



Full wwPDB EM Validation Report ⓘ

Jun 23, 2021 – 06:27 AM BST

PDB ID : 7OF3
EMDB ID : EMD-12868
Title : Structure of a human mitochondrial ribosome large subunit assembly intermediate in complex with MTERF4-NSUN4 (dataset2).
Authors : Hillen, H.S.; Lavdovskaia, E.; Nadler, F.; Hanitsch, E.; Linden, A.; Bohnsack, K.E.; Urlaub, H.; Richter-Dennerlein, R.
Deposited on : 2021-05-04
Resolution : 2.70 Å (reported)
Based on initial model : 5OOL

This is a Full wwPDB EM Validation 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

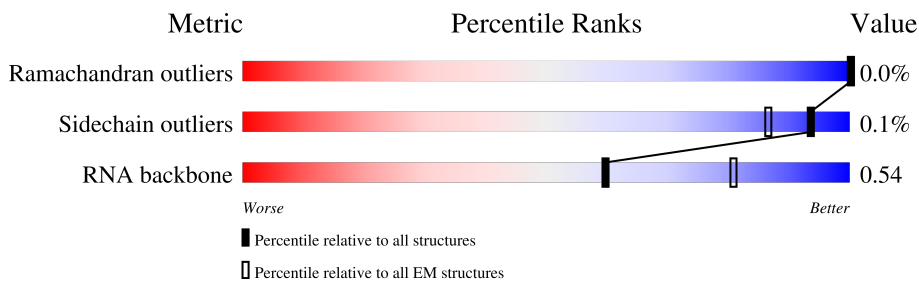
EMDB validation analysis : 0.0.0.dev75
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.20

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 2.70 Å.

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


















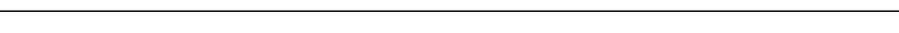
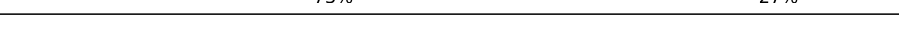



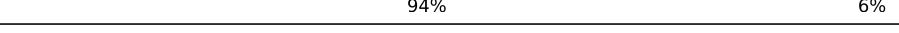




Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	0	188	57% (green), 43% (grey)
2	1	65	80% (green), 20% (grey)
3	2	92	49% (green), 51% (grey)
4	3	188	51% (green), 49% (grey)
5	4	103	36% (green), 64% (grey)
6	5	423	93% (green), 7% (grey)
7	6	380	85% (green), 15% (grey)
8	7	338	85% (green), 15% (grey)

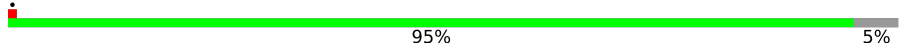
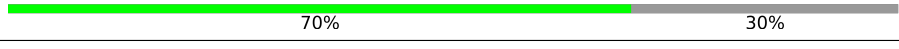
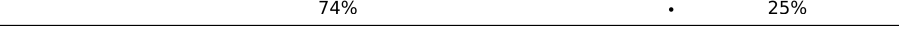
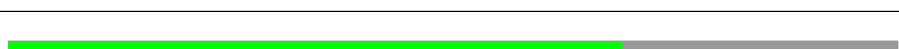



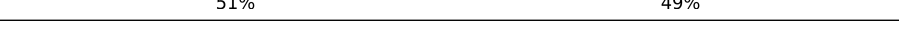



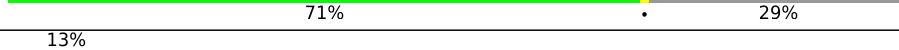

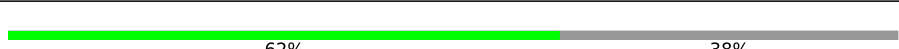


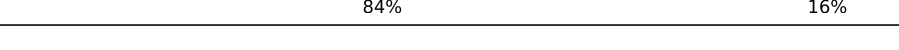






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Mol	Chain	Length	Quality of chain
9	8	206	
10	9	137	
11	A	1559	
12	B	69	
13	C	384	
14	D	305	
15	E	348	
16	F	311	
17	G	381	
18	H	267	
19	I	261	
20	J	192	
21	K	178	
22	L	145	
23	M	296	
24	N	251	
25	O	175	
26	P	180	
27	Q	292	
28	R	149	
29	S	205	
30	T	206	
31	U	153	
32	V	216	
33	W	148	

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Mol	Chain	Length	Quality of chain
34	X	256	 95% 5%
35	Y	250	 70% 30%
36	Z	161	 74% 25%
37	a	142	 57% 42%
38	b	215	 69% 31%
39	c	332	 83% 17%
40	d	306	 67% 33%
41	e	279	 35% 71% 29%
42	f	212	 9% 51% 49%
43	g	166	 78% 22%
44	h	158	 66% 34%
45	i	128	 76% 24%
46	j	123	 69% 31%
47	k	112	 71% 29%
48	m	128	 13% 23% 77%
49	o	102	 78% 22%
50	p	206	 62% 38%
51	q	222	 58% 42%
52	r	196	 74% 26%
53	s	439	 84% 16%
54	u	234	 47% 53%
55	v	70	 15% 97% ..
56	w	156	 15% 50% 49%

2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 101226 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 39S ribosomal protein L32, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	0	108	880	545	172	157	6	0	0

- Molecule 2 is a protein called 39S ribosomal protein L33, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	1	52	433	278	83	70	2	0	0

- Molecule 3 is a protein called 39S ribosomal protein L34, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	2	45	367	227	81	58	1	0	0

- Molecule 4 is a protein called 39S ribosomal protein L35, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	3	95	831	539	162	127	3	0	0

- Molecule 5 is a protein called 39S ribosomal protein L36, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	4	37	333	212	71	47	3	0	0

- Molecule 6 is a protein called 39S ribosomal protein L37, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	5	392	3199	2067	558	563	11	0	0

- Molecule 7 is a protein called 39S ribosomal protein L38, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	6	324	Total	C	N	O	S	0	0
			2723	1743	488	484	8		

- Molecule 8 is a protein called 39S ribosomal protein L39, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	7	287	Total	C	N	O	S	0	0
			2334	1495	397	425	17		

- Molecule 9 is a protein called 39S ribosomal protein L40, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	8	77	Total	C	N	O	S	0	0
			651	413	113	123	2		

- Molecule 10 is a protein called 39S ribosomal protein L41, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	9	117	Total	C	N	O	S	0	0
			947	614	163	168	2		

- Molecule 11 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
11	A	1386	Total	C	N	O	P	0	0
			29436	13209	5322	9519	1386		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	3107	U	UNK	conflict	GB 1025814679

- Molecule 12 is a RNA chain called Mitochondrial tRNAVal.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
12	B	56	Total	C	N	O	P	0	0
			1191	534	214	387	56		

- Molecule 13 is a protein called 5-methylcytosine rRNA methyltransferase NSUN4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	C	327	2595	1651	454	474	16	1	0

- Molecule 14 is a protein called 39S ribosomal protein L2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	D	234	1832	1139	370	314	9	0	0

- Molecule 15 is a protein called 39S ribosomal protein L3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	E	305	2405	1545	418	431	11	0	0

- Molecule 16 is a protein called 39S ribosomal protein L4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	F	250	2013	1294	365	348	6	0	0

- Molecule 17 is a protein called Transcription termination factor 4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	G	238	1943	1243	336	352	12	0	0

- Molecule 18 is a protein called 39S ribosomal protein L9, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
18	H	95	784	498	152	134	0	0

- Molecule 19 is a protein called 39S ribosomal protein L10, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	I	151	1228	795	222	201	10	0	0

- Molecule 20 is a protein called 39S ribosomal protein L11, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	J	140	Total	C	N	O	S	0	0
			1061	680	192	187	2		

- Molecule 21 is a protein called 39S ribosomal protein L13, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	K	177	Total	C	N	O	S	0	0
			1451	934	259	251	7		

- Molecule 22 is a protein called 39S ribosomal protein L14, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	L	115	Total	C	N	O	S	0	0
			889	559	171	154	5		

- Molecule 23 is a protein called 39S ribosomal protein L15, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	M	287	Total	C	N	O	S	0	0
			2305	1472	425	402	6		

- Molecule 24 is a protein called 39S ribosomal protein L16, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	N	183	Total	C	N	O	S	0	0
			1494	960	274	251	9		

- Molecule 25 is a protein called 39S ribosomal protein L17, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	O	152	Total	C	N	O	S	0	0
			1245	784	239	215	7		

- Molecule 26 is a protein called 39S ribosomal protein L18, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	P	141	Total	C	N	O	S	0	0
			1148	719	221	203	5		

- Molecule 27 is a protein called 39S ribosomal protein L19, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	Q	217	1805	1159	317	320	9	0	0

- Molecule 28 is a protein called 39S ribosomal protein L20, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	R	140	1153	732	231	186	4	0	0

- Molecule 29 is a protein called 39S ribosomal protein L21, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	S	156	1251	806	222	219	4	0	0

- Molecule 30 is a protein called 39S ribosomal protein L22, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	T	166	1368	875	254	232	7	0	0

- Molecule 31 is a protein called 39S ribosomal protein L23, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	U	139	1154	734	220	197	3	0	0

- Molecule 32 is a protein called 39S ribosomal protein L24, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	V	191	1568	999	280	281	8	0	0

- Molecule 33 is a protein called 39S ribosomal protein L27, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	W	100	801	518	150	130	3	0	0

- Molecule 34 is a protein called 39S ribosomal protein L28, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	X	243	Total	C	N	O	S	0	0
			2035	1317	351	362	5		

- Molecule 35 is a protein called 39S ribosomal protein L47, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	Y	176	Total	C	N	O	S	0	0
			1517	970	291	252	4		

- Molecule 36 is a protein called 39S ribosomal protein L30, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	Z	120	Total	C	N	O	S	0	0
			978	626	183	166	3		

- Molecule 37 is a protein called 39S ribosomal protein L42, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	a	82	Total	C	N	O	S	0	0
			686	434	124	123	5		

- Molecule 38 is a protein called 39S ribosomal protein L43, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	b	148	Total	C	N	O	S	0	0
			1178	733	229	213	3		

- Molecule 39 is a protein called 39S ribosomal protein L44, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	c	275	Total	C	N	O	S	0	0
			2217	1415	383	410	9		

- Molecule 40 is a protein called 39S ribosomal protein L45, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	d	205	Total	C	N	O	S	0	0
			1702	1103	287	303	9		

- Molecule 41 is a protein called 39S ribosomal protein L46, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	e	197	Total	C	N	O	S	0	0
			1599	1027	277	290	5		

- Molecule 42 is a protein called 39S ribosomal protein L48, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	f	108	Total	C	N	O	S	0	0
			857	549	140	165	3		

- Molecule 43 is a protein called 39S ribosomal protein L49, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	g	129	Total	C	N	O	S	0	0
			1067	690	185	190	2		

- Molecule 44 is a protein called 39S ribosomal protein L50, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	h	105	Total	C	N	O	S	0	0
			862	548	151	160	3		

- Molecule 45 is a protein called 39S ribosomal protein L51, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	i	97	Total	C	N	O	S	0	0
			827	532	165	126	4		

- Molecule 46 is a protein called 39S ribosomal protein L52, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	j	85	Total	C	N	O	S	0	0
			684	423	133	126	2		

- Molecule 47 is a protein called 39S ribosomal protein L53, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	k	80	Total	C	N	O	S	0	0
			627	392	116	114	5		

- Molecule 48 is a protein called 39S ribosomal protein L55, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	m	29	Total	C	N	O	S	0	0
			245	157	48	38	2		

- Molecule 49 is a protein called Ribosomal protein 63, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	o	80	Total	C	N	O	S	0	0
			676	426	134	113	3		

- Molecule 50 is a protein called Peptidyl-tRNA hydrolase ICT1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	p	127	Total	C	N	O	S	0	0
			1058	661	201	192	4		

- Molecule 51 is a protein called Growth arrest and DNA damage-inducible proteins-interacting protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	q	128	Total	C	N	O	S	0	0
			1076	671	208	192	5		

- Molecule 52 is a protein called 39S ribosomal protein S18a, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	r	146	Total	C	N	O	S	0	0
			1203	764	232	199	8		

- Molecule 53 is a protein called 39S ribosomal protein S30, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	s	370	Total	C	N	O	S	0	0
			3036	1946	542	534	14		

- Molecule 54 is a protein called Mitochondrial assembly of ribosomal large subunit protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	u	111	Total	C	N	O	S	0	0
			927	595	155	167	10		

- Molecule 55 is a protein called MIEF1 upstream open reading frame protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
55	v	69	588	372	116	100	0	0

- Molecule 56 is a protein called Acyl carrier protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
56	w	79	638	410	95	128	5	0	0

- Molecule 57 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
57	0	1	1	1	0
57	4	1	1	1	0
57	r	1	1	1	0

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

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
58	A	57	57	57	0
58	g	1	1	1	0

- Molecule 59 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.


- Molecule 1: 39S ribosomal protein L32, mitochondrial

Chain 0:  57% 43%

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

ASP THR SER GLY SER LYS GLU ASN SER SER LEU LEU ASP SER SER ILE PHE TRP MET A79 T136 GLN ASN

- Molecule 2: 39S ribosomal protein L33, mitochondrial

Chain 1:  80% 20%

MET PHE LEU SER ALA VAL PHE PHE ALA LYS SER LYS SER MET L64 L65

- Molecule 3: 39S ribosomal protein L34, mitochondrial

Chain 2:  49% 51%

MET ALA VAL LEU ALA GLY SER LEU LEU LEU VAL PRO THR ARG SER SER ILE ALA ALA LEU LEU LEU GLY ARG TRP LEU GLN PRO ARG TRP LEU LEU GLY PHE PRO ASP ALA TRP GLY LEU LEU THR PRO PRO GLN GLN ALA ARG LYS A48 A92

- Molecule 4: 39S ribosomal protein L35, mitochondrial

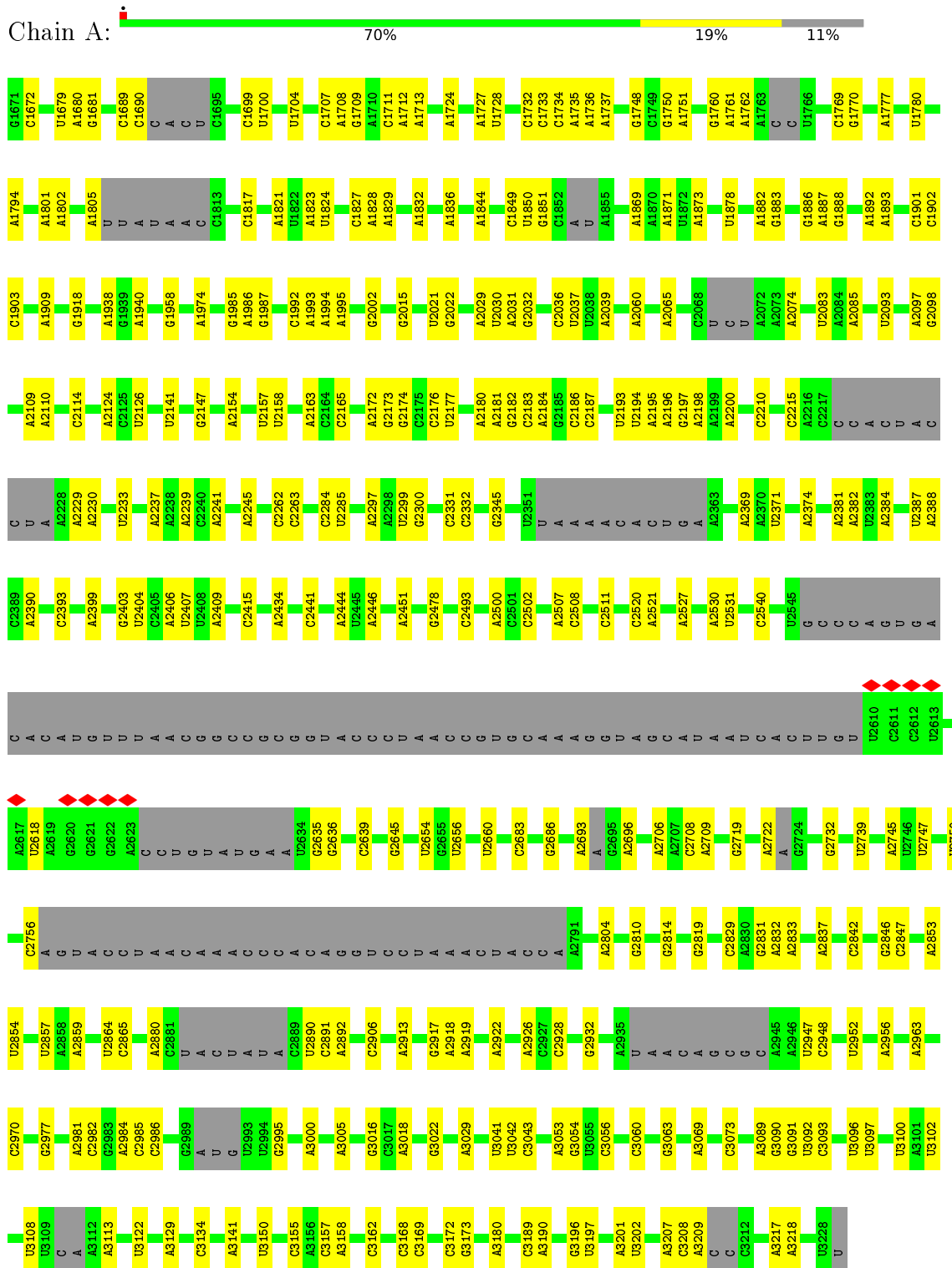
Chain 3:  51% 49%

MET ALA ALA SER ARG PHE ALA GLY ALA CYS VAL HIS ARG THR SER VAL ILE LEU ASN ARG MET ALA PRO ASN VAL LEU LEU PRO SER VAL THR TYR LYS LEU PRO VAL ARG SER L94 V188

- Molecule 5: 39S ribosomal protein L36, mitochondrial

Chain 4:  36% 64%

• Molecule 11: 16S ribosomal RNA



• Molecule 12: Mitochondrial tRNA^{Val}



MET ALA PHE THR GLY LEU TRP GLY PRO PHE THR CYS VAL SER ARG VAL LEU SER HIS CYS PHE SER THR GLY SER LEU SER A31 Y145

- Molecule 23: 39S ribosomal protein L15, mitochondrial

Chain M:  97%

MET ALA GLY PRO LEU GLN GLY GLY A10 R44 S296



- Molecule 24: 39S ribosomal protein L16, mitochondrial

Chain N:  73%  27%

MET TRP ARG LEU VAL ALA ARG ALA SER ALA LEU LEU ARG VAL HIS ASP VAL PRO LEU SER ASP THR ALA LEU PRO ALA ALA VAL LYS THR LEU PRO VAL PRO SER PHE GLU ASP VAL SER ILE PRO K47 R64 GLU PRO LYS ASN S70 I131 THR ARG LYS

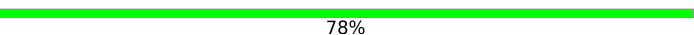
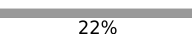
SER VAL GLY HIS ARG MET GLY GLY GLY LYS ALA ILE ASP H49 V251

- Molecule 25: 39S ribosomal protein L17, mitochondrial

Chain O:  87%  13%

MET ARG LEU SER VAL ALA ALA I19 Q160 GLU SER ASN HIS SER GLY HIS THR ALA THR PRO GLY ILE

- Molecule 26: 39S ribosomal protein L18, mitochondrial

Chain P:  78%  22%

MET ALA LEU ARG SER ARG PHE TRP GLY LEU PHE SER VAL CYS ASN PRO GLY CYS ARG ALA LEU LEU SER THR SER SER GLU PRO ALA LYS PRO VAL ASP PRO T39 Y179 GLU

- Molecule 27: 39S ribosomal protein L19, mitochondrial

Chain Q:  74%  26%

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

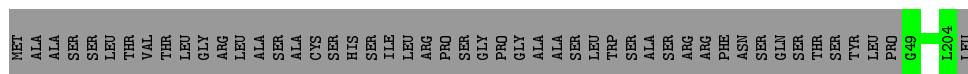
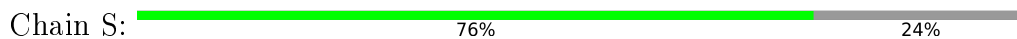
VAL ILE VAL ASP LYS HIS ARG PRO VAL GLU PRO ARG R74 K290 ARG SER

- Molecule 28: 39S ribosomal protein L20, mitochondrial

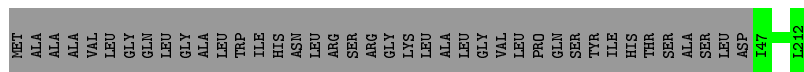
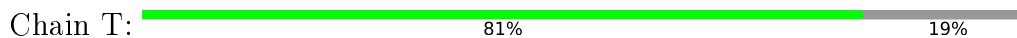
Chain R:  94%  6%

MET VAL PHE LEU THR ALA GLN LEU TRP L10 H149

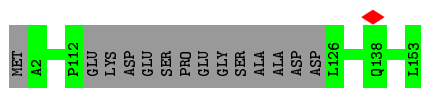
- Molecule 29: 39S ribosomal protein L21, mitochondrial



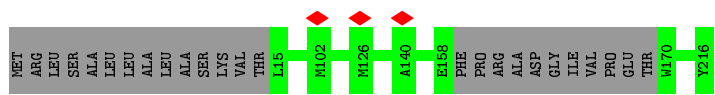
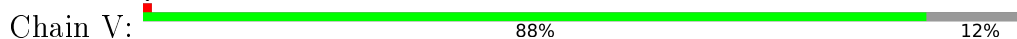
- Molecule 30: 39S ribosomal protein L22, mitochondrial



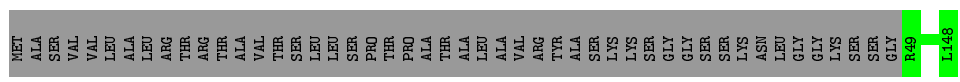
- Molecule 31: 39S ribosomal protein L23, mitochondrial



- Molecule 32: 39S ribosomal protein L24, mitochondrial



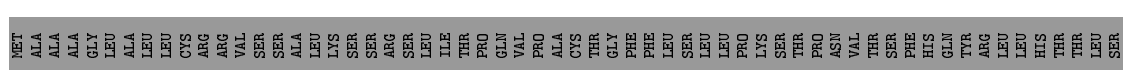
- Molecule 33: 39S ribosomal protein L27, mitochondrial

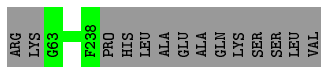


- Molecule 34: 39S ribosomal protein L28, mitochondrial

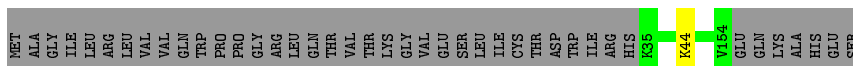


- Molecule 35: 39S ribosomal protein L47, mitochondrial

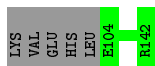
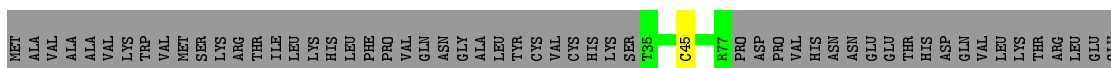




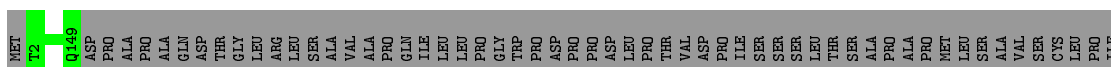
- Molecule 36: 39S ribosomal protein L30, mitochondrial



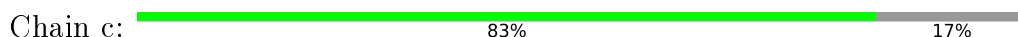
- Molecule 37: 39S ribosomal protein L42, mitochondrial



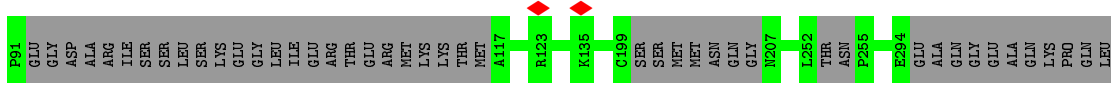
- Molecule 38: 39S ribosomal protein L43, mitochondrial



- Molecule 39: 39S ribosomal protein L44, mitochondrial



- Molecule 40: 39S ribosomal protein L45, mitochondrial



MET
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MET
PRO
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L74
E77
D81
L89
Y90
D91
R92
I93
D94
P95
L98
M101
M105
K106
D107
M120
A121
D124
E125
F128
E129
D132
D146
D150
K151
K152
ASP
VAL
TYR
GLU

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	138715	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	37	Depositor
Minimum defocus (nm)	300	Depositor
Maximum defocus (nm)	2100	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.053	Depositor
Minimum map value	-0.019	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.0046	Depositor
Map size (\AA)	367.49997, 367.49997, 367.49997	wwPDB
Map dimensions	350, 350, 350	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.05, 1.05, 1.05	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	0	0.27	0/895	0.53	0/1201
2	1	0.26	0/438	0.54	0/583
3	2	0.26	0/373	0.56	0/496
4	3	0.28	0/852	0.53	0/1136
5	4	0.30	0/341	0.58	0/451
6	5	0.27	0/3294	0.48	0/4488
7	6	0.27	0/2809	0.51	0/3818
8	7	0.26	0/2391	0.46	0/3234
9	8	0.25	0/665	0.51	0/894
10	9	0.28	0/972	0.49	0/1306
11	A	0.37	0/32925	0.75	1/51219 (0.0%)
12	B	0.21	0/1328	0.74	0/2056
13	C	0.25	0/2655	0.48	0/3601
14	D	0.27	0/1867	0.56	0/2510
15	E	0.29	0/2474	0.46	0/3355
16	F	0.27	0/2071	0.50	0/2817
17	G	0.25	0/1974	0.46	0/2652
18	H	0.26	0/798	0.54	0/1073
19	I	0.25	0/1252	0.49	0/1686
20	J	0.24	0/1077	0.49	0/1452
21	K	0.28	0/1495	0.48	0/2029
22	L	0.26	0/904	0.53	0/1218
23	M	0.28	0/2359	0.52	0/3185
24	N	0.26	0/1533	0.52	0/2061
25	O	0.26	0/1269	0.54	0/1708
26	P	0.25	0/1173	0.53	0/1588
27	Q	0.28	0/1846	0.50	0/2487
28	R	0.28	0/1174	0.55	0/1572
29	S	0.27	0/1276	0.51	0/1729
30	T	0.29	0/1402	0.50	0/1886
31	U	0.28	0/1183	0.54	0/1600
32	V	0.26	0/1609	0.51	0/2179

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	W	0.30	0/823	0.48	0/1113
34	X	0.27	0/2090	0.46	0/2825
35	Y	0.26	0/1552	0.50	0/2079
36	Z	0.27	0/1003	0.48	0/1354
37	a	0.28	0/709	0.51	0/963
38	b	0.28	0/1202	0.56	0/1626
39	c	0.27	0/2264	0.48	0/3059
40	d	0.26	0/1752	0.47	0/2374
41	e	0.24	0/1633	0.48	0/2204
42	f	0.26	0/873	0.43	0/1180
43	g	0.29	0/1102	0.49	0/1503
44	h	0.24	0/884	0.47	0/1203
45	i	0.28	0/849	0.53	0/1135
46	j	0.26	0/698	0.50	0/940
47	k	0.25	0/635	0.54	0/855
48	m	0.23	0/250	0.61	0/336
49	o	0.27	0/693	0.53	0/931
50	p	0.24	0/1071	0.53	0/1433
51	q	0.25	0/1107	0.51	0/1498
52	r	0.27	0/1238	0.52	0/1676
53	s	0.28	0/3114	0.51	0/4225
54	u	0.27	0/949	0.50	0/1281
55	v	0.24	0/597	0.59	0/796
56	w	0.24	0/647	0.42	0/871
All	All	0.30	0/106409	0.60	1/150730 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	2176	C	N3-C2-O2	-5.04	118.37	121.90

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	106/188 (56%)	106 (100%)	0	0	100	100
2	1	50/65 (77%)	50 (100%)	0	0	100	100
3	2	43/92 (47%)	43 (100%)	0	0	100	100
4	3	93/188 (50%)	91 (98%)	2 (2%)	0	100	100
5	4	35/103 (34%)	34 (97%)	1 (3%)	0	100	100
6	5	390/423 (92%)	383 (98%)	7 (2%)	0	100	100
7	6	316/380 (83%)	307 (97%)	9 (3%)	0	100	100
8	7	285/338 (84%)	269 (94%)	16 (6%)	0	100	100
9	8	75/206 (36%)	70 (93%)	5 (7%)	0	100	100
10	9	113/137 (82%)	111 (98%)	2 (2%)	0	100	100
13	C	324/384 (84%)	307 (95%)	17 (5%)	0	100	100
14	D	230/305 (75%)	225 (98%)	5 (2%)	0	100	100
15	E	303/348 (87%)	289 (95%)	14 (5%)	0	100	100
16	F	248/311 (80%)	245 (99%)	3 (1%)	0	100	100
17	G	236/381 (62%)	227 (96%)	9 (4%)	0	100	100
18	H	93/267 (35%)	88 (95%)	5 (5%)	0	100	100
19	I	147/261 (56%)	140 (95%)	7 (5%)	0	100	100
20	J	138/192 (72%)	129 (94%)	9 (6%)	0	100	100
21	K	175/178 (98%)	172 (98%)	3 (2%)	0	100	100
22	L	113/145 (78%)	112 (99%)	1 (1%)	0	100	100
23	M	285/296 (96%)	280 (98%)	5 (2%)	0	100	100
24	N	177/251 (70%)	170 (96%)	7 (4%)	0	100	100
25	O	150/175 (86%)	147 (98%)	3 (2%)	0	100	100
26	P	139/180 (77%)	132 (95%)	7 (5%)	0	100	100
27	Q	215/292 (74%)	209 (97%)	6 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	R	138/149 (93%)	134 (97%)	4 (3%)	0	100	100
29	S	154/205 (75%)	150 (97%)	4 (3%)	0	100	100
30	T	164/206 (80%)	160 (98%)	4 (2%)	0	100	100
31	U	135/153 (88%)	134 (99%)	1 (1%)	0	100	100
32	V	187/216 (87%)	181 (97%)	6 (3%)	0	100	100
33	W	98/148 (66%)	95 (97%)	3 (3%)	0	100	100
34	X	241/256 (94%)	238 (99%)	3 (1%)	0	100	100
35	Y	174/250 (70%)	171 (98%)	3 (2%)	0	100	100
36	Z	118/161 (73%)	116 (98%)	2 (2%)	0	100	100
37	a	78/142 (55%)	76 (97%)	1 (1%)	1 (1%)	12	30
38	b	146/215 (68%)	142 (97%)	4 (3%)	0	100	100
39	c	271/332 (82%)	267 (98%)	4 (2%)	0	100	100
40	d	195/306 (64%)	189 (97%)	6 (3%)	0	100	100
41	e	191/279 (68%)	178 (93%)	13 (7%)	0	100	100
42	f	102/212 (48%)	91 (89%)	11 (11%)	0	100	100
43	g	127/166 (76%)	122 (96%)	5 (4%)	0	100	100
44	h	101/158 (64%)	98 (97%)	3 (3%)	0	100	100
45	i	95/128 (74%)	93 (98%)	2 (2%)	0	100	100
46	j	83/123 (68%)	83 (100%)	0	0	100	100
47	k	76/112 (68%)	71 (93%)	5 (7%)	0	100	100
48	m	27/128 (21%)	18 (67%)	9 (33%)	0	100	100
49	o	78/102 (76%)	78 (100%)	0	0	100	100
50	p	119/206 (58%)	116 (98%)	3 (2%)	0	100	100
51	q	126/222 (57%)	126 (100%)	0	0	100	100
52	r	140/196 (71%)	135 (96%)	5 (4%)	0	100	100
53	s	366/439 (83%)	359 (98%)	7 (2%)	0	100	100
54	u	109/234 (47%)	99 (91%)	10 (9%)	0	100	100
55	v	67/70 (96%)	65 (97%)	2 (3%)	0	100	100
56	w	77/156 (49%)	71 (92%)	6 (8%)	0	100	100
All	All	8462/11756 (72%)	8192 (97%)	269 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
37	a	45	CYS

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	97/164 (59%)	97 (100%)	0	100	100
2	1	49/60 (82%)	49 (100%)	0	100	100
3	2	39/72 (54%)	39 (100%)	0	100	100
4	3	88/166 (53%)	88 (100%)	0	100	100
5	4	36/89 (40%)	36 (100%)	0	100	100
6	5	353/368 (96%)	353 (100%)	0	100	100
7	6	286/332 (86%)	285 (100%)	1 (0%)	92	98
8	7	263/303 (87%)	262 (100%)	1 (0%)	91	97
9	8	70/190 (37%)	70 (100%)	0	100	100
10	9	99/112 (88%)	99 (100%)	0	100	100
13	C	284/328 (87%)	284 (100%)	0	100	100
14	D	192/245 (78%)	192 (100%)	0	100	100
15	E	260/290 (90%)	260 (100%)	0	100	100
16	F	217/262 (83%)	217 (100%)	0	100	100
17	G	221/350 (63%)	221 (100%)	0	100	100
18	H	86/228 (38%)	85 (99%)	1 (1%)	71	88
19	I	139/232 (60%)	139 (100%)	0	100	100
20	J	113/150 (75%)	113 (100%)	0	100	100
21	K	155/156 (99%)	155 (100%)	0	100	100
22	L	98/124 (79%)	98 (100%)	0	100	100
23	M	245/249 (98%)	244 (100%)	1 (0%)	91	97
24	N	156/211 (74%)	156 (100%)	0	100	100
25	O	133/150 (89%)	133 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
26	P	123/155 (79%)	123 (100%)	0	100	100
27	Q	199/256 (78%)	199 (100%)	0	100	100
28	R	118/126 (94%)	118 (100%)	0	100	100
29	S	141/180 (78%)	141 (100%)	0	100	100
30	T	146/176 (83%)	146 (100%)	0	100	100
31	U	124/135 (92%)	124 (100%)	0	100	100
32	V	171/191 (90%)	171 (100%)	0	100	100
33	W	83/119 (70%)	83 (100%)	0	100	100
34	X	219/229 (96%)	218 (100%)	1 (0%)	88	96
35	Y	159/223 (71%)	159 (100%)	0	100	100
36	Z	111/147 (76%)	110 (99%)	1 (1%)	78	92
37	a	78/133 (59%)	78 (100%)	0	100	100
38	b	130/186 (70%)	130 (100%)	0	100	100
39	c	241/288 (84%)	241 (100%)	0	100	100
40	d	190/274 (69%)	190 (100%)	0	100	100
41	e	171/236 (72%)	171 (100%)	0	100	100
42	f	95/188 (50%)	95 (100%)	0	100	100
43	g	119/148 (80%)	119 (100%)	0	100	100
44	h	100/148 (68%)	100 (100%)	0	100	100
45	i	86/110 (78%)	86 (100%)	0	100	100
46	j	68/97 (70%)	68 (100%)	0	100	100
47	k	71/90 (79%)	70 (99%)	1 (1%)	67	86
48	m	27/113 (24%)	27 (100%)	0	100	100
49	o	69/87 (79%)	69 (100%)	0	100	100
50	p	117/181 (65%)	117 (100%)	0	100	100
51	q	110/178 (62%)	110 (100%)	0	100	100
52	r	133/169 (79%)	133 (100%)	0	100	100
53	s	326/381 (86%)	326 (100%)	0	100	100
54	u	105/200 (52%)	105 (100%)	0	100	100
55	v	59/60 (98%)	58 (98%)	1 (2%)	60	84
56	w	73/136 (54%)	72 (99%)	1 (1%)	67	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	7641/10171 (75%)	7632 (100%)	9 (0%)	93 98

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	6	52	ARG
8	7	319	ARG
18	H	72	ARG
23	M	44	ARG
34	X	23	ARG
36	Z	44	LYS
47	k	73	ARG
55	v	41	LYS
56	w	106	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
6	5	160	HIS
6	5	384	GLN
7	6	234	HIS
16	F	103	GLN
29	S	118	ASN
49	o	94	HIS
51	q	130	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
11	A	1368/1559 (87%)	295 (21%)	16 (1%)
12	B	51/69 (73%)	18 (35%)	1 (1%)
All	All	1419/1628 (87%)	313 (22%)	17 (1%)

All (313) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
11	A	1672	C
11	A	1679	U
11	A	1680	A

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Mol	Chain	Res	Type
11	A	1681	G
11	A	1689	C
11	A	1690	C
11	A	1699	C
11	A	1700	U
11	A	1704	U
11	A	1707	C
11	A	1708	A
11	A	1709	G
11	A	1711	C
11	A	1712	A
11	A	1713	A
11	A	1724	A
11	A	1727	A
11	A	1728	U
11	A	1732	C
11	A	1733	C
11	A	1734	C
11	A	1735	A
11	A	1736	A
11	A	1737	A
11	A	1748	G
11	A	1750	G
11	A	1751	A
11	A	1760	G
11	A	1761	A
11	A	1762	A
11	A	1769	C
11	A	1770	G
11	A	1777	A
11	A	1780	U
11	A	1794	A
11	A	1801	A
11	A	1802	A
11	A	1805	A
11	A	1817	C
11	A	1821	A
11	A	1823	A
11	A	1824	U
11	A	1827	C
11	A	1828	A
11	A	1829	A

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Mol	Chain	Res	Type
11	A	1832	A
11	A	1836	A
11	A	1844	A
11	A	1849	C
11	A	1850	U
11	A	1851	G
11	A	1869	A
11	A	1871	A
11	A	1873	A
11	A	1878	U
11	A	1882	A
11	A	1883	G
11	A	1886	G
11	A	1887	A
11	A	1888	G
11	A	1892	A
11	A	1893	A
11	A	1901	C
11	A	1902	C
11	A	1903	C
11	A	1909	A
11	A	1918	G
11	A	1938	A
11	A	1940	A
11	A	1958	G
11	A	1974	A
11	A	1985	G
11	A	1987	G
11	A	1992	C
11	A	1993	A
11	A	1994	A
11	A	1995	A
11	A	2002	G
11	A	2015	G
11	A	2021	U
11	A	2022	G
11	A	2029	A
11	A	2030	U
11	A	2031	A
11	A	2032	G
11	A	2036	C
11	A	2037	U

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Mol	Chain	Res	Type
11	A	2039	A
11	A	2060	A
11	A	2065	A
11	A	2074	A
11	A	2083	U
11	A	2085	A
11	A	2093	U
11	A	2097	A
11	A	2098	G
11	A	2109	A
11	A	2110	A
11	A	2114	C
11	A	2124	A
11	A	2126	U
11	A	2141	U
11	A	2147	G
11	A	2154	A
11	A	2157	U
11	A	2158	U
11	A	2163	A
11	A	2165	C
11	A	2172	A
11	A	2173	G
11	A	2174	G
11	A	2177	U
11	A	2180	A
11	A	2181	A
11	A	2182	G
11	A	2183	C
11	A	2184	A
11	A	2187	C
11	A	2193	U
11	A	2194	U
11	A	2195	A
11	A	2196	A
11	A	2197	G
11	A	2198	A
11	A	2200	A
11	A	2210	C
11	A	2215	C
11	A	2229	A
11	A	2230	A

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Mol	Chain	Res	Type
11	A	2233	U
11	A	2237	A
11	A	2239	A
11	A	2241	A
11	A	2245	A
11	A	2262	C
11	A	2263	C
11	A	2284	C
11	A	2285	U
11	A	2297	A
11	A	2299	U
11	A	2300	G
11	A	2331	C
11	A	2332	C
11	A	2345	G
11	A	2369	A
11	A	2371	U
11	A	2374	A
11	A	2381	A
11	A	2382	A
11	A	2384	A
11	A	2387	U
11	A	2388	A
11	A	2390	A
11	A	2393	C
11	A	2399	A
11	A	2404	U
11	A	2406	A
11	A	2407	U
11	A	2409	A
11	A	2415	C
11	A	2434	A
11	A	2441	C
11	A	2444	A
11	A	2446	A
11	A	2451	A
11	A	2478	G
11	A	2493	C
11	A	2500	A
11	A	2502	C
11	A	2507	A
11	A	2508	C

Continued on next page...

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Mol	Chain	Res	Type
11	A	2511	C
11	A	2520	C
11	A	2521	A
11	A	2527	A
11	A	2531	U
11	A	2540	C
11	A	2618	U
11	A	2635	G
11	A	2636	G
11	A	2639	C
11	A	2645	G
11	A	2654	U
11	A	2656	U
11	A	2660	U
11	A	2683	C
11	A	2686	G
11	A	2693	A
11	A	2696	A
11	A	2706	A
11	A	2708	C
11	A	2709	A
11	A	2719	G
11	A	2722	A
11	A	2732	G
11	A	2739	U
11	A	2745	A
11	A	2747	U
11	A	2750	U
11	A	2756	C
11	A	2804	A
11	A	2810	G
11	A	2814	G
11	A	2819	G
11	A	2829	C
11	A	2831	G
11	A	2832	A
11	A	2833	A
11	A	2837	A
11	A	2842	C
11	A	2846	G
11	A	2847	C
11	A	2853	A

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Mol	Chain	Res	Type
11	A	2854	U
11	A	2857	U
11	A	2859	A
11	A	2864	U
11	A	2865	C
11	A	2880	A
11	A	2890	U
11	A	2891	C
11	A	2892	A
11	A	2906	C
11	A	2913	A
11	A	2917	G
11	A	2918	A
11	A	2919	A
11	A	2922	A
11	A	2926	A
11	A	2928	C
11	A	2932	G
11	A	2947	U
11	A	2948	C
11	A	2952	U
11	A	2956	A
11	A	2963	A
11	A	2970	C
11	A	2977	G
11	A	2981	A
11	A	2982	C
11	A	2984	A
11	A	2985	C
11	A	2986	C
11	A	2995	G
11	A	3000	A
11	A	3005	A
11	A	3016	G
11	A	3018	A
11	A	3022	G
11	A	3029	A
11	A	3041	U
11	A	3042	U
11	A	3043	C
11	A	3053	A
11	A	3054	G

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Mol	Chain	Res	Type
11	A	3056	C
11	A	3060	C
11	A	3063	G
11	A	3069	A
11	A	3073	C
11	A	3089	A
11	A	3090	G
11	A	3091	G
11	A	3093	C
11	A	3096	U
11	A	3097	U
11	A	3100	U
11	A	3102	U
11	A	3108	U
11	A	3113	A
11	A	3122	U
11	A	3129	A
11	A	3134	C
11	A	3141	A
11	A	3150	U
11	A	3155	C
11	A	3157	C
11	A	3158	A
11	A	3162	C
11	A	3168	C
11	A	3169	C
11	A	3172	C
11	A	3173	G
11	A	3180	A
11	A	3189	C
11	A	3190	A
11	A	3196	G
11	A	3197	U
11	A	3201	A
11	A	3202	U
11	A	3207	A
11	A	3208	C
11	A	3209	A
11	A	3217	A
11	A	3218	A
12	B	1607	U
12	B	1608	G

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Mol	Chain	Res	Type
12	B	1609	U
12	B	1611	G
12	B	1614	U
12	B	1615	A
12	B	1625	A
12	B	1631	C
12	B	1632	U
12	B	1633	U
12	B	1640	A
12	B	1641	G
12	B	1644	G
12	B	1645	A
12	B	1649	C
12	B	1650	A
12	B	1651	A
12	B	1669	G

All (17) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
11	A	1708	A
11	A	1823	A
11	A	1986	A
11	A	1994	A
11	A	2031	A
11	A	2182	G
11	A	2186	C
11	A	2403	G
11	A	2507	A
11	A	2530	A
11	A	2635	G
11	A	2890	U
11	A	2891	C
11	A	2947	U
11	A	3092	U
11	A	3196	G
12	B	1607	U

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 63 ligands modelled in this entry, 61 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
59	GTP	A	3359	-	26,34,34	1.05	1 (3%)	33,54,54	2.10	4 (12%)
59	GTP	A	3358	-	26,34,34	1.04	1 (3%)	33,54,54	2.12	5 (15%)

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
59	GTP	A	3359	-	-	0/18/38/38	0/3/3/3
59	GTP	A	3358	-	-	0/18/38/38	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
59	A	3359	GTP	C6-N1	3.96	1.39	1.33
59	A	3358	GTP	C6-N1	3.94	1.39	1.33

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
59	A	3358	GTP	C5-C6-N1	-8.86	111.31	123.43
59	A	3359	GTP	C5-C6-N1	-8.77	111.43	123.43
59	A	3358	GTP	C6-N1-C2	5.96	125.40	115.93
59	A	3359	GTP	C6-N1-C2	5.78	125.12	115.93
59	A	3358	GTP	C2-N3-C4	-2.83	112.12	115.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
59	A	3359	GTP	C2-N3-C4	-2.80	112.16	115.36
59	A	3358	GTP	N3-C2-N1	-2.76	123.55	127.22
59	A	3359	GTP	N3-C2-N1	-2.62	123.72	127.22
59	A	3358	GTP	O4'-C1'-C2'	-2.27	103.61	106.93

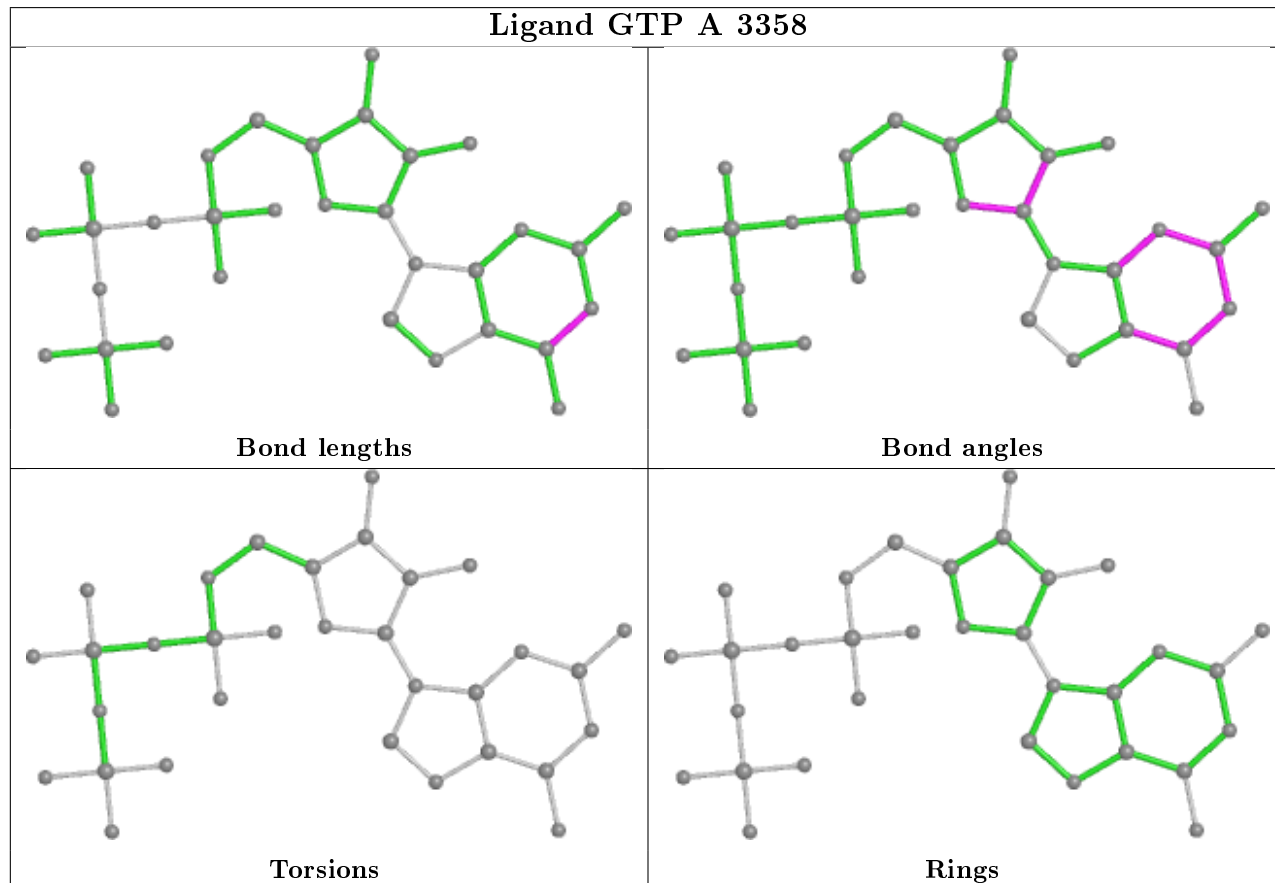
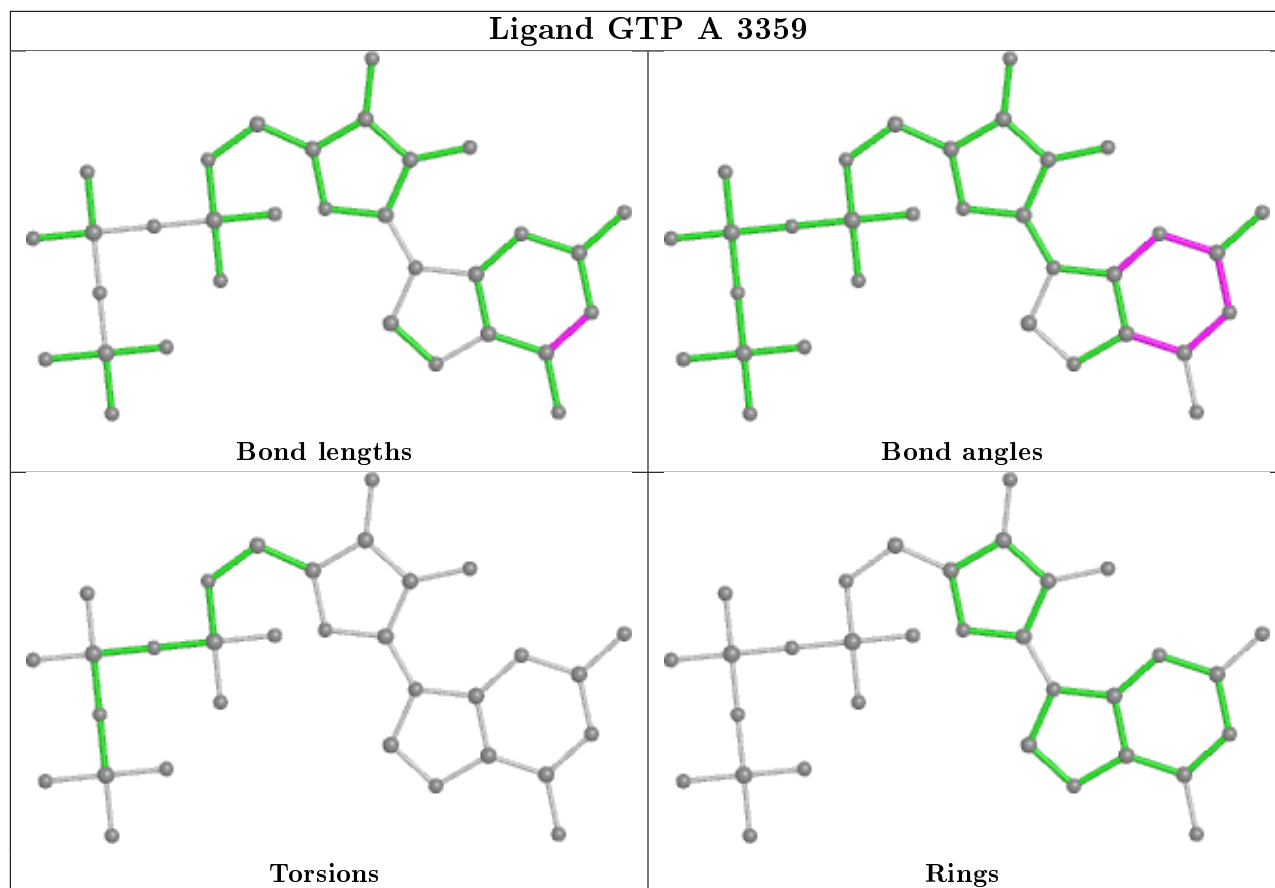
There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

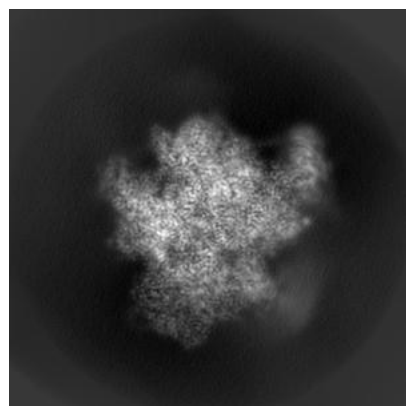
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-12868. These allow visual inspection of the internal detail of the map and identification of artifacts.

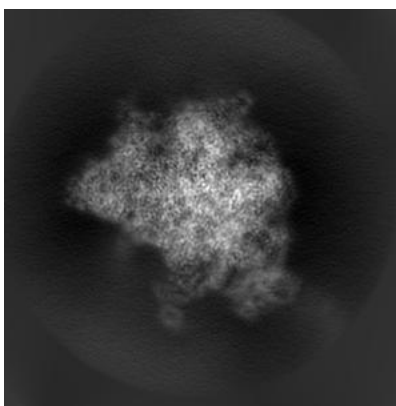
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

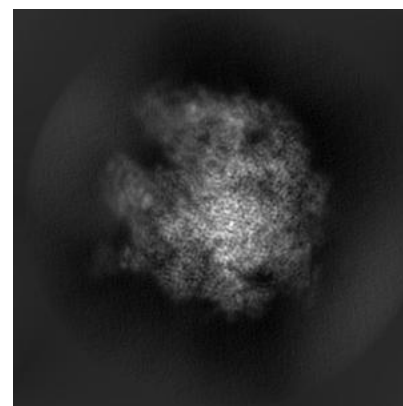
6.1.1 Primary map



X

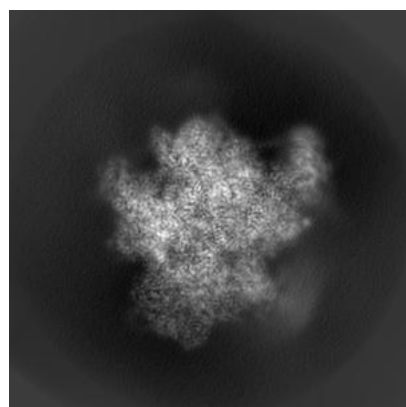


Y

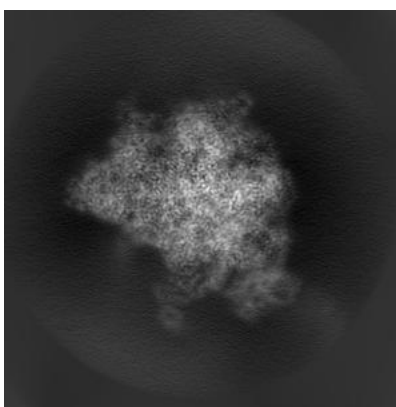


Z

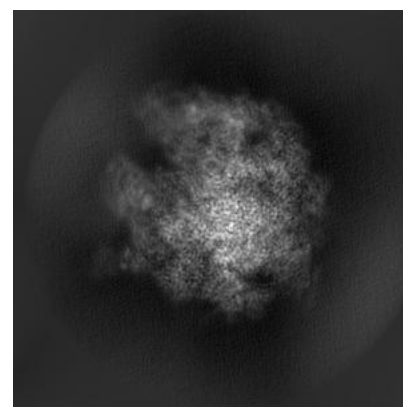
6.1.2 Raw map



X



Y

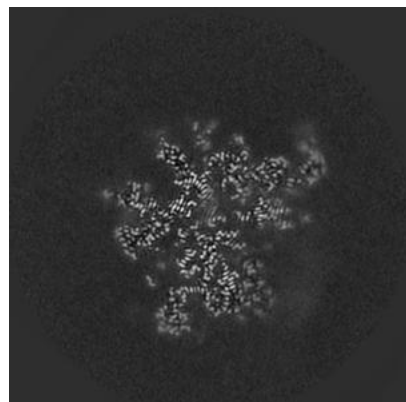


Z

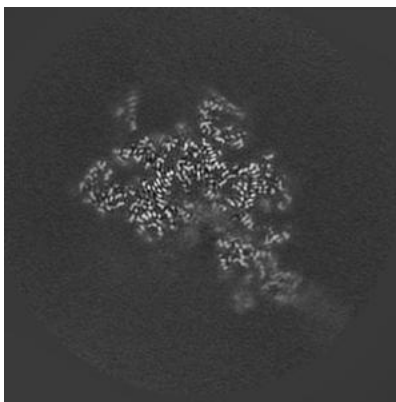
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

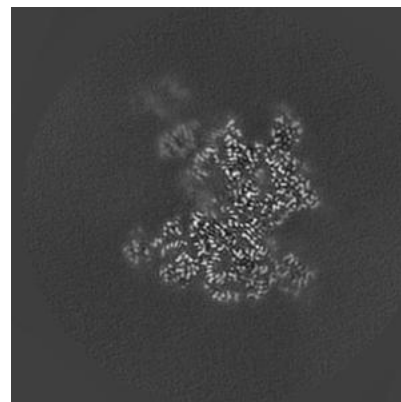
6.2.1 Primary map



X Index: 175

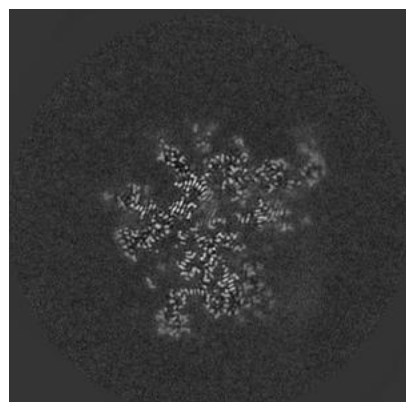


Y Index: 175

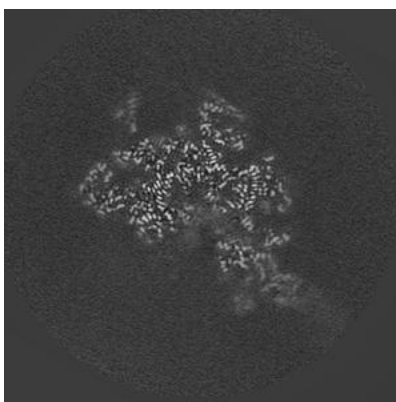


Z Index: 175

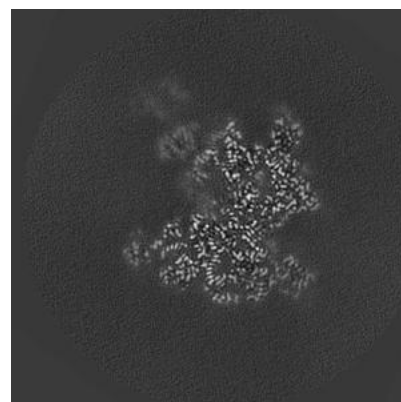
6.2.2 Raw map



X Index: 175



Y Index: 175

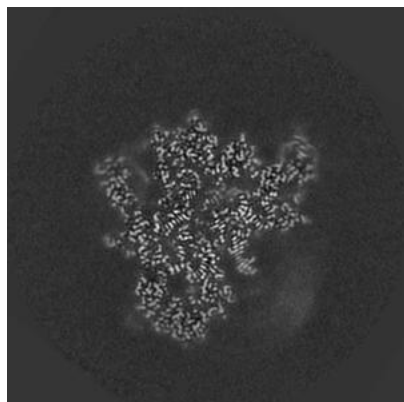


Z Index: 175

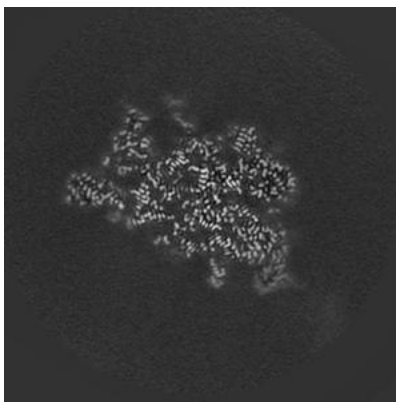
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

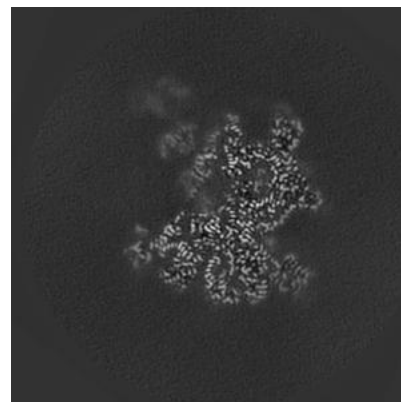
6.3.1 Primary map



X Index: 188

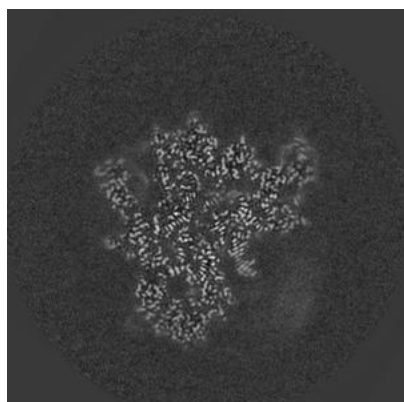


Y Index: 159

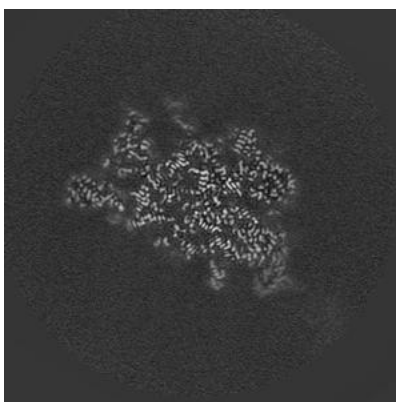


Z Index: 177

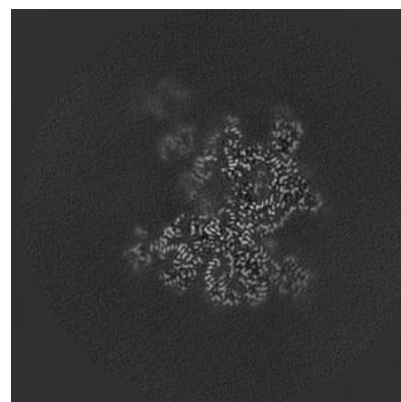
6.3.2 Raw map



X Index: 188



Y Index: 159

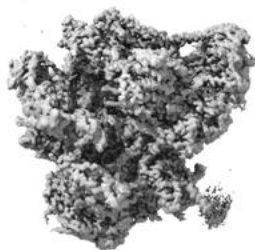


Z Index: 177

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

6.4 Orthogonal surface views [i](#)

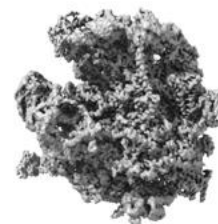
6.4.1 Primary map



X



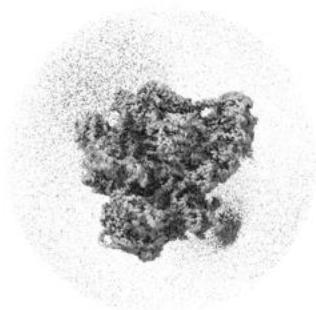
Y



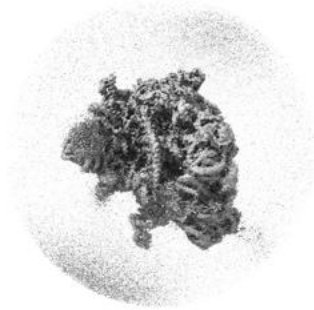
Z

The images above show the 3D surface view of the map at the recommended contour level 0.0046. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

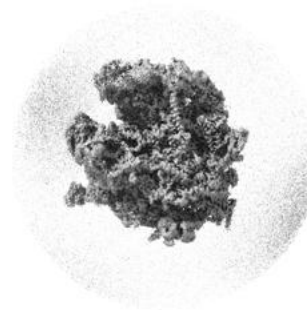
6.4.2 Raw map



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.

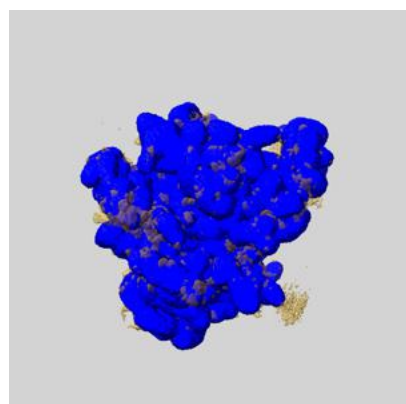
6.5 Mask visualisation [i](#)

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

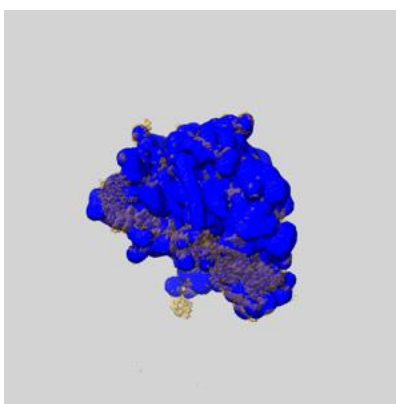
A mask typically either:

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

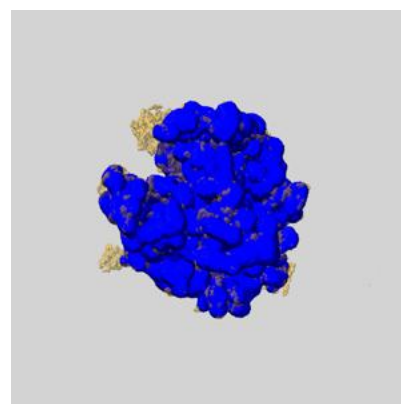
6.5.1 emd_12868_msk_1.map [i](#)



X



Y

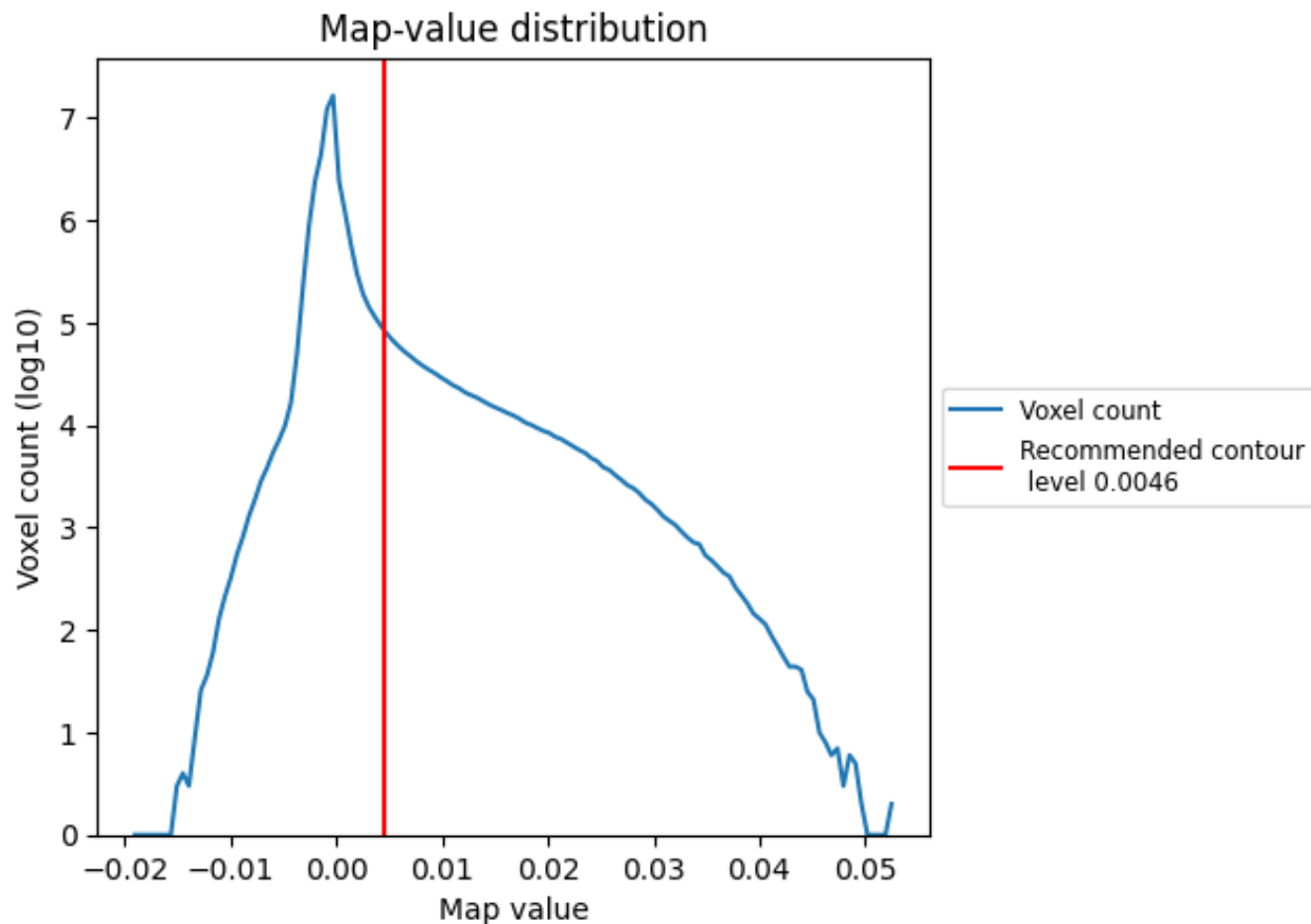


Z

7 Map analysis [i](#)

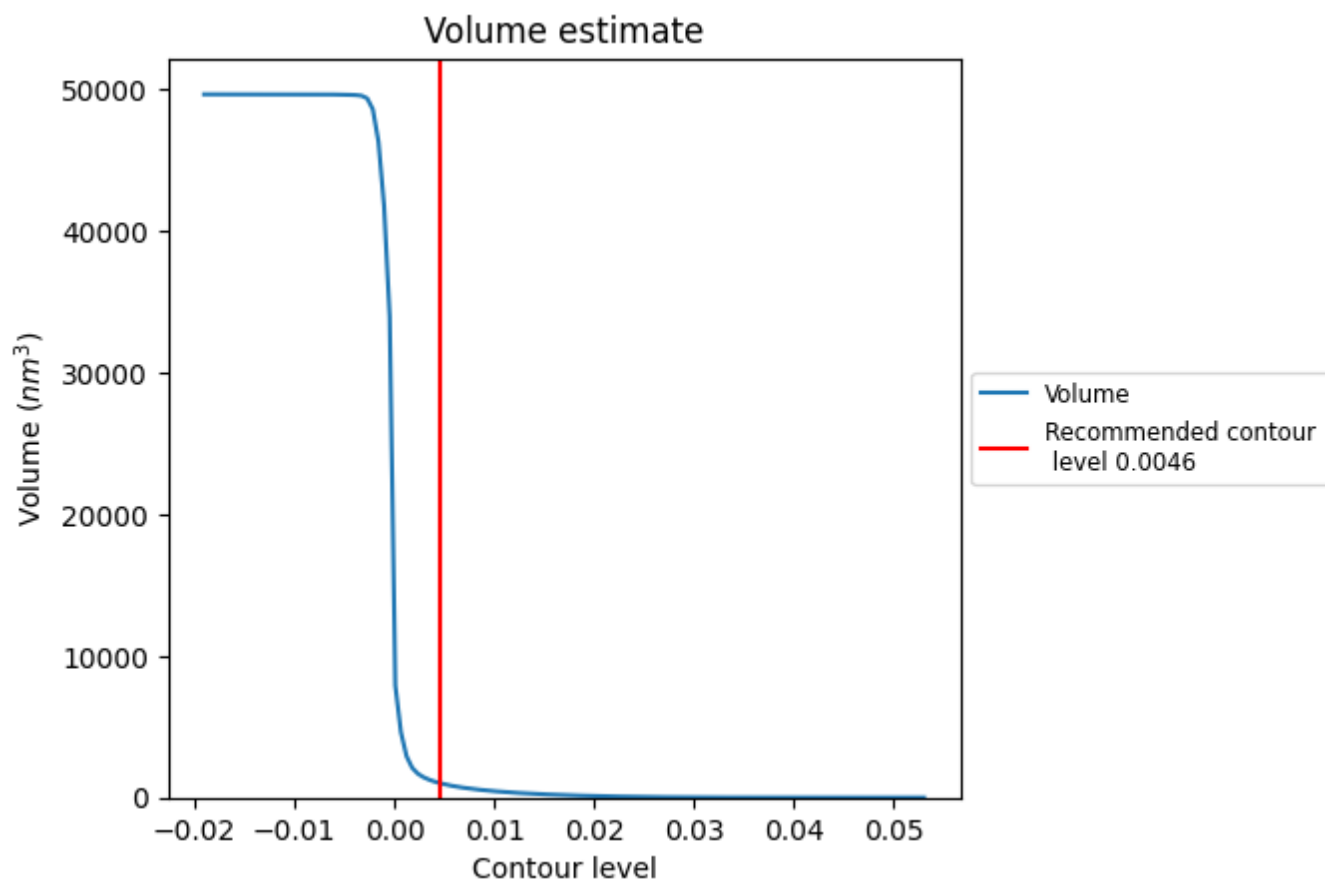
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

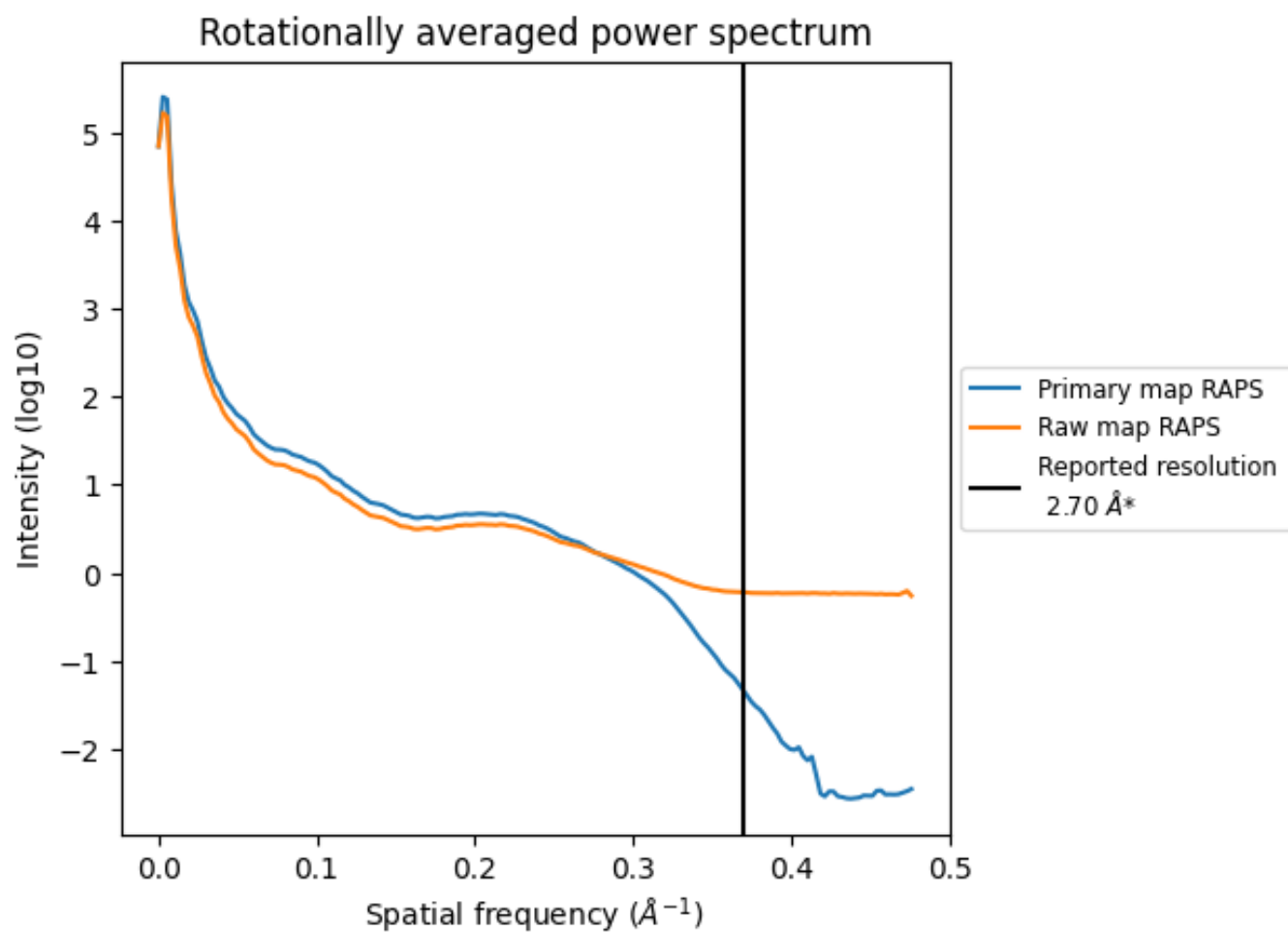
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1010 nm³; this corresponds to an approximate mass of 912 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum [\(i\)](#)

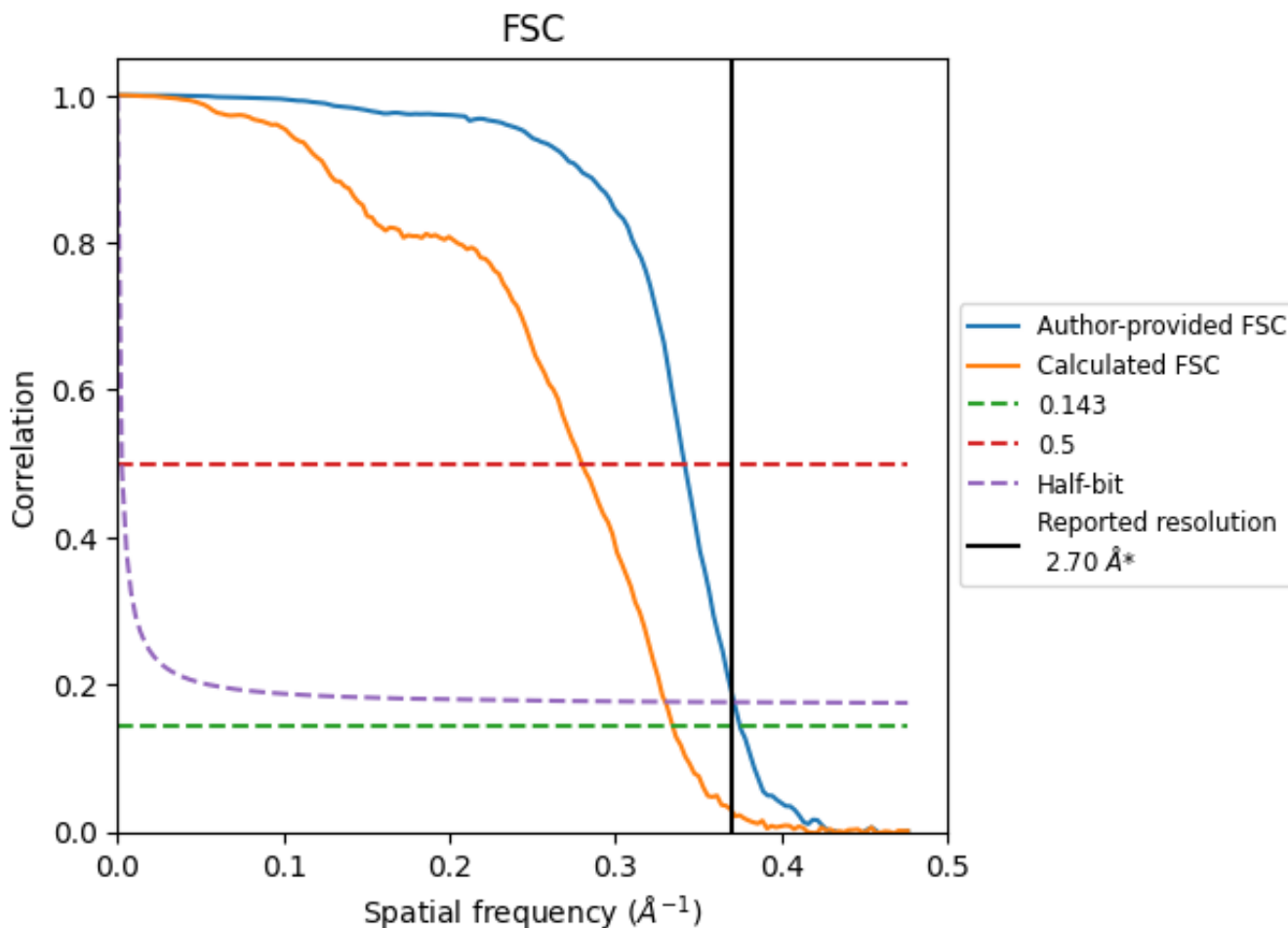


*Reported resolution corresponds to spatial frequency of 0.370 Å⁻¹

8 Fourier-Shell correlation [\(i\)](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [\(i\)](#)



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

8.2 Resolution estimates [i](#)

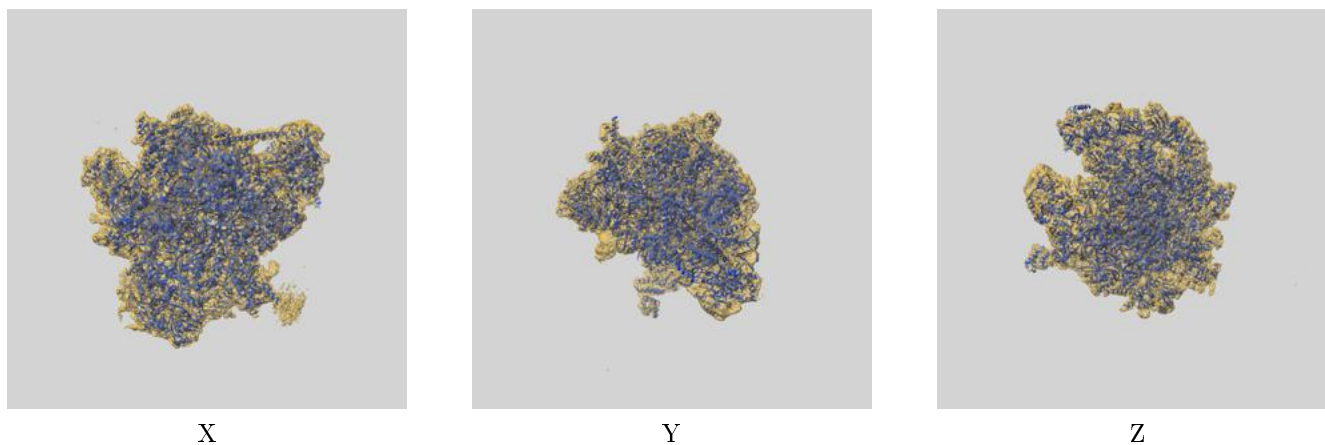
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.70	-	-
Author-provided FSC curve	2.67	2.93	2.69
Calculated*	2.99	3.57	3.03

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.99 differs from the reported value 2.7 by more than 10 %

9 Map-model fit [i](#)

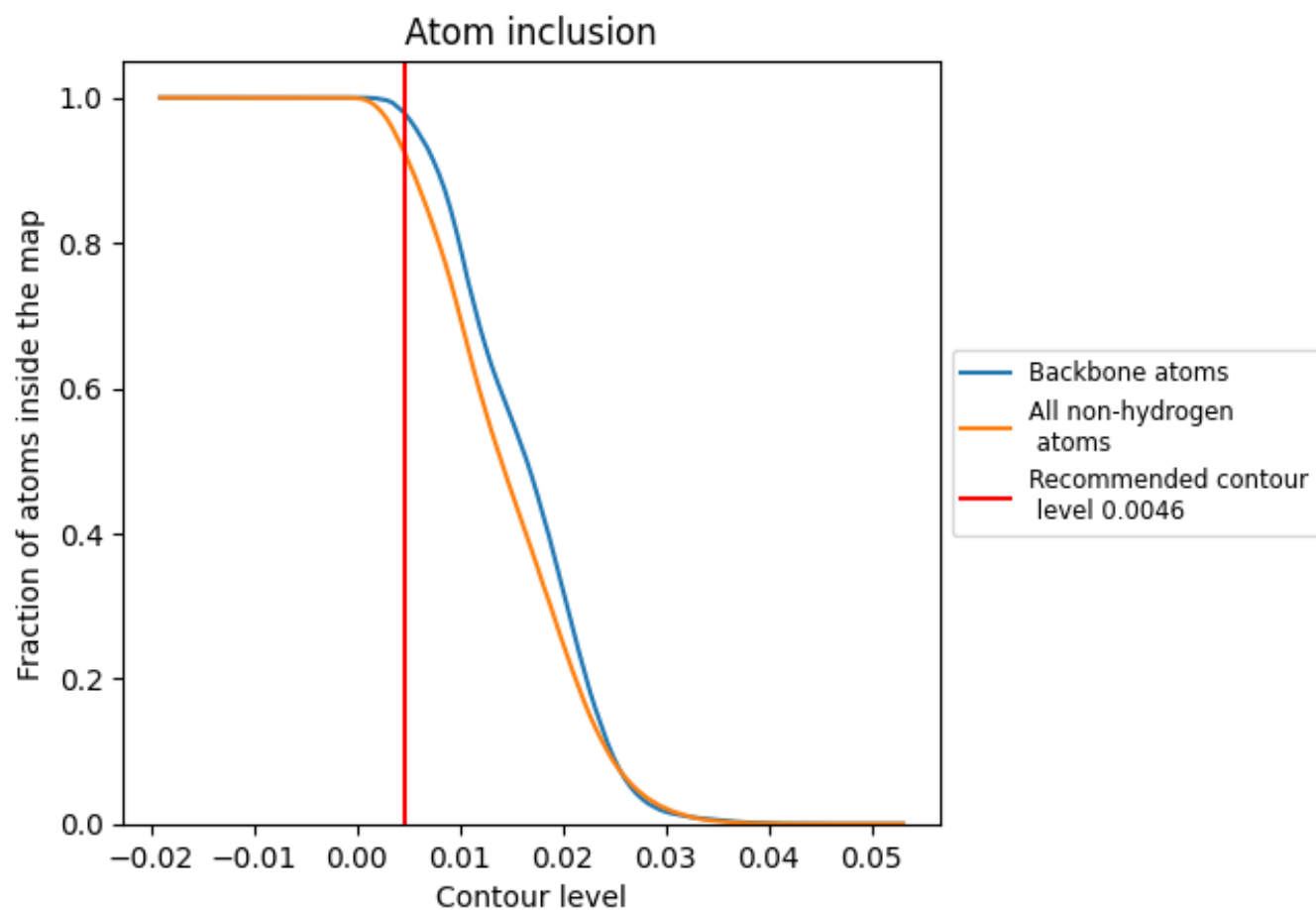
This section contains information regarding the fit between EMDB map EMD-12868 and PDB model 7OF3. Per-residue inclusion information can be found in section 3 on page 15.

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.0046 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 93% of all non-hydrogen atoms, are inside the map.