



wwPDB EM Validation Summary Report ⓘ

Jun 5, 2025 – 02:24 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 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.dev118
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0rc1
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) : 2.43.1

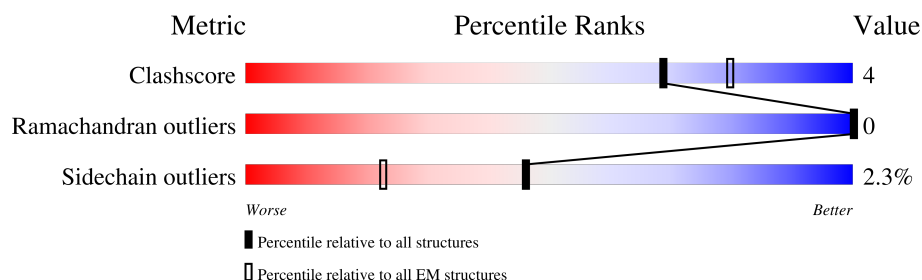
1 Overall quality at a glance

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)
Clashscore	210492	15764
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	
1	a	612	
2	B	732	
2	b	732	
3	C	302	
3	c	302	
4	D	336	
4	E	336	

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Mol	Chain	Length	Quality of chain
4	d	336	
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	51	

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		

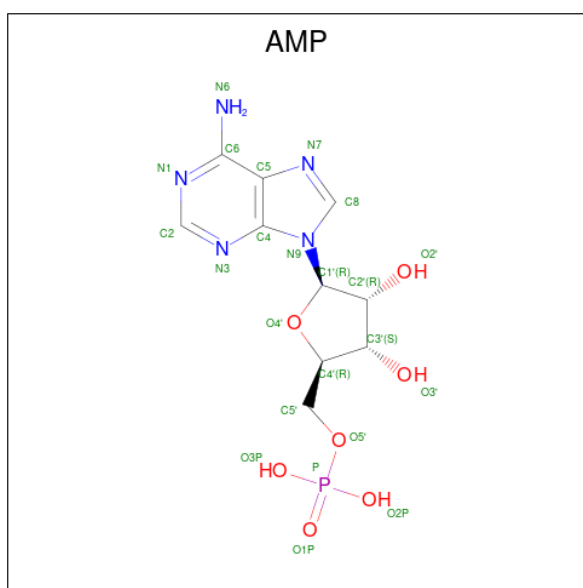
- Molecule 9 is a DNA chain called DNA (35-MER).

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		

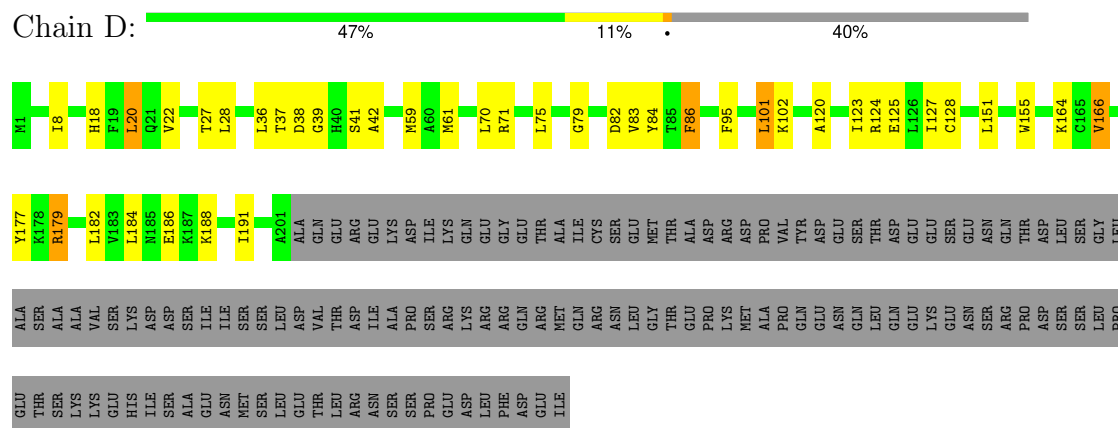
- Molecule 11 is ADENOSINE MONOPHOSPHATE (CCD ID: AMP) (formula: C₁₀H₁₄N₅O₇P) (labeled as "Ligand of Interest" by depositor).



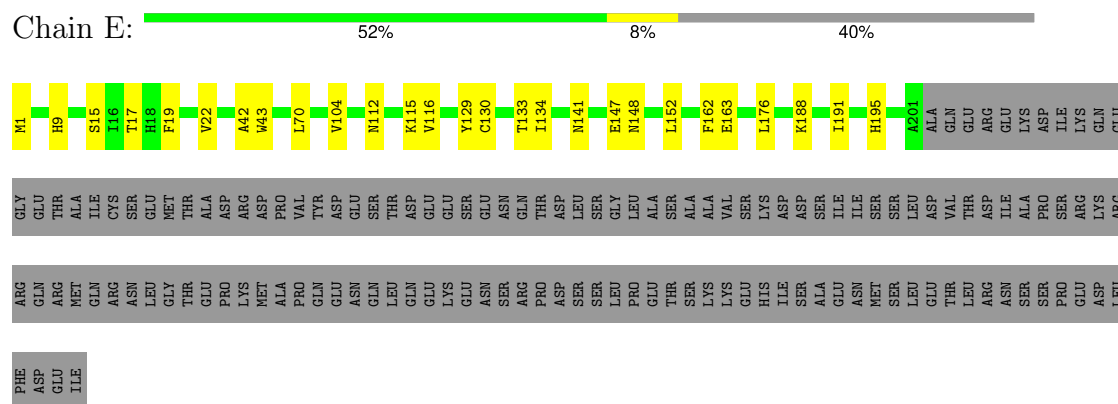
Mol	Chain	Residues	Atoms					AltConf
11	L	1	Total	C	N	O	P	0
			23	10	5	7	1	

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

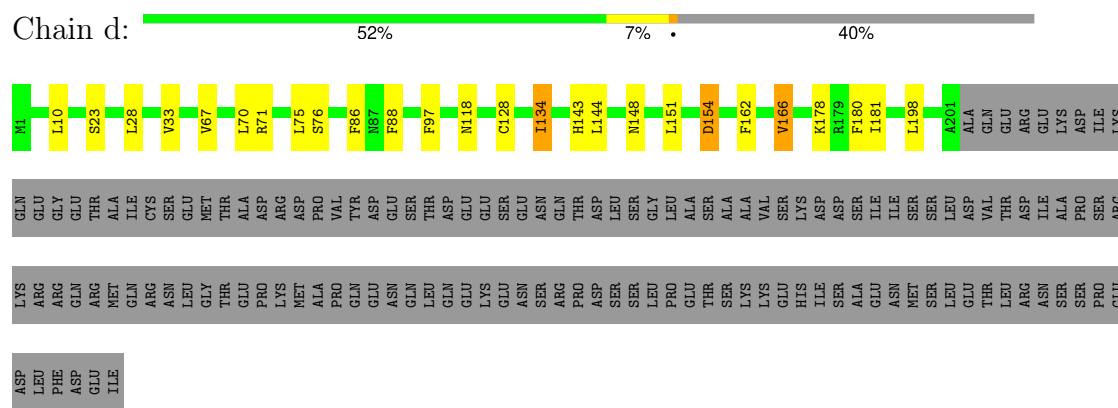
Mol	Chain	Residues	Atoms		AltConf
12	L	1	Total	Mg	0
			1	1	



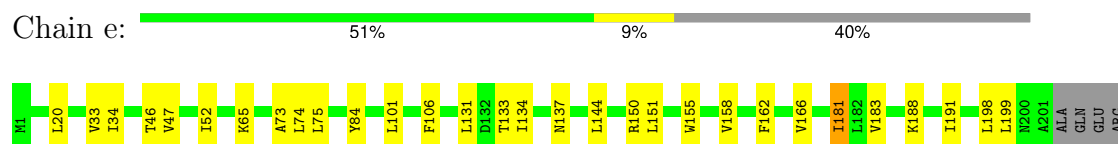
- Molecule 4: DNA repair protein XRCC4



- Molecule 4: DNA repair protein XRCC4




- Molecule 4: DNA repair protein XRCC4



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

• Molecule 5: DNA ligase 4

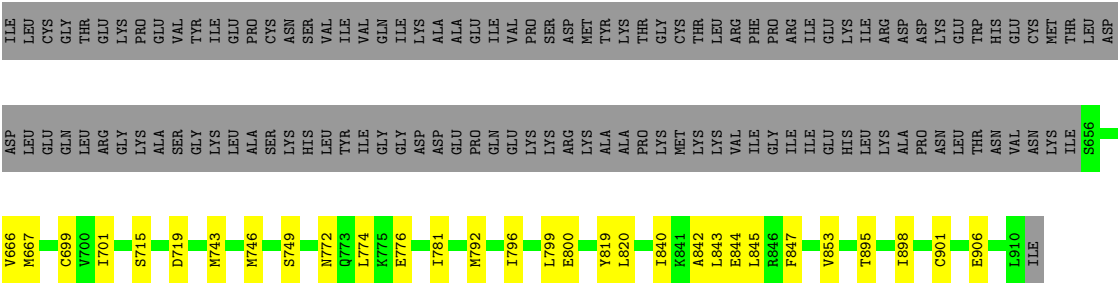
Chain F:  87% 7% 5%

ILE	R681	E684	V690	V700	I707	I712	H718	V721	W725	L726	P740	M743	M746	D759	G760	Y761	Y765	L774	V777	I781	I796	E800	W805	M812	L820	I840	K841	A842	F847	V853	V860	E902	L910									
	V499	S504	I559	K560	A561	C574	E582	L599	L610	I617	GLY	ASP	GLU	PRO	GLN	GLY	LYS	LYS	ALA	PRO	LYS	MET	LYS	VAL	ILE	ILE	GLU	HIS	LEU	LYS	ALA	PRO	ASN	THR	ASN	VAL	ASN	LYS	ILE	S656	D677	C685
GLY	PRO	VAL	MET	ALA	ALA	SER	GLN	THR	S7	S21	T114	P115	T116	L151	L171	L174	D255	I259	E260	M281	F319	T339	K348	F349	K352	L360	V372	L377	I388	T394	M430	V431	W447	L448	I464	H482	C485					

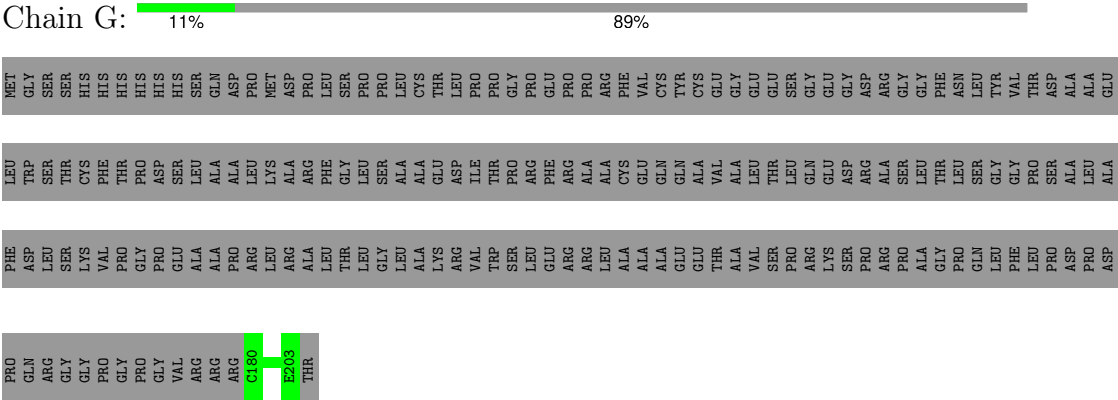
• Molecule 5: DNA ligase 4

Chain f:  25% 72%

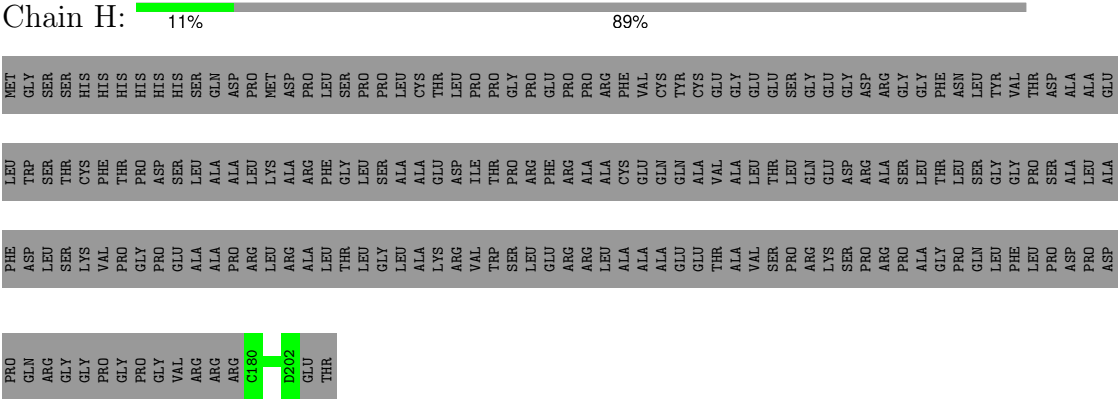
GLY	PRO	VAL	MET	ALA	ALA	SER	GLN	THR	SER	THR	LYS	GLY
LEU	ASN	GLU	GLN	ILE	ASP	TYR	CYS	GLY	THR	ASP	THR	LYS
GLY	ILE	ILE	THR	PHE	THR	VAL	THR	GLY	GLN	ALA	THR	LYS
ASP	ASP	ASP	THR	GLY	ASP	ALA	GLY	GLY	GLY	SER	ASP	LYS
LYS	LYS	ARG	CYS	GLN	GLN	GLY	GLY	ASP	THR	PHE	TYR	LYS
ALA	ALA	GLU	ALA	GLU	PHE	VAL	THR	THR	ILE	ALA	PRO	THR
GLY	GLY	ASP	ASP	GLY	ASP	GLY	GLU	GLY	ARG	ILE	MET	GLN
ILE	ILE	VAL	MET	GLY	VAL	VAL	GLY	ILE	MET	ALA	ARG	THR
LYS	MET	VAL	LEU	SER	ILE	VAL	SER	TYR	ILE	THR	LEU	VAL
PRO	PRO	VAL	PRO	PRO	ALA	VAL	THR	THR	ALA	PHE	LEU	ALA
PRO	PRO	GLN	GLU	GLU	THR	ASN	PHE	THR	ASP	LEU	PRO	SER
GLY	PRO	LEU	PRO	GLY	GLY	ASN	THR	THR	LYS	GLN	VAL	HIS
GLU	GLU	LEU	LYS	GLY	ASP	LYS	ILE	ILE	ASP	PRO	LEU	PRO
LYS	LYS	SER	LEU	ILE	ILE	LYS	HIS	THR	LEU	ARG	GLU	PHE
PRO	PRO	VAL	LEU	VAL	ILE	GLY	GLY	GLY	GLU	GLY	ASP	ALA
PRO	PRO	TYR	SER	TYR	THR	GLY	HIS	THR	VAL	VAL	ARG	ASP
VAL	VAL	GLY	GLY	GLY	THR	GLY	ARG	THR	GLY	GLY	LEU	ILE
GLY	GLY	TRP	GLY	TRP	GLY	GLY	GLY	GLY	GLY	GLY	GLY	THR
GLY	GLY	LEU	GLY	TRP	THR	ILE	TRP	ILE	GLY	THR	GLY	GLN
GLY	GLY	LEU	GLY	TRP	THR	ILE	TRP	ILE	GLY	THR	GLY	GLN
GLY	GLY	LEU	GLY	TRP	THR	ILE	TRP	ILE	GLY	THR	GLY	GLN
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GLY	GLY	LEU	GLY	TRP	THR	ILE	TRP	ILE	GLY	THR	GLY	GLN
GLY	GLY	LEU	GLY	TRP	THR	ILE	TRP	ILE	GLY	THR	GLY	GLN
GLY	GLY	LEU	GLY	TRP	THR	ILE	TRP	ILE	GLY	THR	GLY	GLN
GLY	GLY	LEU	GLY	TRP	THR	ILE	TRP	ILE	GLY	THR	GLY	GLN
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GLY	GLY	LEU	GLY	TRP	THR	ILE	TRP	ILE	GLY	THR	GLY	GLN
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GLY	GLY	LEU	GLY	TRP	THR	ILE	TRP	ILE	GLY	THR	GLY	GLN
GLY	GLY	LEU	GLY	TRP	THR	ILE	TRP	ILE	GLY	THR	GLY	GLN
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GLY	GLY	LEU	GLY	TRP	THR	ILE	TRP	ILE	GLY	THR	GLY	GLN
GLY	GLY	LEU	GLY	TRP	THR	ILE	TRP	ILE	GLY	THR	GLY	GLN
GLY	GLY	LEU	GLY	TRP	THR	ILE	TRP	ILE	GLY	THR	GLY	GLN
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GLY	GLY	LEU	GLY	TRP	THR	ILE	TRP	ILE	GLY	THR	GLY	GLN
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GLY	GLY	LEU	GLY	TRP	THR	ILE	TRP	ILE	GLY	THR	GLY	GLN
GLY	GLY	LEU	GLY	TRP	THR	ILE	TRP	ILE	GLY	THR	GLY	GLN
GLY	GLY	LEU	GLY	TRP	THR	ILE	TRP	ILE	GLY	THR	GLY	GLN
GLY	GLY	LEU	GLY	TRP	THR	ILE	TRP	ILE	GLY	THR	GLY	GLN
GLY	GLY	LEU	GLY	TRP	THR	ILE	TRP	ILE	GLY	THR	GLY	GLN
GLY	GLY	LEU	GLY	TRP	THR	ILE	TRP	ILE	GLY	THR	GLY	GLN
GLY	GLY	LEU	GLY	TRP	THR	ILE	TRP	ILE	GLY	THR	GLY	GLN
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GLY	GLY	LEU	GLY	TRP	THR	ILE	TRP	ILE	GLY	THR	GLY	GLN
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GLY	GLY	LEU	GLY	TRP	THR	ILE	TRP	ILE	GLY	THR	GLY	GLN
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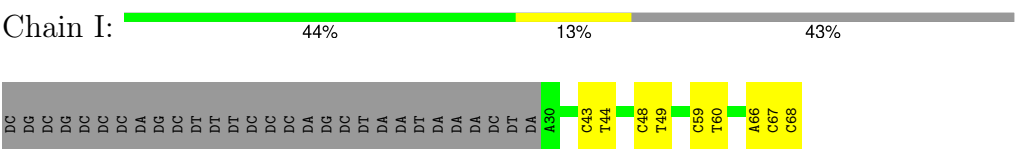
• Molecule 6: Protein PAXX



• Molecule 6: Protein PAXX

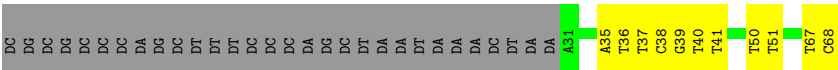


• Molecule 7: DNA (39-MER)

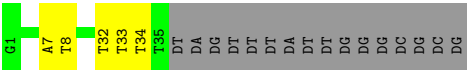


• Molecule 8: DNA (38-MER)

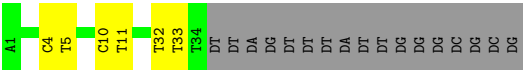




● Molecule 9: DNA (35-MER)



● Molecule 10: DNA (34-MER)



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: AMP, MG

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	0.15	0/4252	0.26	0/5728
1	a	0.15	0/4175	0.25	0/5626
2	B	0.14	0/4196	0.26	0/5661
2	b	0.14	0/4173	0.24	0/5631
3	C	0.15	0/1926	0.28	0/2610
3	c	0.15	0/1914	0.28	0/2594
4	D	0.15	0/1657	0.32	0/2228
4	E	0.15	0/1657	0.32	0/2228
4	d	0.16	0/1657	0.31	0/2228
4	e	0.16	0/1657	0.32	0/2228
5	F	0.14	0/7111	0.26	0/9587
5	f	0.11	0/2118	0.25	0/2862
6	G	0.12	0/178	0.20	0/238
6	H	0.13	0/169	0.22	0/226
7	I	0.20	0/883	0.43	0/1358
8	J	0.21	0/869	0.43	0/1338
9	K	0.21	0/812	0.43	0/1253
10	L	0.22	0/785	0.44	0/1210
All	All	0.15	0/40189	0.29	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](#)

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	4169	0	4230	21	0
1	a	4094	0	4161	20	0
2	B	4115	0	4156	32	0
2	b	4092	0	4130	31	0
3	C	1887	0	1901	18	0
3	c	1876	0	1891	17	0
4	D	1628	0	1620	32	0
4	E	1628	0	1620	21	0
4	d	1628	0	1620	18	0
4	e	1628	0	1620	29	0
5	F	6959	0	6963	42	0
5	f	2069	0	2011	19	0
6	G	174	0	166	0	0
6	H	165	0	160	0	0
7	I	790	0	440	6	0
8	J	776	0	428	6	0
9	K	722	0	396	3	0
10	L	700	0	385	3	0
11	L	23	0	12	1	0
12	L	1	0	0	0	0
All	All	39124	0	37910	272	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 4.

The worst 5 of 272 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)
4:d:144:LEU:HD23	4:e:144:LEU:HD22	1.67	0.77
4:d:162:PHE:HD2	5:f:843:LEU:HD23	1.52	0.74
5:F:820:LEU:HD22	5:F:842:ALA:HB2	1.71	0.72
3:c:100:VAL:HG12	3:c:101:ALA:H	1.57	0.69
4:e:20:LEU:HD21	4:e:74:LEU:HD22	1.72	0.69

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	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%)	460 (98%)	8 (2%)	56	78
1	a	460/550 (84%)	452 (98%)	8 (2%)	56	78
2	B	464/649 (72%)	456 (98%)	8 (2%)	56	78
2	b	462/649 (71%)	454 (98%)	8 (2%)	56	78
3	C	210/264 (80%)	207 (99%)	3 (1%)	62	81
3	c	209/264 (79%)	207 (99%)	2 (1%)	73	86
4	D	180/303 (59%)	168 (93%)	12 (7%)	13	40
4	E	180/303 (59%)	174 (97%)	6 (3%)	33	62
4	d	180/303 (59%)	170 (94%)	10 (6%)	17	46
4	e	180/303 (59%)	177 (98%)	3 (2%)	56	78
5	F	771/810 (95%)	757 (98%)	14 (2%)	54	76
5	f	231/810 (28%)	221 (96%)	10 (4%)	25	55
6	G	19/173 (11%)	19 (100%)	0	100	100
6	H	18/173 (10%)	18 (100%)	0	100	100
All	All	4032/6104 (66%)	3940 (98%)	92 (2%)	46	70

5 of 92 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	a	409	TYR
4	d	67	VAL
2	b	13	CYS
2	b	244	SER
4	d	143	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
5	F	173	GLN
5	F	816	HIS
5	F	773	GLN
6	G	187	ASN
2	B	411	HIS

5.3.3 RNA ⓘ

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 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:

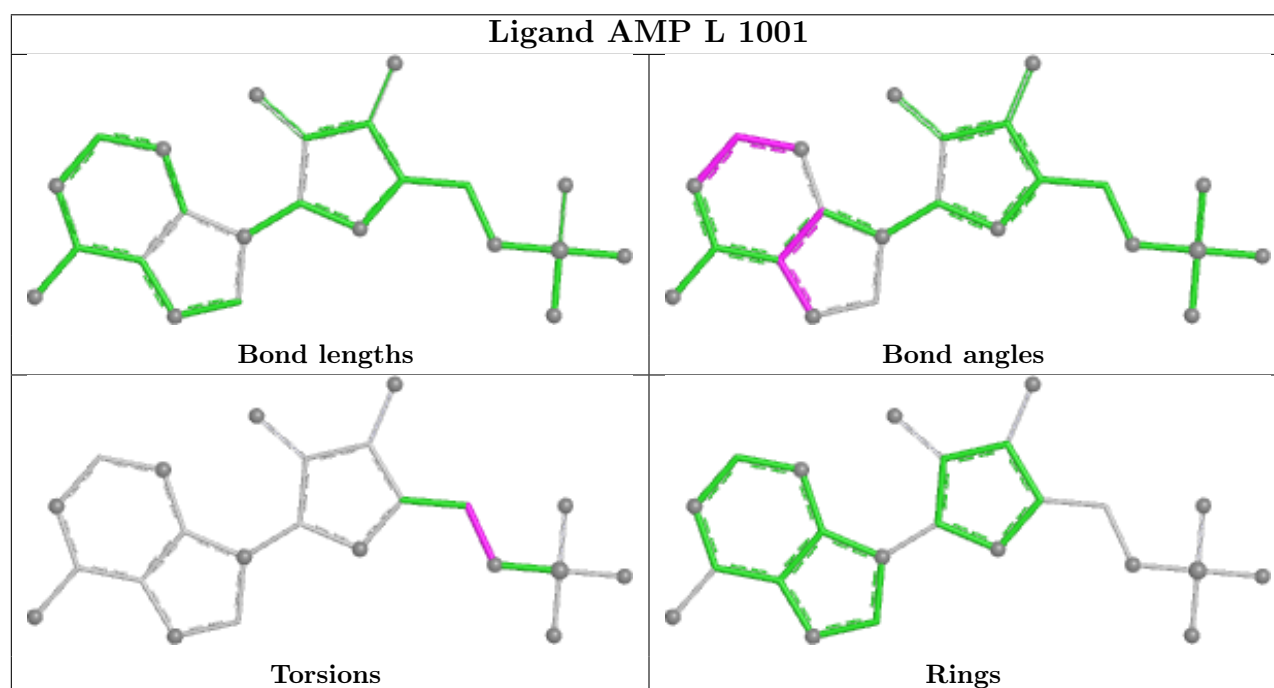
Mol	Chain	Res	Type	Atoms
11	L	1001	AMP	C4'-C5'-O5'-P

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	L	1001	AMP	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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

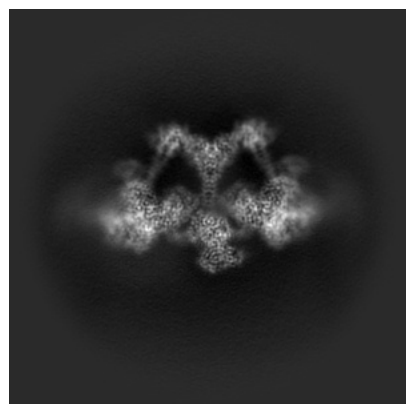
6 Map visualisation [i](#)

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.

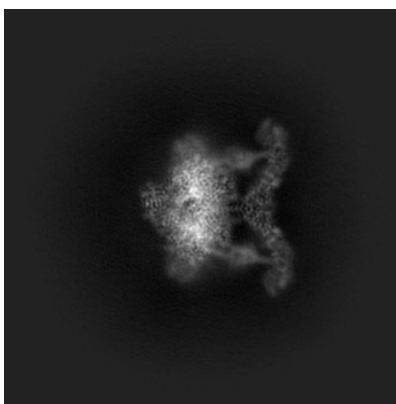
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

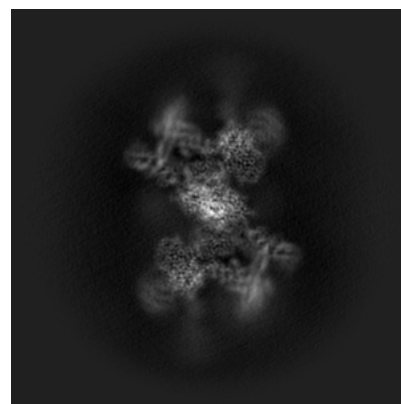
6.1.1 Primary map



X

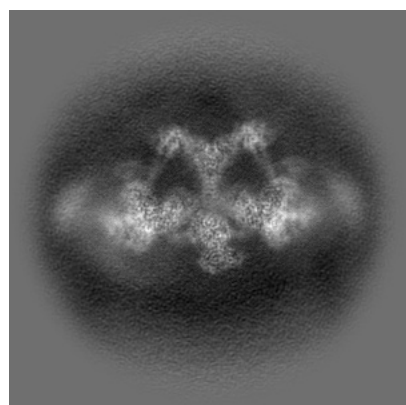


Y

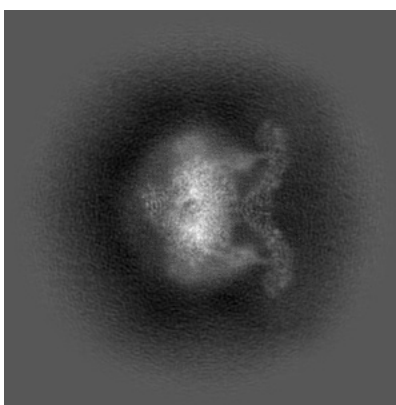


Z

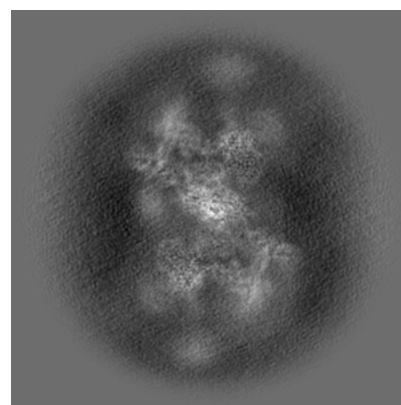
6.1.2 Raw map



X



Y

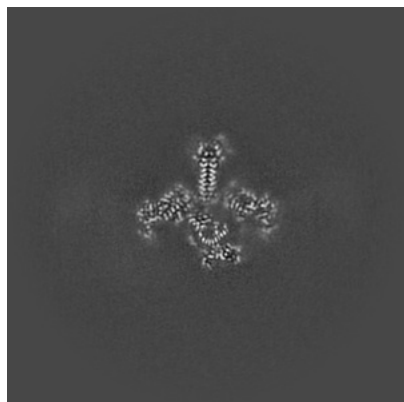


Z

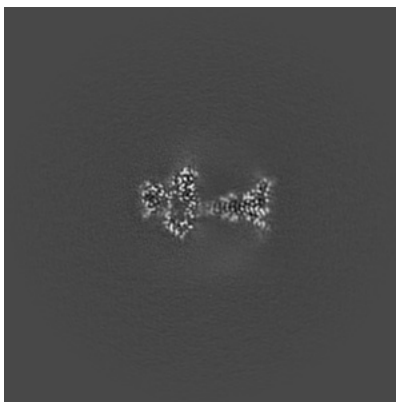
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

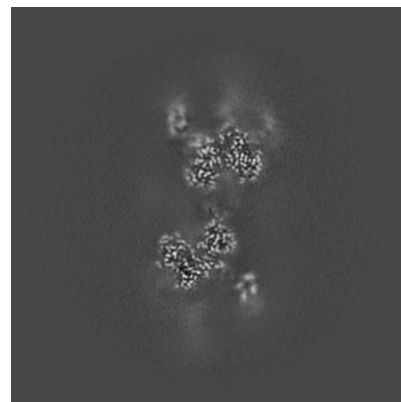
6.2.1 Primary map



X Index: 256

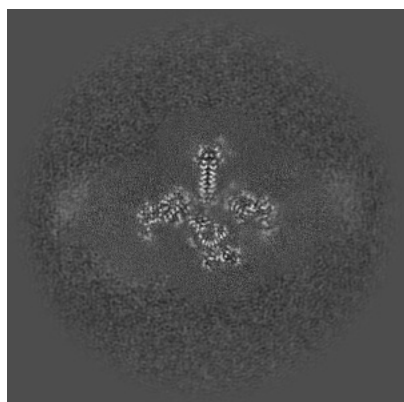


Y Index: 256

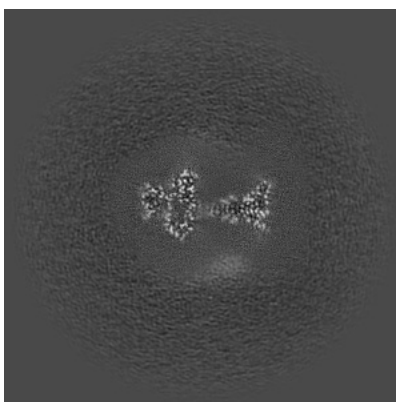


Z Index: 256

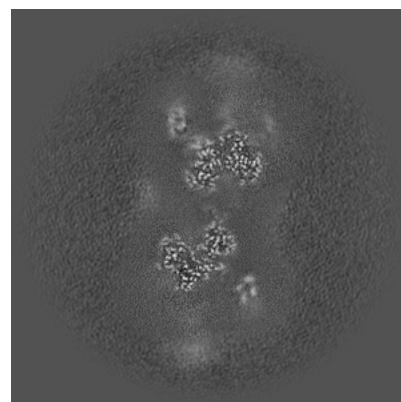
6.2.2 Raw map



X Index: 256



Y Index: 256



Z Index: 256

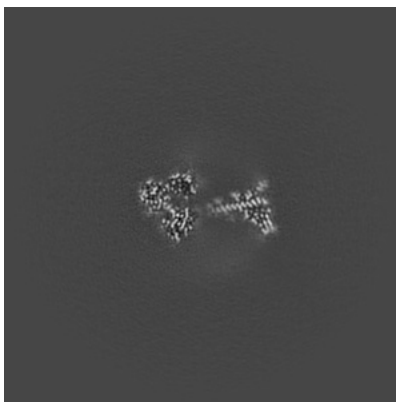
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

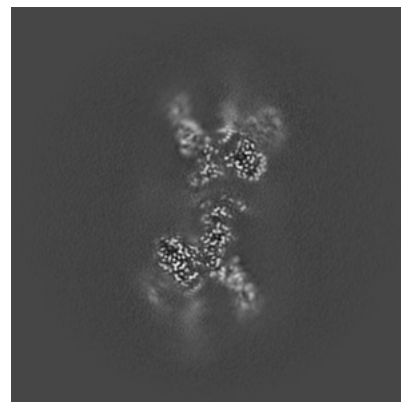
6.3.1 Primary map



X Index: 271

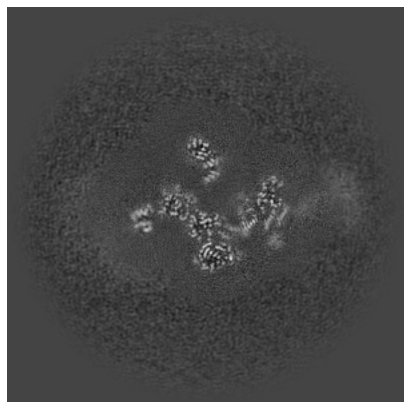


Y Index: 263

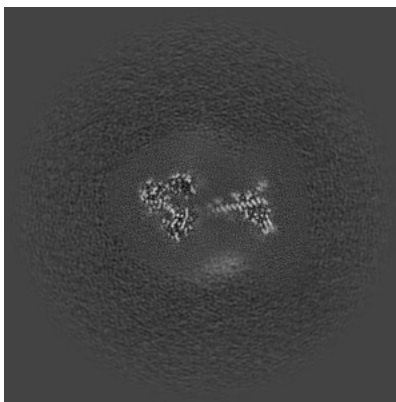


Z Index: 247

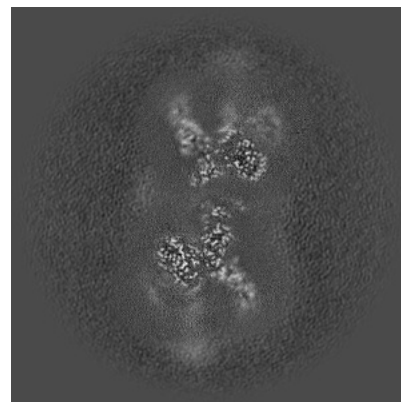
6.3.2 Raw map



X Index: 271



Y Index: 263

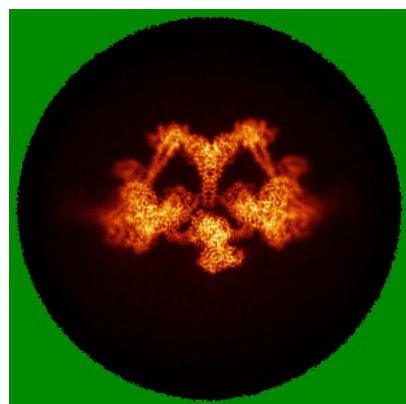


Z Index: 248

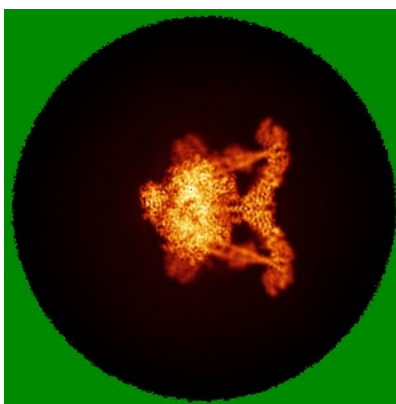
The images above show the largest variance slices of the map in three orthogonal directions.

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

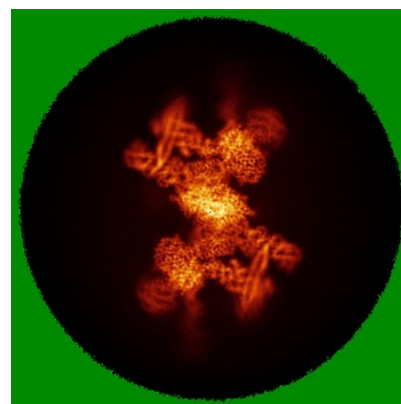
6.4.1 Primary map



X

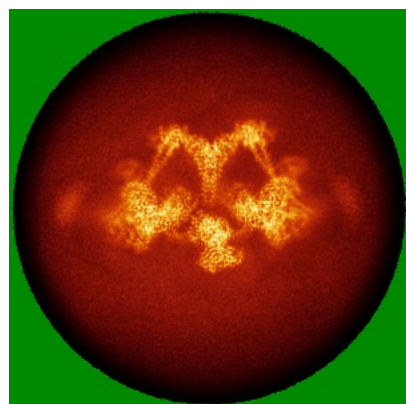


Y

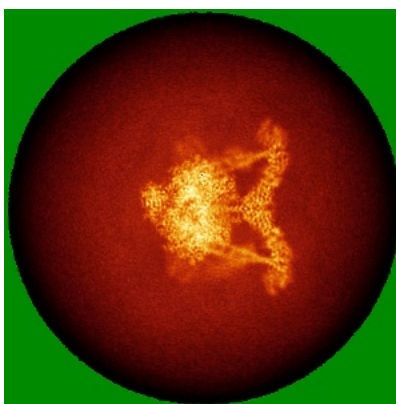


Z

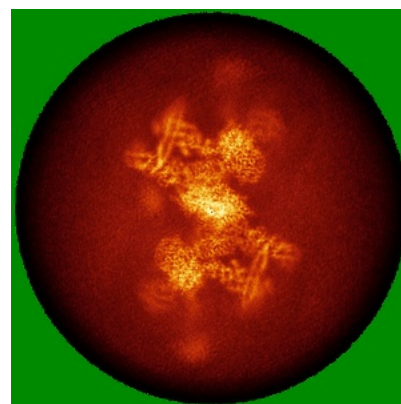
6.4.2 Raw map



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

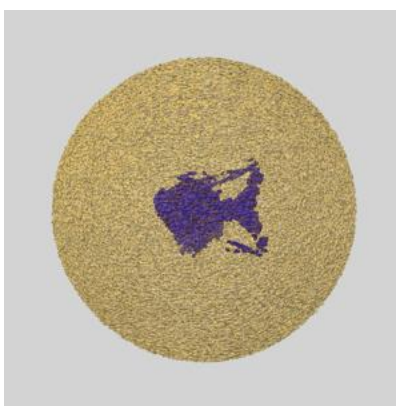
A mask typically either:

- 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

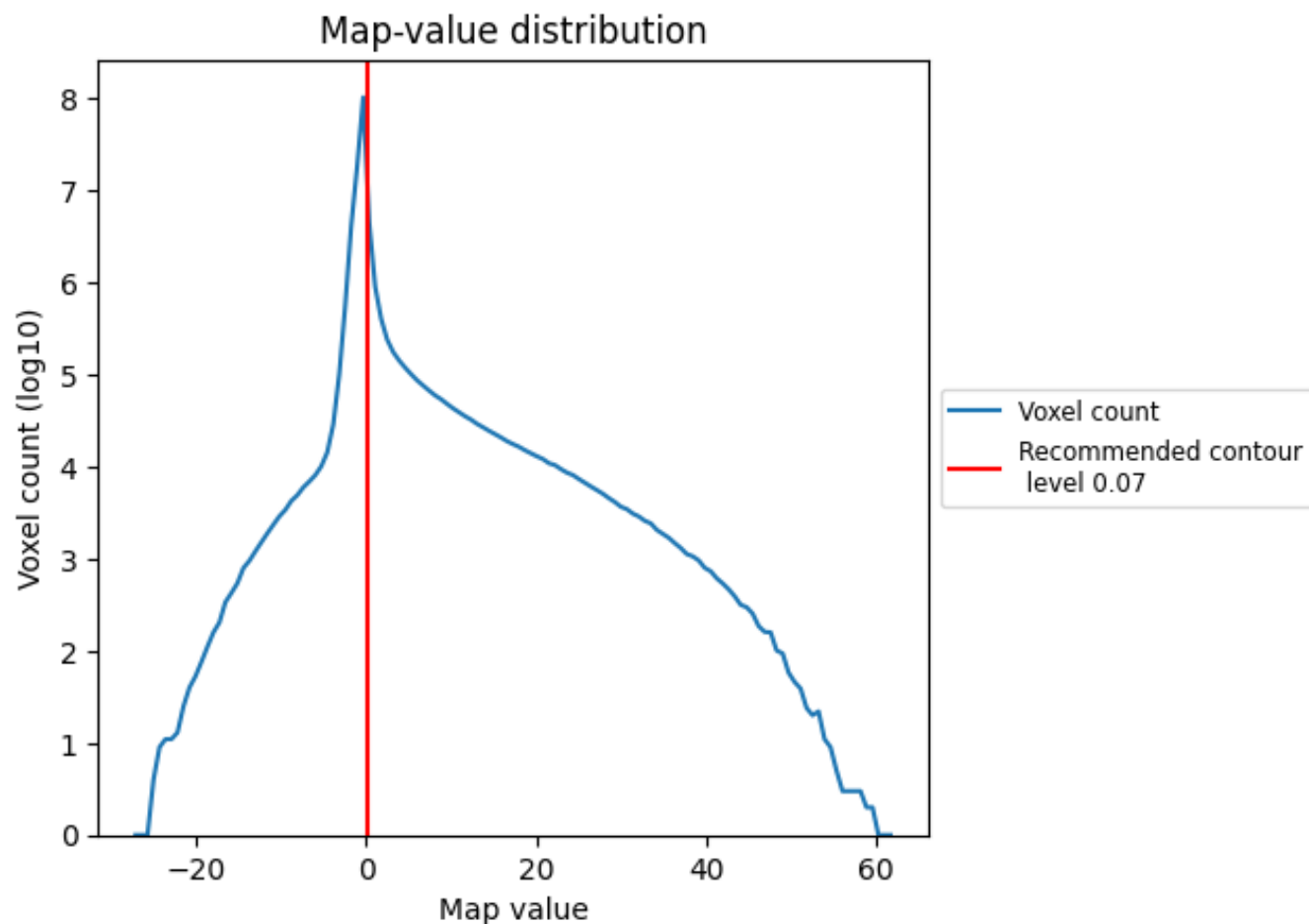


Z

7 Map analysis [i](#)

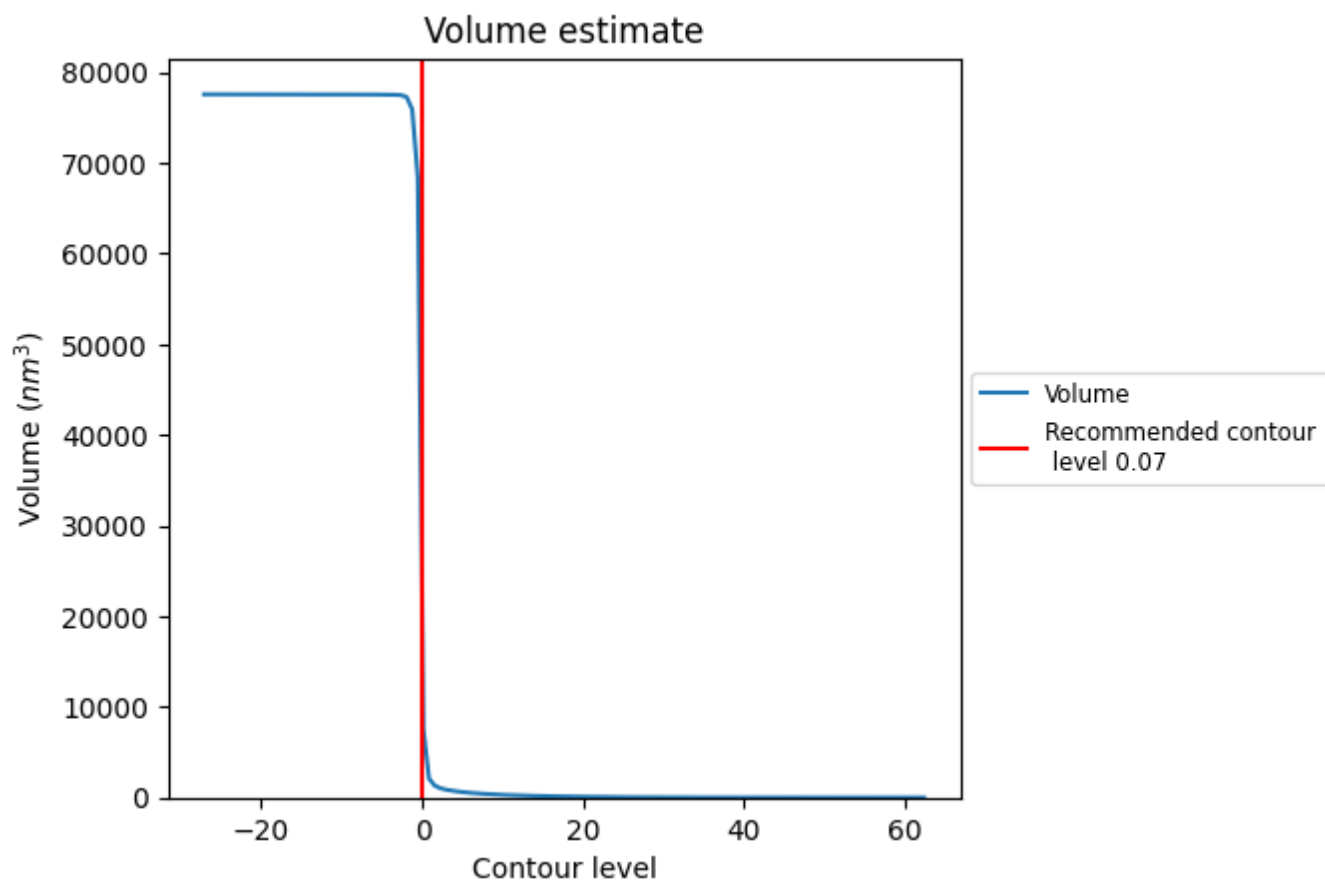
This section contains the results of statistical analysis of the map.

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.

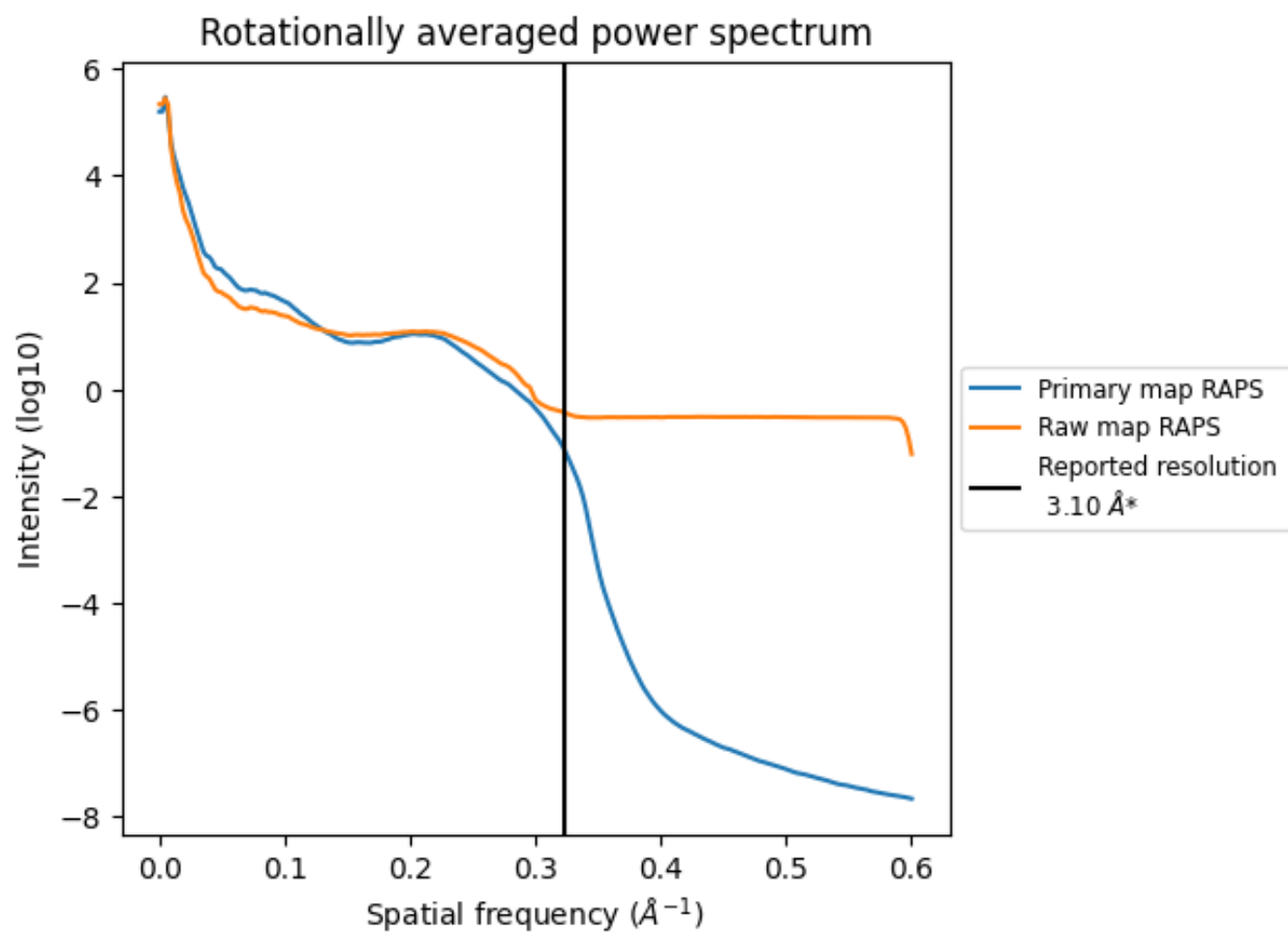
7.2 Volume estimate [i](#)



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 ⓘ

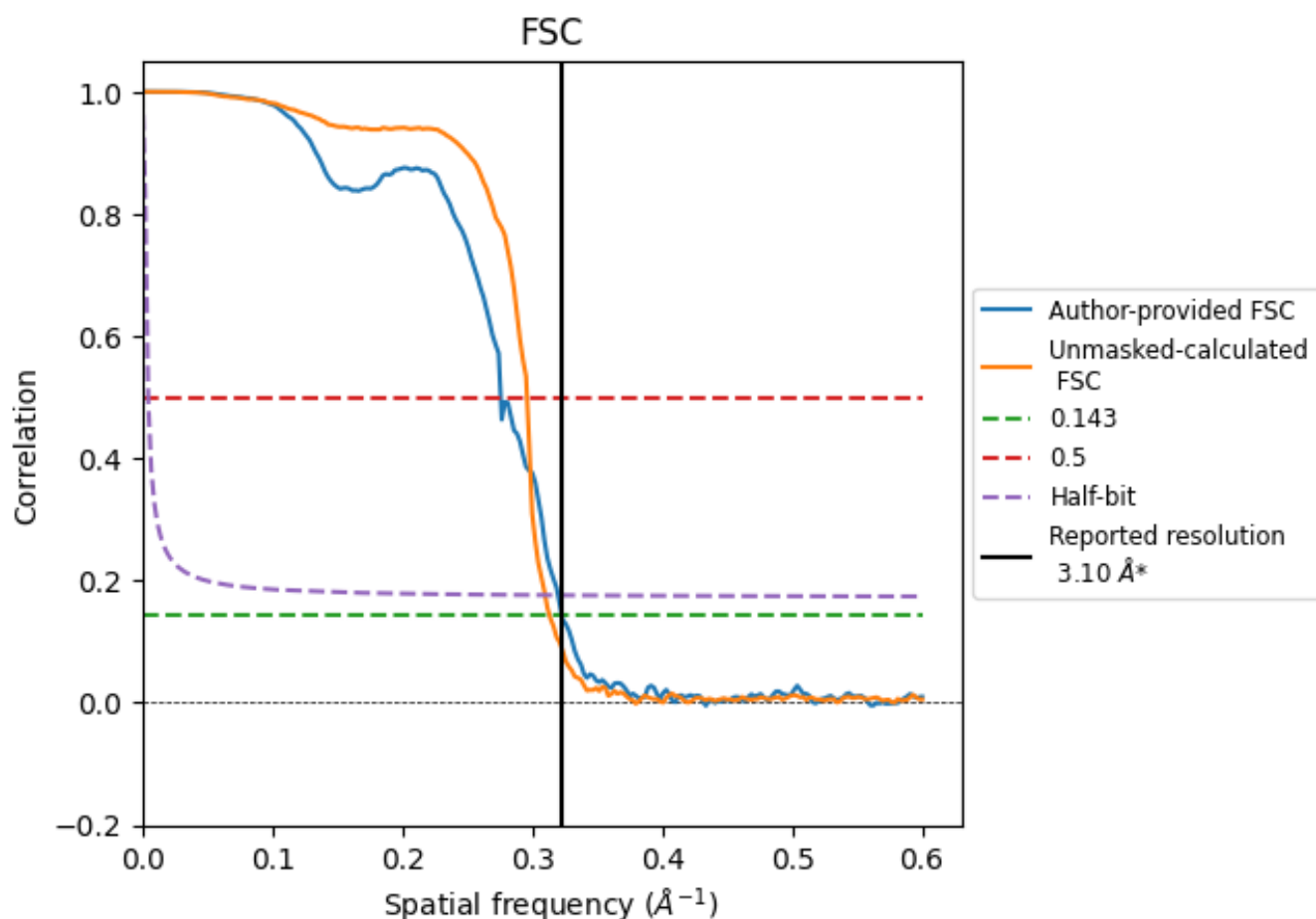


*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

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 0.323 \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](#)

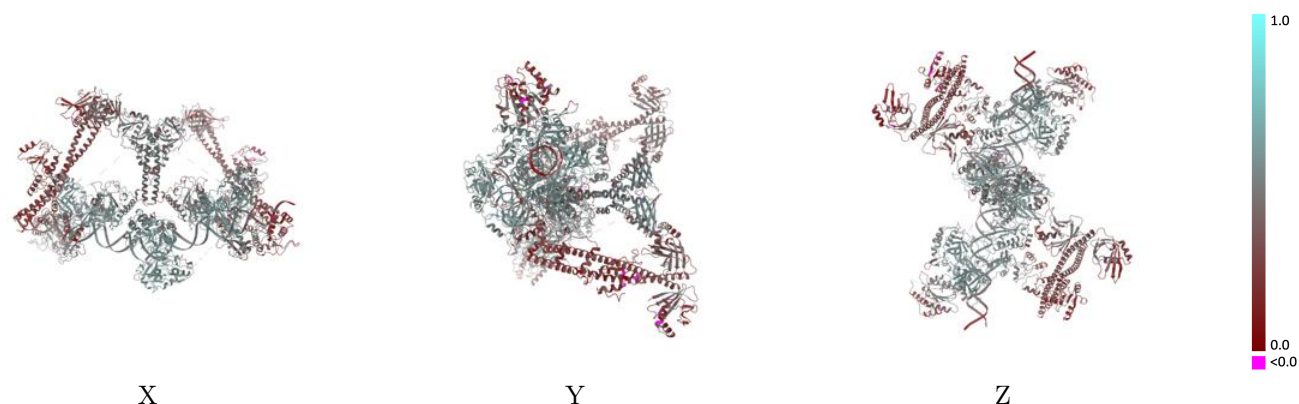
This section contains information regarding the fit between EMDB map EMD-49110 and PDB model 9N83. Per-residue inclusion information can be found in [section 3](#) on [page 8](#).

9.1 Map-model overlay [i](#)



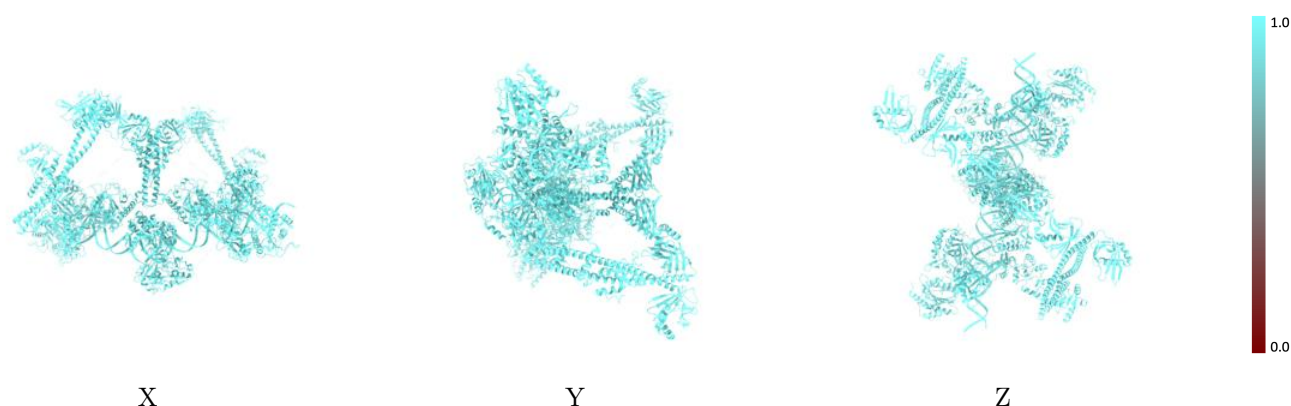
The images above show the 3D surface view of the map at the recommended contour level 0.07 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



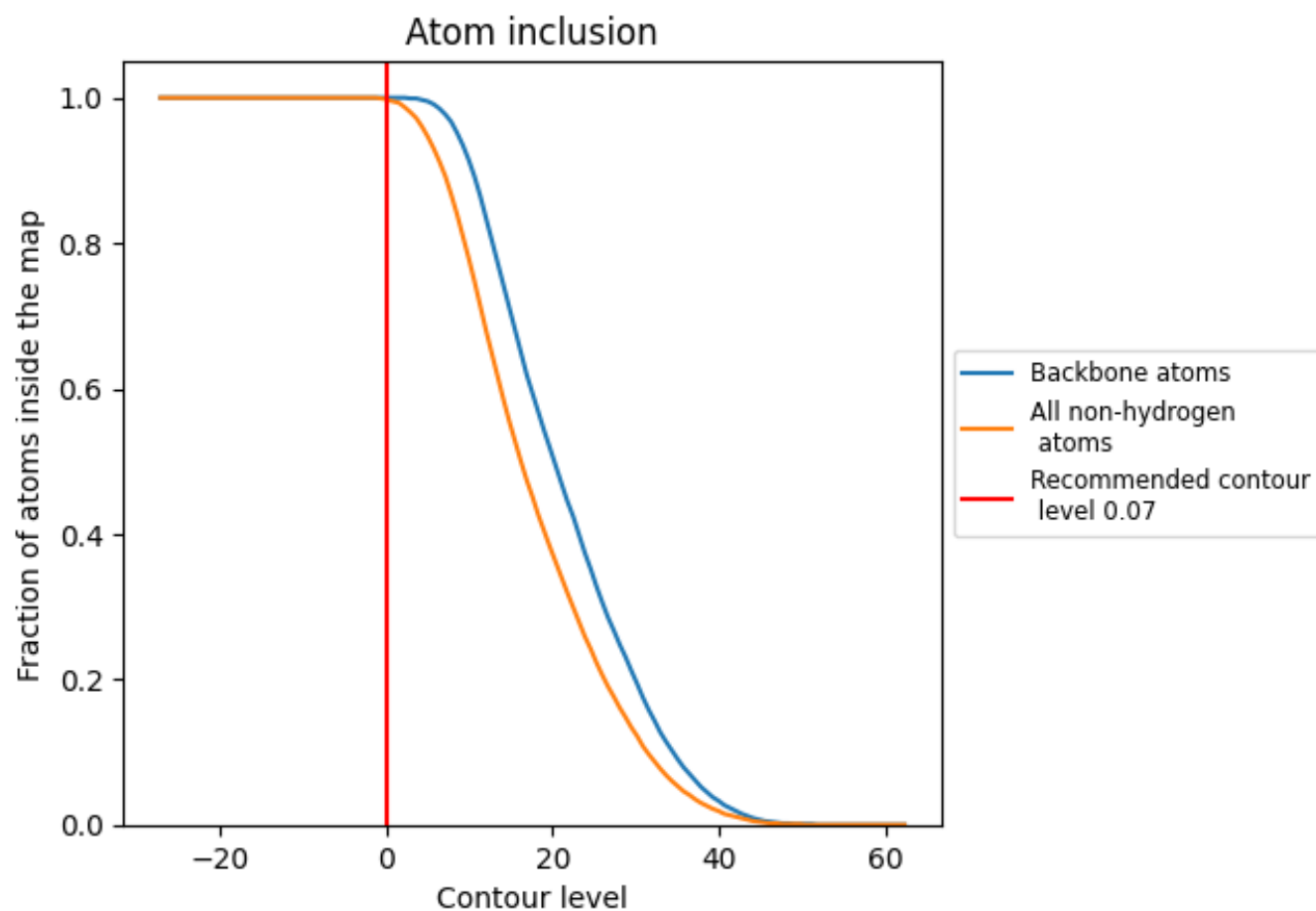
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

