



Full wwPDB EM Validation Report ⓘ

Jun 23, 2021 – 06:28 AM BST

PDB ID : 7OF4
EMDB ID : EMD-12869
Title : Structure of mature human mitochondrial ribosome large subunit in complex with GTPBP6 (PTC conformation 1).
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:

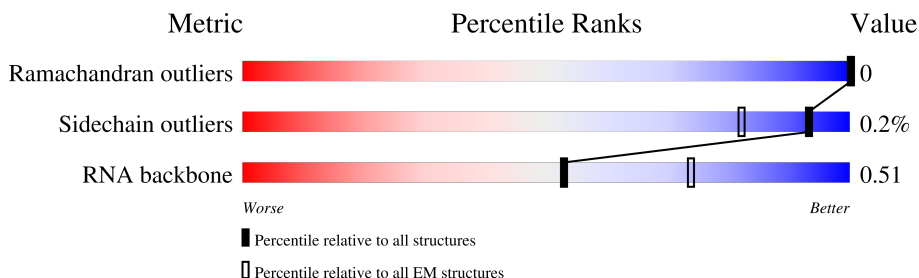
EMDB validation analysis : 0.0.0.dev75
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) :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


















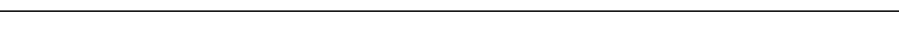
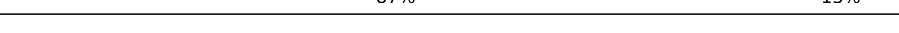


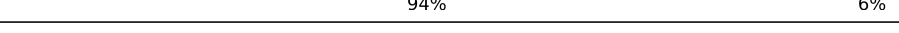





Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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% 43%
2	1	65	80% 20%
3	2	92	49% 51%
4	3	188	51% 49%
5	4	103	36% 64%
6	5	423	92% 7%
7	6	380	85% 15%
8	7	338	84% 15%
















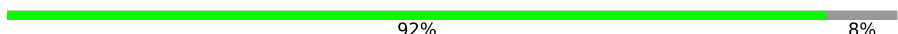




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Mol	Chain	Length	Quality of chain
9	8	206	
10	9	137	
11	A	1559	
12	B	69	
13	C	516	
14	D	305	
15	E	348	
16	F	311	
17	H	267	
18	I	261	
19	J	192	
20	K	178	
21	L	145	
22	M	296	
23	N	251	
24	O	175	
25	P	180	
26	Q	292	
27	R	149	
28	S	205	
29	T	206	
30	U	153	
31	V	216	
32	W	148	
33	X	256	

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Mol	Chain	Length	Quality of chain
34	Y	250	 70% 30%
35	Z	161	 74% 25%
36	a	142	 58% 42%
37	b	215	 69% 31%
38	c	332	 83% 17%
39	d	306	 68% 32%
40	e	279	 39% 71% 29%
41	f	212	 7% 50% 50%
42	g	166	 78% 22%
43	h	158	 66% 34%
44	i	128	 76% 24%
45	j	123	 67% 32%
46	k	112	 71% 29%
47	l	138	 17% 83%
48	m	128	 19% 34% 65%
49	o	102	 92% 8%
50	p	206	 62% 38%
51	q	222	 54% 46%
52	r	196	 80% 20%
53	s	439	 84% 16%

2 Entry composition

There are 56 unique types of molecules in this entry. The entry contains 100322 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	1463	Total	C	N	O	P	0	0
			31075	13943	5609	10060	1463		

- Molecule 12 is a RNA chain called mitochondrial tRNA^{Val}.

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 Putative GTP-binding protein 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	C	422	Total	C	N	O	S	0	0
			3313	2097	607	596	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	D	236	Total	C	N	O	S	0	0
			1842	1145	373	315	9		

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

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

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

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

- Molecule 17 is a protein called 39S ribosomal protein L9, mitochondrial.

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

- Molecule 18 is a protein called 39S ribosomal protein L10, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	I	158	Total	C	N	O	S	0	0
			1283	828	235	210	10		

- Molecule 19 is a protein called 39S ribosomal protein L11, mitochondrial.

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

- Molecule 20 is a protein called 39S ribosomal protein L13, mitochondrial.

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

- Molecule 21 is a protein called 39S ribosomal protein L14, mitochondrial.

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

- Molecule 22 is a protein called 39S ribosomal protein L15, mitochondrial.

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

- Molecule 23 is a protein called 39S ribosomal protein L16, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	N	205	Total	C	N	O	S	0	0
			1654	1056	308	280	10		

- Molecule 24 is a protein called 39S ribosomal protein L17, mitochondrial.

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

- Molecule 25 is a protein called 39S ribosomal protein L18, mitochondrial.

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

- Molecule 26 is a protein called 39S ribosomal protein L19, mitochondrial.

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

- Molecule 27 is a protein called 39S ribosomal protein L20, mitochondrial.

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

- Molecule 28 is a protein called 39S ribosomal protein L21, mitochondrial.

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

- Molecule 29 is a protein called 39S ribosomal protein L22, mitochondrial.

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

- Molecule 30 is a protein called 39S ribosomal protein L23, mitochondrial.

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

- Molecule 31 is a protein called 39S ribosomal protein L24, mitochondrial.

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

- Molecule 32 is a protein called 39S ribosomal protein L27, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	W	109	859	552	162	142	3	0	0

- Molecule 33 is a protein called 39S ribosomal protein L28, mitochondrial.

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

- Molecule 34 is a protein called 39S ribosomal protein L47, mitochondrial.

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

- Molecule 35 is a protein called 39S ribosomal protein L30, mitochondrial.

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

- Molecule 36 is a protein called 39S ribosomal protein L42, mitochondrial.

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

- Molecule 37 is a protein called 39S ribosomal protein L43, mitochondrial.

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

- Molecule 38 is a protein called 39S ribosomal protein L44, mitochondrial.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
39	d	208	1731	1121	295	306	9	0	0

- Molecule 40 is a protein called 39S ribosomal protein L46, mitochondrial.

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

- Molecule 41 is a protein called 39S ribosomal protein L48, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
41	f	105	834	535	136	160	3	0	0

- Molecule 42 is a protein called 39S ribosomal protein L49, mitochondrial.

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

- Molecule 43 is a protein called 39S ribosomal protein L50, mitochondrial.

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

- Molecule 44 is a protein called 39S ribosomal protein L51, mitochondrial.

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

- Molecule 45 is a protein called 39S ribosomal protein L52, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
45	j	84	679	420	132	125	2	0	0

- Molecule 46 is a protein called 39S ribosomal protein L53, mitochondrial.

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

- Molecule 47 is a protein called 39S ribosomal protein L54, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
47	l	23	221	137	52	32	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
48	m	45	372	232	76	62	2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
49	o	94	Total	C	N	O	S	0	0
			797	501	165	128	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	120	Total	C	N	O	S	0	0
			1011	633	194	179	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
52	r	157	Total	C	N	O	S	0	0
			1287	817	247	215	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		

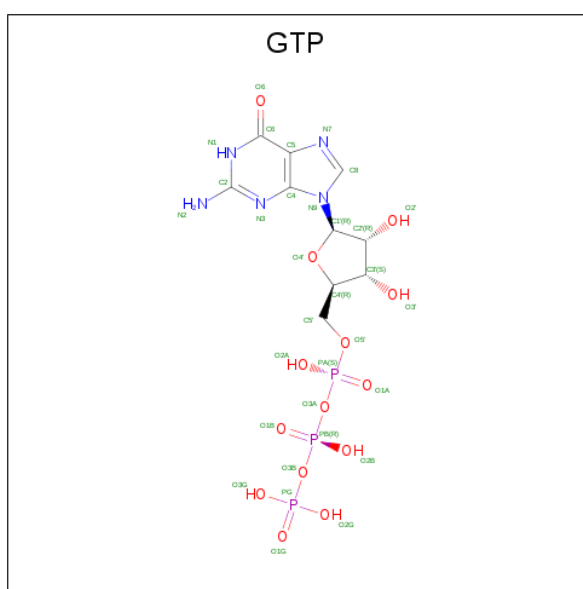
- Molecule 54 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
54	0	1	Total	Zn	0
			1	1	
54	4	1	Total	Zn	0
			1	1	
54	r	1	Total	Zn	0
			1	1	

- Molecule 55 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
55	A	86	Total Mg 86 86	0
55	C	1	Total Mg 1 1	0
55	E	1	Total Mg 1 1	0
55	g	1	Total Mg 1 1	0

- Molecule 56 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



Mol	Chain	Residues	Atoms				AltConf	
			Total	C	N	O		P
56	A	1	Total 64	C 20	N 10	O 28	P 6	0
56	A	1	Total 64	C 20	N 10	O 28	P 6	0
56	C	1	Total 32	C 10	N 5	O 14	P 3	0

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 LEU LEU ARG LEU LYS LYS LEU PRO PRO GLN SER ARG ARG PRO GLY PHE PRO PRO PRO TRP GLY PRO ALA ALA VAL VAL GLN GLY PRO PRO 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 K14 L65

- Molecule 3: 39S ribosomal protein L34, mitochondrial

Chain 2:  49% 51%

MET ALA VAL LEU ALA GLY SER LEU LEU LEU PRO THR ARG SER SER 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 ALA ARG LYS A48 H92

- Molecule 4: 39S ribosomal protein L35, mitochondrial

Chain 3:  51% 49%

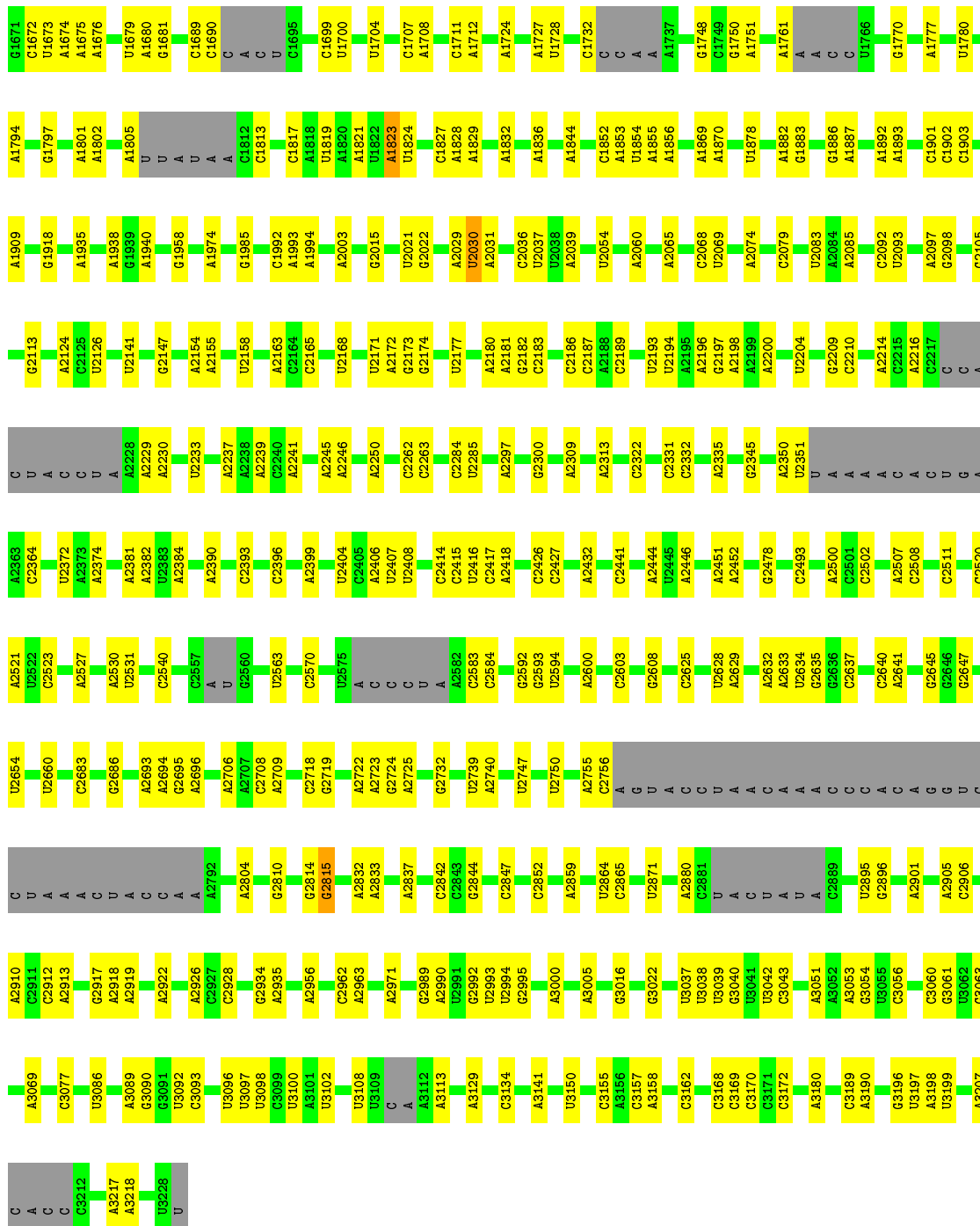
MET ALA ALA SER ARG PHE ALA GLY ALA CYS VAL HIS THR SER VAL ILE LEU ASN ARG MET ALA PRO ASN VAL LEU LEU PRO SER VAL THR TYR LYS PRO CYS VAL SER ASN ALA SER ILE LEU SER LEU ALA THR SER LEU LEU THR ARG VAL L94 V188

- Molecule 5: 39S ribosomal protein L36, mitochondrial

Chain 4:  36% 64%

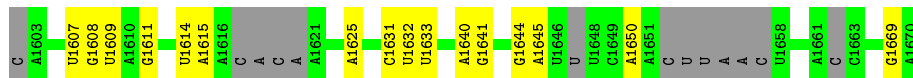
• Molecule 11: 16S ribosomal RNA

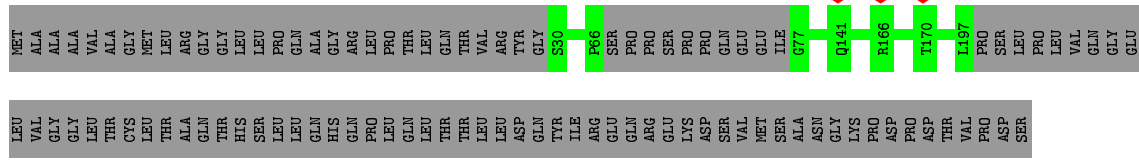
Chain A: 



• Molecule 12: mitochondrial tRNAVal

Chain B: 





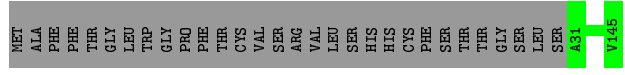
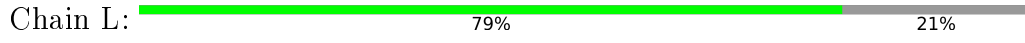
- Molecule 19: 39S ribosomal protein L11, mitochondrial



- Molecule 20: 39S ribosomal protein L13, mitochondrial



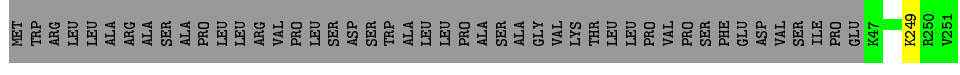
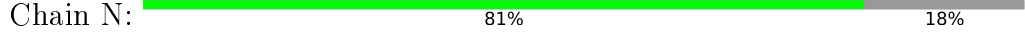
- Molecule 21: 39S ribosomal protein L14, mitochondrial



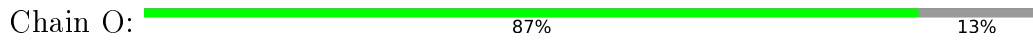
- Molecule 22: 39S ribosomal protein L15, mitochondrial

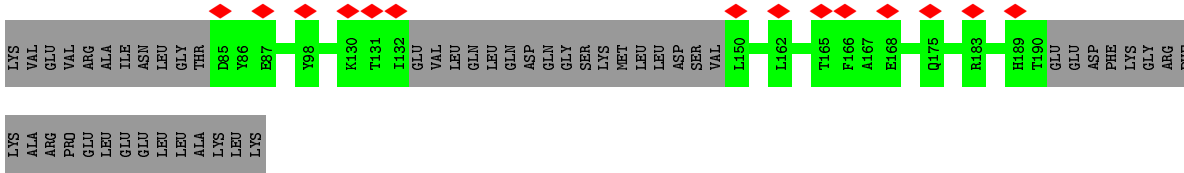


- Molecule 23: 39S ribosomal protein L16, mitochondrial

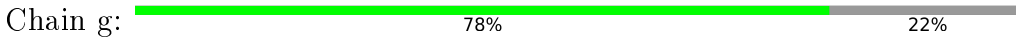


- Molecule 24: 39S ribosomal protein L17, mitochondrial





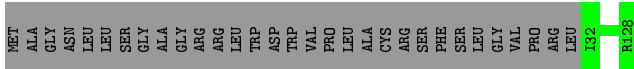
- Molecule 42: 39S ribosomal protein L49, mitochondrial



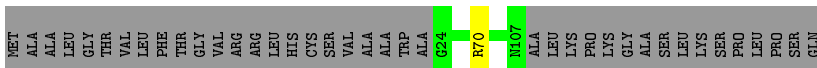
- Molecule 43: 39S ribosomal protein L50, mitochondrial



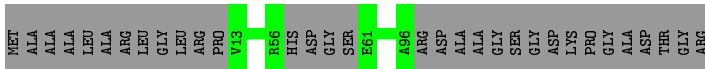
- Molecule 44: 39S ribosomal protein L51, mitochondrial



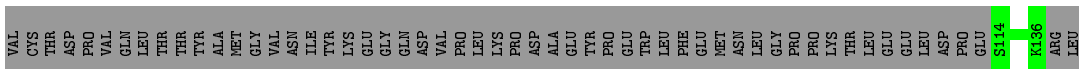
- Molecule 45: 39S ribosomal protein L52, mitochondrial



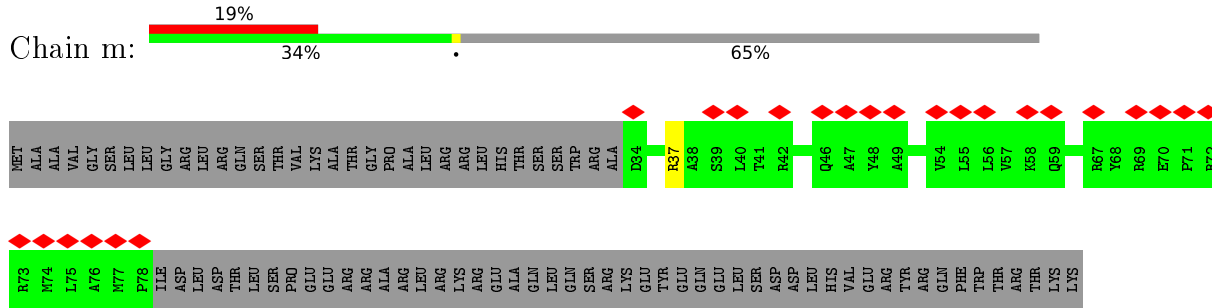
- Molecule 46: 39S ribosomal protein L53, mitochondrial



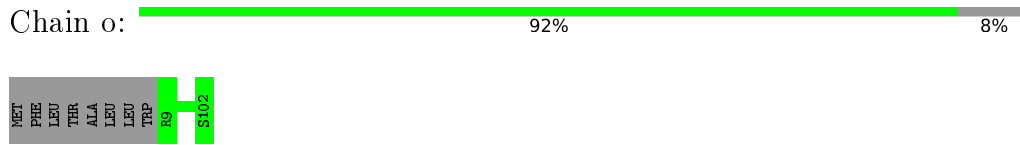
- Molecule 47: 39S ribosomal protein L54, mitochondrial



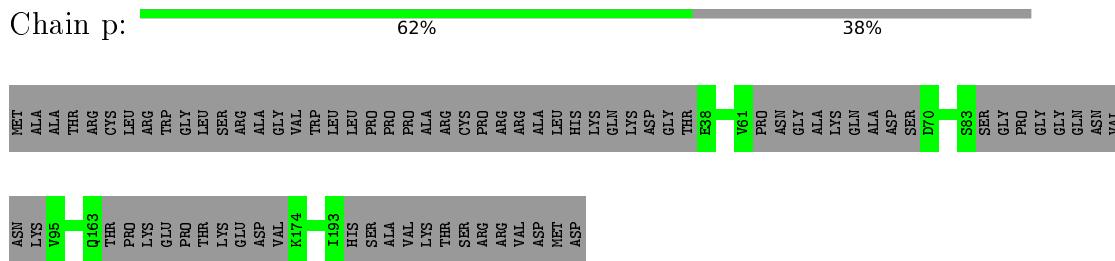
- Molecule 48: 39S ribosomal protein L55, mitochondrial



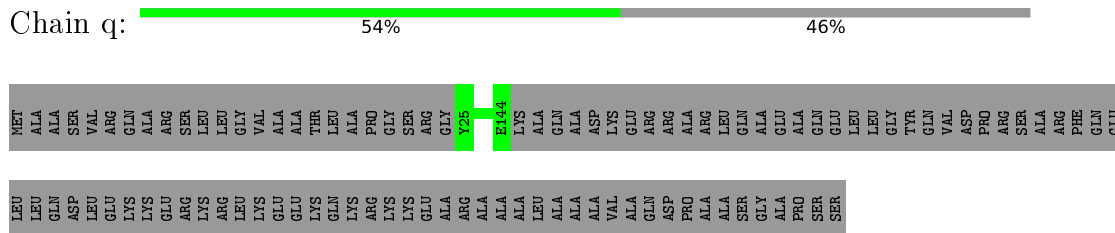
- Molecule 49: Ribosomal protein 63, mitochondrial



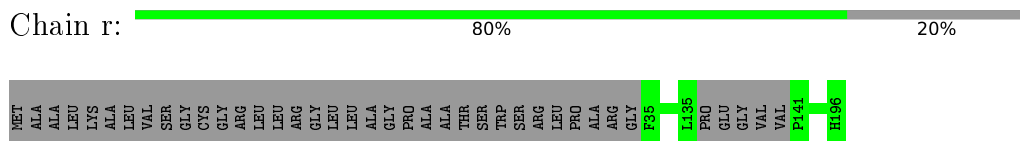
- Molecule 50: Peptidyl-tRNA hydrolase ICT1, mitochondrial



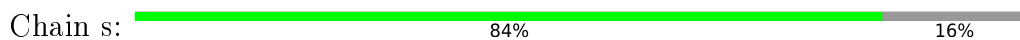
- Molecule 51: Growth arrest and DNA damage-inducible proteins-interacting protein 1



- Molecule 52: 39S ribosomal protein S18a, mitochondrial



- Molecule 53: 39S ribosomal protein S30, mitochondrial



MET ALA ALA ALA ARG CYS TRP ARG ARG PRO LEU LEU ARG GLY PRO ARG ARG LEU LEU SER LEU LEU HIS THR ALA ALA ASN ALA ALA ALA THR ALA THR THR THR THR CYS GLN ASP VAL ALA ALA THR PRO V41 P119 PRO PRO ALA GLU PRO GLU PRO GLU PRO GLU PRO GLU PRO GLU PRO GLU PRO GLU ALA

LEU ASP LEU A140 K430 GLU GLU LYS SER GLN LEU LEU GLU ASN

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	137890	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 ($e^-/\text{\AA}^2$)	36	Depositor
Minimum defocus (nm)	300	Depositor
Maximum defocus (nm)	2800	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.053	Depositor
Minimum map value	-0.014	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.004	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

5.1 Standard geometry

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

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	0.30	0/895	0.55	0/1201
2	1	0.28	0/438	0.57	0/583
3	2	0.29	0/373	0.56	0/496
4	3	0.32	0/852	0.52	0/1136
5	4	0.33	0/341	0.58	0/451
6	5	0.29	0/3294	0.49	0/4488
7	6	0.29	0/2809	0.52	0/3818
8	7	0.29	0/2391	0.47	0/3234
9	8	0.24	0/665	0.50	0/894
10	9	0.31	0/972	0.48	0/1306
11	A	0.49	0/34684	0.76	5/53971 (0.0%)
12	B	0.24	0/1328	0.74	0/2056
13	C	0.26	0/3375	0.51	0/4571
14	D	0.30	0/1879	0.57	0/2527
15	E	0.31	0/2474	0.47	0/3355
16	F	0.31	0/2071	0.52	0/2817
17	H	0.27	0/798	0.54	0/1073
18	I	0.26	0/1308	0.51	0/1761
19	J	0.25	0/1077	0.51	0/1452
20	K	0.30	0/1495	0.47	0/2029
21	L	0.29	0/904	0.52	0/1218
22	M	0.31	0/2359	0.53	0/3185
23	N	0.30	0/1697	0.53	0/2281
24	O	0.29	0/1269	0.56	0/1708
25	P	0.28	0/1173	0.54	0/1588
26	Q	0.29	0/1846	0.50	0/2487
27	R	0.31	0/1174	0.54	0/1572
28	S	0.30	0/1276	0.53	0/1729
29	T	0.32	0/1402	0.50	0/1886
30	U	0.30	0/1183	0.54	0/1600
31	V	0.28	0/1609	0.51	0/2179
32	W	0.34	0/881	0.49	0/1188

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	X	0.29	0/2090	0.46	0/2825
34	Y	0.29	0/1552	0.50	0/2079
35	Z	0.28	0/1003	0.47	0/1354
36	a	0.30	0/709	0.49	0/963
37	b	0.30	0/1202	0.56	0/1626
38	c	0.29	0/2264	0.47	0/3059
39	d	0.28	0/1781	0.49	0/2410
40	e	0.24	0/1633	0.49	0/2204
41	f	0.27	0/850	0.46	0/1150
42	g	0.31	0/1102	0.50	0/1503
43	h	0.26	0/884	0.47	0/1203
44	i	0.31	0/849	0.53	0/1135
45	j	0.28	0/693	0.51	0/933
46	k	0.24	0/635	0.50	0/855
47	l	0.23	0/226	0.58	0/299
48	m	0.23	0/379	0.63	0/510
49	o	0.30	0/818	0.58	0/1097
50	p	0.26	0/1071	0.53	0/1433
51	q	0.27	0/1042	0.52	0/1413
52	r	0.29	0/1325	0.52	0/1793
53	s	0.31	0/3114	0.51	0/4225
All	All	0.37	0/105514	0.62	5/149909 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	1852	C	C2-N1-C1'	6.13	125.54	118.80
11	A	2030	U	C2-N1-C1'	5.89	124.77	117.70
11	A	2523	C	C2-N1-C1'	5.89	125.28	118.80
11	A	2523	C	N1-C2-O2	5.24	122.04	118.90
11	A	1823	A	P-O3'-C3'	5.15	125.88	119.70

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%)	49 (98%)	1 (2%)	0	100	100
3	2	43/92 (47%)	42 (98%)	1 (2%)	0	100	100
4	3	93/188 (50%)	89 (96%)	4 (4%)	0	100	100
5	4	35/103 (34%)	34 (97%)	1 (3%)	0	100	100
6	5	390/423 (92%)	380 (97%)	10 (3%)	0	100	100
7	6	316/380 (83%)	304 (96%)	12 (4%)	0	100	100
8	7	285/338 (84%)	268 (94%)	17 (6%)	0	100	100
9	8	75/206 (36%)	71 (95%)	4 (5%)	0	100	100
10	9	113/137 (82%)	113 (100%)	0	0	100	100
13	C	420/516 (81%)	405 (96%)	15 (4%)	0	100	100
14	D	234/305 (77%)	227 (97%)	7 (3%)	0	100	100
15	E	303/348 (87%)	290 (96%)	13 (4%)	0	100	100
16	F	248/311 (80%)	241 (97%)	7 (3%)	0	100	100
17	H	93/267 (35%)	90 (97%)	3 (3%)	0	100	100
18	I	154/261 (59%)	141 (92%)	13 (8%)	0	100	100
19	J	138/192 (72%)	123 (89%)	15 (11%)	0	100	100
20	K	175/178 (98%)	170 (97%)	5 (3%)	0	100	100
21	L	113/145 (78%)	109 (96%)	4 (4%)	0	100	100
22	M	285/296 (96%)	279 (98%)	6 (2%)	0	100	100
23	N	203/251 (81%)	200 (98%)	3 (2%)	0	100	100
24	O	150/175 (86%)	149 (99%)	1 (1%)	0	100	100
25	P	139/180 (77%)	135 (97%)	4 (3%)	0	100	100
26	Q	215/292 (74%)	209 (97%)	6 (3%)	0	100	100
27	R	138/149 (93%)	135 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	S	154/205 (75%)	148 (96%)	6 (4%)	0	100	100
29	T	164/206 (80%)	160 (98%)	4 (2%)	0	100	100
30	U	135/153 (88%)	132 (98%)	3 (2%)	0	100	100
31	V	187/216 (87%)	180 (96%)	7 (4%)	0	100	100
32	W	107/148 (72%)	106 (99%)	1 (1%)	0	100	100
33	X	241/256 (94%)	238 (99%)	3 (1%)	0	100	100
34	Y	174/250 (70%)	171 (98%)	3 (2%)	0	100	100
35	Z	118/161 (73%)	116 (98%)	2 (2%)	0	100	100
36	a	78/142 (55%)	77 (99%)	1 (1%)	0	100	100
37	b	146/215 (68%)	143 (98%)	3 (2%)	0	100	100
38	c	271/332 (82%)	267 (98%)	4 (2%)	0	100	100
39	d	198/306 (65%)	190 (96%)	8 (4%)	0	100	100
40	e	191/279 (68%)	179 (94%)	12 (6%)	0	100	100
41	f	99/212 (47%)	89 (90%)	10 (10%)	0	100	100
42	g	127/166 (76%)	124 (98%)	3 (2%)	0	100	100
43	h	101/158 (64%)	96 (95%)	5 (5%)	0	100	100
44	i	95/128 (74%)	94 (99%)	1 (1%)	0	100	100
45	j	82/123 (67%)	80 (98%)	2 (2%)	0	100	100
46	k	76/112 (68%)	75 (99%)	1 (1%)	0	100	100
47	l	21/138 (15%)	21 (100%)	0	0	100	100
48	m	43/128 (34%)	36 (84%)	7 (16%)	0	100	100
49	o	92/102 (90%)	89 (97%)	3 (3%)	0	100	100
50	p	119/206 (58%)	116 (98%)	3 (2%)	0	100	100
51	q	118/222 (53%)	117 (99%)	1 (1%)	0	100	100
52	r	153/196 (78%)	149 (97%)	4 (3%)	0	100	100
53	s	366/439 (83%)	359 (98%)	7 (2%)	0	100	100
All	All	8170/11185 (73%)	7911 (97%)	259 (3%)	0	100	100

There are no Ramachandran outliers to report.

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%)	352 (100%)	1 (0%)	92	98
7	6	286/332 (86%)	285 (100%)	1 (0%)	92	98
8	7	263/303 (87%)	261 (99%)	2 (1%)	81	93
9	8	70/190 (37%)	69 (99%)	1 (1%)	67	86
10	9	99/112 (88%)	99 (100%)	0	100	100
13	C	360/424 (85%)	360 (100%)	0	100	100
14	D	190/245 (78%)	190 (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	H	86/228 (38%)	86 (100%)	0	100	100
18	I	145/232 (62%)	145 (100%)	0	100	100
19	J	113/150 (75%)	113 (100%)	0	100	100
20	K	155/156 (99%)	155 (100%)	0	100	100
21	L	98/124 (79%)	98 (100%)	0	100	100
22	M	245/249 (98%)	244 (100%)	1 (0%)	91	97
23	N	172/211 (82%)	171 (99%)	1 (1%)	86	95
24	O	133/150 (89%)	133 (100%)	0	100	100
25	P	123/155 (79%)	123 (100%)	0	100	100
26	Q	199/256 (78%)	199 (100%)	0	100	100
27	R	118/126 (94%)	118 (100%)	0	100	100
28	S	141/180 (78%)	141 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
29	T	146/176 (83%)	146 (100%)	0	100	100
30	U	124/135 (92%)	124 (100%)	0	100	100
31	V	171/191 (90%)	170 (99%)	1 (1%)	86	95
32	W	89/119 (75%)	89 (100%)	0	100	100
33	X	219/229 (96%)	218 (100%)	1 (0%)	88	96
34	Y	159/223 (71%)	159 (100%)	0	100	100
35	Z	111/147 (76%)	110 (99%)	1 (1%)	78	92
36	a	78/133 (59%)	78 (100%)	0	100	100
37	b	130/186 (70%)	130 (100%)	0	100	100
38	c	241/288 (84%)	241 (100%)	0	100	100
39	d	193/274 (70%)	193 (100%)	0	100	100
40	e	171/236 (72%)	171 (100%)	0	100	100
41	f	93/188 (50%)	93 (100%)	0	100	100
42	g	119/148 (80%)	119 (100%)	0	100	100
43	h	100/148 (68%)	100 (100%)	0	100	100
44	i	86/110 (78%)	86 (100%)	0	100	100
45	j	68/97 (70%)	67 (98%)	1 (2%)	65	86
46	k	71/90 (79%)	71 (100%)	0	100	100
47	l	23/116 (20%)	23 (100%)	0	100	100
48	m	40/113 (35%)	39 (98%)	1 (2%)	47	76
49	o	80/87 (92%)	80 (100%)	0	100	100
50	p	117/181 (65%)	117 (100%)	0	100	100
51	q	104/178 (58%)	104 (100%)	0	100	100
52	r	143/169 (85%)	143 (100%)	0	100	100
53	s	326/381 (86%)	326 (100%)	0	100	100
All	All	7337/9637 (76%)	7325 (100%)	12 (0%)	93	98

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	5	412	ARG
7	6	52	ARG
8	7	54	ARG

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Mol	Chain	Res	Type
8	7	319	ARG
9	8	120	LYS
22	M	44	ARG
23	N	249	LYS
31	V	145	ARG
33	X	23	ARG
35	Z	44	LYS
45	j	70	ARG
48	m	37	ARG

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

Mol	Chain	Res	Type
28	S	118	ASN
39	d	47	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
11	A	1450/1559 (93%)	328 (22%)	17 (1%)
12	B	51/69 (73%)	16 (31%)	1 (1%)
All	All	1501/1628 (92%)	344 (22%)	18 (1%)

All (344) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
11	A	1672	C
11	A	1673	U
11	A	1674	A
11	A	1675	A
11	A	1676	A
11	A	1679	U
11	A	1680	A
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

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Mol	Chain	Res	Type
11	A	1708	A
11	A	1711	C
11	A	1712	A
11	A	1724	A
11	A	1727	A
11	A	1728	U
11	A	1732	C
11	A	1748	G
11	A	1750	G
11	A	1751	A
11	A	1761	A
11	A	1770	G
11	A	1777	A
11	A	1780	U
11	A	1794	A
11	A	1797	G
11	A	1801	A
11	A	1802	A
11	A	1805	A
11	A	1813	C
11	A	1817	C
11	A	1819	U
11	A	1821	A
11	A	1823	A
11	A	1824	U
11	A	1827	C
11	A	1828	A
11	A	1829	A
11	A	1832	A
11	A	1836	A
11	A	1844	A
11	A	1853	A
11	A	1854	U
11	A	1855	A
11	A	1856	A
11	A	1869	A
11	A	1870	A
11	A	1878	U
11	A	1882	A
11	A	1883	G
11	A	1886	G
11	A	1887	A

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Mol	Chain	Res	Type
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	1935	A
11	A	1938	A
11	A	1940	A
11	A	1958	G
11	A	1974	A
11	A	1985	G
11	A	1992	C
11	A	1993	A
11	A	1994	A
11	A	2003	A
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	2036	C
11	A	2037	U
11	A	2039	A
11	A	2054	U
11	A	2060	A
11	A	2065	A
11	A	2068	C
11	A	2069	U
11	A	2074	A
11	A	2079	C
11	A	2083	U
11	A	2085	A
11	A	2092	C
11	A	2093	U
11	A	2097	A
11	A	2098	G
11	A	2105	G
11	A	2113	G
11	A	2124	A

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Mol	Chain	Res	Type
11	A	2126	U
11	A	2141	U
11	A	2147	G
11	A	2154	A
11	A	2155	A
11	A	2158	U
11	A	2163	A
11	A	2165	C
11	A	2168	U
11	A	2171	U
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	2187	C
11	A	2189	C
11	A	2193	U
11	A	2194	U
11	A	2196	A
11	A	2197	G
11	A	2198	A
11	A	2200	A
11	A	2204	U
11	A	2210	C
11	A	2214	A
11	A	2216	A
11	A	2229	A
11	A	2230	A
11	A	2233	U
11	A	2237	A
11	A	2239	A
11	A	2241	A
11	A	2245	A
11	A	2246	A
11	A	2250	A
11	A	2262	C
11	A	2263	C
11	A	2284	C

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Mol	Chain	Res	Type
11	A	2285	U
11	A	2297	A
11	A	2300	G
11	A	2309	A
11	A	2313	A
11	A	2322	C
11	A	2331	C
11	A	2332	C
11	A	2335	A
11	A	2345	G
11	A	2350	A
11	A	2351	U
11	A	2364	C
11	A	2372	U
11	A	2374	A
11	A	2381	A
11	A	2382	A
11	A	2384	A
11	A	2390	A
11	A	2393	C
11	A	2396	C
11	A	2399	A
11	A	2404	U
11	A	2406	A
11	A	2407	U
11	A	2408	U
11	A	2414	C
11	A	2415	C
11	A	2416	U
11	A	2417	C
11	A	2418	A
11	A	2426	C
11	A	2427	C
11	A	2432	A
11	A	2441	C
11	A	2444	A
11	A	2446	A
11	A	2451	A
11	A	2452	A
11	A	2478	G
11	A	2493	C
11	A	2500	A

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Mol	Chain	Res	Type
11	A	2502	C
11	A	2507	A
11	A	2508	C
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	2563	U
11	A	2570	C
11	A	2583	C
11	A	2584	C
11	A	2592	G
11	A	2593	G
11	A	2594	U
11	A	2600	A
11	A	2603	C
11	A	2608	G
11	A	2625	C
11	A	2628	U
11	A	2629	A
11	A	2632	A
11	A	2633	A
11	A	2634	U
11	A	2635	G
11	A	2637	C
11	A	2640	C
11	A	2641	A
11	A	2645	G
11	A	2647	G
11	A	2654	U
11	A	2660	U
11	A	2683	C
11	A	2686	G
11	A	2693	A
11	A	2694	A
11	A	2695	G
11	A	2696	A
11	A	2706	A
11	A	2708	C
11	A	2709	A

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Mol	Chain	Res	Type
11	A	2718	C
11	A	2719	G
11	A	2722	A
11	A	2723	A
11	A	2724	G
11	A	2725	A
11	A	2732	G
11	A	2739	U
11	A	2740	A
11	A	2747	U
11	A	2750	U
11	A	2755	A
11	A	2756	C
11	A	2804	A
11	A	2810	G
11	A	2814	G
11	A	2815	OMG
11	A	2832	A
11	A	2833	A
11	A	2837	A
11	A	2842	C
11	A	2844	G
11	A	2847	C
11	A	2852	C
11	A	2859	A
11	A	2864	U
11	A	2865	C
11	A	2871	U
11	A	2880	A
11	A	2895	U
11	A	2896	G
11	A	2901	A
11	A	2906	C
11	A	2910	A
11	A	2912	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

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Mol	Chain	Res	Type
11	A	2934	G
11	A	2935	A
11	A	2956	A
11	A	2962	C
11	A	2963	A
11	A	2971	A
11	A	2989	G
11	A	2990	A
11	A	2992	G
11	A	2994	U
11	A	2995	G
11	A	3000	A
11	A	3005	A
11	A	3016	G
11	A	3022	G
11	A	3037	U
11	A	3038	U
11	A	3042	U
11	A	3043	C
11	A	3051	A
11	A	3053	A
11	A	3054	G
11	A	3056	C
11	A	3060	C
11	A	3061	G
11	A	3063	G
11	A	3069	A
11	A	3077	C
11	A	3086	U
11	A	3089	A
11	A	3090	G
11	A	3092	U
11	A	3093	C
11	A	3096	U
11	A	3097	U
11	A	3098	U
11	A	3100	U
11	A	3102	U
11	A	3108	U
11	A	3113	A
11	A	3129	A
11	A	3134	C

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Mol	Chain	Res	Type
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	3170	C
11	A	3172	C
11	A	3180	A
11	A	3189	C
11	A	3190	A
11	A	3196	G
11	A	3197	U
11	A	3198	A
11	A	3199	U
11	A	3207	A
11	A	3217	A
11	A	3218	A
12	B	1607	U
12	B	1608	G
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	1650	A
12	B	1669	G

All (18) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
11	A	1823	A
11	A	2030	U

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Mol	Chain	Res	Type
11	A	2186	C
11	A	2209	G
11	A	2245	A
11	A	2284	C
11	A	2507	A
11	A	2530	A
11	A	2693	A
11	A	2694	A
11	A	2814	G
11	A	2895	U
11	A	2905	A
11	A	2993	U
11	A	3092	U
11	A	3097	U
11	A	3198	A
12	B	1607	U

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

3 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	OMG	A	2815	11	18,26,27	1.15	2 (11%)	20,38,41	2.13	6 (30%)
11	OMU	A	3039	11	14,22,23	0.91	1 (7%)	14,31,34	0.98	0
11	OMG	A	3040	11	18,26,27	1.05	2 (11%)	20,38,41	2.42	6 (30%)

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
11	OMG	A	2815	11	-	5/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	OMU	A	3039	11	-	0/7/27/28	0/2/2/2
11	OMG	A	3040	11	-	0/5/27/28	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	2815	OMG	C6-C5	3.95	1.48	1.41
11	A	3040	OMG	C6-C5	2.99	1.46	1.41
11	A	3039	OMU	C2-N3	-2.33	1.33	1.38
11	A	2815	OMG	C5-C4	2.21	1.46	1.40
11	A	3040	OMG	C5-C4	2.02	1.46	1.40

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	3040	OMG	C6-N1-C2	5.09	124.02	115.93
11	A	2815	OMG	C2-N3-C4	4.99	121.05	115.36
11	A	3040	OMG	C6-C5-C4	-4.87	116.15	120.80
11	A	3040	OMG	C5-C6-N1	-4.35	117.48	123.43
11	A	3040	OMG	N3-C2-N1	-4.23	121.58	127.22
11	A	3040	OMG	C2-N3-C4	4.22	120.17	115.36
11	A	2815	OMG	C5-C6-N1	-3.83	118.19	123.43
11	A	2815	OMG	C6-N1-C2	3.83	122.02	115.93
11	A	2815	OMG	C6-C5-C4	-3.62	117.34	120.80
11	A	2815	OMG	N3-C2-N1	-3.15	123.02	127.22
11	A	2815	OMG	C4-C5-N7	-2.66	106.63	109.40
11	A	3040	OMG	C1'-N9-C4	-2.25	122.68	126.64

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	A	2815	OMG	O4'-C4'-C5'-O5'
11	A	2815	OMG	C1'-C2'-O2'-CM2
11	A	2815	OMG	C4'-C5'-O5'-P
11	A	2815	OMG	C3'-C2'-O2'-CM2
11	A	2815	OMG	C3'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 95 ligands modelled in this entry, 92 are monoatomic - leaving 3 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
56	GTP	C	601	55	26,34,34	1.05	1 (3%)	33,54,54	2.14	5 (15%)
56	GTP	A	3388	-	26,34,34	1.04	1 (3%)	33,54,54	2.12	4 (12%)
56	GTP	A	3387	-	26,34,34	1.04	1 (3%)	33,54,54	2.13	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
56	GTP	C	601	55	-	1/18/38/38	0/3/3/3
56	GTP	A	3388	-	-	0/18/38/38	0/3/3/3
56	GTP	A	3387	-	-	0/18/38/38	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	A	3388	GTP	C6-N1	3.95	1.39	1.33
56	A	3387	GTP	C6-N1	3.91	1.39	1.33
56	C	601	GTP	C6-N1	3.91	1.39	1.33

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	C	601	GTP	C5-C6-N1	-8.84	111.34	123.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	A	3387	GTP	C5-C6-N1	-8.82	111.36	123.43
56	A	3388	GTP	C5-C6-N1	-8.82	111.37	123.43
56	A	3387	GTP	C6-N1-C2	5.92	125.34	115.93
56	C	601	GTP	C6-N1-C2	5.87	125.26	115.93
56	A	3388	GTP	C6-N1-C2	5.86	125.25	115.93
56	C	601	GTP	C2-N3-C4	-2.98	111.95	115.36
56	A	3387	GTP	C2-N3-C4	-2.84	112.12	115.36
56	A	3388	GTP	C2-N3-C4	-2.77	112.19	115.36
56	C	601	GTP	O4'-C1'-C2'	-2.77	102.89	106.93
56	A	3387	GTP	N3-C2-N1	-2.76	123.54	127.22
56	A	3388	GTP	N3-C2-N1	-2.73	123.58	127.22
56	C	601	GTP	N3-C2-N1	-2.65	123.68	127.22
56	A	3387	GTP	O4'-C1'-C2'	-2.36	103.47	106.93

There are no chirality outliers.

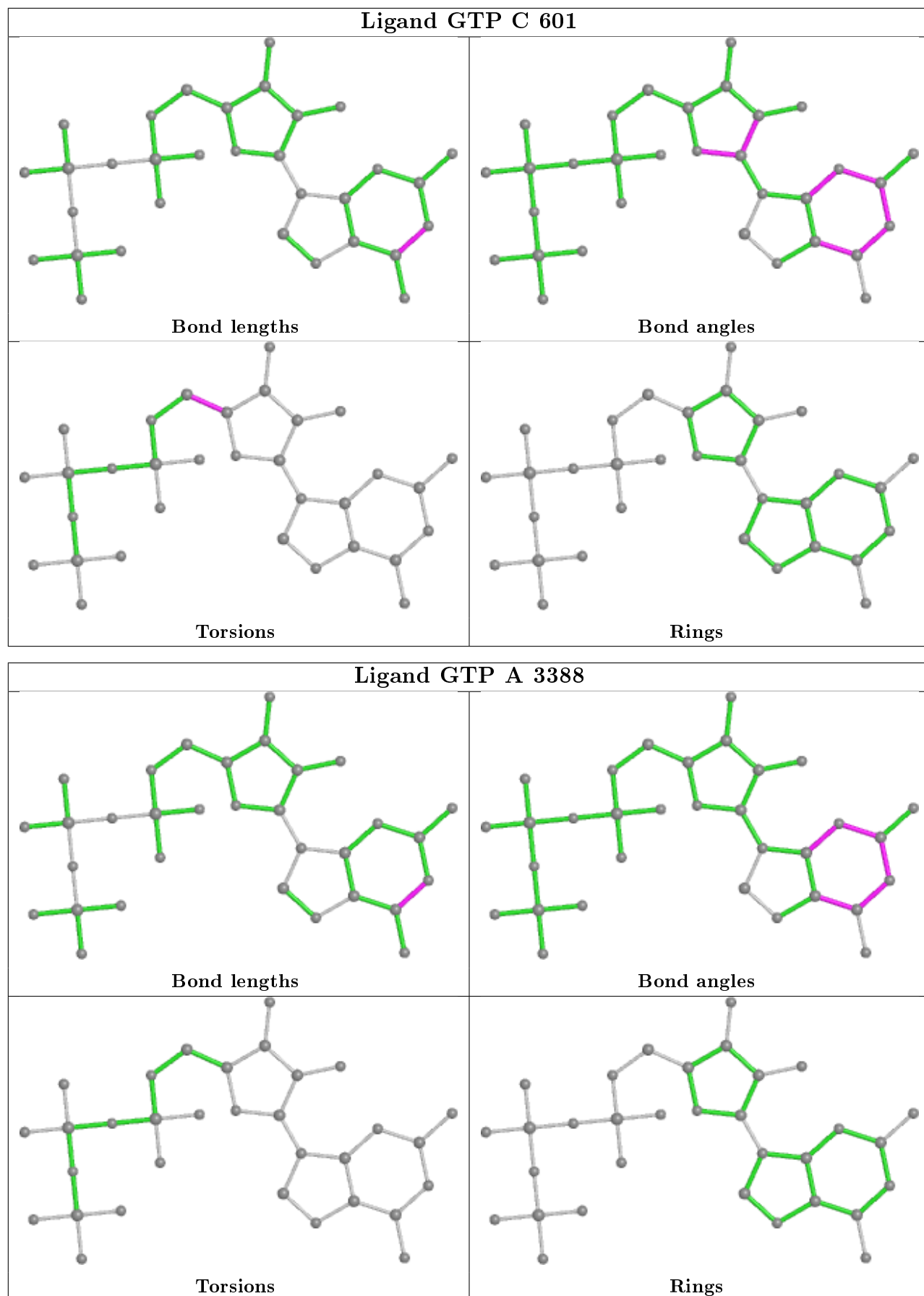
All (1) torsion outliers are listed below:

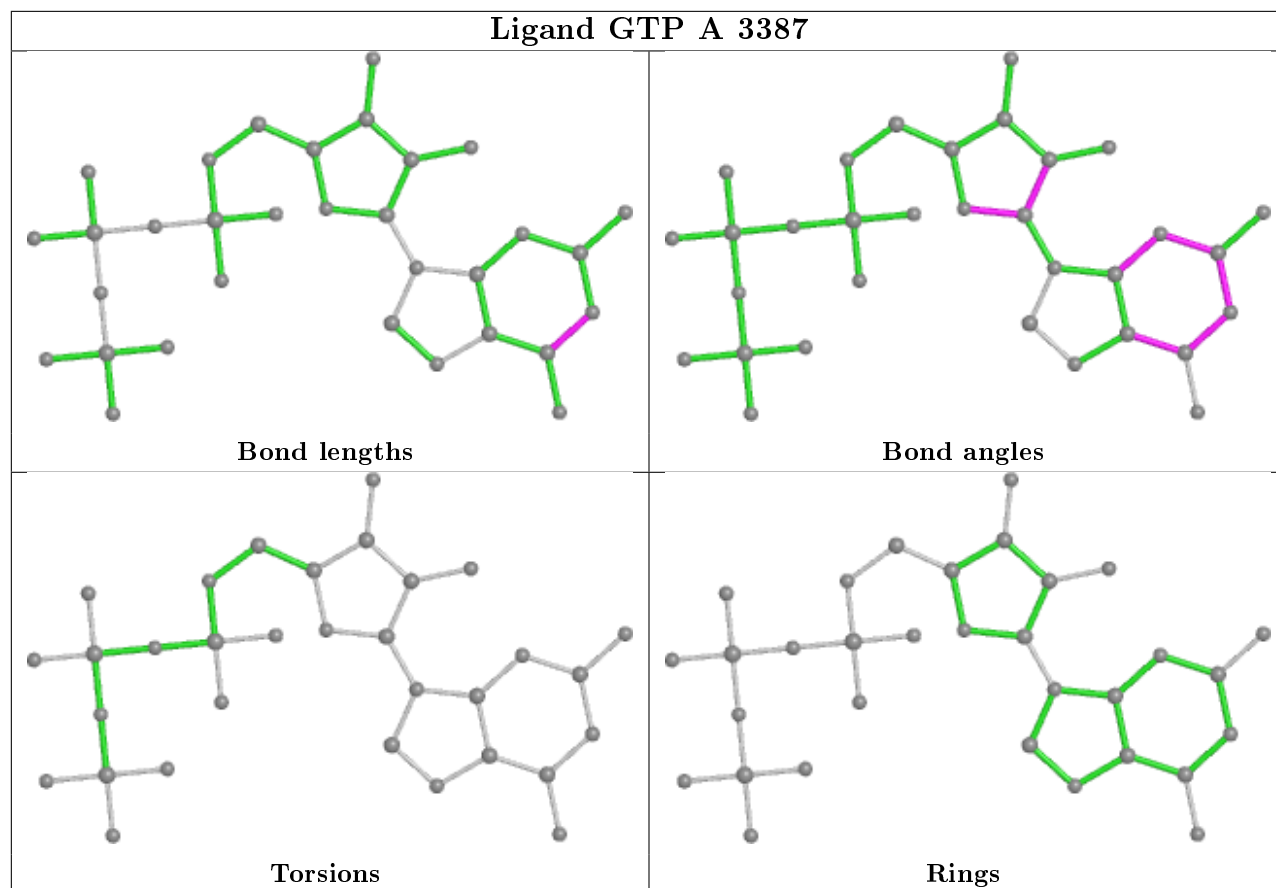
Mol	Chain	Res	Type	Atoms
56	C	601	GTP	O4'-C4'-C5'-O5'

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.

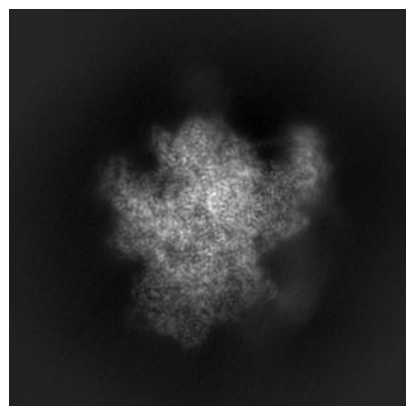
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-12869. These allow visual inspection of the internal detail of the map and identification of artifacts.

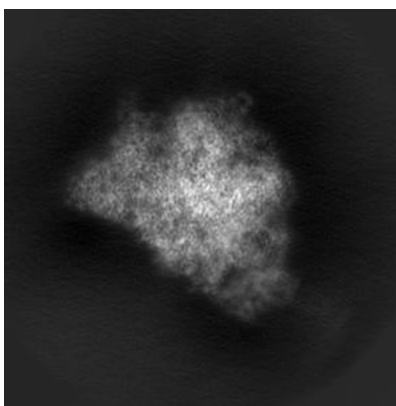
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

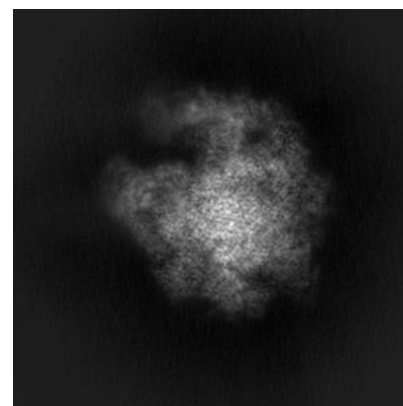
6.1.1 Primary map



X

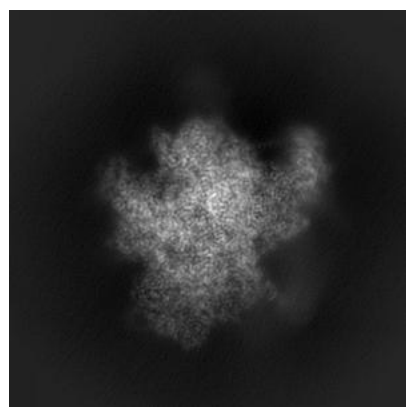


Y

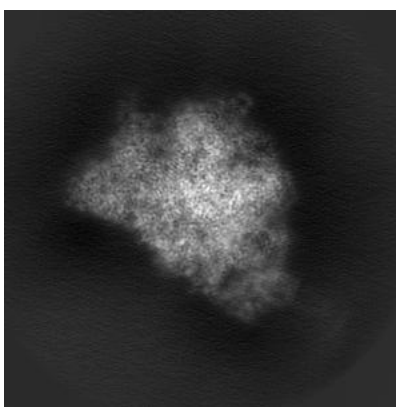


Z

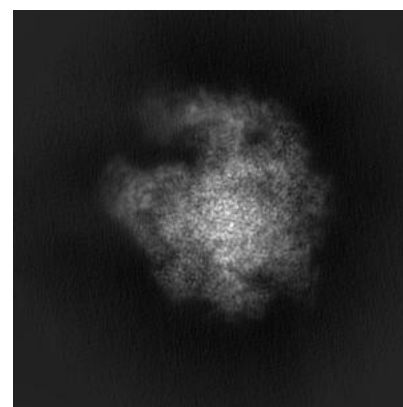
6.1.2 Raw map



X



Y

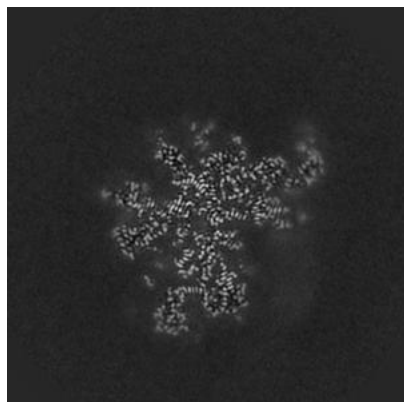


Z

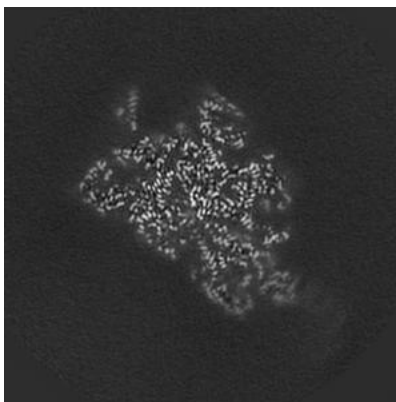
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

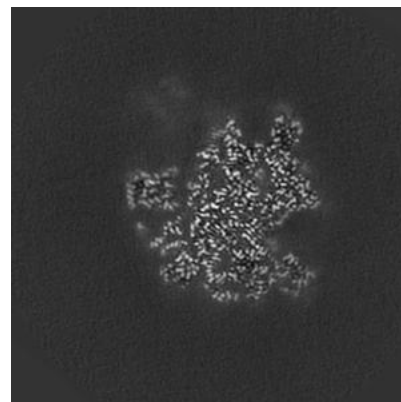
6.2.1 Primary map



X Index: 175

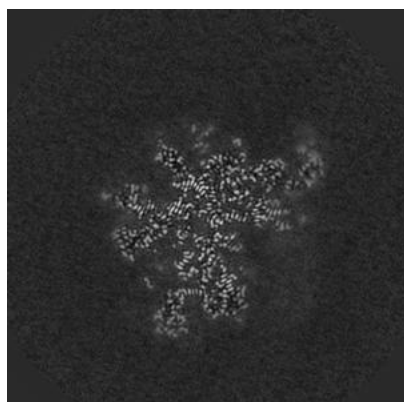


Y Index: 175

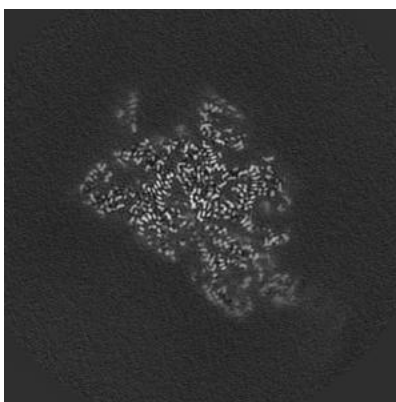


Z Index: 175

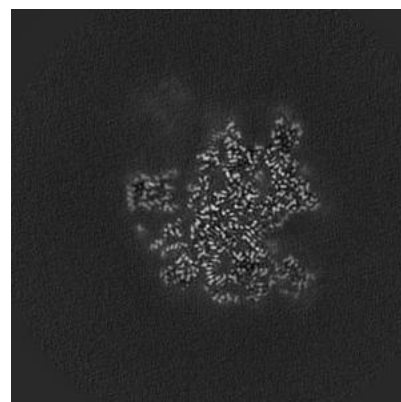
6.2.2 Raw map



X Index: 175



Y Index: 175

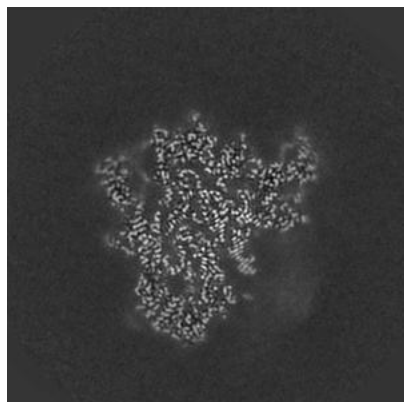


Z Index: 175

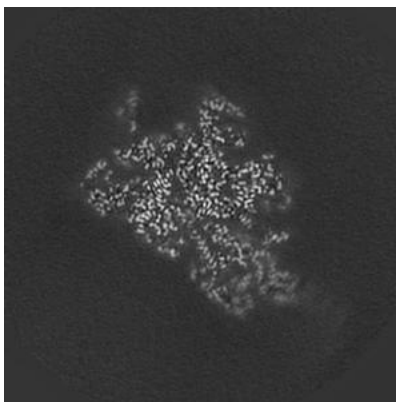
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

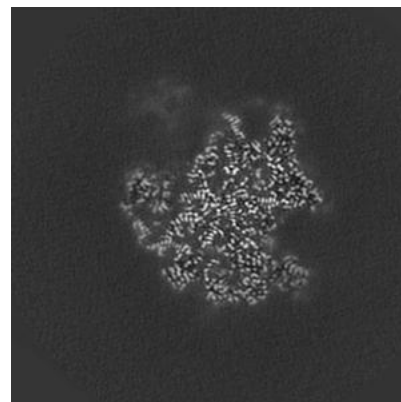
6.3.1 Primary map



X Index: 187

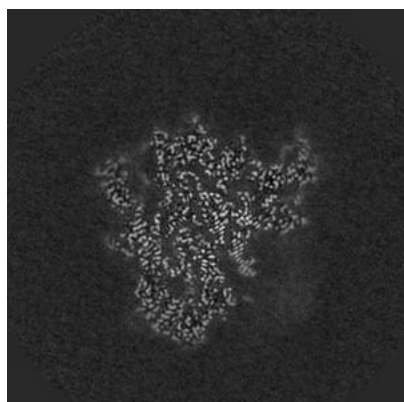


Y Index: 176

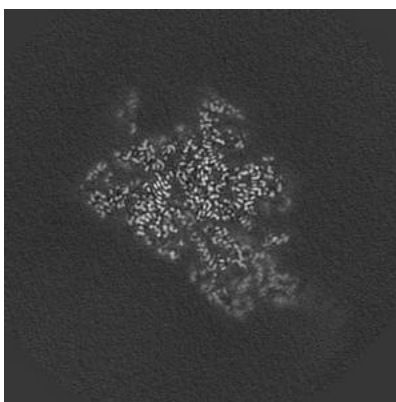


Z Index: 179

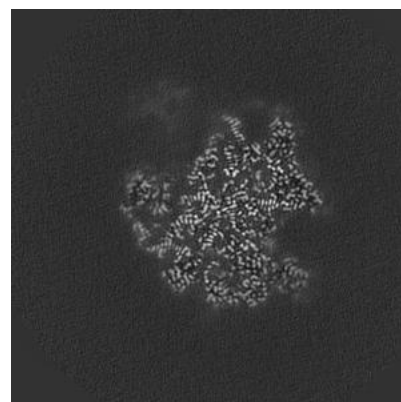
6.3.2 Raw map



X Index: 187



Y Index: 176

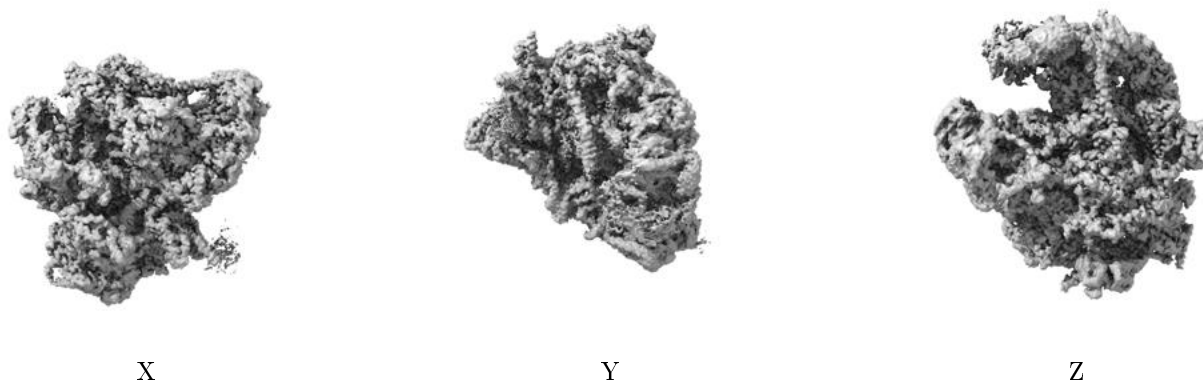


Z Index: 179

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

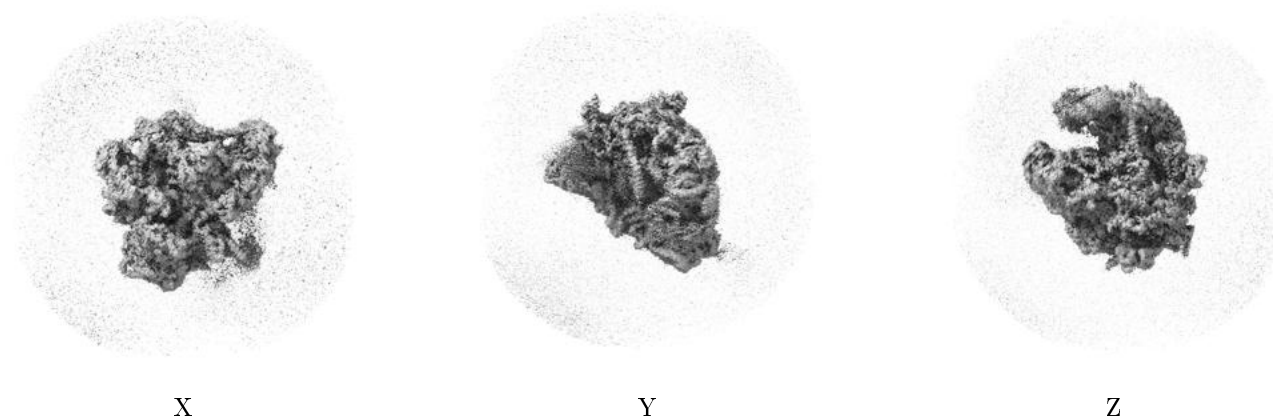
6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.004. 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



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.

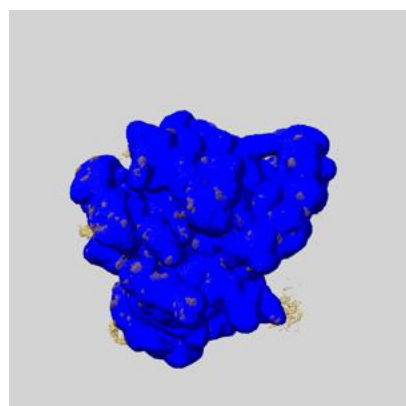
6.5 Mask visualisation [i](#)

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

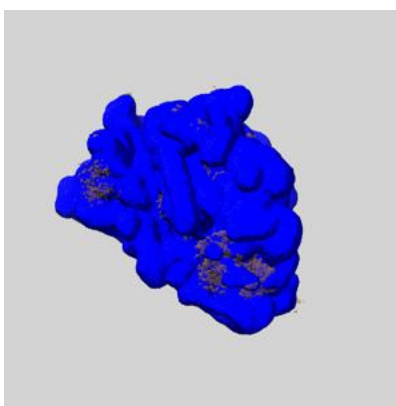
A mask typically either:

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

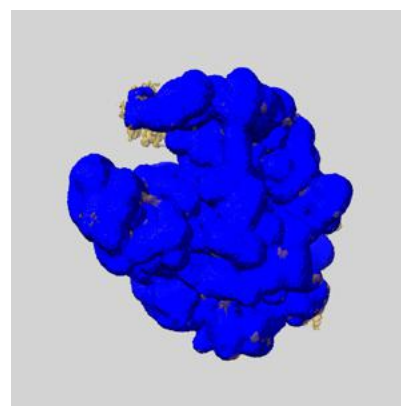
6.5.1 emd_12869_msk_1.map [i](#)



X



Y

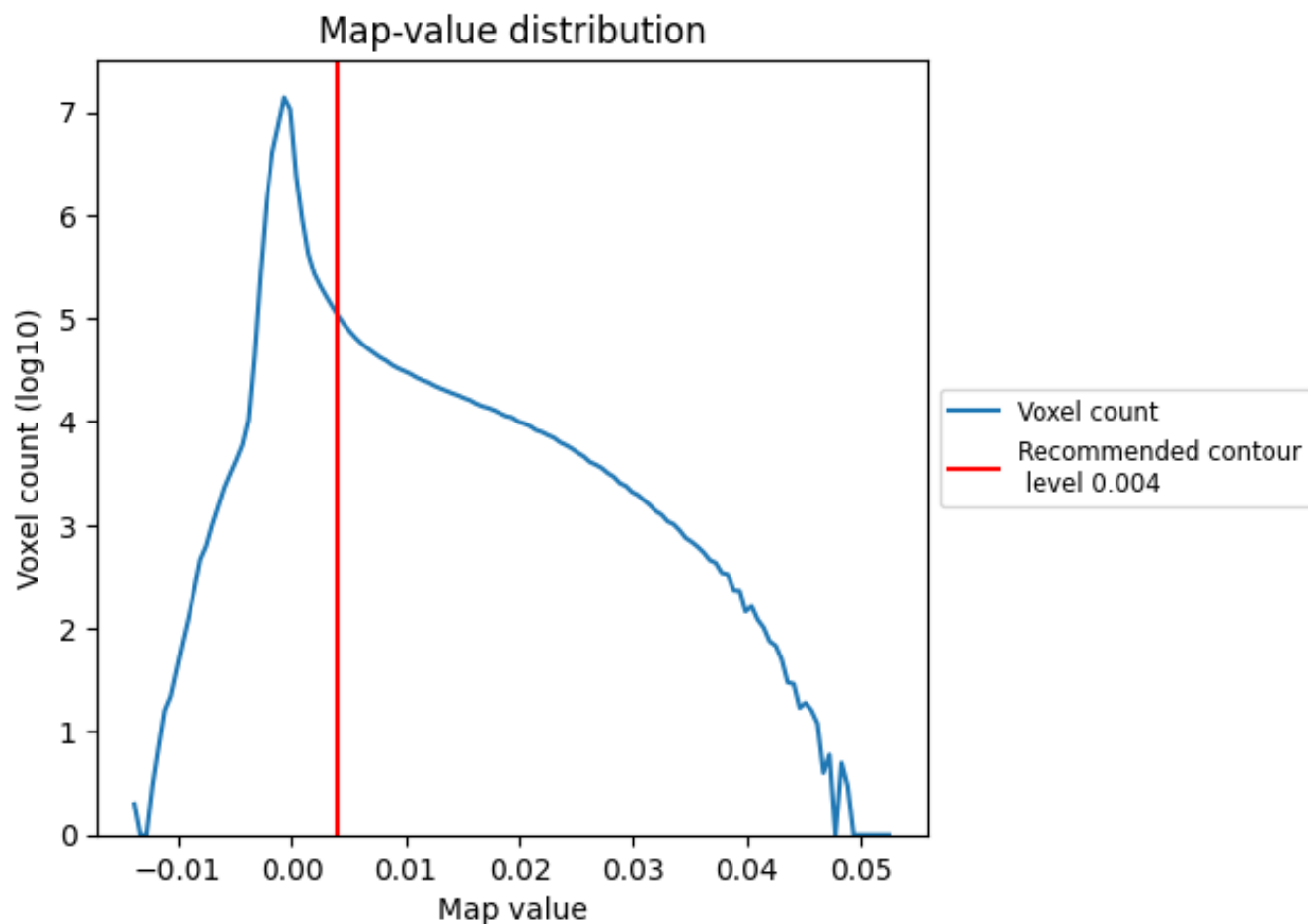


Z

7 Map analysis [i](#)

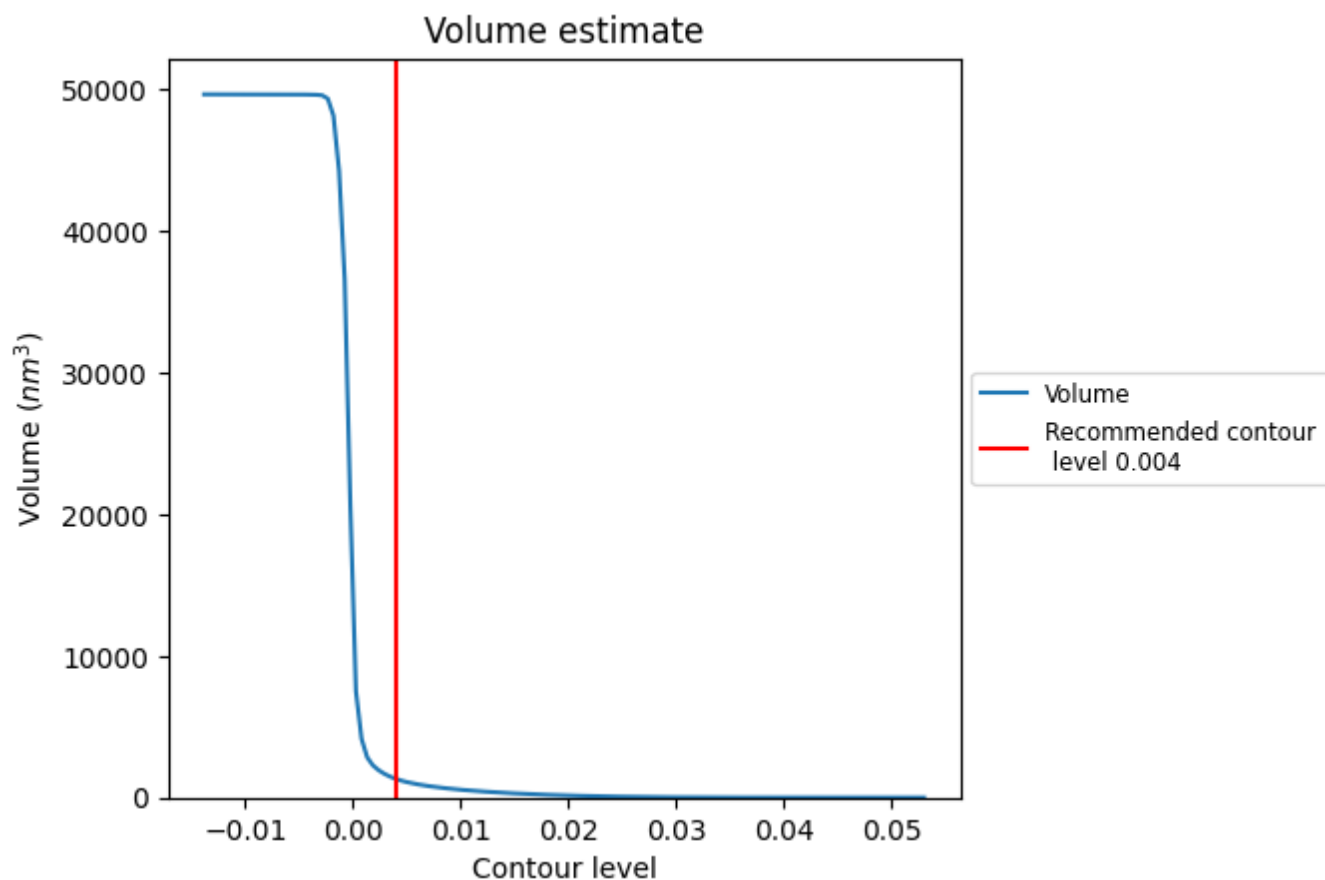
This section contains the results of statistical analysis of the map.

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.

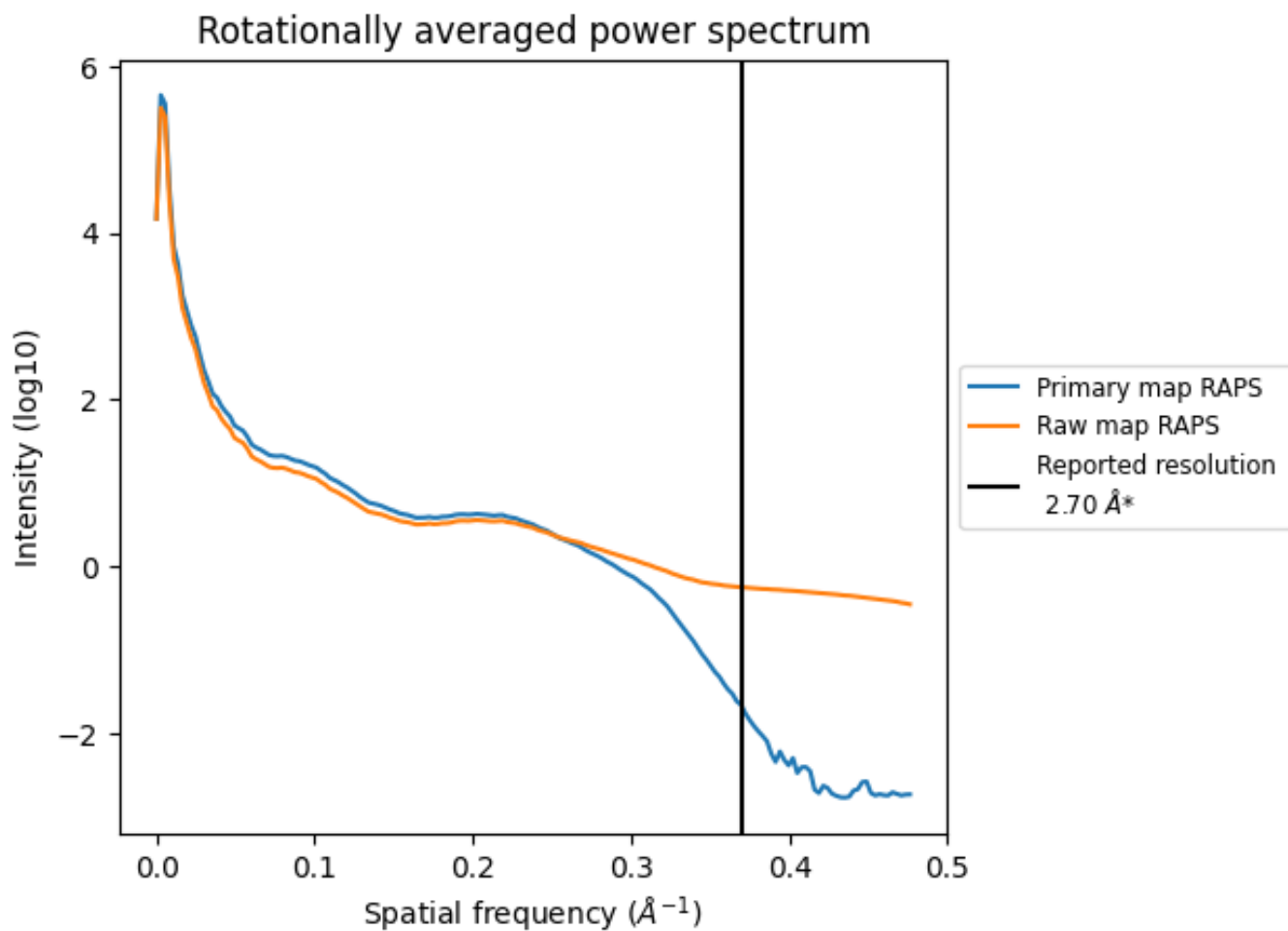
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 1320 nm³; this corresponds to an approximate mass of 1193 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

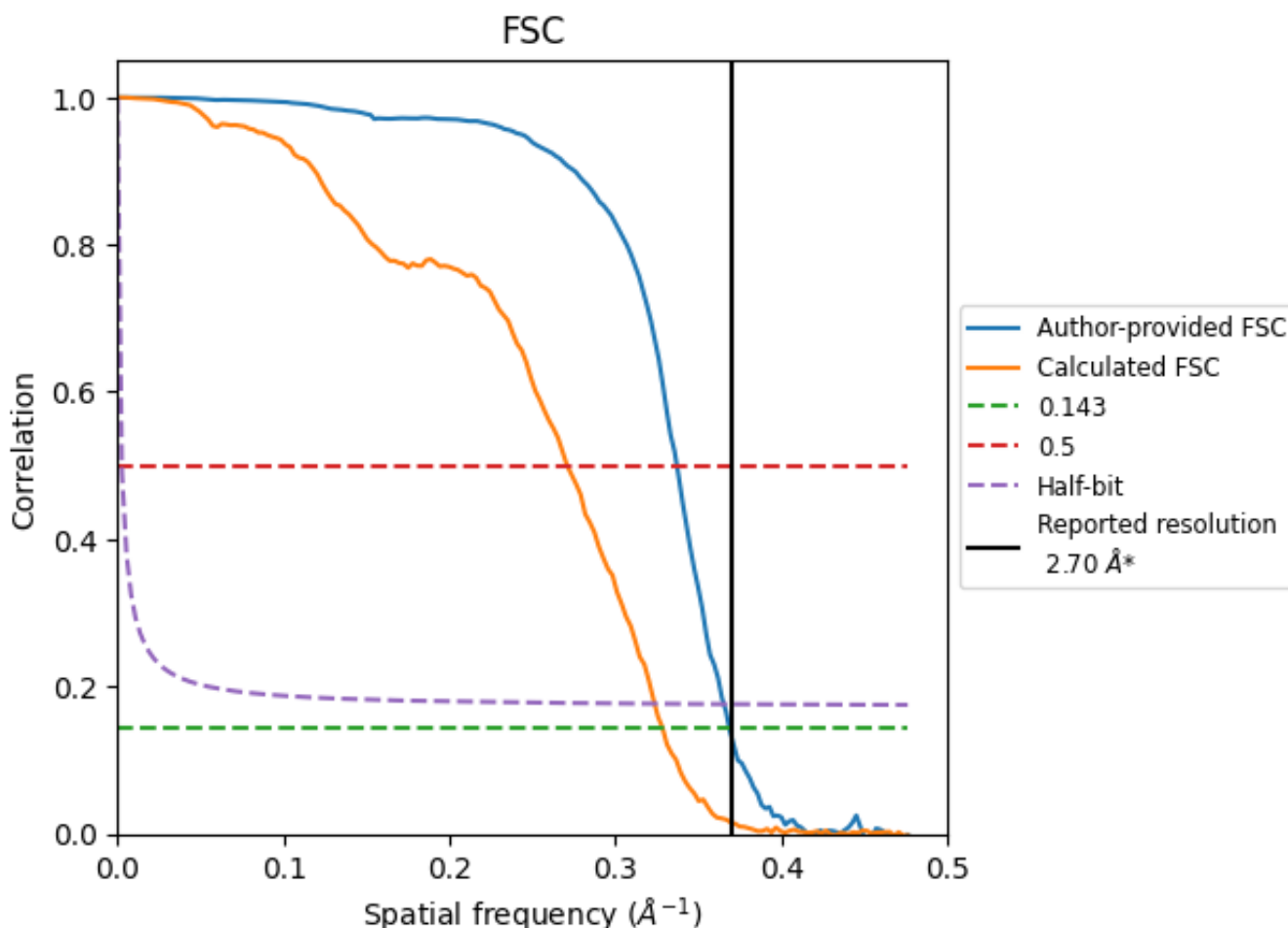


*Reported resolution corresponds to spatial frequency of 0.370 Å⁻¹

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](#)

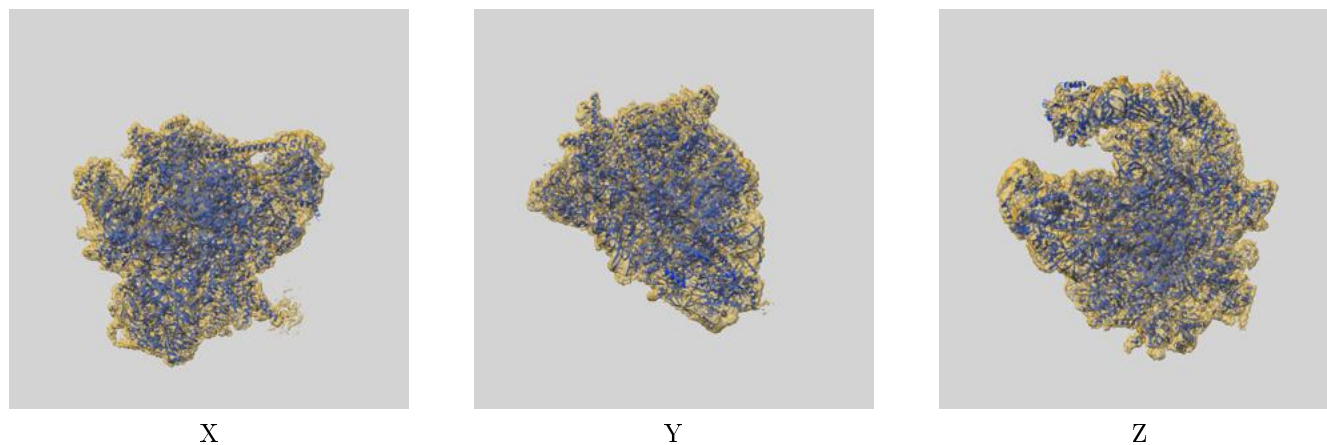
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.70	-	-
Author-provided FSC curve	2.71	2.97	2.74
Calculated*	3.04	3.69	3.09

*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 3.04 differs from the reported value 2.7 by more than 10 %

9 Map-model fit [i](#)

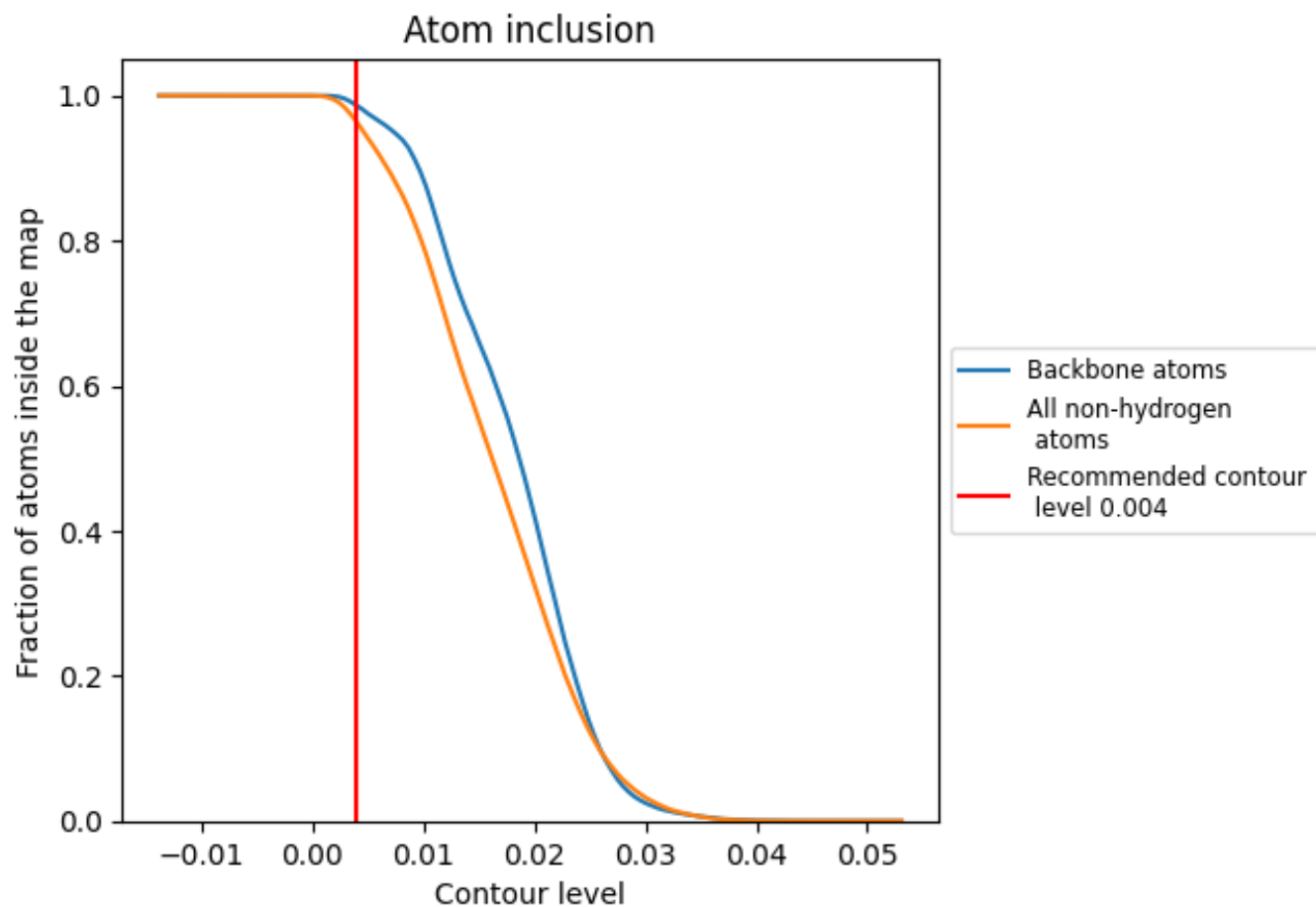
This section contains information regarding the fit between EMDB map EMD-12869 and PDB model 7OF4. Per-residue inclusion information can be found in section 3 on page 14.

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.004 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, 99% of all backbone atoms, 96% of all non-hydrogen atoms, are inside the map.