



wwPDB EM Validation Summary Report ⓘ

Apr 20, 2026 – 01:45 pm BST

PDB ID : 9TZE / pdb_00009tze
EMDB ID : EMD-56466
Title : 70S Coxiella burnetii Ribosome with Doxycycline and HPFcold
Authors : Stuart, W.S.; Isupov, M.N.; Harmer, N.J.
Deposited on : 2026-01-22
Resolution : 2.48 Å (reported)
Based on initial model : .

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 : 1.8.4, CSD as541be (2020)
MolProbity : **FAILED**
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

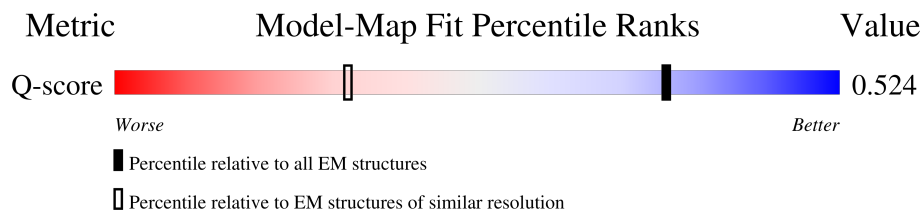
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.48 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	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Q-score	25397	6178 (1.98 - 2.98)

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition

There are 58 unique types of molecules in this entry. The entry contains 142356 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 RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1535	Total	C	N	O	P	0	0
			32928	14693	6016	10684	1535		

- Molecule 2 is a protein called Small ribosomal subunit protein uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	206	Total	C	N	O	S	0	0
			1641	1037	314	286	4		

- Molecule 3 is a protein called Small ribosomal subunit protein uS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	205	Total	C	N	O	S	0	0
			1659	1045	309	298	7		

- Molecule 4 is a protein called Small ribosomal subunit protein uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	158	Total	C	N	O	S	0	0
			1153	723	213	211	6		

- Molecule 5 is a protein called Small ribosomal subunit protein bS6.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	106	Total	C	N	O	S	0	0
			867	545	159	158	5		

- Molecule 6 is a protein called Small ribosomal subunit protein uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	162	Total	C	N	O	S	0	0
			1291	808	254	224	5		

- Molecule 7 is a protein called Small ribosomal subunit protein uS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	130	Total	C	N	O	S	0	0
			1017	634	182	194	7		

- Molecule 8 is a protein called Small ribosomal subunit protein uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	125	Total	C	N	O	S	0	0
			981	607	197	175	2		

- Molecule 9 is a protein called Small ribosomal subunit protein uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	102	Total	C	N	O	S	0	0
			828	517	157	153	1		

- Molecule 10 is a protein called Small ribosomal subunit protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	119	Total	C	N	O	S	0	0
			915	558	190	162	5		

- Molecule 11 is a protein called Small ribosomal subunit protein uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	123	Total	C	N	O	S	0	0
			958	586	204	166	2		

- Molecule 12 is a protein called Small ribosomal subunit protein uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	M	115	Total	C	N	O	S	0	0
			907	557	187	160	3		

- Molecule 13 is a protein called Small ribosomal subunit protein uS14.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	N	98	Total	C	N	O	S	0	0
			800	496	167	132	5		

- Molecule 14 is a protein called Small ribosomal subunit protein uS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	O	88	Total	C	N	O	S	0	0
			716	448	141	125	2		

- Molecule 15 is a protein called Small ribosomal subunit protein bS16.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	106	Total	C	N	O	S	0	0
			865	542	174	146	3		

- Molecule 16 is a protein called Small ribosomal subunit protein uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Q	83	Total	C	N	O	S	0	0
			669	415	131	119	4		

- Molecule 17 is a protein called Small ribosomal subunit protein bS18.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	R	65	Total	C	N	O	S	0	0
			524	331	94	95	4		

- Molecule 18 is a protein called Small ribosomal subunit protein uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	S	84	Total	C	N	O	S	0	0
			668	419	131	114	4		

- Molecule 19 is a protein called Small ribosomal subunit protein bS20.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	T	86	Total	C	N	O	S	0	0
			669	405	144	120			

- Molecule 20 is a protein called Small ribosomal subunit protein bS21.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	U	68	Total	C	N	O	S	0	0
			565	354	111	97	3		

- Molecule 21 is a protein called Coxiellaceae Large Subunit Peptide (CLaSP).

Mol	Chain	Residues	Atoms				AltConf	Trace
21	Z	16	Total	C	N	O	0	0
			133	82	34	17		

- Molecule 22 is a protein called Large ribosomal subunit protein bL33.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	0	68	Total	C	N	O	S	0	0
			550	349	99	99	3		

- Molecule 23 is a protein called Large ribosomal subunit protein uL24.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	1	105	Total	C	N	O	0	0
			813	512	153	148		

- Molecule 24 is a protein called Large ribosomal subunit protein uL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	2	116	Total	C	N	O	S	0	0
			913	566	188	157	2		

- Molecule 25 is a protein called Large ribosomal subunit protein bL36.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	3	38	Total	C	N	O	S	0	0
			307	183	73	46	5		

- Molecule 26 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	b	117	Total	C	N	O	P	0	0
			2488	1112	445	815	116		

- Molecule 27 is a protein called Large ribosomal subunit protein bL19.

Mol	Chain	Residues	Atoms				AltConf	Trace
27	c	113	Total	C	N	O	0	0
			919	573	184	162		

- Molecule 28 is a protein called Large ribosomal subunit protein uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	d	211	Total	C	N	O	S	0	0
			1596	995	298	298	5		

- Molecule 29 is a protein called Large ribosomal subunit protein bL20.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	e	118	Total	C	N	O	S	0	0
			941	595	194	151	1		

- Molecule 30 is a protein called Large ribosomal subunit protein uL5.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	f	182	Total	C	N	O	S	0	0
			1457	930	258	261	8		

- Molecule 31 is a protein called Large ribosomal subunit protein uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	g	174	Total	C	N	O	S	0	0
			1310	818	245	243	4		

- Molecule 32 is a protein called Large ribosomal subunit protein bL21.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	h	104	Total	C	N	O	S	0	0
			813	511	150	148	4		

- Molecule 33 is a protein called Large ribosomal subunit protein uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	i	141	Total	C	N	O	S	0	0
			1108	707	206	193	2		

- Molecule 34 is a protein called Large ribosomal subunit protein uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	j	110	Total	C	N	O	S	0	0
			839	516	165	154	4		

- Molecule 35 is a protein called Large ribosomal subunit protein uL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	k	143	Total	C	N	O	S	0	0
			1076	672	217	185	2		

- Molecule 36 is a protein called Large ribosomal subunit protein bL17.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	m	119	Total	C	N	O	S	0	0
			967	605	195	162	5		

- Molecule 37 is a protein called Large ribosomal subunit protein uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	o	274	Total	C	N	O	S	0	0
			2131	1314	443	368	6		

- Molecule 38 is a protein called Large ribosomal subunit protein bL9.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	q	45	Total	C	N	O	S	0	0
			339	221	59	58	1		

- Molecule 39 is a protein called Large ribosomal subunit protein uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	r	63	Total	C	N	O	S	0	0
			522	324	106	91	1		

- Molecule 40 is a protein called Large ribosomal subunit protein uL16.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	s	137	Total	C	N	O	S	0	0
			1090	688	215	182	5		

- Molecule 41 is a protein called Large ribosomal subunit protein uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	t	56	Total	C	N	O	S	0	0
			449	281	86	78	4		

- Molecule 42 is a protein called Large ribosomal subunit protein bL25.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	u	191	Total	C	N	O	S	0	0
			1486	940	260	281	5		

- Molecule 43 is a protein called Large ribosomal subunit protein bL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	v	54	Total	C	N	O	S	0	0
			436	263	95	76	2		

- Molecule 44 is a protein called Large ribosomal subunit protein uL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	w	205	Total	C	N	O	S	0	0
			1571	974	296	296	5		

- Molecule 45 is a protein called Large ribosomal subunit protein uL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	x	122	Total	C	N	O	S	0	0
			948	594	184	165	5		

- Molecule 46 is a protein called Large ribosomal subunit protein bL34.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	y	44	Total	C	N	O	S	0	0
			374	224	91	57	2		

- Molecule 47 is a protein called Large ribosomal subunit protein bL35.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	z	62	Total	C	N	O	S	0	0
			500	308	110	80	2		

- Molecule 48 is a protein called Large ribosomal subunit protein bL31.

Mol	Chain	Residues	Atoms				AltConf	Trace
48	4	10	Total	C	N	O	0	0
			93	61	19	13		

- Molecule 49 is a protein called Ribosome hibernation promoting factor.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	9	175	Total	C	N	O	S	0	0
			1412	892	253	262	5		

- Molecule 50 is a protein called Large ribosomal subunit protein bL27.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	8	77	Total	C	N	O	S	0	0
			613	381	124	105	3		

- Molecule 51 is a protein called Large ribosomal subunit protein uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	7	91	Total	C	N	O	S	0	0
			732	464	135	130	3		

- Molecule 52 is a protein called Large ribosomal subunit protein bL28.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	6	77	Total	C	N	O	S	0	0
			631	395	128	106	2		

- Molecule 53 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	a	2873	Total	C	N	O	P	3	0
			61677	27530	11292	19979	2876		

- Molecule 54 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
54	A	52	Total	Mg	0
			52	52	
54	b	1	Total	Mg	0
			1	1	
54	d	1	Total	Mg	0
			1	1	
54	o	1	Total	Mg	0
			1	1	
54	9	1	Total	Mg	0
			1	1	
54	a	164	Total	Mg	0
			164	164	

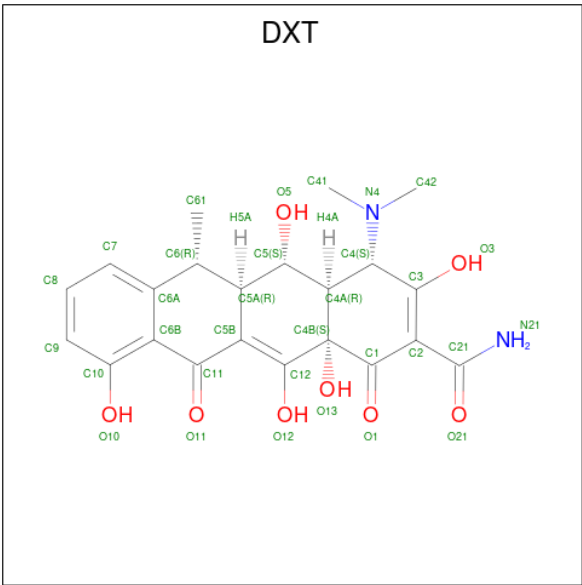
- Molecule 55 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
55	A	34	Total 34	K 34	0
55	b	1	Total 1	K 1	0
55	d	1	Total 1	K 1	0
55	o	1	Total 1	K 1	0
55	s	1	Total 1	K 1	0
55	v	1	Total 1	K 1	0
55	w	1	Total 1	K 1	0
55	a	127	Total 127	K 127	0

- Molecule 56 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
56	N	1	Total 1	Zn 1	0
56	R	1	Total 1	Zn 1	0
56	3	1	Total 1	Zn 1	0

- Molecule 57 is (4S,4AR,5S,5AR,6R,12AS)-4-(DIMETHYLAMINO)-3,5,10,12,12A-PENTAHYDROXY-6-METHYL-1,11-DIOXO-1,4,4A,5,5A,6,11,12A-OCTAHYDROTETRACENE-2-CARBOXAMIDE (CCD ID: DXT) (formula: C₂₂H₂₄N₂O₈) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
57	a	1	Total	C	N	O	0
			32	22	2	8	
57	a	1	Total	C	N	O	0
			32	22	2	8	
57	a	1	Total	C	N	O	0
			32	22	2	8	

- Molecule 58 is water.

Mol	Chain	Residues	Atoms		AltConf
58	A	6	Total	O	0
			6	6	
58	K	1	Total	O	0
			1	1	
58	M	1	Total	O	0
			1	1	
58	a	7	Total	O	0
			7	7	

MolProbity failed to run properly - this section is therefore empty.

3 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	44196	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 ($e^-/\text{\AA}^2$)	45	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.467	Depositor
Minimum map value	-0.127	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.018	Depositor
Recommended contour level	0.078	Depositor
Map size (Å)	423.99997, 423.99997, 423.99997	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

4 Model quality [i](#)

4.1 Standard geometry [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.2 Too-close contacts [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3.2 Protein sidechains [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA [i](#)

MolProbity failed to run properly - this section is therefore empty.

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

17 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	4OC	A	1399	1	20,23,24	0.89	1 (5%)	26,32,35	1.26	4 (15%)
53	PSU	a	1933	53	18,21,22	1.44	3 (16%)	22,30,33	1.85	5 (22%)
1	UR3	A	1495	1	19,22,23	1.26	3 (15%)	26,32,35	1.76	6 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
53	PSU	a	2520	55,53	18,21,22	1.86	4 (22%)	22,30,33	3.28	6 (27%)
1	MA6	A	1515	1	23,26,27	1.57	5 (21%)	34,38,41	2.15	11 (32%)
1	2MG	A	962	1	23,26,27	1.25	2 (8%)	32,38,41	2.37	8 (25%)
53	OMU	a	2568	53,54	19,22,23	1.20	2 (10%)	26,31,34	1.84	6 (23%)
53	PSU	a	2621	53	18,21,22	1.41	3 (16%)	22,30,33	1.87	5 (22%)
53	2MA	a	2519	53,54	22,25,26	1.55	4 (18%)	33,37,40	2.12	8 (24%)
1	MA6	A	1516	1	23,26,27	1.66	4 (17%)	34,38,41	2.23	11 (32%)
1	5MC	A	963	1	18,22,23	1.05	1 (5%)	26,32,35	1.31	4 (15%)
1	G7M	A	524	1	23,26,27	2.33	5 (21%)	35,39,42	2.99	10 (28%)
53	PSU	a	2596	55,53	18,21,22	1.49	2 (11%)	22,30,33	1.81	5 (22%)
53	PSU	a	961	53	18,21,22	1.41	3 (16%)	22,30,33	1.88	4 (18%)
53	OMG	a	2267	55,53	23,26,27	1.21	3 (13%)	33,38,41	2.08	9 (27%)
53	PSU	a	1927	53	18,21,22	1.44	2 (11%)	22,30,33	1.77	4 (18%)
1	2MG	A	1513	1	23,26,27	1.26	3 (13%)	32,38,41	2.37	9 (28%)

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
1	4OC	A	1399	1	-	0/9/29/30	0/2/2/2
53	PSU	a	1933	53	-	0/7/25/26	0/2/2/2
1	UR3	A	1495	1	-	0/7/25/26	0/2/2/2
53	PSU	a	2520	55,53	-	0/7/25/26	0/2/2/2
1	MA6	A	1515	1	-	3/11/29/30	0/3/3/3
1	2MG	A	962	1	-	3/9/27/28	0/3/3/3
53	OMU	a	2568	53,54	-	0/9/27/28	0/2/2/2
53	PSU	a	2621	53	-	2/7/25/26	0/2/2/2
53	2MA	a	2519	53,54	-	2/7/25/26	0/3/3/3
1	MA6	A	1516	1	-	6/11/29/30	0/3/3/3
1	5MC	A	963	1	-	2/7/25/26	0/2/2/2
1	G7M	A	524	1	-	3/7/25/26	0/3/3/3
53	PSU	a	2596	55,53	-	0/7/25/26	0/2/2/2
53	PSU	a	961	53	-	0/7/25/26	0/2/2/2
53	OMG	a	2267	55,53	-	1/9/27/28	0/3/3/3
53	PSU	a	1927	53	-	0/7/25/26	0/2/2/2
1	2MG	A	1513	1	-	2/9/27/28	0/3/3/3

The worst 5 of 50 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	524	G7M	C8-N7	7.30	1.46	1.33
53	a	2520	PSU	O2-C2	5.37	1.34	1.23
1	A	1516	MA6	C5-C4	4.91	1.48	1.39
1	A	1515	MA6	C5-C4	4.83	1.48	1.39
1	A	524	G7M	C5-N7	-4.82	1.33	1.39

The worst 5 of 115 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	a	2520	PSU	O2-C2-N1	-12.02	109.55	122.79
1	A	1513	2MG	C2-N3-C4	7.90	121.83	112.04
1	A	962	2MG	C2-N3-C4	7.85	121.78	112.04
1	A	524	G7M	CN7-N7-C8	-7.67	113.00	124.84
53	a	2519	2MA	C5-C4-N3	-7.18	119.11	127.19

There are no chirality outliers.

5 of 24 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	524	G7M	C3'-C4'-C5'-O5'
1	A	962	2MG	N1-C2-N2-CM2
1	A	962	2MG	N3-C2-N2-CM2
1	A	963	5MC	O4'-C4'-C5'-O5'
1	A	1513	2MG	N1-C2-N2-CM2

There are no ring outliers.

No monomer is involved in short contacts.

4.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

4.6 Ligand geometry [i](#)

Of 393 ligands modelled in this entry, 390 are monoatomic - leaving 3 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
57	DXT	a	3302	54	33,35,35	1.00	2 (6%)	42,57,57	1.47	8 (19%)
57	DXT	a	3303	54	33,35,35	1.31	3 (9%)	42,57,57	1.20	5 (11%)
57	DXT	a	3301	54	33,35,35	1.19	3 (9%)	42,57,57	1.49	9 (21%)

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
57	DXT	a	3302	54	-	8/8/74/74	0/4/4/4
57	DXT	a	3303	54	-	8/8/74/74	0/4/4/4
57	DXT	a	3301	54	-	6/8/74/74	0/4/4/4

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	a	3303	DXT	C4B-C1	-3.63	1.50	1.55
57	a	3303	DXT	C4B-C12	-3.62	1.48	1.52
57	a	3302	DXT	C21-N21	3.33	1.42	1.33
57	a	3301	DXT	C21-N21	3.31	1.42	1.33
57	a	3301	DXT	C4B-C1	-3.29	1.50	1.55

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	a	3301	DXT	C11-C5B-C12	-3.86	115.75	118.80
57	a	3303	DXT	C1-C4B-C12	-3.82	105.41	109.88
57	a	3302	DXT	C10-C6B-C6A	3.65	122.83	118.97
57	a	3302	DXT	O11-C11-C6B	-3.64	115.10	121.99
57	a	3301	DXT	C5A-C5-C4A	3.24	116.03	110.62

There are no chirality outliers.

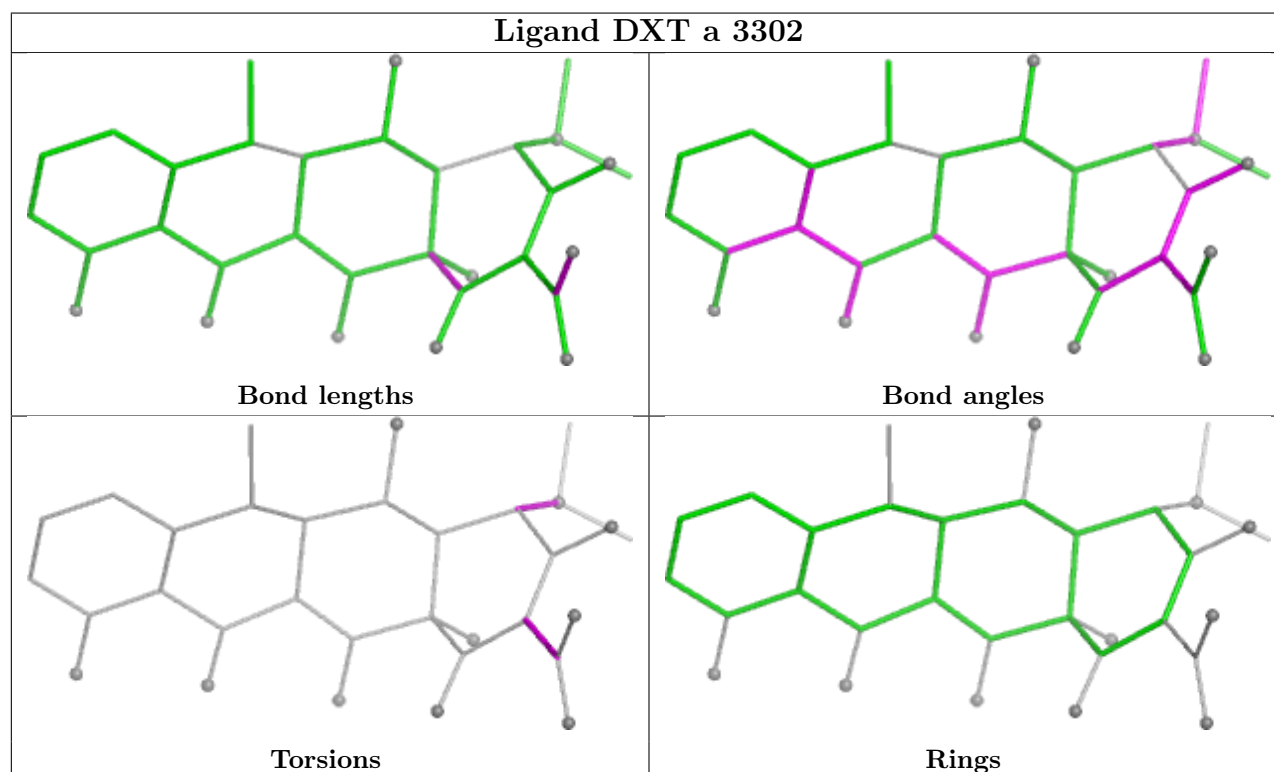
5 of 22 torsion outliers are listed below:

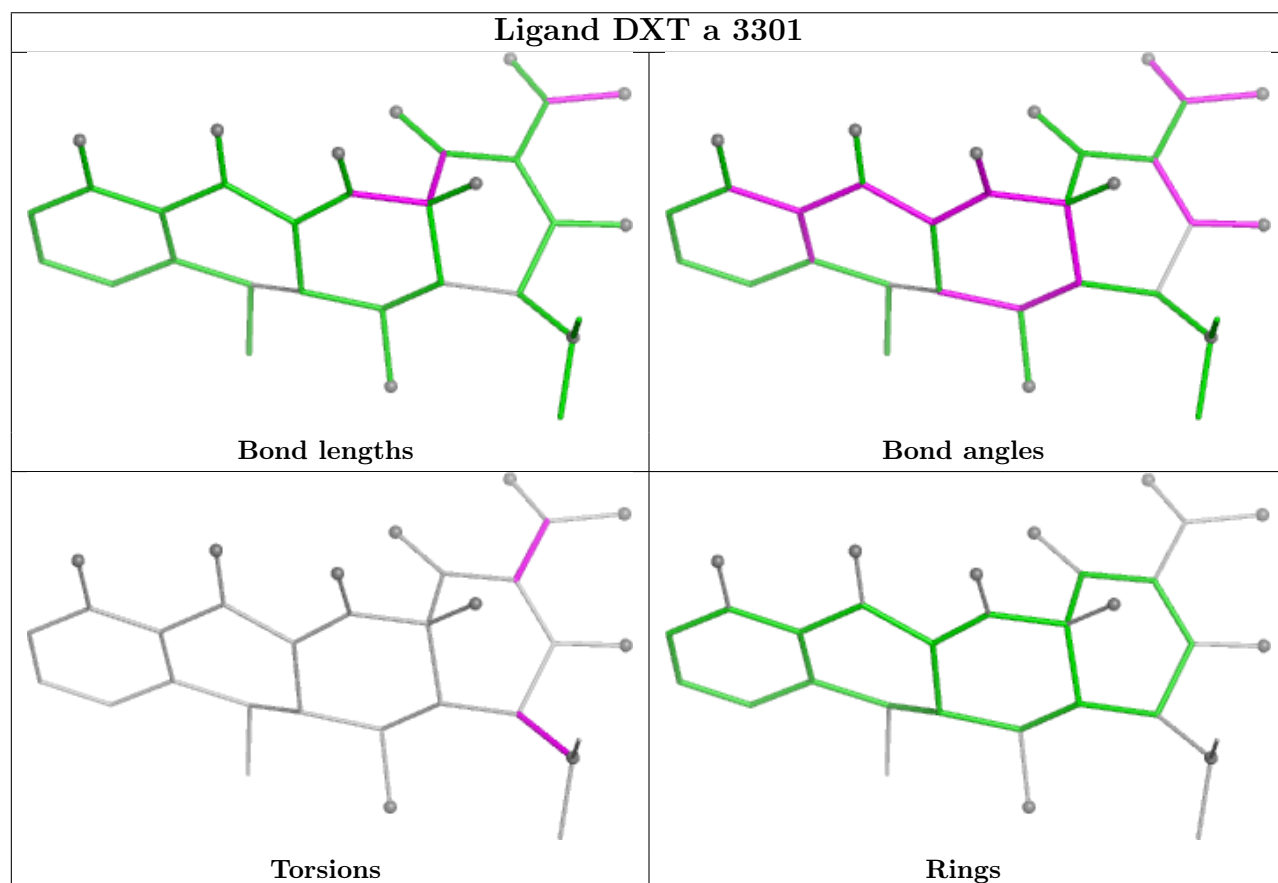
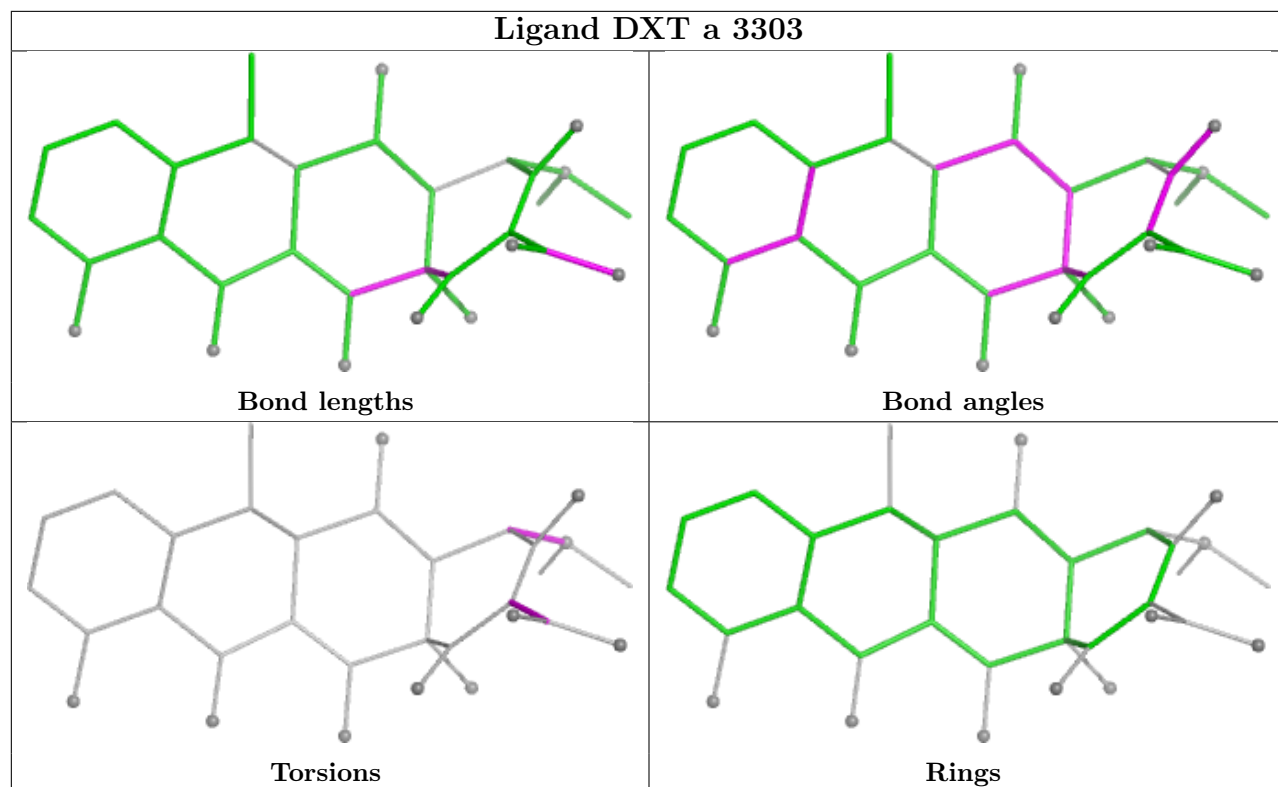
Mol	Chain	Res	Type	Atoms
57	a	3301	DXT	C1-C2-C21-O21
57	a	3301	DXT	C1-C2-C21-N21
57	a	3301	DXT	C3-C2-C21-O21
57	a	3301	DXT	C3-C2-C21-N21
57	a	3301	DXT	C4A-C4-N4-C42

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.





4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

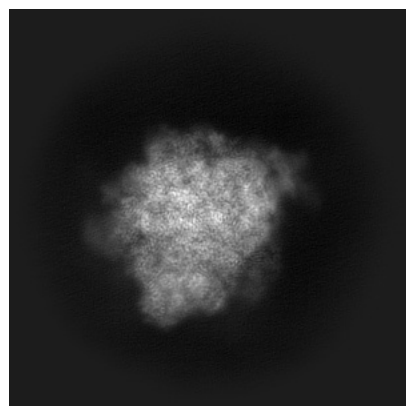
5 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-56466. These allow visual inspection of the internal detail of the map and identification of artifacts.

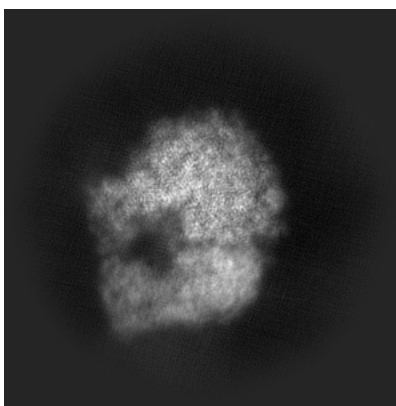
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

5.1 Orthogonal projections [i](#)

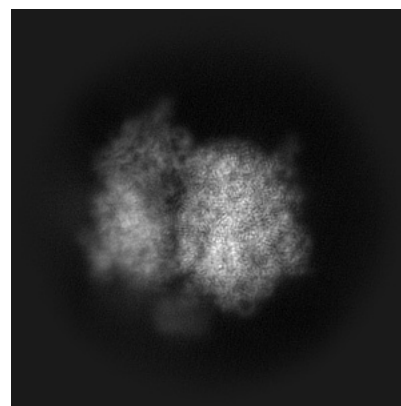
5.1.1 Primary map



X

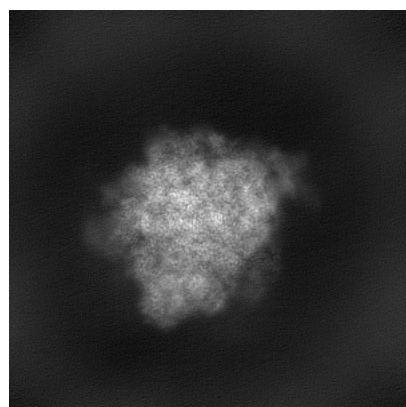


Y

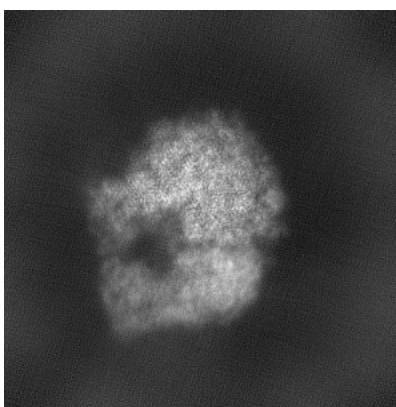


Z

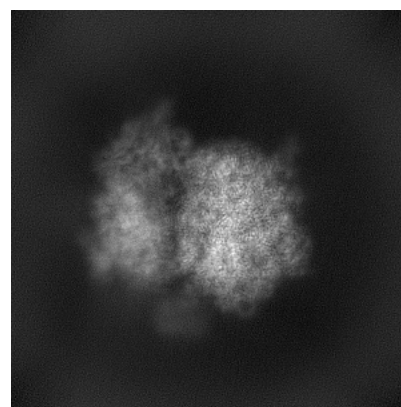
5.1.2 Raw map



X



Y

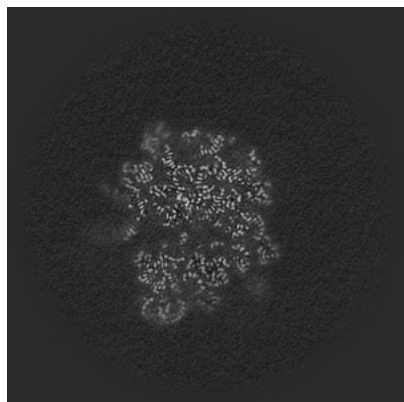


Z

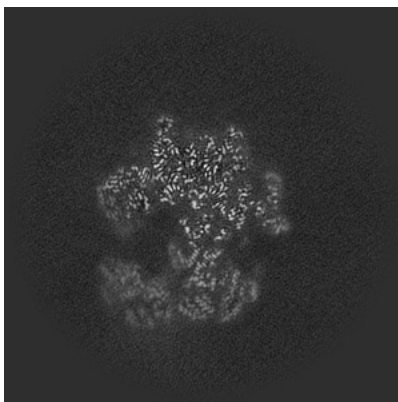
The images above show the map projected in three orthogonal directions.

5.2 Central slices [i](#)

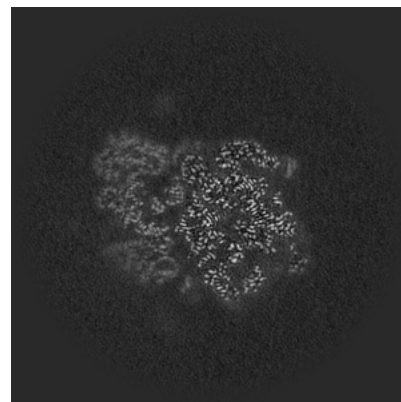
5.2.1 Primary map



X Index: 200

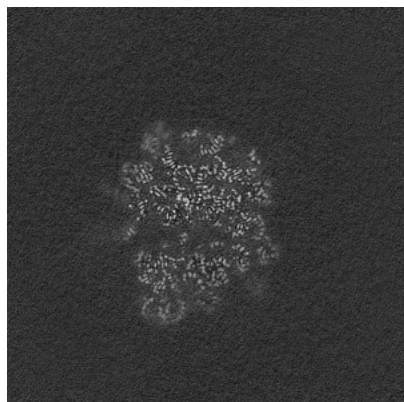


Y Index: 200

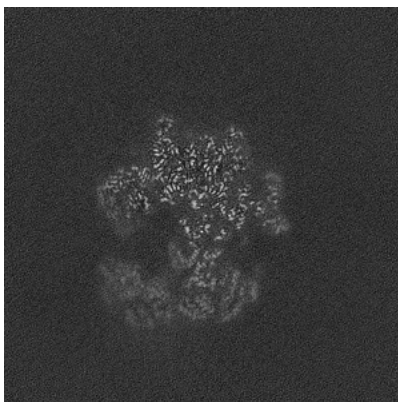


Z Index: 200

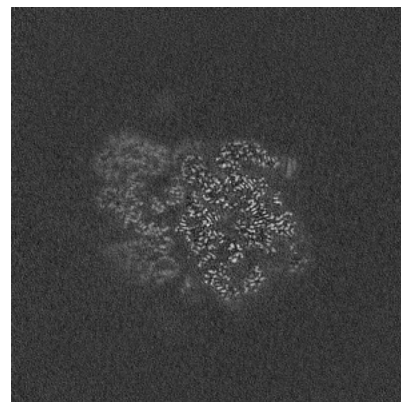
5.2.2 Raw map



X Index: 200



Y Index: 200

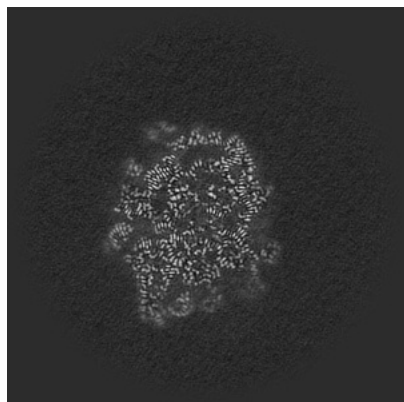


Z Index: 200

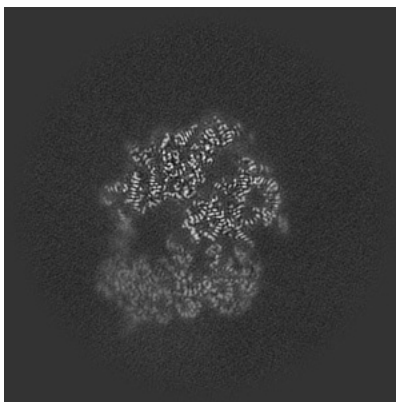
The images above show central slices of the map in three orthogonal directions.

5.3 Largest variance slices [i](#)

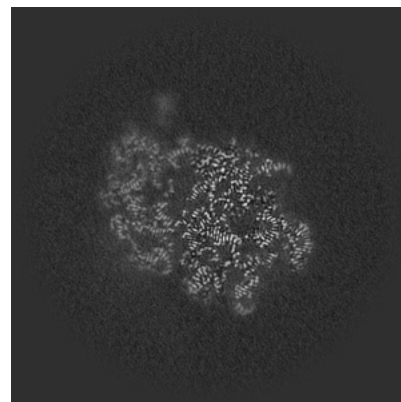
5.3.1 Primary map



X Index: 209

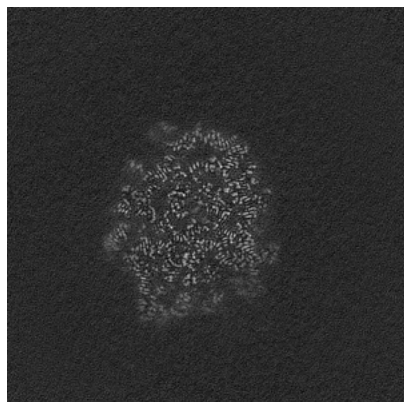


Y Index: 185

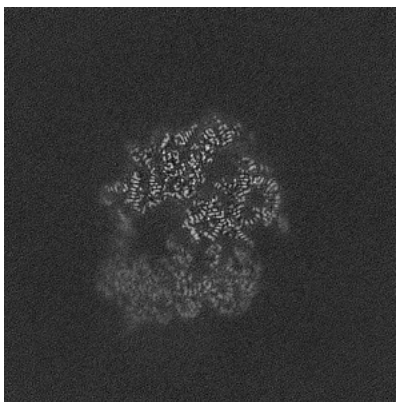


Z Index: 209

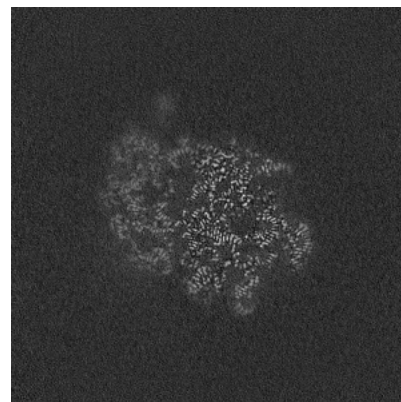
5.3.2 Raw map



X Index: 211



Y Index: 185

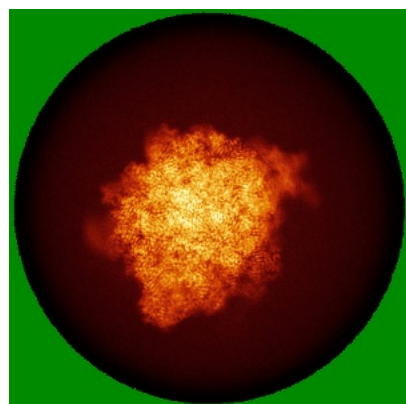


Z Index: 209

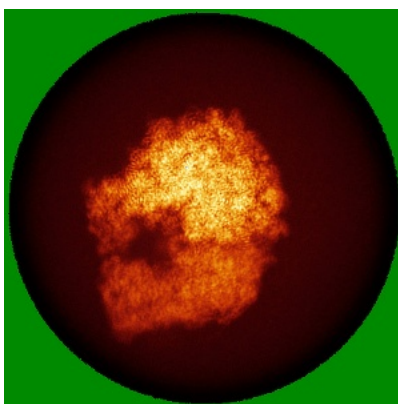
The images above show the largest variance slices of the map in three orthogonal directions.

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

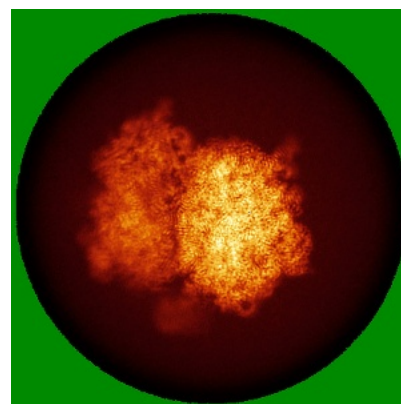
5.4.1 Primary map



X

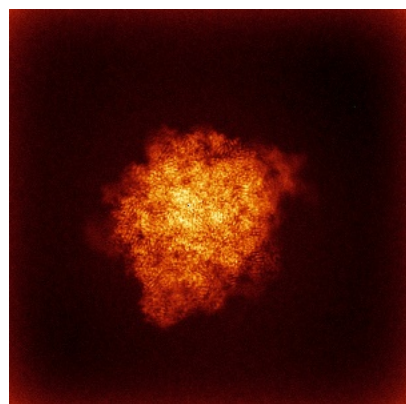


Y

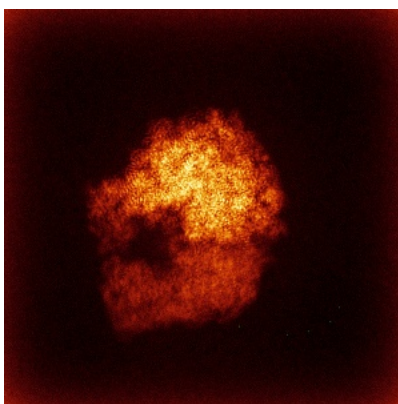


Z

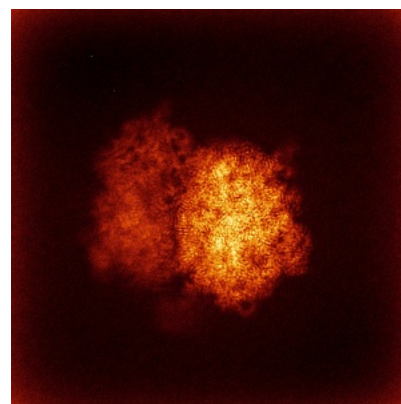
5.4.2 Raw map



X



Y

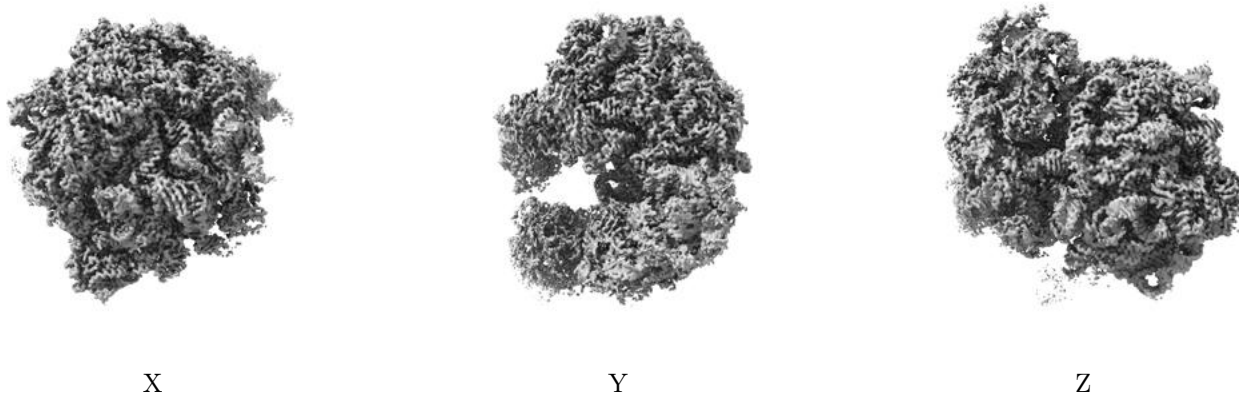


Z

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.

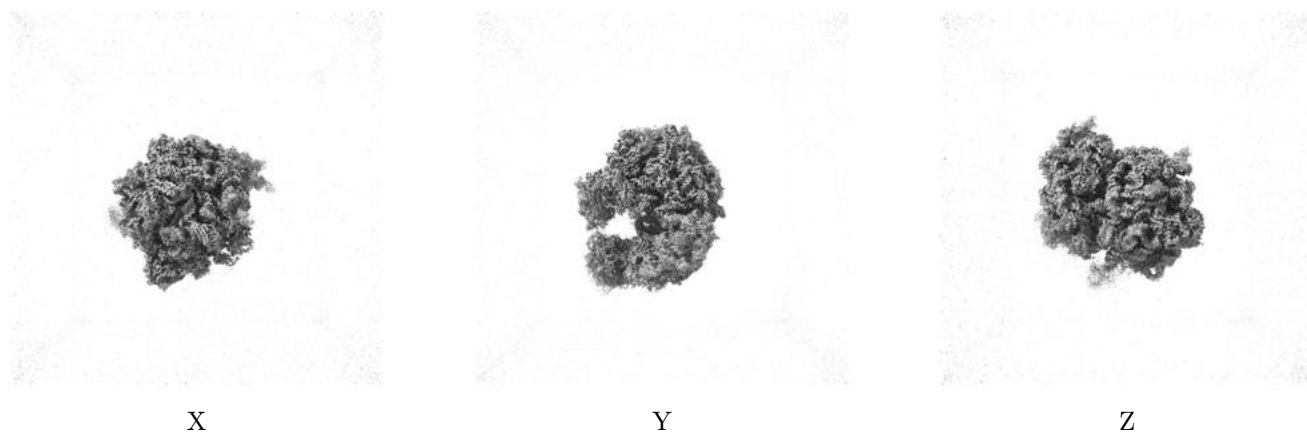
5.5 Orthogonal surface views [i](#)

5.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.078. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

5.5.2 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.

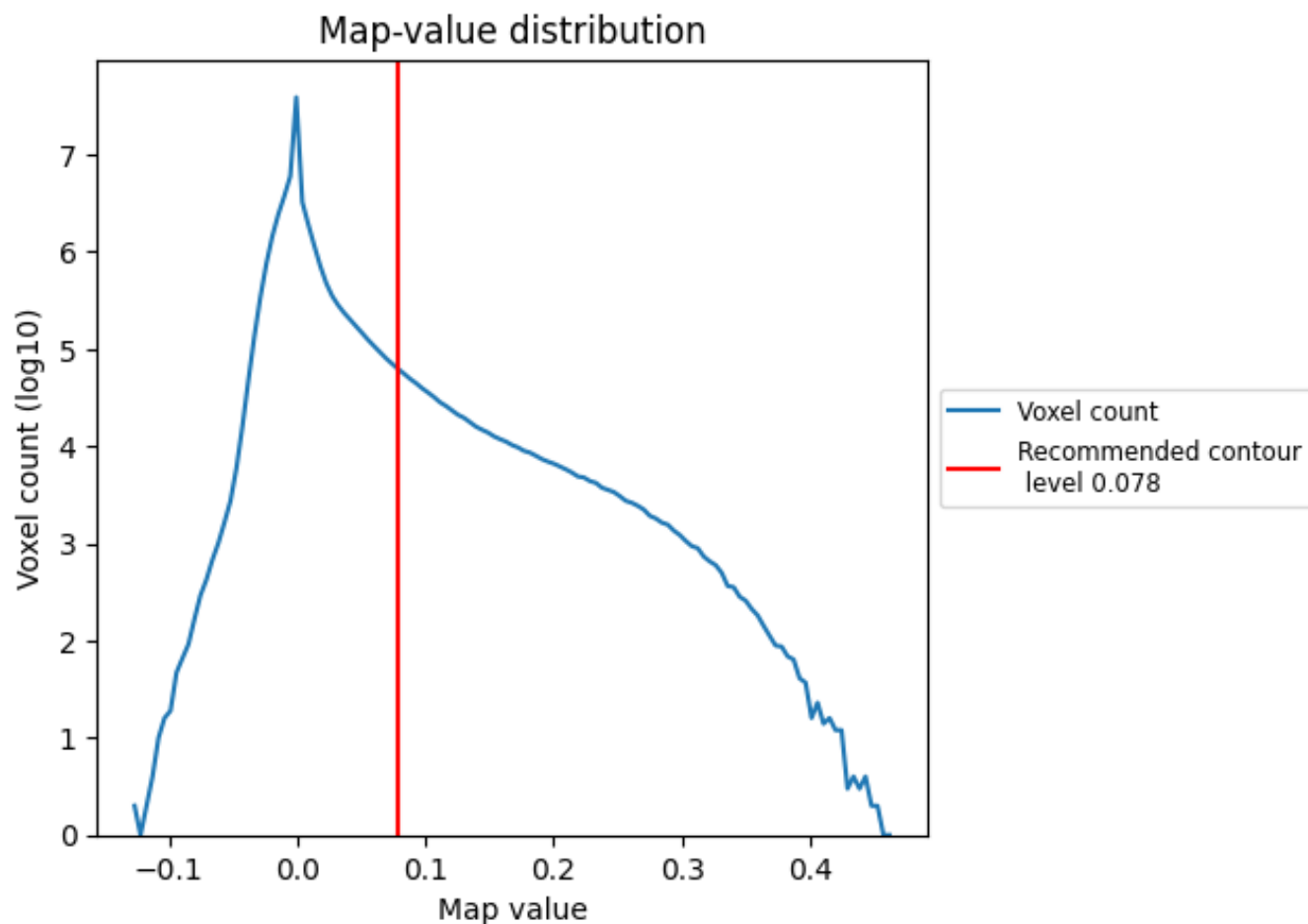
5.6 Mask visualisation [i](#)

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

6 Map analysis [i](#)

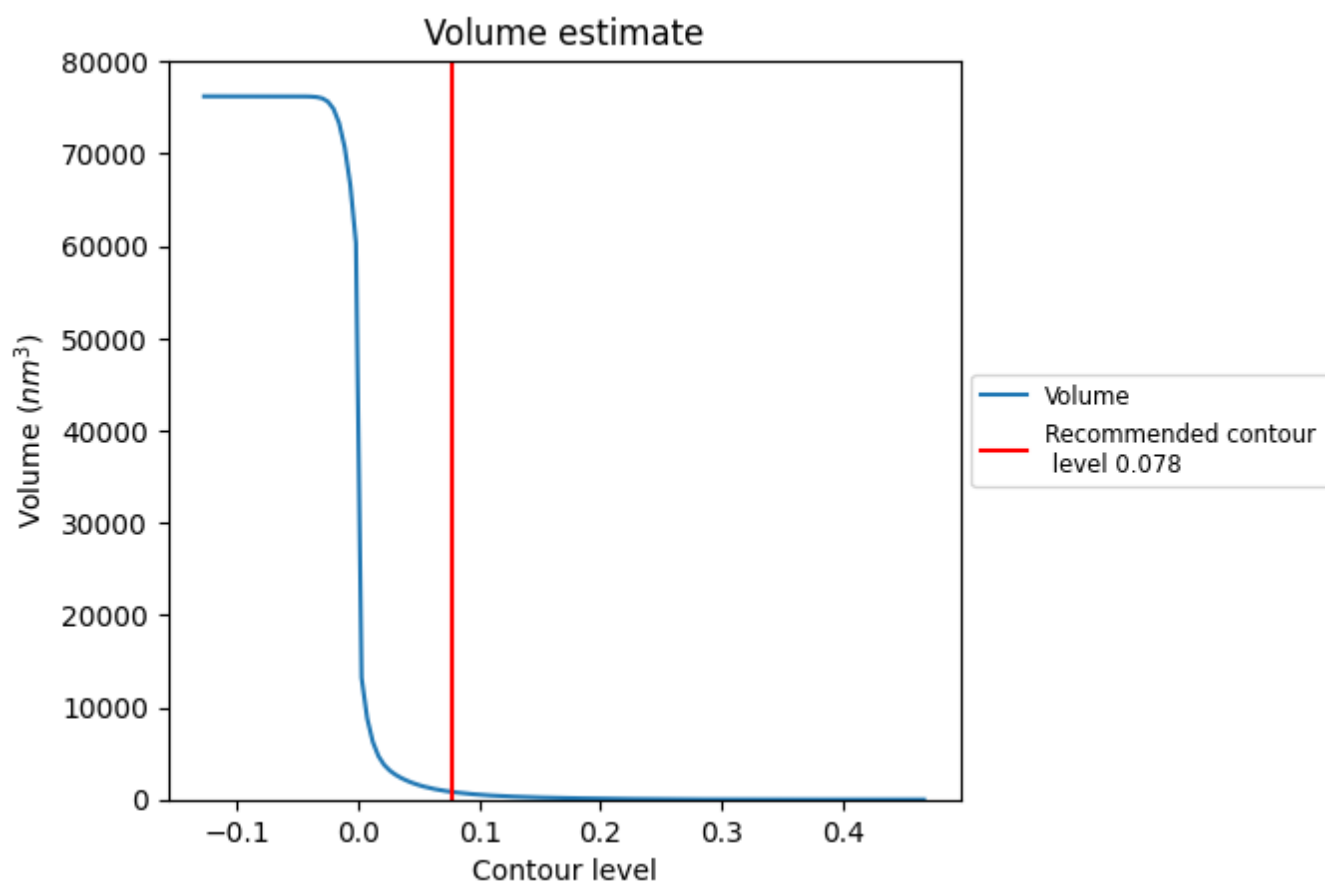
This section contains the results of statistical analysis of the map.

6.1 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.

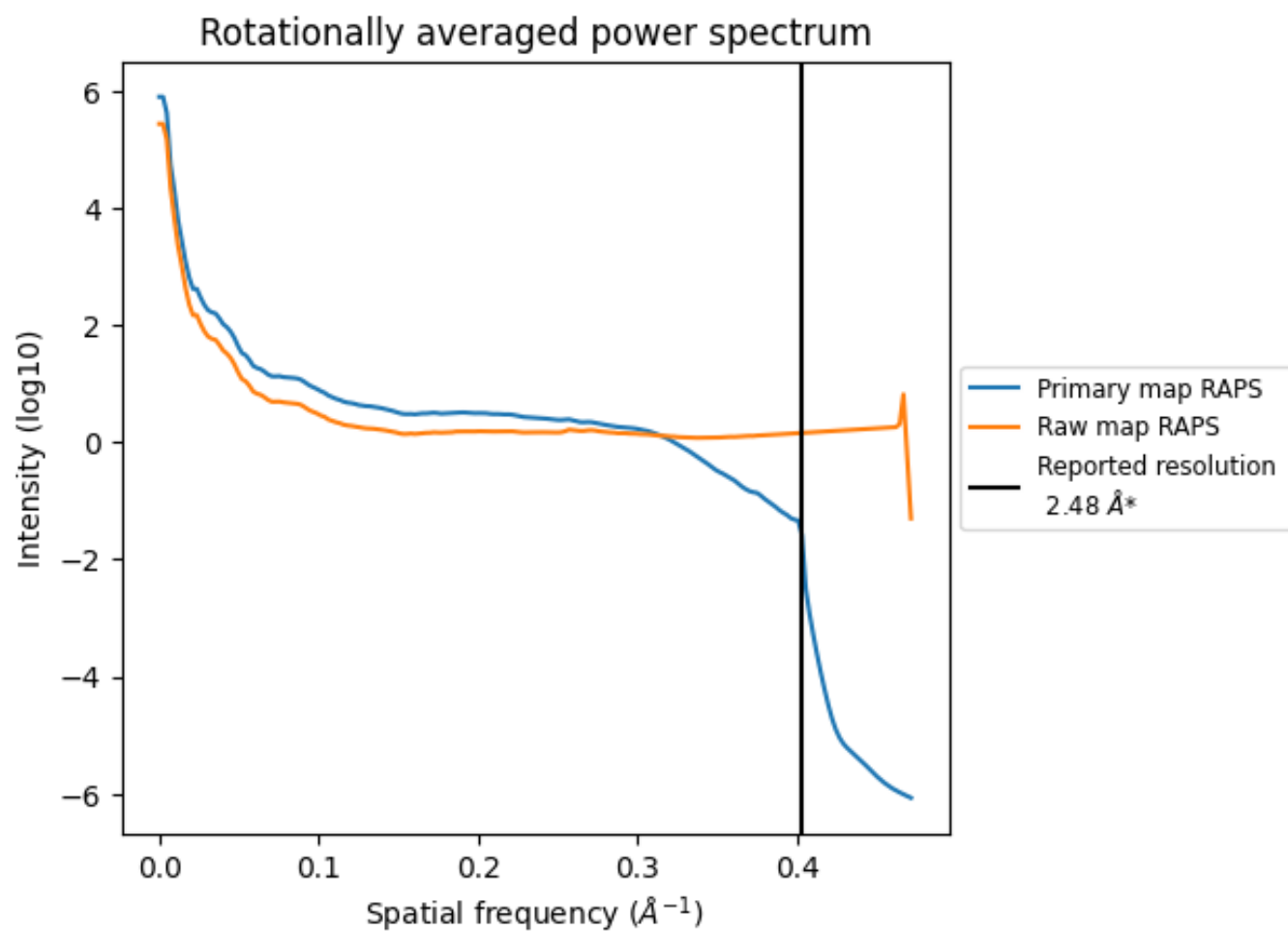
6.2 Volume estimate [i](#)



The volume at the recommended contour level is 819 nm³; this corresponds to an approximate mass of 740 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.

6.3 Rotationally averaged power spectrum ⓘ

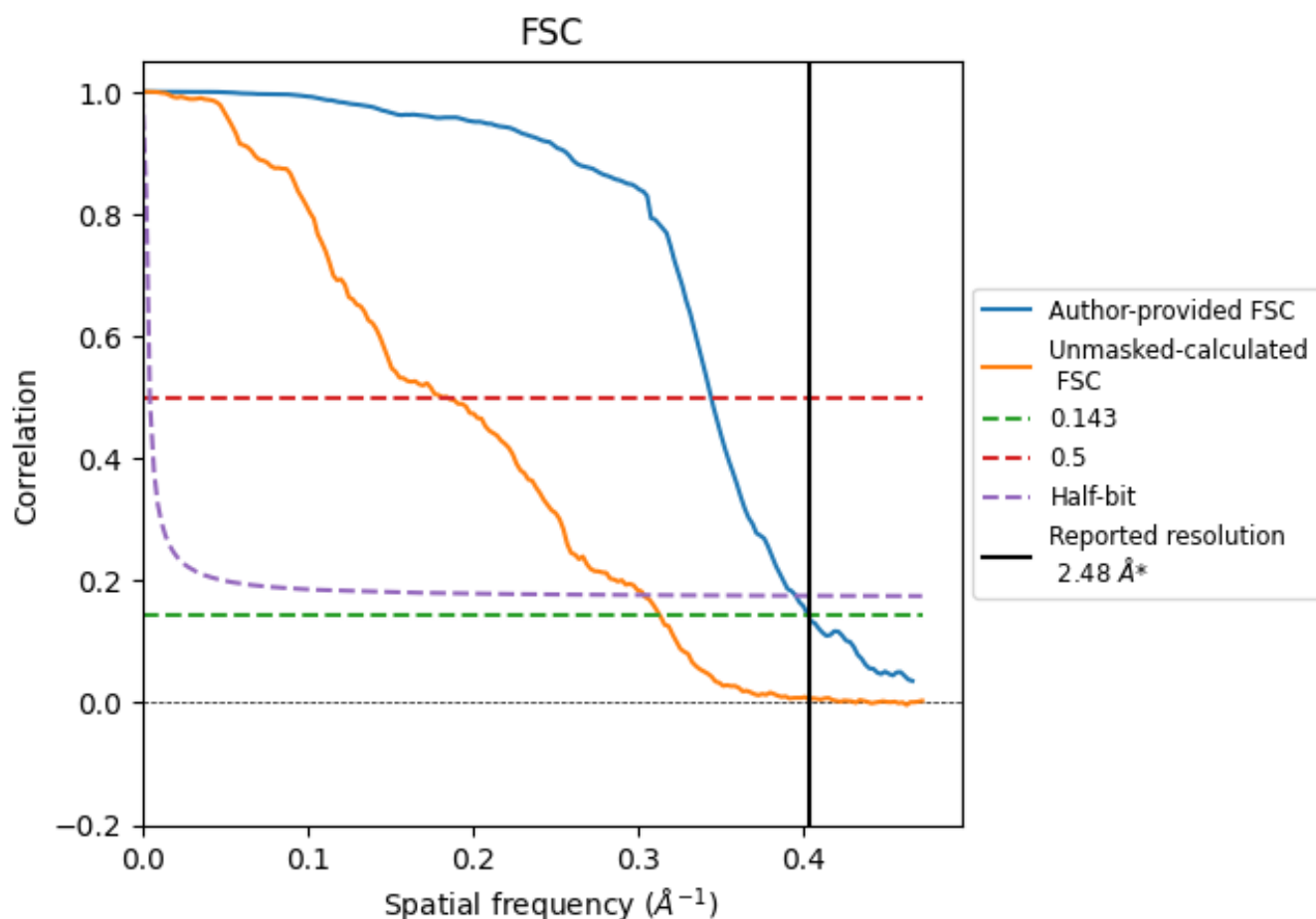


*Reported resolution corresponds to spatial frequency of 0.403 Å⁻¹

7 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.

7.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.403 \AA^{-1}

7.2 Resolution estimates [i](#)

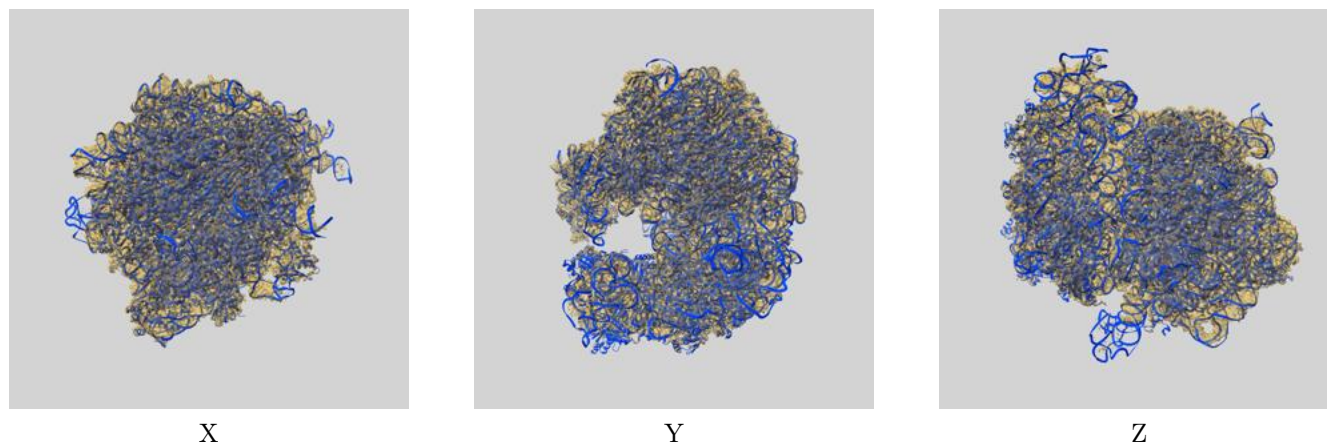
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.48	-	-
Author-provided FSC curve	2.48	2.91	2.53
Unmasked-calculated*	3.19	5.51	3.30

*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 3.19 differs from the reported value 2.48 by more than 10 %

8 Map-model fit [i](#)

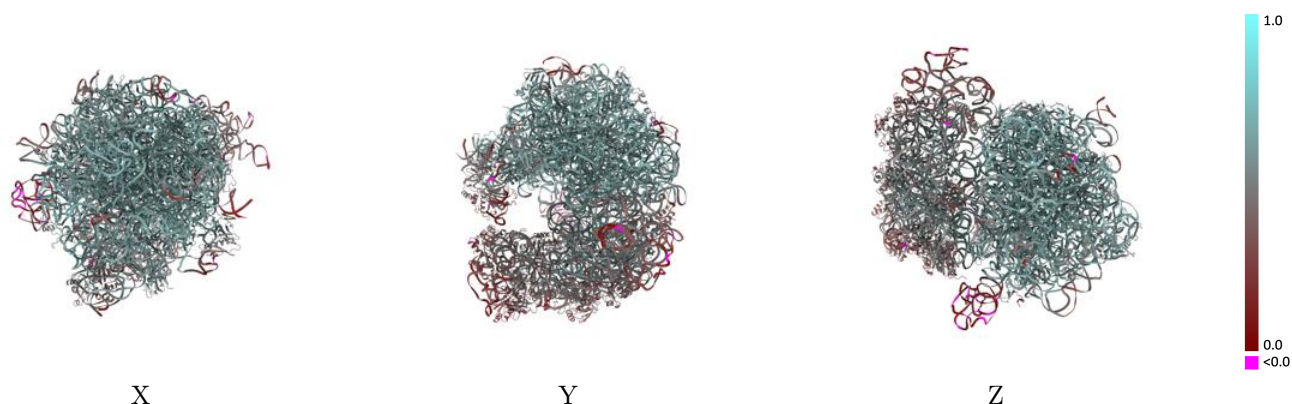
This section contains information regarding the fit between EMDB map EMD-56466 and PDB model 9TZE. Per-residue inclusion information can be found in section ?? on page ??.

8.1 Map-model overlay [i](#)



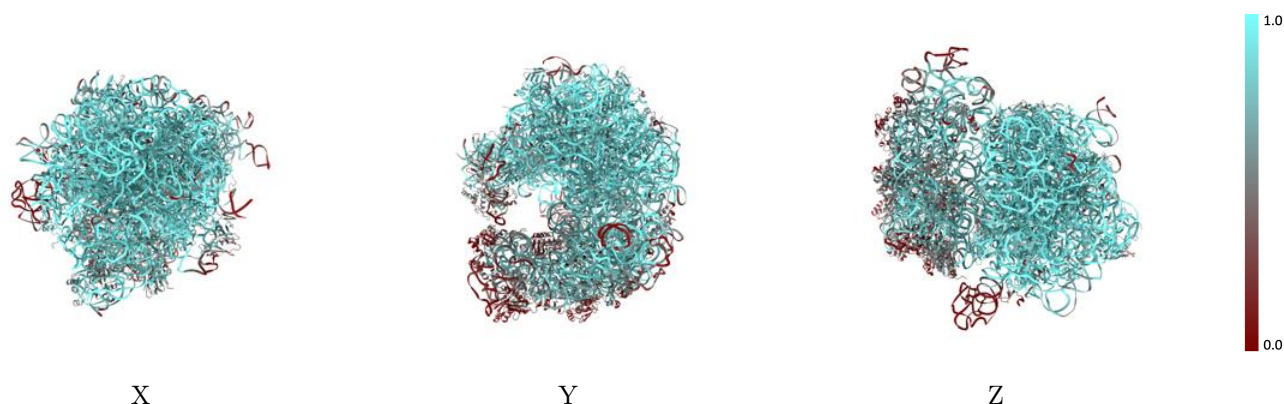
The images above show the 3D surface view of the map at the recommended contour level 0.078 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



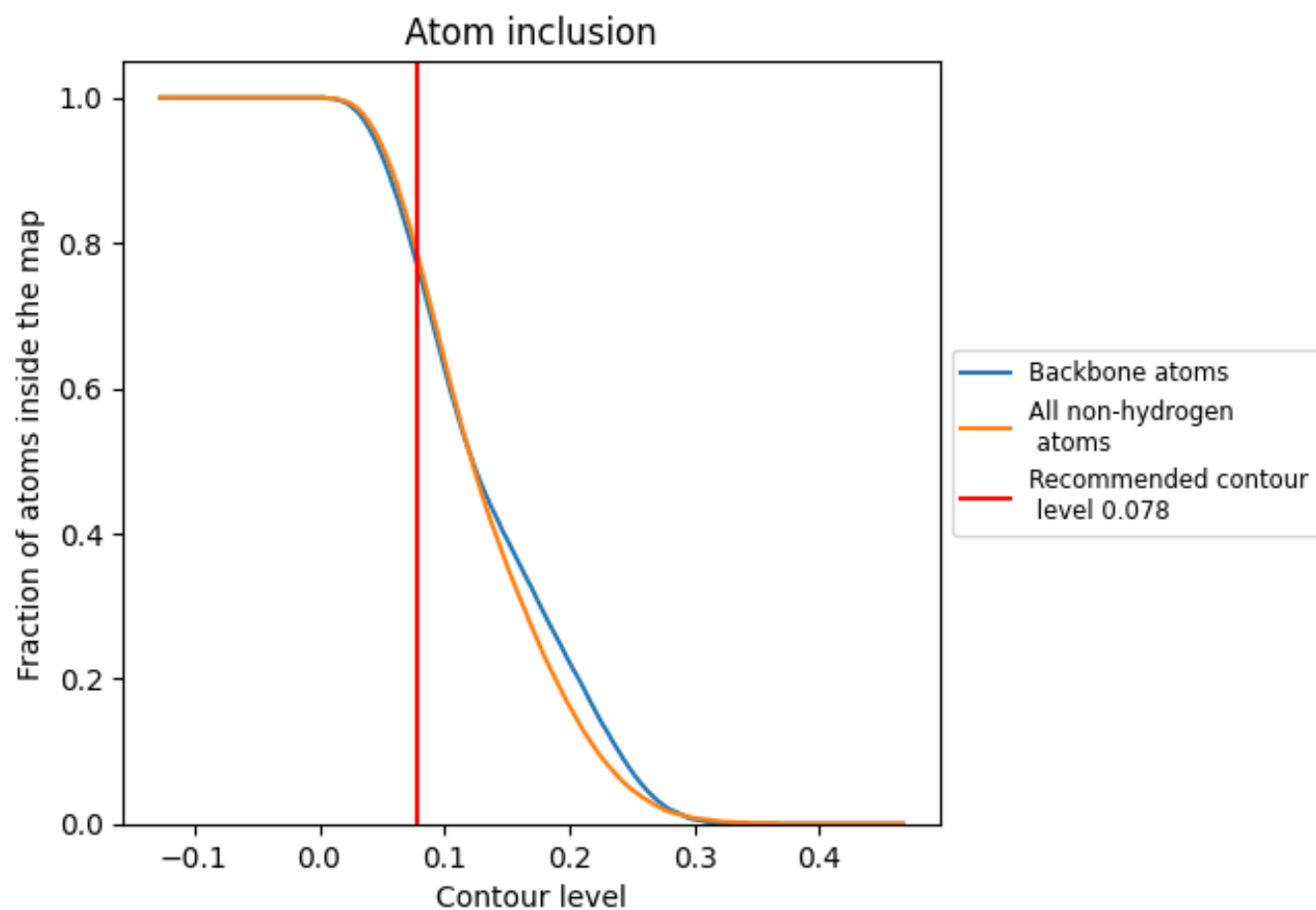
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

8.3 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 (0.078).







































































8.4 Atom inclusion [i](#)



At the recommended contour level, 77% of all backbone atoms, 79% of all non-hydrogen atoms, are inside the map.

8.5 Map-model fit summary ⓘ







































The table lists the average atom inclusion at the recommended contour level (0.078) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7870	 0.5240
0	 0.8210	 0.5780
1	 0.7010	 0.5230
2	 0.7280	 0.5020
3	 0.8970	 0.5930
4	 0.0570	 0.1560
6	 0.8420	 0.5820
7	 0.8230	 0.5670
8	 0.8950	 0.5990
9	 0.1220	 0.3340
A	 0.7710	 0.4670
C	 0.3040	 0.3520
D	 0.3920	 0.4020
E	 0.5950	 0.4860
F	 0.4220	 0.3930
G	 0.2440	 0.3440
H	 0.5750	 0.4720
I	 0.3160	 0.3390
J	 0.2170	 0.2940
K	 0.5290	 0.4530
L	 0.5330	 0.4730
M	 0.3100	 0.3720
N	 0.3600	 0.3590
O	 0.5680	 0.4720
P	 0.4730	 0.4100
Q	 0.5110	 0.4640
R	 0.5190	 0.4300
S	 0.1690	 0.3150
T	 0.5030	 0.4190
U	 0.3180	 0.3690
Z	 0.8960	 0.6030
a	 0.9150	 0.5810
b	 0.8860	 0.5050
c	 0.8250	 0.5670
d	 0.8930	 0.6050



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
e	 0.9290	 0.6190
f	 0.4120	 0.2910
g	 0.5460	 0.4740
h	 0.8320	 0.5910
i	 0.9170	 0.6100
j	 0.8760	 0.6000
k	 0.8640	 0.5870
m	 0.9260	 0.6160
o	 0.8920	 0.6110
q	 0.3390	 0.4610
r	 0.7190	 0.5080
s	 0.8450	 0.5960
t	 0.8940	 0.5990
u	 0.5550	 0.4950
v	 0.9020	 0.6080
w	 0.8220	 0.5740
x	 0.8470	 0.5850
y	 0.9520	 0.6370
z	 0.9400	 0.6220