wwPDB EM Validation Summary Report (i)

Jun 2, 2025 – 03:01 pm BST

PDB ID	:	9HQV / pdb_00009hqv
EMDB ID	:	EMD-52348
Title	:	Cryo-EM structure of the small subunit of the mitochondrial ribosome from Toxoplasma gondii
Authors	:	Tobiasson, V.; Shikha, S.; Muhleip, A.
Deposited on	:	2024-12-17
Resolution	:	2.52 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 (i) 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 (i)) were used in the production of this report:

EMDB validation analysis	:	0.0.1.dev118
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	FAILED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.52 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 (i)

There are 90 unique types of molecules in this entry. The entry contains 246248 atoms, of which 117783 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 Enoyl-CoA hydratase/isomerase family protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	BA	526	8318	2671	4127	743	760	17	0	0

- Molecule 2 is a protein called mS75.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
2	BB	25	489	133	269	58	27	2	0	0

- Molecule 3 is a protein called Pentatricopeptide repeat domain-containing protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
3	BC	382	6119	1920	3081	576	533	9	0	0

- Molecule 4 is a protein called mS92.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
4	BD	144	2408	786	1206	215	194	7	0	0

- Molecule 5 is a protein called Ribosomal protein, uS2m.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
5	Ba	129	1978	634	994	174	169	7	0	0

- Molecule 6 is a protein called Putative 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
6	Bb	783	12689	4048	6338	1143	1143	17	0	0

- Molecule 7 is a protein called Putative mitochondrial ribosomal protein s6-2.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	Bc	114	Total	C	H	N	O	S	0	0
			1916	610	964	184	154	4		

- Molecule 8 is a protein called Putative ribosomal protein S8.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	Bd	129	Total	C	H	N	O	S	0	0
			2122	659	1085	195	172	11		

- Molecule 9 is a protein called Putative ribosomal protein S9.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	Be	161	Total	C	H	N	O	S	0	0
			2544	797	1270	244	222	11		

- Molecule 10 is a protein called uS10m.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	Bf	186	Total	C	H	N	O	S	0	0
			3055	976	1530	284	259	6		

- Molecule 11 is a protein called Putative ribosomal protein S11.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	Bg	150	Total	C	H	N	O	S	0	0
			2442	743	1245	252	197	5		

- Molecule 12 is a protein called Putative 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	Bh	199	Total	C	H	N	O	S	0	0
			3374	1038	1723	332	275	6		

- Molecule 13 is a protein called us13m.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	Bi	102	Total	C	H	N	O	S	0	0
			1688	512	875	158	136	7		

- Molecule 14 is a protein called Putative ribosomal protein S14.

Mol	Chain	Residues	Atoms						AltConf	Trace
14	Bj	112	Total	C	H	N	O	S	0	0
			1863	589	944	180	143	7		

- Molecule 15 is a protein called Putative 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms						AltConf	Trace
15	Bk	270	Total	C	H	N	O	S	0	0
			4582	1439	2326	441	366	10		

- Molecule 16 is a protein called Putative 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms						AltConf	Trace
16	Bl	154	Total	C	H	N	O	S	0	0
			2574	809	1314	238	206	7		

- Molecule 17 is a protein called Putative ribosomal protein S17.

Mol	Chain	Residues	Atoms						AltConf	Trace
17	Bm	106	Total	C	H	N	O	S	0	0
			1840	591	920	174	150	5		

- Molecule 18 is a protein called Putative ribosomal protein S18.

Mol	Chain	Residues	Atoms						AltConf	Trace
18	Bn	335	Total	C	H	N	O	S	0	0
			5542	1749	2760	518	502	13		

- Molecule 19 is a protein called Ribosomal protein, bS21m.

Mol	Chain	Residues	Atoms						AltConf	Trace
19	Bo	92	Total	C	H	N	O	S	0	0
			1556	494	779	152	128	3		

- Molecule 20 is a protein called mS23.

Mol	Chain	Residues	Atoms						AltConf	Trace
20	Bp	221	Total	C	H	N	O	S	0	0
			3514	1099	1765	330	309	11		

- Molecule 21 is a protein called Mitochondrial ribosomal protein, mS26.

Mol	Chain	Residues	Atoms						AltConf	Trace
21	Bq	413	Total	C	H	N	O	S	0	0
			6898	2121	3520	640	610	7		

- Molecule 22 is a protein called Small ribosomal subunit protein mS29.

Mol	Chain	Residues	Atoms						AltConf	Trace
22	Br	418	Total	C	H	N	O	S	0	0
			6851	2180	3414	628	619	10		

- Molecule 23 is a protein called DNA double-strand break repair rad50 ATPase.

Mol	Chain	Residues	Atoms						AltConf	Trace
23	Bs	333	Total	C	H	N	O	S	0	0
			5405	1693	2725	503	477	7		

- Molecule 24 is a protein called mS34.

Mol	Chain	Residues	Atoms						AltConf	Trace
24	Bt	211	Total	C	H	N	O	S	0	0
			3551	1157	1783	340	270	1		

- Molecule 25 is a protein called Small ribosomal subunit protein mS35 mitochondrial conserved domain-containing protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
25	Bu	201	Total	C	H	N	O	S	0	0
			3272	1031	1638	302	296	5		

- Molecule 26 is a protein called CHCH domain-containing protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
26	Bv	134	Total	C	H	N	O	S	0	0
			2197	697	1098	208	186	8		

- Molecule 27 is a protein called Mitochondrial mRNA-processing protein COX24 C-terminal domain-containing protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
27	Bx	67	Total	C	H	N	O	S	0	0
			1306	394	692	133	84	3		

- Molecule 28 is a protein called Homeodomain-like containing protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
28	By	262	Total	C	H	N	O	S	0	0
			4338	1410	2157	370	395	6		

- Molecule 29 is a protein called mS45.

Mol	Chain	Residues	Atoms						AltConf	Trace
29	Bz	202	Total	C	H	N	O	S	0	0
			3408	1085	1705	311	301	6		

- Molecule 30 is a protein called UNK1.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Ua	20	Total	C	H	N	O	0	0
			182	60	82	20	20		

- Molecule 31 is a protein called UNK2.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	Ub	7	Total	C	H	N	O	0	0
			76	23	39	7	7		

- Molecule 32 is a protein called UNK3.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Uc	10	Total	C	H	N	O	0	0
			92	30	42	10	10		

- Molecule 33 is a protein called UNK4.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	Ud	72	Total	C	H	N	O	0	0
			713	232	329	80	72		

- Molecule 34 is a protein called Chain Uh.

Mol	Chain	Residues	Atoms						AltConf	Trace
34	Uh	56	Total	C	H	N	O	S	0	0
			837	261	417	79	78	2		

- Molecule 35 is a protein called Unknown peptide.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	Ui	13	Total 119	C 39	H 54	N 13	O 13	0	0
35	Uk	13	Total 119	C 39	H 54	N 13	O 13	0	0

- Molecule 36 is a protein called Chain Uj.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	Uj	60	Total 542	C 180	H 242	N 60	O 60	0	0

- Molecule 37 is a protein called GLY-ARG-SER-LYS-VAL-LEU-ILE-ARG-ARG-LEU-LYS-GLU-ARG-ALA-LYS-LYS-GLU-ALA-GLU-LYS-LYS-ALA.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	Ul	22	Total 396	C 112	H 215	N 40	O 29	0	0

- Molecule 38 is a protein called ARG-ALA-GLU-LEU-VAL-ALA-ALA-GLN-VAL-ARG-GLU-LYS-LEU-ALA-ILE-LYS-MET-ALA-ASN-ALA-LEU-ALA.

Mol	Chain	Residues	Atoms						AltConf	Trace
38	Um	22	Total 350	C 103	H 186	N 32	O 28	S 1	0	0

- Molecule 39 is a protein called Chain Un.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	Un	24	Total 393	C 122	H 198	N 35	O 38	0	0

- Molecule 40 is a protein called chain Uo.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	Uo	26	Total 236	C 78	H 106	N 26	O 26	0	0

- Molecule 41 is a protein called chain Up.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	Up	24	Total 218	C 72	H 98	N 24	O 24	0	0

- Molecule 42 is a protein called chain Uq.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	Uq	32	Total	C	H	N	O	0	0
			305	104	136	33	32		

- Molecule 43 is a protein called mS117.

Mol	Chain	Residues	Atoms						AltConf	Trace
43	Ya	339	Total	C	H	N	O	S	0	0
			5396	1716	2683	488	499	10		

- Molecule 44 is a protein called ATP-dependent Clp protease proteolytic subunit,related protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
44	Yb	553	Total	C	H	N	O	S	0	0
			9019	2849	4544	821	784	21		

- Molecule 45 is a protein called mS119.

Mol	Chain	Residues	Atoms						AltConf	Trace
45	Yc	137	Total	C	H	N	O	S	0	0
			2114	667	1064	187	192	4		

- Molecule 46 is a protein called mS120.

Mol	Chain	Residues	Atoms						AltConf	Trace
46	Yd	296	Total	C	H	N	O	S	0	0
			4928	1576	2449	457	439	7		

- Molecule 47 is a protein called mS121.

Mol	Chain	Residues	Atoms						AltConf	Trace
47	Ye	240	Total	C	H	N	O	S	0	0
			3896	1245	1940	376	329	6		

- Molecule 48 is a protein called Macro domain-containing protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
48	Yf	466	Total	C	H	N	O	S	0	0
			7377	2345	3705	675	643	9		

- Molecule 49 is a protein called Thioredoxin domain-containing protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
49	Yg	556	Total	C	H	N	O	S	0	0
			8596	2732	4279	768	800	17		

- Molecule 50 is a protein called mS124.

Mol	Chain	Residues	Atoms						AltConf	Trace
50	Yh	122	Total	C	H	N	O	S	0	0
			1979	643	984	192	158	2		

- Molecule 51 is a protein called mS125.

Mol	Chain	Residues	Atoms						AltConf	Trace
51	Yi	628	Total	C	H	N	O	S	0	0
			9914	3121	5001	870	905	17		

- Molecule 52 is a protein called DnaJ domain-containing protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
52	Yj	64	Total	C	H	N	O	S	0	0
			1094	348	547	104	94	1		

- Molecule 53 is a protein called RAP domain-containing protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
53	Yk	733	Total	C	H	N	O	S	0	0
			11754	3688	5969	1064	1004	29		

- Molecule 54 is a protein called mS128.

Mol	Chain	Residues	Atoms						AltConf	Trace
54	Yl	93	Total	C	H	N	O	S	0	0
			1529	514	747	125	140	3		

- Molecule 55 is a protein called RAP domain-containing protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
55	Ym	498	Total	C	H	N	O	S	0	0
			7815	2434	3971	693	704	13		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Ym	200	ARG	GLY	conflict	UNP A0A7J6K7K5

- Molecule 56 is a protein called AP2 domain transcription factor AP2IX-6.

Mol	Chain	Residues	Atoms						AltConf	Trace
56	Yn	205	Total	C	H	N	O	S	0	0
			3396	1056	1709	349	274	8		

- Molecule 57 is a protein called mS131.

Mol	Chain	Residues	Atoms						AltConf	Trace
57	Yo	277	Total	C	H	N	O	S	0	0
			4591	1452	2290	440	396	13		

- Molecule 58 is a protein called mS132.

Mol	Chain	Residues	Atoms						AltConf	Trace
58	Yp	123	Total	C	H	N	O	S	0	0
			1957	599	1001	190	159	8		

- Molecule 59 is a protein called Acylphosphatase-like domain-containing protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
59	Yr	225	Total	C	H	N	O	S	0	0
			3688	1155	1852	351	324	6		

- Molecule 60 is a protein called mS135.

Mol	Chain	Residues	Atoms						AltConf	Trace
60	Ys	172	Total	C	H	N	O	S	0	0
			2889	908	1451	278	247	5		

- Molecule 61 is a protein called mS136.

Mol	Chain	Residues	Atoms						AltConf	Trace
61	Yt	132	Total	C	H	N	O	S	0	0
			2180	688	1094	203	189	6		

- Molecule 62 is a protein called mS137.

Mol	Chain	Residues	Atoms						AltConf	Trace
62	Yu	36	Total	C	H	N	O	S	0	0
			617	180	319	69	48	1		

- Molecule 63 is a protein called mS133.

Mol	Chain	Residues	Atoms						AltConf	Trace
63	Yq	123	Total	C	H	N	O	S	0	0
			1974	621	1009	183	159	2		

- Molecule 64 is a RNA chain called SSU-1.

Mol	Chain	Residues	Atoms						AltConf	Trace
64	SA	91	Total	C	H	N	O	P	0	0
			2904	866	977	342	628	91		

- Molecule 65 is a RNA chain called SSU-2.

Mol	Chain	Residues	Atoms						AltConf	Trace
65	SB	28	Total	C	H	N	O	P	0	0
			917	273	304	121	191	28		

- Molecule 66 is a RNA chain called SSU-3.

Mol	Chain	Residues	Atoms						AltConf	Trace
66	SC	23	Total	C	H	N	O	P	0	0
			747	224	248	97	155	23		

- Molecule 67 is a RNA chain called SSU-4.

Mol	Chain	Residues	Atoms						AltConf	Trace
67	SD	47	Total	C	H	N	O	P	0	0
			1505	448	503	176	331	47		

- Molecule 68 is a RNA chain called SSU-5.

Mol	Chain	Residues	Atoms						AltConf	Trace
68	SE	73	Total	C	H	N	O	P	0	0
			2357	705	787	298	494	73		

- Molecule 69 is a RNA chain called SSU-6.

Mol	Chain	Residues	Atoms						AltConf	Trace
69	SF	120	Total	C	H	N	O	P	0	0
			3854	1149	1293	470	822	120		

- Molecule 70 is a RNA chain called SSU-7.

Mol	Chain	Residues	Atoms						AltConf	Trace
70	SG	26	Total	C	H	N	O	P	0	0
			824	245	275	88	190	26		

- Molecule 71 is a RNA chain called SSU-8.

Mol	Chain	Residues	Atoms						AltConf	Trace
71	SH	25	Total	C	H	N	O	P	0	0
			815	244	271	108	167	25		

- Molecule 72 is a RNA chain called SSU-9.

Mol	Chain	Residues	Atoms						AltConf	Trace
72	SI	53	Total	C	H	N	O	P	0	0
			1713	514	572	221	353	53		

- Molecule 73 is a RNA chain called SSU-10.

Mol	Chain	Residues	Atoms						AltConf	Trace
73	SJ	93	Total	C	H	N	O	P	0	0
			2989	889	1001	360	646	93		

- Molecule 74 is a RNA chain called SSU-11.

Mol	Chain	Residues	Atoms						AltConf	Trace
74	SK	114	Total	C	H	N	O	P	0	0
			3633	1080	1218	413	808	114		

- Molecule 75 is a RNA chain called SSU-12.

Mol	Chain	Residues	Atoms						AltConf	Trace
75	SL	28	Total	C	H	N	O	P	0	0
			892	265	298	99	202	28		

- Molecule 76 is a RNA chain called SSU-13.

Mol	Chain	Residues	Atoms						AltConf	Trace
76	SM	75	Total	C	H	N	O	P	0	0
			2388	710	803	272	528	75		

- Molecule 77 is a RNA chain called SSU-14.

Mol	Chain	Residues	Atoms						AltConf	Trace
77	SN	24	Total	C	H	N	O	P	0	0
			789	236	263	110	156	24		

- Molecule 78 is a RNA chain called SSU-15.

Mol	Chain	Residues	Atoms						AltConf	Trace
78	SO	16	Total	C	H	N	O	P	0	0
			514	154	173	64	107	16		

- Molecule 79 is a RNA chain called SSU-16.

Mol	Chain	Residues	Atoms						AltConf	Trace
79	SP	33	Total	C	H	N	O	P	0	0
			1066	318	358	135	222	33		

- Molecule 80 is a RNA chain called SSU-17.

Mol	Chain	Residues	Atoms						AltConf	Trace
80	SQ	56	Total	C	H	N	O	P	0	0
			1808	537	605	222	388	56		

- Molecule 81 is a RNA chain called SSU-18.

Mol	Chain	Residues	Atoms						AltConf	Trace
81	SR	34	Total	C	H	N	O	P	0	0
			1084	322	368	127	233	34		

- Molecule 82 is a RNA chain called SSU-19.

Mol	Chain	Residues	Atoms						AltConf	Trace
82	SS	12	Total	C	H	N	O	P	0	0
			386	114	131	46	83	12		

- Molecule 83 is a RNA chain called SSU-20.

Mol	Chain	Residues	Atoms						AltConf	Trace
83	ST	24	Total	C	H	N	O	P	0	0
			786	234	261	104	163	24		

- Molecule 84 is a RNA chain called SSU-21.

Mol	Chain	Residues	Atoms						AltConf	Trace
84	SU	54	Total	C	H	N	O	P	0	0
			1756	523	586	227	366	54		

- Molecule 85 is a RNA chain called tRNA E-site.

Mol	Chain	Residues	Atoms						AltConf	Trace
85	TP	21	Total	C	H	N	O	P	0	0
			671	200	224	77	149	21		

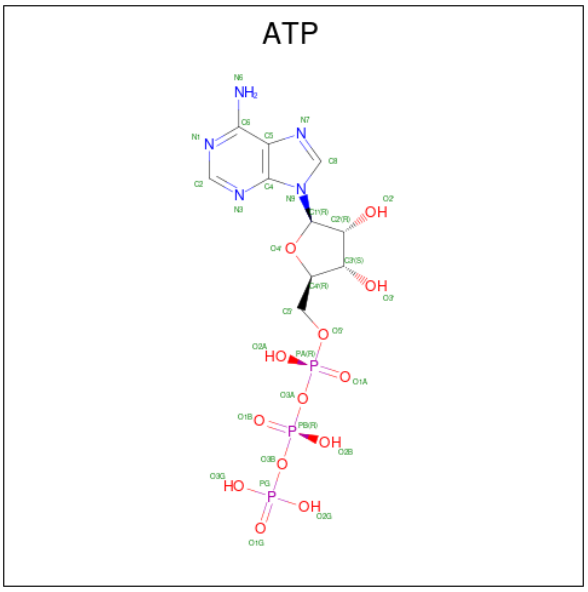
- Molecule 86 is a RNA chain called Chain UC.

Mol	Chain	Residues	Atoms						AltConf	Trace
86	UC	31	Total	C	H	N	O	P	0	0
			993	297	330	117	218	31		

- Molecule 87 is a protein called mS138.

Mol	Chain	Residues	Atoms						AltConf	Trace
87	Yv	101	Total	C	H	N	O	S	0	0
			1692	534	869	159	128	2		

- Molecule 88 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
88	Br	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	

- Molecule 89 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
89	Br	1	Total	Mg	0
			1	1	

- Molecule 90 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
90	Yp	1	Total	Zn	0
			1	1	

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

3 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	375745	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 ($e^-/Å^2$)	36	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	1600	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	1.540	Depositor
Minimum map value	-0.949	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.034	Depositor
Recommended contour level	0.15	Depositor
Map size (Å)	581.0, 581.0, 581.0	wwPDB
Map dimensions	700, 700, 700	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83, 0.83, 0.83	Depositor

4 Model quality

4.1 Standard geometry

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

4.2 Too-close contacts

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

4.3 Torsion angles

4.3.1 Protein backbone

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

4.3.2 Protein sidechains

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

4.3.3 RNA

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

4.4 Non-standard residues in protein, DNA, RNA chains

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

4.5 Carbohydrates

There are no oligosaccharides in this entry.

4.6 Ligand geometry

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 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	$\#\|Z\| > 2$
88	ATP	Br	601	89	26,33,33	0.60	0	31,52,52	1.05	2 (6%)

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
88	ATP	Br	601	89	-	7/18/38/38	0/3/3/3

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
88	Br	601	ATP	C5-C6-N6	2.25	123.77	120.35
88	Br	601	ATP	PB-O3B-PG	2.04	139.84	132.83

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
88	Br	601	ATP	PB-O3B-PG-O2G
88	Br	601	ATP	C3'-C4'-C5'-O5'
88	Br	601	ATP	O4'-C4'-C5'-O5'
88	Br	601	ATP	PA-O3A-PB-O1B
88	Br	601	ATP	PG-O3B-PB-O2B

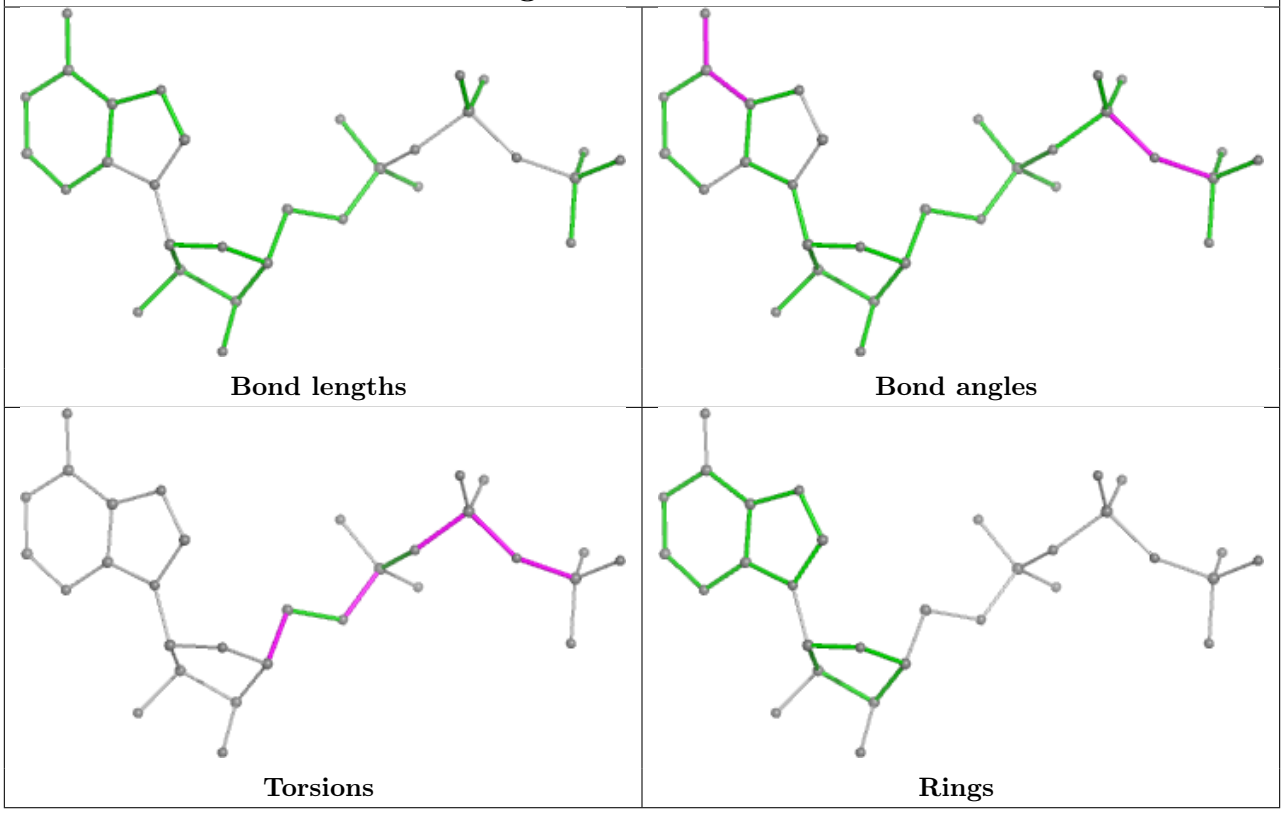
There are no ring outliers.

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 then 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.

Ligand ATP Br 601



4.7 Other polymers (i)

There are no such residues in this entry.

4.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
77	SN	1
74	SK	1
34	Uh	1
79	SP	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	SN	20:A	O3'	26:A	P	27.13
1	SK	16:U	O3'	23:C	P	20.39
1	Uh	30:ALA	C	36:GLU	N	12.46
1	SP	11:A	O3'	16:A	P	10.49

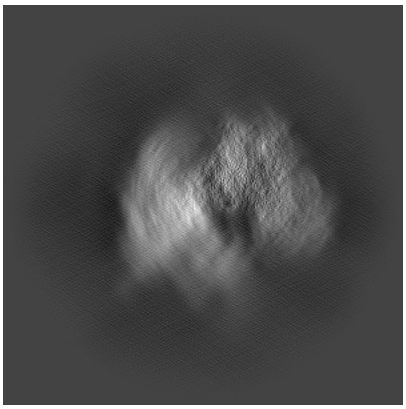
5 Map visualisation

This section contains visualisations of the EMDB entry EMD-52348. These allow visual inspection of the internal detail of the map and identification of artifacts.

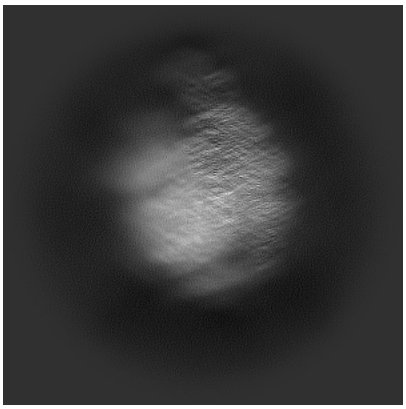
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

5.1 Orthogonal projections

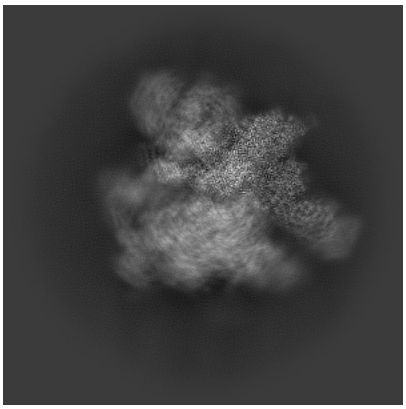
5.1.1 Primary map



X

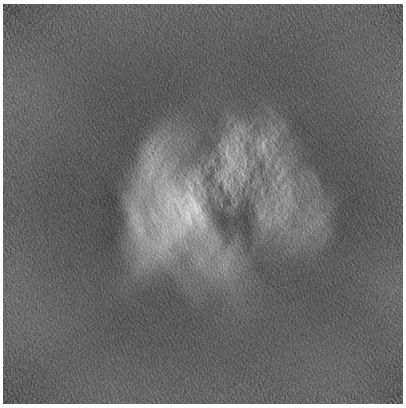


Y

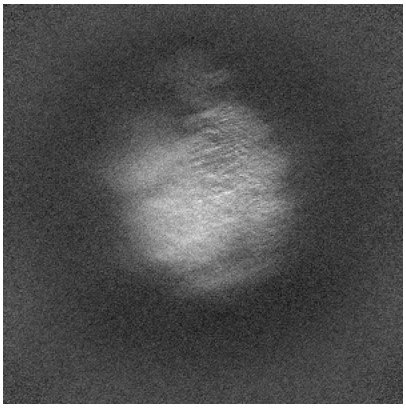


Z

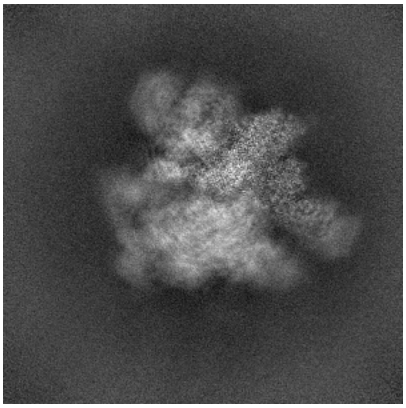
5.1.2 Raw map



X



Y

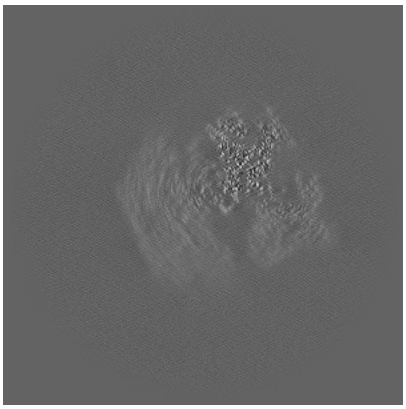


Z

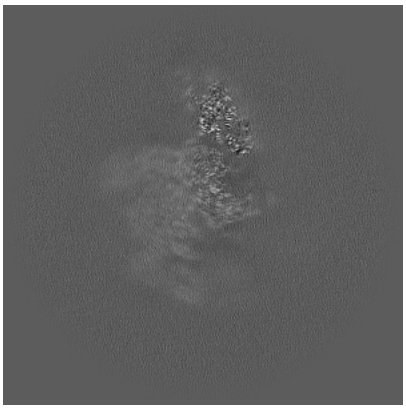
The images above show the map projected in three orthogonal directions.

5.2 Central slices (i)

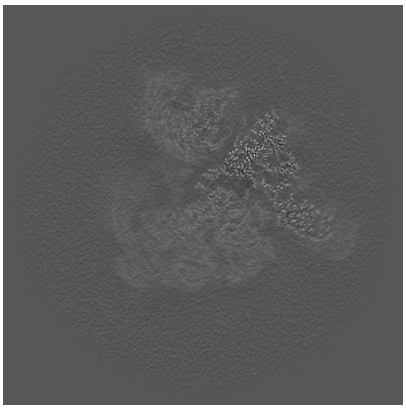
5.2.1 Primary map



X Index: 350

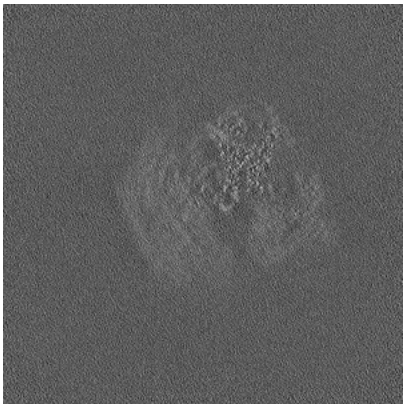


Y Index: 350

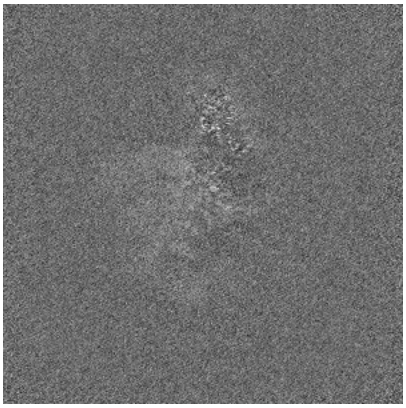


Z Index: 350

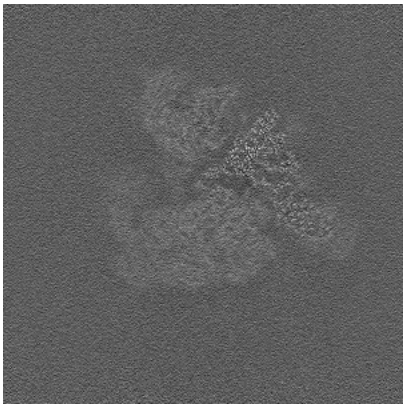
5.2.2 Raw map



X Index: 350



Y Index: 350

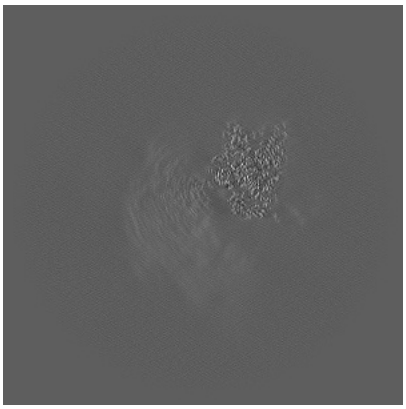


Z Index: 350

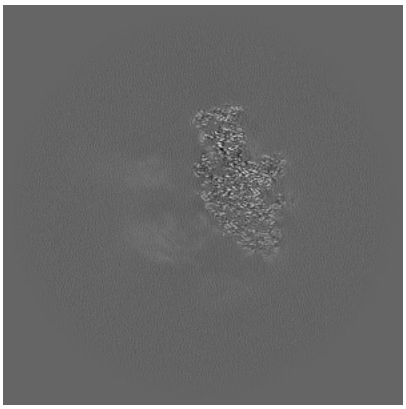
The images above show central slices of the map in three orthogonal directions.

5.3 Largest variance slices (i)

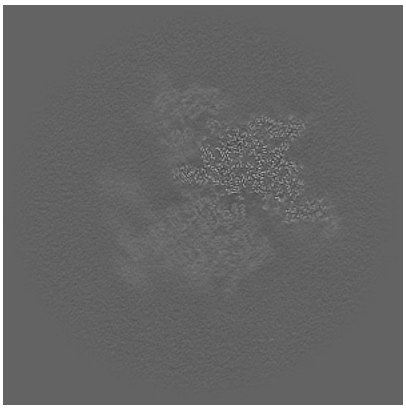
5.3.1 Primary map



X Index: 416

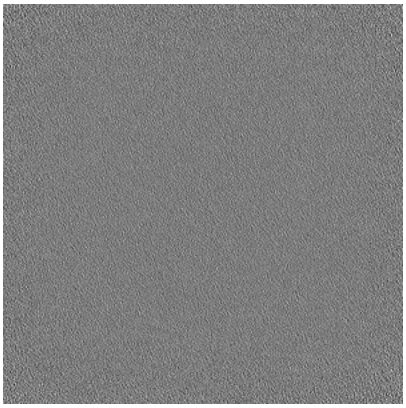


Y Index: 410

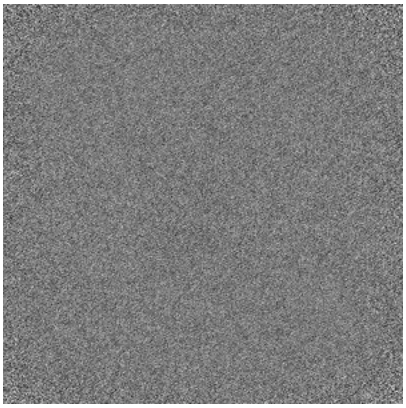


Z Index: 384

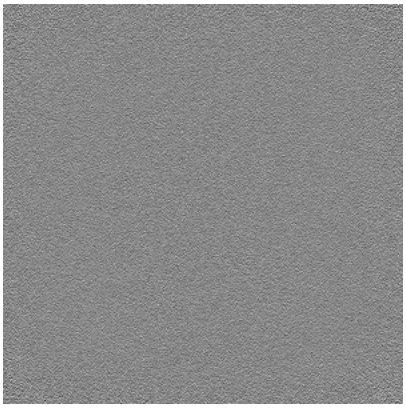
5.3.2 Raw map



X Index: 0



Y Index: 0

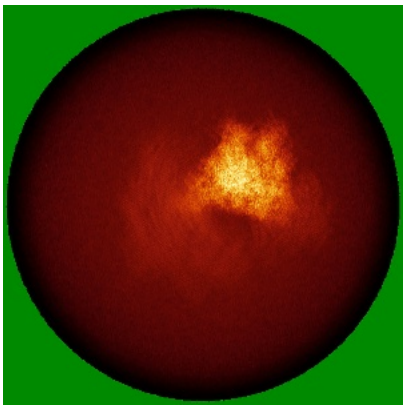


Z Index: 0

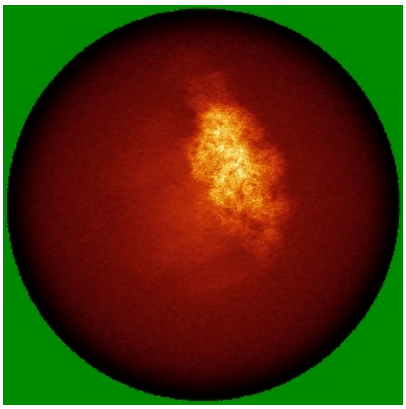
The images above show the largest variance slices of the map in three orthogonal directions.

5.4 Orthogonal standard-deviation projections (False-color) (i)

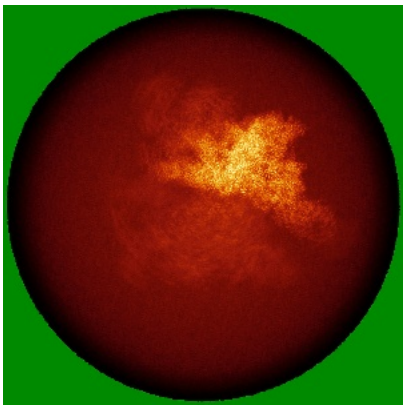
5.4.1 Primary map



X

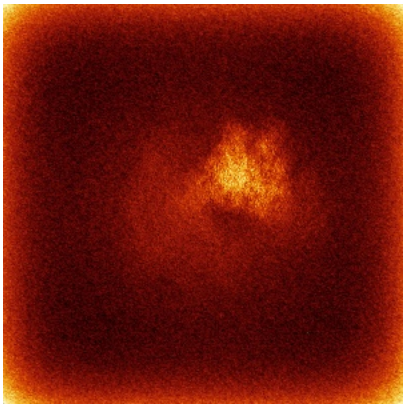


Y

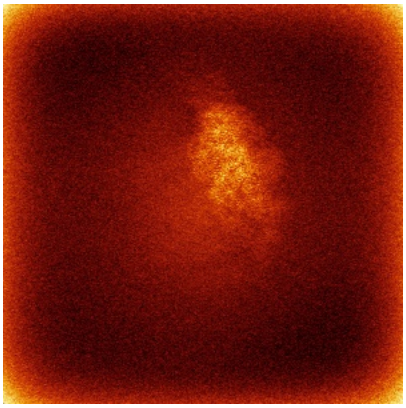


Z

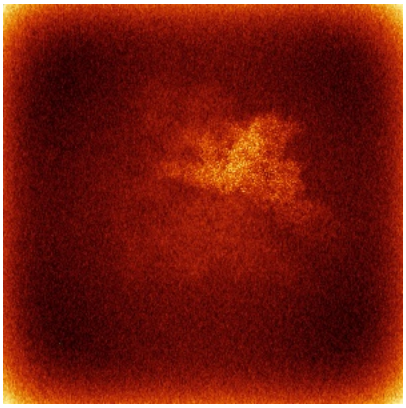
5.4.2 Raw map



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.

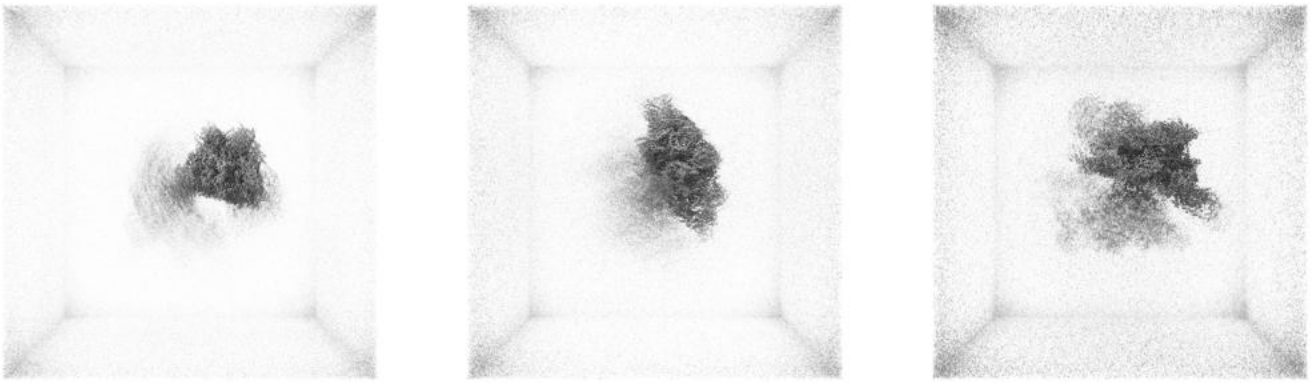
5.5 Orthogonal surface views (i)

5.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.15. 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



X Y Z

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

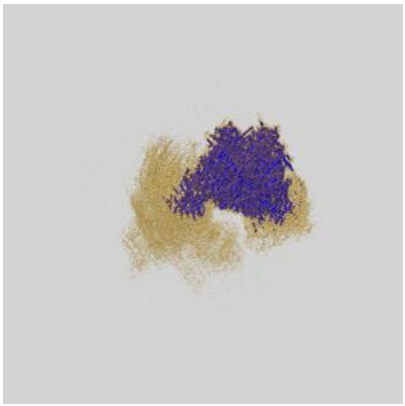
5.6 Mask visualisation (i)

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

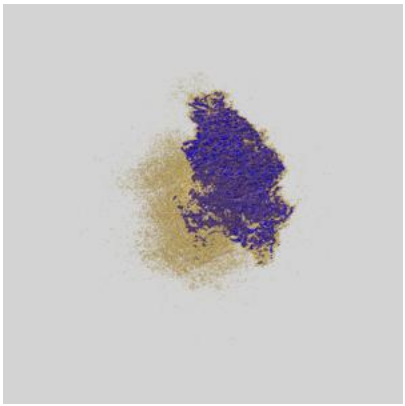
A mask typically either:

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

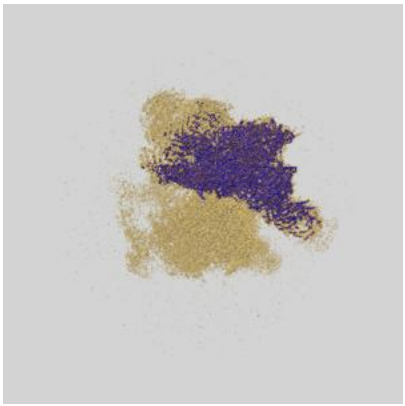
5.6.1 emd_52348_msk_1.map (i)



X



Y

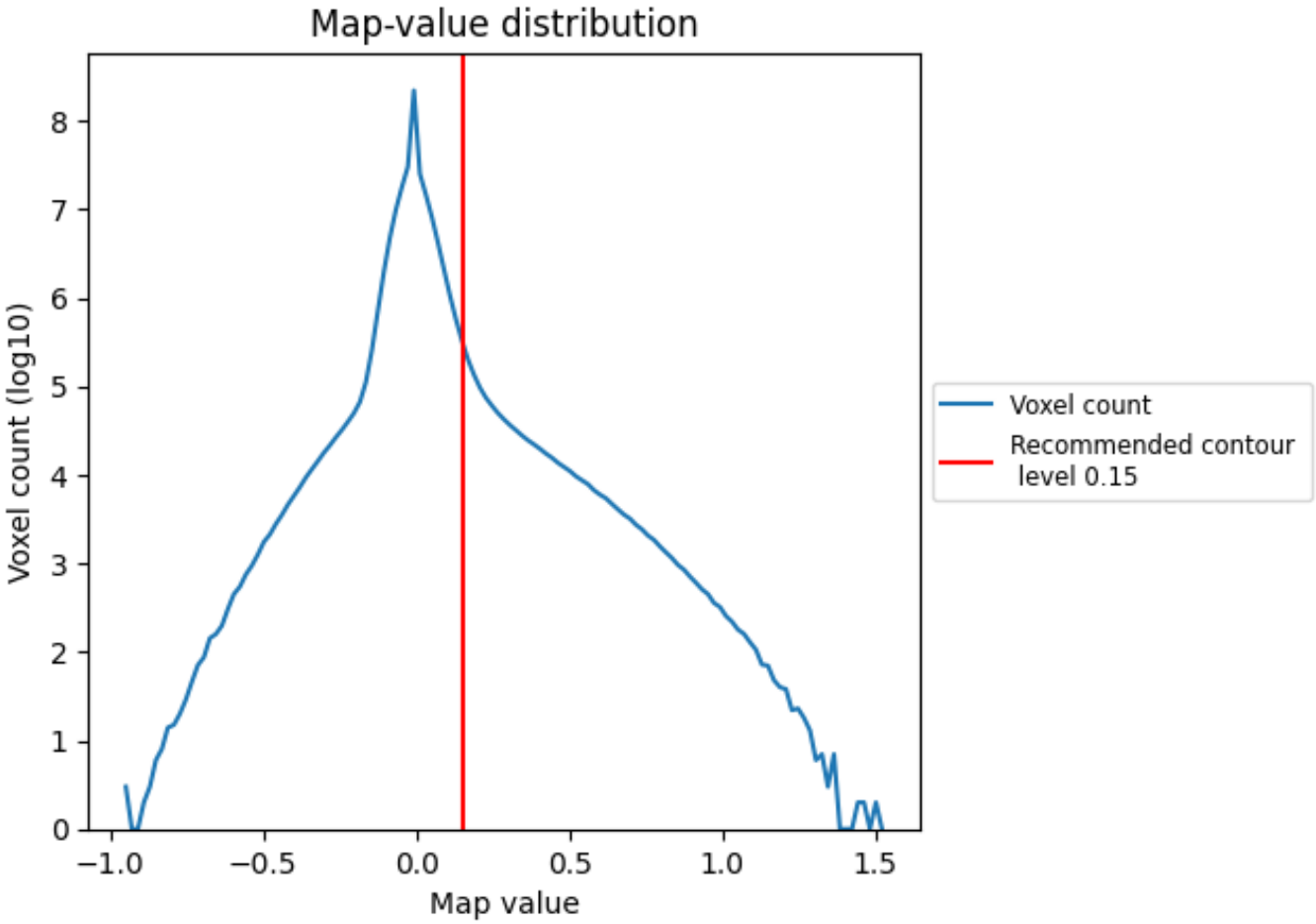


Z

6 Map analysis

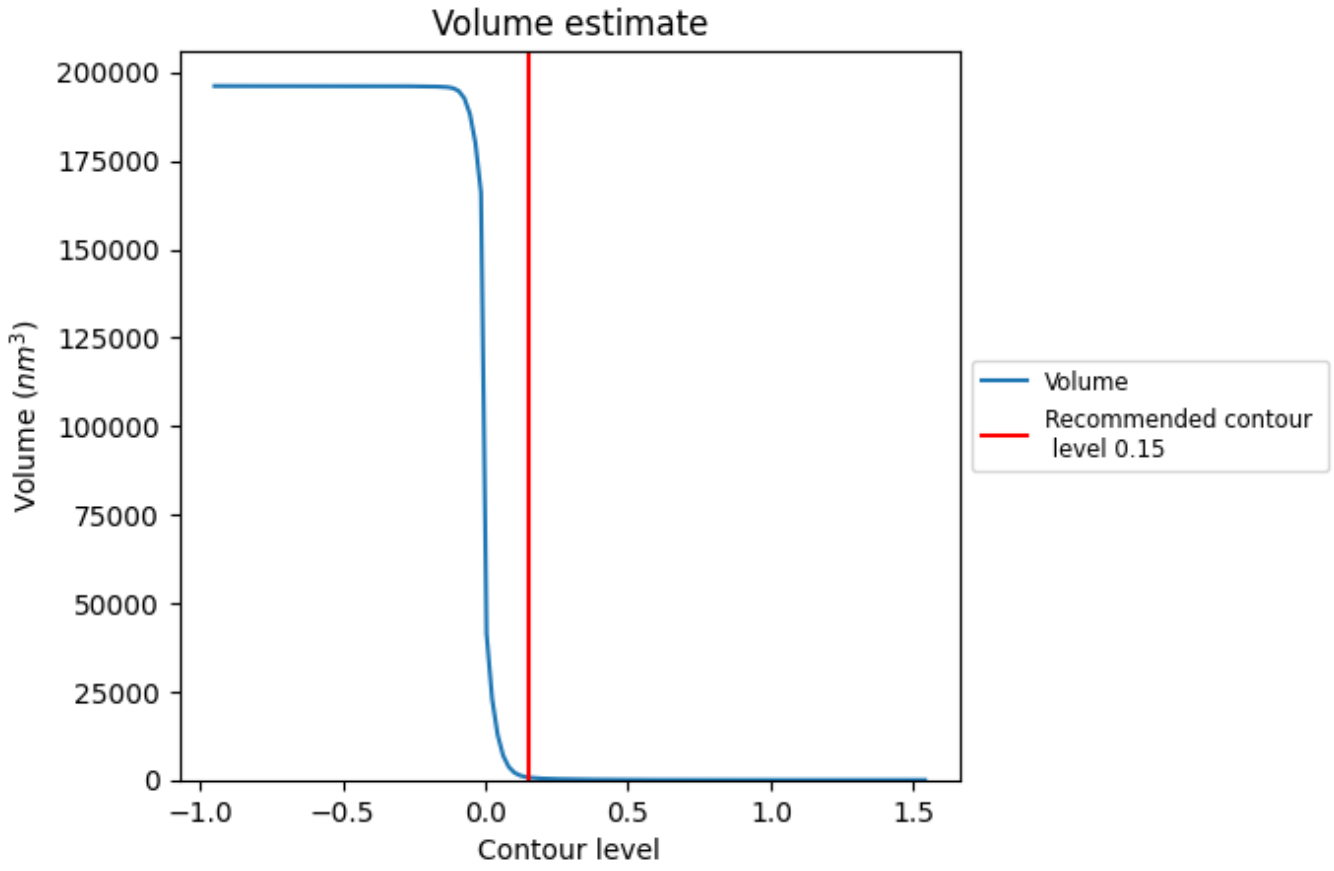
This section contains the results of statistical analysis of the map.

6.1 Map-value distribution



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.

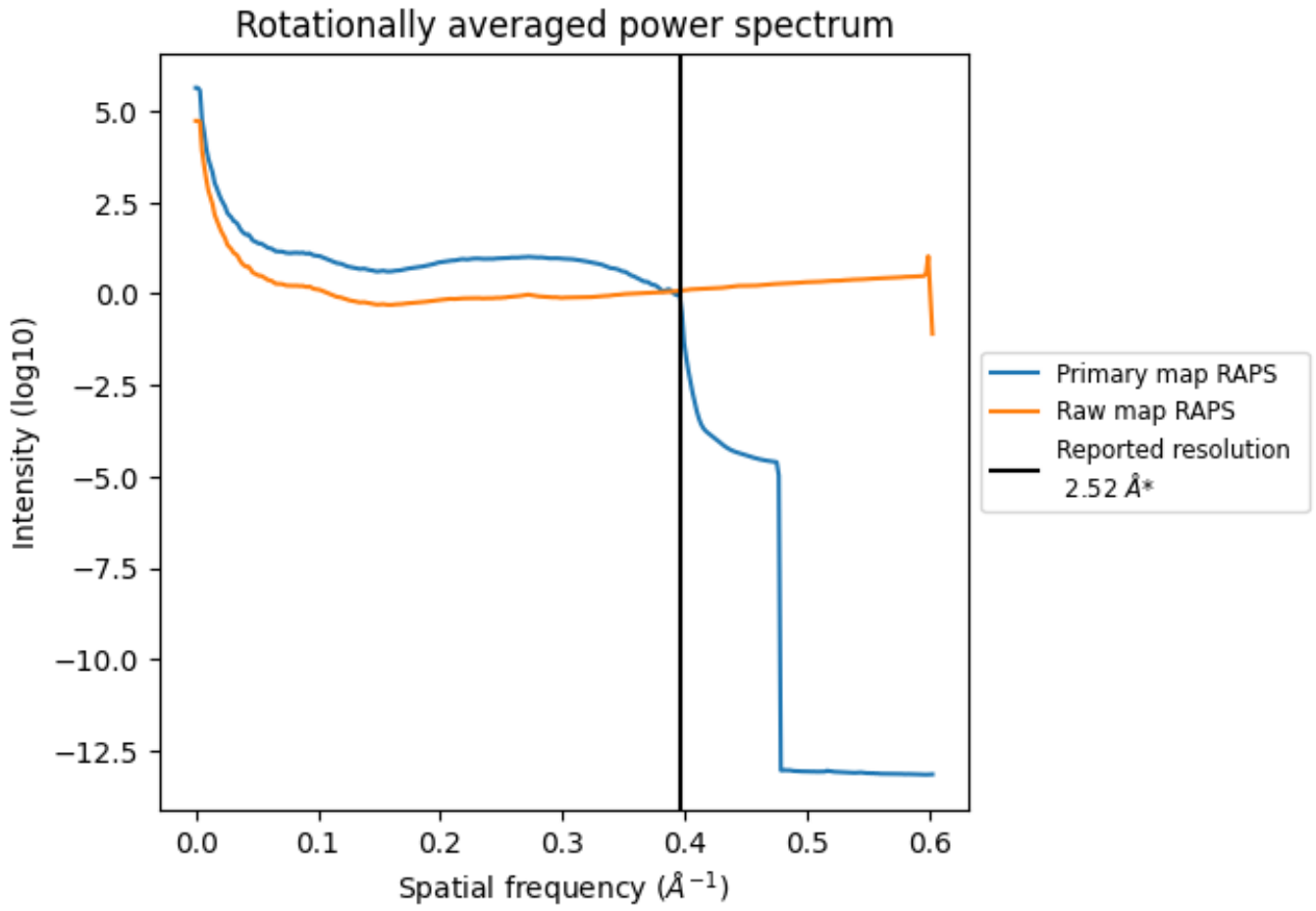
6.2 Volume estimate (i)



The volume at the recommended contour level is 747 nm^3; this corresponds to an approximate mass of 675 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)

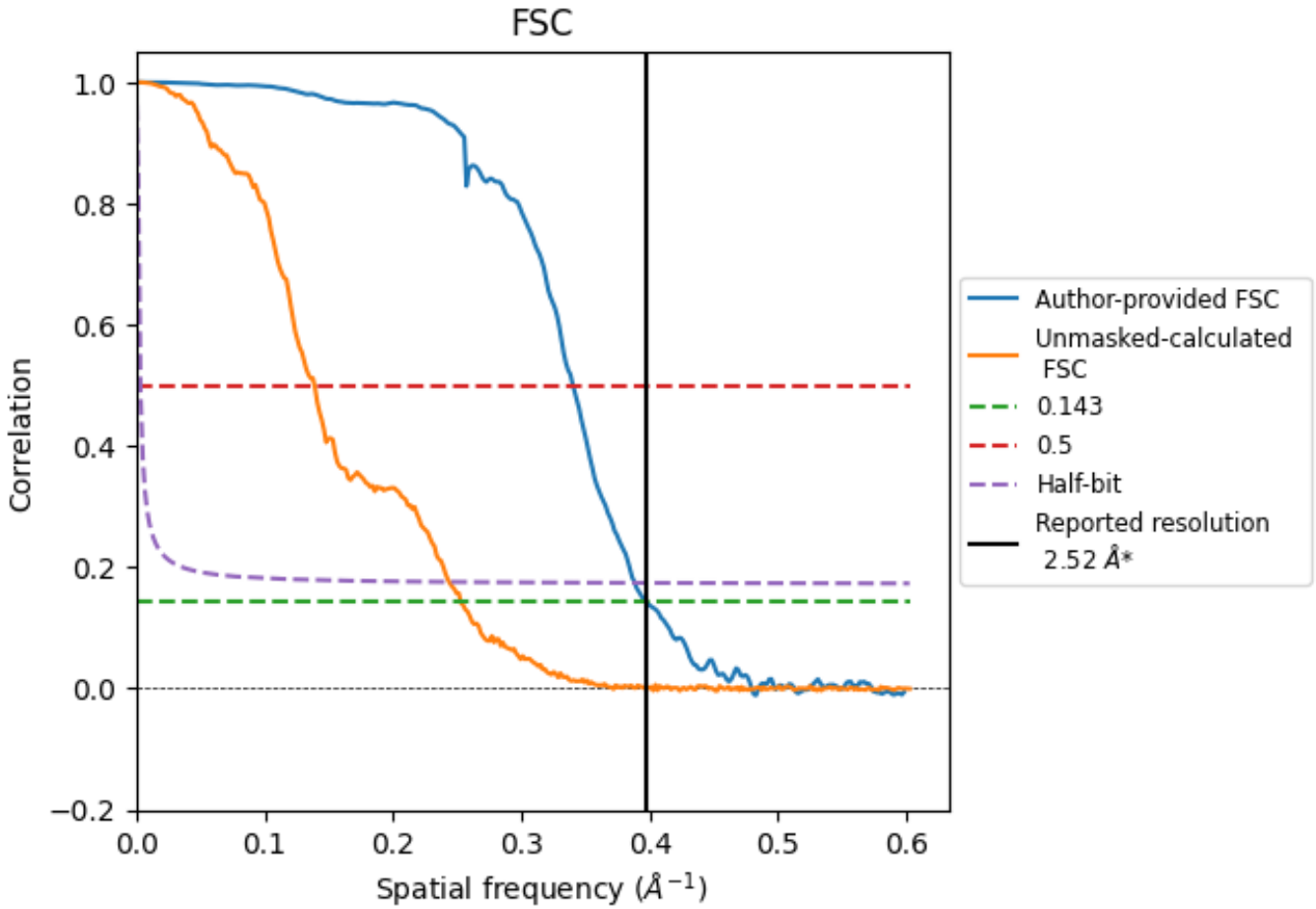


*Reported resolution corresponds to spatial frequency of 0.397 Å^{-1}

7 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.397 Å^{-1}

7.2 Resolution estimates (i)

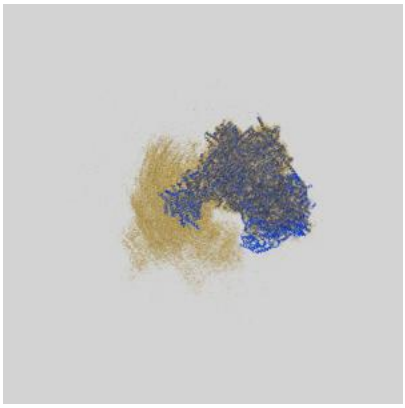
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.52	-	-
Author-provided FSC curve	2.52	2.94	2.58
Unmasked-calculated*	3.96	7.20	4.10

*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 3.96 differs from the reported value 2.52 by more than 10 %

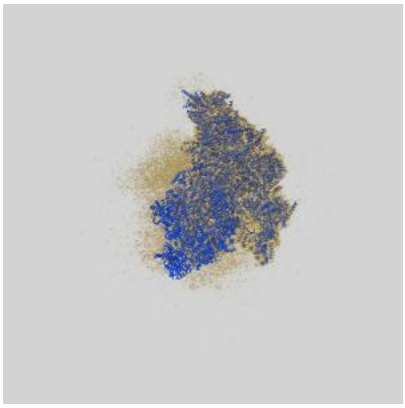
8 Map-model fit

This section contains information regarding the fit between EMDB map EMD-52348 and PDB model 9HQV. Per-residue inclusion information can be found in section ?? on page ??.

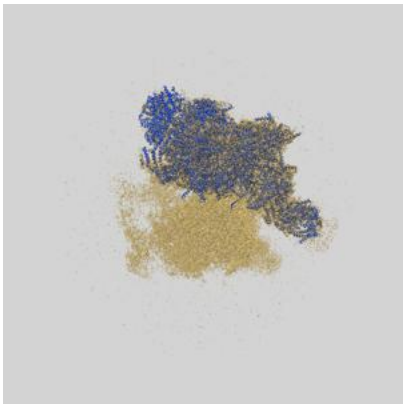
8.1 Map-model overlay



X



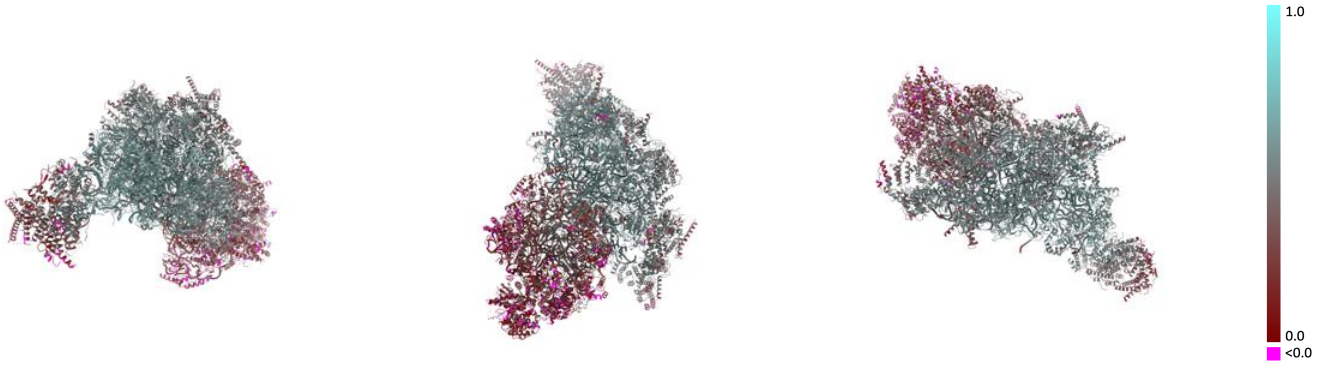
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.15 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.

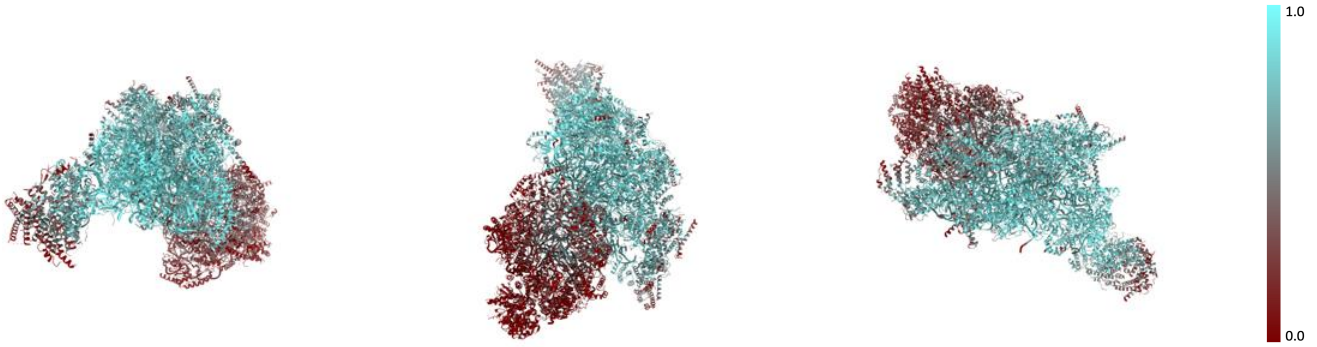
8.2 Q-score mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according 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.

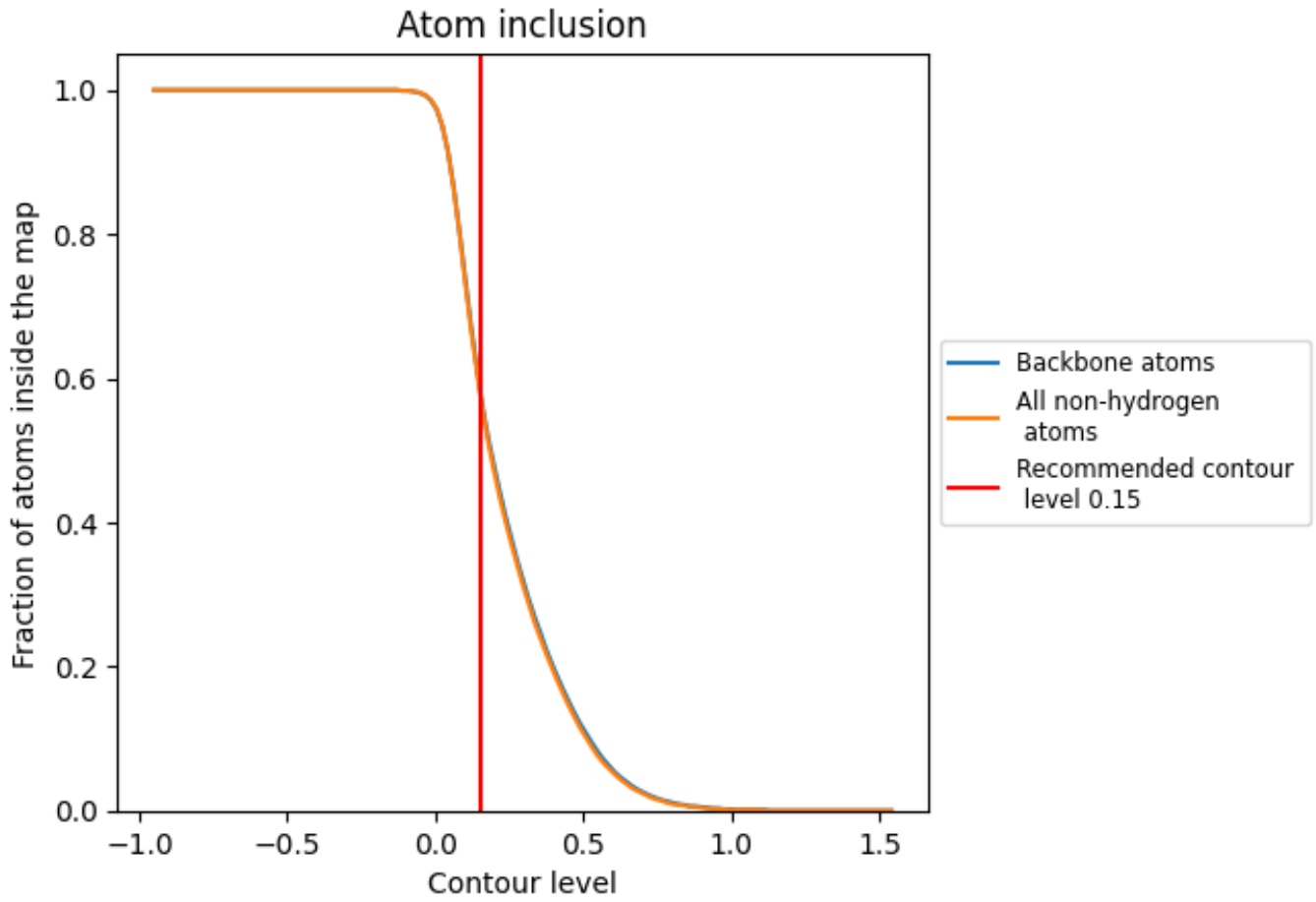
8.3 Atom inclusion mapped to coordinate model



X Y Z

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 (0.15).

8.4 Atom inclusion (i)



At the recommended contour level, 59% of all backbone atoms, 58% 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 (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5830	0.4310
BA	0.7930	0.5180
BB	0.2650	0.3560
BC	0.5450	0.4010
BD	0.3660	0.3850
Ba	0.8690	0.5670
Bb	0.5260	0.4130
Bc	0.8940	0.5760
Bd	0.9420	0.6070
Be	0.3410	0.3490
Bf	0.3920	0.3660
Bg	0.8380	0.5600
Bh	0.8580	0.5840
Bi	0.0620	0.2010
Bj	0.2960	0.3250
Bk	0.9000	0.5820
Bl	0.8680	0.5770
Bm	0.9350	0.6150
Bn	0.7730	0.5220
Bo	0.8420	0.5640
Bp	0.8180	0.5350
Bq	0.7570	0.5210
Br	0.1130	0.1770
Bs	0.2300	0.2820
Bt	0.8560	0.5770
Bu	0.1680	0.2410
Bv	0.6030	0.4420
Bx	0.7940	0.5690
By	0.8420	0.5570
Bz	0.9240	0.5940
SA	0.8550	0.5470
SB	0.9220	0.5970
SC	0.8000	0.5450
SD	0.9480	0.5980
SE	0.8180	0.5540

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Chain	Atom inclusion	Q-score
SF	0.9180	0.5830
SG	0.8670	0.5390
SH	0.8490	0.5360
SI	0.8370	0.5250
SJ	0.9000	0.5580
SK	0.6840	0.4520
SL	0.4830	0.3800
SM	0.3070	0.2610
SN	0.2800	0.2320
SO	0.4580	0.3390
SP	0.3560	0.2660
SQ	0.4960	0.3310
SR	0.7930	0.5570
SS	0.8240	0.4840
ST	0.8460	0.5360
SU	0.8850	0.5670
TP	0.0510	0.2020
UC	0.0330	0.1010
Ua	0.7900	0.5160
Ub	0.4050	0.4100
Uc	0.7800	0.5040
Ud	0.6870	0.4220
Uh	0.0730	0.2190
Ui	0.0460	0.1920
Uj	0.2270	0.2640
Uk	0.0000	0.1710
Ul	0.3870	0.4150
Um	0.4190	0.3180
Un	0.1600	0.3260
Uo	0.7150	0.4550
Up	0.7330	0.5070
Uq	0.7980	0.4840
Ya	0.8510	0.5660
Yb	0.6030	0.4530
Yc	0.8280	0.5630
Yd	0.7740	0.5130
Ye	0.8570	0.5580
Yf	0.8330	0.5430
Yg	0.7330	0.5020
Yh	0.9050	0.6050
Yi	0.1080	0.1880
Yj	0.7640	0.5440

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Chain	Atom inclusion	Q-score
Yk	0.5190	0.3910
Yl	0.1140	0.1940
Ym	0.0450	0.1520
Yn	0.2720	0.3110
Yo	0.1050	0.2450
Yp	0.1330	0.2430
Yq	0.3660	0.3580
Yr	0.6380	0.4910
Ys	0.0350	0.1200
Yt	0.0330	0.1250
Yu	0.8970	0.5890
Yv	0.8800	0.5810