R161	C165	R209	ALA	GLN	GLU	THR	GLU	LYS	ILE	LYS	GLU	GLY	THR	ALA	ILE	CYS	SER	GLU	MET	THR	ALA

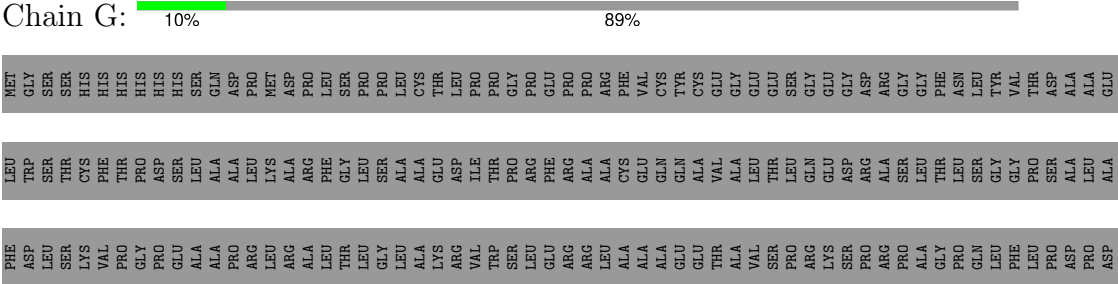
ASP	GLY	GLN	GLY	GLY	SER
MET	PRO		T362		
TYR	VAL			CYS	THR
LYS	MET		C365		
THR	ALA			MET	
GLY	ALA		E453	LYS	
CYS	SER	THR		GLU	
THR	GLN	VAL		LEU	
LEU	SER	TYR		LEU	
ARG	THR	GLY		ASP	
PHE	SER	LEU		LEU	
PRO	Q8	MET		GLY	
ARG	S12	ASP		LEU	
ILE	S21	GLU		LEU	
GLU	S21	LEU		ALA	
LYS	D51	ASP		LYS	
ILE		ILE		TYR	
ARG	T114	LEU		TRP	
ASP	PRO	ILE		TRP	
ASP	THR	VAL		LYS	
LYS	GLY	GLY		ALA	
GLU	THR	GLY		PHE	
TRP	THR	TYR		HIS	
HIS	HIS	ARG		ARG	
GLU	GLY	TRP		LYS	
CYS	ASP	LYS		ALA	
MET	ALA	GLY		PRO	
THR	ALA	GLY		PRO	
LEU	G123	SER	ARG	SER	
ASP	N209	GLY		SER	
ASP	D210	GLY		ILE	
LEU		MET		LEU	
GLU	D220	SER		CYS	
GLN		GLY		GLY	
LEU	M263	THR	HIS	THR	
ARG		GLU		GLU	
GLY	S267	LYS	PHE	LYS	
LYS		LEU		PRO	
ALA	M281	CYS	VAL	PRO	
SER		ALA	VAL	ASN	
GLY	C326	ALA	TYR	VAL	
LYS		GLU	ILE	VAL	
LEU	M343	LYS	GLU	ILE	
ALA	Q344	PRO	GLU	VAL	
SER	K345	PRO	ASN	GLN	
LYS		PRO	CYS	ILE	
HIS		SER	LYS	LYS	
LEU		VAL	VAL	ALA	
TYR		ILE	VAL	ALA	
ILE		VAL	GLN	GLU	
GLY		LYS	ILE	ILE	
ASP		PHE	LYS	VAL	
ASP		HIS	HIS	GLU	
GLU		THR	THR	PRO	
PRO		LEU	LEU	GLN	
GLN		ARG	ARG	ILE	
GLU		SER	VAL	VAL	
LYS		GLY	PRO	PRO	
VAL		VAL	GLY	SER	



● Molecule 5: DNA ligase 4

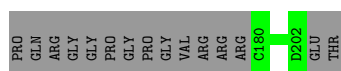
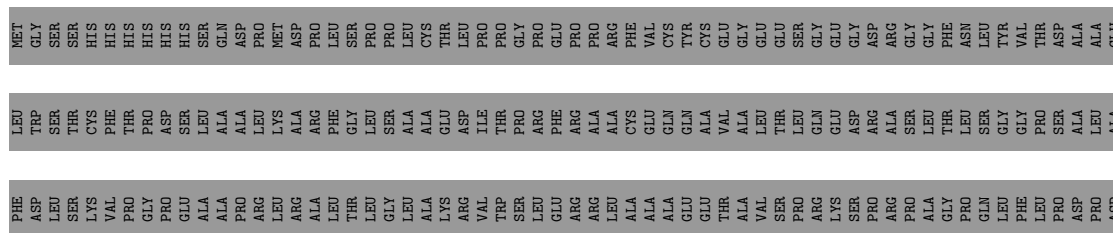


● Molecule 6: Protein PAXX



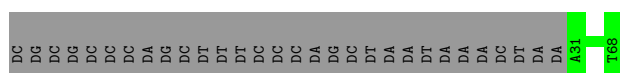
- Molecule 6: Protein PAXX

Chain H:  11% 89%



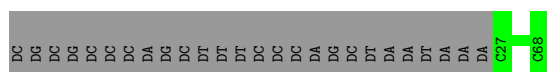
- Molecule 7: DNA (38-MER)

Chain I:  56% 44%



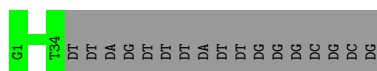
- Molecule 8: DNA (42-MER)

Chain J:  62% 38%



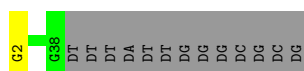
- Molecule 9: DNA (34-MER)

Chain K:  67% 33%



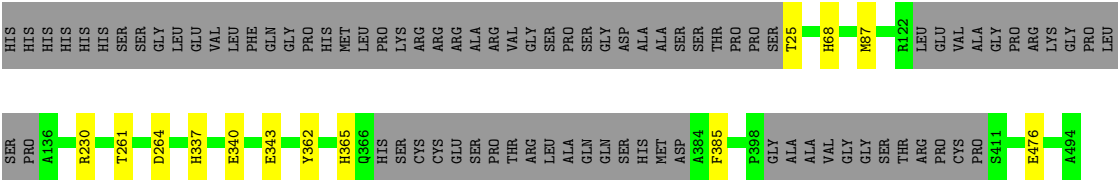
- Molecule 10: DNA (37-MER)

Chain L:  72% • 26%



- Molecule 11: DNA-directed DNA/RNA polymerase mu

Chain M:  81% • 16%



● Molecule 11: DNA-directed DNA/RNA polymerase mu



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	671447	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 ( $e^-/\text{\AA}^2$ )	47.42	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	1200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.586	Depositor
Minimum map value	-0.200	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.012	Depositor
Recommended contour level	0.06	Depositor
Map size (Å)	426.496, 426.496, 426.496	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.833, 0.833, 0.833	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, DZ4

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	0.25	0/4252	0.47	0/5728
1	a	0.25	0/4175	0.47	0/5626
2	B	0.25	0/4196	0.47	0/5661
2	b	0.25	0/4181	0.46	0/5642
3	C	0.24	0/1926	0.46	0/2610
3	c	0.24	0/1907	0.45	0/2584
4	D	0.25	0/1662	0.45	0/2235
4	E	0.26	0/1657	0.47	0/2228
4	d	0.26	0/1652	0.45	0/2221
4	e	0.25	0/1652	0.46	0/2221
5	F	0.24	0/5617	0.45	0/7568
5	f	0.25	0/2118	0.46	0/2862
6	G	0.25	0/169	0.36	0/226
6	H	0.26	0/169	0.37	0/226
7	I	0.50	0/861	0.94	0/1325
8	J	0.51	0/960	0.93	0/1478
9	K	0.55	0/790	0.92	0/1219
10	L	0.65	1/855 (0.1%)	0.97	0/1317
11	M	0.25	0/3468	0.50	0/4695
11	m	0.26	0/749	0.55	0/1017
All	All	0.28	1/43016 (0.0%)	0.53	0/58689

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	L	2	DG	OP3-P	-10.57	1.48	1.61

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

Due to software issues we are unable to calculate clashes - this section is therefore empty.

## 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	512/612 (84%)	500 (98%)	12 (2%)	0	100	100
1	a	505/612 (82%)	496 (98%)	9 (2%)	0	100	100
2	B	509/732 (70%)	500 (98%)	9 (2%)	0	100	100
2	b	507/732 (69%)	503 (99%)	4 (1%)	0	100	100
3	C	234/302 (78%)	224 (96%)	10 (4%)	0	100	100
3	c	231/302 (76%)	223 (96%)	8 (4%)	0	100	100
4	D	200/336 (60%)	193 (96%)	7 (4%)	0	100	100
4	E	199/336 (59%)	195 (98%)	4 (2%)	0	100	100
4	d	198/336 (59%)	196 (99%)	2 (1%)	0	100	100
4	e	198/336 (59%)	192 (97%)	6 (3%)	0	100	100
5	F	671/914 (73%)	657 (98%)	14 (2%)	0	100	100
5	f	253/914 (28%)	244 (96%)	9 (4%)	0	100	100
6	G	21/218 (10%)	21 (100%)	0	0	100	100
6	H	21/218 (10%)	21 (100%)	0	0	100	100
11	M	420/512 (82%)	404 (96%)	16 (4%)	0	100	100
11	m	94/512 (18%)	93 (99%)	1 (1%)	0	100	100
All	All	4773/7924 (60%)	4662 (98%)	111 (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	468/550 (85%)	459 (98%)	9 (2%)	52	82
1	a	460/550 (84%)	450 (98%)	10 (2%)	47	79
2	B	464/649 (72%)	457 (98%)	7 (2%)	60	86
2	b	463/649 (71%)	451 (97%)	12 (3%)	41	75
3	C	210/264 (80%)	198 (94%)	12 (6%)	17	46
3	c	208/264 (79%)	202 (97%)	6 (3%)	37	71
4	D	180/303 (59%)	172 (96%)	8 (4%)	24	56
4	E	180/303 (59%)	164 (91%)	16 (9%)	8	25
4	d	180/303 (59%)	175 (97%)	5 (3%)	38	72
4	e	180/303 (59%)	174 (97%)	6 (3%)	33	67
5	F	611/810 (75%)	592 (97%)	19 (3%)	35	69
5	f	231/810 (28%)	218 (94%)	13 (6%)	17	47
6	G	18/173 (10%)	17 (94%)	1 (6%)	17	47
6	H	18/173 (10%)	18 (100%)	0	100	100
11	M	360/428 (84%)	347 (96%)	13 (4%)	30	64
11	m	77/428 (18%)	73 (95%)	4 (5%)	19	50
All	All	4308/6960 (62%)	4167 (97%)	141 (3%)	35	67

All (141) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	53	SER
1	A	92	LYS
1	A	206	LYS
1	A	252	ARG
1	A	258	ARG
1	A	360	HIS
1	A	409	TYR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	450	GLU
2	B	89	ASP
2	B	249	CYS
2	B	306	LEU
2	B	309	ASP
2	B	323	PHE
2	B	400	ARG
2	B	432	GLN
3	C	26	LYS
3	C	47	GLU
3	C	49	VAL
3	C	89	HIS
3	C	107	ARG
3	C	110	SER
3	C	129	SER
3	C	132	SER
3	C	167	TYR
3	C	176	ARG
3	C	182	GLU
3	C	188	SER
4	D	66	TYR
4	D	84	TYR
4	D	87	ASN
4	D	140	LYS
4	D	142	GLU
4	D	165	CYS
4	D	166	VAL
4	D	184	LEU
4	E	17	THR
4	E	18	HIS
4	E	21	GLN
4	E	53	SER
4	E	63	LYS
4	E	93	CYS
4	E	96	PHE
4	E	105	SER
4	E	118	ASN
4	E	153	ARG
4	E	157	ASP
4	E	162	PHE
4	E	165	CYS
4	E	190	LYS

*Continued on next page...*

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Mol	Chain	Res	Type
4	E	193	SER
4	E	200	ASN
5	F	12	SER
5	F	21	SER
5	F	51	ASP
5	F	209	ASN
5	F	210	ASP
5	F	220	ASP
5	F	263	MET
5	F	267	SER
5	F	281	MET
5	F	326	CYS
5	F	343	MET
5	F	365	CYS
5	F	739	GLN
5	F	743	MET
5	F	848	HIS
5	F	862	HIS
5	F	871	ARG
5	F	905	GLU
5	F	906	GLU
6	G	200	ASP
11	M	25	THR
11	M	68	HIS
11	M	87	MET
11	M	230	ARG
11	M	261	THR
11	M	264	ASP
11	M	337	HIS
11	M	340	GLU
11	M	343	GLU
11	M	362	TYR
11	M	365	HIS
11	M	385	PHE
11	M	476	GLU
1	a	192	ASP
1	a	200	LEU
1	a	257	SER
1	a	312	LEU
1	a	319	SER
1	a	351	LYS
1	a	357	LYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	a	409	TYR
1	a	427	VAL
1	a	516	LYS
2	b	20	MET
2	b	66	ASN
2	b	83	LEU
2	b	87	ASP
2	b	97	LYS
2	b	246	HIS
2	b	286	LYS
2	b	296	CYS
2	b	323	PHE
2	b	339	CYS
2	b	465	LYS
2	b	525	LYS
3	c	1	MET
3	c	37	LEU
3	c	42	GLN
3	c	74	CYS
3	c	188	SER
3	c	202	CYS
4	d	23	SER
4	d	63	LYS
4	d	164	LYS
4	d	167	SER
4	d	175	ASP
4	e	7	ARG
4	e	38	ASP
4	e	55	GLU
4	e	106	PHE
4	e	161	ARG
4	e	165	CYS
5	f	662	VAL
5	f	667	MET
5	f	673	GLN
5	f	681	ARG
5	f	747	CYS
5	f	757	GLU
5	f	759	ASP
5	f	764	SER
5	f	765	TYR
5	f	770	ASP

*Continued on next page...*

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Mol	Chain	Res	Type
5	f	847	PHE
5	f	848	HIS
5	f	901	CYS
11	m	62	CYS
11	m	71	MET
11	m	94	CYS
11	m	95	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	264	ASN
2	B	517	ASN
4	E	21	GLN
5	F	200	GLN
5	F	227	GLN
11	M	329	HIS
1	a	65	GLN
2	b	104	GLN
3	c	17	GLN
3	c	133	GLN

### 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 2 ligands modelled in this entry, 1 is 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	$\# Z  > 2$
13	DZ4	M	502	12	28,32,32	1.18	2 (7%)	33,50,50	1.21	2 (6%)

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
13	DZ4	M	502	12	-	3/15/34/34	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	M	502	DZ4	C8-N7	-2.49	1.30	1.34
13	M	502	DZ4	C4-N3	-2.15	1.32	1.35

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	M	502	DZ4	N3-C2-N1	-4.56	122.48	128.67
13	M	502	DZ4	C2'-C1'-N9	-2.12	109.70	114.61

There are no chirality outliers.

All (3) torsion outliers are listed below:

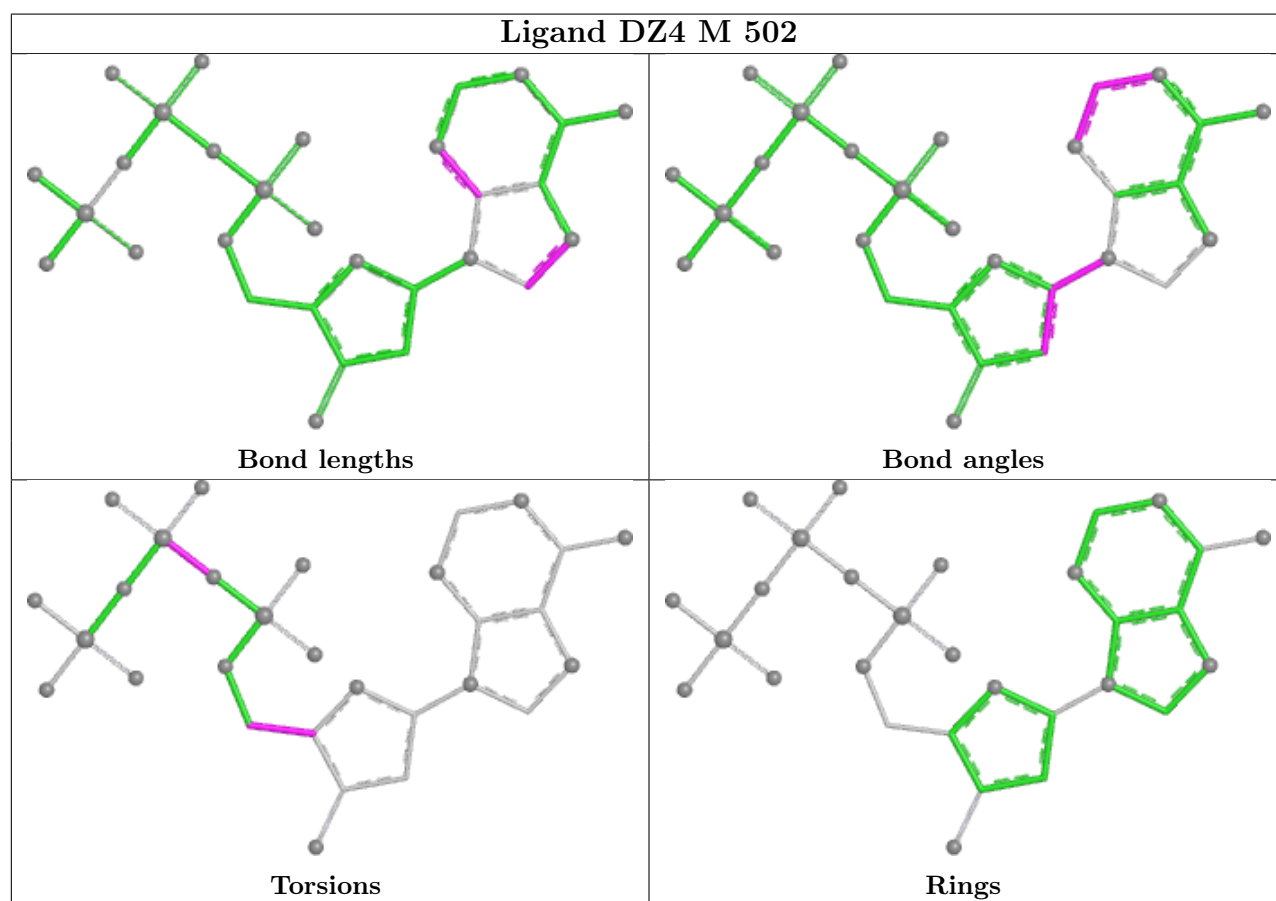
Mol	Chain	Res	Type	Atoms
13	M	502	DZ4	O4'-C4'-C5'-O5'
13	M	502	DZ4	C3'-C4'-C5'-O5'
13	M	502	DZ4	PA-N3A-PB-O1B

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.

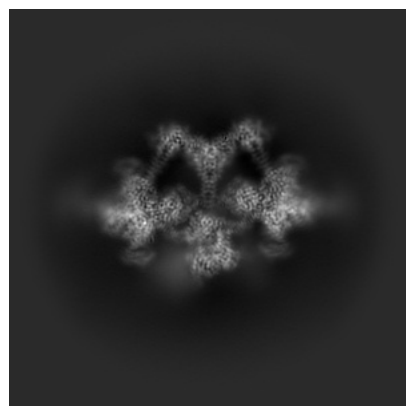
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-49108. These allow visual inspection of the internal detail of the map and identification of artifacts.

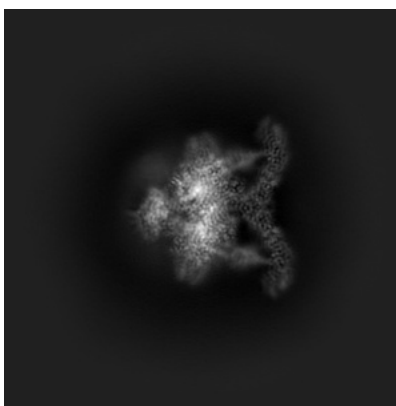
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

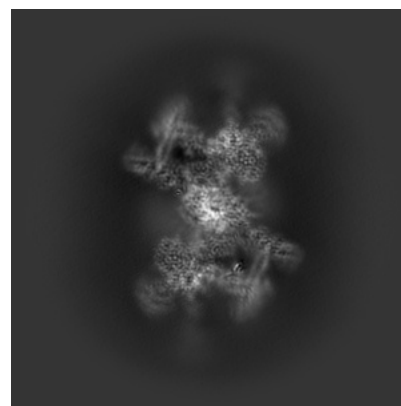
#### 6.1.1 Primary map



X

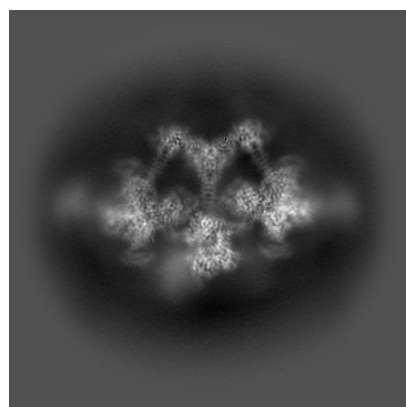


Y

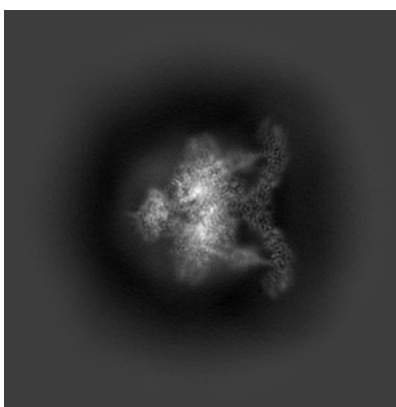


Z

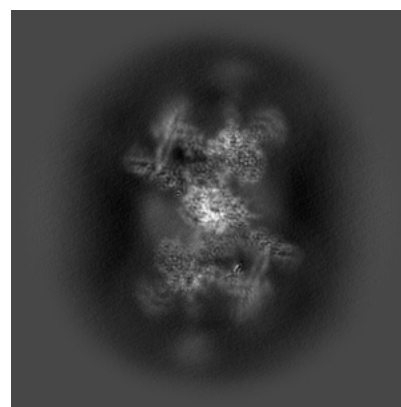
#### 6.1.2 Raw map



X



Y

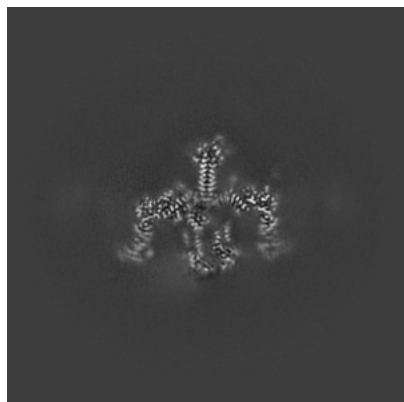


Z

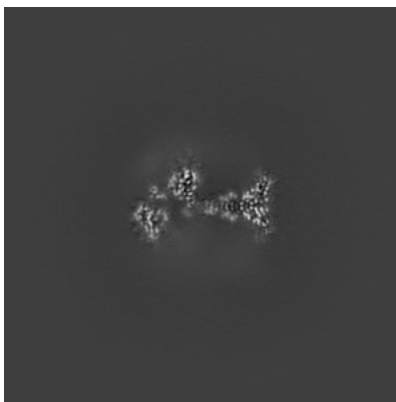
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

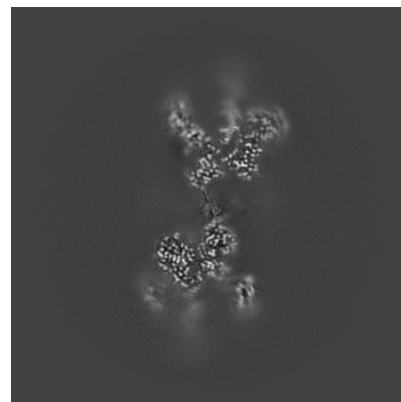
### 6.2.1 Primary map



X Index: 256

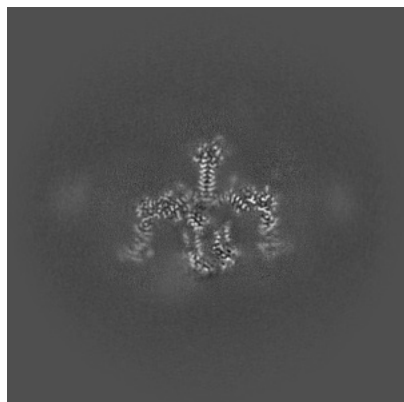


Y Index: 256

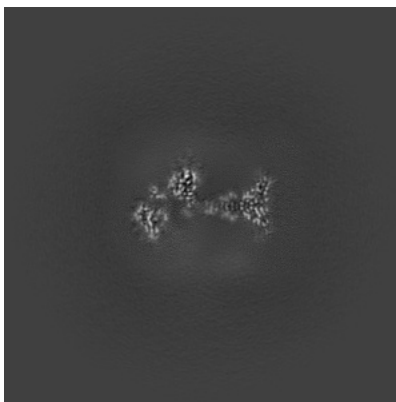


Z Index: 256

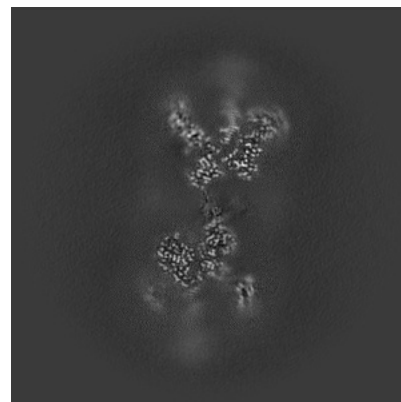
### 6.2.2 Raw map



X Index: 256



Y Index: 256

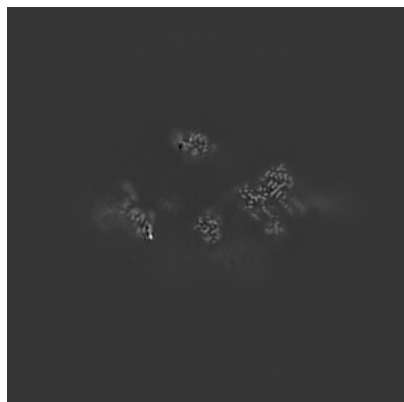


Z Index: 256

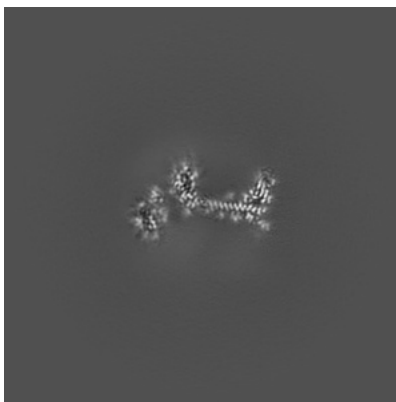
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

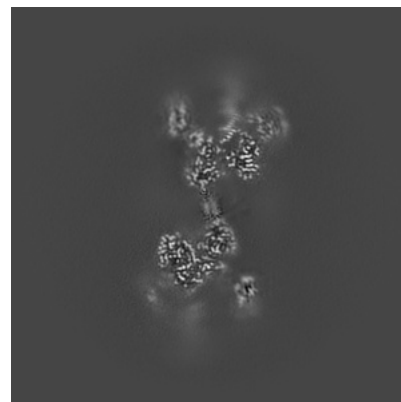
### 6.3.1 Primary map



X Index: 289

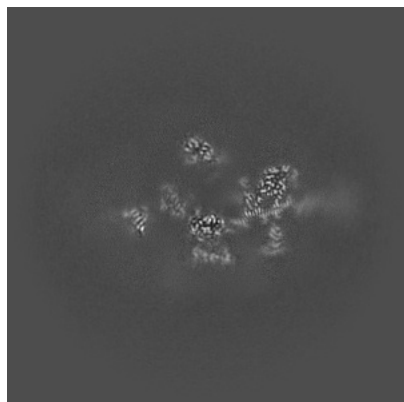


Y Index: 251

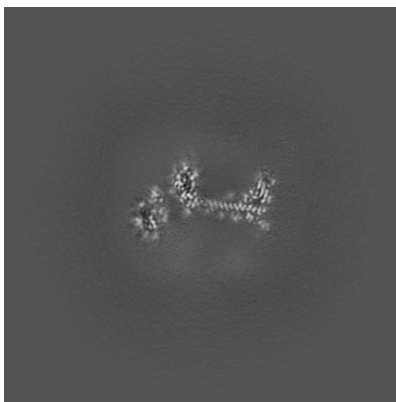


Z Index: 259

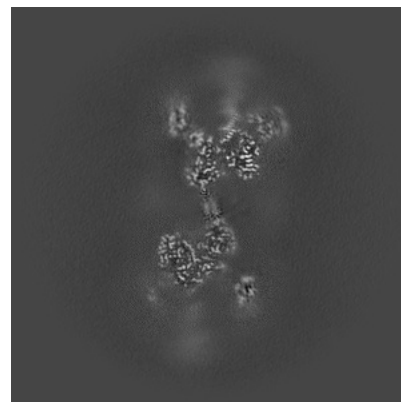
### 6.3.2 Raw map



X Index: 278



Y Index: 251

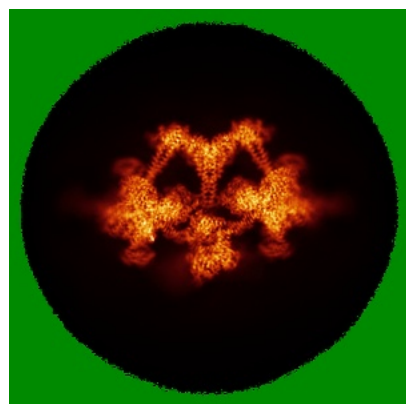


Z Index: 259

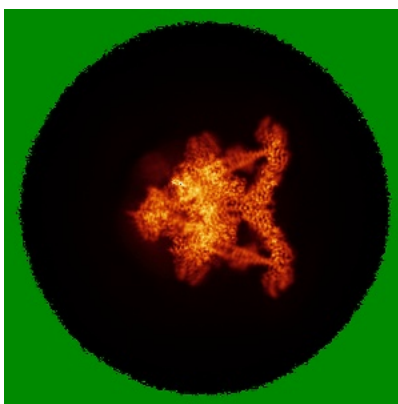
The images above show the largest variance slices of the map in three orthogonal directions.

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

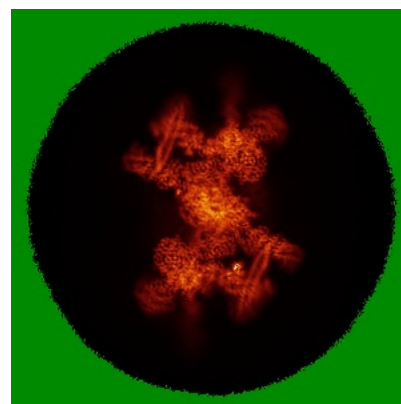
### 6.4.1 Primary map



X

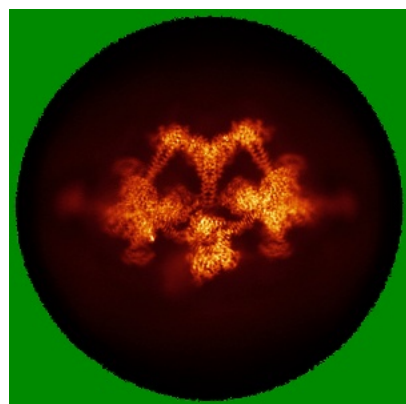


Y

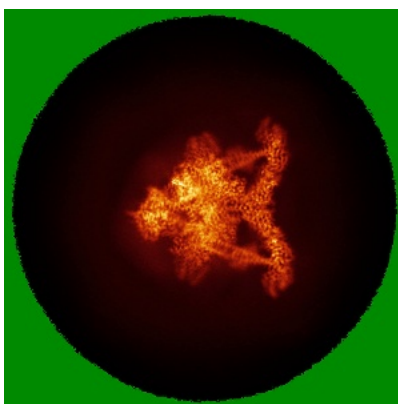


Z

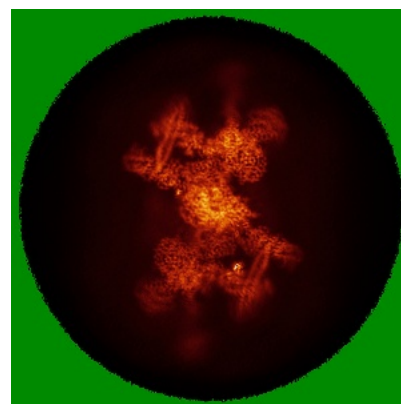
### 6.4.2 Raw map



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



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.06. 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



X



Y



Z

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

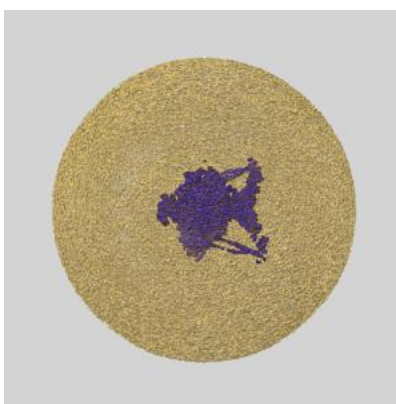
A mask typically either:

- 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\_49108\_msk\_1.map [i](#)



X



Y

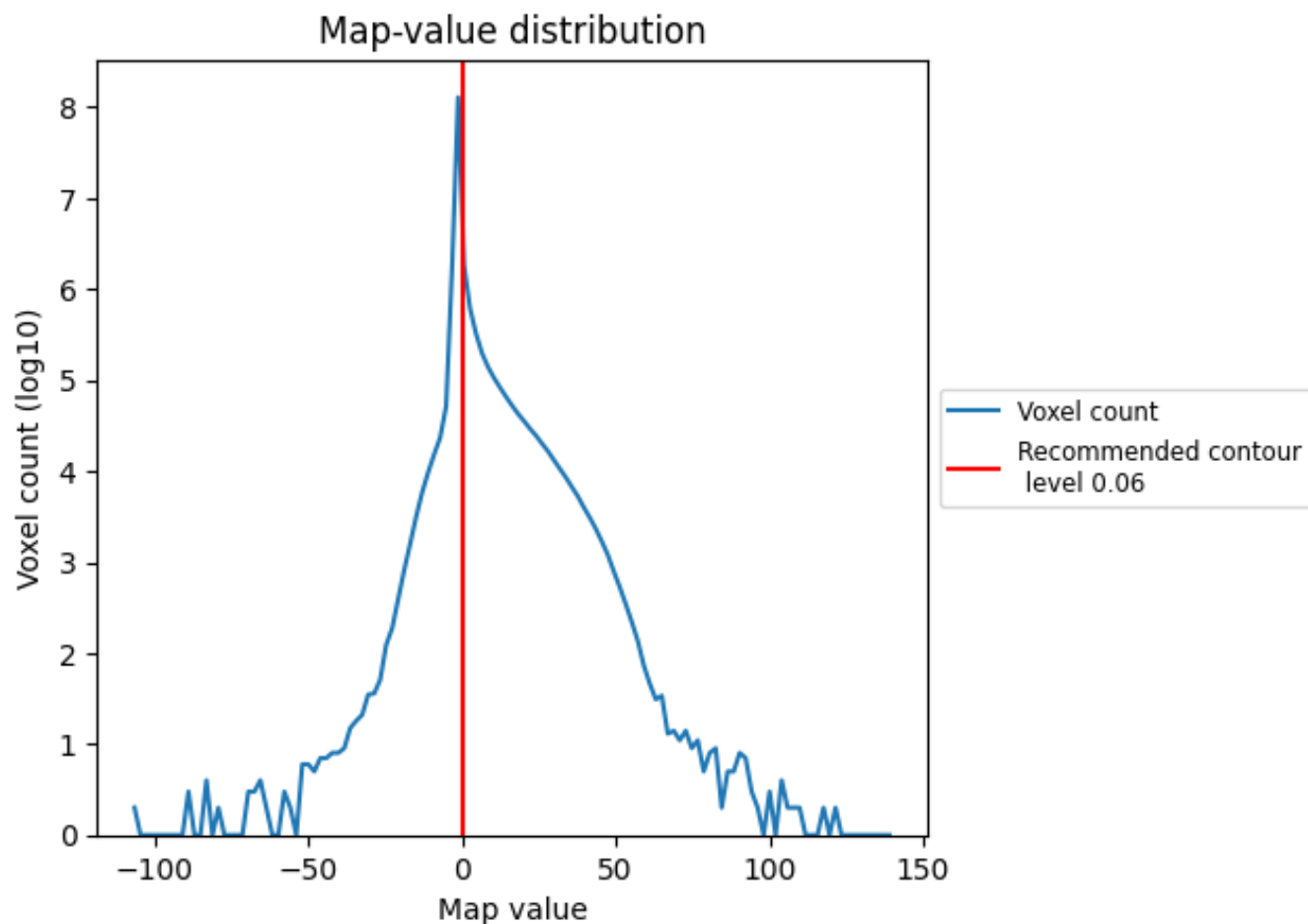


Z

## 7 Map analysis [i](#)

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

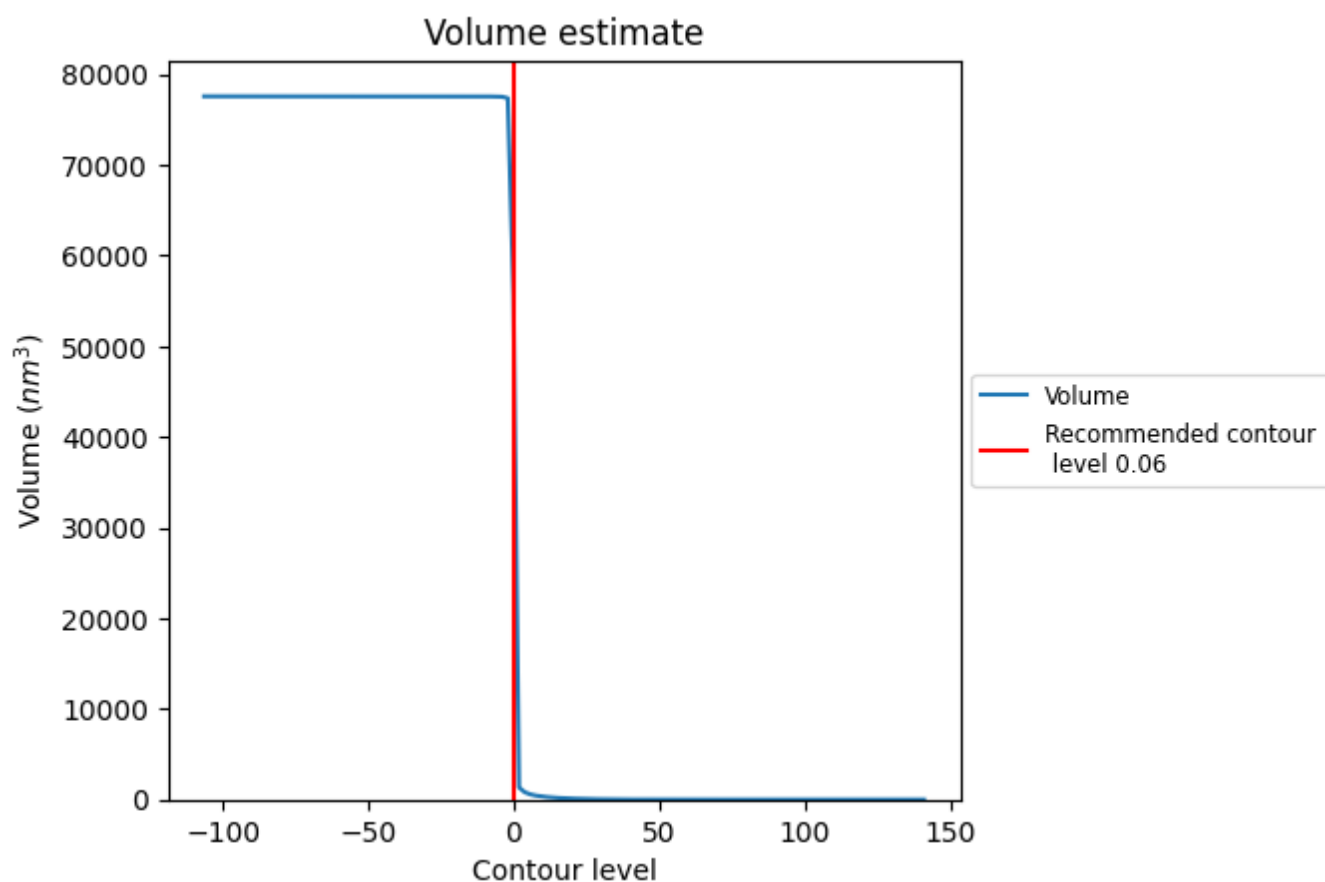
### 7.1 Map-value distribution [i](#)



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.



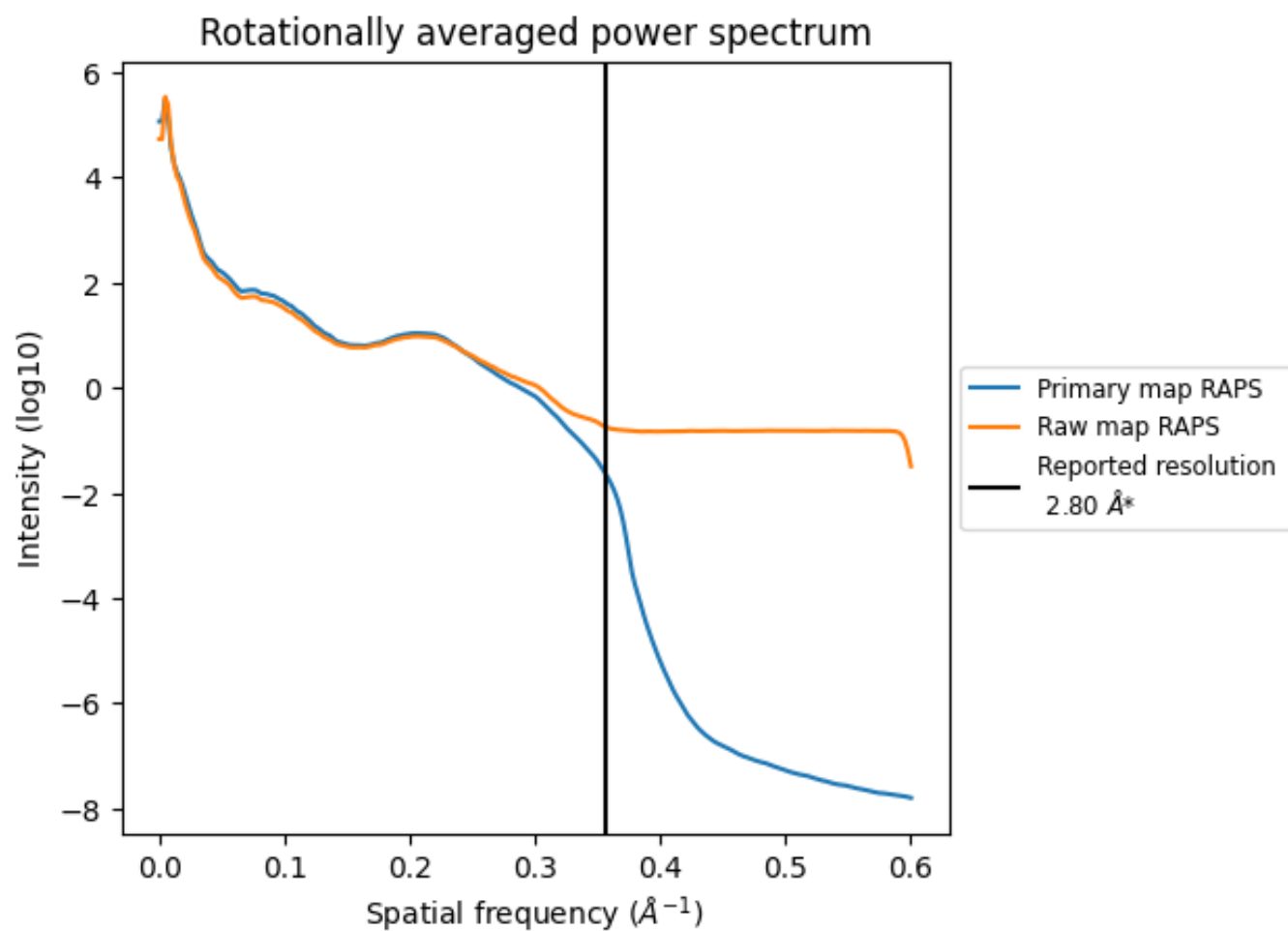
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 50910 nm<sup>3</sup>; this corresponds to an approximate mass of 45988 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 ⓘ

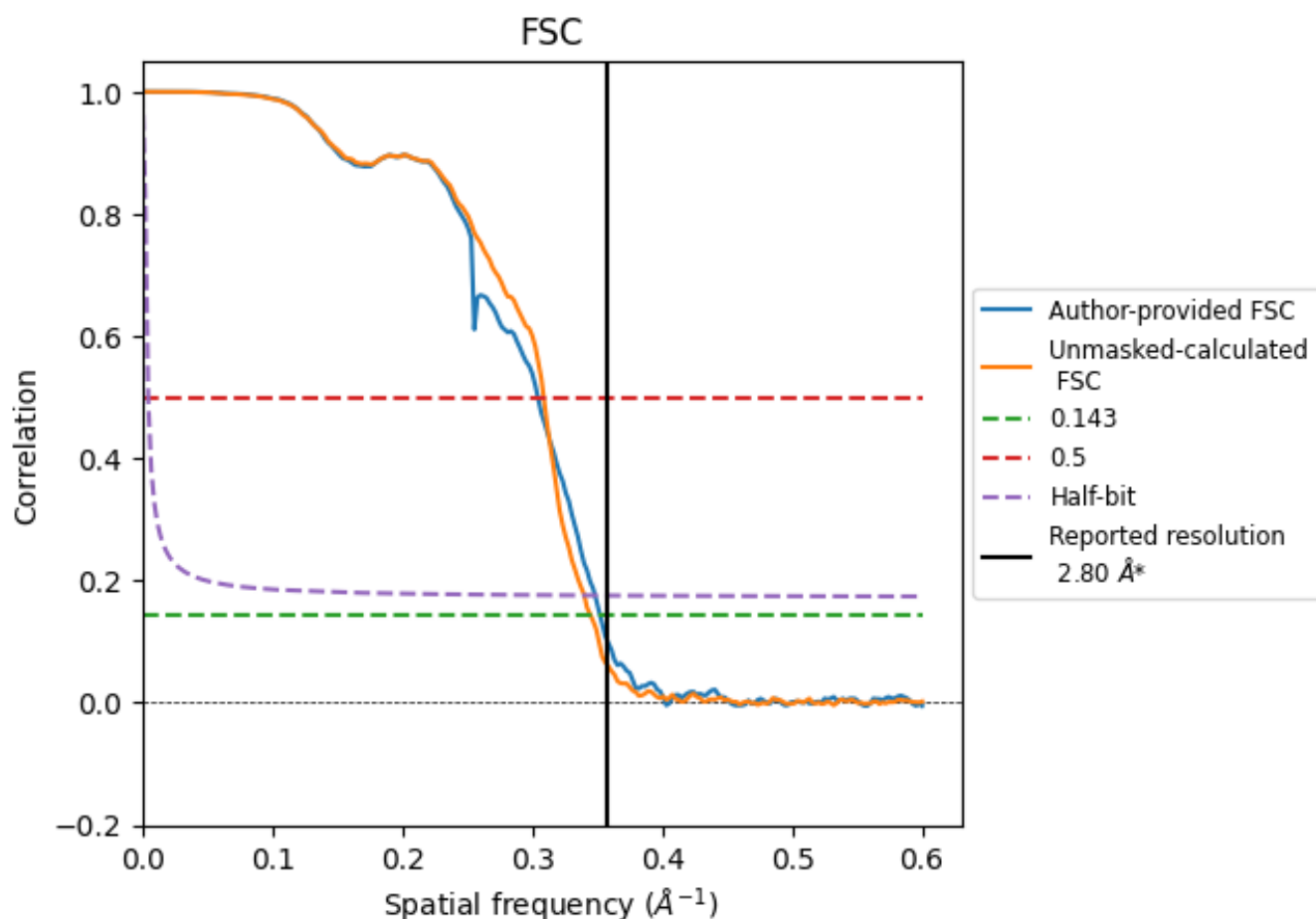


\*Reported resolution corresponds to spatial frequency of 0.357 Å<sup>-1</sup>

## 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 0.357  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

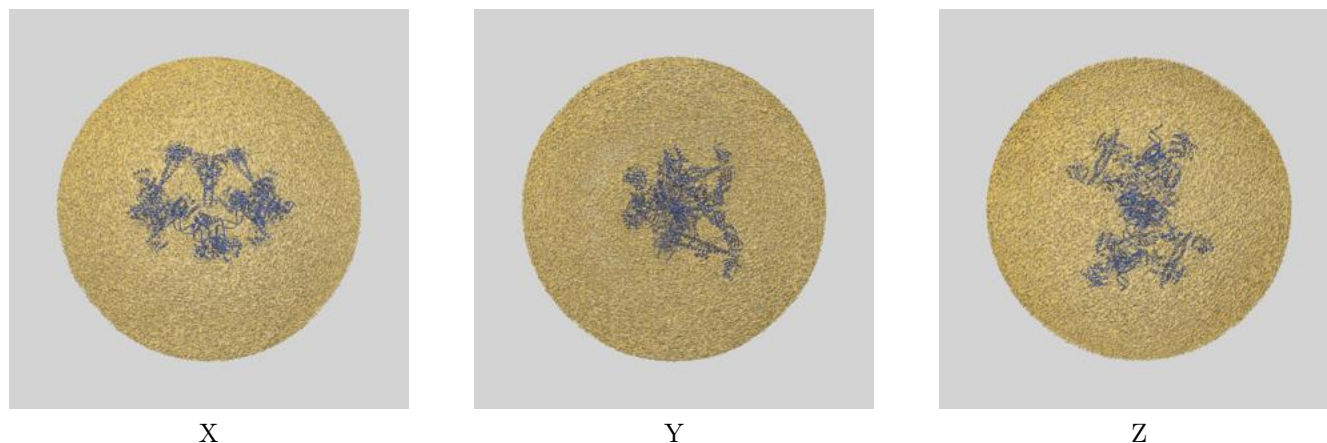
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.80	-	-
Author-provided FSC curve	2.84	3.28	2.87
Unmasked-calculated*	2.90	3.24	2.94

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

## 9 Map-model fit [i](#)

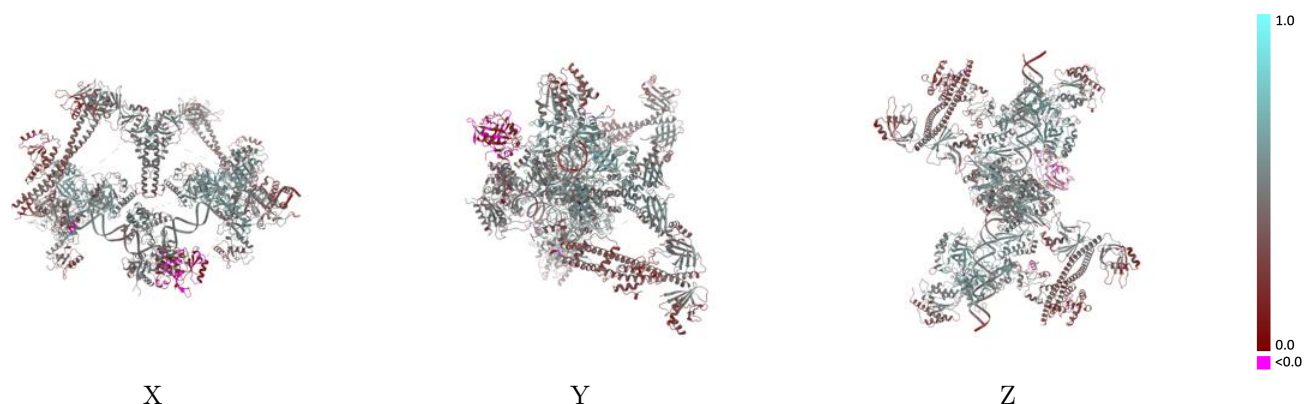
This section contains information regarding the fit between EMDB map EMD-49108 and PDB model 9N81. Per-residue inclusion information can be found in [section 3](#) on [page 10](#).

### 9.1 Map-model overlay [i](#)



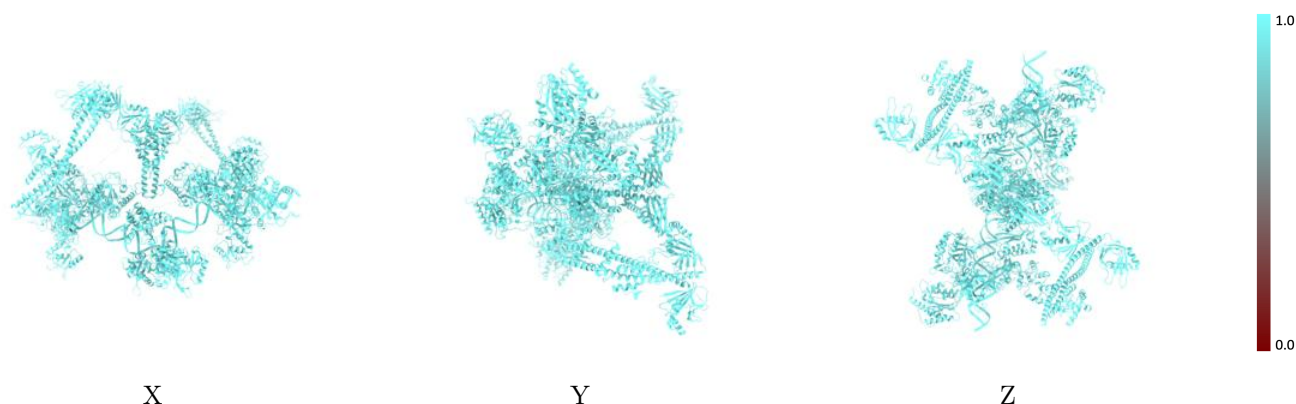
The images above show the 3D surface view of the map at the recommended contour level 0.06 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



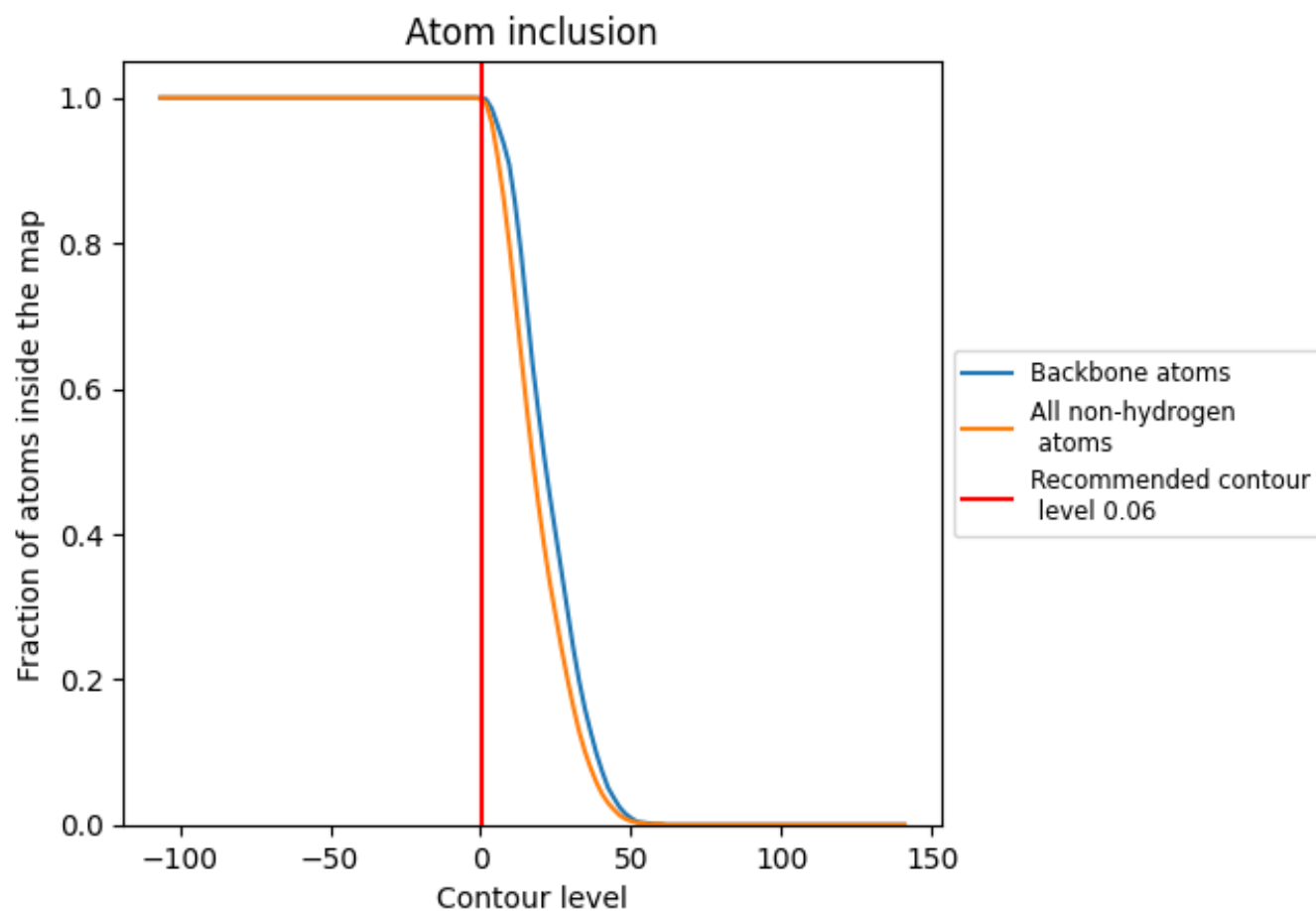
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.06).











































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 100% of all backbone atoms, 100% 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 (0.06) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9980	 0.4410
A	 0.9980	 0.5350
B	 1.0000	 0.4960
C	 0.9970	 0.4780
D	 0.9980	 0.3510
E	 0.9940	 0.4050
F	 0.9990	 0.3040
G	 1.0000	 0.5440
H	 0.9940	 0.5160
I	 1.0000	 0.4240
J	 1.0000	 0.4510
K	 1.0000	 0.4590
L	 1.0000	 0.4690
M	 0.9990	 0.4470
a	 0.9990	 0.5400
b	 1.0000	 0.5020
c	 0.9980	 0.4690
d	 0.9980	 0.3650
e	 0.9980	 0.4190
f	 0.9960	 0.2980
m	 0.9940	 0.3680

