



Full wwPDB EM Validation Report ⓘ

Apr 15, 2025 – 07:47 PM EDT

PDB ID : 9N83 / pdb_00009n83
EMDB ID : EMD-49110
Title : The ligation complex in the NHEJ pathway
Authors : Li, J.; Liu, L.; Gellert, M.; Yang, W.
Deposited on : 2025-02-07
Resolution : 3.10 Å (reported)
Based on initial model : 9CQ6

This is a Full wwPDB EM Validation 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:

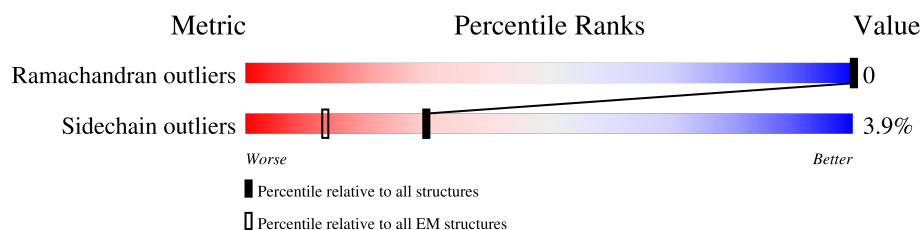
EMDB validation analysis : 0.0.1.dev117
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, 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 3.10 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 ≥ 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	82% 16%
1	a	612	81% 17%
2	B	732	68% 30%
2	b	732	68% 30%
3	C	302	75% 21%
3	c	302	77% 22%
4	D	336	55% 40%
4	E	336	56% 40%
4	d	336	56% 40%

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Mol	Chain	Length	Quality of chain
4	e	336	 57% 40%
5	F	914	 92% 5%
5	f	914	 27% 72%
6	G	218	 11% 89%
6	H	218	 10% 89%
7	I	68	 57% 43%
8	J	68	 56% 44%
9	K	51	 69% 31%
10	L	51	 67% 33%

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 39124 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	510	Total	C	N	O	S	0	0
			4092	2617	685	767	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	236	Total	C	N	O	S	0	0
			1876	1200	315	346	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	201	Total	C	N	O	S	0	0
			1628	1031	278	312	7		
4	E	201	Total	C	N	O	S	0	0
			1628	1031	278	312	7		
4	d	201	Total	C	N	O	S	0	0
			1628	1031	278	312	7		
4	e	201	Total	C	N	O	S	0	0
			1628	1031	278	312	7		

- Molecule 5 is a protein called DNA ligase 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	866	Total	C	N	O	S	0	0
			6959	4429	1192	1292	46		
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	24	Total	C	N	O	S	0	0
			174	110	28	35	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 (39-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	39	Total	C	N	O	P	0	0
			790	379	137	235	39		

- Molecule 8 is a DNA chain called DNA (38-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
8	J	38	Total	C	N	O	P	0	0
			776	371	139	228	38		

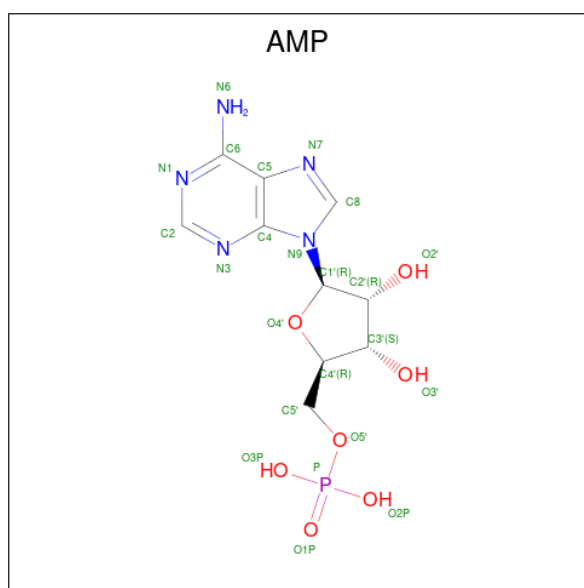
- Molecule 9 is a DNA chain called DNA (35-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
9	K	35	Total	C	N	O	P	0	0
			722	345	138	205	34		

- Molecule 10 is a DNA chain called DNA (34-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
10	L	34	Total	C	N	O	P	0	0
			700	334	128	204	34		

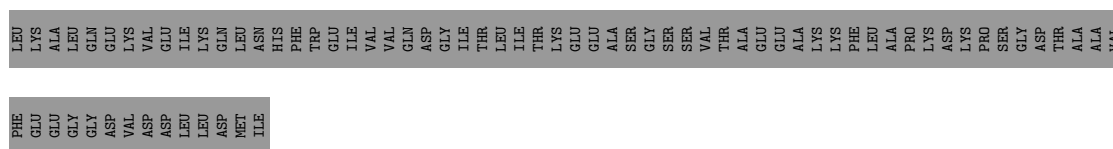
- Molecule 11 is ADENOSINE MONOPHOSPHATE (CCD ID: AMP) (formula: C₁₀H₁₄N₅O₇P) (labeled as "Ligand of Interest" by depositor).



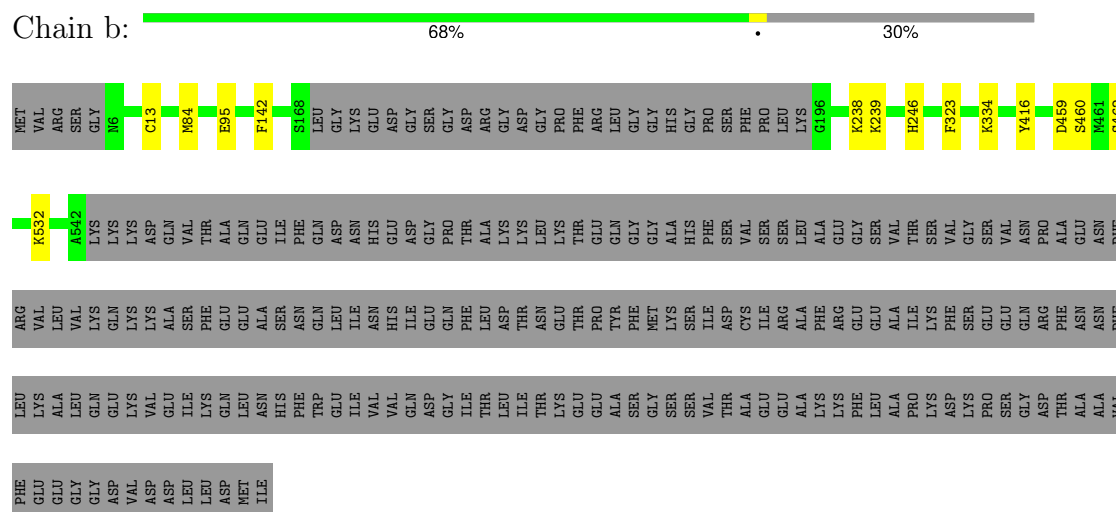
Mol	Chain	Residues	Atoms					AltConf
11	L	1	Total	C	N	O	P	0
			23	10	5	7	1	

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

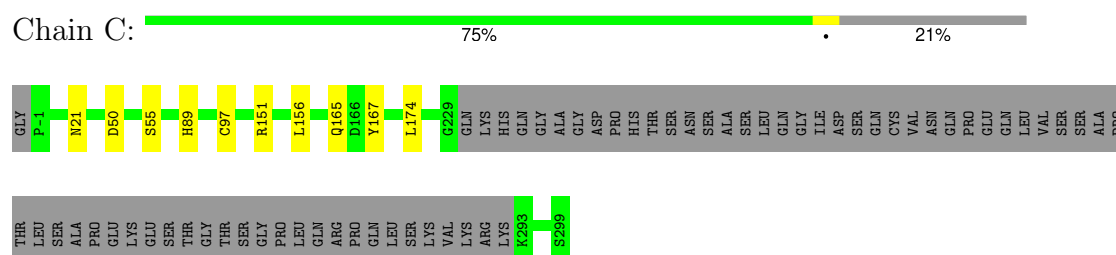
Mol	Chain	Residues	Atoms		AltConf
12	L	1	Total	Mg	0
			1	1	



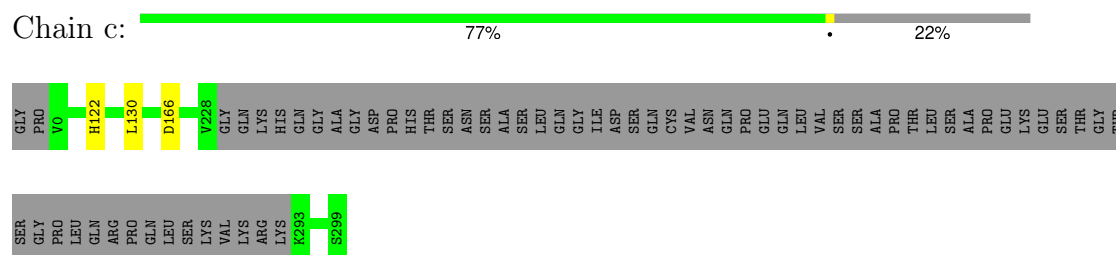
- Molecule 2: X-ray repair cross-complementing protein 5



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



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



- Molecule 4: DNA repair protein XRCC4



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

• Molecule 4: DNA repair protein XRCC4

Chain E:  56% 40%

H1	S15	V22	F88	F106	N112	E117	L126	D132	H143	R161	F162	E163	R192	K197	A201	ALA	GLN	GLU	ARG	GLU	LYS	ASP	PRO	SER	ILE	LYS	GLN	GLU	GLY	GLU	THR	ALA	ILE	CYS	SER	SER	GLU	THR	ALA	ALA	ASP	ARG	LYS	PRO	VAL	PRO	GLN	TYR	ASP	GLU	ASN
THR	ASP	GLU	SER	GLU	ASN	GLN	THR	ASP	LEU	GLY	LEU	ALA	ALA	VAL	SER	LYS	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	

LEU	GLN	GLY	LYS	ASN	SER	ARG	PRO	ASP	SER	SER	PRO	LEU	PRO	THR	SER	LYS	LYS	GLY	HIS	ILE	ILE	ALA	ASN	MET	SER	SER	GLU	THR	LEU	ARG	ASN	ASP	PHE	GLY	ILE	GLN	MET	ARG	ASN	GLY	THR	VAL	PRO	LYS	PRO	GLN	GLU	ASN
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• Molecule 4: DNA repair protein XRCC4

Chain d:  56% 40%

H1	F32	M59	S76	F86	S89	F96	H143	H148	D154	C165	Y177	K187	A201	ALA	GLN	GLU	ARG	GLU	LYS	ASP	ILE	LYS	GLN	GLU	GLY	GLU	THR	ALA	ILE	CYS	SER	GLU	MET	THR	ALA	ASP	ARG	ASP	PRO	VAL	GLN	ASP	GLU	SER	THR
GLU	GLU	ASN	THR	LEU	GLY	ALA	ALA	VAL	LYS	ASP	ILE	ILE	SER	LEU	ASP	VAL	THR	ASP	ILE	ALA	SER	ARG	LYS	ARG	ARG	GLN	ARG	MET	GLN	ARG	ASN	LEU	GLY	THR	GLU	PRO	LYS	MET	ALA	PRO	GLN	GLU	ASN	GLN	LEU

GLU	LYS	GLU	ASN	ARG	PRO	ASP	SER	PRO	GLY	THR	LYS	HIS	ILE	SER	GLU	ASN	MET	SER	LEU	GLU	THR	VAL	THR	LEU	ARG	ASN	SER	ASP	LEU	PHE	GLY	ILE	GLN	ARG	ASN	LEU	THR	VAL	GLN	GLY	THR	ASP	GLU	LYS
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• Molecule 4: DNA repair protein XRCC4

Chain e:  57% 40%

SER	ASN	GLN	THR	ASP	LEU	SER	GLY	LEU	ALA	SER	ALA	VAL	SER	LYS	ASP	ASP	ASP	ILE	ILE	SER	SER	LEU	ASP	VAL	THR	ASP	ILE	ALA	PRO	SER	ARG	LYS	ARG	GLN	GLU	THR	ALA	ILE	CYS	GLY	SER	GLU	MET	THR	THR	ALA	ASP	ARG	ALA	PRO	VAL	TYR	ASP	GLN	ASN	GLN	LEU	THR	ASP	GLU
H1	K4	D38	G39	H40	K65	E69	S76	F106	F111	E147	V166	K197	A201	ALA	GLN	GLU	ARG	GLU	LYS	ASP	ILE	LYS	GLN	GLU	GLY	THR	ALA	ILE	CYS	SER	GLU	MET	THR	ALA	ASP	ARG	ALA	PRO	VAL	TYR	ASP	GLN	ASN	GLN	LEU	THR	ASP	GLU												

GLU	ASN	SER	ARG	PRO	ASP	SER	PRO	GLY	THR	SER	LYS	LYS	HIS	ILE	SER	ALA	ASN	MET	SER	LEU	GLU	THR	VAL	THR	ARG	ASN	SER	PRO	GLU	ASP	PHE	ASP	GLU	ILE	GLN	ARG	ASN	LEU	THR	VAL	GLN	GLY	THR	ASP	GLU
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• Molecule 5: DNA ligase 4

Chain F:  92% 5%

GLY	PRO	VAL	MET	ALA	ALA	SER	GLN	THR	S7	S21	S29	L138	K162	K261	D322	E331	K345	K352	L360	H379	T394	K442	H482	S504	S537	R580	I617	GLY	GLY	ASP	ASP	GLU	PRO	GLN	GLU	LYS	LYS	ARG	LYS	ALA	
PRO	LYS	MET	LYS	VAL	ILE	GLY	ILE	HIS	GLU	LEU	LYS	ALA	ASN	THR	ASN	VAL	ASN	LYS	ILE	S656	S668	Y688	H718	F742	M743	I840	E891	L910	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE

[illegible]

DC	DG	DC	DG	DC	DC	DC	DA	DG	DC	DC	DC	DC	DC	DC	DC	DC	DA	DA	DC	DA	DA	DA	DC	DC	DC	DA	A30	C68
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DC
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DA
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DC
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DA
A31
C68

G1	T35	DT	DA	DG	DT	DT	DT	DA	DT	DT	DG	DG	DG	DC	DG	DC	DG
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A1	T34	DT	DT	DA	DG	DT	DT	DT	DA	DT	DT	DG	DG	DG	DC	DG	DC	DG
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	109389	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 ($e^-/\text{\AA}^2$)	47.39	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	0.583	Depositor
Minimum map value	-0.232	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.014	Depositor
Recommended contour level	0.07	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, AMP

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	0.28	0/4252	0.48	0/5728
1	a	0.29	0/4175	0.48	0/5626
2	B	0.27	0/4196	0.48	0/5661
2	b	0.27	0/4173	0.48	0/5631
3	C	0.27	0/1926	0.48	0/2610
3	c	0.28	0/1914	0.48	0/2594
4	D	0.28	0/1657	0.49	0/2228
4	E	0.28	0/1657	0.50	0/2228
4	d	0.28	0/1657	0.49	0/2228
4	e	0.29	0/1657	0.50	0/2228
5	F	0.27	0/7111	0.48	0/9587
5	f	0.25	0/2118	0.47	0/2862
6	G	0.27	0/178	0.37	0/238
6	H	0.27	0/169	0.36	0/226
7	I	0.54	0/883	0.93	0/1358
8	J	0.56	0/869	0.93	0/1338
9	K	0.56	0/812	0.91	0/1253
10	L	0.57	0/785	0.93	0/1210
All	All	0.31	0/40189	0.54	0/54834

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](#)

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%)	491 (96%)	21 (4%)	0	100	100
1	a	505/612 (82%)	493 (98%)	12 (2%)	0	100	100
2	B	509/732 (70%)	497 (98%)	12 (2%)	0	100	100
2	b	506/732 (69%)	498 (98%)	8 (2%)	0	100	100
3	C	234/302 (78%)	225 (96%)	9 (4%)	0	100	100
3	c	232/302 (77%)	225 (97%)	7 (3%)	0	100	100
4	D	199/336 (59%)	193 (97%)	6 (3%)	0	100	100
4	E	199/336 (59%)	193 (97%)	6 (3%)	0	100	100
4	d	199/336 (59%)	190 (96%)	9 (4%)	0	100	100
4	e	199/336 (59%)	192 (96%)	7 (4%)	0	100	100
5	F	862/914 (94%)	830 (96%)	32 (4%)	0	100	100
5	f	253/914 (28%)	242 (96%)	11 (4%)	0	100	100
6	G	22/218 (10%)	22 (100%)	0	0	100	100
6	H	21/218 (10%)	20 (95%)	1 (5%)	0	100	100
All	All	4452/6900 (64%)	4311 (97%)	141 (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	468/550 (85%)	455 (97%)	13 (3%)	38	66
1	a	460/550 (84%)	448 (97%)	12 (3%)	41	68
2	B	464/649 (72%)	449 (97%)	15 (3%)	34	63
2	b	462/649 (71%)	448 (97%)	14 (3%)	36	64
3	C	210/264 (80%)	200 (95%)	10 (5%)	21	51
3	c	209/264 (79%)	206 (99%)	3 (1%)	62	81
4	D	180/303 (59%)	165 (92%)	15 (8%)	9	33
4	E	180/303 (59%)	166 (92%)	14 (8%)	10	35
4	d	180/303 (59%)	168 (93%)	12 (7%)	13	40
4	e	180/303 (59%)	169 (94%)	11 (6%)	15	43
5	F	771/810 (95%)	747 (97%)	24 (3%)	35	63
5	f	231/810 (28%)	219 (95%)	12 (5%)	19	48
6	G	19/173 (11%)	18 (95%)	1 (5%)	19	48
6	H	18/173 (10%)	17 (94%)	1 (6%)	17	46
All	All	4032/6104 (66%)	3875 (96%)	157 (4%)	30	58

All (157) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	66	CYS
1	A	114	LYS
1	A	162	SER
1	A	229	LEU
1	A	254	ARG
1	A	303	PHE
1	A	316	THR
1	A	398	CYS
1	A	409	TYR
1	A	441	ASP
1	A	462	MET
1	A	471	PHE
1	A	496	ASP
2	B	84	MET
2	B	215	LEU
2	B	249	CYS
2	B	295	TYR
2	B	323	PHE
2	B	346	CYS

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Mol	Chain	Res	Type
2	B	432	GLN
2	B	437	SER
2	B	459	ASP
2	B	460	SER
2	B	465	LYS
2	B	471	ASP
2	B	473	LEU
2	B	526	SER
2	B	541	GLU
3	C	21	ASN
3	C	50	ASP
3	C	55	SER
3	C	89	HIS
3	C	97	CYS
3	C	151	ARG
3	C	156	LEU
3	C	165	GLN
3	C	167	TYR
3	C	174	LEU
4	D	27	THR
4	D	84	TYR
4	D	86	PHE
4	D	94	TYR
4	D	95	PHE
4	D	96	PHE
4	D	99	LYS
4	D	101	LEU
4	D	143	HIS
4	D	162	PHE
4	D	165	CYS
4	D	169	LYS
4	D	179	ARG
4	D	185	ASN
4	D	186	GLU
4	E	15	SER
4	E	22	VAL
4	E	88	PHE
4	E	106	PHE
4	E	112	ASN
4	E	117	GLU
4	E	126	LEU
4	E	132	ASP

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Mol	Chain	Res	Type
4	E	143	HIS
4	E	161	ARG
4	E	162	PHE
4	E	163	GLU
4	E	192	ARG
4	E	197	LYS
5	F	21	SER
5	F	29	SER
5	F	138	LEU
5	F	162	LYS
5	F	261	LYS
5	F	322	ASP
5	F	331	GLU
5	F	345	LYS
5	F	352	LYS
5	F	360	LEU
5	F	379	HIS
5	F	394	THR
5	F	442	LYS
5	F	482	HIS
5	F	504	SER
5	F	537	SER
5	F	580	ARG
5	F	668	SER
5	F	688	TYR
5	F	718	HIS
5	F	742	PHE
5	F	743	MET
5	F	840	ILE
5	F	891	GLU
6	G	184	SER
6	H	180	CYS
1	a	36	ASP
1	a	53	SER
1	a	61	ASP
1	a	109	ASP
1	a	162	SER
1	a	200	LEU
1	a	257	SER
1	a	319	SER
1	a	320	GLN
1	a	409	TYR

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Mol	Chain	Res	Type
1	a	435	VAL
1	a	453	MET
2	b	13	CYS
2	b	84	MET
2	b	95	GLU
2	b	142	PHE
2	b	238	LYS
2	b	239	LYS
2	b	246	HIS
2	b	323	PHE
2	b	334	LYS
2	b	416	TYR
2	b	459	ASP
2	b	460	SER
2	b	462	SER
2	b	532	LYS
3	c	122	HIS
3	c	130	LEU
3	c	166	ASP
4	d	32	PHE
4	d	59	MET
4	d	76	SER
4	d	86	PHE
4	d	89	SER
4	d	96	PHE
4	d	143	HIS
4	d	148	ASN
4	d	154	ASP
4	d	165	CYS
4	d	177	TYR
4	d	187	LYS
4	e	4	LYS
4	e	38	ASP
4	e	40	HIS
4	e	65	LYS
4	e	69	GLU
4	e	76	SER
4	e	106	PHE
4	e	111	PHE
4	e	147	GLU
4	e	166	VAL
4	e	197	LYS

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Mol	Chain	Res	Type
5	f	673	GLN
5	f	685	PHE
5	f	699	CYS
5	f	704	SER
5	f	715	SER
5	f	728	GLU
5	f	749	SER
5	f	781	ILE
5	f	845	LEU
5	f	846	ARG
5	f	851	LYS
5	f	906	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	293	ASN
2	B	256	ASN
3	C	133	GLN
4	D	145	GLN
4	E	18	HIS
5	F	173	GLN
5	F	773	GLN
1	a	65	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	$\# Z > 2$
11	AMP	L	1001	10	21,25,25	0.73	0	23,38,38	1.26	2 (8%)

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
11	AMP	L	1001	10	-	1/6/26/26	0/3/3/3

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	L	1001	AMP	N3-C2-N1	-4.02	123.21	128.67
11	L	1001	AMP	C4-C5-N7	-2.46	106.73	109.34

There are no chirality outliers.

All (1) torsion outliers are listed below:

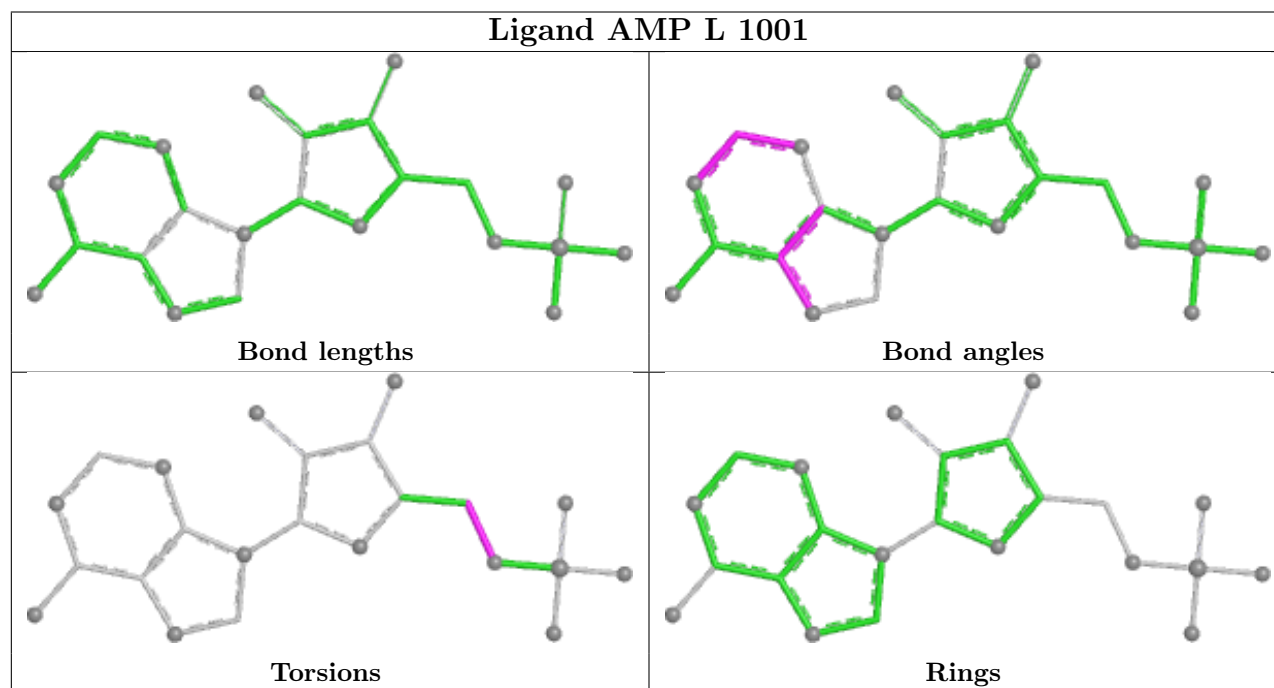
Mol	Chain	Res	Type	Atoms
11	L	1001	AMP	C4'-C5'-O5'-P

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.

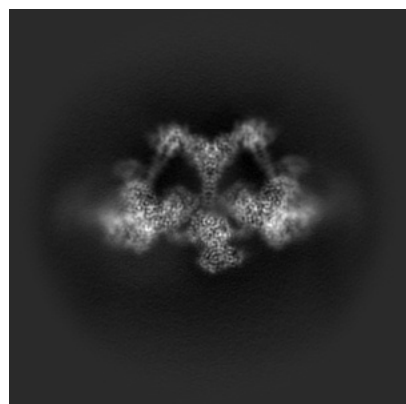
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-49110. These allow visual inspection of the internal detail of the map and identification of artifacts.

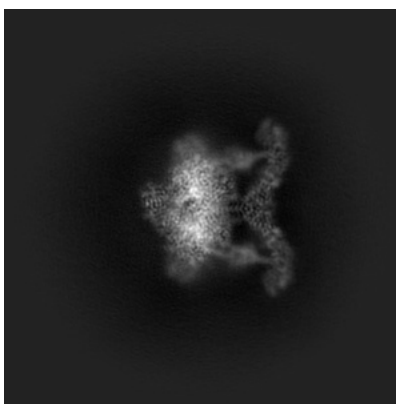
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

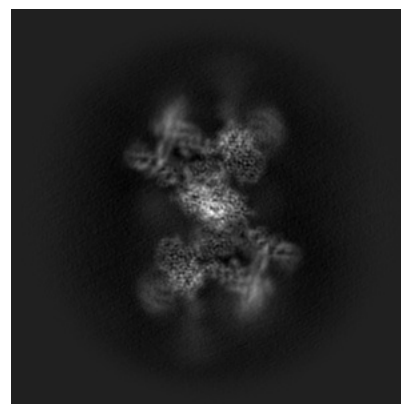
6.1.1 Primary map



X

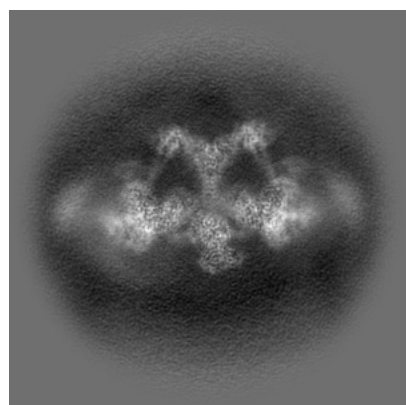


Y

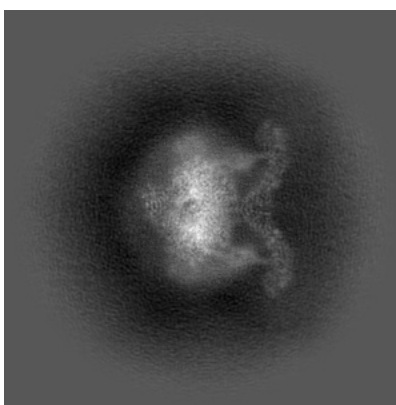


Z

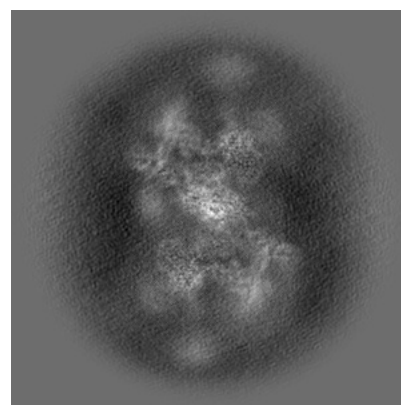
6.1.2 Raw map



X



Y

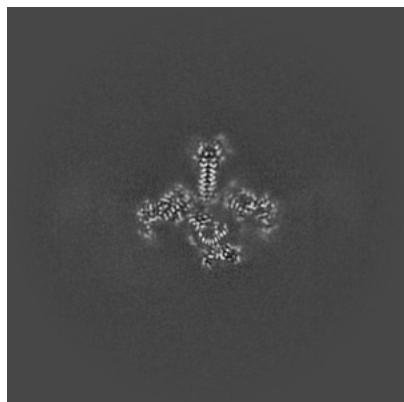


Z

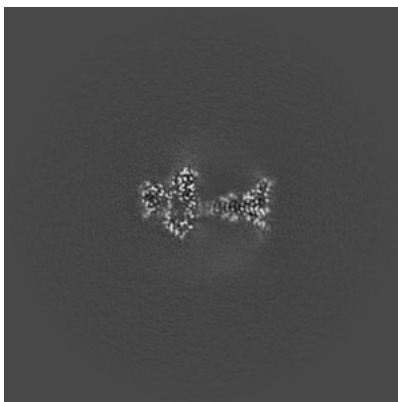
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

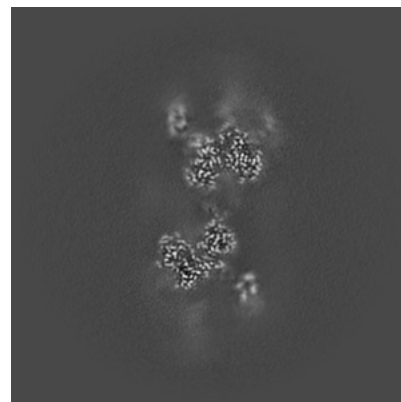
6.2.1 Primary map



X Index: 256

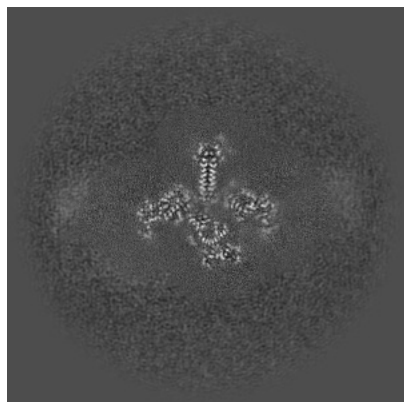


Y Index: 256

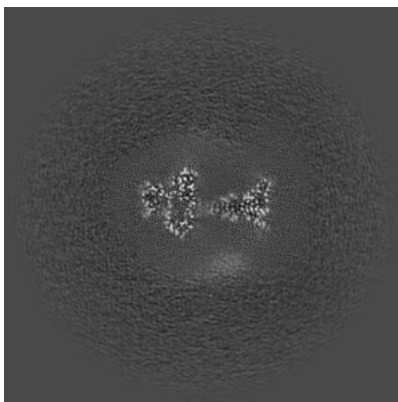


Z Index: 256

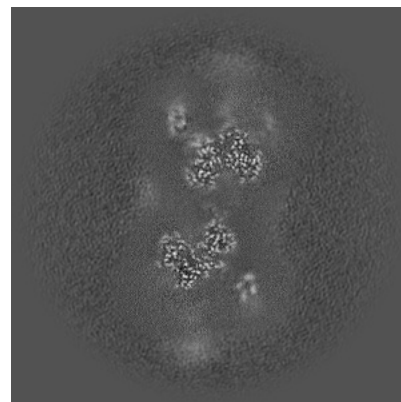
6.2.2 Raw map



X Index: 256



Y Index: 256



Z Index: 256

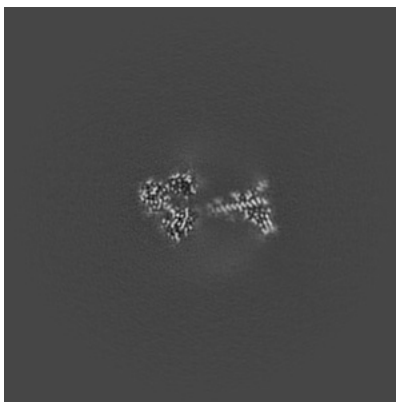
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

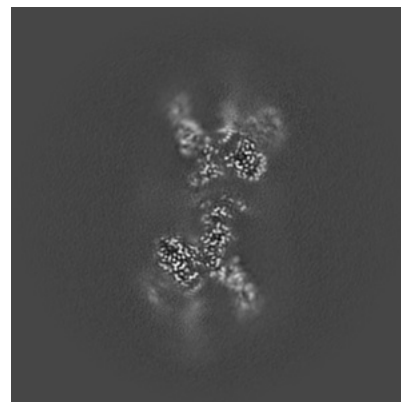
6.3.1 Primary map



X Index: 271

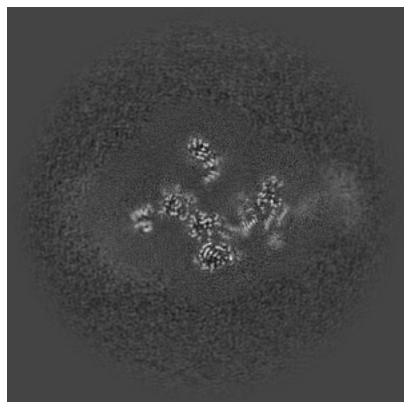


Y Index: 263

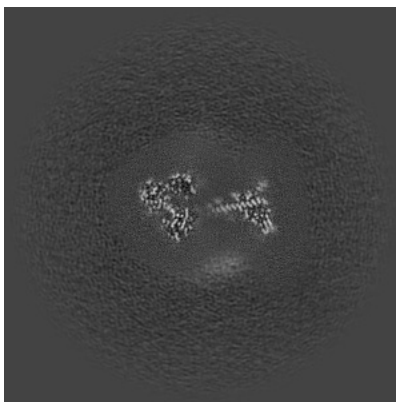


Z Index: 247

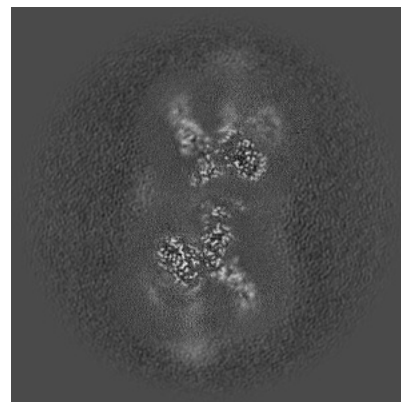
6.3.2 Raw map



X Index: 271



Y Index: 263

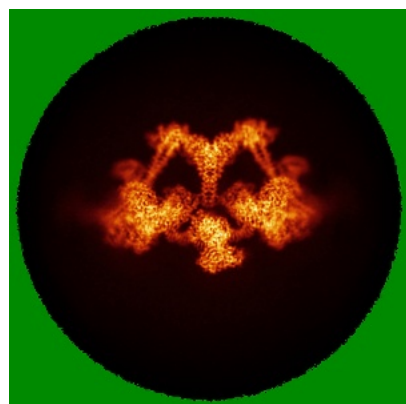


Z Index: 248

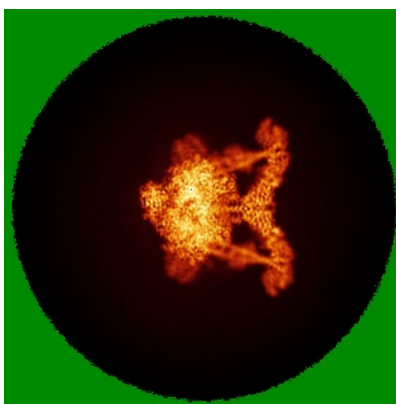
The images above show the largest variance slices of the map in three orthogonal directions.

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

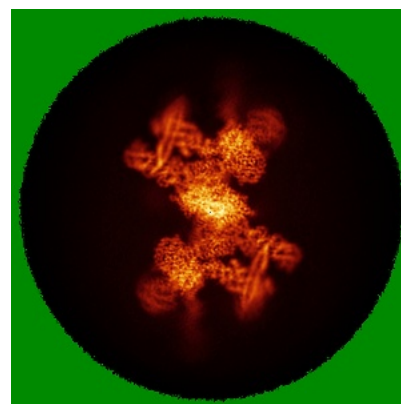
6.4.1 Primary map



X

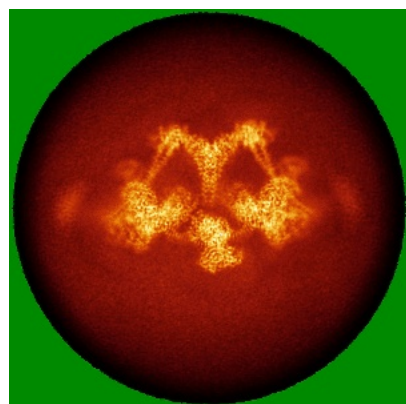


Y

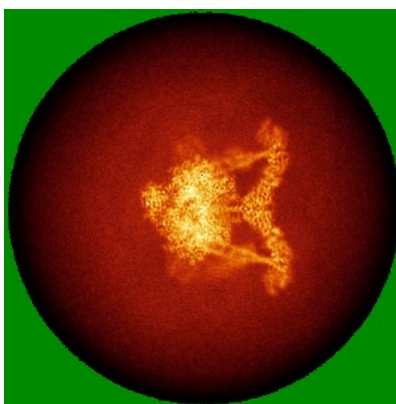


Z

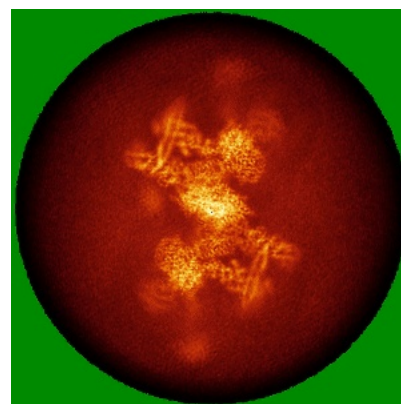
6.4.2 Raw map



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



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.07. 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

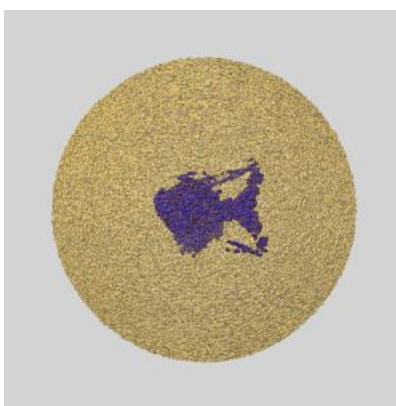
A mask typically either:

- 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_49110_msk_1.map [i](#)



X



Y

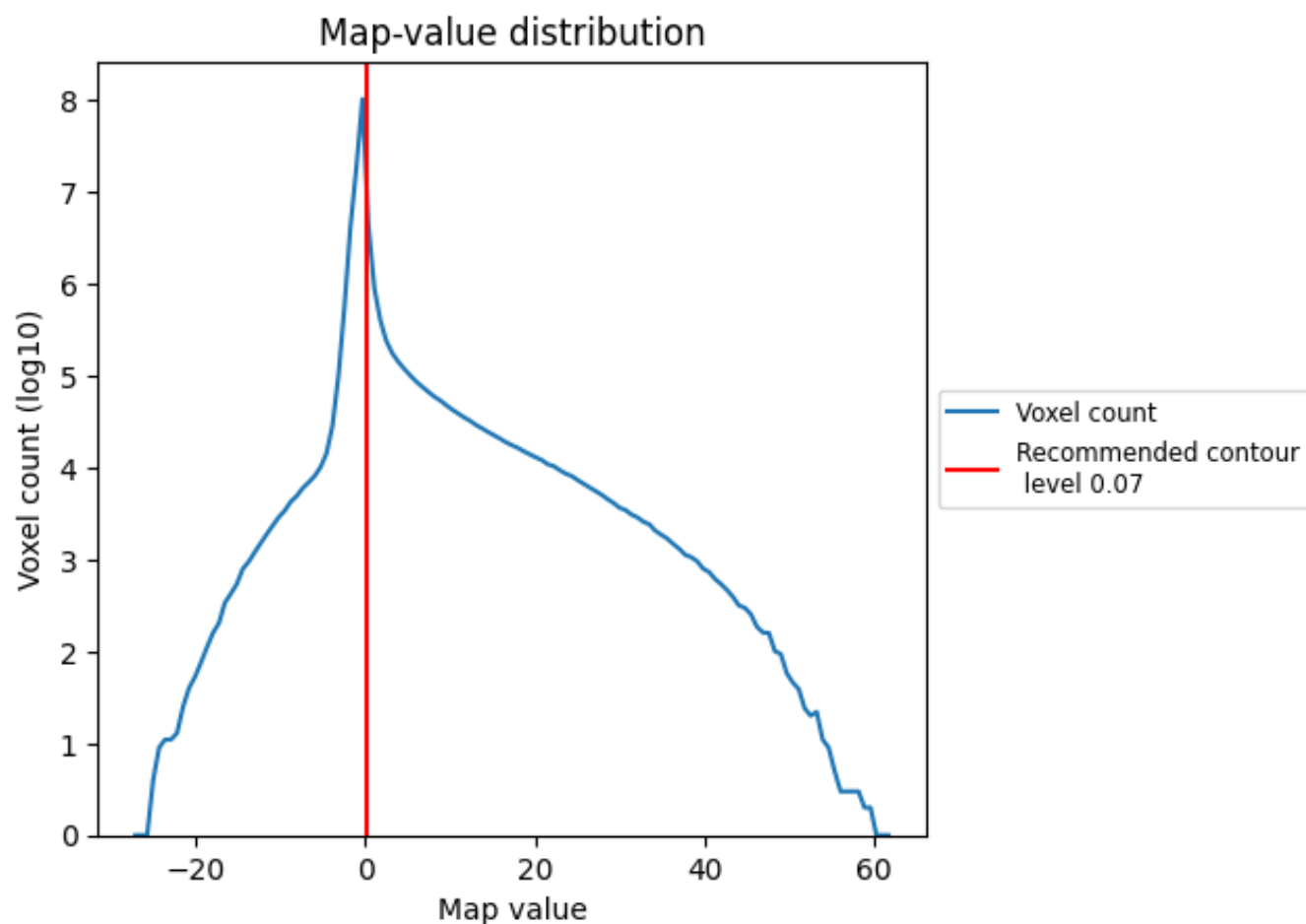


Z

7 Map analysis [i](#)

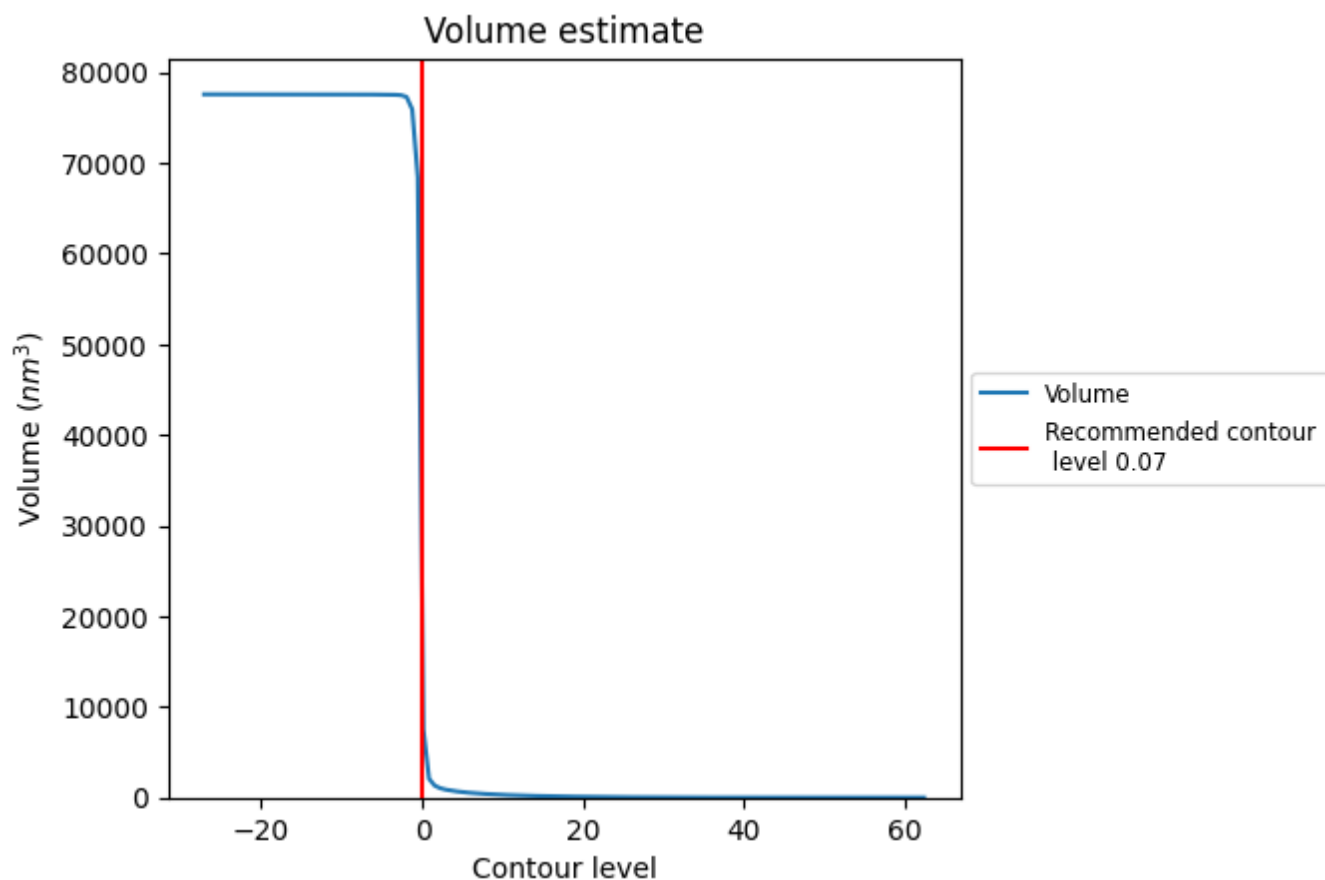
This section contains the results of statistical analysis of the map.

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.

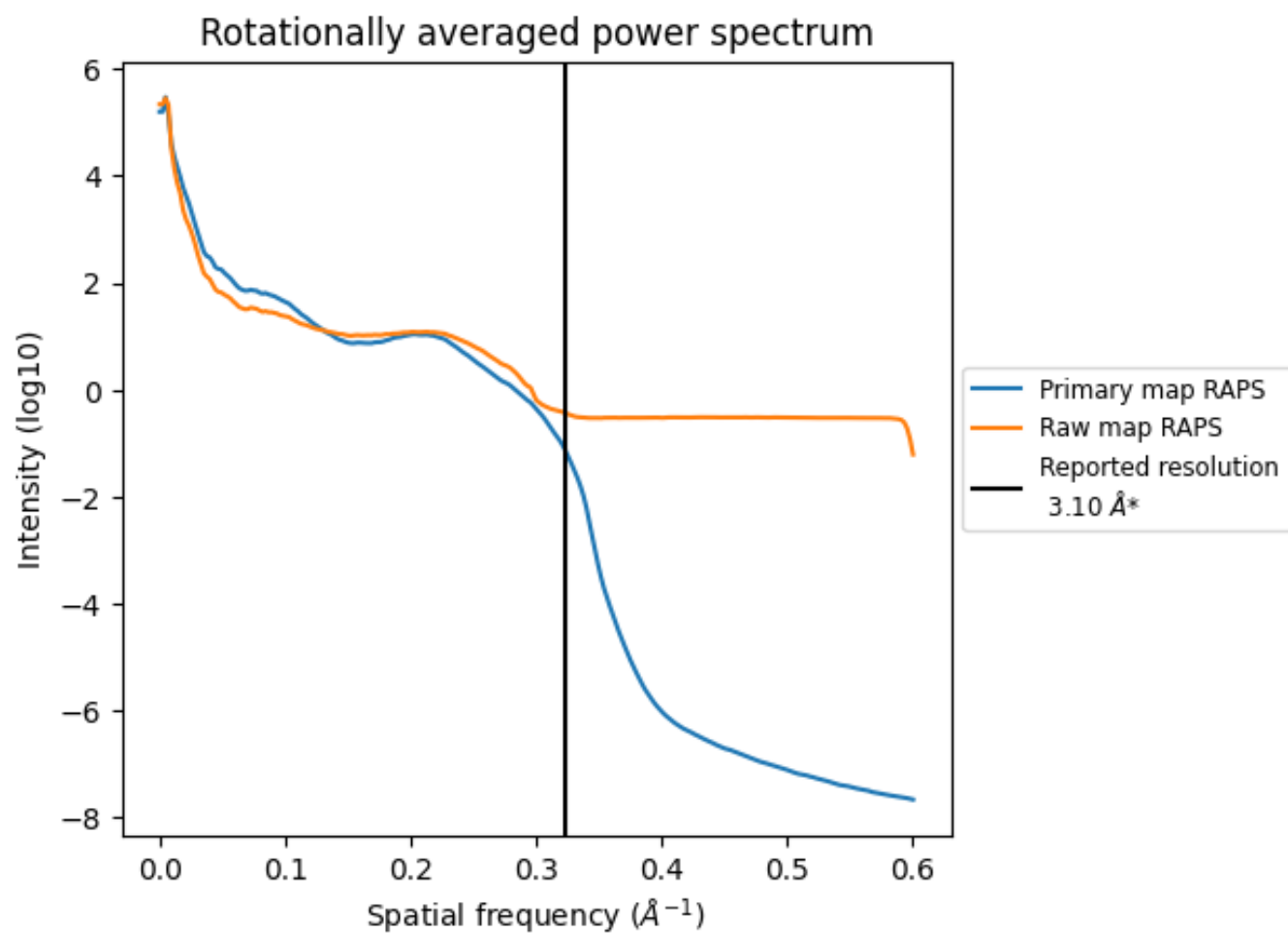
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 15311 nm^3 ; this corresponds to an approximate mass of 13831 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 ⓘ

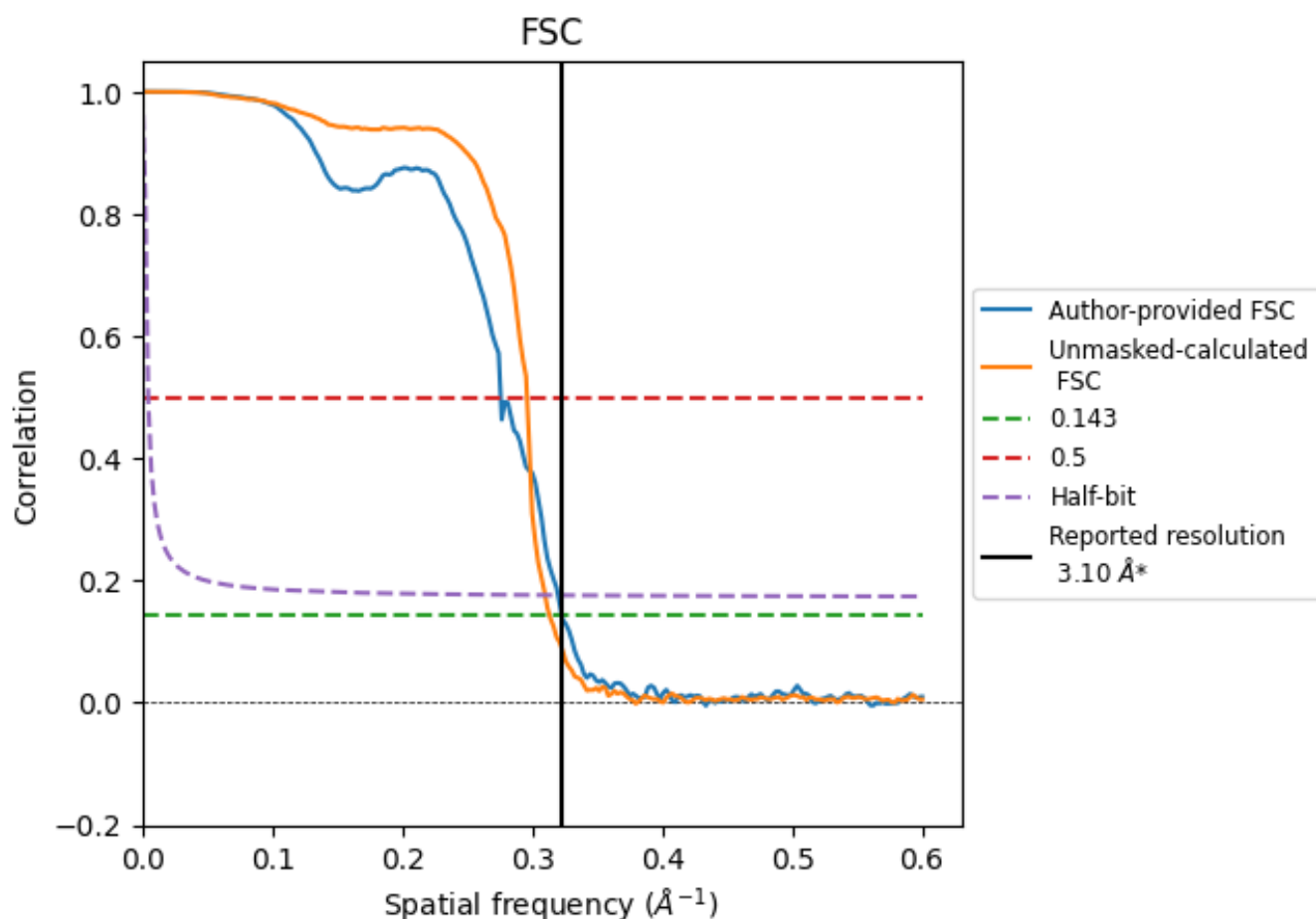


*Reported resolution corresponds to spatial frequency of 0.323 \AA^{-1}

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.323 \AA^{-1}

8.2 Resolution estimates [i](#)

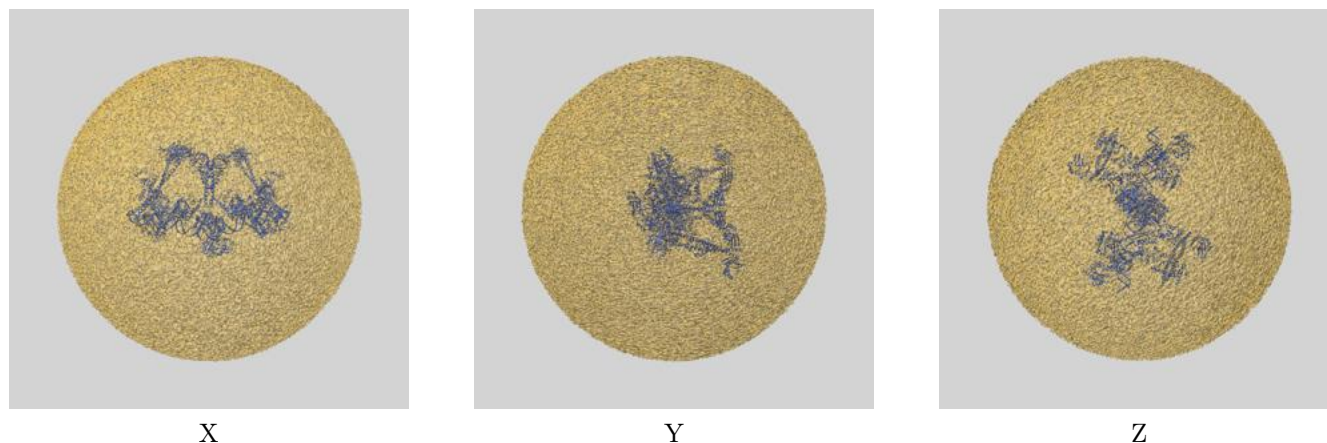
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.10	3.62	3.12
Unmasked-calculated*	3.19	3.38	3.22

*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-49110 and PDB model 9N83. Per-residue inclusion information can be found in [section 3](#) on [page 8](#).

9.1 Map-model overlay [i](#)



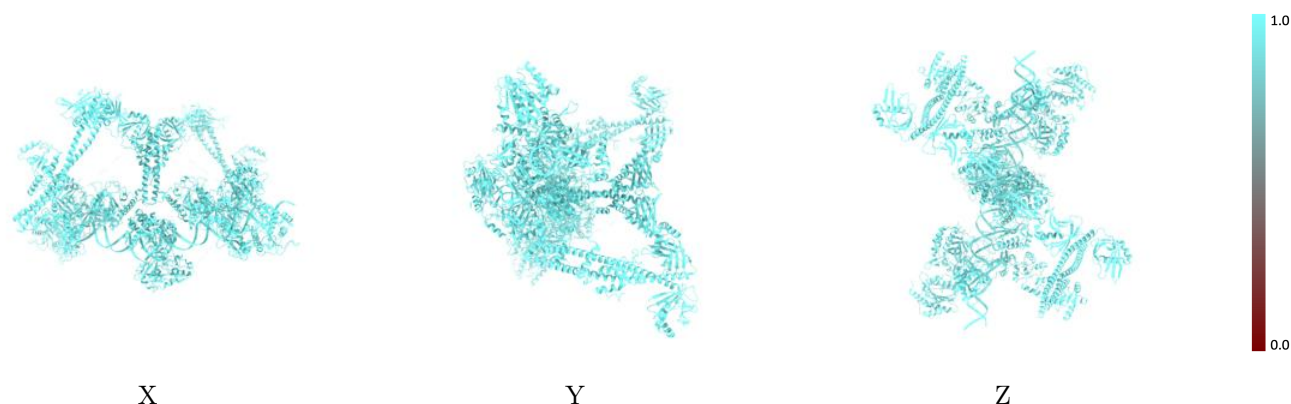
The images above show the 3D surface view of the map at the recommended contour level 0.07 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



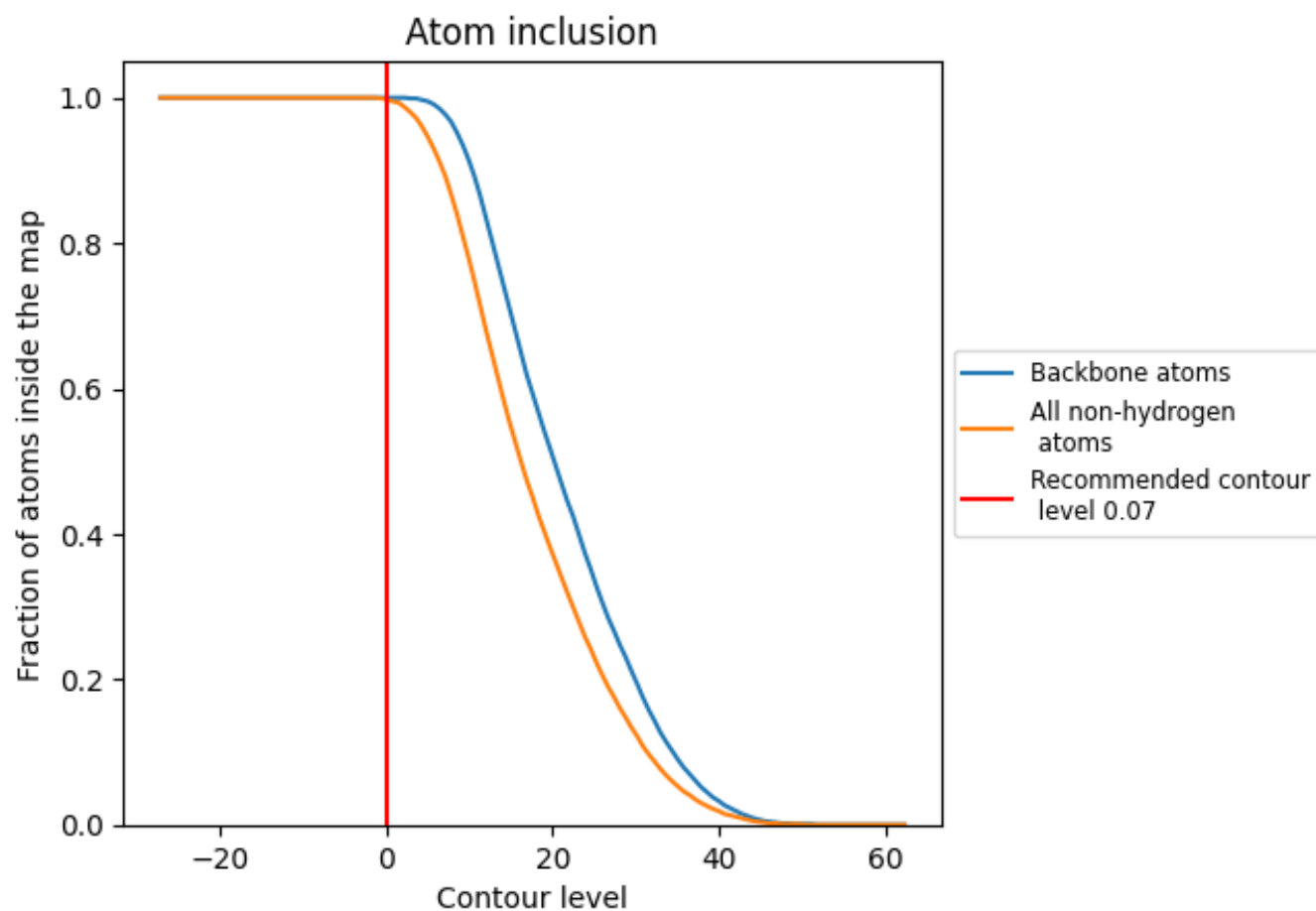
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.07).







































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 (0.07) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9980	 0.4330
A	 0.9980	 0.4950
B	 0.9990	 0.4330
C	 0.9940	 0.4640
D	 0.9960	 0.2760
E	 0.9950	 0.3160
F	 0.9960	 0.4570
G	 0.9940	 0.4860
H	 1.0000	 0.5310
I	 1.0000	 0.4560
J	 1.0000	 0.4540
K	 1.0000	 0.4600
L	 0.9990	 0.4460
a	 0.9990	 0.5240
b	 1.0000	 0.4580
c	 0.9960	 0.4720
d	 0.9980	 0.2990
e	 0.9980	 0.3460
f	 0.9990	 0.2790

