



## wwPDB EM Validation Summary Report ⓘ

Apr 15, 2025 – 07:29 PM EDT

PDB ID : 9N82 / pdb\_00009n82  
EMDB ID : EMD-49109  
Title : The ligation (AMP-Lys) complex in the NHEJ pathway  
Authors : Li, J.; Liu, L.; Gellert, M.; Yang, W.  
Deposited on : 2025-02-07  
Resolution : 3.30 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](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

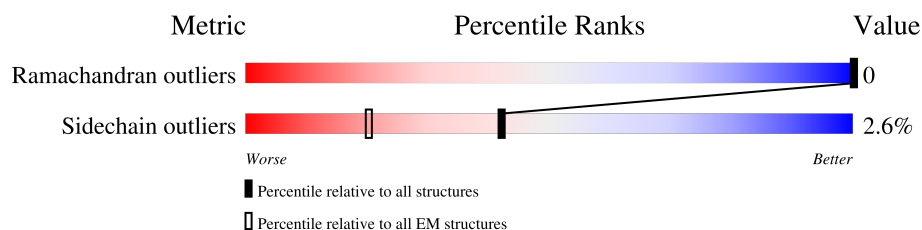
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.30 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	82% 17%
2	B	732	68% 30%
2	b	732	69% 30%
3	C	302	76% 21%
3	c	302	76% 22%
4	D	336	57% 40%
4	E	336	58% 40%
4	d	336	57% 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	51	

## 2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 37812 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	699	Total	C	N	O	S	0	0
			5648	3591	971	1053	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	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		

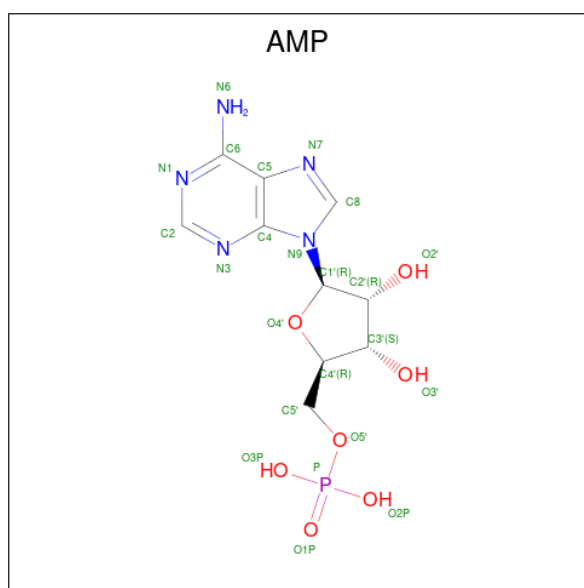
- Molecule 9 is a DNA chain called DNA (35-MER).

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
			701	334	128	205	34		

- Molecule 11 is ADENOSINE MONOPHOSPHATE (CCD ID: AMP) (formula: C<sub>10</sub>H<sub>14</sub>N<sub>5</sub>O<sub>7</sub>P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
11	F	1	Total	C	N	O	P	0
			22	10	5	6	1	







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

● Molecule 4: DNA repair protein XRCC4

Chain E: 

58%

40%

H1 K4 D68 S76 F97 E98 K99 H443 K197 A201  
GLN GLU ARG  
GLU GLU  
LYS LYS  
ASP ASP  
SER SER  
ILE ILE  
LYS LYS  
GLN GLN  
GLU GLU  
GLY GLY  
THR THR  
ALA ALA  
ILE ILE  
CYS CYS  
SER SER  
MET MET  
THR THR  
ALA ALA  
ASP ASP  
ARG ARG  
PRO PRO  
VAL VAL  
TTR TTR  
GLU GLU  
SER SER  
GLU GLU  
ASN ASN  
SER SER  
ASN ASN  
THR THR  
LEU LEU  
SER SER

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

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ASN ASN  
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ARG ARG  
ASN ASN  
SER SER  
SER SER  
PRO PRO  
GLU GLU  
ASP ASP  
PHE PHE  
GLU GLU  
ILE ILE

● Molecule 4: DNA repair protein XRCC4

Chain d: 

57%

40%

H1 E13 H18 Q21 V67 S92 C130 D157 Y177 A201  
ALA GLN  
GLU GLU  
ARG ARG  
GLU GLU  
LYS LYS  
ASP ASP  
ILE ILE  
SER SER  
SER SER  
LEU LEU  
ASP ASP  
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THR THR  
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GLU GLU  
MET MET  
SER SER  
SER SER  
LEU LEU  
THR THR  
GLU GLU  
ASP ASP  
PHE PHE  
GLU GLU  
ILE ILE

● Molecule 4: DNA repair protein XRCC4

Chain e: 

59%

40%

H1 K63 S89 F106 Y129 A201  
ALA GLN  
GLU GLU  
ARG ARG  
GLU GLU  
LYS LYS  
ASP ASP  
ILE ILE  
SER SER  
SER SER  
LEU LEU  
THR THR  
VAL VAL  
GLN GLN  
CYS CYS  
SER SER  
GLU GLU  
MET MET  
THR THR  
ALA ALA  
ASP ASP  
ARG ARG  
PRO PRO  
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GLU GLU  
LYS LYS  
ASN ASN  
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ALA ALA  
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SER SER  
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SER SER  
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SER SER  
ALA ALA  
GLU GLU  
ASN ASN  
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SER SER  
LEU LEU  
THR THR  
GLU GLU  
THR THR  
LEU LEU  
ASN ASN  
SER SER  
SER SER  
PRO PRO  
GLU GLU  
ASP ASP  
PHE PHE  
LEU LEU  
SER SER  
GLU GLU  
ILE ILE

● Molecule 5: DNA ligase 4

Chain F: 

75%

24%

GLY PRO  
VAL VAL  
MET MET  
ALA ALA  
SER SER  
GLN GLN  
THR THR  
S7 S21 H57 M68 T116 D150 N158 D359 F367 Q404 H409 P452  
GLU TYR  
VAL VAL  
SER SER  
GLY GLY  
LEU LEU  
MET MET  
ASP ASP  
GLU GLU  
LYS LYS  
LEU LEU  
ASP ASP  
ILE ILE  
LEU LEU  
ILE ILE  
VAL VAL  
GLY GLY  
GLY GLY  
TYR TYR  
TRP TRP  
GLY GLY  
LYS LYS  
CYS CYS  
MET MET  
THR THR  
GLY GLY  
VAL VAL  
MET MET

SER HIS  
PHE PHE  
LEU LEU  
CYS CYS  
VAL VAL  
VAL VAL  
ALA ALA  
GLU GLU  
LYS LYS  
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PRO PRO  
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LYS LYS  
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SER SER  
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THR THR  
LYS LYS  
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GLY GLY  
CYS CYS  
VAL VAL  
SER SER  
LEU LEU  
MET MET  
GLY GLY  
CYS CYS

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



Chain f:  27% . 72%



Chain G:  11% 89%

PRO	GLN	ARG	GLY	GLY	PRO	GLY	PRO	GLY	VAL	ARG	ARG	ARG	C180	E183	E203	THR
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- Molecule 6: Protein PAXX

Chain H:  11% 89%

LEU	TRP	SER	THR	THR	PHE	THR	PRO	ASP	SER	SER	LEU	ALA	ALA	LEU	LYS	ALA	ARG	ARG	PHE	GLY	LEU	SER	ALA	ALA	ALA	GLU	ASP	ILE	THR	THR	ARG	ARG	PHE	ARG	ALA	ALA	CYS	CYS	GLN	GLN	VAL	ALA	ALA	LEU	ALA	LEU	THR	LEU	GLN	GLN	ASP	ARG	ALA	SER	LEU	THR	LEU	LEU	SER	GLY	GLY	PRO	SER	ALA	ALA	LEU	ALA
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PHE ASP LEU LEU SER LYS VAL PRO GLY GLU GLU ALA ALA PRO ARG ARG LEU LEU ARG ALA LEU THR LEU LEU LEU LYS ARG ARG VAL TRP SER SER LEU LEU ALA ALA ALA GLU GLU GLU THR THR VAL VAL SER ARG ARG PRO PRO PRO GLY GLY PRO PRO ASP ASP

PRO	GLN	ARG	GLY	GLY	PRO	GLY	PRO	GLY	VAL	ARG	ARG	ARG	C180	D202	GLU	THR
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- Molecule 7: DNA (39-MER)

Chain I:  57% 43%

DC
DG
DC
DG
DC
DC
DC
DA
DG
DT
DT
DT
DC
DC
DC
DA
DG
DC
DT
DA
DA
DA
DT
DA
DA
DC
DT
DT
DA
A30
C68

- Molecule 8: DNA (38-MER)

Chain J:  56% 44%

DC
DG
DC
DG
DC
DC
DA
DG
DC
DT
DT
DT
DC
DC
DA
DG
DC
DT
DA
DA
DT
DA
DA
DA
DC
DT
DA
DA
A31
C68

- Molecule 9: DNA (35-MER)

Chain K:  69% 31%

G1	T35	DT	DA	DG	DT	DT	DT	DT	DA	DT	DT	DG	DG	DG	DC	DC	DC	DG
----	-----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----

- Molecule 10: DNA (34-MER)

Chain L:  65% 33%

A1	T34	DT	DT	DA	DG	DT	DT	DT	DA	DT	DT	DG	DG	DG	DC	DG	DC	DG
----	-----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	78835	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	0.550	Depositor
Minimum map value	-0.181	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.013	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

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	0.48	0/5626
2	B	0.25	0/4196	0.47	0/5661
2	b	0.25	0/4173	0.46	0/5631
3	C	0.25	0/1926	0.50	0/2610
3	c	0.25	0/1914	0.48	0/2594
4	D	0.27	0/1657	0.52	0/2228
4	E	0.27	0/1657	0.51	0/2228
4	d	0.28	0/1657	0.50	0/2228
4	e	0.27	0/1657	0.50	0/2228
5	F	0.26	0/5767	0.48	0/7775
5	f	0.24	0/2118	0.46	0/2862
6	G	0.26	0/178	0.36	0/238
6	H	0.25	0/169	0.36	0/226
7	I	0.52	0/883	0.94	0/1358
8	J	0.51	0/869	0.93	0/1338
9	K	0.53	0/812	0.91	0/1253
10	L	0.64	1/786 (0.1%)	0.94	0/1210
All	All	0.29	1/38846 (0.0%)	0.54	0/53022

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	L	1	DA	OP3-P	-10.71	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 [i](#)

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

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	512/612 (84%)	500 (98%)	12 (2%)	0	100	100
1	a	505/612 (82%)	499 (99%)	6 (1%)	0	100	100
2	B	509/732 (70%)	501 (98%)	8 (2%)	0	100	100
2	b	506/732 (69%)	499 (99%)	7 (1%)	0	100	100
3	C	234/302 (78%)	224 (96%)	10 (4%)	0	100	100
3	c	232/302 (77%)	226 (97%)	6 (3%)	0	100	100
4	D	199/336 (59%)	195 (98%)	4 (2%)	0	100	100
4	E	199/336 (59%)	194 (98%)	5 (2%)	0	100	100
4	d	199/336 (59%)	191 (96%)	8 (4%)	0	100	100
4	e	199/336 (59%)	196 (98%)	3 (2%)	0	100	100
5	F	695/914 (76%)	665 (96%)	30 (4%)	0	100	100
5	f	253/914 (28%)	247 (98%)	6 (2%)	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	4285/6900 (62%)	4179 (98%)	106 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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%)	458 (98%)	10 (2%)	48	70
1	a	460/550 (84%)	452 (98%)	8 (2%)	56	74
2	B	464/649 (72%)	453 (98%)	11 (2%)	44	68
2	b	462/649 (71%)	455 (98%)	7 (2%)	60	77
3	C	210/264 (80%)	202 (96%)	8 (4%)	28	56
3	c	209/264 (79%)	203 (97%)	6 (3%)	37	63
4	D	180/303 (59%)	170 (94%)	10 (6%)	17	45
4	E	180/303 (59%)	173 (96%)	7 (4%)	27	55
4	d	180/303 (59%)	172 (96%)	8 (4%)	24	52
4	e	180/303 (59%)	176 (98%)	4 (2%)	47	69
5	F	626/810 (77%)	609 (97%)	17 (3%)	40	65
5	f	231/810 (28%)	226 (98%)	5 (2%)	47	69
6	G	19/173 (11%)	18 (95%)	1 (5%)	19	47
6	H	18/173 (10%)	18 (100%)	0	100	100
All	All	3887/6104 (64%)	3785 (97%)	102 (3%)	42	66

5 of 102 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	F	742	PHE
1	a	523	ASP
5	f	759	ASP
5	F	754	PHE
1	a	95	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	232	HIS
1	A	293	ASN

### 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](#)

1 ligand is modelled in this entry.

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	F	1001	-	17,24,25	0.77	0	16,35,38	1.37	2 (12%)

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	F	1001	-	-	0/3/25/26	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	F	1001	AMP	N3-C2-N1	-4.22	122.94	128.67
11	F	1001	AMP	C4-C5-N7	-2.58	106.61	109.34

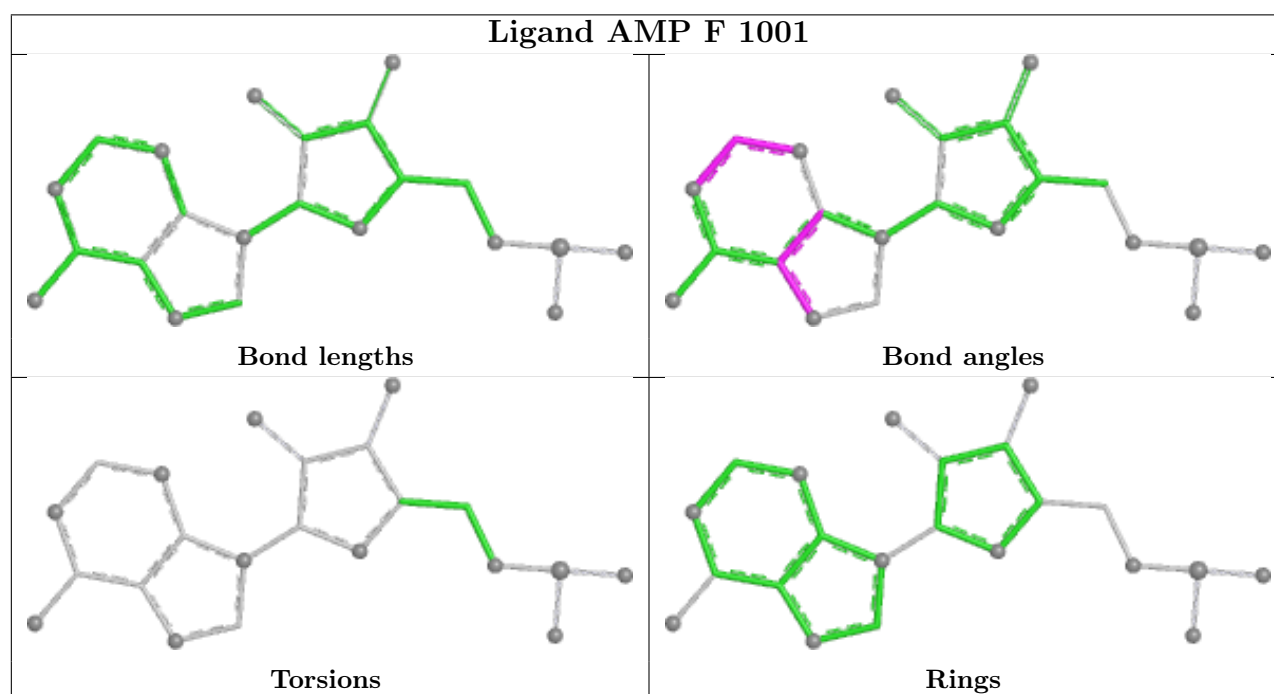
There are no chirality outliers.

There are no torsion outliers.

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.

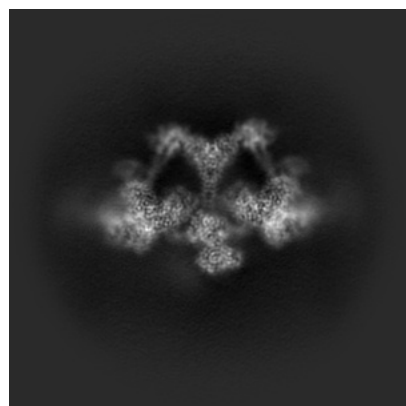
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-49109. These allow visual inspection of the internal detail of the map and identification of artifacts.

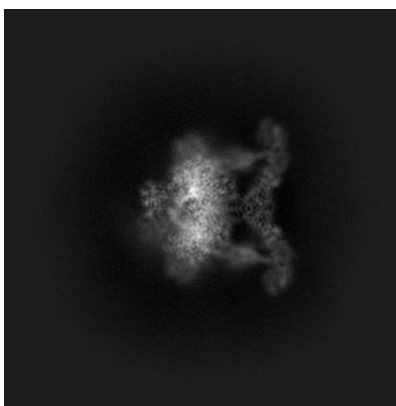
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

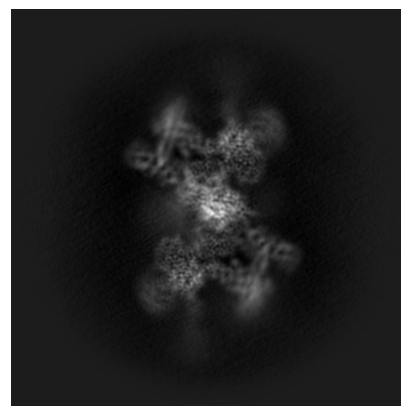
#### 6.1.1 Primary map



X

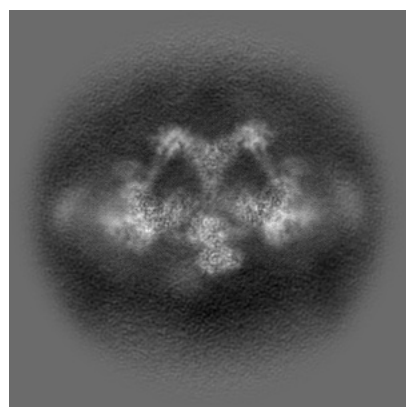


Y

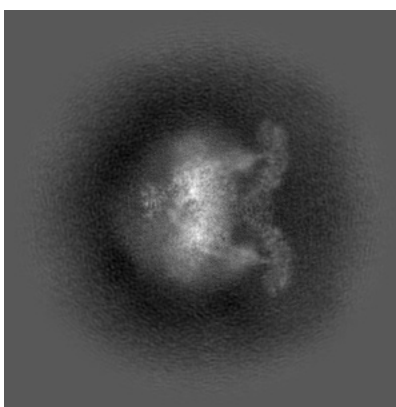


Z

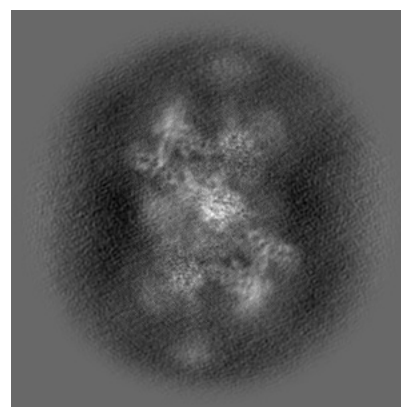
#### 6.1.2 Raw map



X



Y

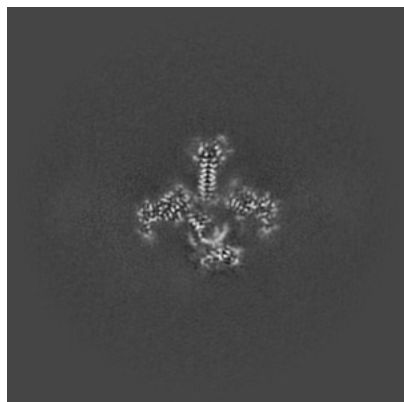


Z

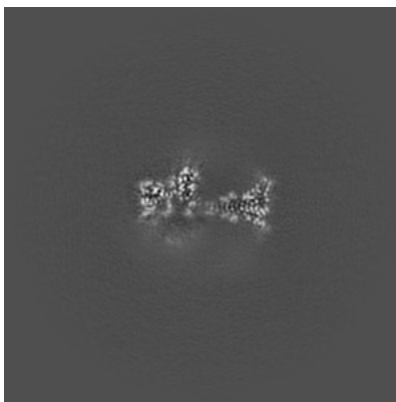
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

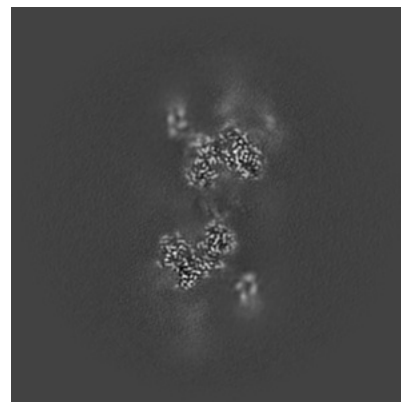
### 6.2.1 Primary map



X Index: 256

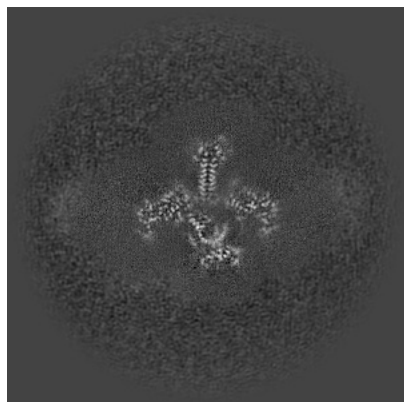


Y Index: 256

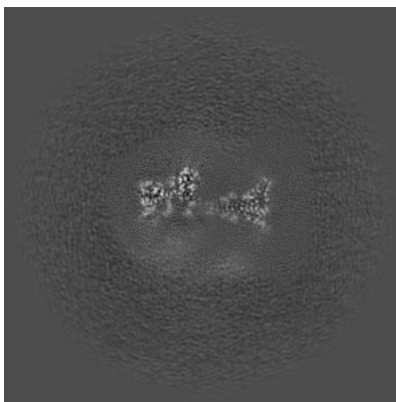


Z Index: 256

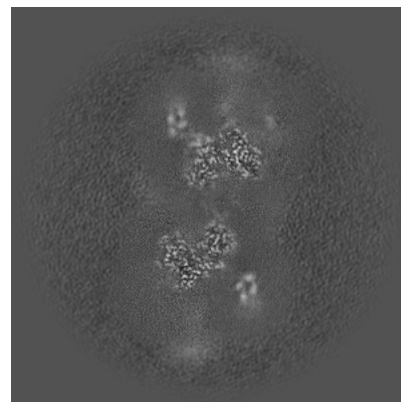
### 6.2.2 Raw map



X Index: 256



Y Index: 256

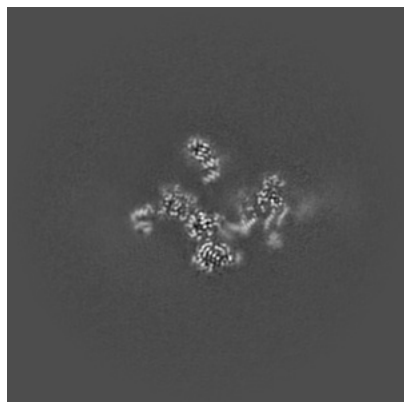


Z Index: 256

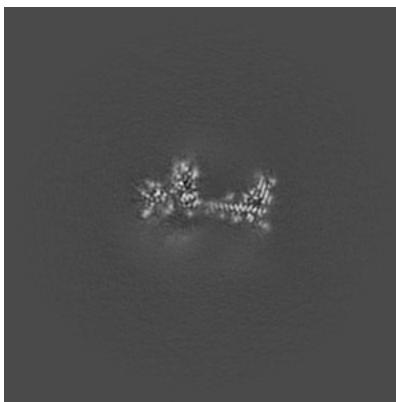
The images above show central slices of the map in three orthogonal directions.

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

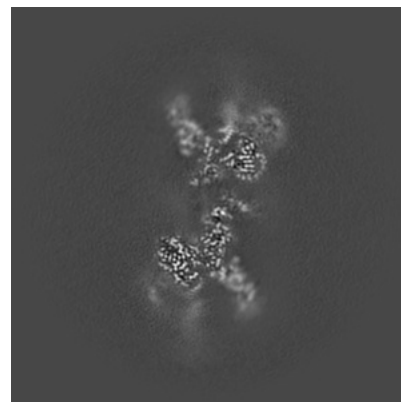
### 6.3.1 Primary map



X Index: 271

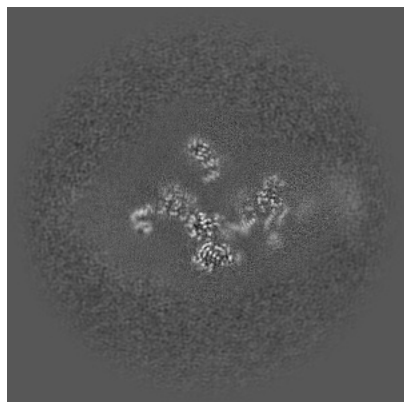


Y Index: 252

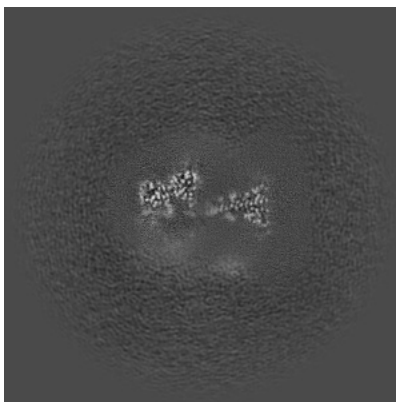


Z Index: 247

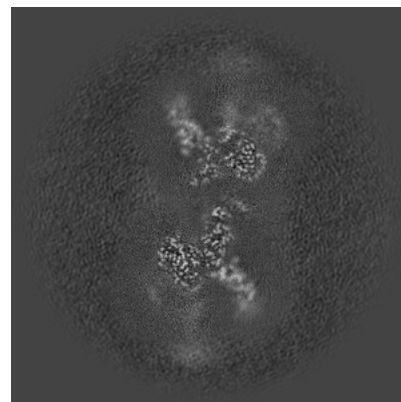
### 6.3.2 Raw map



X Index: 271



Y Index: 259

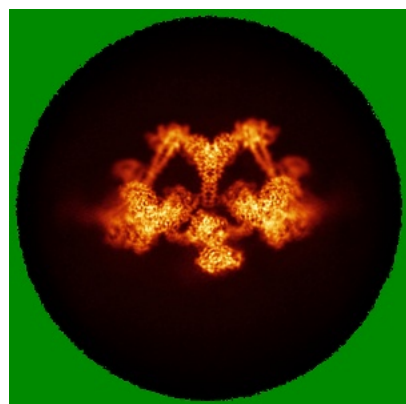


Z Index: 248

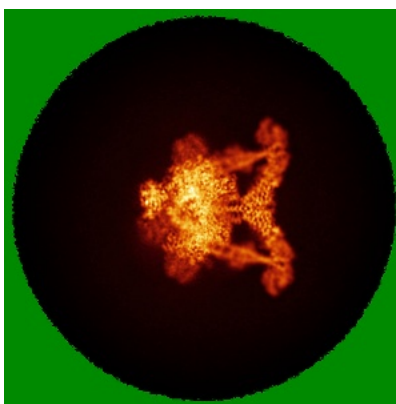
The images above show the largest variance slices of the map in three orthogonal directions.

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

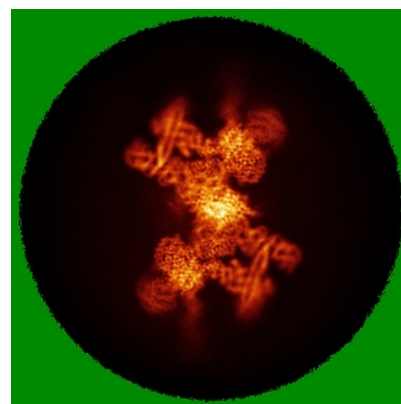
### 6.4.1 Primary map



X

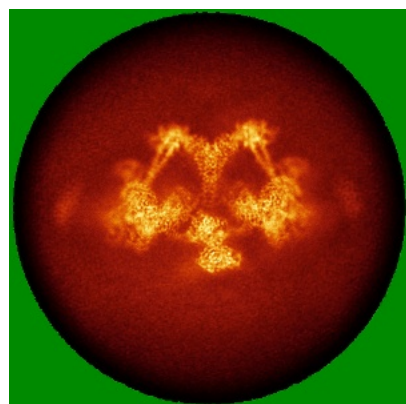


Y

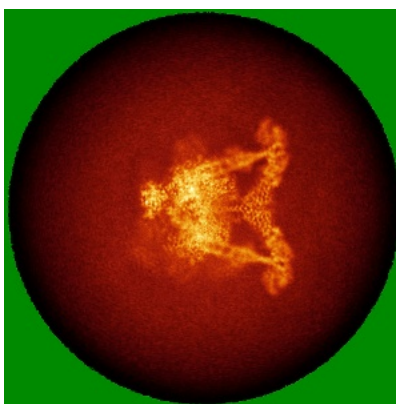


Z

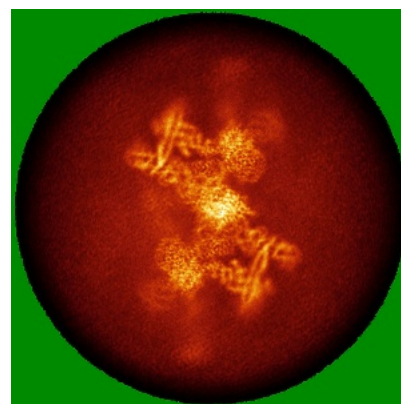
### 6.4.2 Raw map



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\_49109\_msk\_1.map [i](#)



X



Y



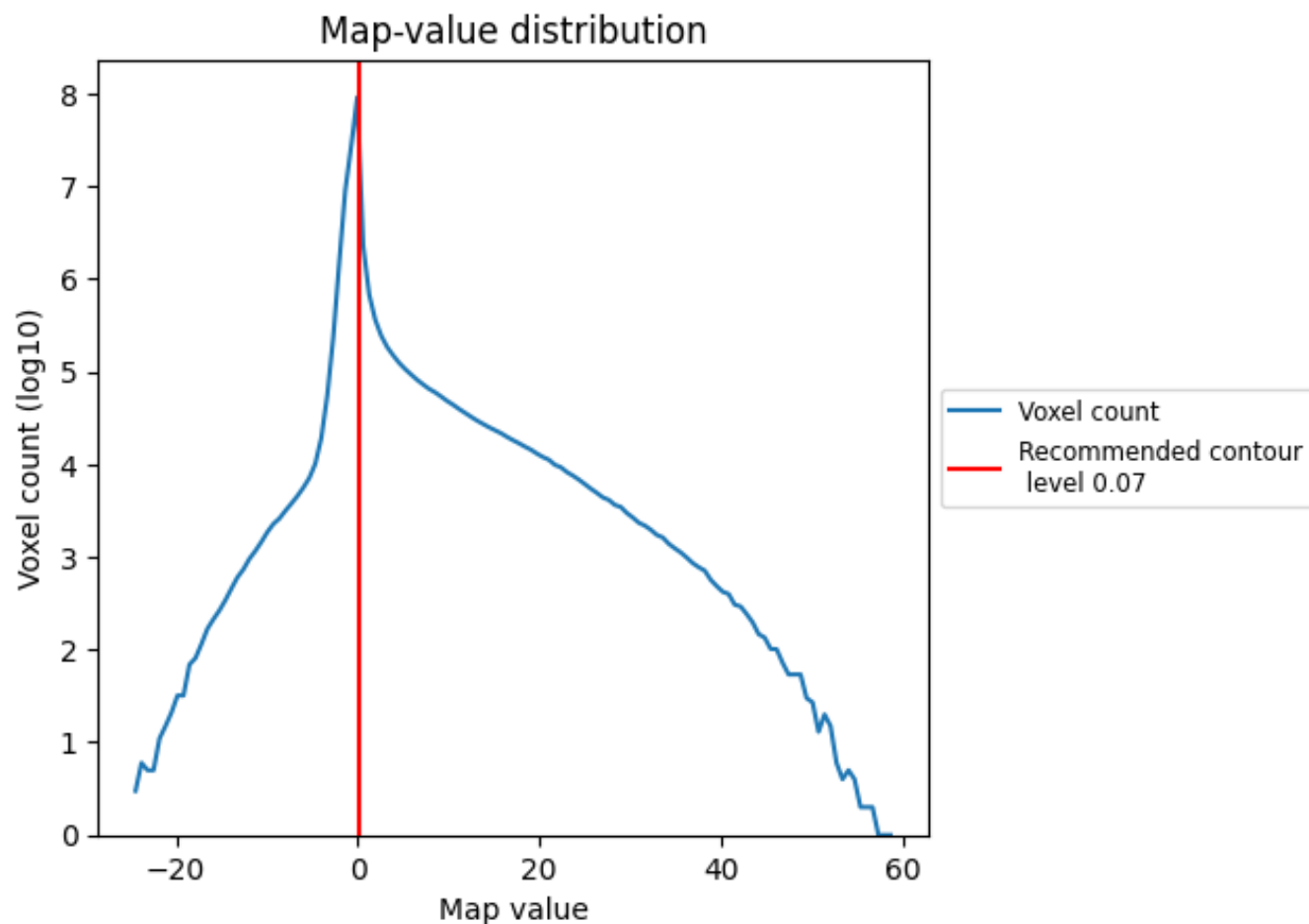
Z



## 7 Map analysis [i](#)

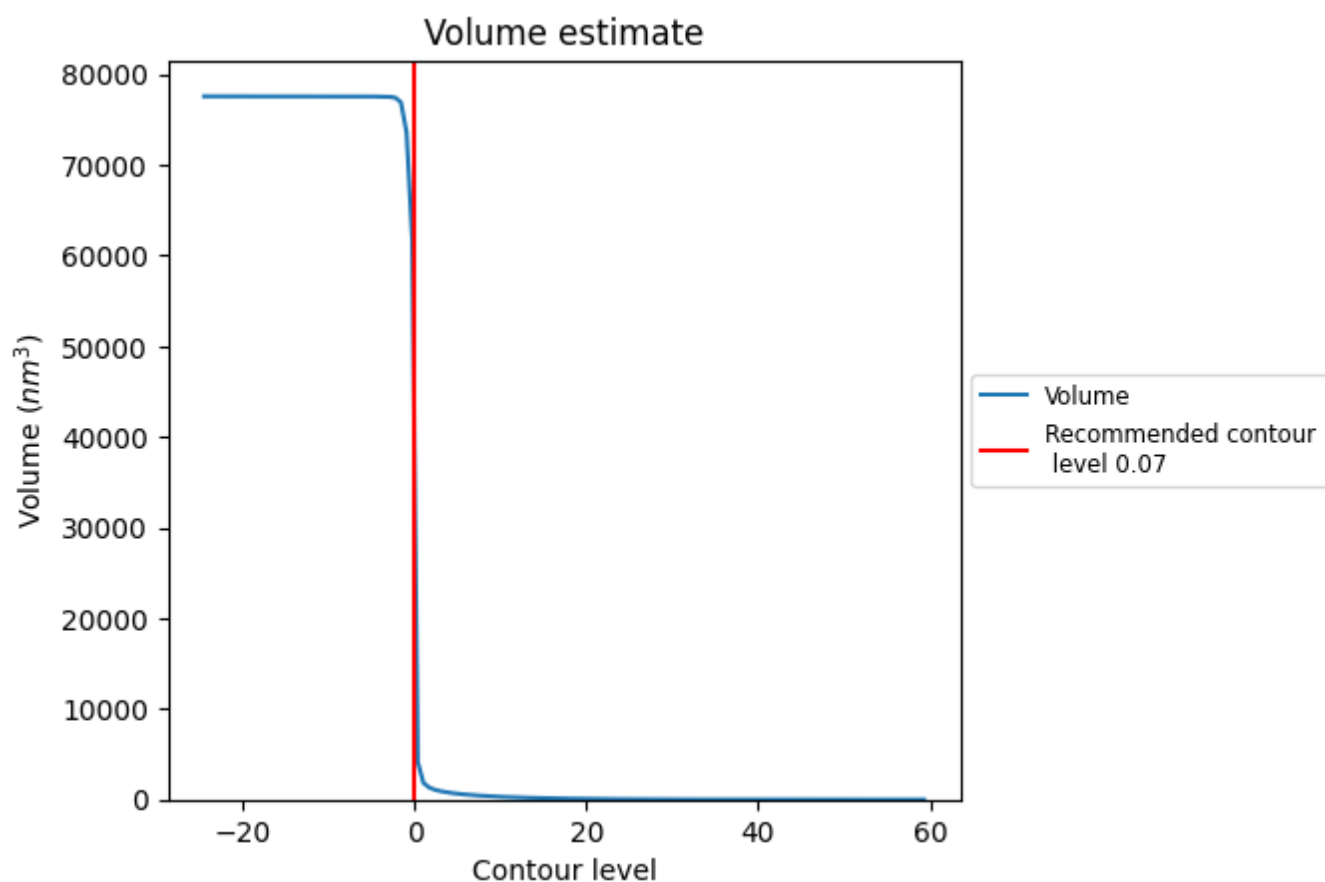
This section contains the results of statistical analysis of the map.

### 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.

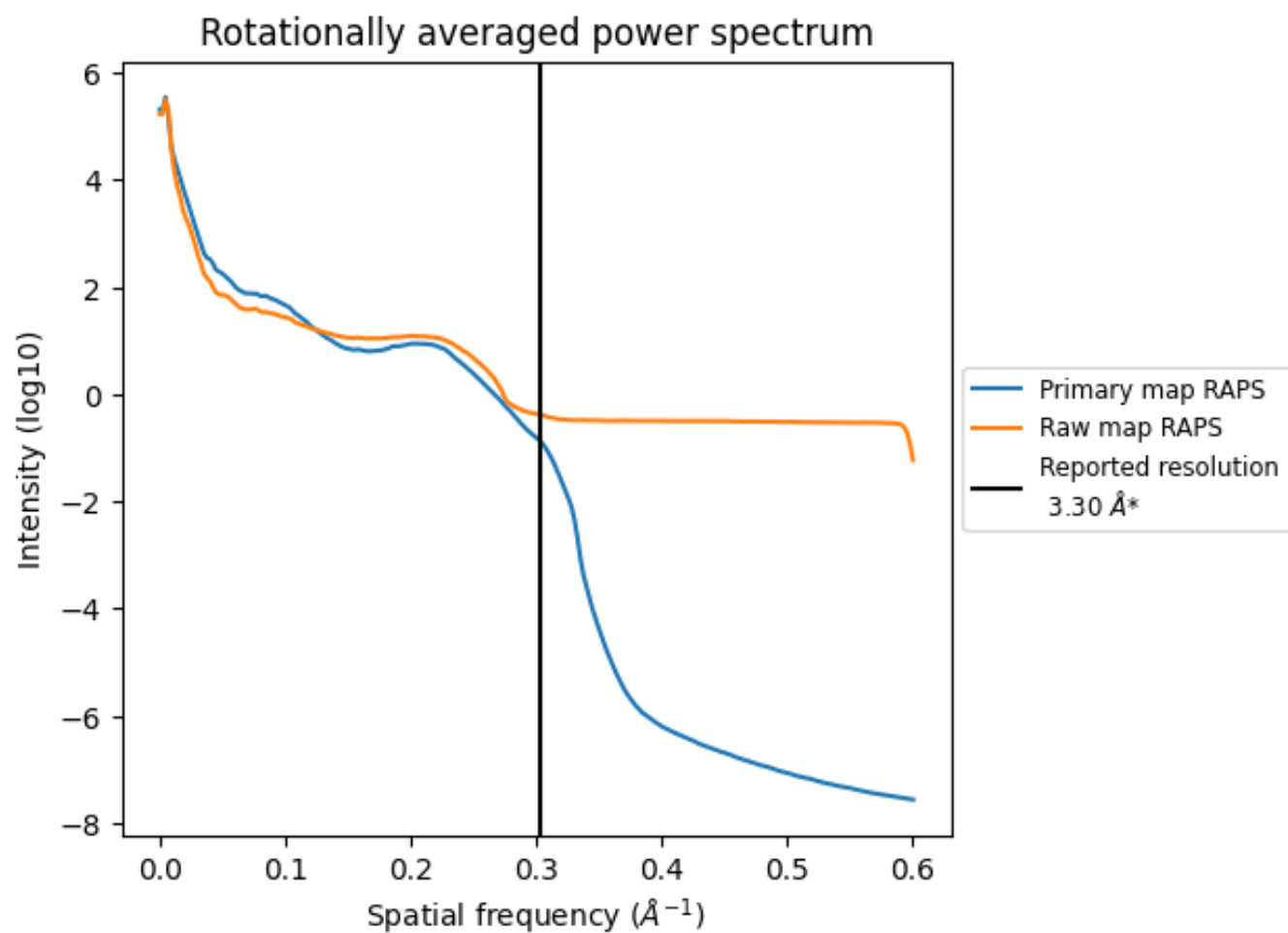
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 33482  $\text{nm}^3$ ; this corresponds to an approximate mass of 30245 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 ⓘ

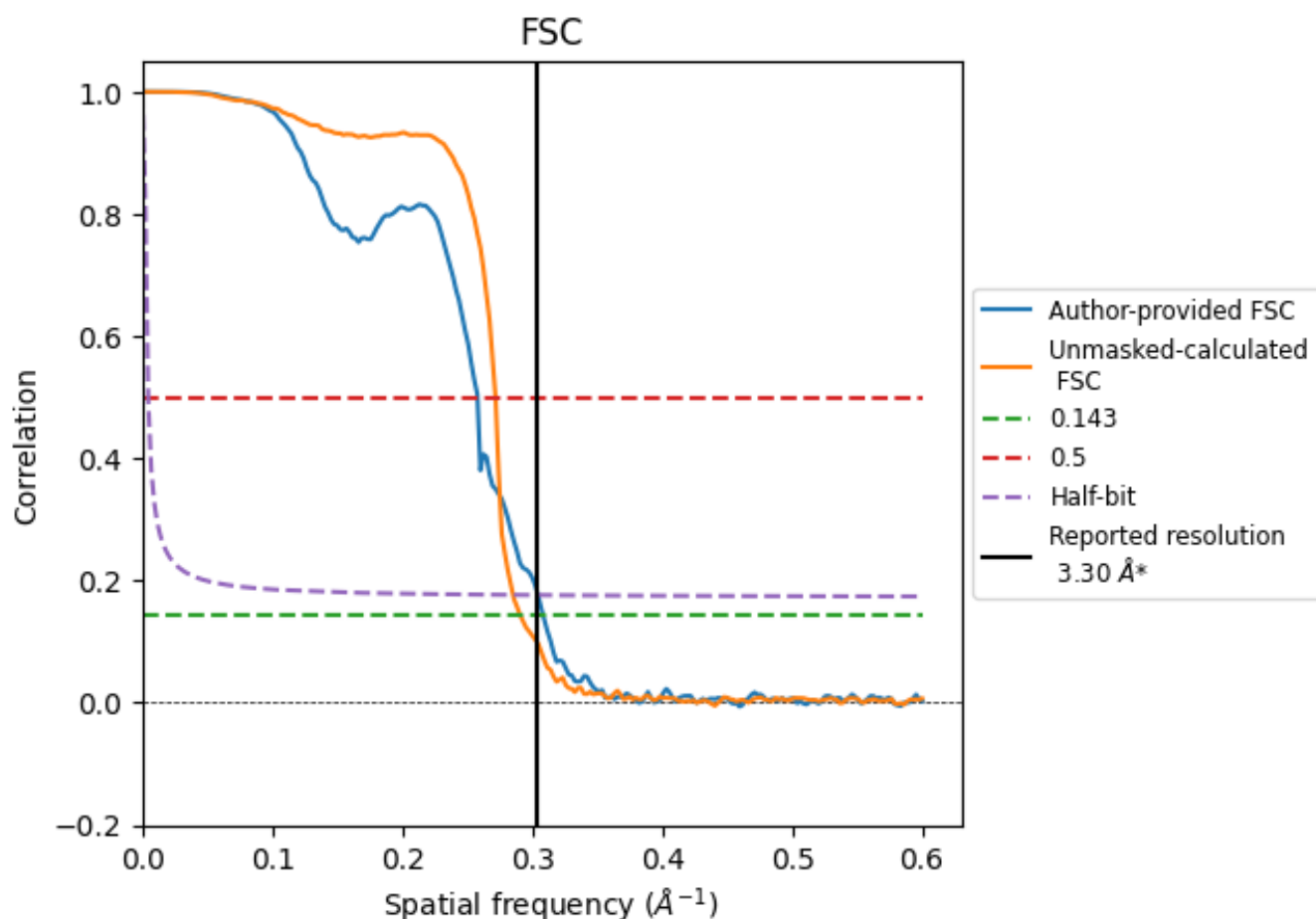


\*Reported resolution corresponds to spatial frequency of 0.303 Å<sup>-1</sup>

## 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  $0.303 \text{ \AA}^{-1}$

## 8.2 Resolution estimates [i](#)

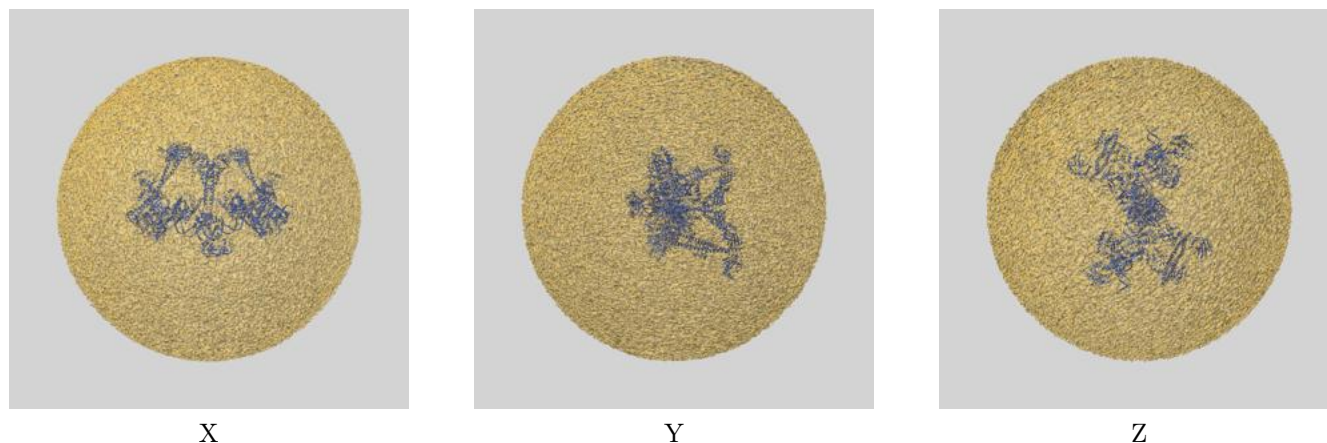
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.24	3.88	3.28
Unmasked-calculated*	3.44	3.68	3.50

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

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

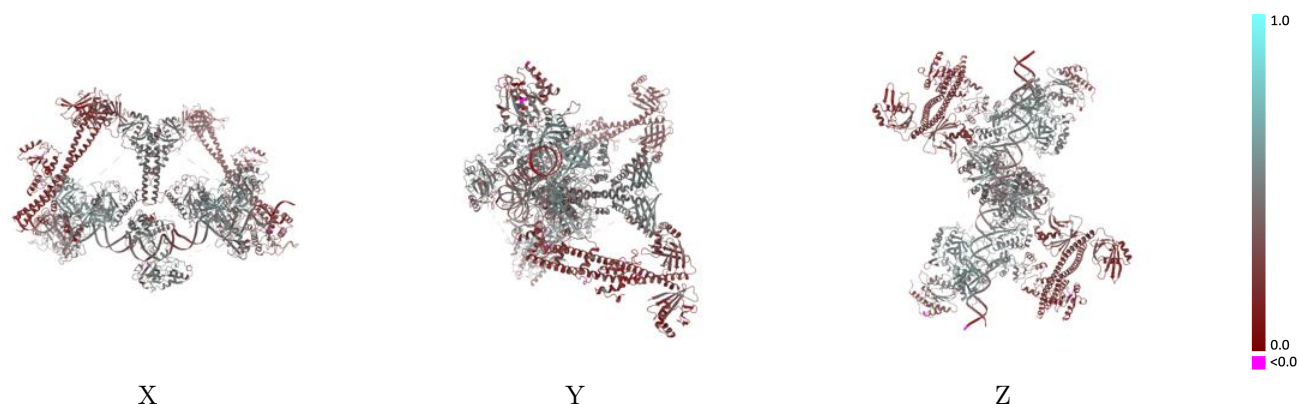
This section contains information regarding the fit between EMDB map EMD-49109 and PDB model 9N82. Per-residue inclusion information can be found in [section 3](#) on [page 8](#).

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



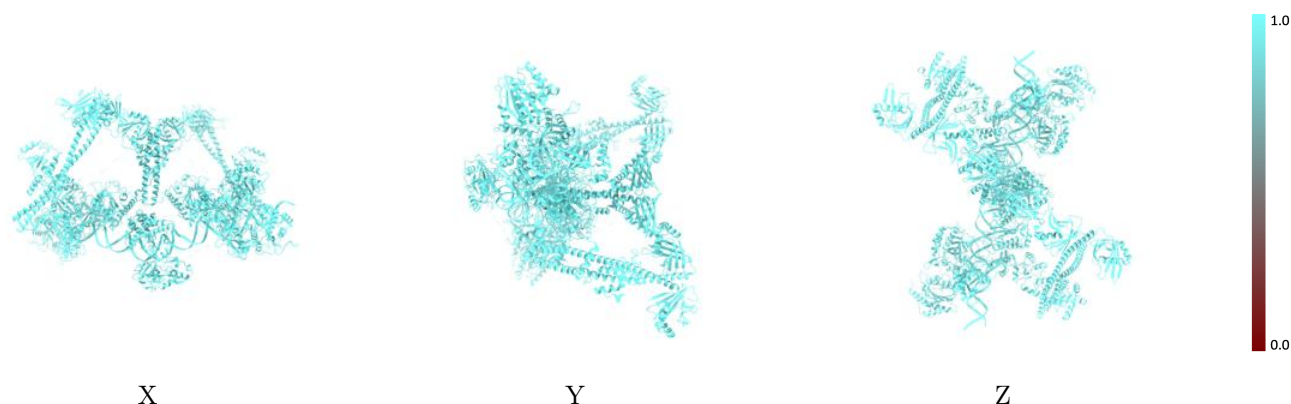
The images above show the 3D surface view of the map at the recommended contour level 0.07 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



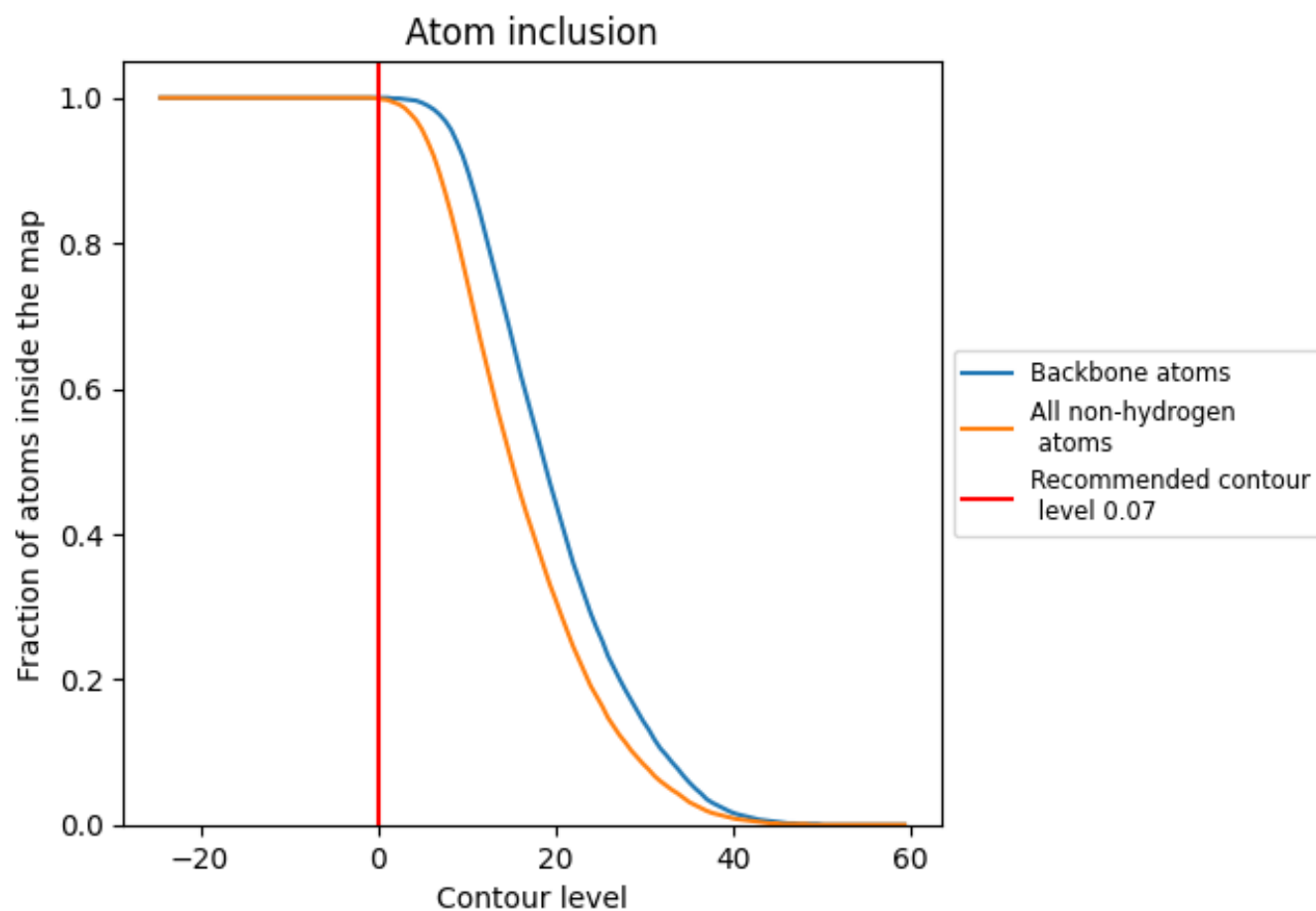
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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	 0.9990	 0.3900
A	 1.0000	 0.4760
B	 1.0000	 0.4290
C	 0.9990	 0.4470
D	 0.9980	 0.2310
E	 0.9980	 0.2610
F	 0.9950	 0.3660
G	 0.9940	 0.4800
H	 1.0000	 0.5020
I	 1.0000	 0.3800
J	 1.0000	 0.3310
K	 1.0000	 0.3850
L	 1.0000	 0.3440
a	 1.0000	 0.5030
b	 1.0000	 0.4480
c	 1.0000	 0.4400
d	 0.9990	 0.2320
e	 1.0000	 0.2720
f	 0.9990	 0.2440

