



wwPDB EM Validation Summary Report ⓘ

Jul 7, 2024 – 07:38 pm BST

PDB ID : 7OOB
EMDB ID : EMD-13009
Title : Pol II-CSB-CSA-DDB1-UVSSA-ADPBeF3 (Structure2)
Authors : Kokic, G.; Cramer, P.
Deposited on : 2021-05-27
Resolution : 2.70 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:

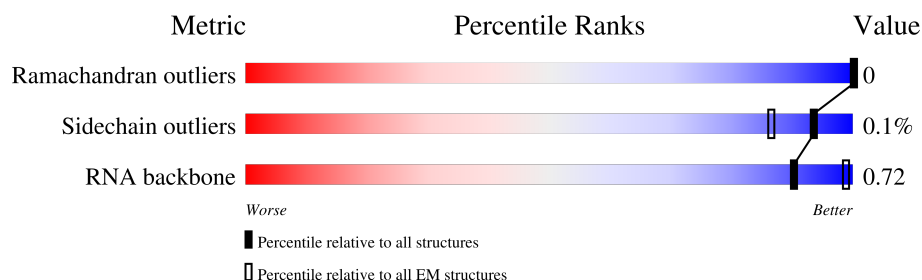
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.70 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	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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	1970	<div> <div>8%</div> <div>71%</div> <div>28%</div> </div>
2	B	1174	<div> <div>11%</div> <div>96%</div> <div>.</div> </div>
3	C	275	<div> <div>.</div> <div>94%</div> <div>5%</div> </div>
4	D	142	<div> <div>66%</div> <div>89%</div> <div>11%</div> </div>
5	E	210	<div> <div>6%</div> <div>99%</div> </div>
6	F	127	<div> <div>6%</div> <div>65%</div> <div>35%</div> </div>
7	G	172	<div> <div>74%</div> <div>99%</div> <div>.</div> </div>
8	H	150	<div> <div>.</div> <div>99%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
9	I	125	
10	J	67	
11	K	117	
12	L	58	
13	b	1496	
14	d	1143	
15	N	47	
16	T	47	
17	P	10	
18	a	396	

2 Entry composition [i](#)

There are 22 unique types of molecules in this entry. The entry contains 90756 atoms, of which 44495 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 DNA-directed RNA polymerase II subunit RPB1.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	1412	Total	C	H	N	O	S	0	0
			22494	7033	11315	2002	2074	70		

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	B	1131	Total	C	H	N	O	S	0	0
			18140	5727	9088	1592	1669	64		

- Molecule 3 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	C	260	Total	C	H	N	O	S	0	0
			4120	1309	2031	359	415	6		

- Molecule 4 is a protein called RPOL4c domain-containing protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	D	126	Total	C	H	N	O	S	0	0
			2046	642	1016	175	209	4		

- Molecule 5 is a protein called DNA-directed RNA polymerase II subunit E.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	E	209	Total	C	H	N	O	S	0	0
			3457	1089	1737	300	323	8		

- Molecule 6 is a protein called DNA-directed RNA polymerase II subunit F.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	F	82	Total	C	H	N	O	S	0	0
			1341	418	684	113	121	5		

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit RPB7.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	G	171	Total	C	H	N	O	S	0	0
			2709	875	1358	219	249	8		

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	H	148	Total	C	H	N	O	S	0	0
			2333	750	1147	194	237	5		

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	I	117	Total	C	H	N	O	S	0	0
			1828	587	879	169	182	11		

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	J	67	Total	C	H	N	O	S	0	0
			1086	345	553	90	92	6		

- Molecule 11 is a protein called RNA_pol_L_2 domain-containing protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	K	115	Total	C	H	N	O	S	0	0
			1862	593	942	152	173	2		

- Molecule 12 is a protein called RNA polymerase II subunit K.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	L	46	Total	C	H	N	O	S	0	0
			781	241	393	75	66	6		

- Molecule 13 is a protein called DNA excision repair protein ERCC-6.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	b	520	Total	C	H	N	O	S	0	0
			8561	2746	4302	746	746	21		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
b	-2	SER	-	expression tag	UNP Q03468
b	-1	ASN	-	expression tag	UNP Q03468
b	0	ALA	-	expression tag	UNP Q03468

- Molecule 14 is a protein called DNA damage-binding protein 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
14	d	781	Total	C	H	N	O	S	0	0
			12317	3919	6153	1038	1173	34		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
d	-2	SER	-	expression tag	UNP Q16531
d	-1	ASN	-	expression tag	UNP Q16531
d	0	ALA	-	expression tag	UNP Q16531

- Molecule 15 is a DNA chain called NTS.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	N	35	Total	C	N	O	P	0	0
			727	344	142	206	35		

- Molecule 16 is a DNA chain called TS.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	T	47	Total	C	N	O	P	0	0
			947	453	159	288	47		

- Molecule 17 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
17	P	10	Total	C	H	N	O	P	0	0
			329	98	109	45	67	10		

- Molecule 18 is a protein called DNA excision repair protein ERCC-8.

Mol	Chain	Residues	Atoms						AltConf	Trace
18	a	365	Total	C	H	N	O	S	0	0
			5626	1775	2777	507	548	19		

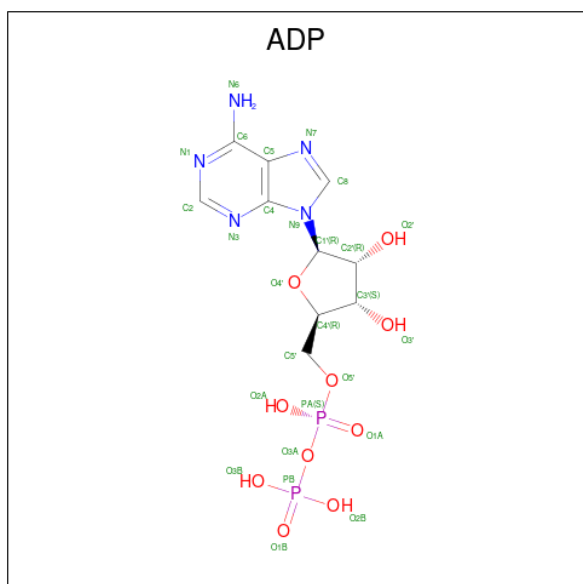
- Molecule 19 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
19	A	2	Total	Zn	0
			2	2	
19	B	1	Total	Zn	0
			1	1	
19	C	1	Total	Zn	0
			1	1	
19	I	2	Total	Zn	0
			2	2	
19	J	1	Total	Zn	0
			1	1	
19	L	1	Total	Zn	0
			1	1	

- Molecule 20 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

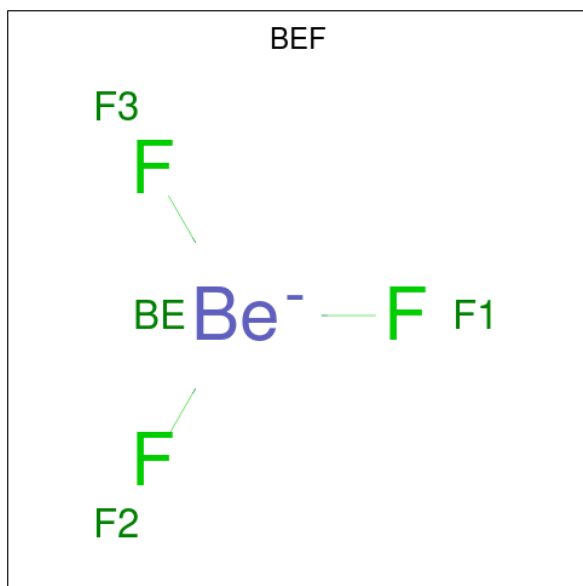
Mol	Chain	Residues	Atoms		AltConf
20	A	1	Total	Mg	0
			1	1	
20	b	1	Total	Mg	0
			1	1	

- Molecule 21 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



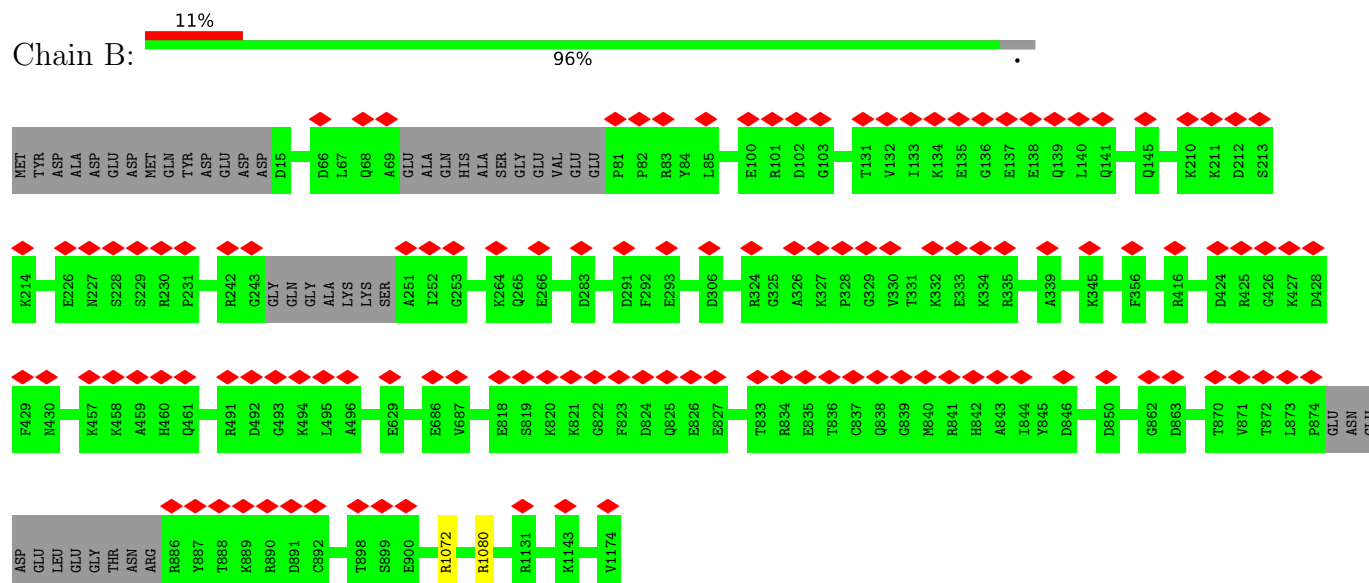
Mol	Chain	Residues	Atoms						AltConf
21	b	1	Total	C	H	N	O	P	0
			38	10	11	5	10	2	

- Molecule 22 is BERYLLIUM TRIFLUORIDE ION (three-letter code: BEF) (formula: BeF_3).

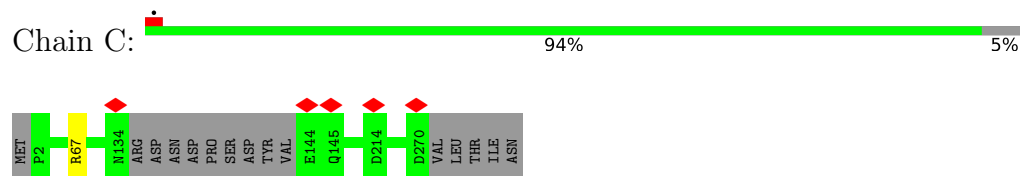


Mol	Chain	Residues	Atoms			AltConf
			Total	Be	F	
22	b	1	4	1	3	0

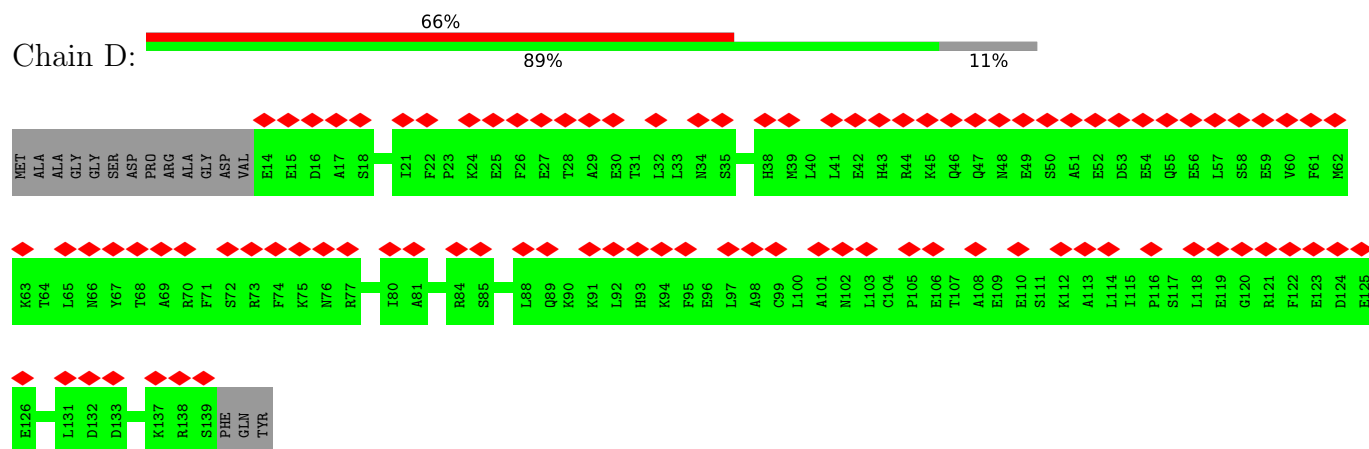
- Molecule 2: DNA-directed RNA polymerase subunit beta



- Molecule 3: DNA-directed RNA polymerase II subunit RPB3

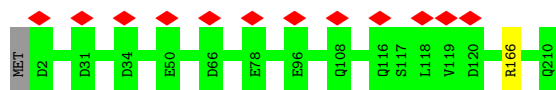


- Molecule 4: RPOL4c domain-containing protein

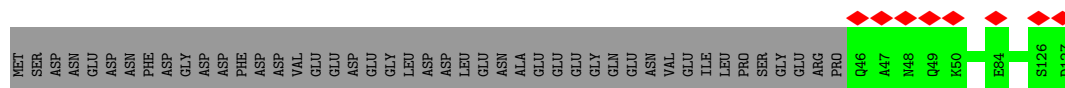


- Molecule 5: DNA-directed RNA polymerase II subunit E





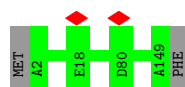
- Molecule 6: DNA-directed RNA polymerase II subunit F



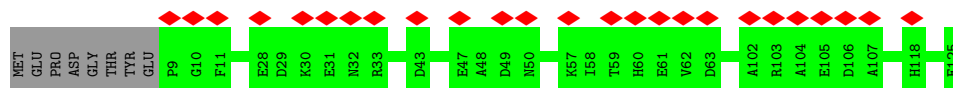
- Molecule 7: DNA-directed RNA polymerase II subunit RPB7



- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3




- Molecule 9: DNA-directed RNA polymerase II subunit RPB9



- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5



- Molecule 11: RNA_pol_L_2 domain-containing protein

- Chain L: 

MET ASP THR GLN LYS ASP VAL GLN PRO PRO LYS GLN Q13 P14 K29 S30 R31 D32 R58

- Chain b:  35% 65%

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

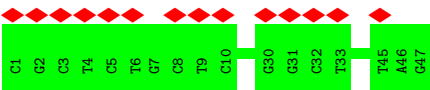
ALA	PRO	ALA	PRO	VAL	THR	PRO	PRO	ALA	ALA	PRO	VAL	GLN	ASN	LYS	ASN	LYS	ASN	PRO	ASN	LYS	SER	LEU	LEU	GLY	GLU	ARG	LYS	LEU	GLN	PHE	GLN	GLN	GLN	GLY	LYS	VAL	ALA	ALA	ARG	ARG	PRO	TRP	GLU
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[illegible][illegible]

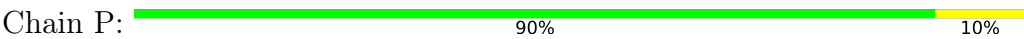
Amino Acid	Percentage (%)
LYS	10
ARG	10
LEU	10
LYS	10
LEU	10
GLU	10
ASP	5
ASP	5
SER	5
SER	5
GLU	5
GLU	5
SER	5
D490	5
F493	5
D494	5
R555	5
THR	5
ARG	5
GLY	5
SER	5
ASN	5
ASN	5
TYR	5
R562	5
D633	5
R666	5
K729	5
D749	5
V750	5
K751	5
M752	5
V786	5
N790	5
G791	5
E792	5
F812	5
S813	5
G814	5
GLY	5
PRO	1
LYS	1
ASN	1
LEU	1
LYS	1
GLY	1
LEU	1
PRO	1
ASP	1
ASP	1
GLU	1
LEU	1
SER	1

[illegible]

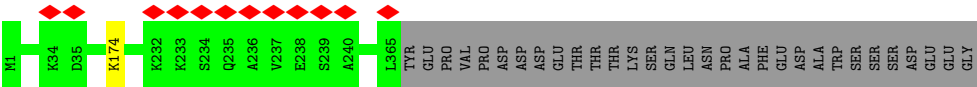
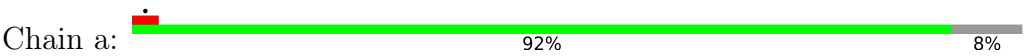
LEU	SER	VAL	ILE	SER	GLY	ASN	GLY	GLU	CYS	SER	ASN	SER	SER	GLY	THR	GLY	LYS	THR	SER	SER	MET	PRO	SER	GLY	ASP	GLU	GLY	SER	SER	ILE	ASP	GLU	LYS	LEU	GLY	LEU	SER	TYR	PRO	SER	GLN	ALA	ALA	GLN	THR	THR	ASN	LYS	GLU	GLU	ALA	PHE	TRP	PHE
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● Molecule 17: RNA



● Molecule 18: DNA excision repair protein ERCC-8



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	100000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	41.2	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.241	Depositor
Minimum map value	-0.116	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	419.99997, 419.99997, 419.99997	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, BEF, ZN, ADP

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	0.30	0/11382	0.53	1/15368 (0.0%)
2	B	0.32	0/9233	0.54	0/12463
3	C	0.34	0/2132	0.56	1/2896 (0.0%)
4	D	0.28	0/1043	0.47	0/1400
5	E	0.29	0/1751	0.53	0/2366
6	F	0.31	0/667	0.49	0/901
7	G	0.27	0/1382	0.56	0/1874
8	H	0.33	0/1207	0.53	0/1628
9	I	0.30	0/972	0.54	0/1316
10	J	0.32	0/542	0.51	0/730
11	K	0.30	0/939	0.49	0/1271
12	L	0.33	0/394	0.59	0/524
13	b	0.36	0/4362	0.60	0/5890
14	d	0.34	0/6271	0.59	0/8470
15	N	0.54	0/817	0.87	0/1258
16	T	0.60	0/1056	0.97	0/1624
17	P	0.50	0/247	0.89	0/384
18	a	0.35	0/2908	0.59	0/3939
All	All	0.34	0/47305	0.58	2/64302 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
13	b	0	1
14	d	0	1
18	a	0	1
All	All	0	4

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	67	ARG	NE-CZ-NH2	-5.63	117.48	120.30
1	A	483	ARG	CG-CD-NE	5.27	122.87	111.80

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	538	VAL	Peptide
18	a	174	LYS	Peptide
13	b	493	PHE	Peptide
14	d	884	ILE	Peptide

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	1402/1970 (71%)	1365 (97%)	37 (3%)	0	100	100
2	B	1123/1174 (96%)	1076 (96%)	47 (4%)	0	100	100
3	C	256/275 (93%)	249 (97%)	7 (3%)	0	100	100
4	D	124/142 (87%)	119 (96%)	5 (4%)	0	100	100
5	E	207/210 (99%)	204 (99%)	3 (1%)	0	100	100
6	F	80/127 (63%)	75 (94%)	5 (6%)	0	100	100
7	G	169/172 (98%)	165 (98%)	4 (2%)	0	100	100
8	H	146/150 (97%)	142 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	I	115/125 (92%)	111 (96%)	4 (4%)	0	100	100
10	J	65/67 (97%)	65 (100%)	0	0	100	100
11	K	113/117 (97%)	111 (98%)	2 (2%)	0	100	100
12	L	44/58 (76%)	40 (91%)	4 (9%)	0	100	100
13	b	512/1496 (34%)	477 (93%)	35 (7%)	0	100	100
14	d	765/1143 (67%)	721 (94%)	44 (6%)	0	100	100
18	a	363/396 (92%)	343 (94%)	20 (6%)	0	100	100
All	All	5484/7622 (72%)	5263 (96%)	221 (4%)	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	1242/1749 (71%)	1240 (100%)	2 (0%)	93	98
2	B	992/1027 (97%)	990 (100%)	2 (0%)	93	98
3	C	237/252 (94%)	237 (100%)	0	100	100
4	D	116/126 (92%)	116 (100%)	0	100	100
5	E	191/192 (100%)	190 (100%)	1 (0%)	88	96
6	F	71/111 (64%)	71 (100%)	0	100	100
7	G	152/153 (99%)	152 (100%)	0	100	100
8	H	129/131 (98%)	129 (100%)	0	100	100
9	I	105/112 (94%)	105 (100%)	0	100	100
10	J	56/56 (100%)	56 (100%)	0	100	100
11	K	104/106 (98%)	104 (100%)	0	100	100
12	L	43/55 (78%)	43 (100%)	0	100	100
13	b	466/1299 (36%)	465 (100%)	1 (0%)	93	98
14	d	686/1001 (68%)	686 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	a	320/348 (92%)	320 (100%)	0	100	100
All	All	4910/6718 (73%)	4904 (100%)	6 (0%)	93	98

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	1080	ARG
5	E	166	ARG
13	b	729	LYS
1	A	1101	GLN
1	A	241	ARG

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

Mol	Chain	Res	Type
13	b	616	HIS
18	a	229	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
17	P	9/10 (90%)	1 (11%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
17	P	9	G

There are no RNA pucker outliers to report.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 12 ligands modelled in this entry, 10 are monoatomic - leaving 2 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	$\# Z > 2$
22	BEF	b	1502	-	0,3,3	-	-	-		
21	ADP	b	1501	20	24,29,29	0.87	0	29,45,45	1.40	4 (13%)

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
21	ADP	b	1501	20	-	2/12/32/32	0/3/3/3

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	b	1501	ADP	N3-C2-N1	-3.88	122.61	128.68
21	b	1501	ADP	PA-O3A-PB	-2.46	124.40	132.83
21	b	1501	ADP	C3'-C2'-C1'	2.35	104.52	100.98
21	b	1501	ADP	N6-C6-N1	2.05	122.83	118.57

There are no chirality outliers.

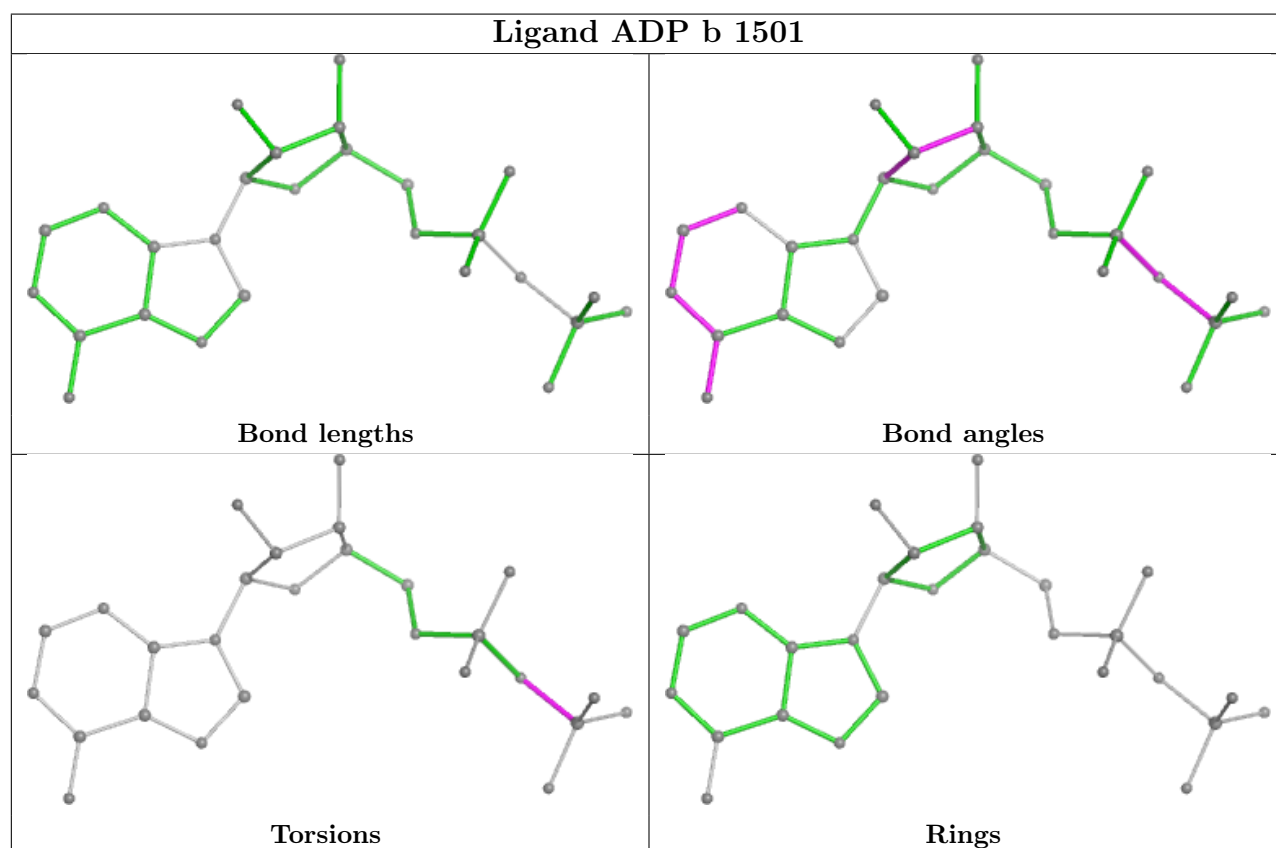
All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
21	b	1501	ADP	PA-O3A-PB-O1B
21	b	1501	ADP	PA-O3A-PB-O3B

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.

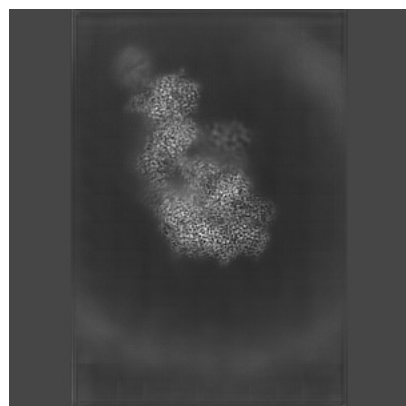
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-13009. These allow visual inspection of the internal detail of the map and identification of artifacts.

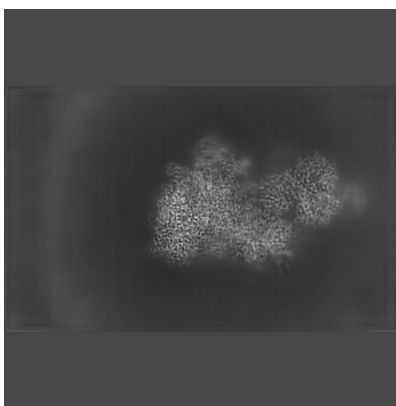
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

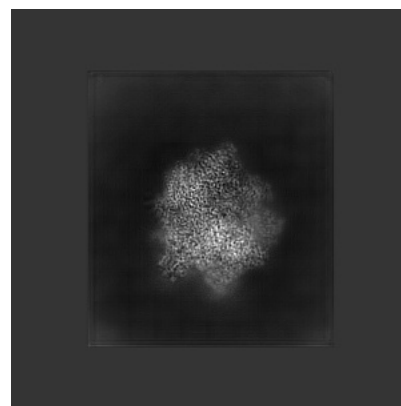
6.1.1 Primary map



X

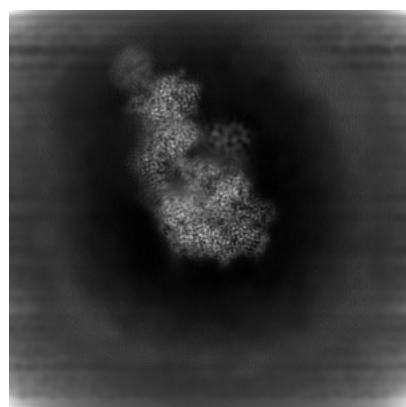


Y

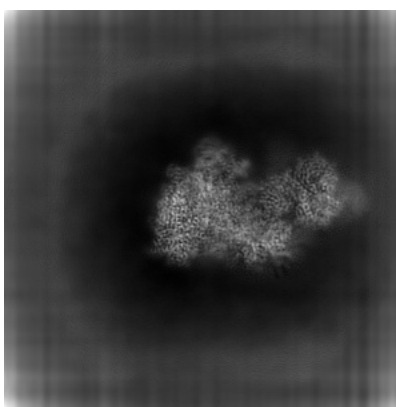


Z

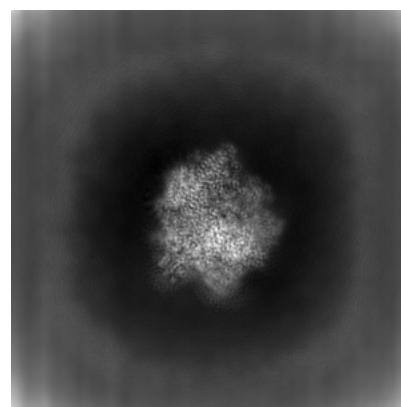
6.1.2 Raw map



X



Y

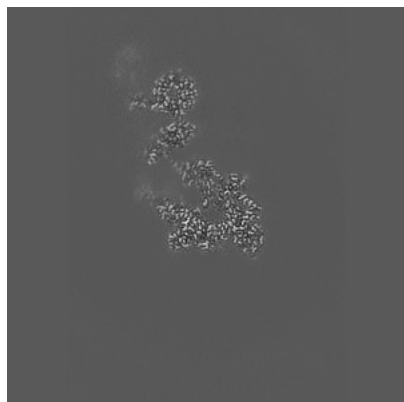


Z

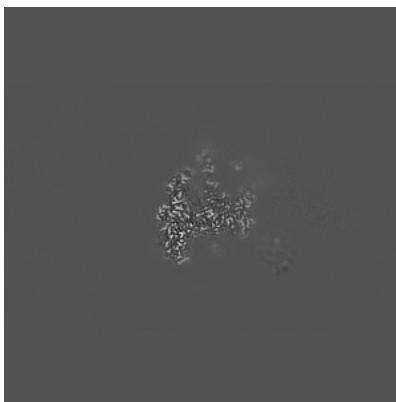
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

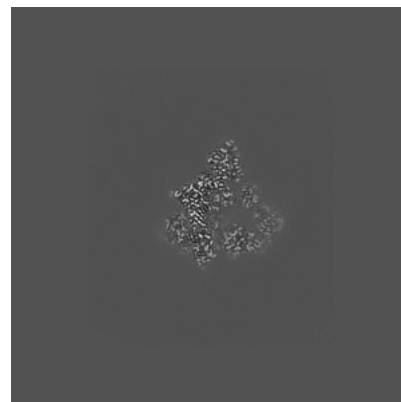
6.2.1 Primary map



X Index: 200

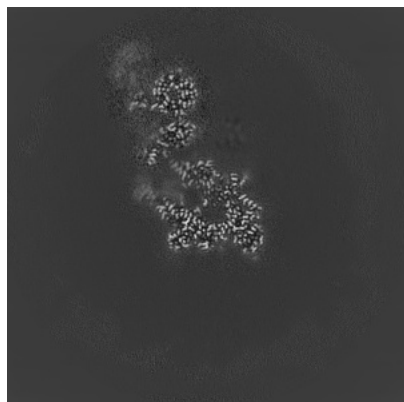


Y Index: 200

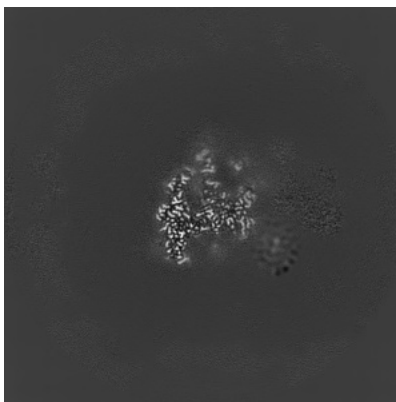


Z Index: 200

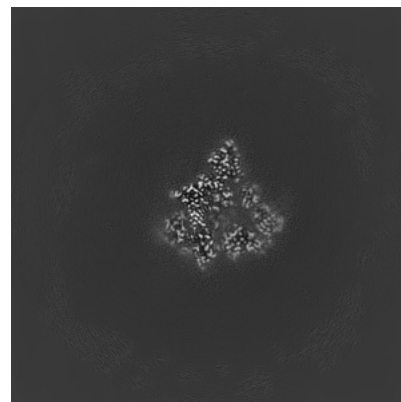
6.2.2 Raw map



X Index: 200



Y Index: 200

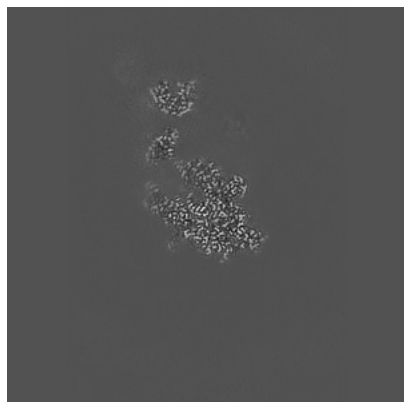


Z Index: 200

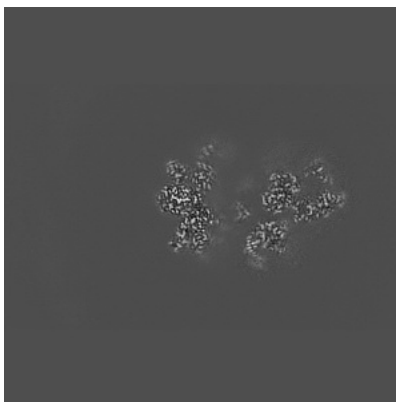
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

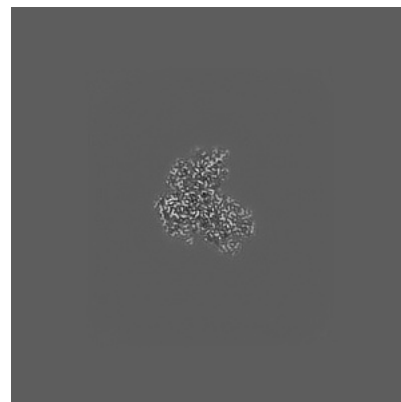
6.3.1 Primary map



X Index: 191

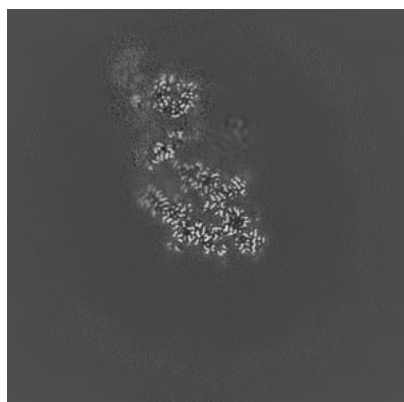


Y Index: 172

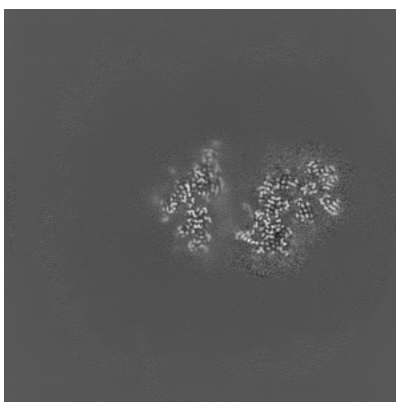


Z Index: 174

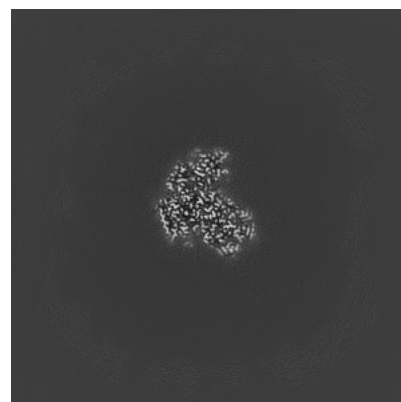
6.3.2 Raw map



X Index: 195



Y Index: 164

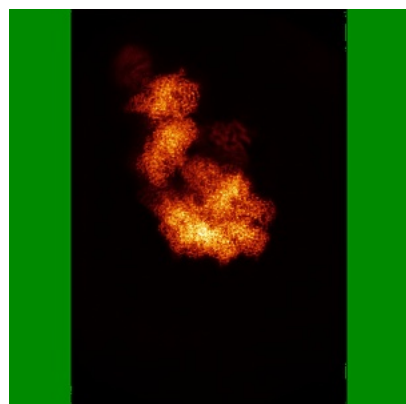


Z Index: 173

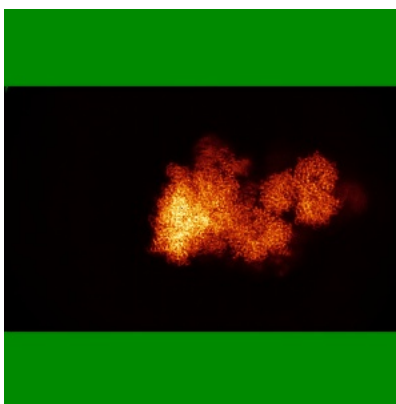
The images above show the largest variance slices of the map in three orthogonal directions.

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

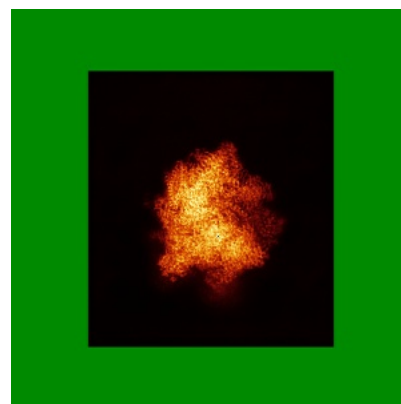
6.4.1 Primary map



X

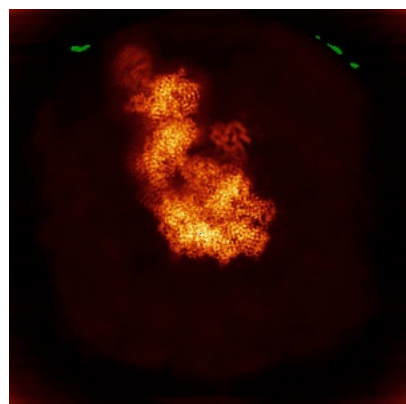


Y

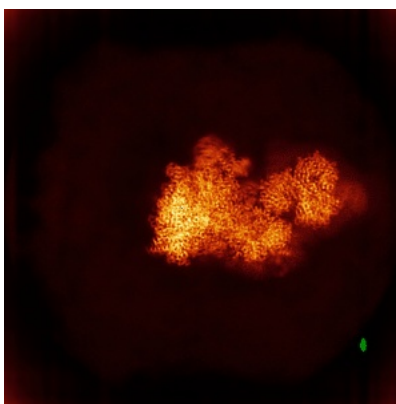


Z

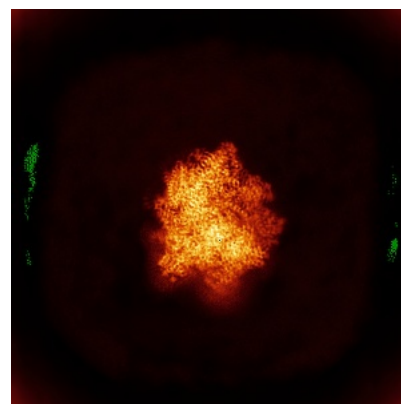
6.4.2 Raw map



X



Y

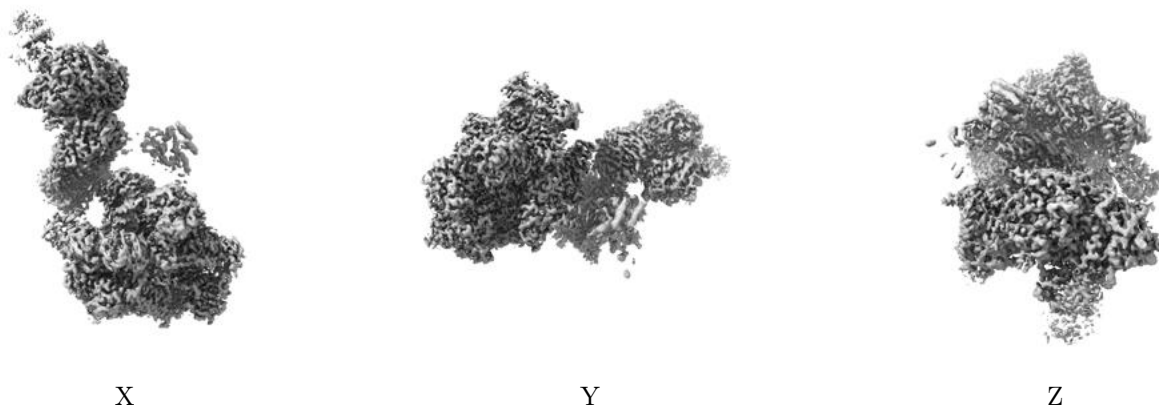


Z

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.

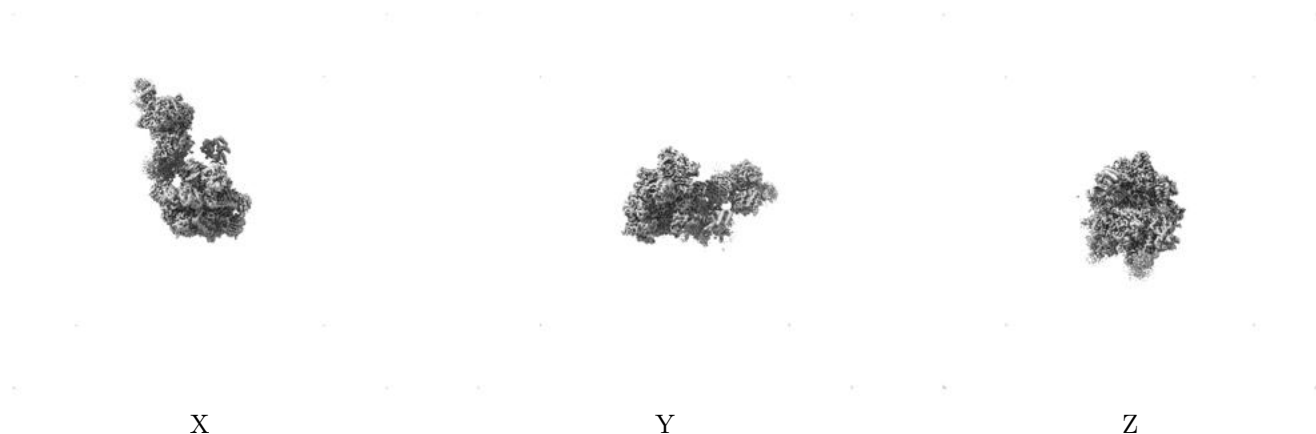
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.02. 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.

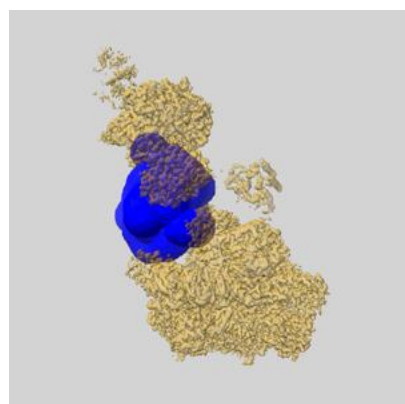
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

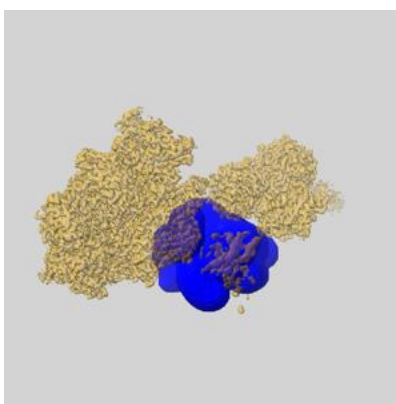
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

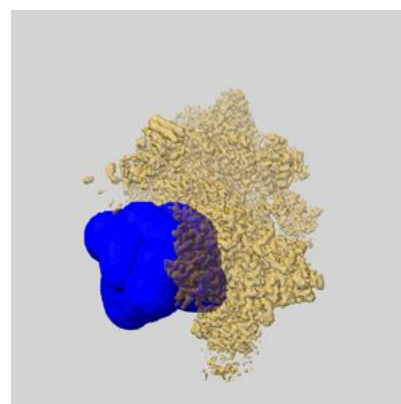
6.6.1 emd_13009_msk_4.map [i](#)



X

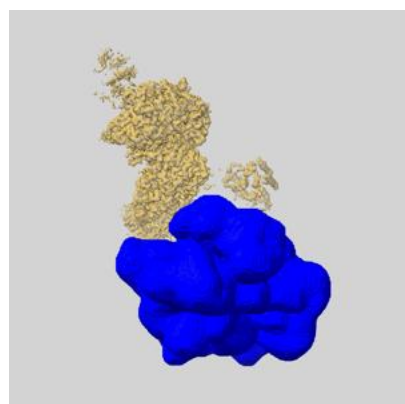


Y

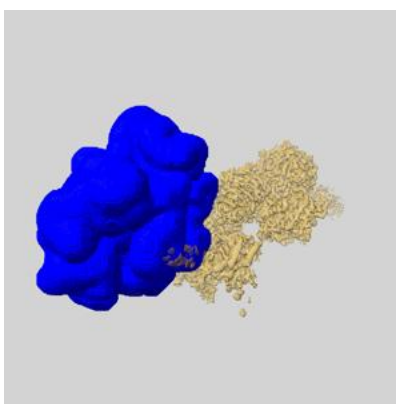


Z

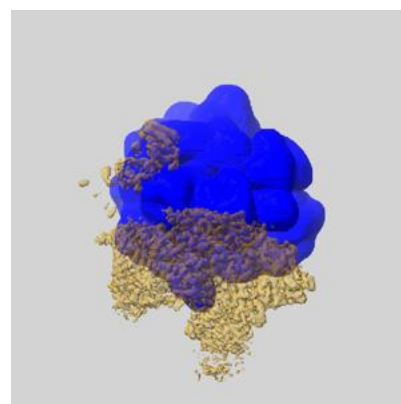
6.6.2 emd_13009_msk_3.map [i](#)



X

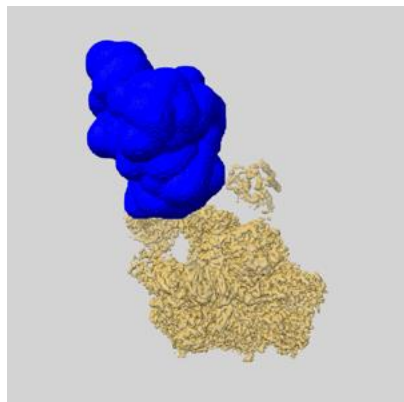


Y

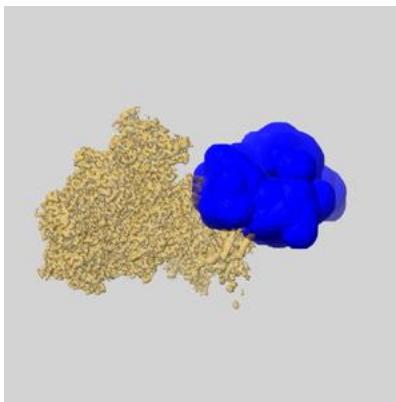


Z

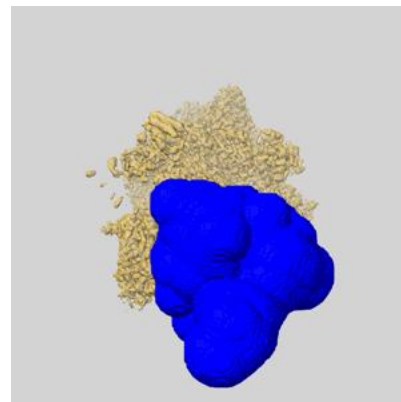
6.6.3 emd_13009_msk_2.map [i](#)



X

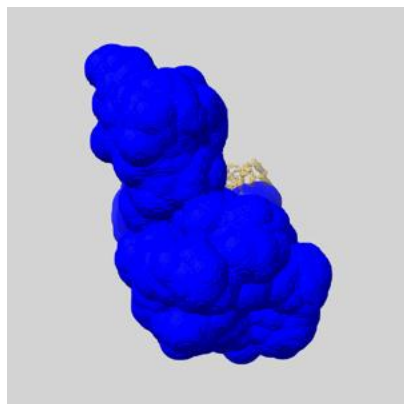


Y

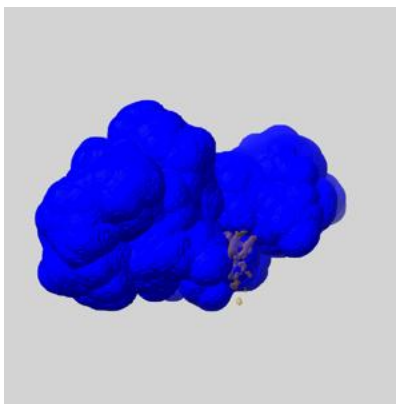


Z

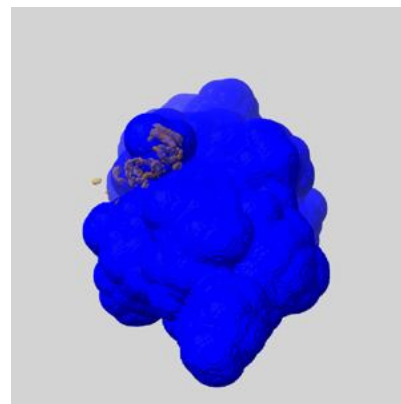
6.6.4 emd_13009_msk_1.map [i](#)



X



Y

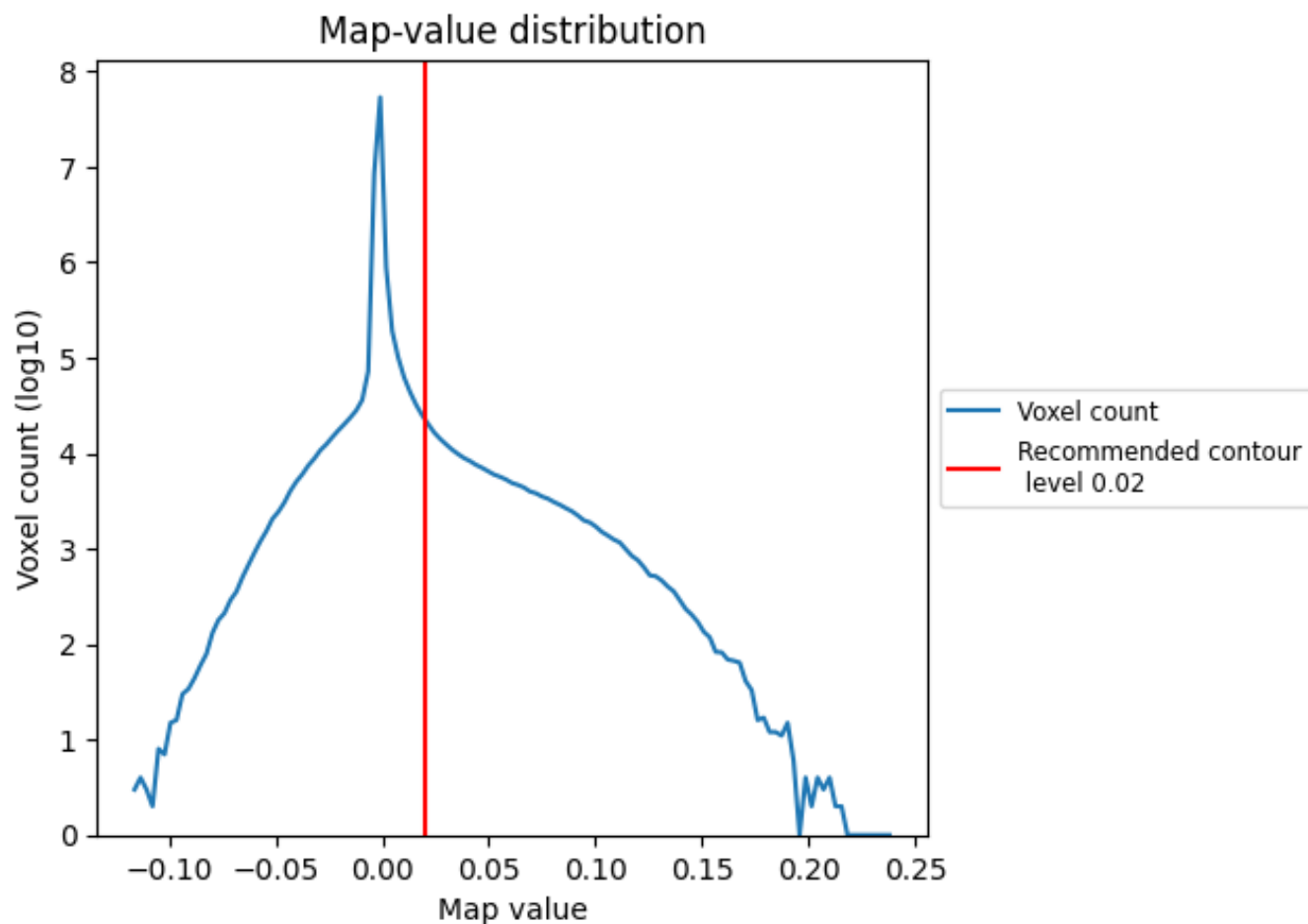


Z

7 Map analysis [i](#)

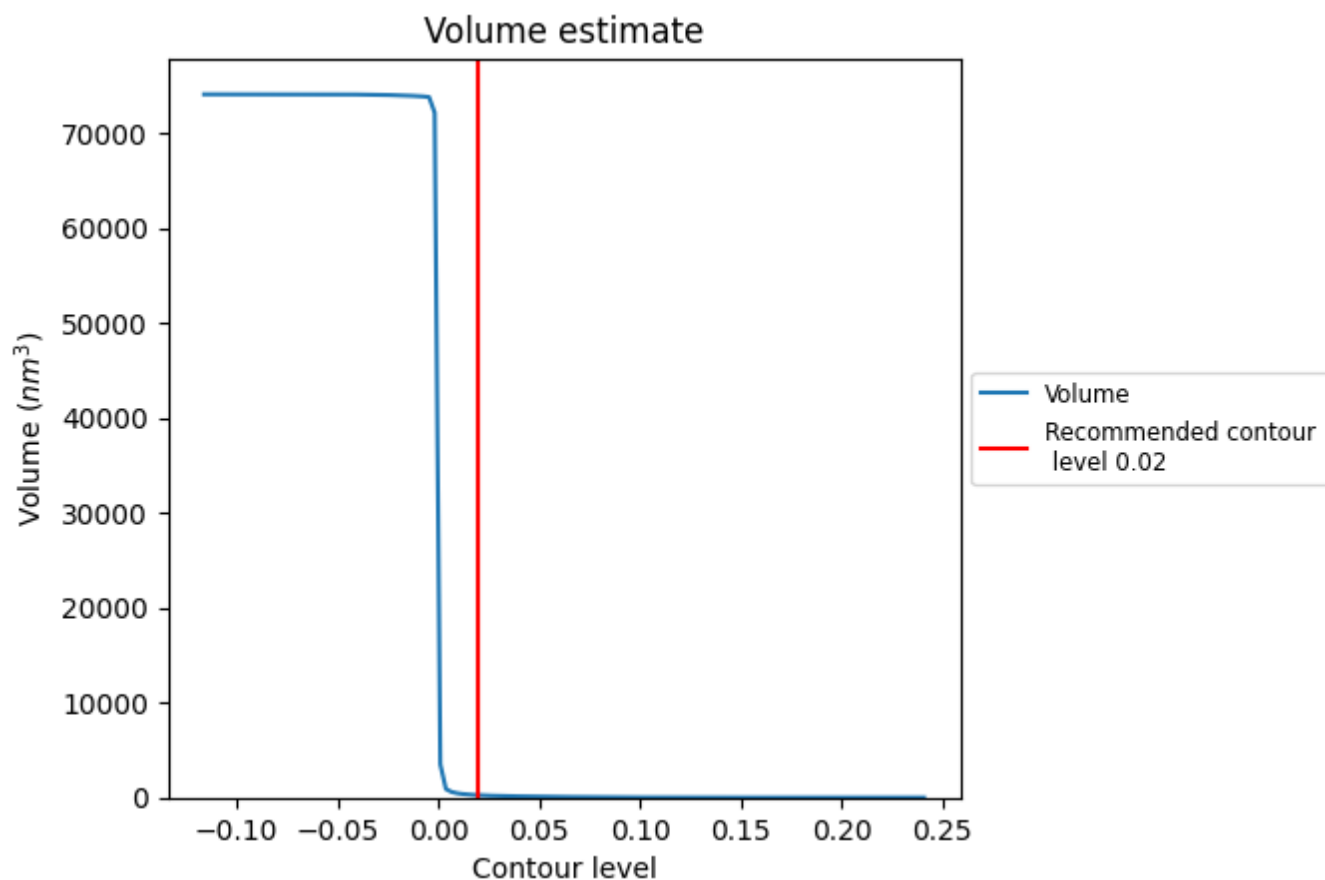
This section contains the results of statistical analysis of the map.

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.

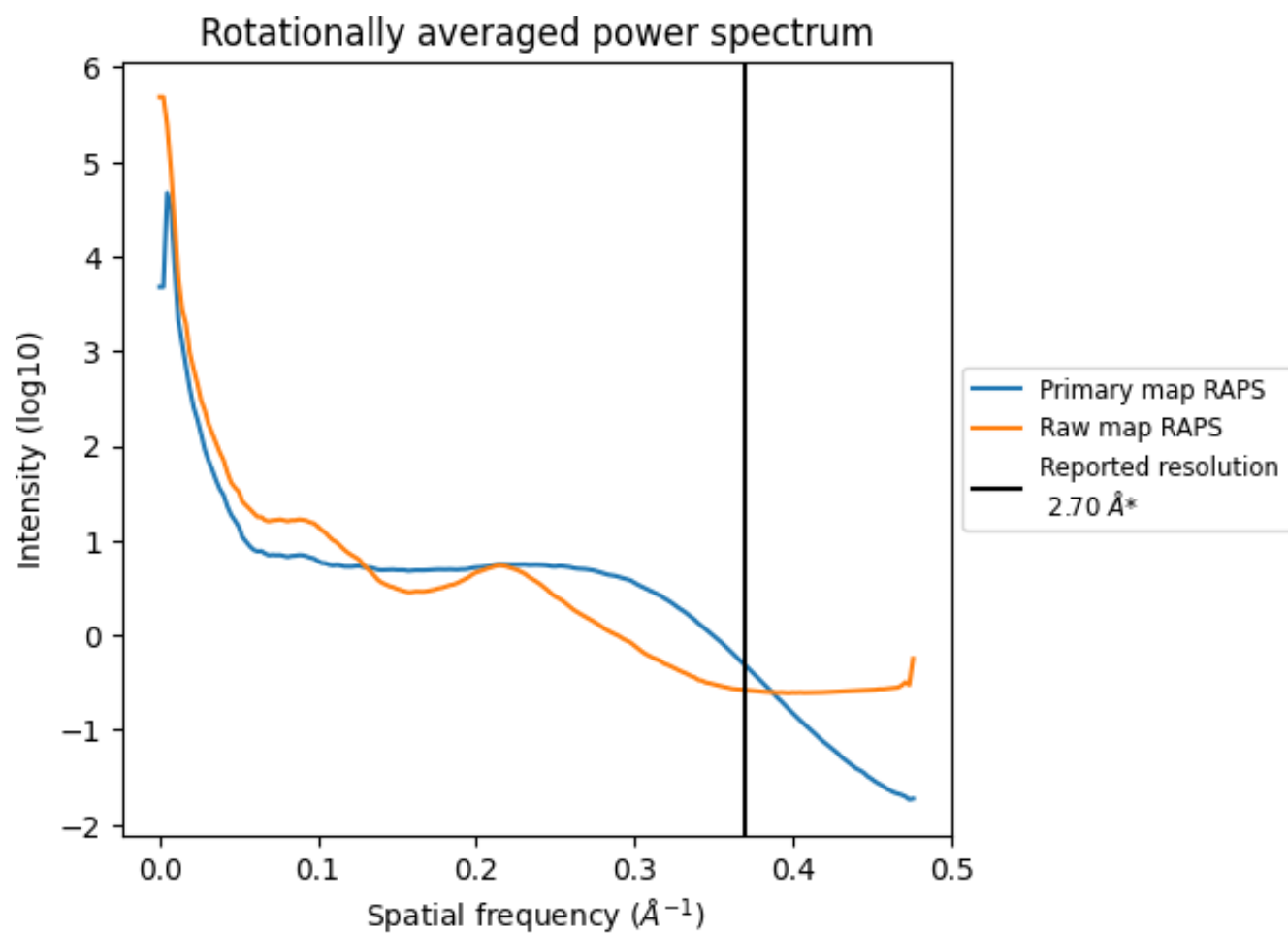
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 247 nm^3 ; this corresponds to an approximate mass of 223 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 ⓘ

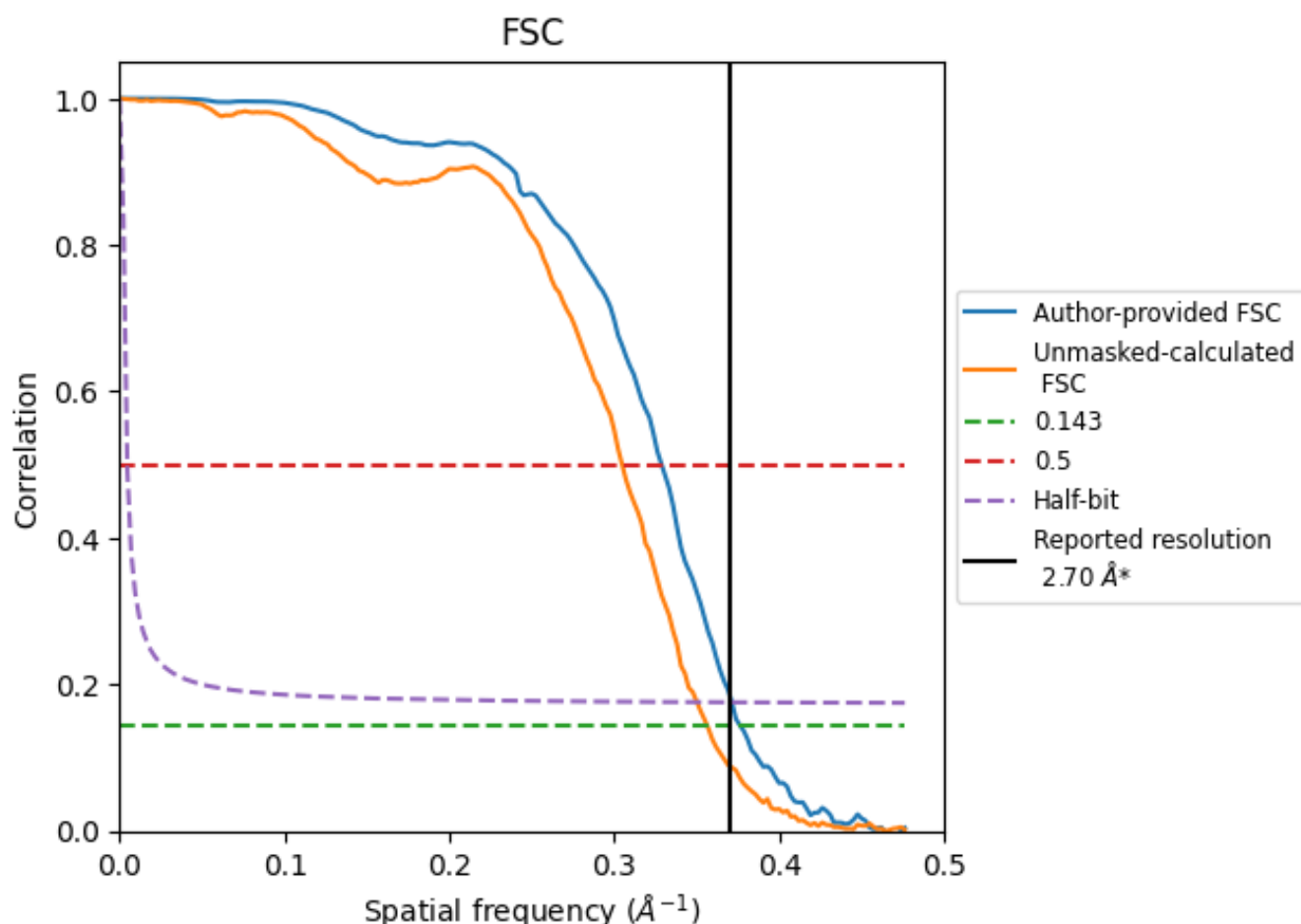


*Reported resolution corresponds to spatial frequency of 0.370 Å⁻¹

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 0.370 \AA^{-1}

8.2 Resolution estimates [i](#)

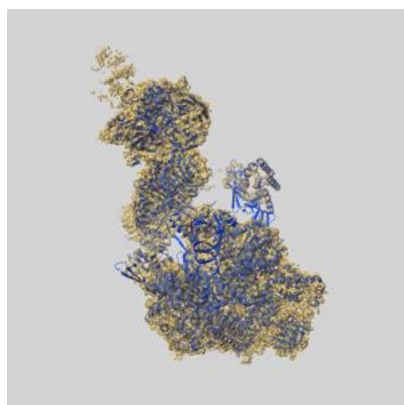
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.70	-	-
Author-provided FSC curve	2.66	3.04	2.69
Unmasked-calculated*	2.81	3.28	2.86

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

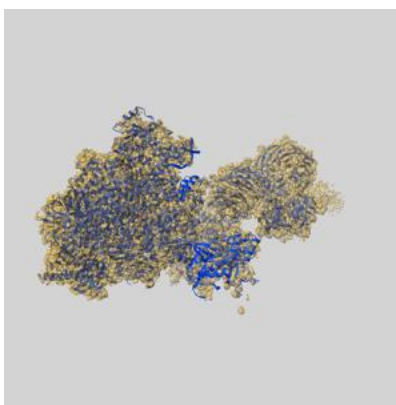
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-13009 and PDB model 7OOB. Per-residue inclusion information can be found in [section 3](#) on [page 9](#).

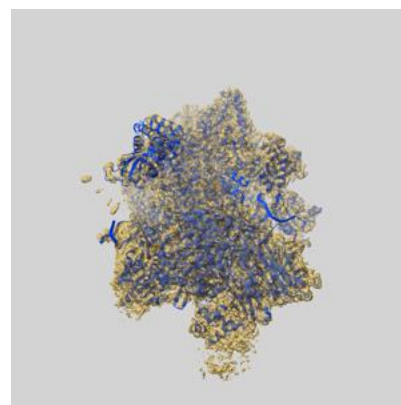
9.1 Map-model overlay [i](#)



X



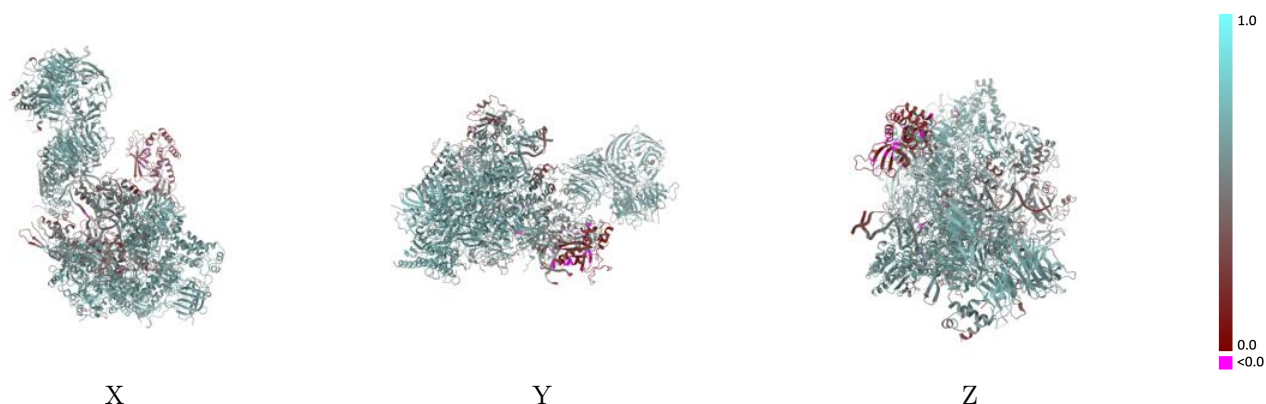
Y



Z

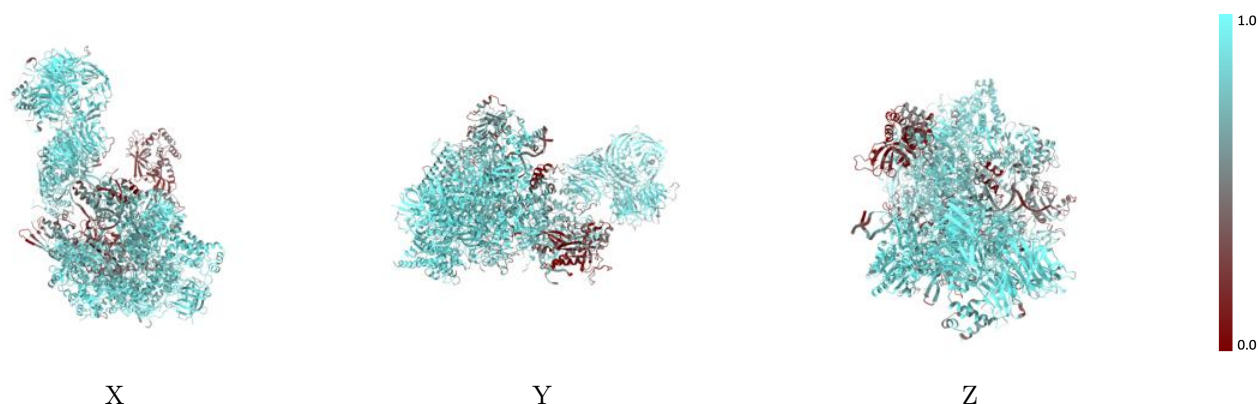
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



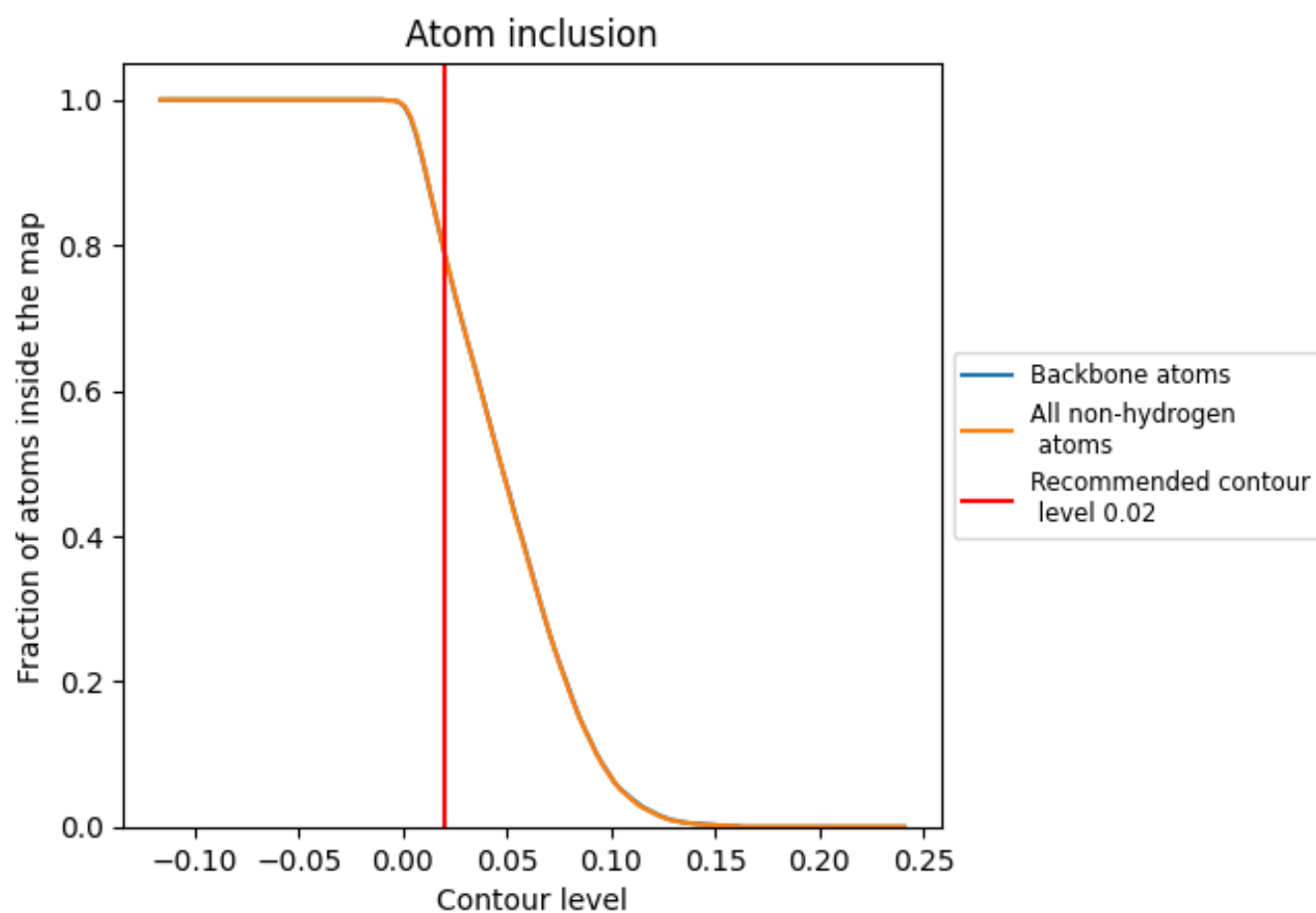
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.02).







































9.4 Atom inclusion [i](#)



At the recommended contour level, 79% of all backbone atoms, 79% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7900	 0.5660
A	 0.7980	 0.5810
B	 0.8190	 0.5900
C	 0.8980	 0.6280
D	 0.2350	 0.1820
E	 0.7920	 0.5690
F	 0.8510	 0.6030
G	 0.2930	 0.2910
H	 0.8820	 0.6130
I	 0.6810	 0.5050
J	 0.9230	 0.6540
K	 0.9060	 0.6290
L	 0.7180	 0.5180
N	 0.5750	 0.4840
P	 0.9500	 0.6530
T	 0.6470	 0.4900
a	 0.8700	 0.5970
b	 0.8640	 0.5760
d	 0.8650	 0.5880

