



wwPDB EM Validation Summary Report ⓘ

Apr 16, 2024 – 10:20 am BST

PDB ID : 6YSR
EMDB ID : EMD-10905
Title : Structure of the P+9 stalled ribosome complex
Authors : Chan, K.-H.; Petrychenko, V.; Mueller, C.; Maracci, C.; Holtkamp, W.; Wilson, D.N.; Fischer, N.; Rodnina, M.V.
Deposited on : 2020-04-23
Resolution : 3.10 Å (reported)
Based on initial models : 5AFI, 4RB7

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 : **FAILED**
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) : 2.36

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.10 Å.

There are no overall percentile quality scores available for this entry.

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

2 Entry composition

There are 62 unique types of molecules in this entry. The entry contains 145959 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 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	0	56	444	269	94	80	1	0	0

- Molecule 2 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	1	50	409	263	75	71	0	0

- Molecule 3 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	2	46	377	228	90	57	2	0	0

- Molecule 4 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	3	64	504	323	105	74	2	0	0

- Molecule 5 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	4	38	302	185	65	48	4	0	0

- Molecule 6 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
6	5	131	647	385	131	131	0	0

- Molecule 7 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	6	66	522	323	99	94	6	0	0

- Molecule 8 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
8	A	2903	62336	27815	11468	20150	2903	0	0

- Molecule 9 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
9	B	120	2570	1144	468	838	120	0	0

- Molecule 10 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	C	271	2082	1288	423	364	7	0	0

- Molecule 11 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	D	209	1565	979	288	294	4	0	0

- Molecule 12 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	E	201	1552	974	283	290	5	0	0

- Molecule 13 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	F	177	1410	899	249	256	6	0	0

- Molecule 14 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	G	176	1323	832	243	246	2	0	0

- Molecule 15 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	H	149	1111	699	197	214	1	0	0

- Molecule 16 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
16	I	141	693	411	141	141	0	0

- Molecule 17 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	J	142	1129	714	212	199	4	0	0

- Molecule 18 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	K	122	938	587	180	165	6	0	0

- Molecule 19 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	L	143	1045	649	206	189	1	0	0

- Molecule 20 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	M	136	1074	686	205	177	6	0	0

- Molecule 21 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	N	120	960	593	196	166	5	0	0

- Molecule 22 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	O	116	892	552	178	162		0	0

- Molecule 23 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	P	114	917	574	179	163	1	0	0

- Molecule 24 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	Q	117	947	604	192	151		0	0

- Molecule 25 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	R	103	816	516	153	145	2	0	0

- Molecule 26 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	S	110	857	532	166	156	3	0	0

- Molecule 27 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	T	93	738	466	139	131	2	0	0

- Molecule 28 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	U	102	Total	C	N	O	0	0
			779	492	146	141		

- Molecule 29 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	V	94	Total	C	N	O	S	0	0
			753	479	137	134	3		

- Molecule 30 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	W	75	Total	C	N	O	S	0	0
			575	356	116	102	1		

- Molecule 31 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	X	77	Total	C	N	O	S	0	0
			625	388	129	106	2		

- Molecule 32 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Y	63	Total	C	N	O	S	0	0
			509	313	99	95	2		

- Molecule 33 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	Z	58	Total	C	N	O	S	0	0
			449	281	87	79	2		

- Molecule 34 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	a	1539	Total	C	N	O	P	0	0
			33028	14738	6052	10699	1539		

- Molecule 35 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	b	218	1704	1081	305	311	7	0	0

- Molecule 36 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	c	206	1624	1028	305	288	3	0	0

- Molecule 37 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	d	205	1643	1026	315	298	4	0	0

- Molecule 38 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
38	e	157	1141	709	218	208	6	0	0

- Molecule 39 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
39	f	100	817	515	148	148	6	0	0

- Molecule 40 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
40	g	151	1181	735	227	215	4	0	0

- Molecule 41 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
41	h	129	979	616	173	184	6	0	0

- Molecule 42 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
42	i	127	1022	634	206	179	3	0	0

- Molecule 43 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
43	j	98	786	493	150	142	1	0	0

- Molecule 44 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
44	k	116	869	535	173	158	3	0	0

- Molecule 45 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
45	l	123	955	590	196	165	4	0	0

- Molecule 46 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
46	m	114	883	546	178	156	3	0	0

- Molecule 47 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
47	n	101	799	498	165	133	3	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
n	35	ALA	-	insertion	UNP C3SR07

- Molecule 48 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	o	88	Total	C	N	O	S	0	0
			714	439	144	130	1		

- Molecule 49 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	p	82	Total	C	N	O	S	0	0
			649	406	128	114	1		

- Molecule 50 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	q	80	Total	C	N	O	S	0	0
			648	411	121	113	3		

- Molecule 51 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	r	65	Total	C	N	O	S	0	0
			535	339	100	95	1		

- Molecule 52 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	s	82	Total	C	N	O	S	0	0
			658	421	125	110	2		

- Molecule 53 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	t	85	Total	C	N	O	S	0	0
			665	411	137	114	3		

- Molecule 54 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	u	65	Total	C	N	O	S	0	0
			506	313	105	87	1		

- Molecule 55 is a protein called P-site fMet-Phe-tRNA(Phe).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
55	v	2	19	14	2	2	1	0	0

- Molecule 56 is a RNA chain called P-site fMet-Phe-tRNA(Phe).

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	N	O	P	S		
56	w	76	1631	731	291	531	76	2	0	0

- Molecule 57 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
57	x	15	314	141	49	109	15	0	0

- Molecule 58 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
58	0	1	Total 1	Mg 1	0
58	6	1	Total 1	Mg 1	0
58	A	236	Total 236	Mg 236	0
58	B	5	Total 5	Mg 5	0
58	O	1	Total 1	Mg 1	0
58	Q	1	Total 1	Mg 1	0
58	T	1	Total 1	Mg 1	0
58	a	82	Total 82	Mg 82	0
58	g	1	Total 1	Mg 1	0
58	w	3	Total 3	Mg 3	0

- Molecule 59 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
59	4	1	Total	Zn	0
			1	1	
59	6	1	Total	Zn	0
			1	1	

- Molecule 60 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		AltConf
60	A	1	Total	Cl	0
			1	1	

- Molecule 61 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		AltConf
61	A	1	Total	Na	0
			1	1	
61	V	1	Total	Na	0
			1	1	

- Molecule 62 is water.

Mol	Chain	Residues	Atoms		AltConf
62	A	1	Total	O	0
			1	1	
62	a	1	Total	O	0
			1	1	

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, C1	Depositor
Number of particles used	25347	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)	200	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	59000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	15.609	Depositor
Minimum map value	-7.539	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	0.035	Depositor
Map size (Å)	334.08, 334.08, 334.08	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.6525, 0.6525, 0.6525	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](#)

41 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
56	PSU	w	32	56	18,21,22	1.00	1 (5%)	22,30,33	1.64	5 (22%)
8	PSU	A	1911	8	18,21,22	1.08	2 (11%)	22,30,33	1.77	4 (18%)
56	4SU	w	8	56	18,21,22	3.61	7 (38%)	26,30,33	2.22	4 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	PSU	A	2605	8	18,21,22	1.33	2 (11%)	22,30,33	1.89	4 (18%)
8	5MC	A	747	26,8	18,22,23	3.62	7 (38%)	26,32,35	1.13	2 (7%)
8	OMC	A	2498	8,58	19,22,23	2.86	7 (36%)	26,31,34	0.82	0
8	2MG	A	1835	8	18,26,27	2.57	7 (38%)	16,38,41	1.50	4 (25%)
8	G7M	A	2069	8	20,26,27	3.93	9 (45%)	17,39,42	1.14	2 (11%)
8	PSU	A	746	8,58	18,21,22	1.09	2 (11%)	22,30,33	1.78	4 (18%)
34	2MG	a	966	34	18,26,27	2.60	7 (38%)	16,38,41	1.59	4 (25%)
34	2MG	a	1207	34	18,26,27	2.59	7 (38%)	16,38,41	1.39	4 (25%)
56	MIA	w	37	56	24,31,32	2.46	4 (16%)	26,44,47	2.93	9 (34%)
8	OMG	A	2251	8,56	18,26,27	2.46	8 (44%)	19,38,41	1.46	4 (21%)
34	5MC	a	967	34	18,22,23	3.69	7 (38%)	26,32,35	1.00	2 (7%)
34	2MG	a	1516	34	18,26,27	2.63	7 (38%)	16,38,41	1.47	4 (25%)
8	PSU	A	2604	8	18,21,22	1.33	2 (11%)	22,30,33	1.98	5 (22%)
34	5MC	a	1407	34	18,22,23	3.65	7 (38%)	26,32,35	0.99	1 (3%)
8	2MG	A	2445	8	18,26,27	2.58	7 (38%)	16,38,41	1.56	4 (25%)
56	PSU	w	55	56	18,21,22	1.04	1 (5%)	22,30,33	1.84	5 (22%)
8	3TD	A	1915	8,58	18,22,23	4.33	5 (27%)	22,32,35	1.65	3 (13%)
8	PSU	A	1917	8	18,21,22	1.03	1 (5%)	22,30,33	1.78	4 (18%)
8	5MU	A	1939	8	19,22,23	4.67	7 (36%)	28,32,35	3.75	10 (35%)
8	OMU	A	2552	8	19,22,23	2.92	8 (42%)	26,31,34	1.79	5 (19%)
34	MA6	a	1518	34	18,26,27	1.01	1 (5%)	19,38,41	2.65	2 (10%)
34	UR3	a	1498	34	19,22,23	2.63	6 (31%)	26,32,35	1.49	3 (11%)
8	6MZ	A	2030	8	18,25,26	2.12	3 (16%)	16,36,39	2.32	3 (18%)
56	5MU	w	54	56	19,22,23	4.80	7 (36%)	28,32,35	3.65	9 (32%)
56	G7M	w	46	56	20,26,27	2.46	7 (35%)	17,39,42	1.07	1 (5%)
8	PSU	A	955	8,58	18,21,22	1.09	1 (5%)	22,30,33	1.85	5 (22%)
8	6MZ	A	1618	8	18,25,26	2.13	3 (16%)	16,36,39	2.06	3 (18%)
56	PSU	w	39	56	18,21,22	1.01	1 (5%)	22,30,33	1.75	3 (13%)
8	1MG	A	745	8	18,26,27	2.63	4 (22%)	19,39,42	1.39	3 (15%)
34	4OC	a	1402	34	20,23,24	2.97	8 (40%)	26,32,35	0.92	2 (7%)
8	2MA	A	2503	8,58	17,25,26	2.38	5 (29%)	17,37,40	1.43	3 (17%)
8	PSU	A	2457	8	18,21,22	1.01	2 (11%)	22,30,33	1.95	6 (27%)
8	PSU	A	2580	8	18,21,22	1.08	2 (11%)	22,30,33	1.92	5 (22%)
34	PSU	a	516	34,58	18,21,22	0.93	2 (11%)	22,30,33	1.76	5 (22%)
34	MA6	a	1519	34	18,26,27	1.02	1 (5%)	19,38,41	2.78	2 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	5MC	A	1962	8	18,22,23	3.63	7 (38%)	26,32,35	1.03	2 (7%)
8	PSU	A	2504	8	18,21,22	1.02	1 (5%)	22,30,33	1.90	5 (22%)
34	G7M	a	527	34	20,26,27	4.02	10 (50%)	17,39,42	1.04	1 (5%)

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
56	PSU	w	32	56	-	2/7/25/26	0/2/2/2
8	PSU	A	1911	8	-	0/7/25/26	0/2/2/2
56	4SU	w	8	56	-	0/7/25/26	0/2/2/2
8	PSU	A	2605	8	-	1/7/25/26	0/2/2/2
8	5MC	A	747	26,8	-	4/7/25/26	0/2/2/2
8	OMC	A	2498	8,58	-	0/9/27/28	0/2/2/2
8	2MG	A	1835	8	-	2/5/27/28	0/3/3/3
8	G7M	A	2069	8	-	1/3/25/26	0/3/3/3
8	PSU	A	746	8,58	-	1/7/25/26	0/2/2/2
34	2MG	a	966	34	-	0/5/27/28	0/3/3/3
34	2MG	a	1207	34	-	0/5/27/28	0/3/3/3
56	MIA	w	37	56	-	3/11/33/34	0/3/3/3
8	OMG	A	2251	8,56	-	3/5/27/28	0/3/3/3
34	5MC	a	967	34	-	0/7/25/26	0/2/2/2
34	2MG	a	1516	34	-	0/5/27/28	0/3/3/3
8	PSU	A	2604	8	-	1/7/25/26	0/2/2/2
34	5MC	a	1407	34	-	0/7/25/26	0/2/2/2
8	2MG	A	2445	8	-	2/5/27/28	0/3/3/3
56	PSU	w	55	56	-	1/7/25/26	0/2/2/2
8	3TD	A	1915	8,58	-	3/7/25/26	0/2/2/2
8	PSU	A	1917	8	-	0/7/25/26	0/2/2/2
8	5MU	A	1939	8	-	0/7/25/26	0/2/2/2
8	OMU	A	2552	8	-	2/9/27/28	0/2/2/2
34	MA6	a	1518	34	-	0/7/29/30	0/3/3/3
34	UR3	a	1498	34	-	2/7/25/26	0/2/2/2
8	6MZ	A	2030	8	-	2/5/27/28	0/3/3/3
56	5MU	w	54	56	-	2/7/25/26	0/2/2/2
56	G7M	w	46	56	-	3/3/25/26	0/3/3/3
8	PSU	A	955	8,58	-	0/7/25/26	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	6MZ	A	1618	8	-	1/5/27/28	0/3/3/3
56	PSU	w	39	56	-	3/7/25/26	0/2/2/2
8	1MG	A	745	8	-	0/3/25/26	0/3/3/3
34	4OC	a	1402	34	-	2/9/29/30	0/2/2/2
8	2MA	A	2503	8,58	-	2/3/25/26	0/3/3/3
8	PSU	A	2457	8	-	0/7/25/26	0/2/2/2
8	PSU	A	2580	8	-	0/7/25/26	0/2/2/2
34	PSU	a	516	34,58	-	3/7/25/26	0/2/2/2
34	MA6	a	1519	34	-	1/7/29/30	0/3/3/3
8	5MC	A	1962	8	-	0/7/25/26	0/2/2/2
8	PSU	A	2504	8	-	0/7/25/26	0/2/2/2
34	G7M	a	527	34	-	3/3/25/26	0/3/3/3

The worst 5 of 193 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	1915	3TD	C6-C5	13.20	1.50	1.35
56	w	54	5MU	C2-N1	10.85	1.55	1.38
56	w	54	5MU	C6-N1	10.39	1.55	1.38
8	A	1939	5MU	C2-N1	10.23	1.54	1.38
8	A	1939	5MU	C6-N1	10.22	1.55	1.38

The worst 5 of 156 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	1939	5MU	C5-C4-N3	12.36	125.86	115.31
56	w	54	5MU	C5-C4-N3	12.15	125.69	115.31
8	A	1939	5MU	C5-C6-N1	-10.72	112.31	123.34
34	a	1519	MA6	N1-C6-N6	-10.32	106.19	117.06
56	w	54	5MU	C5-C6-N1	-10.32	112.72	123.34

There are no chirality outliers.

5 of 50 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	1618	6MZ	N1-C6-N6-C9
8	A	1915	3TD	C2'-C1'-C5-C4
8	A	1915	3TD	O4'-C1'-C5-C4
8	A	1915	3TD	O4'-C1'-C5-C6
8	A	2030	6MZ	O4'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

4.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

4.6 Ligand geometry [i](#)

Of 337 ligands modelled in this entry, 337 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.

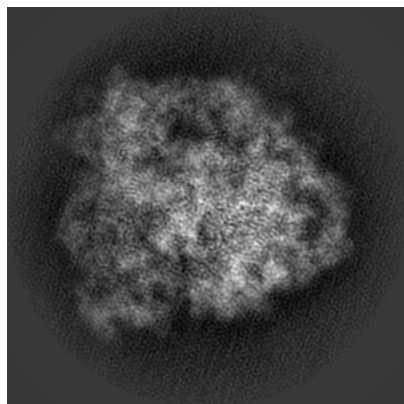
5 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10905. These allow visual inspection of the internal detail of the map and identification of artifacts.

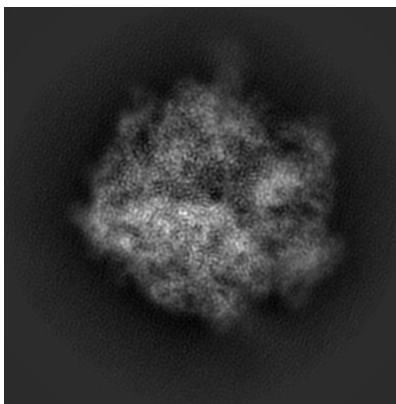
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

5.1 Orthogonal projections [i](#)

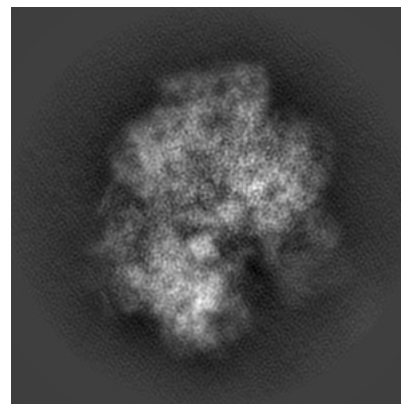
5.1.1 Primary map



X

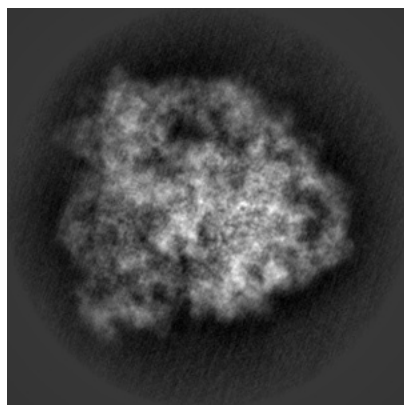


Y

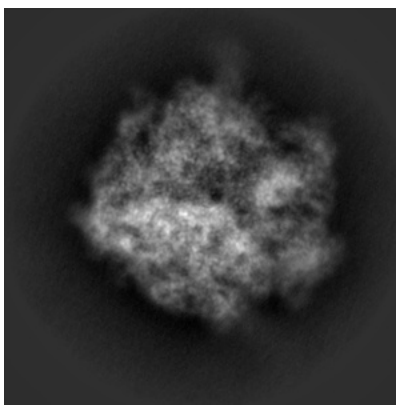


Z

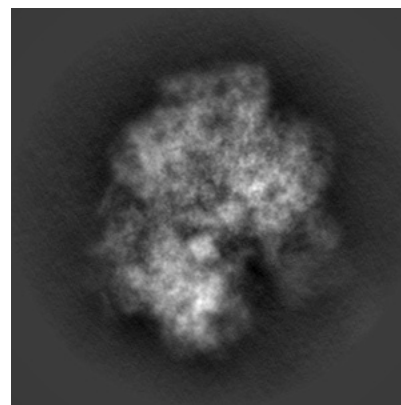
5.1.2 Raw map



X



Y

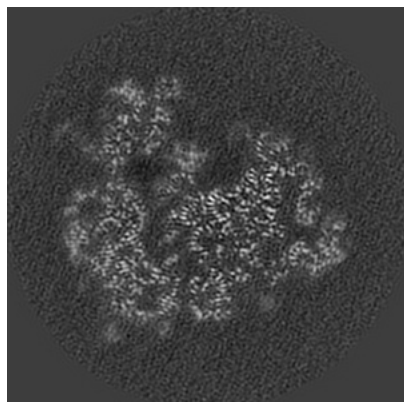


Z

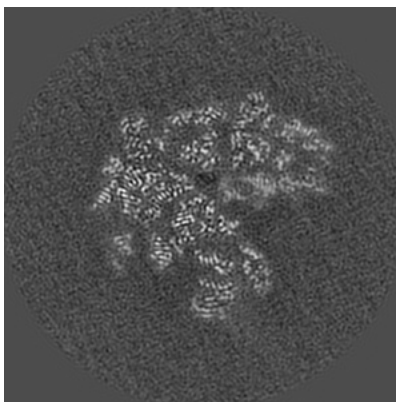
The images above show the map projected in three orthogonal directions.

5.2 Central slices [i](#)

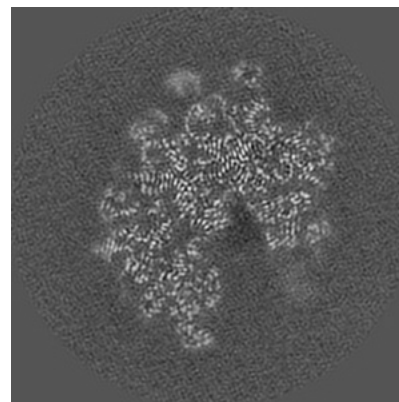
5.2.1 Primary map



X Index: 256

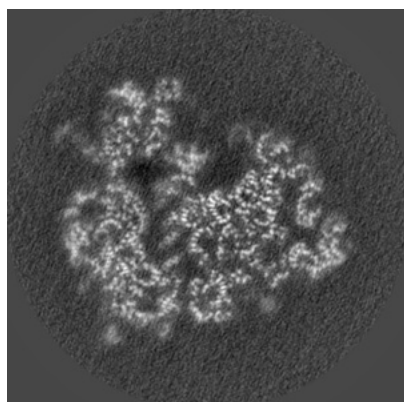


Y Index: 256

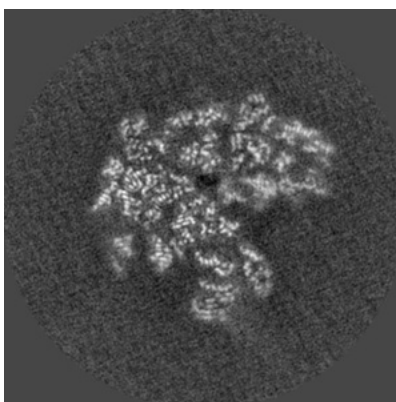


Z Index: 256

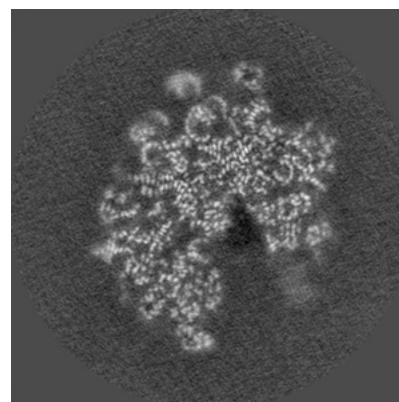
5.2.2 Raw map



X Index: 144



Y Index: 144

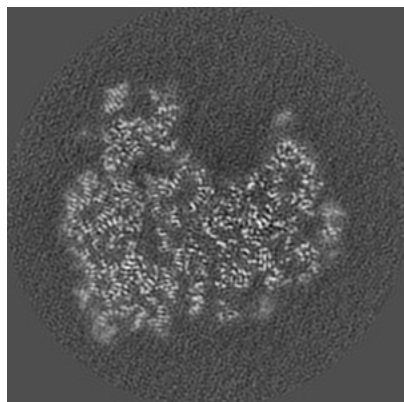


Z Index: 144

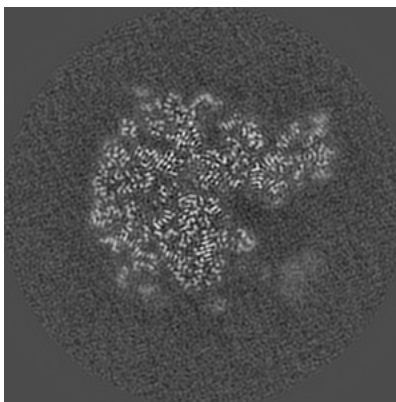
The images above show central slices of the map in three orthogonal directions.

5.3 Largest variance slices [i](#)

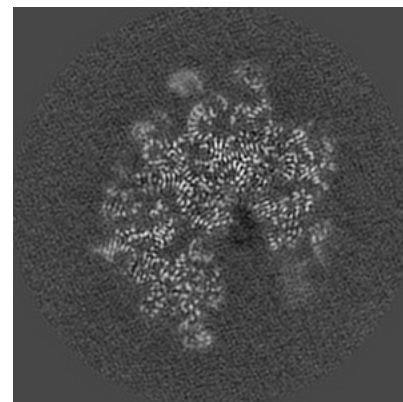
5.3.1 Primary map



X Index: 241

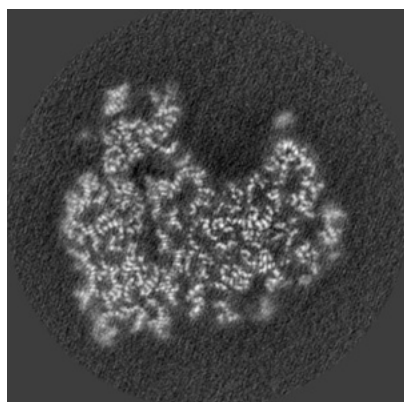


Y Index: 285

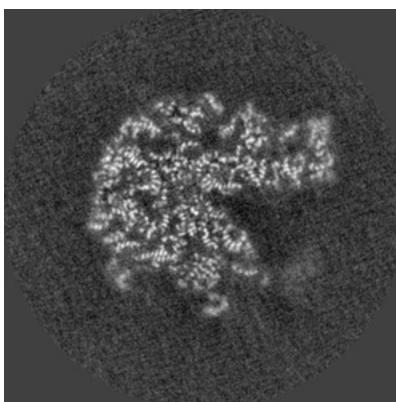


Z Index: 258

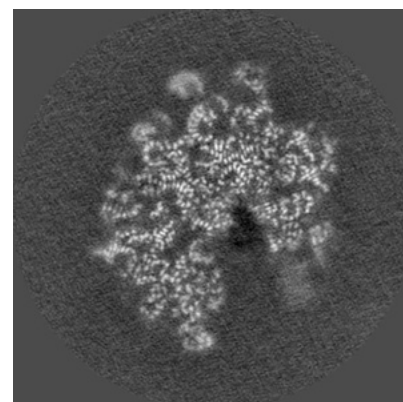
5.3.2 Raw map



X Index: 136



Y Index: 157

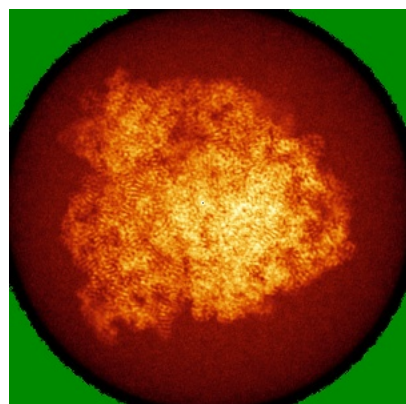


Z Index: 145

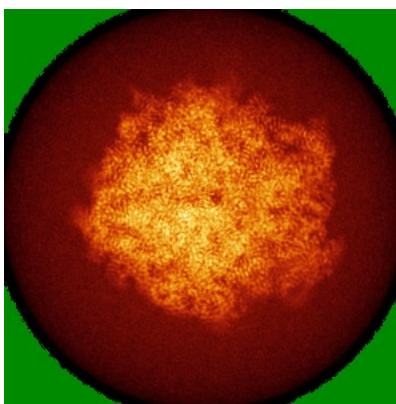
The images above show the largest variance slices of the map in three orthogonal directions.

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

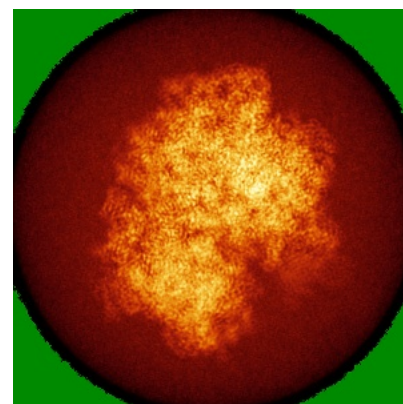
5.4.1 Primary map



X

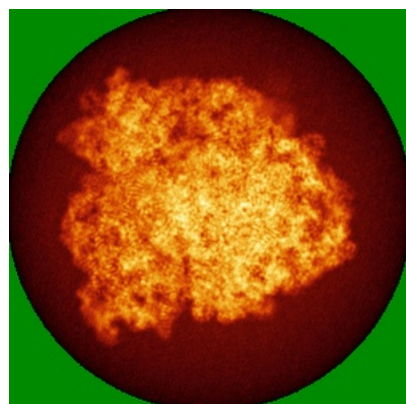


Y

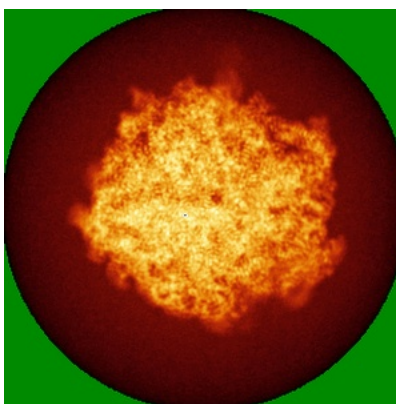


Z

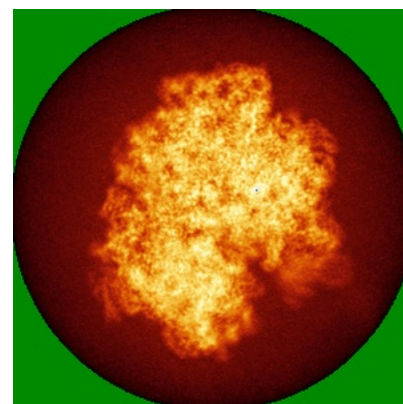
5.4.2 Raw map



X



Y

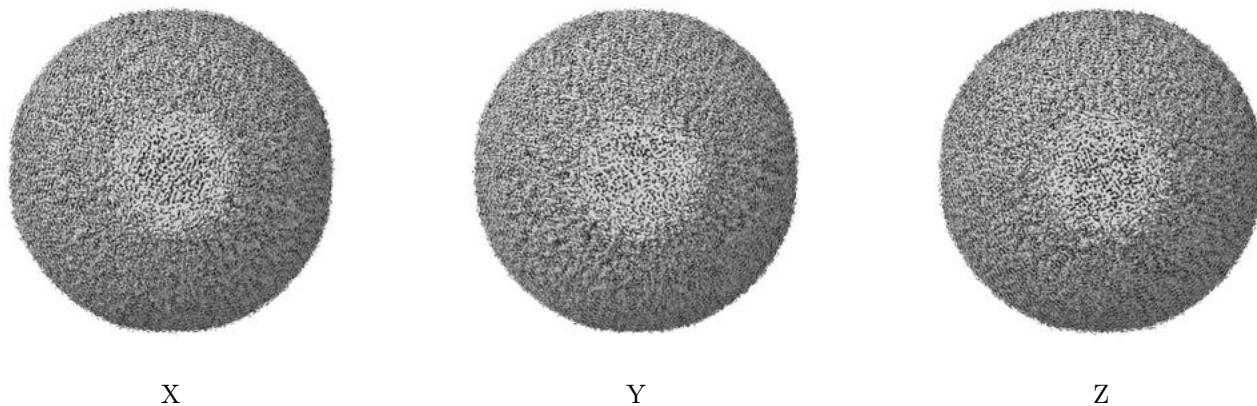


Z

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 0.035. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

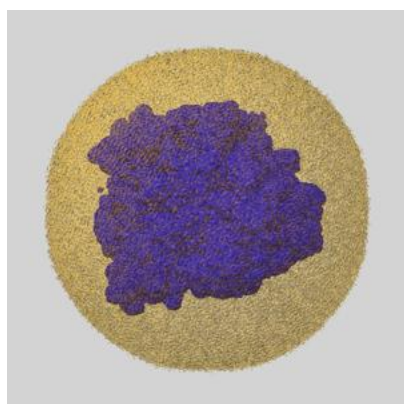
5.6 Mask visualisation [i](#)

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

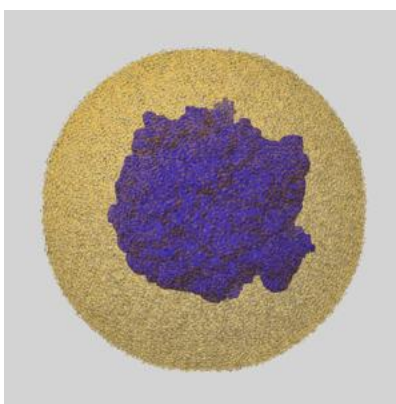
A mask typically either:

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

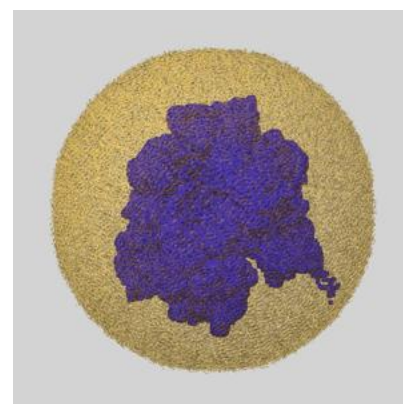
5.6.1 emd_10905_msk_1.map [i](#)



X



Y

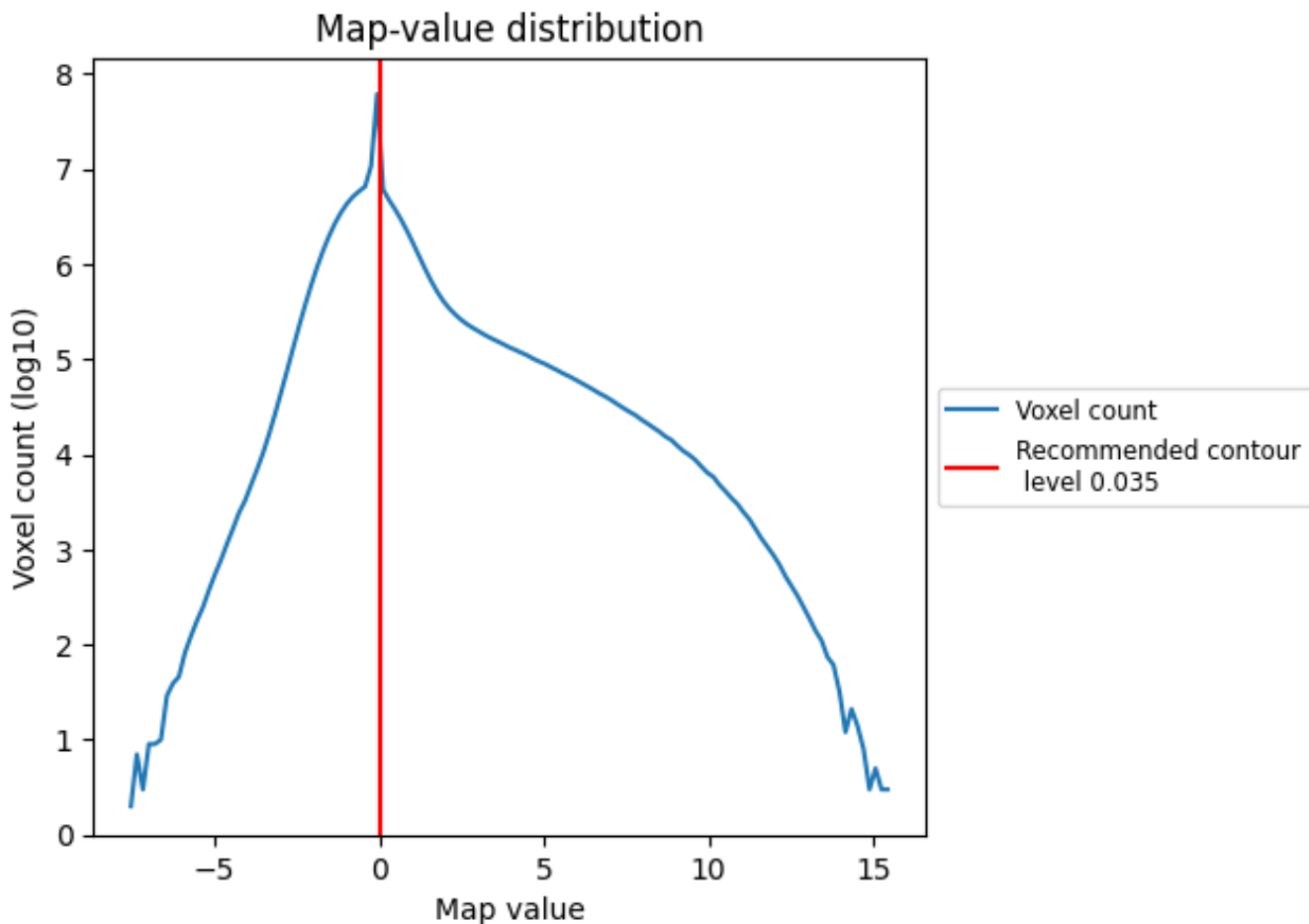


Z

6 Map analysis [i](#)

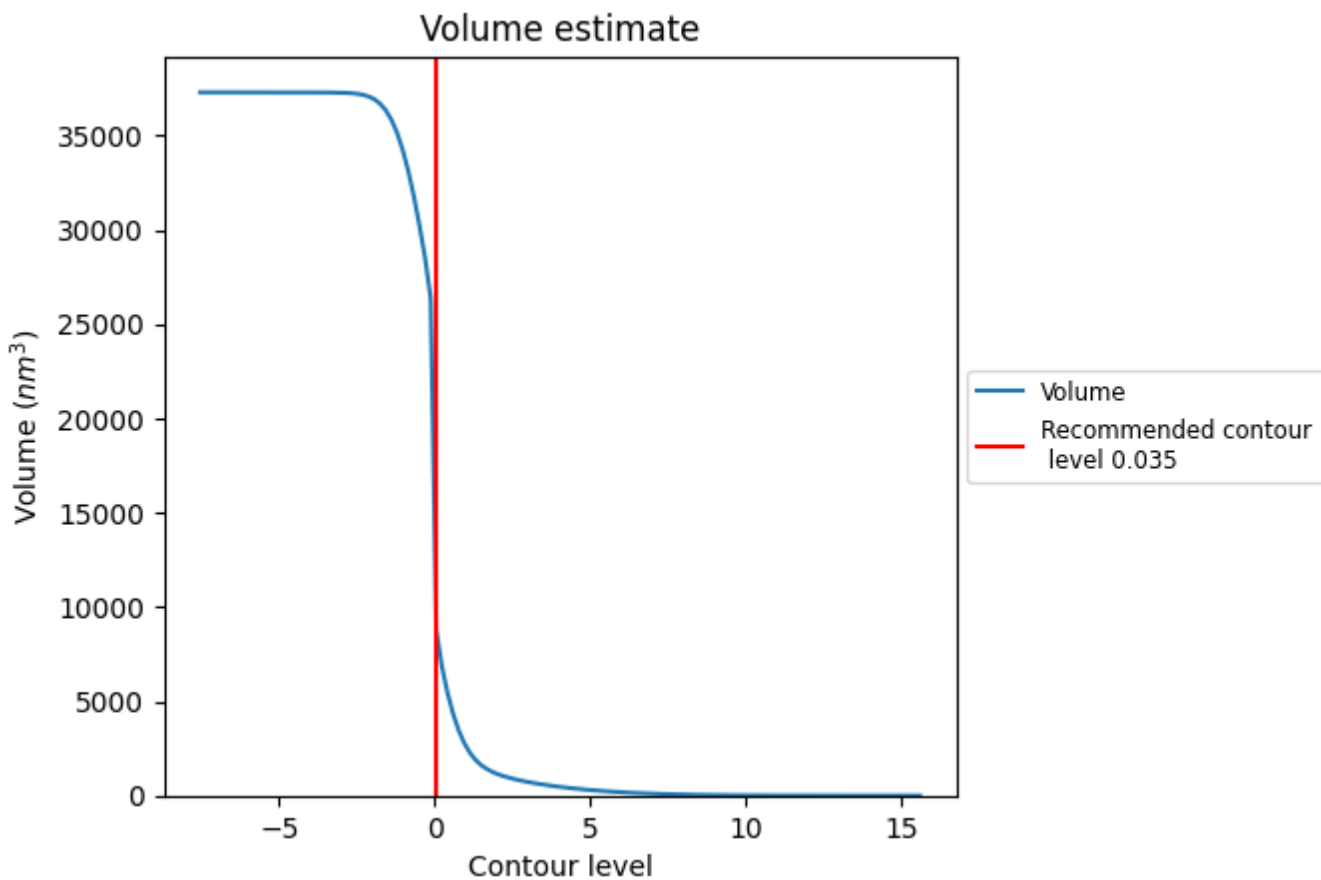
This section contains the results of statistical analysis of the map.

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.

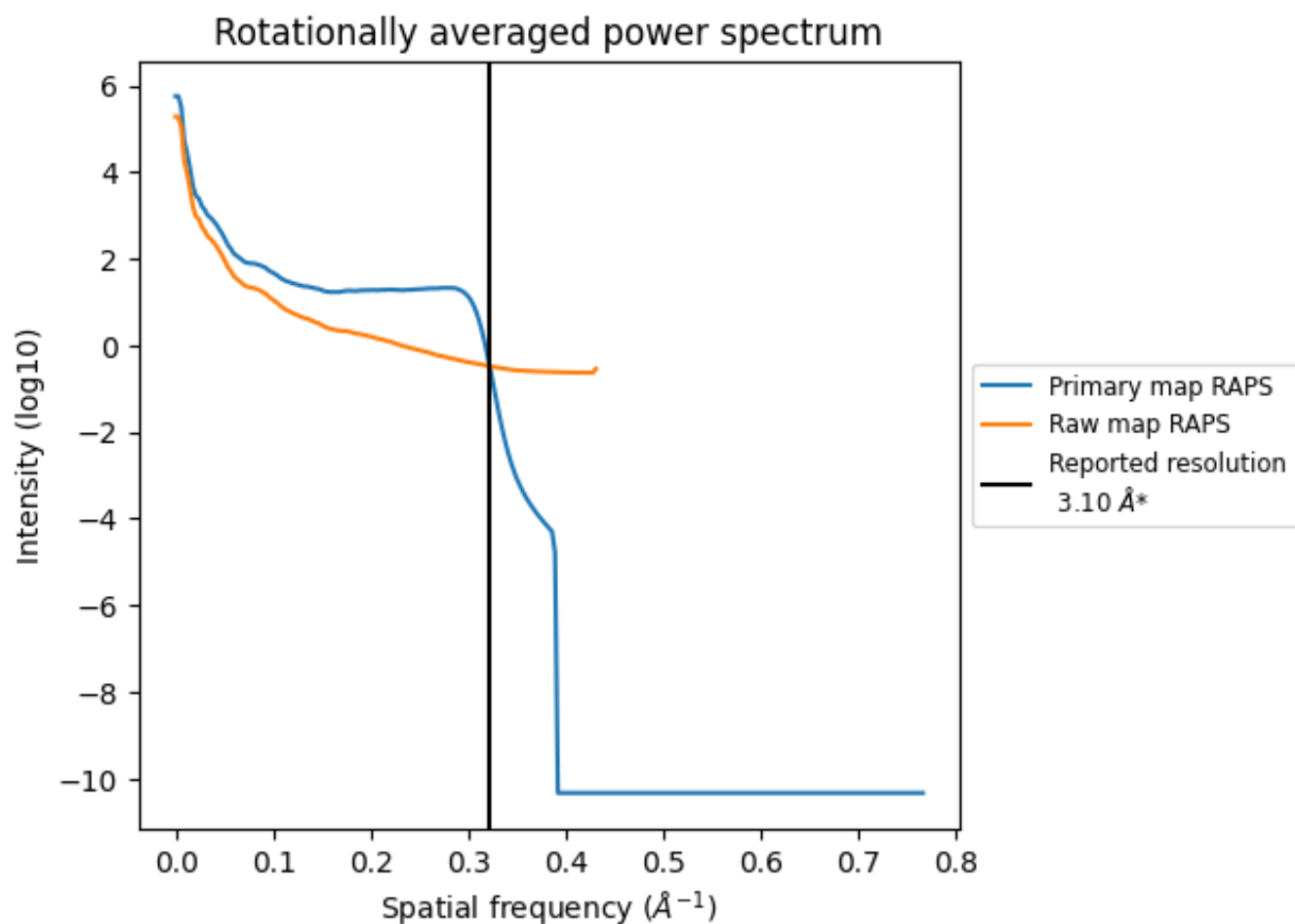
6.2 Volume estimate [i](#)



The volume at the recommended contour level is 10850 nm^3 ; this corresponds to an approximate mass of 9801 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 [i](#)

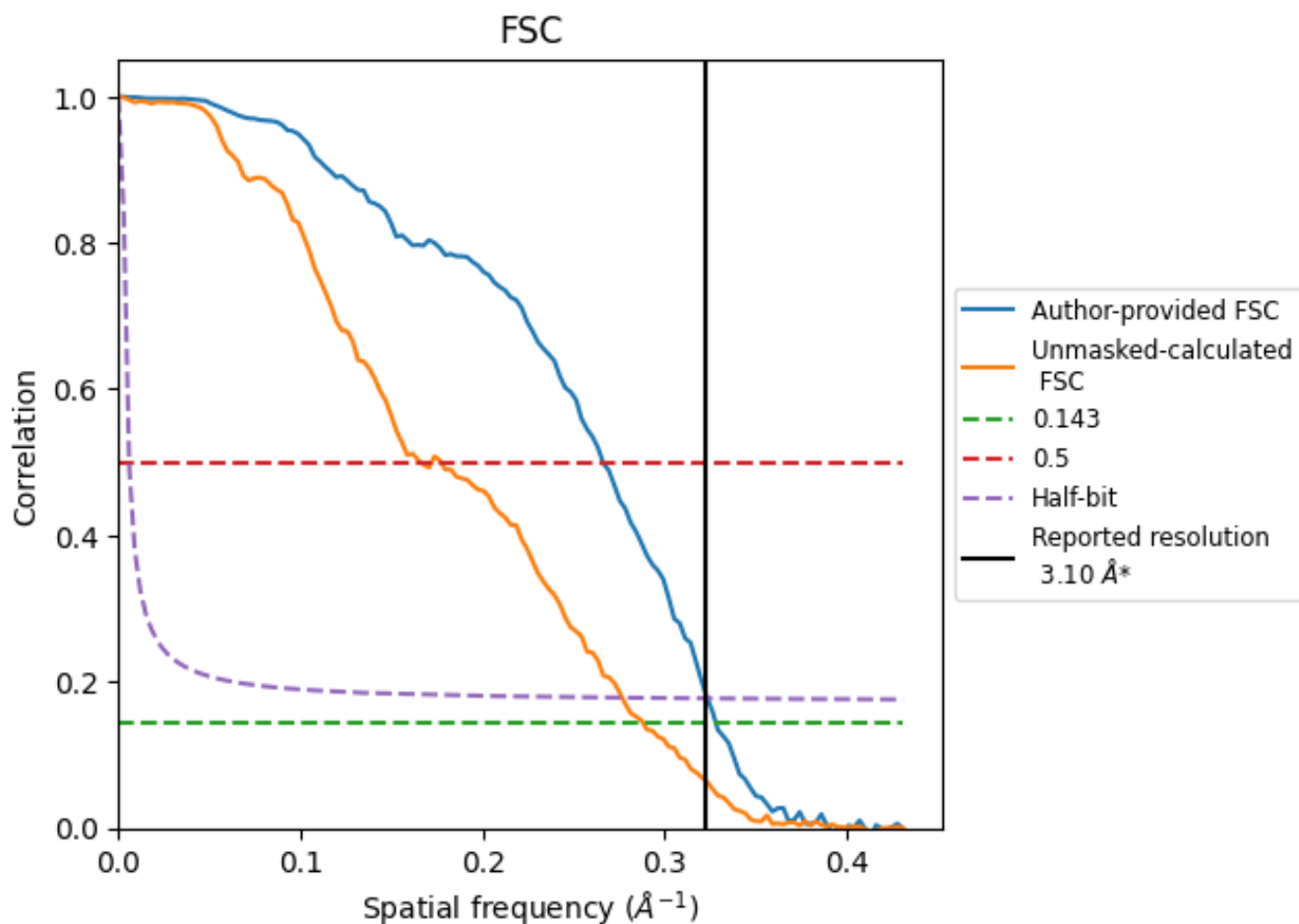


*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

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 0.323 Å⁻¹

7.2 Resolution estimates [i](#)

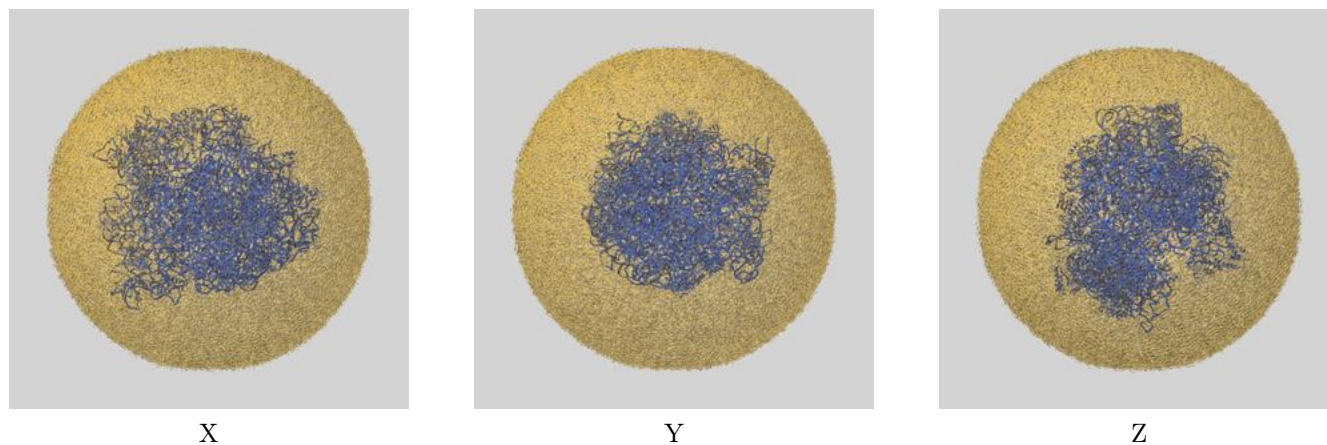
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.05	3.76	3.09
Unmasked-calculated*	3.47	6.02	3.61

*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 3.47 differs from the reported value 3.1 by more than 10 %

8 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-10905 and PDB model 6YSR. Per-residue inclusion information can be found in section ?? on page ??.

8.1 Map-model overlay [i](#)

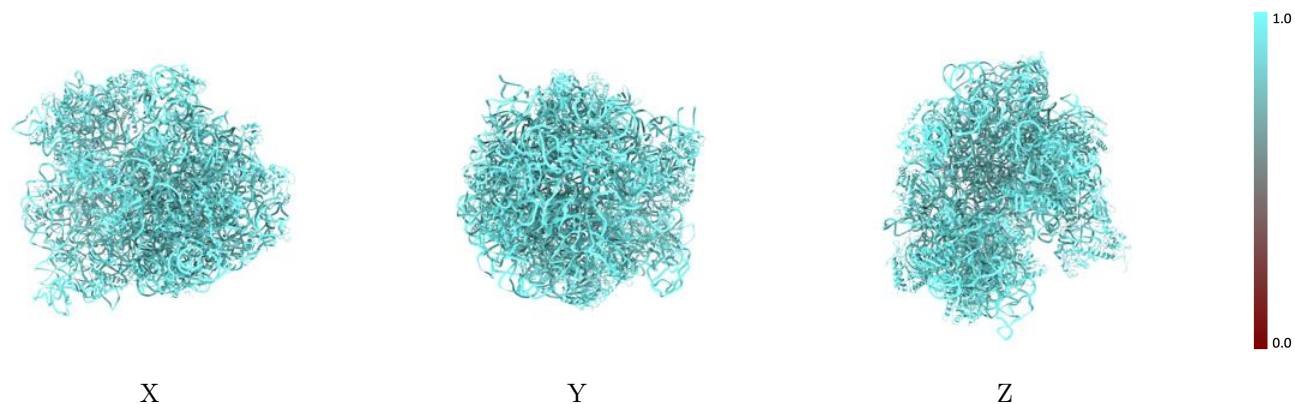


The images above show the 3D surface view of the map at the recommended contour level 0.035 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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

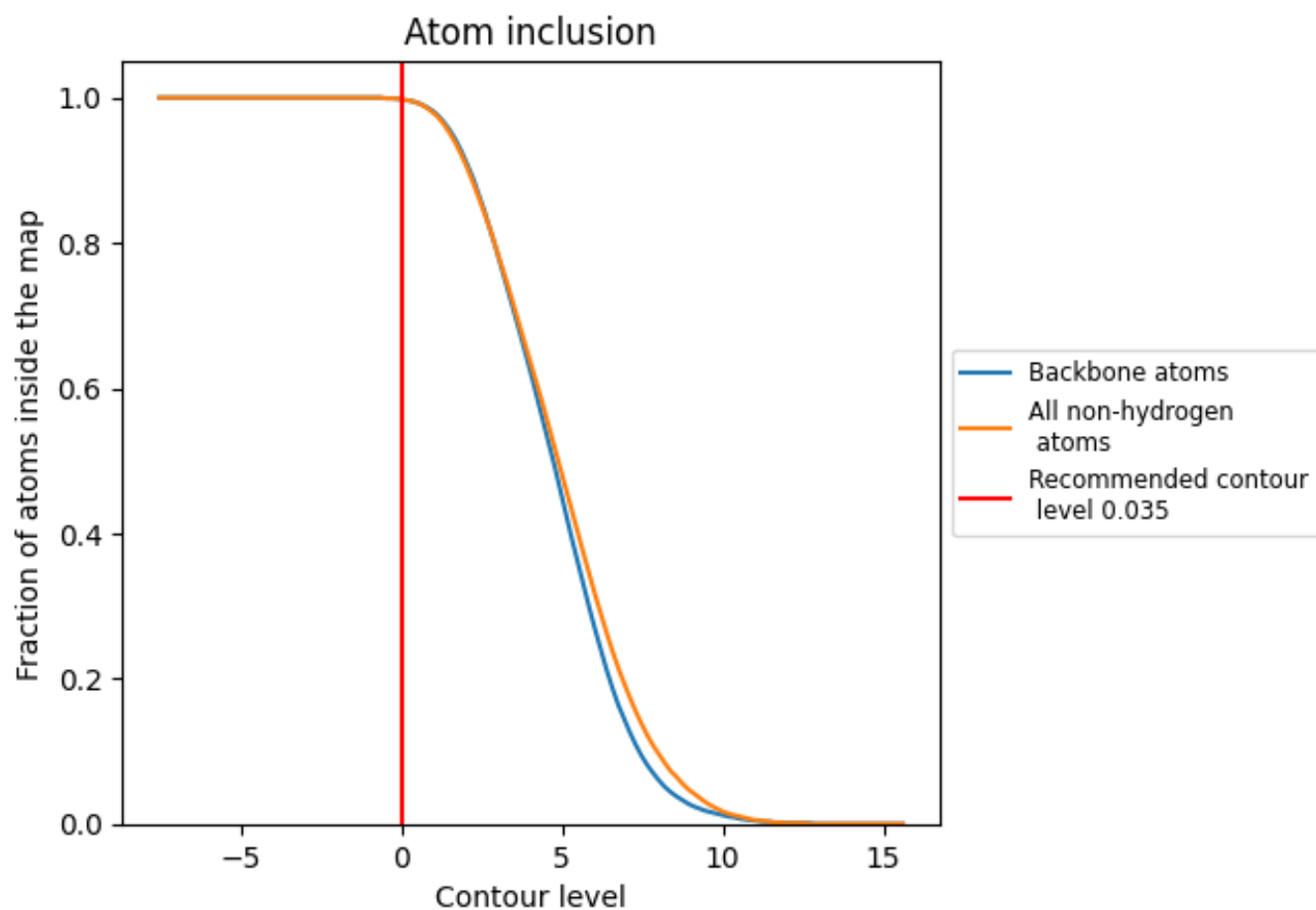
This section was not generated.

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 (0.035).




































8.4 Atom inclusion [i](#)



At the recommended contour level, 100% of all backbone atoms, 100% 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 (0.035) and Q-score for the entire model and for each chain.

Chain	Atom inclusion
All	 0.9980
0	 0.9980
1	 1.0000
2	 0.9940
3	 0.9960
4	 0.9930
5	 0.9710
6	 0.9920
A	 0.9980
B	 1.0000
C	 0.9980
D	 0.9970
E	 0.9990
F	 0.9960
G	 0.9970
H	 0.9750
I	 0.9670
J	 1.0000
K	 0.9970
L	 0.9960
M	 0.9990
N	 1.0000
O	 0.9990
P	 0.9990
Q	 0.9970
R	 1.0000
S	 0.9950
T	 1.0000
U	 0.9990
V	 0.9970
W	 0.9930
X	 0.9970
Y	 0.9980
Z	 1.0000
a	 1.0000



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Chain	Atom inclusion
b	 0.9920
c	 0.9980
d	 0.9970
e	 0.9990
f	 0.9960
g	 0.9970
h	 0.9960
i	 1.0000
j	 0.9970
k	 0.9950
l	 0.9910
m	 0.9990
n	 1.0000
o	 0.9970
p	 0.9980
q	 0.9980
r	 0.9960
s	 0.9980
t	 0.9950
u	 0.9960
v	 0.8420
w	 1.0000
x	 0.9780