



wwPDB EM Validation Summary Report ⓘ

Mar 23, 2026 – 07:07 PM UTC

PDB ID : 8DS9 / pdb_00008ds9
EMDB ID : EMD-27686
Title : LRRC8A:C in MSPE3D1 nanodisc top focus
Authors : Kern, D.M.; Brohawn, S.G.
Deposited on : 2022-07-21
Resolution : 3.17 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

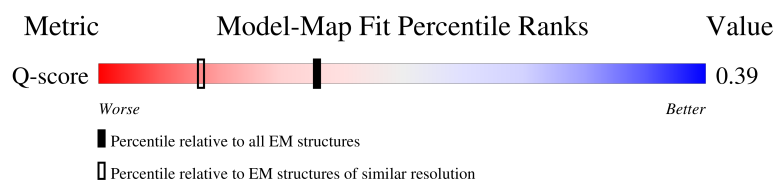
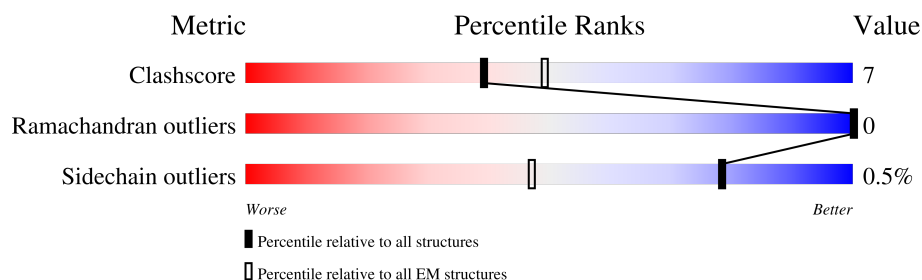
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.17 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14465 (2.67 - 3.67)

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	911	 17% 5% 78%
1	B	911	 18% 78%
1	C	911	 29% 6% 65%
1	D	911	 27% 7% 65%

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Mol	Chain	Length	Quality of chain
1	E	911	<div><div><div></div><div></div><div></div><div></div></div><div>5%17%5%78%</div></div>
2	F	813	<div><div><div></div><div></div><div></div><div></div></div><div>19%5%77%</div></div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12039 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 Volume-regulated anion channel subunit LRRC8A, Soluble cytochrome b562.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	197	Total	C	N	O	S	0	0
			1662	1116	258	273	15		
1	B	197	Total	C	N	O	S	0	0
			1662	1116	258	273	15		
1	C	320	Total	C	N	O	S	0	0
			2685	1771	431	466	17		
1	D	316	Total	C	N	O	S	0	0
			2646	1747	424	458	17		
1	E	197	Total	C	N	O	S	0	0
			1662	1116	258	273	15		

There are 85 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	68D	TRP	-	linker	UNP Q80WG5
A	68E	ALA	-	linker	UNP Q80WG5
A	68F	ALA	-	linker	UNP Q80WG5
A	68G	SER	-	linker	UNP Q80WG5
A	68H	SER	-	linker	UNP Q80WG5
A	68O	TRP	MET	conflict	UNP P0ABE7
A	72F	ILE	HIS	conflict	UNP P0ABE7
A	72J	LEU	-	linker	UNP P0ABE7
A	811	SER	-	expression tag	UNP Q80WG5
A	812	ASN	-	expression tag	UNP Q80WG5
A	813	SER	-	expression tag	UNP Q80WG5
A	814	LEU	-	expression tag	UNP Q80WG5
A	815	GLU	-	expression tag	UNP Q80WG5
A	816	VAL	-	expression tag	UNP Q80WG5
A	817	LEU	-	expression tag	UNP Q80WG5
A	818	PHE	-	expression tag	UNP Q80WG5
A	819	GLN	-	expression tag	UNP Q80WG5
B	68D	TRP	-	linker	UNP Q80WG5
B	68E	ALA	-	linker	UNP Q80WG5

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Chain	Residue	Modelled	Actual	Comment	Reference
B	68F	ALA	-	linker	UNP Q80WG5
B	68G	SER	-	linker	UNP Q80WG5
B	68H	SER	-	linker	UNP Q80WG5
B	68O	TRP	MET	conflict	UNP P0ABE7
B	72F	ILE	HIS	conflict	UNP P0ABE7
B	72J	LEU	-	linker	UNP P0ABE7
B	811	SER	-	expression tag	UNP Q80WG5
B	812	ASN	-	expression tag	UNP Q80WG5
B	813	SER	-	expression tag	UNP Q80WG5
B	814	LEU	-	expression tag	UNP Q80WG5
B	815	GLU	-	expression tag	UNP Q80WG5
B	816	VAL	-	expression tag	UNP Q80WG5
B	817	LEU	-	expression tag	UNP Q80WG5
B	818	PHE	-	expression tag	UNP Q80WG5
B	819	GLN	-	expression tag	UNP Q80WG5
C	68D	TRP	-	linker	UNP Q80WG5
C	68E	ALA	-	linker	UNP Q80WG5
C	68F	ALA	-	linker	UNP Q80WG5
C	68G	SER	-	linker	UNP Q80WG5
C	68H	SER	-	linker	UNP Q80WG5
C	68O	TRP	MET	conflict	UNP P0ABE7
C	72F	ILE	HIS	conflict	UNP P0ABE7
C	72J	LEU	-	linker	UNP P0ABE7
C	811	SER	-	expression tag	UNP Q80WG5
C	812	ASN	-	expression tag	UNP Q80WG5
C	813	SER	-	expression tag	UNP Q80WG5
C	814	LEU	-	expression tag	UNP Q80WG5
C	815	GLU	-	expression tag	UNP Q80WG5
C	816	VAL	-	expression tag	UNP Q80WG5
C	817	LEU	-	expression tag	UNP Q80WG5
C	818	PHE	-	expression tag	UNP Q80WG5
C	819	GLN	-	expression tag	UNP Q80WG5
D	68D	TRP	-	linker	UNP Q80WG5
D	68E	ALA	-	linker	UNP Q80WG5
D	68F	ALA	-	linker	UNP Q80WG5
D	68G	SER	-	linker	UNP Q80WG5
D	68H	SER	-	linker	UNP Q80WG5
D	68O	TRP	MET	conflict	UNP P0ABE7
D	72F	ILE	HIS	conflict	UNP P0ABE7
D	72J	LEU	-	linker	UNP P0ABE7
D	811	SER	-	expression tag	UNP Q80WG5
D	812	ASN	-	expression tag	UNP Q80WG5

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Chain	Residue	Modelled	Actual	Comment	Reference
D	813	SER	-	expression tag	UNP Q80WG5
D	814	LEU	-	expression tag	UNP Q80WG5
D	815	GLU	-	expression tag	UNP Q80WG5
D	816	VAL	-	expression tag	UNP Q80WG5
D	817	LEU	-	expression tag	UNP Q80WG5
D	818	PHE	-	expression tag	UNP Q80WG5
D	819	GLN	-	expression tag	UNP Q80WG5
E	68D	TRP	-	linker	UNP Q80WG5
E	68E	ALA	-	linker	UNP Q80WG5
E	68F	ALA	-	linker	UNP Q80WG5
E	68G	SER	-	linker	UNP Q80WG5
E	68H	SER	-	linker	UNP Q80WG5
E	68O	TRP	MET	conflict	UNP P0ABE7
E	72F	ILE	HIS	conflict	UNP P0ABE7
E	72J	LEU	-	linker	UNP P0ABE7
E	811	SER	-	expression tag	UNP Q80WG5
E	812	ASN	-	expression tag	UNP Q80WG5
E	813	SER	-	expression tag	UNP Q80WG5
E	814	LEU	-	expression tag	UNP Q80WG5
E	815	GLU	-	expression tag	UNP Q80WG5
E	816	VAL	-	expression tag	UNP Q80WG5
E	817	LEU	-	expression tag	UNP Q80WG5
E	818	PHE	-	expression tag	UNP Q80WG5
E	819	GLN	-	expression tag	UNP Q80WG5

- Molecule 2 is a protein called Volume-regulated anion channel subunit LRRC8C.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	F	191	Total	C	N	O	S	0	0
			1599	1071	246	264	18		

There are 10 discrepancies between the modelled and reference sequences:

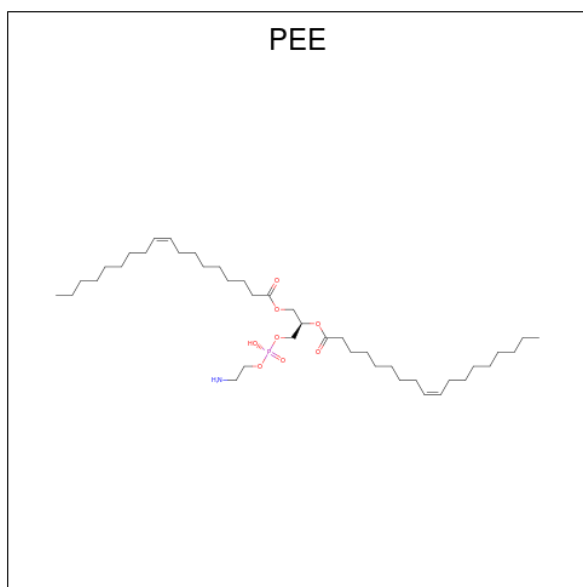
Chain	Residue	Modelled	Actual	Comment	Reference
F	804	SER	-	expression tag	UNP Q8R502
F	805	ASN	-	expression tag	UNP Q8R502
F	806	SER	-	expression tag	UNP Q8R502
F	807	GLU	-	expression tag	UNP Q8R502
F	808	ASN	-	expression tag	UNP Q8R502
F	809	LEU	-	expression tag	UNP Q8R502
F	810	TYR	-	expression tag	UNP Q8R502
F	811	PHE	-	expression tag	UNP Q8R502

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Chain	Residue	Modelled	Actual	Comment	Reference
F	812	GLN	-	expression tag	UNP Q8R502
F	813	GLY	-	expression tag	UNP Q8R502

- Molecule 3 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (CCD ID: PEE) (formula: $C_{41}H_{78}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
3	C	1	Total	C	O			0
			10	8	2			
3	C	1	Total	C	O			0
			12	10	2			
3	D	1	Total	C	N	O	P	0
			44	34	1	8	1	
3	D	1	Total	C	N	O	P	0
			51	41	1	8	1	

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		AltConf
4	A	1	Total	O	0
			1	1	
4	B	1	Total	O	0
			1	1	
4	C	1	Total	O	0
			1	1	
4	D	1	Total	O	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
4	E	1	Total	O	0
			1	1	
4	F	1	Total	O	0
			1	1	

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

- Molecule 1: Volume-regulated anion channel subunit LRRC8A, Soluble cytochrome b562

Chain B:  18% 78%

Protein	Score
PHE	0.00
ASP	0.00
ILE	0.00
LEU	0.00
VAL	0.00
GLY	0.00
GLN	0.00
ILE	0.00
ASP	0.00
ASP	0.00
ALA	0.00
LEU	0.00
LYS	0.00
LEU	0.00
ALA	0.00
ASN	0.00
GLU	0.00
GLY	0.00
VAL	0.00
VAL	0.00
LYS	0.00
GLU	0.00
ALA	0.00
GLN	0.00
ALA	0.00
ALA	0.00
ALA	0.00
GLU	0.00
GLN	0.00
LEU	0.00
LYS	0.00
THR	0.00
ARG	0.00
ASN	0.00
ALA	0.00
TYR	0.00
ILE	0.00
GLN	0.00
LYS	0.00
TYR	0.00
LEU	0.00
ASP	0.00
T92	0.00
Q106	0.00
R117	0.00
L118	0.00
H119	0.00
L130	0.00
L131	0.00
H132	0.00
I136	0.00
F136	0.00
L137	0.00
S140	0.00

[illegible]

SER	GLU	ASP	VAL	GLU	ALA	THR	VAL	PRO	MET	LEU	GLN	ARG	THR	LYS	SER	ARG	ILE	GLU	GLN	GLY	ILE	VAL	ASP	ARG	SER	SER	GLU	THR	GLY	VAL	LEU	ASP	LYS	GLU	GLY	GLU	GLN	ALA	LYS	ALA	LEU	LEU	PHE	GLU	PHE	LYS	VAL	LYS	THR	ARG	PHE	LYS	THR	HIS	VAL	GLU	GLY	GLY	D258	R262
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Position	Number of Mutations
R266	10
Q267	9
T268	8
T269	7
L270	6
K271	5
K274	4
L277	3
T296	2
L299	1
L302	0
R309	0
A315	0
T316	0
L317	0
F318	0
K319	0
I320	0
G333	10
C336	9
L344	10
R345	9
ARG	8
SER	7
LEU	6
LYS	5
LYS	4
TYR	3
TYR	2
PHE	1
GLU	0
ILE	0
SER	0
SER	0
TYR	0
ARG	0
ARG	0
GLU	0
GLU	0
SER	0
SER	0
SER	0
TYR	0
SER	0
SER	0
ASP	0
ASP	0
ILE	0
PRO	0
ASP	0
ASP	0
VAL	0
LYS	0
VAL	0
ASP	0
ASN	0
ASP	0
PHE	0

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

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

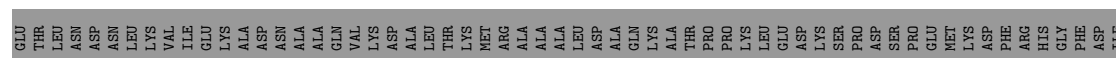
ASN	LEU	ARG	ALA	LEU	HIS	ILE	LYS	PHE	THR	ASP	ILE	LYS	GLU	ILE	PRO	LEU	TRP	ILE	TYR	SER	LEU	LYS	THR	LEU	GLU	GLU	LEU	HIS	LEU	THR	GLY	ASN	SER	ALA	GLU	ASN	ASN	ARG	TYR	ILE	VAL	ILE	ASP	GLY	LEU	ARG	GLU	LEU	LYS	ARG	LEU	LYS	VAL	LEU	ARG	LEU	LYS	SER
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ASN	LEU	SEU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

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	176166	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	4.940	Depositor
Minimum map value	-3.651	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.064	Depositor
Recommended contour level	0.35	Depositor
Map size (Å)	435.968, 435.968, 435.968	wwPDB
Map dimensions	416, 416, 416	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.048, 1.048, 1.048	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: PEE

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	0.21	0/1715	0.43	0/2333
1	B	0.18	0/1715	0.40	0/2333
1	C	0.21	0/2762	0.44	0/3741
1	D	0.24	0/2721	0.47	0/3684
1	E	0.23	0/1715	0.51	0/2333
2	F	0.17	0/1644	0.39	0/2226
All	All	0.21	0/12272	0.45	0/16650

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	1662	0	1657	30	0
1	B	1662	0	1657	20	0
1	C	2685	0	2670	34	0
1	D	2646	0	2642	46	0
1	E	1662	0	1657	32	0
2	F	1599	0	1605	29	0
3	C	22	0	28	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	95	0	147	6	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
All	All	12039	0	12063	174	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

The worst 5 of 174 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)
1:B:309:ARG:HD3	1:C:302:LEU:HD11	1.63	0.80
1:E:291:PHE:HE2	1:E:316:THR:H	1.33	0.76
1:D:46:GLN:HA	1:D:50:ASP:HB2	1.68	0.74
2:F:258:LEU:HA	2:F:261:MET:HE2	1.70	0.72
1:B:39:ALA:HB1	1:B:130:LEU:HD22	1.71	0.71

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	191/911 (21%)	183 (96%)	8 (4%)	0	100	100
1	B	191/911 (21%)	186 (97%)	5 (3%)	0	100	100
1	C	314/911 (34%)	308 (98%)	6 (2%)	0	100	100
1	D	310/911 (34%)	303 (98%)	7 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	191/911 (21%)	183 (96%)	8 (4%)	0	100	100
2	F	185/813 (23%)	183 (99%)	2 (1%)	0	100	100
All	All	1382/5368 (26%)	1346 (97%)	36 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	182/830 (22%)	179 (98%)	3 (2%)	55	72
1	B	182/830 (22%)	181 (100%)	1 (0%)	81	83
1	C	297/830 (36%)	295 (99%)	2 (1%)	76	81
1	D	293/830 (35%)	293 (100%)	0	100	100
1	E	182/830 (22%)	181 (100%)	1 (0%)	81	83
2	F	178/756 (24%)	178 (100%)	0	100	100
All	All	1314/4906 (27%)	1307 (100%)	7 (0%)	78	83

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	23	TRP
1	C	253	HIS
1	E	314	LEU
1	C	263	LEU
1	A	329	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	288	ASN
2	F	112	ASN

Continued on next page...

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Mol	Chain	Res	Type
2	F	288	GLN
1	B	49	GLN
1	B	267	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 ligands are 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	$\# Z > 2$
3	PEE	C	901	-	9,9,50	1.70	2 (22%)	9,9,55	1.63	2 (22%)
3	PEE	D	902	-	50,50,50	1.31	4 (8%)	53,55,55	0.97	1 (1%)
3	PEE	C	902	-	11,11,50	1.93	3 (27%)	11,11,55	1.59	2 (18%)
3	PEE	D	901	-	43,43,50	1.36	4 (9%)	46,48,55	1.05	2 (4%)

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
3	PEE	C	901	-	-	4/7/7/54	-
3	PEE	D	902	-	-	30/54/54/54	-
3	PEE	C	902	-	-	5/9/9/54	-
3	PEE	D	901	-	-	20/47/47/54	-

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	902	PEE	P-O4P	4.78	1.78	1.59
3	D	901	PEE	P-O4P	4.77	1.78	1.59
3	C	902	PEE	O4-C10	4.29	1.36	1.22
3	C	901	PEE	O4-C10	4.29	1.36	1.22
3	D	902	PEE	C39-C38	3.99	1.54	1.31

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	902	PEE	O2P-P-O1P	4.48	133.28	112.44
3	D	901	PEE	O2P-P-O1P	4.46	133.19	112.44
3	C	901	PEE	O2-C10-C11	3.38	124.69	114.00
3	C	902	PEE	O2-C10-C11	3.38	124.67	114.00
3	C	901	PEE	O4-C10-C11	-2.69	114.56	123.09

There are no chirality outliers.

5 of 59 torsion outliers are listed below:

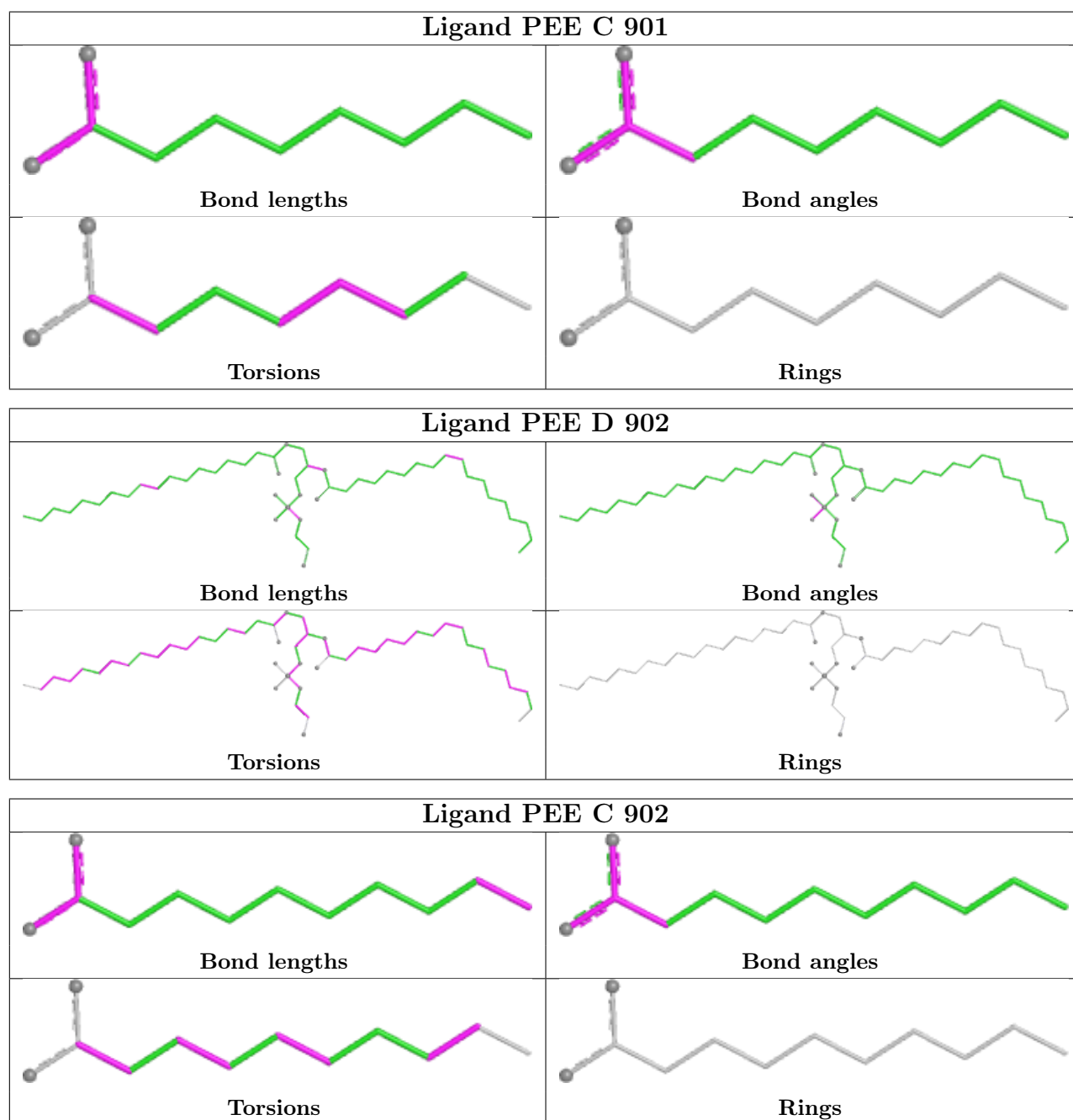
Mol	Chain	Res	Type	Atoms
3	D	901	PEE	C1-O3P-P-O1P
3	D	901	PEE	C1-O3P-P-O4P
3	D	901	PEE	C4-O4P-P-O3P
3	D	901	PEE	C37-C38-C39-C40
3	D	902	PEE	O4-C10-O2-C2

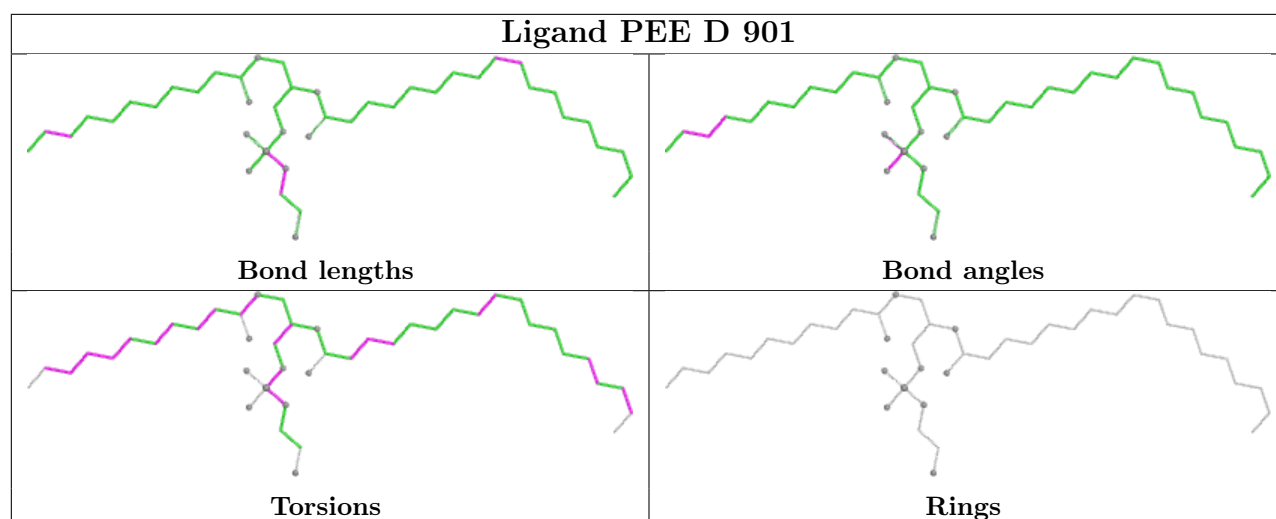
There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	902	PEE	5	0
3	C	902	PEE	1	0
3	D	901	PEE	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

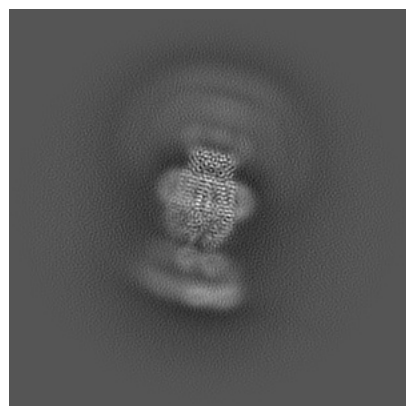
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-27686. These allow visual inspection of the internal detail of the map and identification of artifacts.

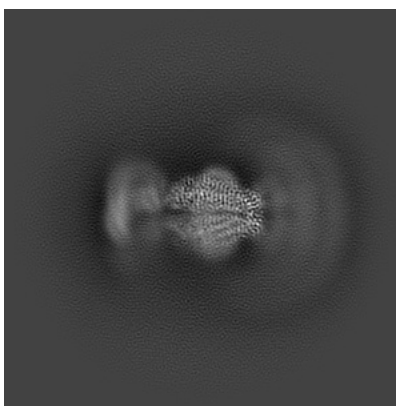
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

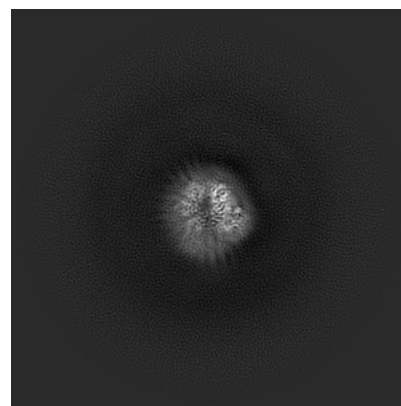
6.1.1 Primary map



X

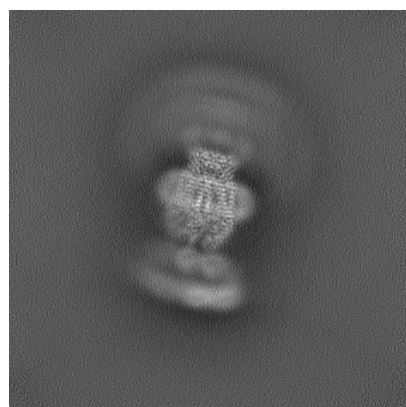


Y

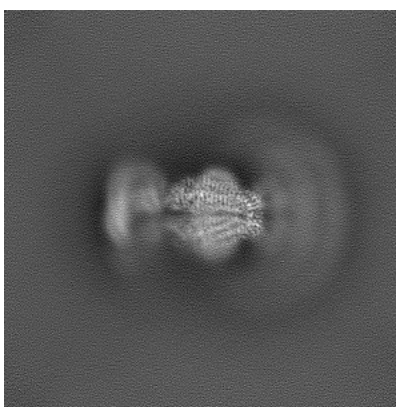


Z

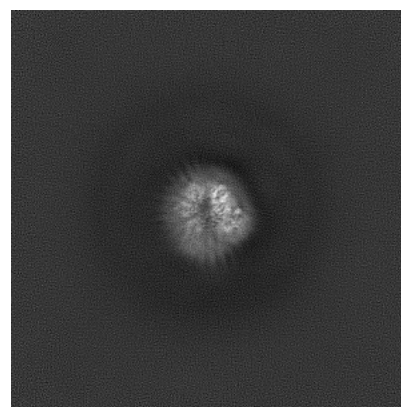
6.1.2 Raw map



X



Y

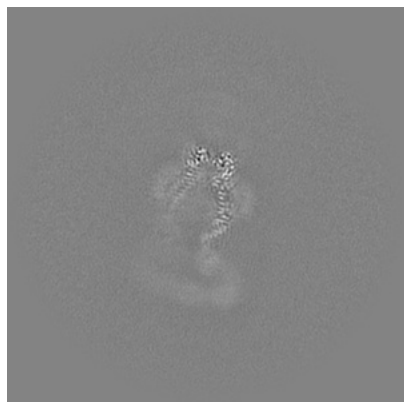


Z

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

6.2 Central slices [i](#)

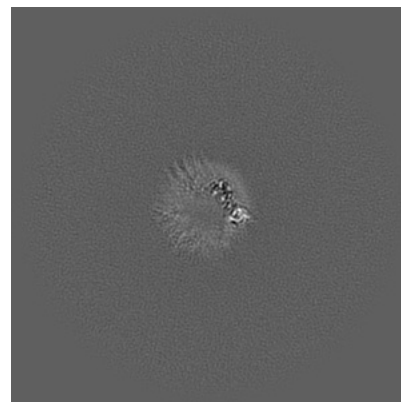
6.2.1 Primary map



X Index: 208



Y Index: 208



Z Index: 208

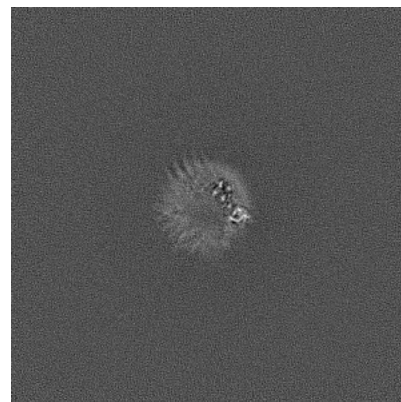
6.2.2 Raw map



X Index: 208



Y Index: 208

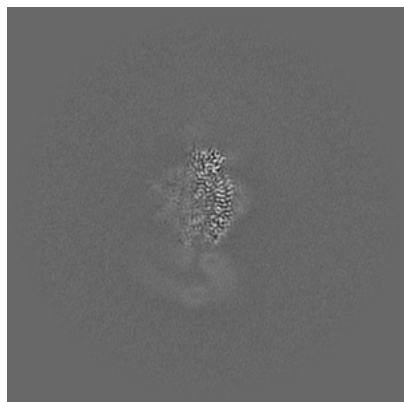


Z Index: 208

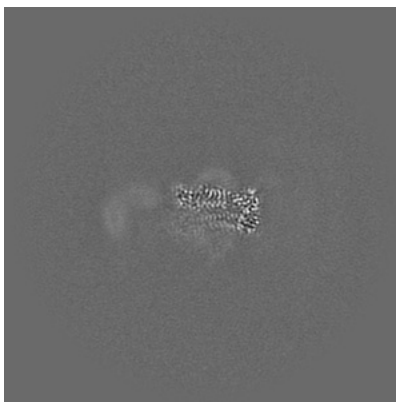
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

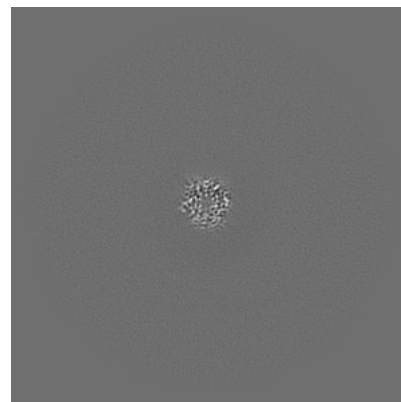
6.3.1 Primary map



X Index: 222

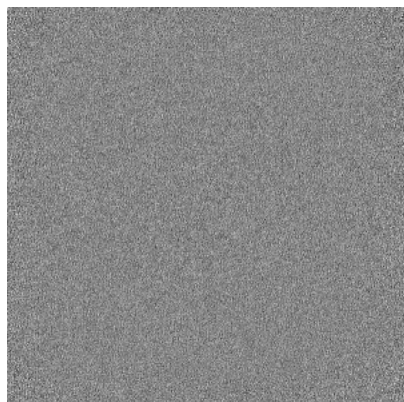


Y Index: 223

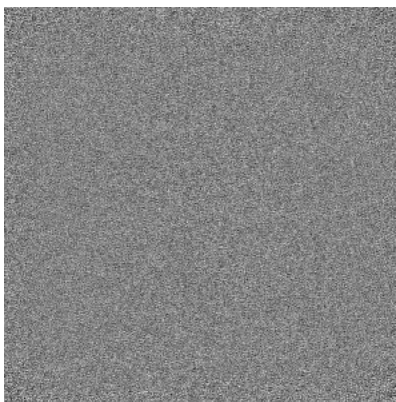


Z Index: 256

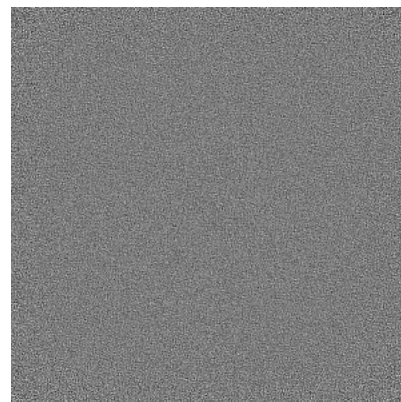
6.3.2 Raw map



X Index: 0



Y Index: 0



Z Index: 0

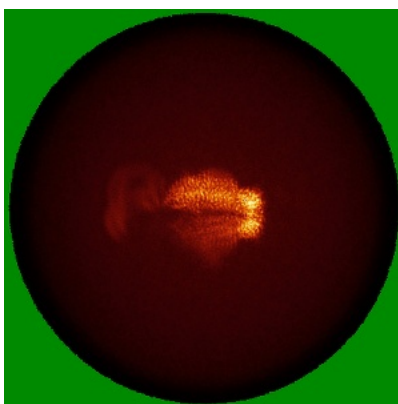
The images above show the largest variance slices of the map in three orthogonal directions.

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

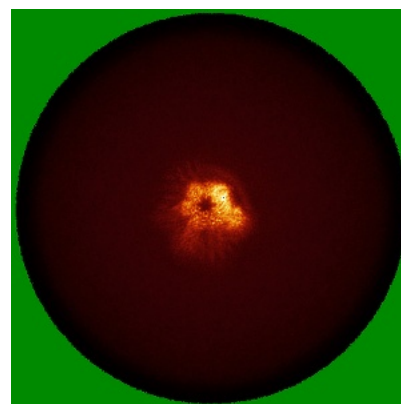
6.4.1 Primary map



X



Y

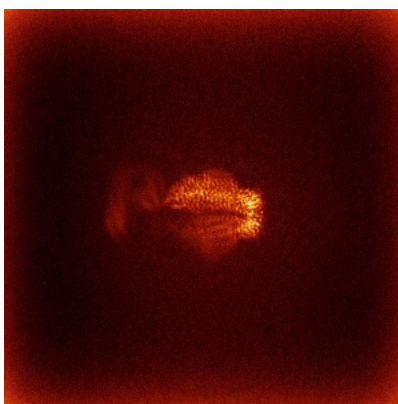


Z

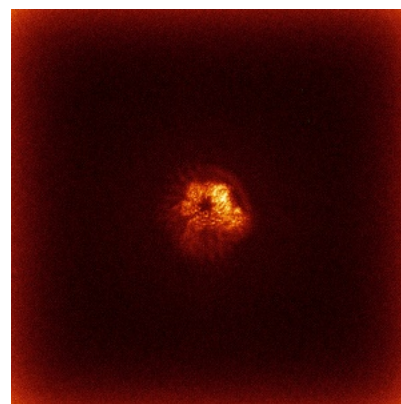
6.4.2 Raw map



X



Y

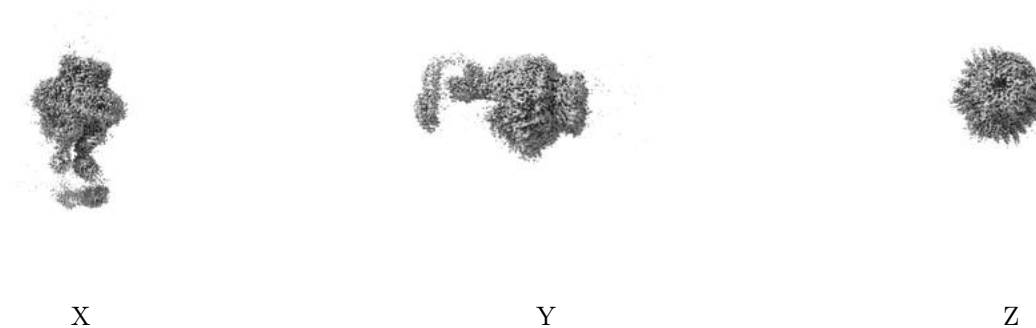


Z

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.

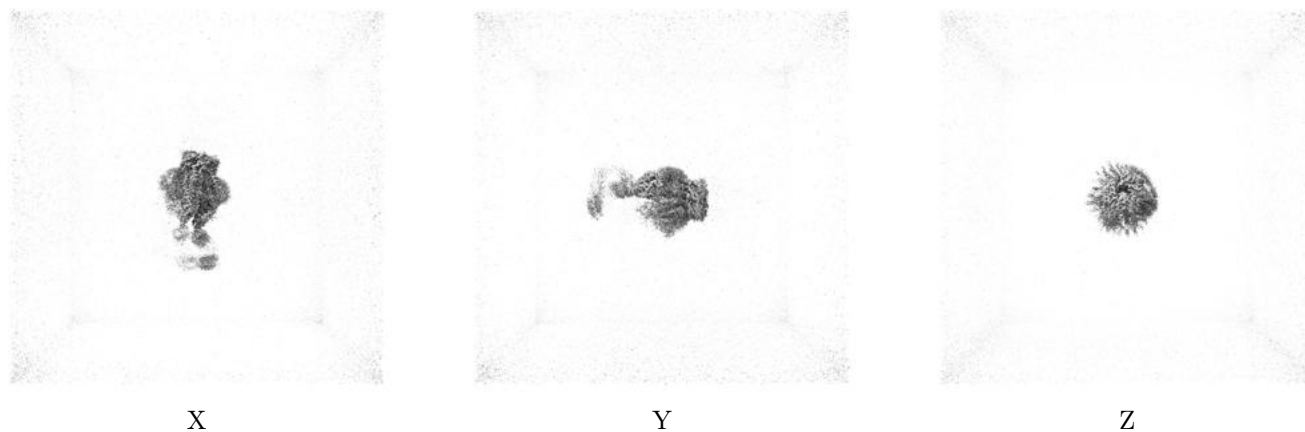
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.35. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

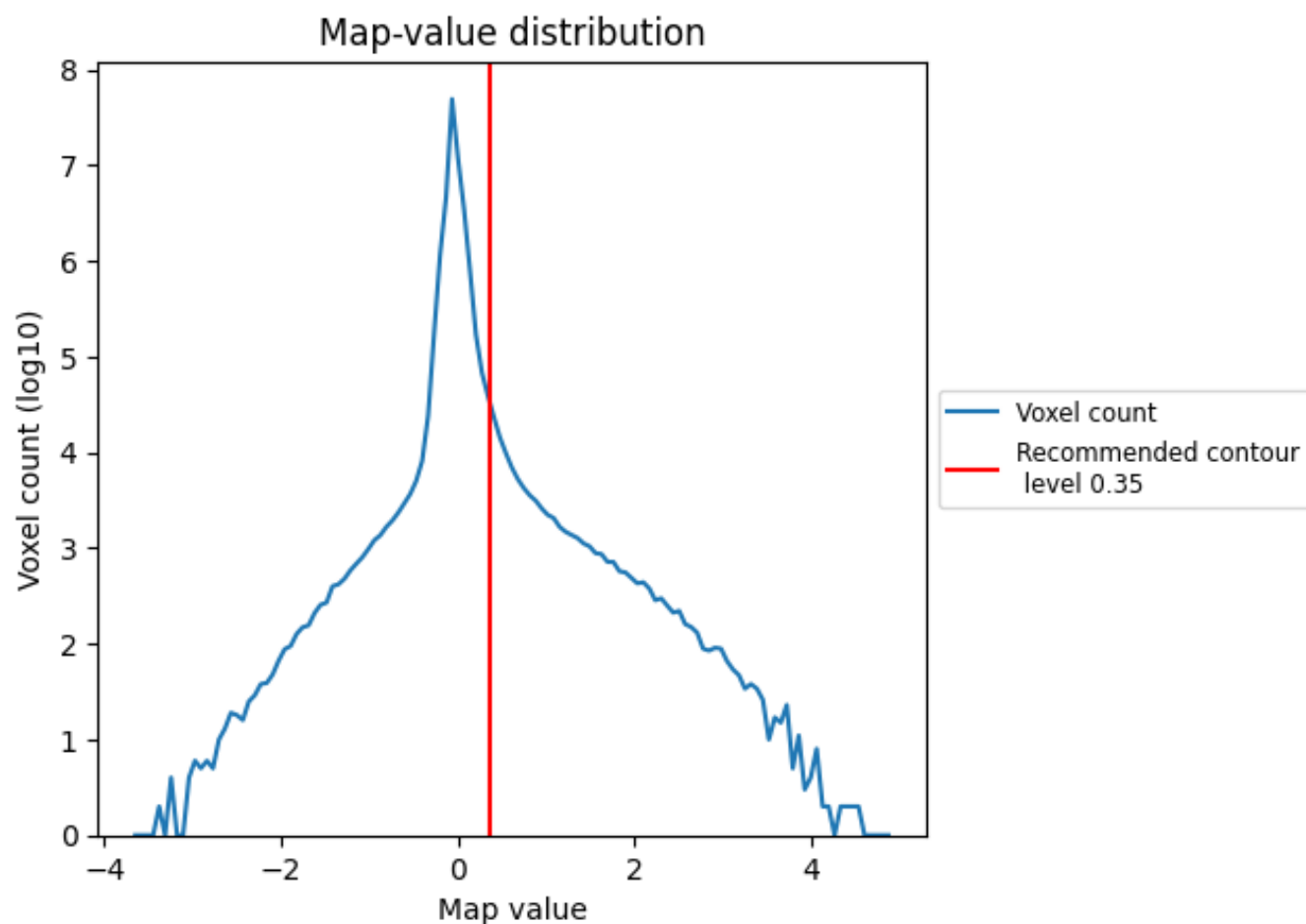
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

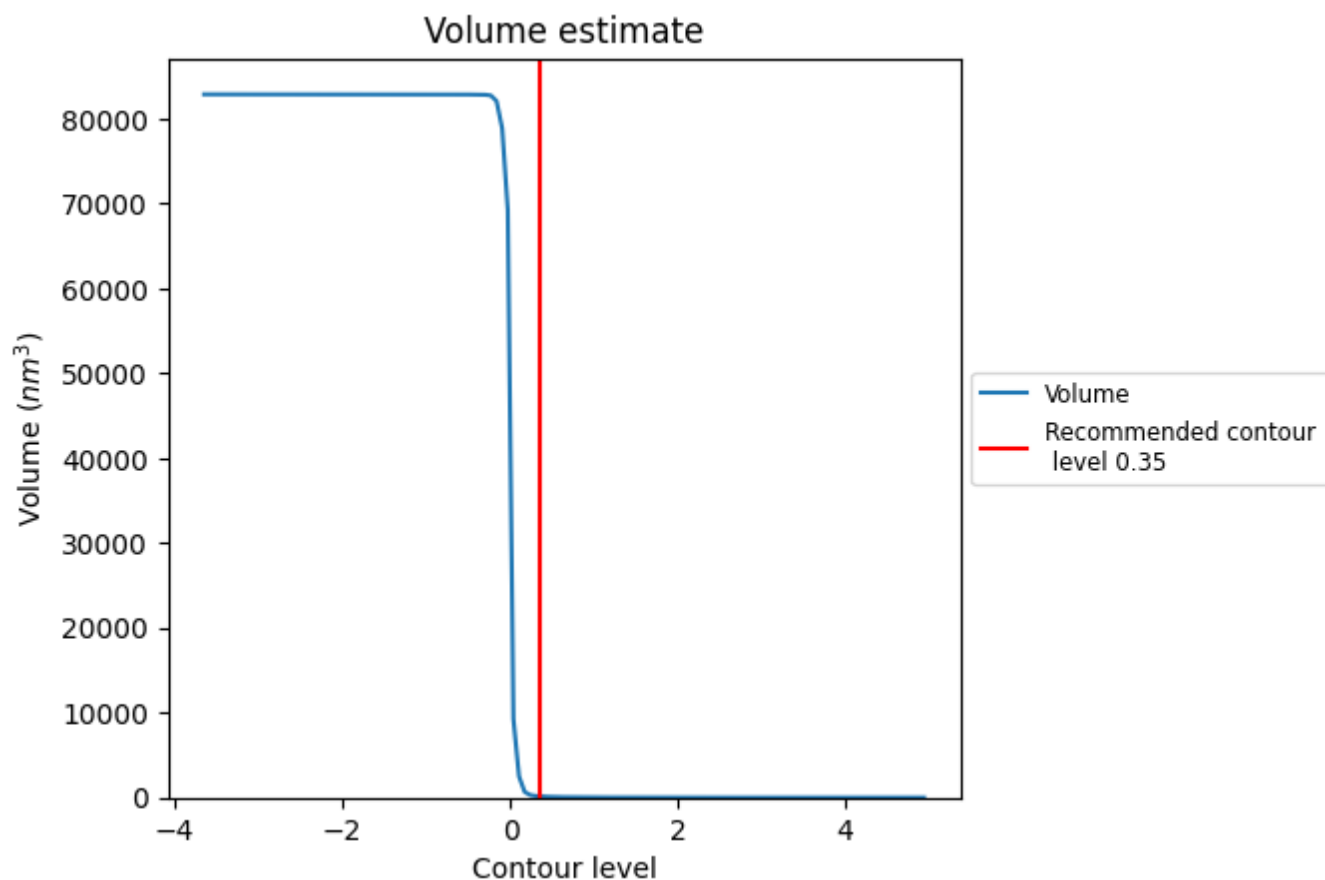
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

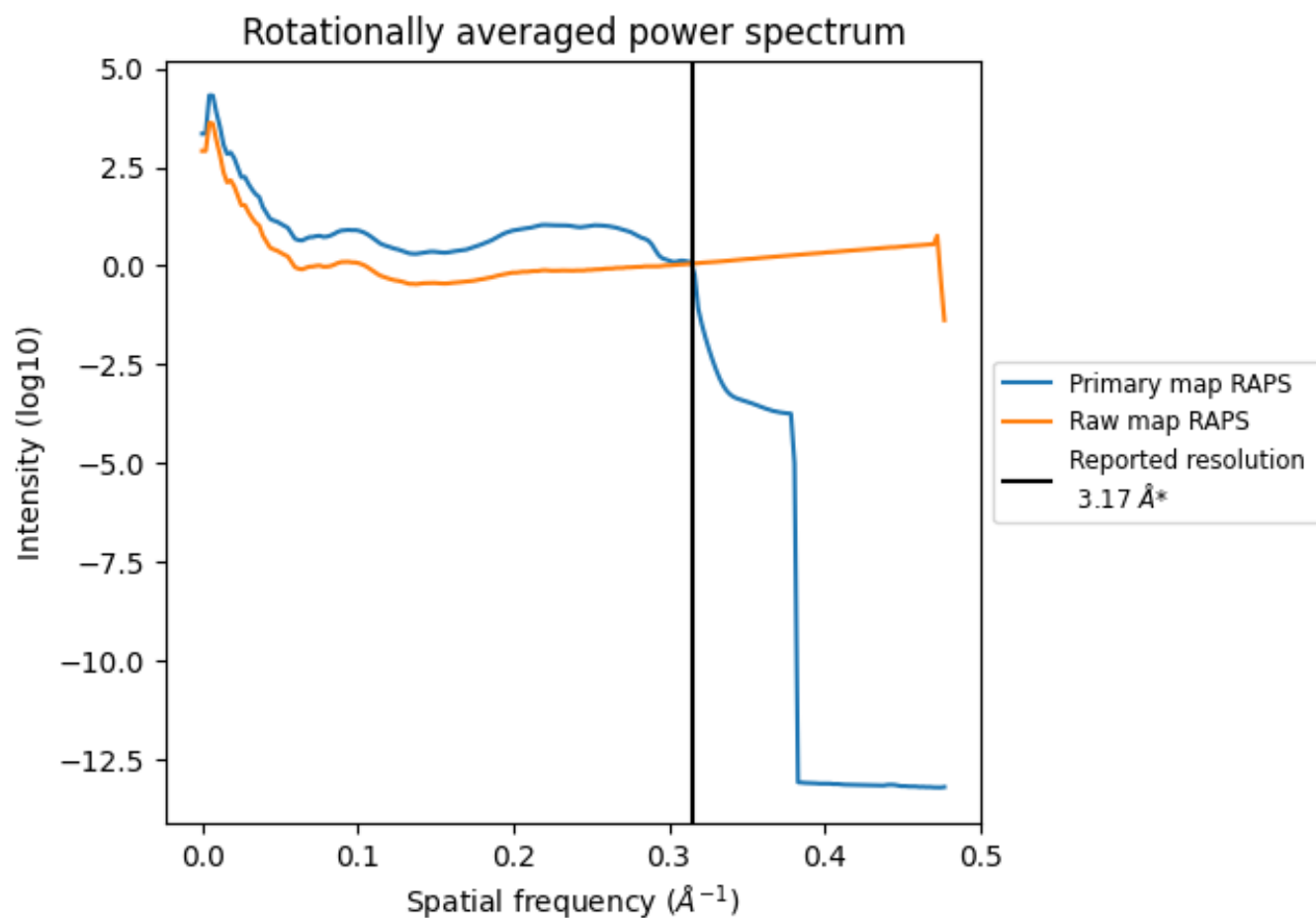
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 149 nm³; this corresponds to an approximate mass of 135 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 ⓘ

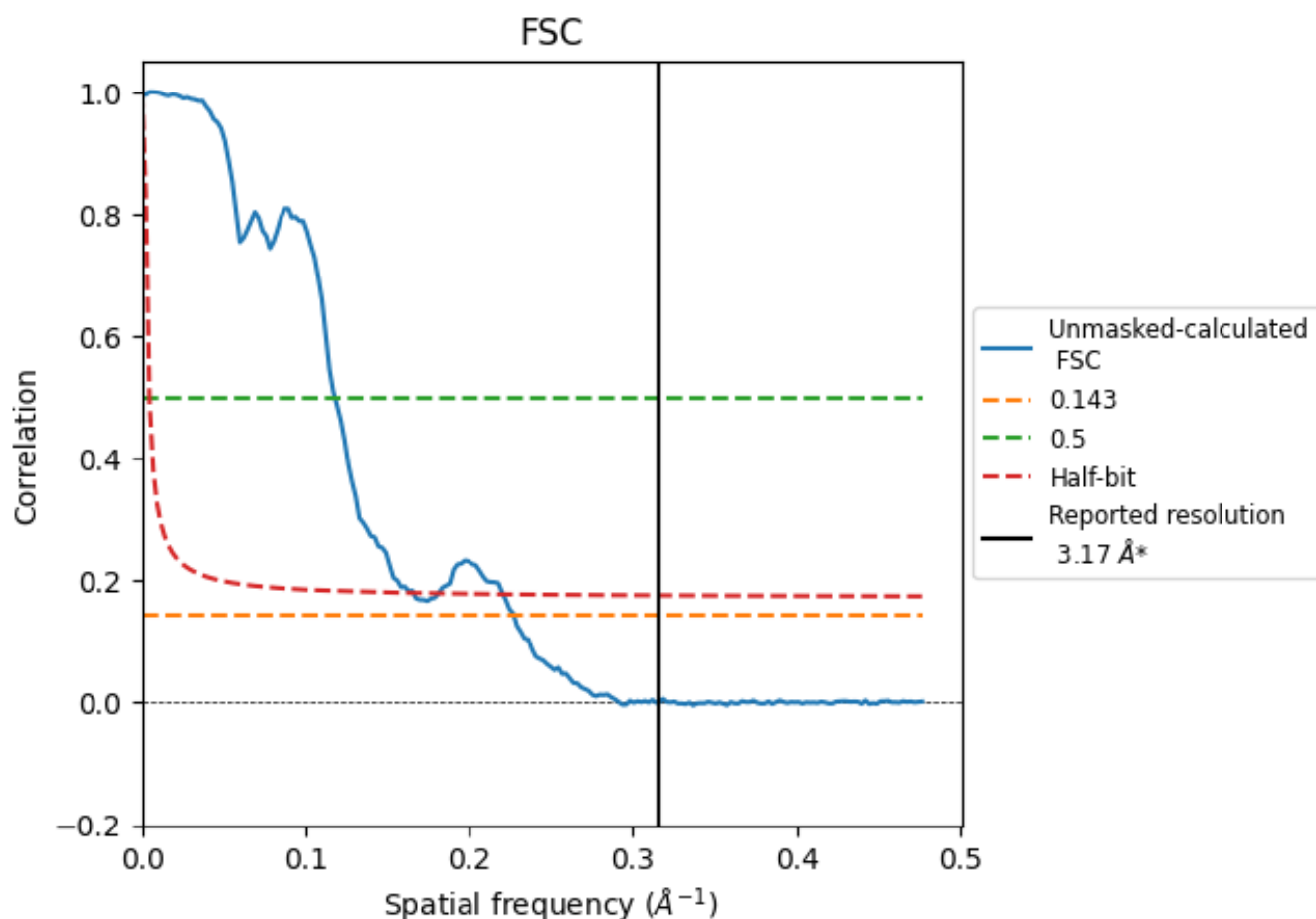


*Reported resolution corresponds to spatial frequency of 0.315 Å⁻¹

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 0.315 Å⁻¹

8.2 Resolution estimates [i](#)

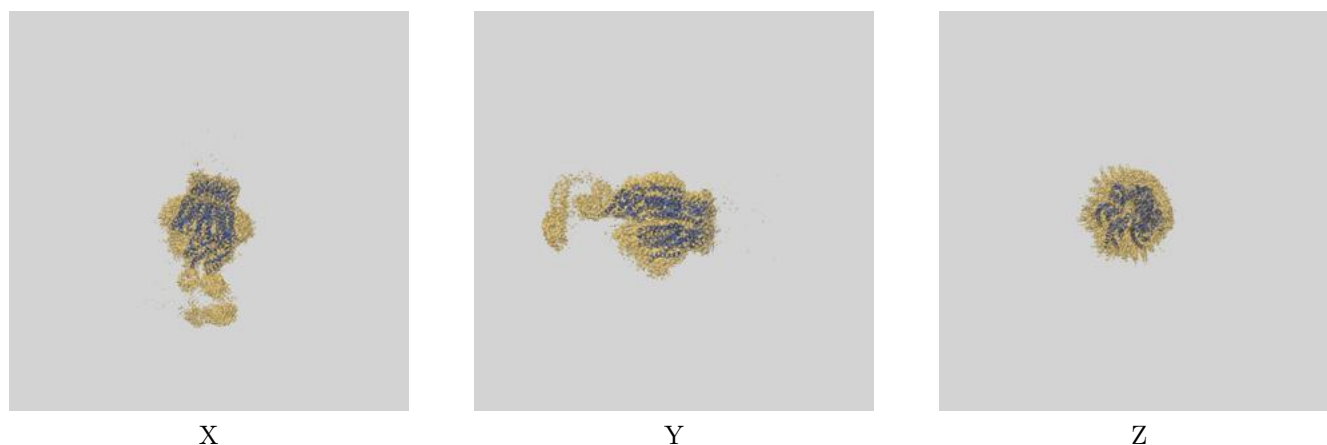
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.17	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.40	8.48	6.03

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.40 differs from the reported value 3.17 by more than 10 %

9 Map-model fit [i](#)

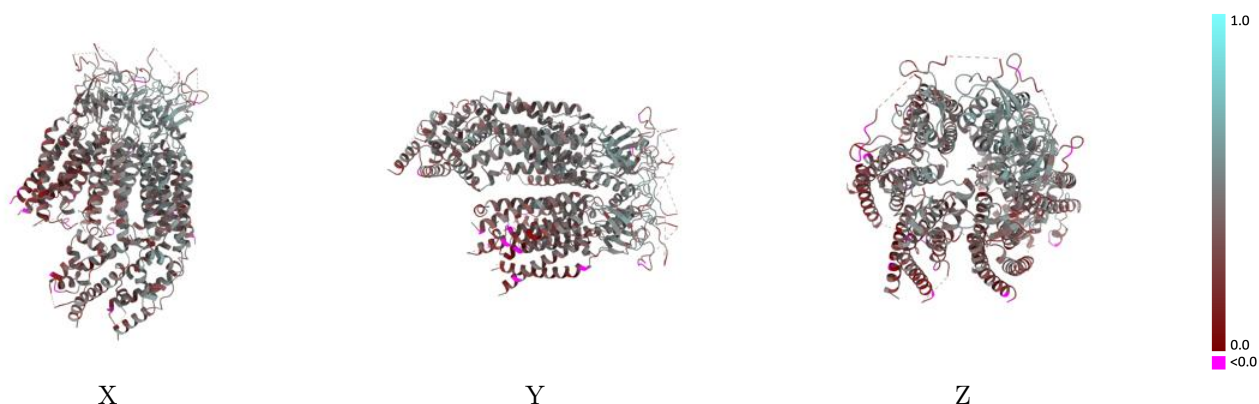
This section contains information regarding the fit between EMDB map EMD-27686 and PDB model 8DS9. Per-residue inclusion information can be found in section [3](#) on page [9](#).

9.1 Map-model overlay [i](#)



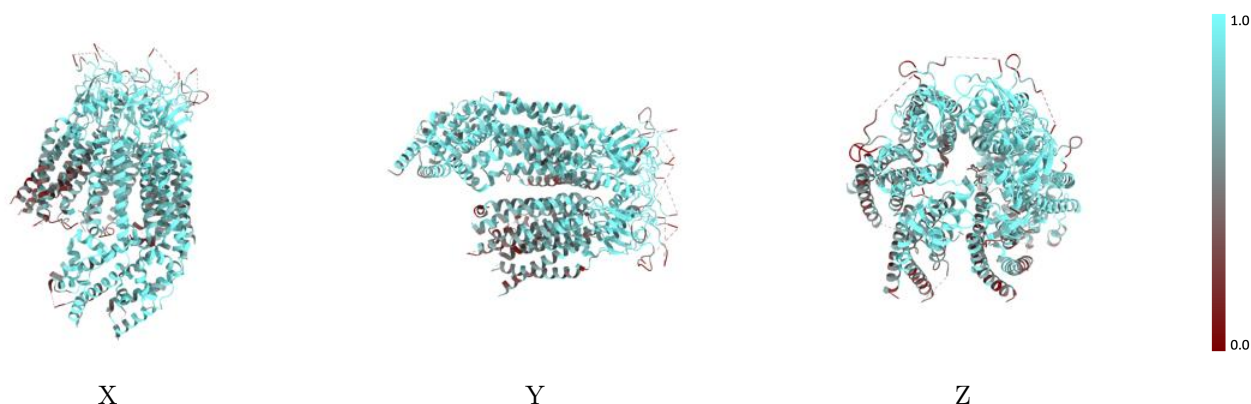
The images above show the 3D surface view of the map at the recommended contour level 0.35 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



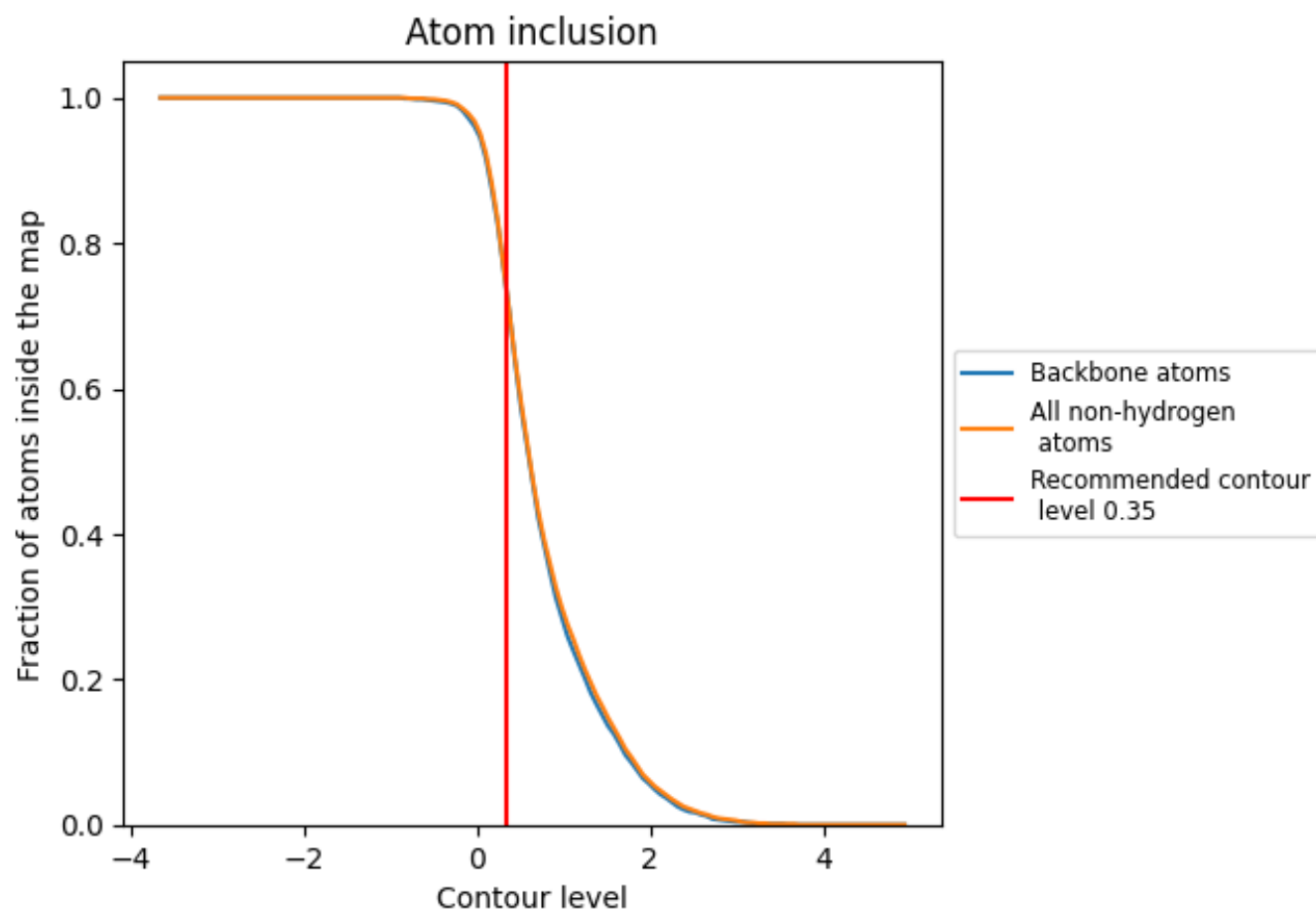
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.35).

9.4 Atom inclusion [i](#)



At the recommended contour level, 73% of all backbone atoms, 73% 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 (0.35) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7310	<div></div> 0.3900
A	<div></div> 0.6390	<div></div> 0.3450
B	<div></div> 0.7020	<div></div> 0.3830
C	<div></div> 0.8360	<div></div> 0.4560
D	<div></div> 0.8090	<div></div> 0.4160
E	<div></div> 0.6530	<div></div> 0.3580
F	<div></div> 0.6820	<div></div> 0.3200

1.0

0.0

<0.0