



## Full wwPDB EM Validation Report ⓘ

Jun 24, 2021 – 06:41 PM BST

PDB ID : 7O9K  
EMDB ID : EMD-12763  
Title : Human mitochondrial ribosome large subunit assembly intermediate with MTERF4-NSUN4, MRM2, MTG1, the MALSU module, GTPBP5 and mtEF-Tu  
Authors : Valentin Gese, G.; Hallberg, B.M.  
Deposited on : 2021-04-16  
Resolution : 3.10 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](mailto: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.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

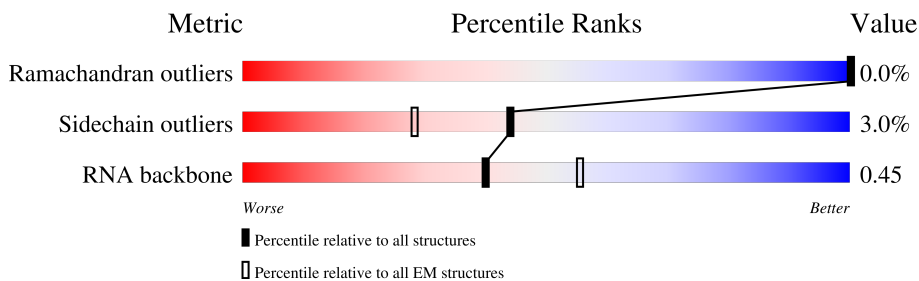
EMDB validation analysis : 0.0.0.dev75  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, 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 3.10 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  $\geq 3$ , 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	
2	a	142	
3	1	65	
4	2	92	
5	3	188	
6	4	103	
7	5	423	
8	6	380	



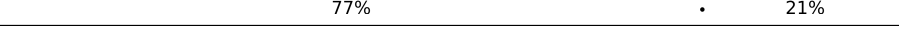
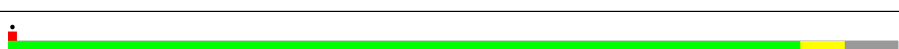



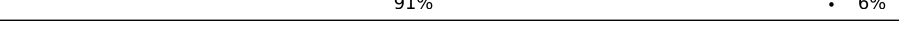



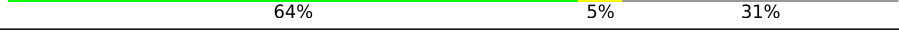

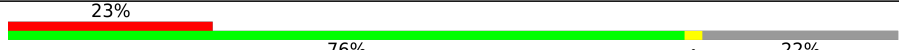


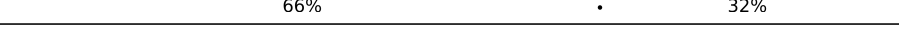







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Mol	Chain	Length	Quality of chain
9	7	338	83% 14%
10	8	206	38% 59%
11	9	137	88% 10%
12	A	1559	68% 23% 8%
13	A1	384	88% 10%
14	B	69	58% 29% 13%
15	A2	381	61% 38%
16	C	334	66% 75% 24%
17	D	305	77% 22%
18	E	348	86% 13%
19	F	311	79% 20%
20	FF	198	32% 35% 65%
20	t1	198	18% 22% 77%
20	t2	198	12% 15% 85%
20	t3	198	15% 15% 85%
20	t4	198	15% 15% 85%
20	t5	198	15% 15% 85%
20	t6	198	14% 14% 86%
21	G	414	79% 19%
22	H	267	35% 64%
23	I	261	21% 78% 19%
24	J	192	12% 68% 28%
25	K	178	98%
26	L	145	74% 5% 21%
27	M	296	94%

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Mol	Chain	Length	Quality of chain
28	N	251	
29	O	175	
30	P	179	
31	Q	292	
32	R	149	
33	S	205	
34	T	212	
35	U	153	
36	V	216	
37	W	148	
38	X	256	
39	Y	250	
40	Z	161	
41	b	215	
42	c	332	
43	d	306	
44	e	279	
45	f	212	
46	g	166	
47	h	158	
48	i	128	
49	j	123	
50	k	112	
51	l	138	
52	m	128	

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Mol	Chain	Length	Quality of chain
53	n	246	<p>34% 75% 23%</p>
54	o	102	<p>86% 11%</p>
55	p	206	<p>61% 38%</p>
56	q	222	<p>59% 39%</p>
57	r	196	<p>76% 21%</p>
58	s	439	<p>83% 16%</p>
59	t	452	<p>31% 84% 16%</p>
60	u	234	<p>56% 43%</p>
61	v	70	<p>90% 7%</p>
62	w	156	<p>16% 52% 44%</p>
63	UNK	28	<p>32% 93% 7%</p>

## 2 Entry composition i

There are 70 unique types of molecules in this entry. The entry contains 115679 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 L42, mitochondrial.

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

- Molecule 3 is a protein called 39S ribosomal protein L33, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	1	52	433	278	83	70	2	0	0

- Molecule 4 is a protein called 39S ribosomal protein L34, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	2	45	367	227	81	58	1	0	0

- Molecule 5 is a protein called 39S ribosomal protein L35, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	3	95	831	539	162	127	3	0	0

- Molecule 6 is a protein called 39S ribosomal protein L36, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	4	38	342	217	72	49	4	0	0

- Molecule 7 is a protein called 39S ribosomal protein L37, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	5	392	3199	2067	558	563	11	0	0

- Molecule 8 is a protein called 39S ribosomal protein L38, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	6	331	2692	1723	480	480	9	0	0

- Molecule 9 is a protein called 39S ribosomal protein L39, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	7	290	2356	1509	400	429	18	0	0

- Molecule 10 is a protein called 39S ribosomal protein L40, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	8	85	719	454	129	134	2	0	0

- Molecule 11 is a protein called 39S ribosomal protein L41, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	9	123	992	642	169	179	2	0	0

- Molecule 12 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
12	A	1436	30486	13680	5498	9872	1436	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	A1	344	2731	1743	476	495	17	0	0

- Molecule 14 is a RNA chain called MT-TRNAVAL.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
14	B	60	1275	572	230	413	60	0	0

- Molecule 15 is a protein called Transcription termination factor 4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	A2	238	1942	1244	336	350	12	0	0

- Molecule 16 is a protein called Mitochondrial ribosome-associated GTPase 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	C	255	1990	1267	349	360	14	0	0

- Molecule 17 is a protein called 39S ribosomal protein L2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	D	237	1851	1151	375	316	9	0	0

- Molecule 18 is a protein called 39S ribosomal protein L3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	E	304	2396	1539	416	430	11	0	0

- Molecule 19 is a protein called 39S ribosomal protein L4, mitochondrial.

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

- Molecule 20 is a protein called 39S ribosomal protein L12, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
20	FF	70	540	348	92	100	0	0
20	t1	46	354	228	56	70	0	0
20	t2	30	238	154	38	46	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
20	t3	30	238	154	38	46	0	0
20	t4	29	229	148	36	45	0	0
20	t5	29	229	148	36	45	0	0
20	t6	27	214	137	34	43	0	0

- Molecule 21 is a protein called Mitochondrial ribosome-associated GTPase 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	G	337	2549	1608	466	467	8	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	407	ASP	-	expression tag	UNP Q9H4K7
G	408	TYR	-	expression tag	UNP Q9H4K7
G	409	LYS	-	expression tag	UNP Q9H4K7
G	410	ASP	-	expression tag	UNP Q9H4K7
G	411	ASP	-	expression tag	UNP Q9H4K7
G	412	ASP	-	expression tag	UNP Q9H4K7
G	413	ASP	-	expression tag	UNP Q9H4K7
G	414	LYS	-	expression tag	UNP Q9H4K7

- Molecule 22 is a protein called 39S ribosomal protein L9, mitochondrial.

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

- Molecule 23 is a protein called 39S ribosomal protein L10, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	I	212	1695	1088	304	292	11	0	0

- Molecule 24 is a protein called 39S ribosomal protein L11, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	J	138	Total	C	N	O	S	0	0
			1050	673	190	185	2		

- Molecule 25 is a protein called 39S ribosomal protein L13, mitochondrial.

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

- Molecule 26 is a protein called 39S ribosomal protein L14, mitochondrial.

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

- Molecule 27 is a protein called 39S ribosomal protein L15, mitochondrial.

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

- Molecule 28 is a protein called 39S ribosomal protein L16, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	N	179	Total	C	N	O	S	0	0
			1457	930	267	251	9		

- Molecule 29 is a protein called 39S ribosomal protein L17, mitochondrial.

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

- Molecule 30 is a protein called Mitochondrial ribosomal protein L18, isoform CRA\_b.

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

- Molecule 31 is a protein called 39S ribosomal protein L19, mitochondrial.

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

- Molecule 32 is a protein called 39S ribosomal protein L20, mitochondrial.

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

- Molecule 33 is a protein called 39S ribosomal protein L21, mitochondrial.

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

- Molecule 34 is a protein called 39S ribosomal protein L22, mitochondrial.

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

- Molecule 35 is a protein called 39S ribosomal protein L23, mitochondrial.

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

- Molecule 36 is a protein called 39S ribosomal protein L24, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	V	202	Total	C	N	O	S	0	0
			1652	1053	294	297	8		

- Molecule 37 is a protein called 39S ribosomal protein L27, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	W	101	Total	C	N	O	S	0	0
			805	520	151	131	3		

- Molecule 38 is a protein called 39S ribosomal protein L28, mitochondrial.

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

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

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

- Molecule 40 is a protein called 39S ribosomal protein L30, mitochondrial.

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

- Molecule 41 is a protein called 39S ribosomal protein L43, mitochondrial.

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

- Molecule 42 is a protein called 39S ribosomal protein L44, mitochondrial.

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

- Molecule 43 is a protein called 39S ribosomal protein L45, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	d	223	Total	C	N	O	S	0	0
			1847	1187	317	330	13		

- Molecule 44 is a protein called 39S ribosomal protein L46, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	e	217	Total	C	N	O	S	0	0
			1762	1124	310	323	5		

- Molecule 45 is a protein called 39S ribosomal protein L48, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
45	f	123	979	625	164	187	3	0	0

- Molecule 46 is a protein called 39S ribosomal protein L49, mitochondrial.

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

- Molecule 47 is a protein called 39S ribosomal protein L50, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
47	h	107	871	551	153	164	3	0	0

- Molecule 48 is a protein called 39S ribosomal protein L51, mitochondrial.

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

- Molecule 49 is a protein called 39S ribosomal protein L52, mitochondrial.

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

- Molecule 50 is a protein called 39S ribosomal protein L53, mitochondrial.

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

- Molecule 51 is a protein called 39S ribosomal protein L54, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
51	l	44	395	251	76	67	1	0	0

- Molecule 52 is a protein called 39S ribosomal protein L55, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
52	m	35	Total	C	N	O	0	0
			287	180	57	50		

- Molecule 53 is a protein called rRNA methyltransferase 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	n	189	Total	C	N	O	S	0	0
			1450	917	259	268	6		

- Molecule 54 is a protein called Ribosomal protein 63, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	o	91	Total	C	N	O	S	0	0
			771	487	156	125	3		

- Molecule 55 is a protein called Peptidyl-tRNA hydrolase ICT1, mitochondrial.

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

- Molecule 56 is a protein called Growth arrest and DNA damage-inducible proteins-interacting protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	q	135	Total	C	N	O	S	0	0
			1134	705	222	202	5		

- Molecule 57 is a protein called 39S ribosomal protein S18a, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	r	155	Total	C	N	O	S	0	0
			1268	806	243	211	8		

- Molecule 58 is a protein called 39S ribosomal protein S30, mitochondrial.

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

- Molecule 59 is a protein called Elongation factor Tu, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
59	t	381	2939	1860	519	545	15	0	0

- Molecule 60 is a protein called Mitochondrial assembly of ribosomal large subunit protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
60	u	133	1092	702	181	199	10	0	0

- Molecule 61 is a protein called MIEF1 upstream open reading frame protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
61	v	68	584	369	115	100	0	0

- Molecule 62 is a protein called Acyl carrier protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
62	w	87	705	452	103	144	6	0	0

- Molecule 63 is a protein called UNK.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
63	UNK	26	130	78	26	26	0	0

- Molecule 64 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
64	0	1	1	1	0
64	4	1	1	1	0

- Molecule 65 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

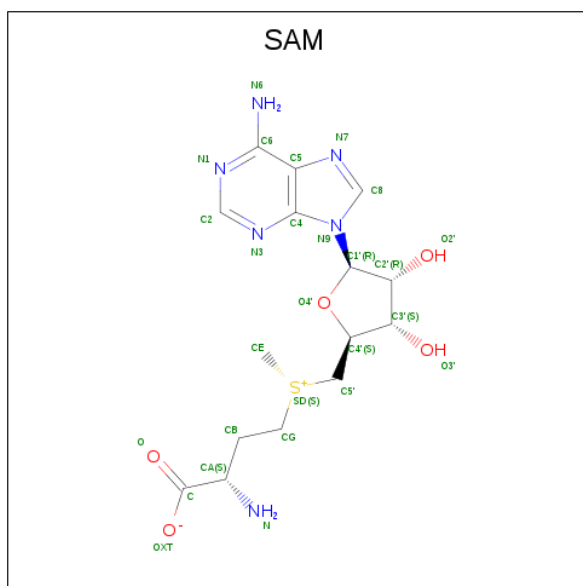
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
65	A	85	85	85	0
65	D	1	1	1	0

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Mol	Chain	Residues	Atoms		AltConf
65	E	1	Total	Mg	0
			1	1	
65	G	2	Total	Mg	0
			2	2	
65	M	1	Total	Mg	0
			1	1	
65	W	1	Total	Mg	0
			1	1	
65	g	1	Total	Mg	0
			1	1	
65	t	1	Total	Mg	0
			1	1	

- Molecule 66 is S-ADENOSYLMETHIONINE (three-letter code: SAM) (formula:  $C_{15}H_{22}N_6O_5S$ ).



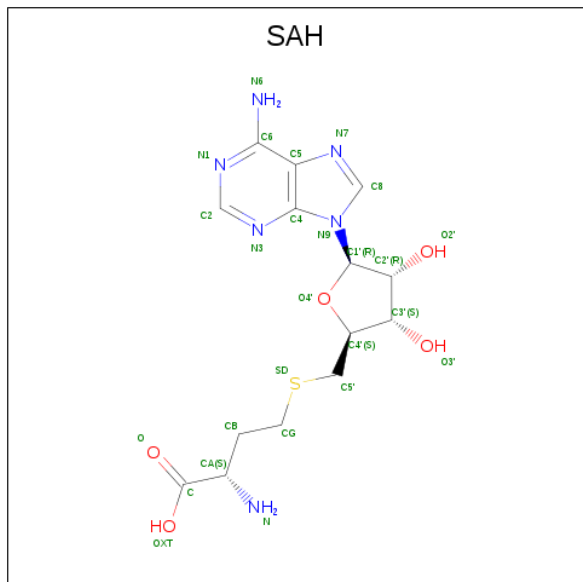
Mol	Chain	Residues	Atoms					AltConf
66	A1	1	Total	C	N	O	S	0
			27	15	6	5	1	

- Molecule 67 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula:  $C_{10}H_{15}N_5O_{11}P_2$ ).



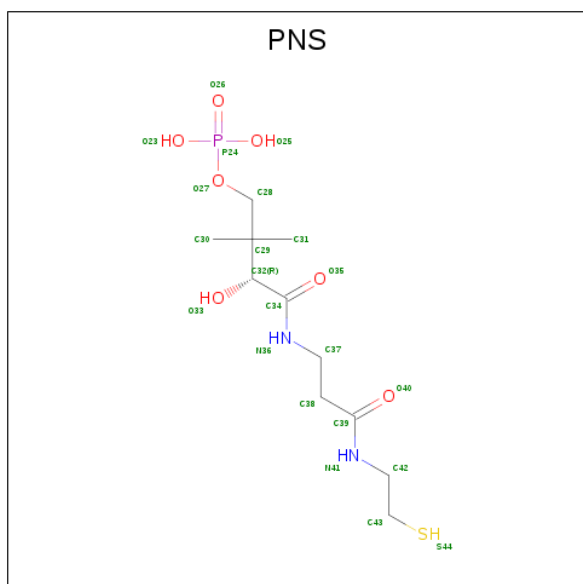


- Molecule 69 is S-ADENOSYL-L-HOMOCYSTEINE (three-letter code: SAH) (formula:  $C_{14}H_{20}N_6O_5S$ ).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	S	
69	n	1	26	14	6	5	1	0

- Molecule 70 is 4'-PHOSPHOPANTETHEINE (three-letter code: PNS) (formula:  $C_{11}H_{23}N_2O_7PS$ ).

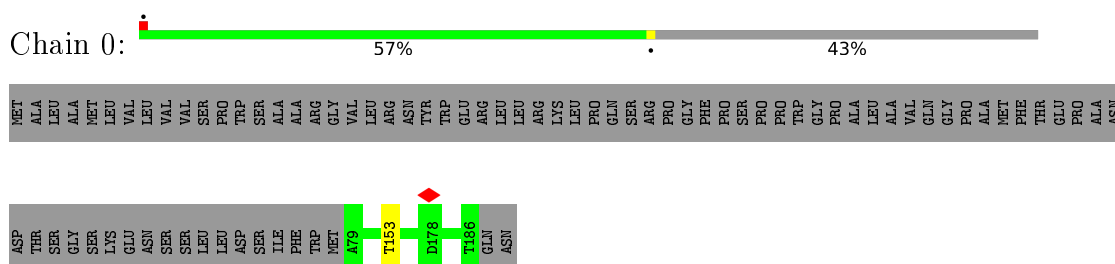


Mol	Chain	Residues	Atoms						AltConf
			Total	C	N	O	P	S	
70	w	1	21	11	2	6	1	1	0

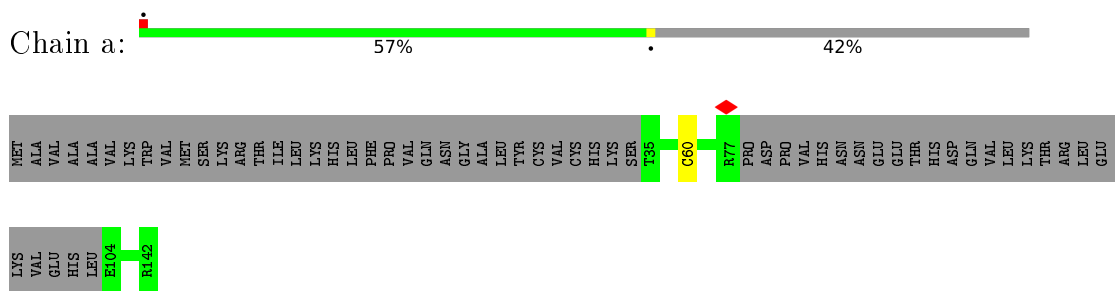
### 3 Residue-property plots [i](#)

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.

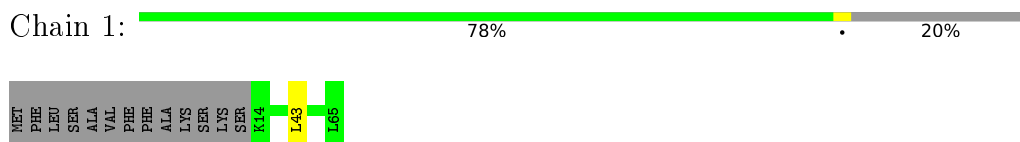
- Molecule 1: 39S ribosomal protein L32, mitochondrial



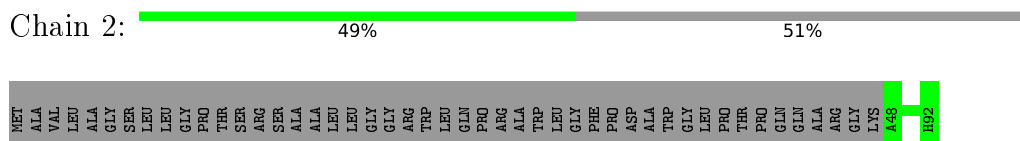
- Molecule 2: 39S ribosomal protein L42, mitochondrial



- Molecule 3: 39S ribosomal protein L33, mitochondrial



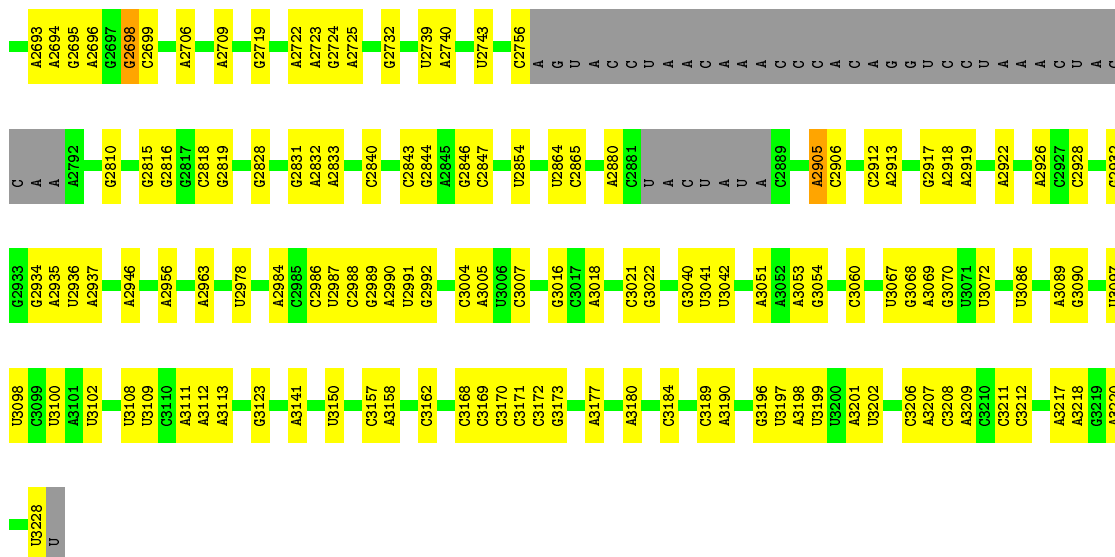
- Molecule 4: 39S ribosomal protein L34, mitochondrial



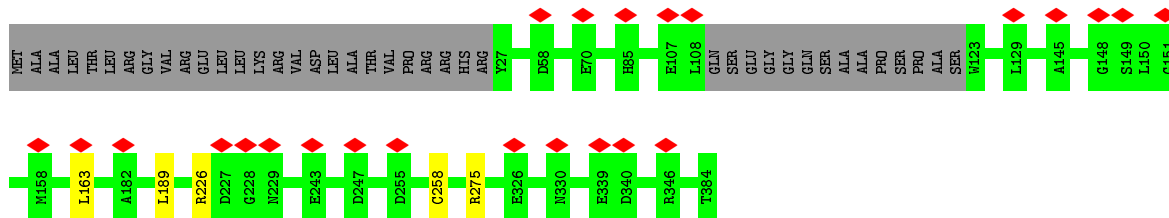
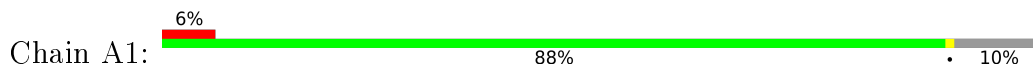
- Molecule 5: 39S ribosomal protein L35, mitochondrial







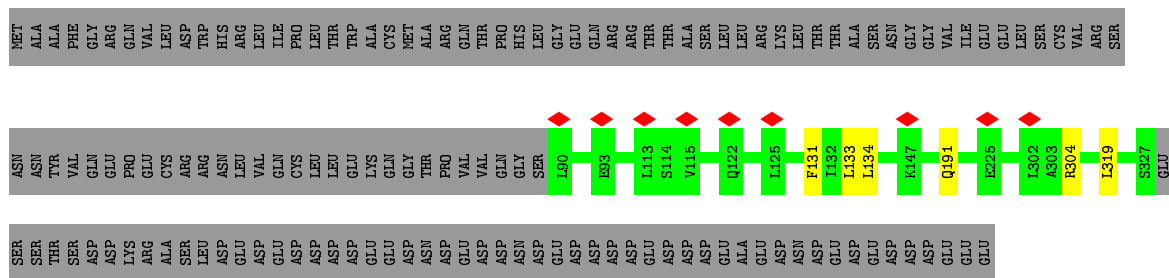
• Molecule 13: 5-methylcytosine rRNA methyltransferase NSUN4



• Molecule 14: MT-TRNAVAL



• Molecule 15: Transcription termination factor 4, mitochondrial



• Molecule 16: Mitochondrial ribosome-associated GTPase 1

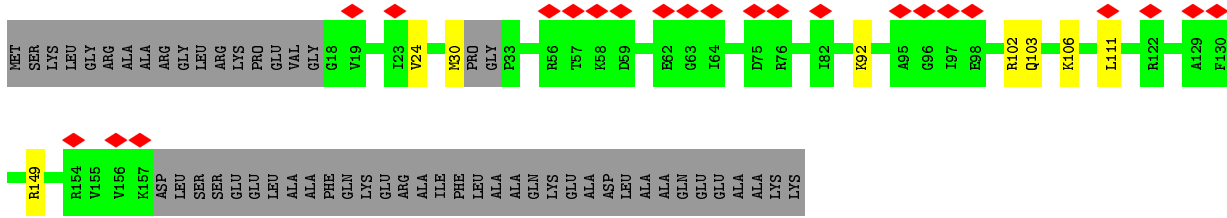












- Molecule 25: 39S ribosomal protein L13, mitochondrial

Chain K: 98%



- Molecule 26: 39S ribosomal protein L14, mitochondrial

Chain L: 74% 5% 21%



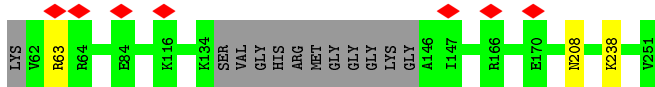
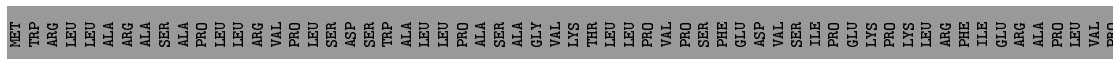
- Molecule 27: 39S ribosomal protein L15, mitochondrial

Chain M: 94%



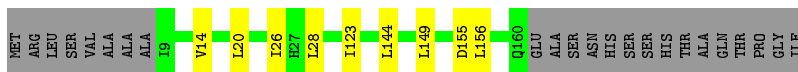
- Molecule 28: 39S ribosomal protein L16, mitochondrial

Chain N: 70% 29%



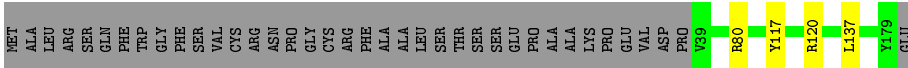
- Molecule 29: 39S ribosomal protein L17, mitochondrial

Chain O: 82% 5% 13%

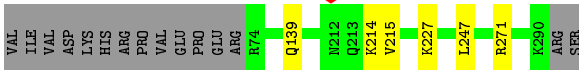
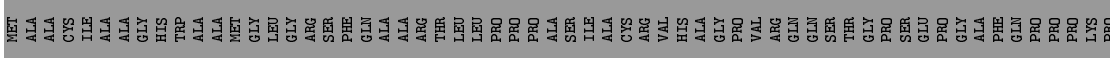


- Molecule 30: Mitochondrial ribosomal protein L18, isoform CRA\_b

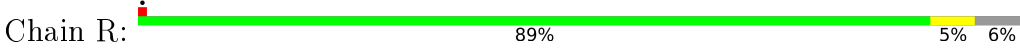
Chain P: 77% 21%



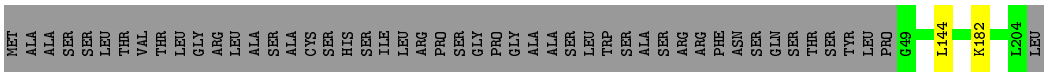
- Molecule 31: 39S ribosomal protein L19, mitochondrial



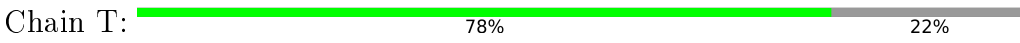
- Molecule 32: 39S ribosomal protein L20, mitochondrial



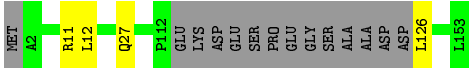
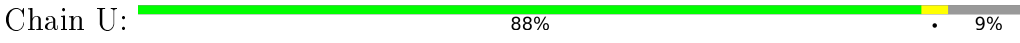
- Molecule 33: 39S ribosomal protein L21, mitochondrial



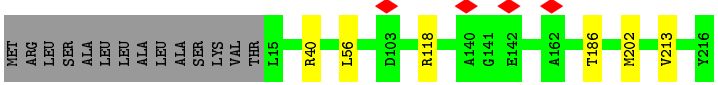
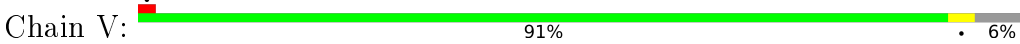
- Molecule 34: 39S ribosomal protein L22, mitochondrial



- Molecule 35: 39S ribosomal protein L23, mitochondrial

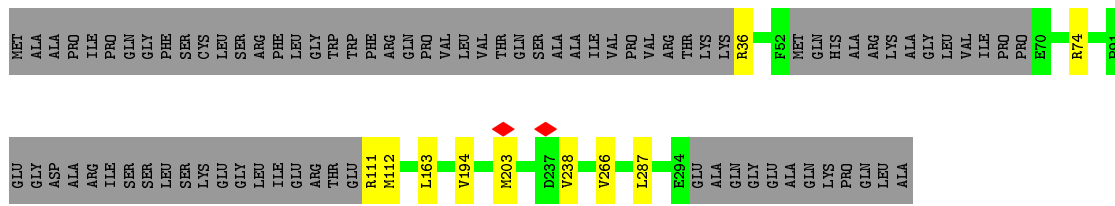


- Molecule 36: 39S ribosomal protein L24, mitochondrial

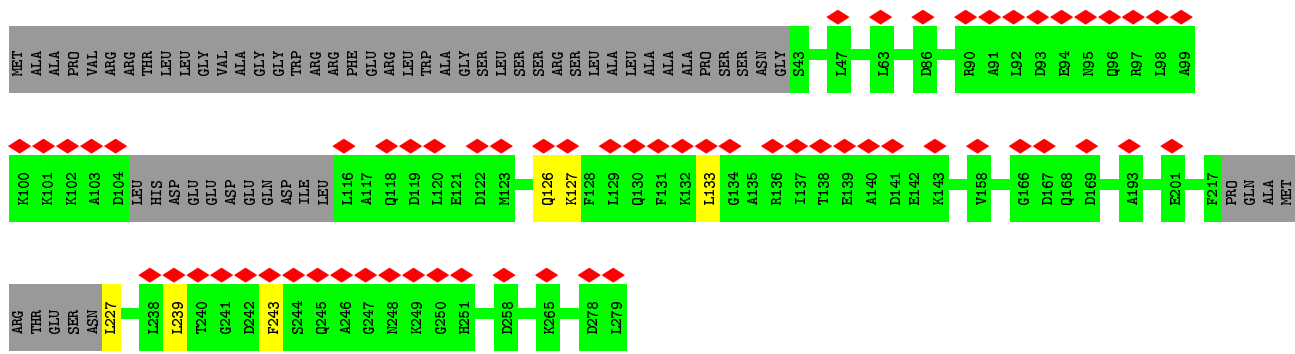
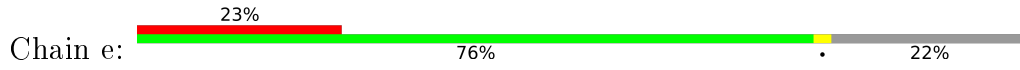


- Molecule 37: 39S ribosomal protein L27, mitochondrial

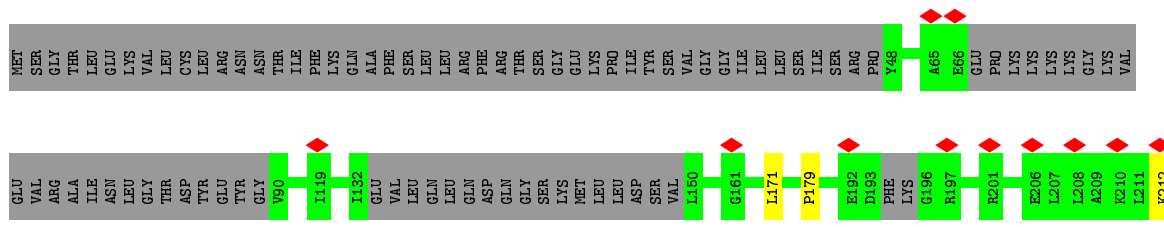




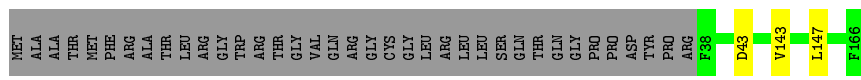
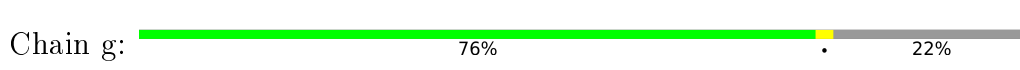
• Molecule 44: 39S ribosomal protein L46, mitochondrial



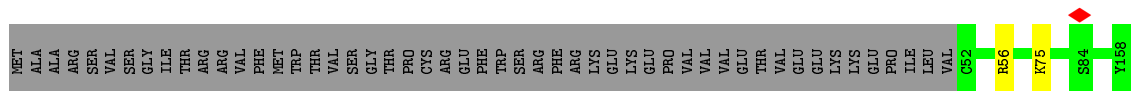
• Molecule 45: 39S ribosomal protein L48, mitochondrial



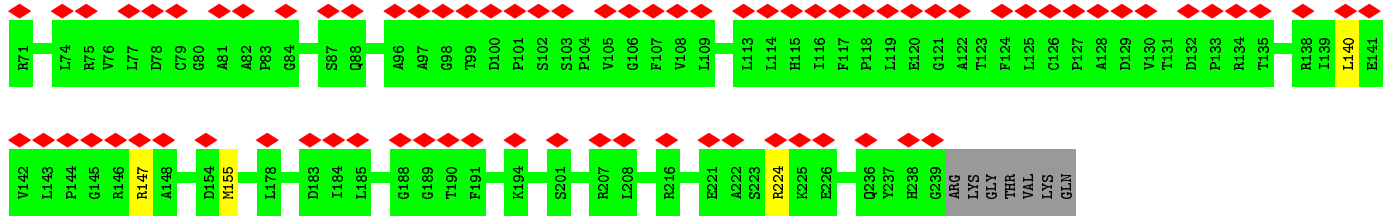
• Molecule 46: 39S ribosomal protein L49, mitochondrial



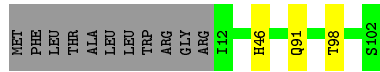
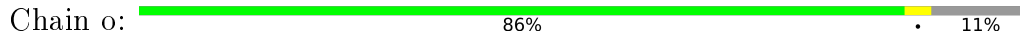
• Molecule 47: 39S ribosomal protein L50, mitochondrial



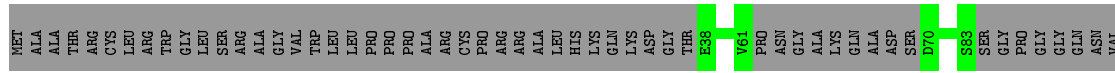




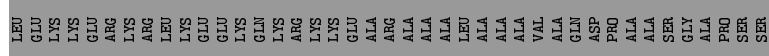
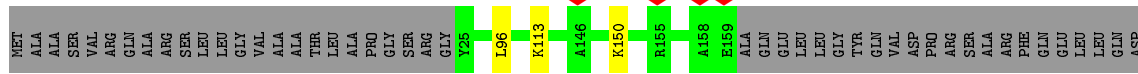
• Molecule 54: Ribosomal protein 63, mitochondrial



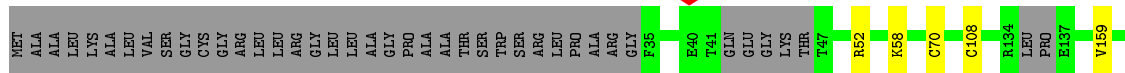
• Molecule 55: Peptidyl-tRNA hydrolase ICT1, mitochondrial



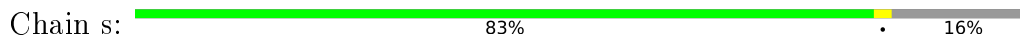
• Molecule 56: Growth arrest and DNA damage-inducible proteins-interacting protein 1



• Molecule 57: 39S ribosomal protein S18a, mitochondrial



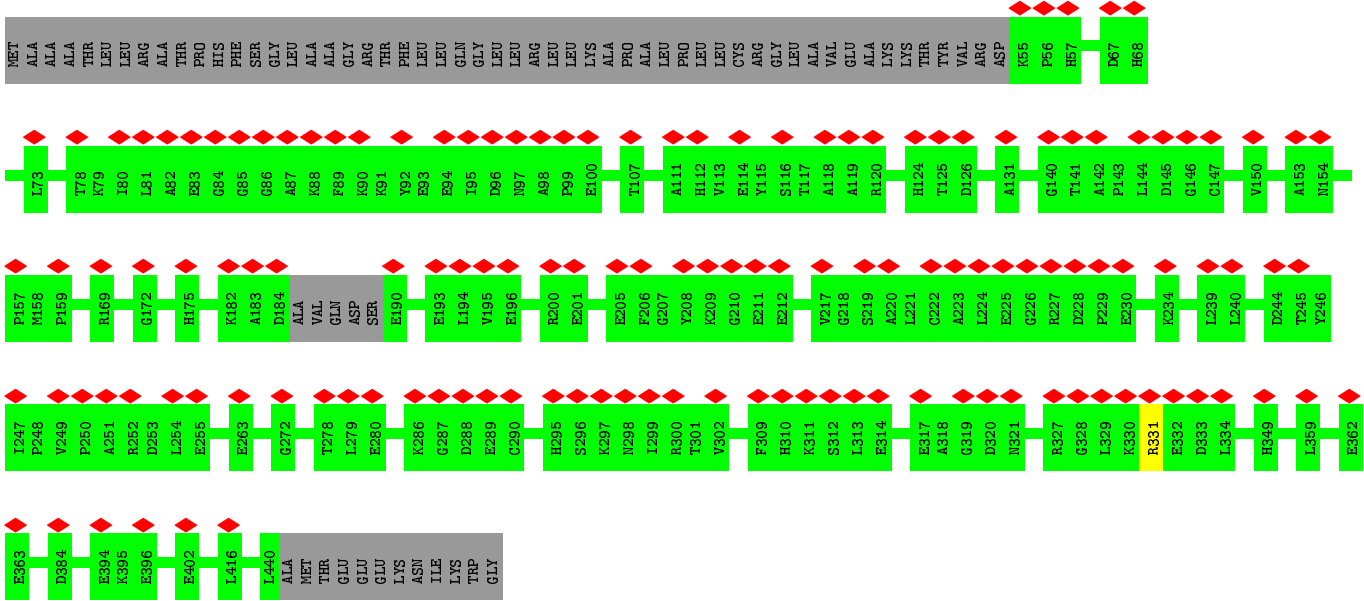
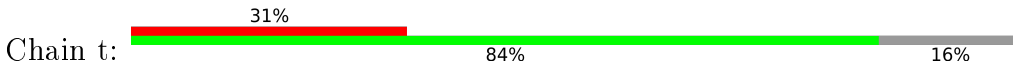
• Molecule 58: 39S ribosomal protein S30, mitochondrial



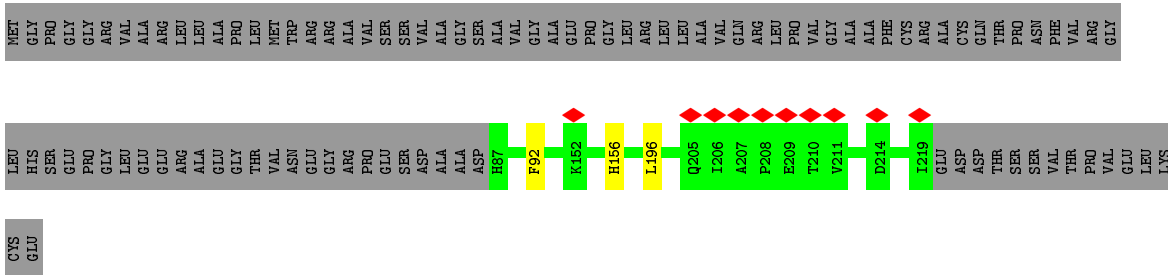




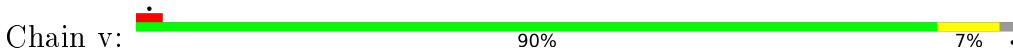
• Molecule 59: Elongation factor Tu, mitochondrial



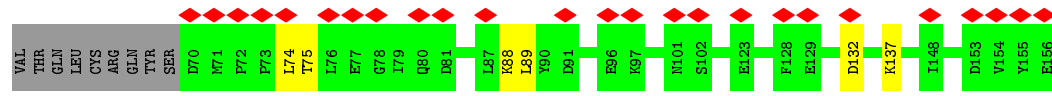
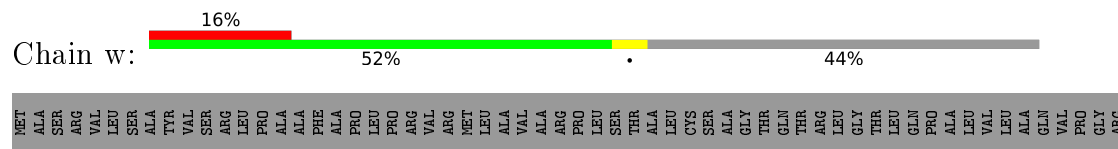
• Molecule 60: Mitochondrial assembly of ribosomal large subunit protein 1



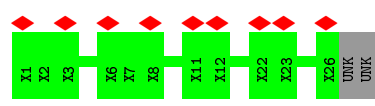
• Molecule 61: MIEF1 upstream open reading frame protein



• Molecule 62: Acyl carrier protein, mitochondrial



• Molecule 63: UNK



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	39495	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	49.2	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.935	Depositor
Minimum map value	-0.278	Depositor
Average map value	0.025	Depositor
Map value standard deviation	0.082	Depositor
Recommended contour level	0.15	Depositor
Map size ( $\text{\AA}$ )	221.34, 280.5, 250.92	wwPDB
Map dimensions	246, 275, 217	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.02, 1.02, 1.02	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: GTP, SAH, OMG, MG, GDP, PNS, SAM, ZN

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	0.34	0/895	0.66	0/1201
2	a	0.29	0/709	0.63	0/963
3	1	0.26	0/438	0.69	0/583
4	2	0.33	0/373	0.68	0/496
5	3	0.27	0/852	0.63	0/1136
6	4	0.39	0/350	0.77	1/461 (0.2%)
7	5	0.27	0/3294	0.62	0/4488
8	6	0.27	0/2779	0.62	0/3787
9	7	0.26	0/2413	0.61	0/3264
10	8	0.26	0/734	0.65	0/986
11	9	0.30	0/1020	0.66	0/1374
12	A	0.49	0/34076	0.76	12/53028 (0.0%)
13	A1	0.27	0/2795	0.62	0/3792
14	B	0.46	0/1423	0.72	0/2206
15	A2	0.26	0/1973	0.62	0/2651
16	C	0.35	0/2020	0.55	0/2724
17	D	0.29	0/1888	0.69	0/2538
18	E	0.28	0/2465	0.63	0/3344
19	F	0.29	0/2071	0.64	0/2817
20	FF	0.25	0/544	0.66	0/730
20	t1	0.44	0/358	0.54	0/486
20	t2	0.22	0/238	0.36	0/319
20	t3	0.21	0/238	0.35	0/319
20	t4	0.22	0/229	0.34	0/308
20	t5	0.21	0/229	0.41	0/308
20	t6	0.22	0/213	0.39	0/286
21	G	0.28	0/2600	0.63	0/3513
22	H	0.27	0/798	0.71	0/1073
23	I	0.28	0/1731	0.62	0/2345
24	J	0.28	0/1064	0.68	0/1431
25	K	0.28	0/1495	0.63	0/2029
26	L	0.28	0/904	0.64	0/1218

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
27	M	0.28	0/2359	0.66	0/3185
28	N	0.27	0/1494	0.64	0/2010
29	O	0.28	0/1269	0.64	0/1708
30	P	0.28	0/1173	0.65	0/1588
31	Q	0.27	0/1846	0.64	0/2487
32	R	0.28	0/1174	0.64	0/1572
33	S	0.27	0/1276	0.68	0/1729
34	T	0.28	0/1402	0.63	0/1886
35	U	0.28	0/1183	0.66	0/1600
36	V	0.27	0/1697	0.64	0/2302
37	W	0.28	0/827	0.65	0/1118
38	X	0.26	0/2090	0.62	0/2825
39	Y	0.26	0/1552	0.63	0/2079
40	Z	0.28	0/1003	0.66	0/1354
41	b	0.30	0/1202	0.67	0/1626
42	c	0.28	0/2264	0.62	0/3059
43	d	0.27	0/1899	0.64	0/2569
44	e	0.27	0/1797	0.66	0/2422
45	f	0.28	0/994	0.62	0/1336
46	g	0.28	0/1102	0.63	0/1503
47	h	0.29	0/894	0.63	0/1217
48	i	0.29	0/849	0.66	0/1135
49	j	0.32	0/698	0.64	0/940
50	k	0.28	0/635	0.68	0/855
51	l	0.26	0/407	0.62	0/547
52	m	0.28	0/292	0.67	0/394
53	n	0.27	0/1480	0.61	0/2013
54	o	0.26	0/792	0.63	0/1064
55	p	0.28	0/1071	0.64	0/1433
56	q	0.27	0/1165	0.62	0/1575
57	r	0.29	0/1305	0.65	0/1767
58	s	0.27	0/3114	0.62	0/4225
59	t	0.26	0/2992	0.63	0/4047
60	u	0.25	0/1119	0.63	0/1516
61	v	0.25	0/593	0.64	0/788
62	w	0.26	0/717	0.60	0/967
All	All	0.35	0/120935	0.67	13/170645 (0.0%)

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	A	1855	A	C2'-C3'-O3'	7.67	126.38	109.50
12	A	2182	G	C2'-C3'-O3'	7.49	125.97	109.50
12	A	1871	A	C2'-C3'-O3'	6.95	124.82	113.70
12	A	2457	A	C2'-C3'-O3'	6.63	124.31	113.70
12	A	2905	A	C2'-C3'-O3'	6.48	124.07	113.70
12	A	2653	C	C4'-C3'-O3'	6.38	125.75	113.00
6	4	79	CYS	CA-CB-SG	-6.16	102.91	114.00
12	A	2620	G	C2'-C3'-O3'	5.90	123.14	113.70
12	A	2543	C	C2'-C3'-O3'	5.75	122.91	113.70
12	A	2347	C	C2'-C3'-O3'	5.72	122.85	113.70
12	A	1958	G	C1'-O4'-C4'	-5.35	105.62	109.90
12	A	2698	G	O4'-C1'-N9	5.35	112.48	108.20
12	A	1770	G	C4'-C3'-C2'	-5.01	97.59	102.60

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 [i](#)

### 5.3.1 Protein backbone [i](#)

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%)	103 (97%)	3 (3%)	0	100	100
2	a	78/142 (55%)	75 (96%)	3 (4%)	0	100	100
3	1	50/65 (77%)	50 (100%)	0	0	100	100
4	2	43/92 (47%)	42 (98%)	1 (2%)	0	100	100
5	3	93/188 (50%)	89 (96%)	4 (4%)	0	100	100
6	4	36/103 (35%)	36 (100%)	0	0	100	100

*Continued on next page...*

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	5	390/423 (92%)	376 (96%)	14 (4%)	0	100	100
8	6	323/380 (85%)	310 (96%)	13 (4%)	0	100	100
9	7	288/338 (85%)	274 (95%)	14 (5%)	0	100	100
10	8	83/206 (40%)	75 (90%)	8 (10%)	0	100	100
11	9	121/137 (88%)	117 (97%)	4 (3%)	0	100	100
13	A1	340/384 (88%)	330 (97%)	10 (3%)	0	100	100
15	A2	236/381 (62%)	233 (99%)	3 (1%)	0	100	100
16	C	251/334 (75%)	245 (98%)	6 (2%)	0	100	100
17	D	235/305 (77%)	225 (96%)	10 (4%)	0	100	100
18	E	302/348 (87%)	288 (95%)	14 (5%)	0	100	100
19	F	248/311 (80%)	243 (98%)	5 (2%)	0	100	100
20	FF	68/198 (34%)	65 (96%)	3 (4%)	0	100	100
20	t1	44/198 (22%)	38 (86%)	4 (9%)	2 (4%)	2	15
20	t2	28/198 (14%)	28 (100%)	0	0	100	100
20	t3	28/198 (14%)	28 (100%)	0	0	100	100
20	t4	27/198 (14%)	27 (100%)	0	0	100	100
20	t5	27/198 (14%)	27 (100%)	0	0	100	100
20	t6	25/198 (13%)	24 (96%)	1 (4%)	0	100	100
21	G	335/414 (81%)	316 (94%)	19 (6%)	0	100	100
22	H	93/267 (35%)	91 (98%)	2 (2%)	0	100	100
23	I	210/261 (80%)	207 (99%)	3 (1%)	0	100	100
24	J	134/192 (70%)	127 (95%)	7 (5%)	0	100	100
25	K	175/178 (98%)	173 (99%)	2 (1%)	0	100	100
26	L	113/145 (78%)	107 (95%)	6 (5%)	0	100	100
27	M	285/296 (96%)	279 (98%)	6 (2%)	0	100	100
28	N	175/251 (70%)	170 (97%)	5 (3%)	0	100	100
29	O	150/175 (86%)	144 (96%)	6 (4%)	0	100	100
30	P	139/179 (78%)	137 (99%)	2 (1%)	0	100	100
31	Q	215/292 (74%)	209 (97%)	6 (3%)	0	100	100
32	R	138/149 (93%)	137 (99%)	1 (1%)	0	100	100
33	S	154/205 (75%)	149 (97%)	5 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
34	T	164/212 (77%)	161 (98%)	3 (2%)	0	100	100
35	U	135/153 (88%)	131 (97%)	4 (3%)	0	100	100
36	V	200/216 (93%)	196 (98%)	4 (2%)	0	100	100
37	W	99/148 (67%)	99 (100%)	0	0	100	100
38	X	241/256 (94%)	239 (99%)	2 (1%)	0	100	100
39	Y	174/250 (70%)	170 (98%)	4 (2%)	0	100	100
40	Z	118/161 (73%)	113 (96%)	5 (4%)	0	100	100
41	b	146/215 (68%)	138 (94%)	8 (6%)	0	100	100
42	c	271/332 (82%)	267 (98%)	4 (2%)	0	100	100
43	d	217/306 (71%)	207 (95%)	10 (5%)	0	100	100
44	e	211/279 (76%)	202 (96%)	9 (4%)	0	100	100
45	f	115/212 (54%)	107 (93%)	7 (6%)	1 (1%)	17	52
46	g	127/166 (76%)	125 (98%)	2 (2%)	0	100	100
47	h	105/158 (66%)	101 (96%)	4 (4%)	0	100	100
48	i	95/128 (74%)	92 (97%)	3 (3%)	0	100	100
49	j	83/123 (68%)	82 (99%)	1 (1%)	0	100	100
50	k	76/112 (68%)	73 (96%)	3 (4%)	0	100	100
51	l	42/138 (30%)	42 (100%)	0	0	100	100
52	m	33/128 (26%)	31 (94%)	2 (6%)	0	100	100
53	n	187/246 (76%)	186 (100%)	1 (0%)	0	100	100
54	o	89/102 (87%)	84 (94%)	5 (6%)	0	100	100
55	p	119/206 (58%)	115 (97%)	4 (3%)	0	100	100
56	q	133/222 (60%)	132 (99%)	1 (1%)	0	100	100
57	r	149/196 (76%)	143 (96%)	6 (4%)	0	100	100
58	s	366/439 (83%)	353 (96%)	13 (4%)	0	100	100
59	t	377/452 (83%)	368 (98%)	9 (2%)	0	100	100
60	u	131/234 (56%)	124 (95%)	7 (5%)	0	100	100
61	v	66/70 (94%)	61 (92%)	5 (8%)	0	100	100
62	w	85/156 (54%)	83 (98%)	2 (2%)	0	100	100
All	All	10140/14731 (69%)	9819 (97%)	318 (3%)	3 (0%)	100	100

All (3) Ramachandran outliers are listed below:



Mol	Chain	Res	Type
20	t1	-3	LYS
45	f	179	PRO
20	t1	1	PRO

### 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%)	96 (99%)	1 (1%)	76	90
2	a	78/133 (59%)	77 (99%)	1 (1%)	69	87
3	1	49/60 (82%)	48 (98%)	1 (2%)	55	80
4	2	39/72 (54%)	39 (100%)	0	100	100
5	3	88/166 (53%)	84 (96%)	4 (4%)	27	60
6	4	37/89 (42%)	35 (95%)	2 (5%)	22	53
7	5	353/368 (96%)	343 (97%)	10 (3%)	43	73
8	6	271/332 (82%)	265 (98%)	6 (2%)	52	78
9	7	266/303 (88%)	257 (97%)	9 (3%)	37	69
10	8	77/190 (40%)	71 (92%)	6 (8%)	12	40
11	9	104/112 (93%)	102 (98%)	2 (2%)	57	81
13	A1	297/328 (90%)	292 (98%)	5 (2%)	60	83
15	A2	221/350 (63%)	215 (97%)	6 (3%)	44	74
16	C	224/287 (78%)	219 (98%)	5 (2%)	52	78
17	D	191/245 (78%)	189 (99%)	2 (1%)	76	90
18	E	259/290 (89%)	255 (98%)	4 (2%)	65	85
19	F	217/262 (83%)	212 (98%)	5 (2%)	50	77
20	FF	58/158 (37%)	58 (100%)	0	100	100
20	t1	40/158 (25%)	38 (95%)	2 (5%)	24	57
20	t2	29/158 (18%)	29 (100%)	0	100	100
20	t3	29/158 (18%)	28 (97%)	1 (3%)	37	69
20	t4	28/158 (18%)	28 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	t5	28/158 (18%)	28 (100%)	0	100	100
20	t6	26/158 (16%)	26 (100%)	0	100	100
21	G	264/328 (80%)	256 (97%)	8 (3%)	41	71
22	H	86/228 (38%)	84 (98%)	2 (2%)	50	77
23	I	194/232 (84%)	185 (95%)	9 (5%)	27	59
24	J	112/150 (75%)	104 (93%)	8 (7%)	14	44
25	K	155/156 (99%)	152 (98%)	3 (2%)	57	81
26	L	98/124 (79%)	91 (93%)	7 (7%)	14	44
27	M	245/249 (98%)	235 (96%)	10 (4%)	30	64
28	N	152/211 (72%)	149 (98%)	3 (2%)	55	80
29	O	133/150 (89%)	124 (93%)	9 (7%)	16	45
30	P	123/154 (80%)	119 (97%)	4 (3%)	38	69
31	Q	199/256 (78%)	193 (97%)	6 (3%)	41	71
32	R	118/126 (94%)	111 (94%)	7 (6%)	19	50
33	S	141/180 (78%)	139 (99%)	2 (1%)	67	86
34	T	146/182 (80%)	145 (99%)	1 (1%)	84	93
35	U	124/135 (92%)	120 (97%)	4 (3%)	39	69
36	V	180/191 (94%)	174 (97%)	6 (3%)	38	69
37	W	83/119 (70%)	80 (96%)	3 (4%)	35	67
38	X	219/229 (96%)	214 (98%)	5 (2%)	50	77
39	Y	159/223 (71%)	154 (97%)	5 (3%)	40	70
40	Z	111/147 (76%)	107 (96%)	4 (4%)	35	67
41	b	130/186 (70%)	120 (92%)	10 (8%)	13	41
42	c	241/288 (84%)	233 (97%)	8 (3%)	38	69
43	d	207/274 (76%)	197 (95%)	10 (5%)	25	58
44	e	188/236 (80%)	182 (97%)	6 (3%)	39	69
45	f	108/188 (57%)	106 (98%)	2 (2%)	57	81
46	g	119/148 (80%)	116 (98%)	3 (2%)	47	75
47	h	101/148 (68%)	99 (98%)	2 (2%)	55	80
48	i	86/110 (78%)	81 (94%)	5 (6%)	20	51
49	j	68/97 (70%)	65 (96%)	3 (4%)	28	61

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
50	k	71/90 (79%)	68 (96%)	3 (4%)	30	62
51	l	43/116 (37%)	41 (95%)	2 (5%)	26	59
52	m	31/113 (27%)	29 (94%)	2 (6%)	17	47
53	n	157/209 (75%)	152 (97%)	5 (3%)	39	69
54	o	78/87 (90%)	75 (96%)	3 (4%)	33	66
55	p	117/181 (65%)	116 (99%)	1 (1%)	78	91
56	q	115/178 (65%)	112 (97%)	3 (3%)	46	74
57	r	141/169 (83%)	135 (96%)	6 (4%)	29	62
58	s	326/381 (86%)	319 (98%)	7 (2%)	53	79
59	t	317/371 (85%)	316 (100%)	1 (0%)	92	96
60	u	123/200 (62%)	120 (98%)	3 (2%)	49	76
61	v	59/60 (98%)	54 (92%)	5 (8%)	10	37
62	w	81/136 (60%)	75 (93%)	6 (7%)	13	42
All	All	9055/12593 (72%)	8781 (97%)	274 (3%)	44	71

All (274) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0	153	THR
2	a	60	CYS
3	1	43	LEU
5	3	103	LYS
5	3	137	THR
5	3	156	LYS
5	3	157	LEU
6	4	76	CYS
6	4	81	LEU
7	5	46	LEU
7	5	55	LEU
7	5	128	LEU
7	5	132	LEU
7	5	280	GLN
7	5	300	ARG
7	5	315	LEU
7	5	316	PHE
7	5	365	ASP
7	5	420	HIS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
8	6	41	ASP
8	6	52	ARG
8	6	184	LEU
8	6	291	TYR
8	6	371	ASP
8	6	379	ILE
9	7	50	LYS
9	7	97	GLU
9	7	143	TRP
9	7	156	ARG
9	7	196	LYS
9	7	204	LYS
9	7	234	LYS
9	7	272	THR
9	7	321	ARG
10	8	97	LYS
10	8	113	ARG
10	8	117	LEU
10	8	125	LYS
10	8	156	LYS
10	8	163	LYS
11	9	55	GLU
11	9	69	LYS
13	A1	163	LEU
13	A1	189	LEU
13	A1	226	ARG
13	A1	258	CYS
13	A1	275	ARG
15	A2	131	PHE
15	A2	133	LEU
15	A2	134	LEU
15	A2	191	GLN
15	A2	304	ARG
15	A2	319	LEU
16	C	60	ILE
16	C	120	LYS
16	C	216	THR
16	C	317	VAL
16	C	318	MET
17	D	187	LEU
17	D	281	TRP
18	E	152	VAL

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
18	E	245	THR
18	E	303	LYS
18	E	346	THR
19	F	70	ARG
19	F	130	GLN
19	F	131	LYS
19	F	263	LEU
19	F	291	SER
21	G	63	LEU
21	G	68	LEU
21	G	123	LYS
21	G	168	ARG
21	G	257	THR
21	G	284	ARG
21	G	298	ARG
21	G	300	ILE
22	H	138	LYS
22	H	145	LEU
23	I	50	VAL
23	I	57	LYS
23	I	78	LEU
23	I	99	CYS
23	I	101	ASN
23	I	122	LEU
23	I	152	MET
23	I	169	ARG
23	I	197	LEU
24	J	24	VAL
24	J	30	MET
24	J	92	LYS
24	J	102	ARG
24	J	103	GLN
24	J	106	LYS
24	J	111	LEU
24	J	149	ARG
25	K	2	SER
25	K	91	THR
25	K	178	LEU
26	L	35	MET
26	L	37	ARG
26	L	77	ILE
26	L	95	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
26	L	99	ARG
26	L	101	ASP
26	L	136	LYS
27	M	43	ARG
27	M	44	ARG
27	M	98	LEU
27	M	134	ARG
27	M	146	ASP
27	M	222	TYR
27	M	239	LYS
27	M	269	LEU
27	M	277	MET
27	M	292	LYS
28	N	63	ARG
28	N	208	ASN
28	N	238	LYS
29	O	14	VAL
29	O	20	LEU
29	O	26	ILE
29	O	28	LEU
29	O	123	ILE
29	O	144	LEU
29	O	149	LEU
29	O	155	ASP
29	O	156	LEU
30	P	80	ARG
30	P	117	TYR
30	P	120	ARG
30	P	137	LEU
31	Q	139	GLN
31	Q	214	LYS
31	Q	215	VAL
31	Q	227	LYS
31	Q	247	LEU
31	Q	271	ARG
32	R	11	ARG
32	R	32	ARG
32	R	40	ARG
32	R	82	LYS
32	R	87	ILE
32	R	104	ASP
32	R	119	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
33	S	144	LEU
33	S	182	LYS
34	T	84	LYS
35	U	11	ARG
35	U	12	LEU
35	U	27	GLN
35	U	126	LEU
36	V	40	ARG
36	V	56	LEU
36	V	118	ARG
36	V	186	THR
36	V	202	MET
36	V	213	VAL
37	W	49	ARG
37	W	88	CYS
37	W	125	VAL
38	X	59	ARG
38	X	87	LEU
38	X	96	LYS
38	X	99	LYS
38	X	161	LEU
39	Y	121	ARG
39	Y	198	ARG
39	Y	202	LEU
39	Y	226	LEU
39	Y	237	LYS
40	Z	41	ILE
40	Z	73	LYS
40	Z	119	ILE
40	Z	141	SER
41	b	4	ARG
41	b	36	ASP
41	b	80	LEU
41	b	86	GLU
41	b	100	LEU
41	b	115	ILE
41	b	119	PHE
41	b	122	ASP
41	b	123	ASN
41	b	141	ARG
42	c	68	TYR
42	c	86	ASP

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
42	c	173	LEU
42	c	193	GLN
42	c	246	LYS
42	c	279	LYS
42	c	280	LEU
42	c	287	GLU
43	d	36	ARG
43	d	74	ARG
43	d	111	ARG
43	d	112	MET
43	d	163	LEU
43	d	194	VAL
43	d	203	MET
43	d	238	VAL
43	d	266	VAL
43	d	287	LEU
44	e	126	GLN
44	e	127	LYS
44	e	133	LEU
44	e	227	LEU
44	e	239	LEU
44	e	243	PHE
45	f	171	LEU
45	f	212	LYS
46	g	43	ASP
46	g	143	VAL
46	g	147	LEU
47	h	56	ARG
47	h	75	LYS
48	i	36	LEU
48	i	37	THR
48	i	80	LEU
48	i	105	ASP
48	i	107	LEU
49	j	67	LYS
49	j	93	LEU
49	j	103	ARG
50	k	34	LEU
50	k	41	LYS
50	k	56	ARG
51	l	110	LEU
51	l	128	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
52	m	40	LEU
52	m	51	LEU
53	n	55	ARG
53	n	140	LEU
53	n	147	ARG
53	n	155	MET
53	n	224	ARG
54	o	46	HIS
54	o	91	GLN
54	o	98	THR
55	p	179	ARG
56	q	96	LEU
56	q	113	LYS
56	q	150	LYS
57	r	52	ARG
57	r	58	LYS
57	r	70	CYS
57	r	108	CYS
57	r	159	VAL
57	r	164	LYS
58	s	52	THR
58	s	66	TRP
58	s	150	LEU
58	s	200	LEU
58	s	230	ARG
58	s	279	GLU
58	s	379	LEU
59	t	331	ARG
20	t1	-3	LYS
20	t1	3	ILE
20	t3	27	LYS
60	u	92	PHE
60	u	156	HIS
60	u	196	LEU
61	v	16	LEU
61	v	29	ASP
61	v	45	LEU
61	v	47	ASP
61	v	61	PHE
62	w	74	LEU
62	w	75	THR
62	w	88	LYS

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Mol	Chain	Res	Type
62	w	89	LEU
62	w	132	ASP
62	w	137	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (56) such sidechains are listed below:

Mol	Chain	Res	Type
4	2	77	GLN
5	3	154	GLN
7	5	96	HIS
7	5	108	HIS
7	5	165	GLN
7	5	385	HIS
8	6	66	GLN
8	6	354	GLN
9	7	298	GLN
10	8	143	GLN
13	A1	317	ASN
13	A1	367	ASN
15	A2	191	GLN
15	A2	255	GLN
16	C	295	GLN
16	C	297	ASN
19	F	103	GLN
23	I	101	ASN
23	I	225	GLN
25	K	26	GLN
25	K	126	HIS
25	K	147	GLN
27	M	26	ASN
27	M	30	ASN
27	M	92	GLN
27	M	264	GLN
28	N	210	GLN
29	O	69	ASN
30	P	147	GLN
32	R	79	HIS
32	R	94	GLN
33	S	84	ASN
34	T	132	HIS
35	U	103	GLN
35	U	138	GLN

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Mol	Chain	Res	Type
38	X	15	GLN
39	Y	99	HIS
39	Y	183	GLN
41	b	120	HIS
42	c	122	ASN
42	c	172	ASN
42	c	193	GLN
43	d	149	HIS
44	e	175	GLN
45	f	111	HIS
45	f	153	HIS
48	i	59	ASN
49	j	63	GLN
53	n	214	ASN
54	o	33	GLN
54	o	94	HIS
58	s	87	GLN
58	s	101	ASN
58	s	239	ASN
60	u	156	HIS
62	w	103	HIS

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
12	A	1427/1559 (91%)	355 (24%)	54 (3%)
14	B	56/69 (81%)	19 (33%)	2 (3%)
All	All	1483/1628 (91%)	374 (25%)	56 (3%)

All (374) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
12	A	1678	C
12	A	1679	U
12	A	1680	A
12	A	1681	G
12	A	1689	C
12	A	1693	C
12	A	1694	U
12	A	1699	C
12	A	1700	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
12	A	1704	U
12	A	1707	C
12	A	1708	A
12	A	1714	C
12	A	1715	C
12	A	1724	A
12	A	1728	U
12	A	1733	C
12	A	1734	C
12	A	1735	A
12	A	1736	A
12	A	1743	U
12	A	1748	G
12	A	1750	G
12	A	1751	A
12	A	1769	C
12	A	1770	G
12	A	1780	U
12	A	1794	A
12	A	1795	A
12	A	1798	A
12	A	1804	A
12	A	1805	A
12	A	1812	C
12	A	1817	C
12	A	1824	U
12	A	1827	C
12	A	1828	A
12	A	1829	A
12	A	1832	A
12	A	1836	A
12	A	1844	A
12	A	1849	C
12	A	1852	C
12	A	1853	A
12	A	1854	U
12	A	1855	A
12	A	1856	A
12	A	1867	A
12	A	1869	A
12	A	1872	U
12	A	1878	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
12	A	1882	A
12	A	1883	G
12	A	1887	A
12	A	1892	A
12	A	1893	A
12	A	1901	C
12	A	1902	C
12	A	1903	C
12	A	1909	A
12	A	1918	G
12	A	1936	A
12	A	1937	A
12	A	1938	A
12	A	1940	A
12	A	1946	C
12	A	1974	A
12	A	1975	U
12	A	1985	G
12	A	1986	A
12	A	1994	A
12	A	1995	A
12	A	2000	C
12	A	2001	C
12	A	2002	G
12	A	2015	G
12	A	2016	C
12	A	2021	U
12	A	2022	G
12	A	2029	A
12	A	2030	U
12	A	2031	A
12	A	2036	C
12	A	2037	U
12	A	2039	A
12	A	2044	A
12	A	2055	U
12	A	2060	A
12	A	2065	A
12	A	2066	C
12	A	2070	C
12	A	2071	U
12	A	2074	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
12	A	2079	C
12	A	2085	A
12	A	2092	C
12	A	2097	A
12	A	2098	G
12	A	2105	G
12	A	2107	G
12	A	2108	G
12	A	2111	C
12	A	2112	A
12	A	2113	G
12	A	2114	C
12	A	2126	U
12	A	2131	A
12	A	2135	A
12	A	2136	C
12	A	2142	A
12	A	2147	G
12	A	2154	A
12	A	2158	U
12	A	2159	U
12	A	2160	A
12	A	2167	A
12	A	2171	U
12	A	2172	A
12	A	2173	G
12	A	2174	G
12	A	2175	C
12	A	2178	A
12	A	2179	A
12	A	2181	A
12	A	2182	G
12	A	2183	C
12	A	2187	C
12	A	2194	U
12	A	2195	A
12	A	2196	A
12	A	2197	G
12	A	2198	A
12	A	2199	A
12	A	2200	A
12	A	2210	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
12	A	2211	U
12	A	2228	A
12	A	2229	A
12	A	2230	A
12	A	2233	U
12	A	2237	A
12	A	2241	A
12	A	2243	A
12	A	2245	A
12	A	2246	A
12	A	2250	A
12	A	2251	A
12	A	2257	C
12	A	2262	C
12	A	2263	C
12	A	2264	A
12	A	2284	C
12	A	2285	U
12	A	2297	A
12	A	2300	G
12	A	2321	A
12	A	2322	C
12	A	2324	U
12	A	2332	C
12	A	2345	G
12	A	2348	A
12	A	2350	A
12	A	2351	U
12	A	2358	A
12	A	2359	C
12	A	2360	U
12	A	2361	G
12	A	2362	A
12	A	2363	A
12	A	2374	A
12	A	2381	A
12	A	2390	A
12	A	2394	A
12	A	2401	A
12	A	2404	U
12	A	2406	A
12	A	2407	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
12	A	2414	C
12	A	2415	C
12	A	2418	A
12	A	2434	A
12	A	2446	A
12	A	2451	A
12	A	2452	A
12	A	2457	A
12	A	2458	A
12	A	2478	G
12	A	2483	U
12	A	2485	U
12	A	2488	C
12	A	2493	C
12	A	2494	C
12	A	2500	A
12	A	2502	C
12	A	2511	C
12	A	2520	C
12	A	2521	A
12	A	2527	A
12	A	2530	A
12	A	2531	U
12	A	2536	G
12	A	2539	A
12	A	2540	C
12	A	2544	C
12	A	2547	C
12	A	2548	C
12	A	2549	C
12	A	2550	A
12	A	2554	A
12	A	2603	C
12	A	2611	C
12	A	2613	U
12	A	2617	A
12	A	2618	U
12	A	2619	A
12	A	2620	G
12	A	2621	G
12	A	2622	G
12	A	2623	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
12	A	2626	U
12	A	2627	G
12	A	2628	U
12	A	2629	A
12	A	2630	U
12	A	2633	A
12	A	2634	U
12	A	2645	G
12	A	2654	U
12	A	2655	G
12	A	2656	U
12	A	2660	U
12	A	2670	C
12	A	2683	C
12	A	2684	C
12	A	2686	G
12	A	2693	A
12	A	2694	A
12	A	2695	G
12	A	2696	A
12	A	2698	G
12	A	2699	C
12	A	2706	A
12	A	2709	A
12	A	2719	G
12	A	2722	A
12	A	2723	A
12	A	2724	G
12	A	2725	A
12	A	2732	G
12	A	2739	U
12	A	2740	A
12	A	2743	U
12	A	2756	C
12	A	2810	G
12	A	2815	G
12	A	2816	G
12	A	2819	G
12	A	2828	G
12	A	2831	G
12	A	2832	A
12	A	2833	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
12	A	2840	C
12	A	2843	C
12	A	2844	G
12	A	2847	C
12	A	2854	U
12	A	2864	U
12	A	2865	C
12	A	2880	A
12	A	2906	C
12	A	2912	C
12	A	2913	A
12	A	2917	G
12	A	2918	A
12	A	2919	A
12	A	2922	A
12	A	2926	A
12	A	2928	C
12	A	2932	G
12	A	2934	G
12	A	2935	A
12	A	2936	U
12	A	2937	A
12	A	2946	A
12	A	2956	A
12	A	2963	A
12	A	2978	U
12	A	2984	A
12	A	2986	C
12	A	2987	U
12	A	2988	C
12	A	2989	G
12	A	2990	A
12	A	2991	U
12	A	2992	G
12	A	3005	A
12	A	3007	C
12	A	3016	G
12	A	3018	A
12	A	3021	C
12	A	3022	G
12	A	3041	U
12	A	3042	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
12	A	3051	A
12	A	3053	A
12	A	3054	G
12	A	3060	C
12	A	3067	U
12	A	3069	A
12	A	3070	G
12	A	3072	U
12	A	3086	U
12	A	3089	A
12	A	3090	G
12	A	3097	U
12	A	3098	U
12	A	3100	U
12	A	3102	U
12	A	3108	U
12	A	3109	U
12	A	3111	A
12	A	3112	A
12	A	3113	A
12	A	3123	G
12	A	3141	A
12	A	3150	U
12	A	3157	C
12	A	3158	A
12	A	3162	C
12	A	3168	C
12	A	3169	C
12	A	3170	C
12	A	3171	C
12	A	3172	C
12	A	3173	G
12	A	3177	A
12	A	3180	A
12	A	3184	C
12	A	3189	C
12	A	3190	A
12	A	3196	G
12	A	3197	U
12	A	3198	A
12	A	3199	U
12	A	3201	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
12	A	3202	U
12	A	3207	A
12	A	3208	C
12	A	3209	A
12	A	3211	C
12	A	3212	C
12	A	3217	A
12	A	3218	A
12	A	3220	A
12	A	3228	U
14	B	1604	G
14	B	1608	G
14	B	1609	U
14	B	1610	A
14	B	1611	G
14	B	1614	U
14	B	1615	A
14	B	1617	C
14	B	1618	A
14	B	1620	A
14	B	1621	A
14	B	1622	A
14	B	1628	C
14	B	1632	U
14	B	1633	U
14	B	1644	G
14	B	1645	A
14	B	1646	U
14	B	1670	A

All (56) RNA pucker outliers are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
12	A	1727	A
12	A	1749	C
12	A	1772	A
12	A	1811	A
12	A	1823	A
12	A	1824	U
12	A	1853	A
12	A	1854	U
12	A	1855	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
12	A	1871	A
12	A	1936	A
12	A	1956	U
12	A	1974	A
12	A	1994	A
12	A	2001	C
12	A	2015	G
12	A	2021	U
12	A	2030	U
12	A	2065	A
12	A	2097	A
12	A	2135	A
12	A	2158	U
12	A	2182	G
12	A	2186	C
12	A	2245	A
12	A	2291	A
12	A	2347	C
12	A	2361	G
12	A	2380	C
12	A	2417	C
12	A	2457	A
12	A	2527	A
12	A	2530	A
12	A	2543	C
12	A	2619	A
12	A	2620	G
12	A	2628	U
12	A	2629	A
12	A	2630	U
12	A	2653	C
12	A	2723	A
12	A	2724	G
12	A	2739	U
12	A	2818	C
12	A	2832	A
12	A	2846	G
12	A	2905	A
12	A	2926	A
12	A	2935	A
12	A	2991	U
12	A	3004	C

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Mol	Chain	Res	Type
12	A	3041	U
12	A	3068	G
12	A	3206	C
14	B	1607	U
14	B	1614	U

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

1 non-standard protein/DNA/RNA residue is 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
12	OMG	A	3040	12	18,26,27	1.44	2 (11%)	20,38,41	2.21	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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	OMG	A	3040	12	-	0/5/27/28	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	A	3040	OMG	C6-C5	4.39	1.48	1.41
12	A	3040	OMG	C5-C4	2.93	1.48	1.40

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	A	3040	OMG	C2-N3-C4	4.79	120.82	115.36
12	A	3040	OMG	C6-N1-C2	4.19	122.58	115.93
12	A	3040	OMG	C5-C6-N1	-4.13	117.78	123.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	A	3040	OMG	C6-C5-C4	-3.94	117.03	120.80
12	A	3040	OMG	N3-C2-N1	-3.41	122.67	127.22
12	A	3040	OMG	C4-C5-N7	-2.12	107.19	109.40

There are no chirality outliers.

There are no torsion outliers.

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 101 ligands modelled in this entry, 95 are monoatomic - leaving 6 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
67	GDP	C	401	-	24,30,30	1.18	2 (8%)	31,47,47	1.99	8 (25%)
69	SAH	n	301	-	21,28,28	0.64	0	20,40,40	0.82	2 (10%)
70	PNS	w	201	62	13,20,21	0.30	0	18,26,29	0.73	0
66	SAM	A1	401	-	21,29,29	0.64	0	18,42,42	0.96	2 (11%)
68	GTP	G	502	65	26,34,34	1.06	1 (3%)	33,54,54	2.04	4 (12%)
67	GDP	t	501	65	24,30,30	1.30	2 (8%)	31,47,47	2.01	8 (25%)

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
67	GDP	C	401	-	-	0/12/32/32	0/3/3/3
69	SAH	n	301	-	-	3/7/31/31	0/3/3/3
70	PNS	w	201	62	-	16/24/26/27	-
66	SAM	A1	401	-	-	3/8/33/33	0/3/3/3
68	GTP	G	502	65	-	2/18/38/38	0/3/3/3
67	GDP	t	501	65	-	0/12/32/32	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
67	t	501	GDP	C6-C5	4.65	1.49	1.41
67	C	401	GDP	C6-C5	4.16	1.48	1.41
68	G	502	GTP	C6-N1	4.09	1.40	1.33
67	t	501	GDP	C5-C4	2.69	1.48	1.40
67	C	401	GDP	C5-C4	2.47	1.47	1.40

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
68	G	502	GTP	C5-C6-N1	-8.69	111.55	123.43
68	G	502	GTP	C6-N1-C2	5.80	125.14	115.93
67	t	501	GDP	C2-N3-C4	5.40	121.52	115.36
67	C	401	GDP	C2-N3-C4	5.07	121.14	115.36
67	C	401	GDP	C5-C6-N1	-4.02	117.93	123.43
67	C	401	GDP	C6-N1-C2	3.99	122.27	115.93
67	t	501	GDP	C6-N1-C2	3.99	122.26	115.93
67	t	501	GDP	C6-C5-C4	-3.95	117.03	120.80
67	t	501	GDP	C5-C6-N1	-3.66	118.43	123.43
67	C	401	GDP	PA-O3A-PB	-3.62	120.40	132.83
67	C	401	GDP	C6-C5-C4	-3.57	117.39	120.80
67	t	501	GDP	N3-C2-N1	-3.56	122.47	127.22
67	C	401	GDP	N3-C2-N1	-3.27	122.86	127.22
67	C	401	GDP	C3'-C2'-C1'	3.15	105.73	100.98
67	t	501	GDP	C3'-C2'-C1'	2.84	105.26	100.98
68	G	502	GTP	N3-C2-N1	-2.84	123.44	127.22
67	t	501	GDP	C4-C5-N7	-2.69	106.60	109.40
67	t	501	GDP	PA-O3A-PB	-2.62	123.83	132.83
67	C	401	GDP	C4-C5-N7	-2.62	106.67	109.40
68	G	502	GTP	C2-N3-C4	-2.49	112.52	115.36
69	n	301	SAH	C3'-C2'-C1'	2.17	104.25	100.98
66	A1	401	SAM	C3'-C2'-C1'	2.10	104.14	100.98
69	n	301	SAH	C5-C6-N6	2.01	123.40	120.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
66	A1	401	SAM	C5-C6-N6	2.00	123.40	120.35

There are no chirality outliers.

All (24) torsion outliers are listed below:

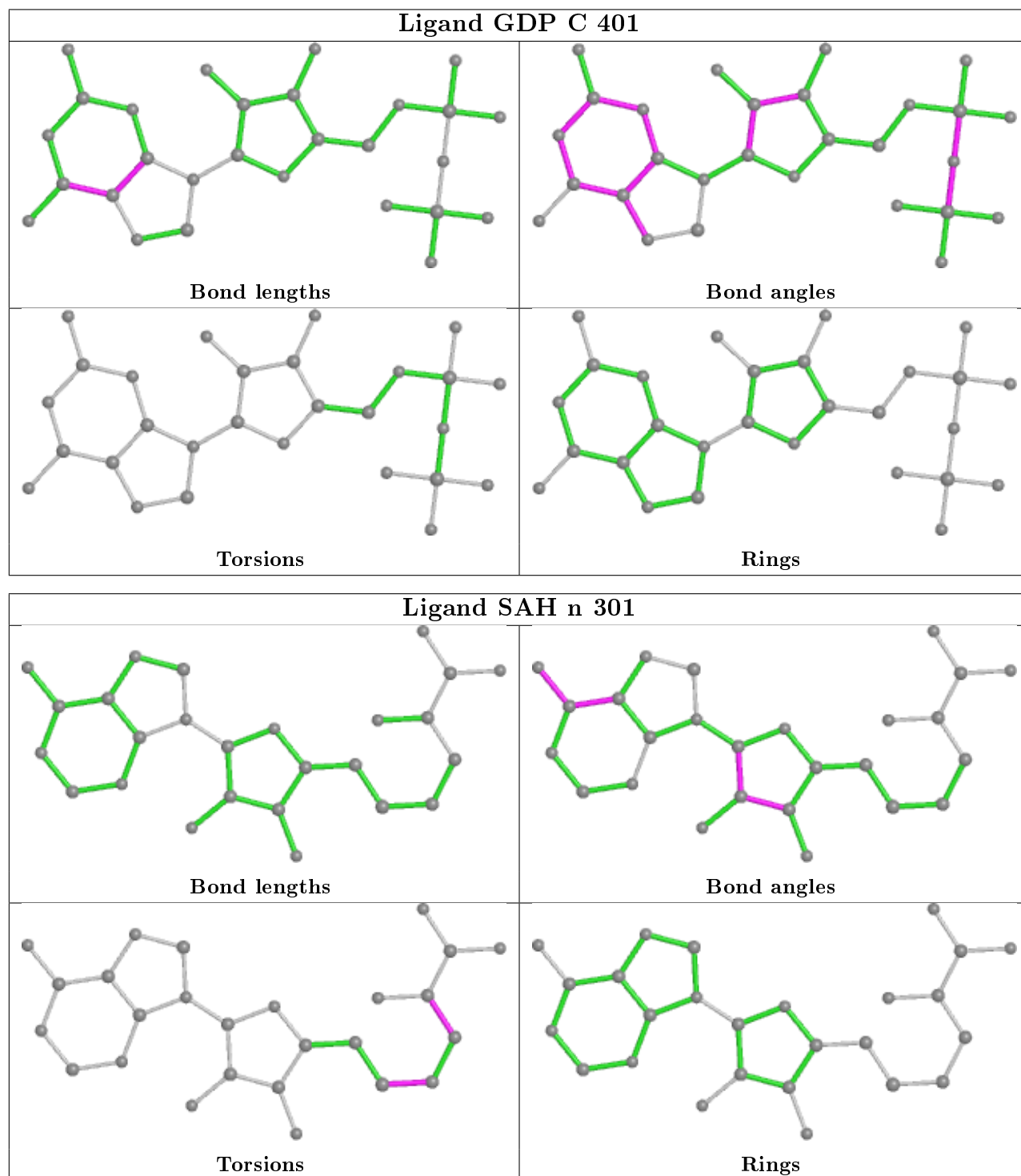
Mol	Chain	Res	Type	Atoms
66	A1	401	SAM	N-CA-CB-CG
66	A1	401	SAM	C-CA-CB-CG
66	A1	401	SAM	CA-CB-CG-SD
69	n	301	SAH	C-CA-CB-CG
70	w	201	PNS	O27-C28-C29-C31
70	w	201	PNS	O27-C28-C29-C32
70	w	201	PNS	C28-C29-C32-C34
70	w	201	PNS	O33-C32-C34-N36
70	w	201	PNS	C32-C34-N36-C37
70	w	201	PNS	O35-C34-N36-C37
70	w	201	PNS	N36-C37-C38-C39
70	w	201	PNS	O40-C39-N41-C42
70	w	201	PNS	O27-C28-C29-C30
70	w	201	PNS	C38-C39-N41-C42
70	w	201	PNS	O33-C32-C34-O35
70	w	201	PNS	N41-C42-C43-S44
70	w	201	PNS	C30-C29-C32-C34
70	w	201	PNS	C31-C29-C32-C34
69	n	301	SAH	N-CA-CB-CG
69	n	301	SAH	CB-CG-SD-C5'
68	G	502	GTP	O4'-C4'-C5'-O5'
68	G	502	GTP	PA-O3A-PB-O2B
70	w	201	PNS	C37-C38-C39-O40
70	w	201	PNS	C37-C38-C39-N41

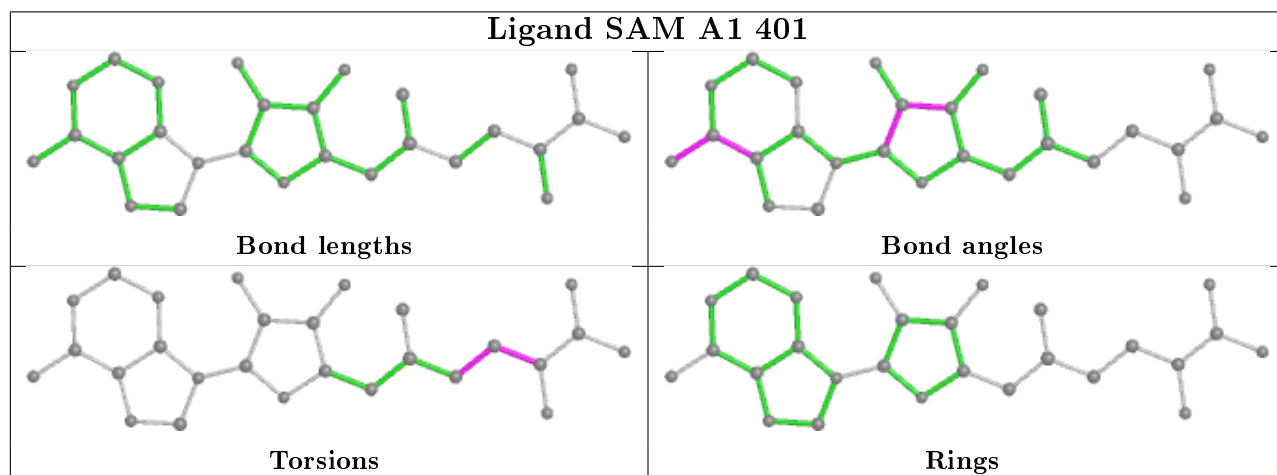
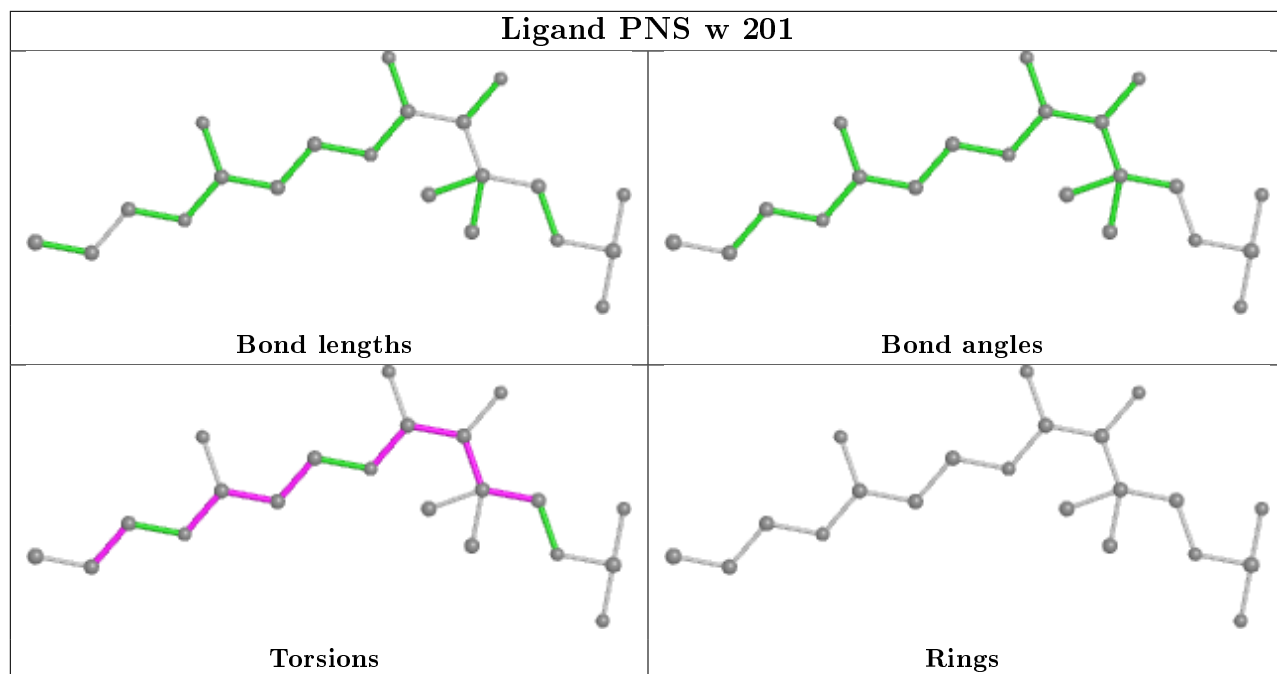
There are no ring outliers.

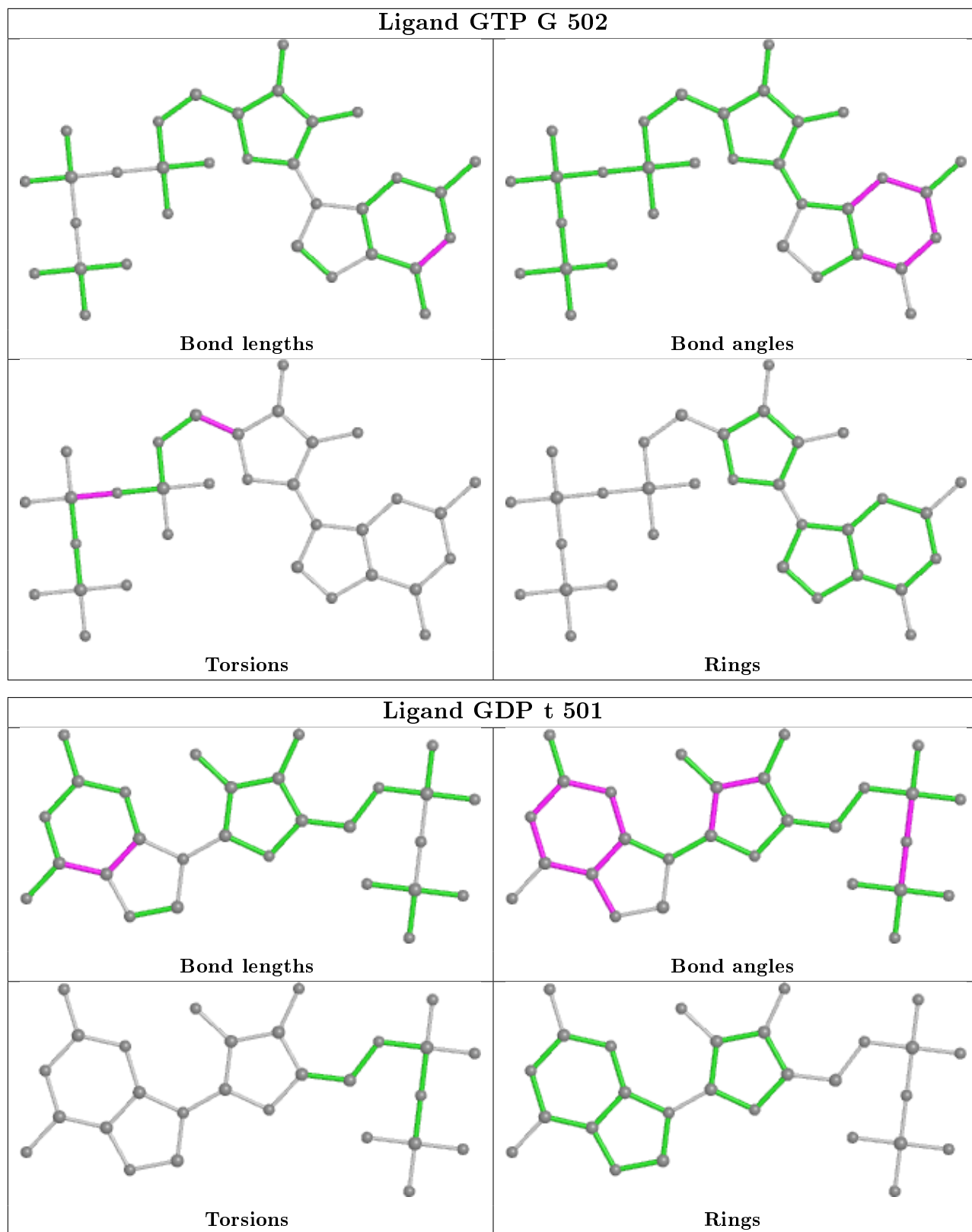
No monomer is involved in short contacts.

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

There are no chain breaks in this entry.

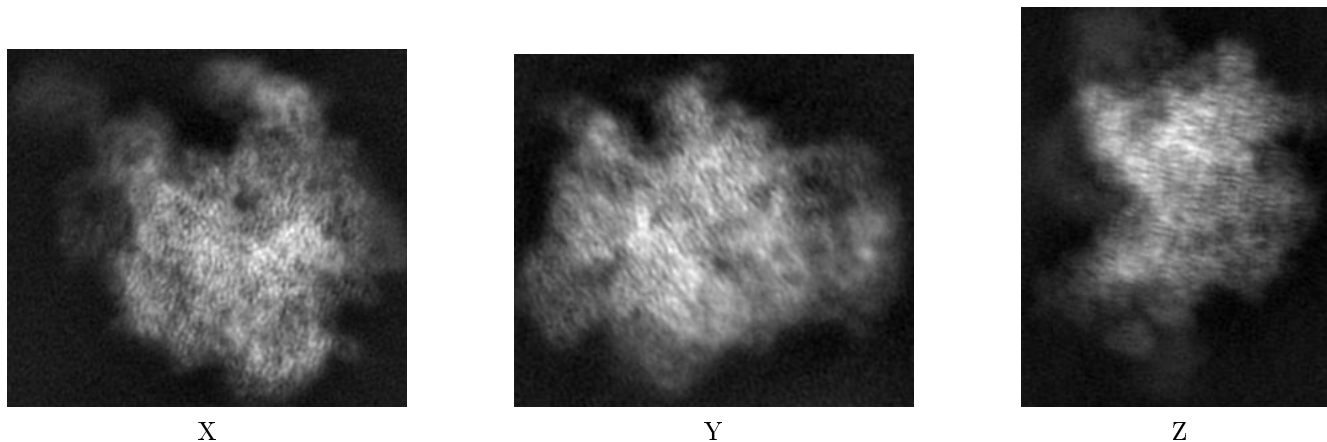
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-12763. These allow visual inspection of the internal detail of the map and identification of artifacts.

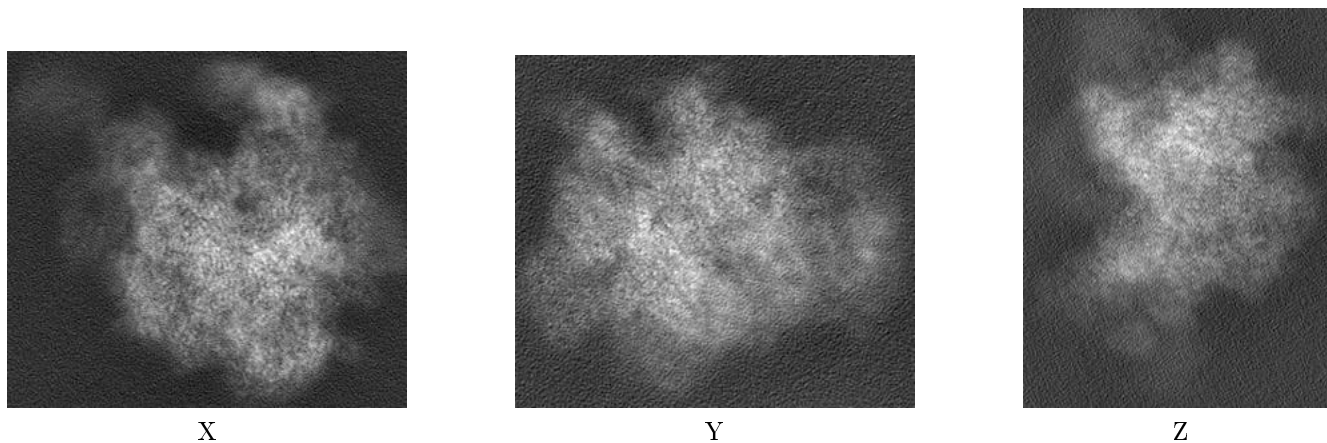
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

#### 6.1.1 Primary map



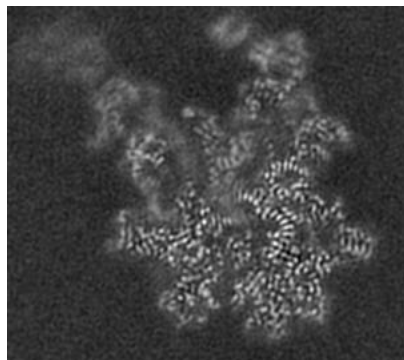
#### 6.1.2 Raw map



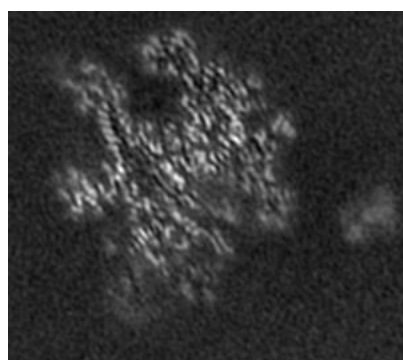
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

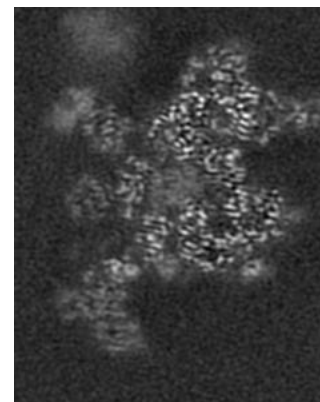
### 6.2.1 Primary map



X Index: 108

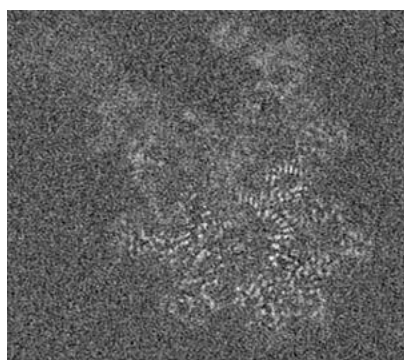


Y Index: 137

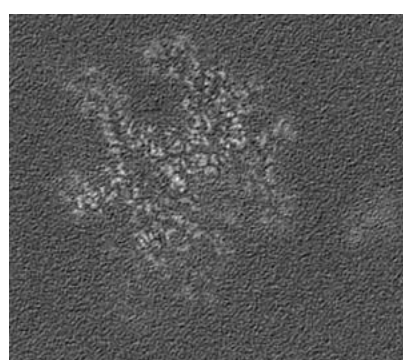


Z Index: 123

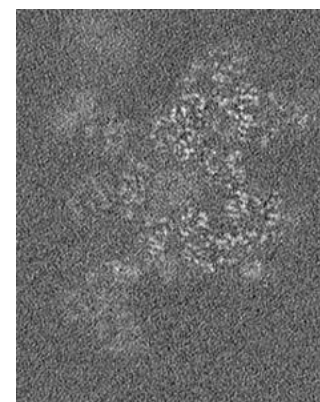
### 6.2.2 Raw map



X Index: 108



Y Index: 138



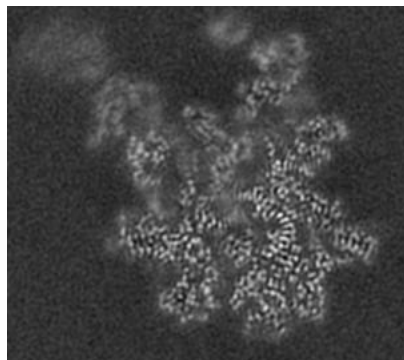
Z Index: 123

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

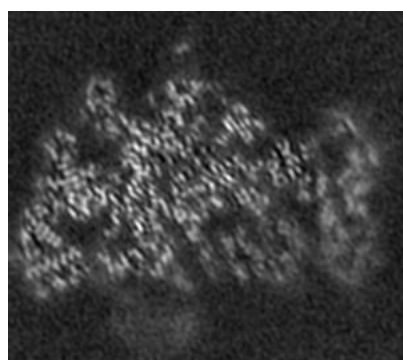


## 6.3 Largest variance slices [i](#)

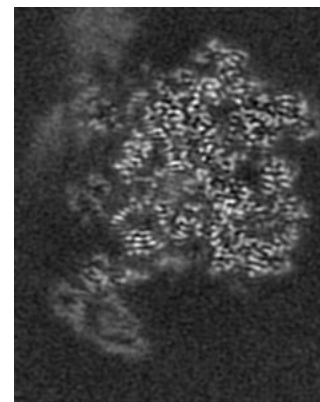
### 6.3.1 Primary map



X Index: 106

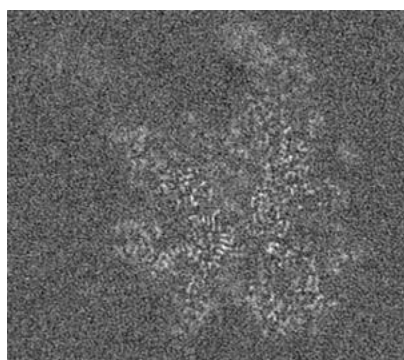


Y Index: 181

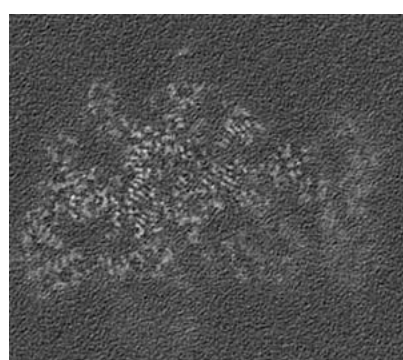


Z Index: 113

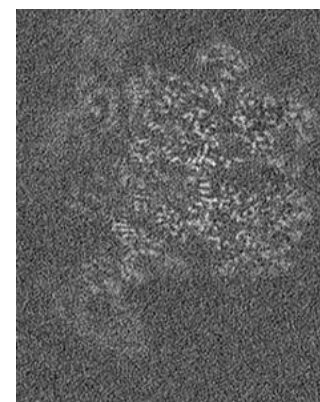
### 6.3.2 Raw map



X Index: 117



Y Index: 182



Z Index: 110

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



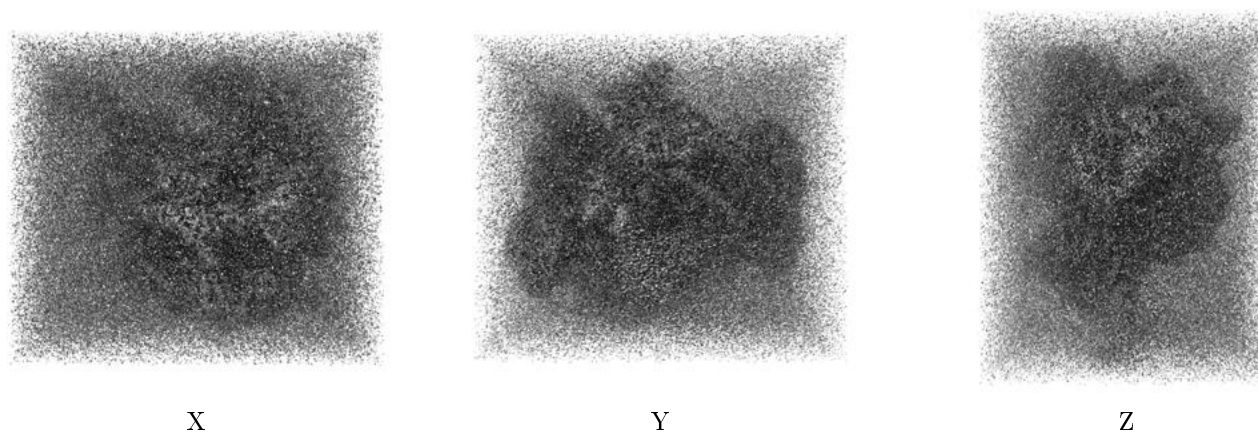
## 6.4 Orthogonal surface views [i](#)

### 6.4.1 Primary map



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

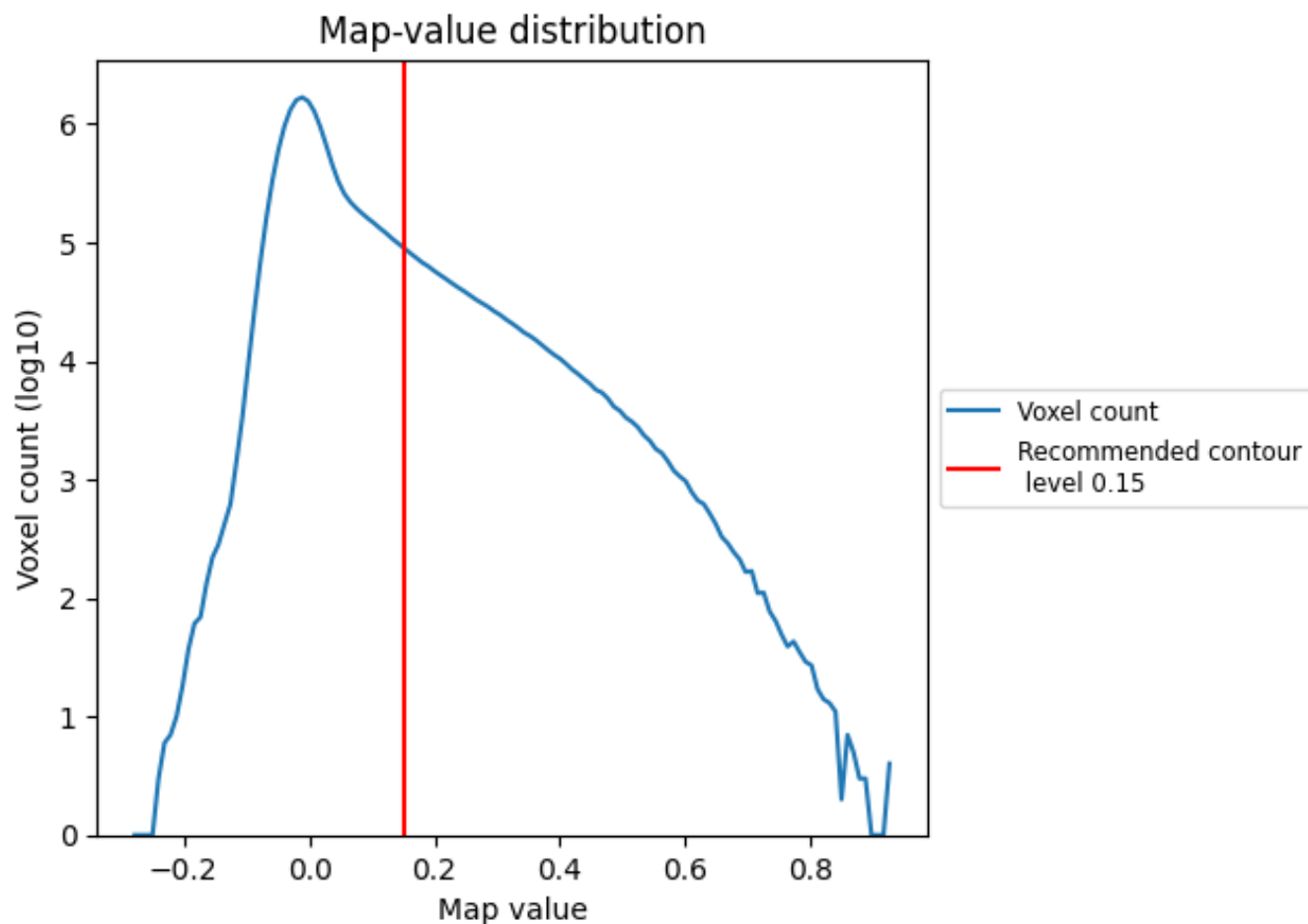
## 6.5 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

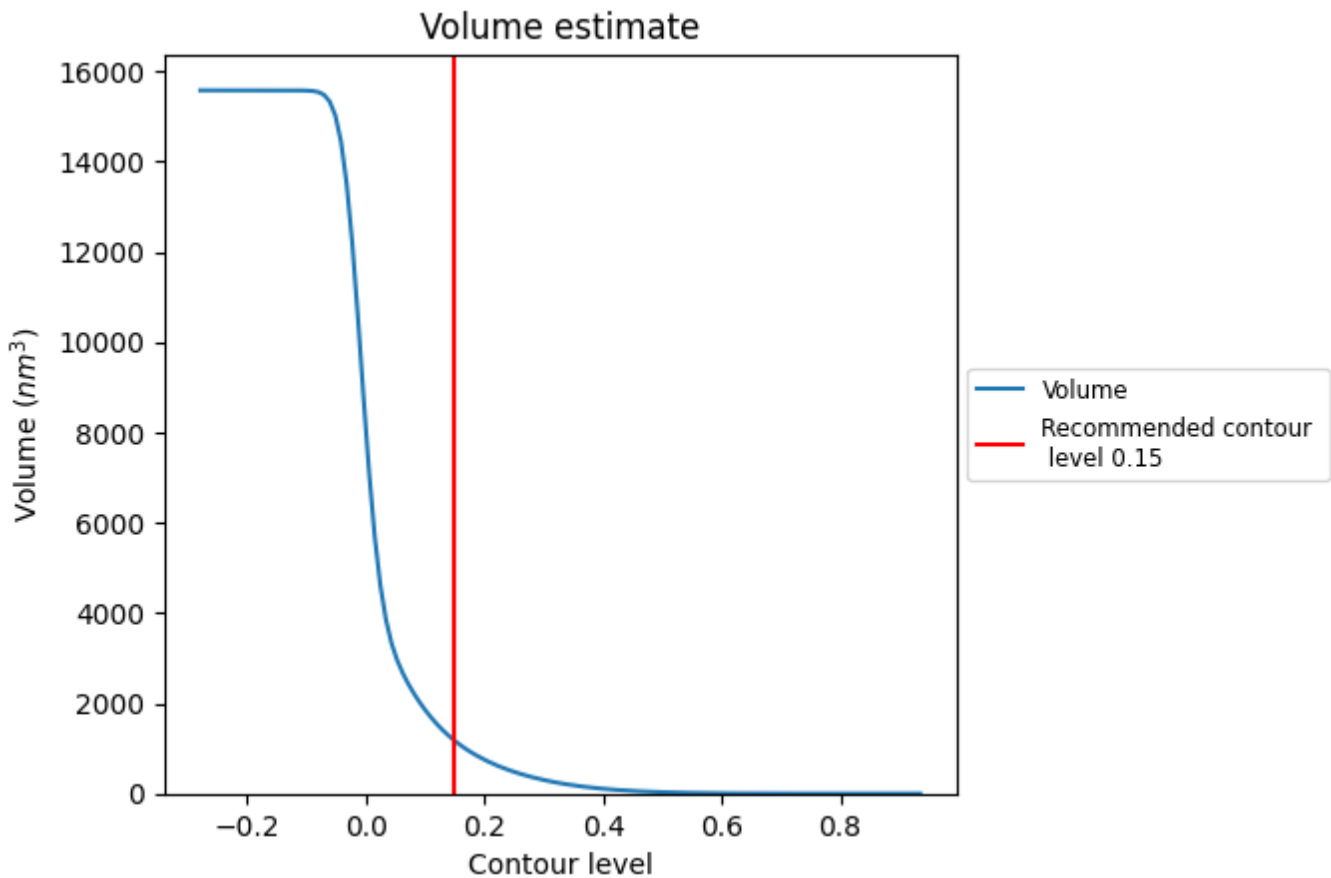
This section contains the results of statistical analysis of the map.

### 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 1174 nm<sup>3</sup>; this corresponds to an approximate mass of 1061 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.

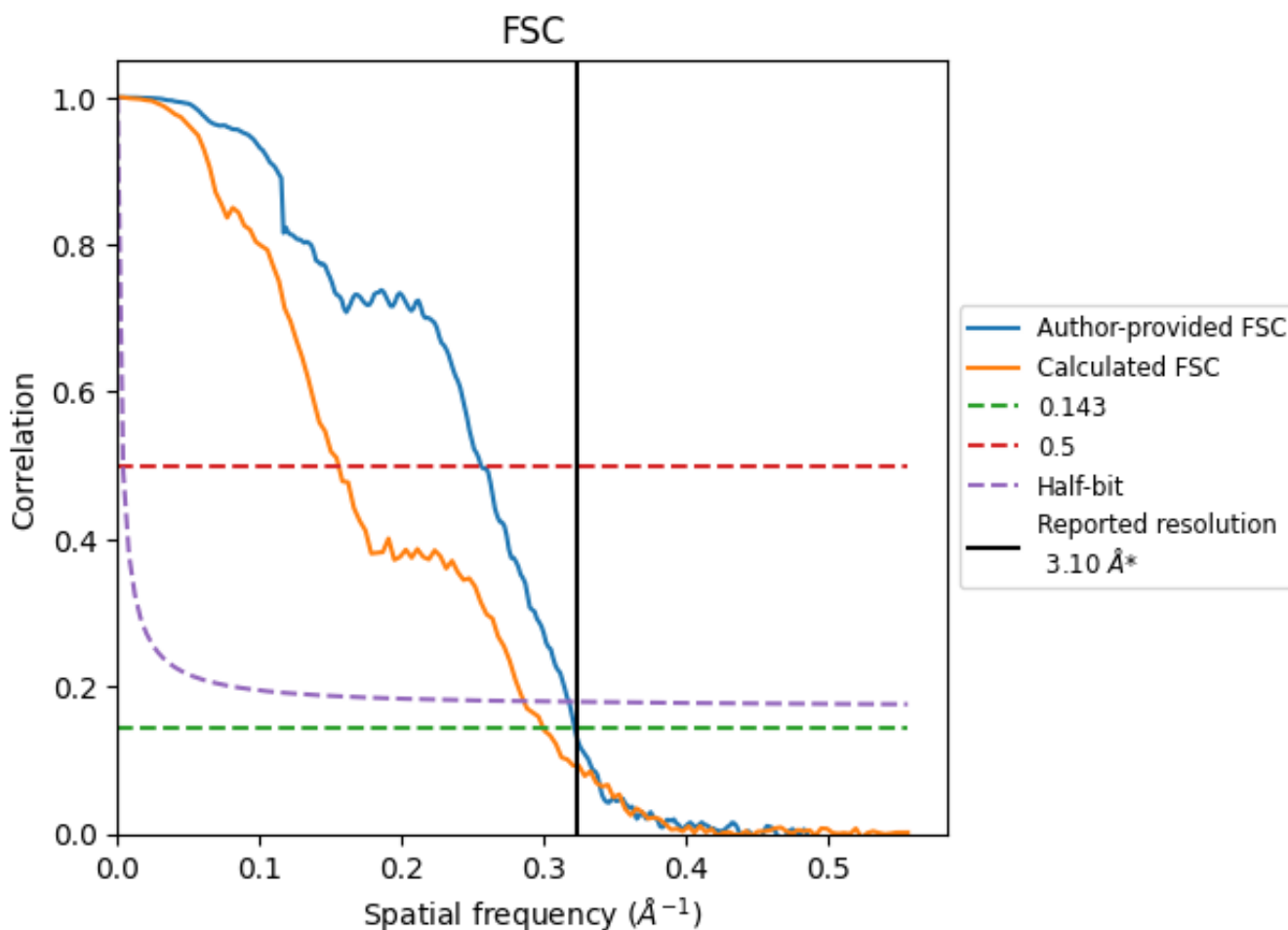
## 7.3 Rotationally averaged power spectrum [i](#)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

## 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 0.323 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

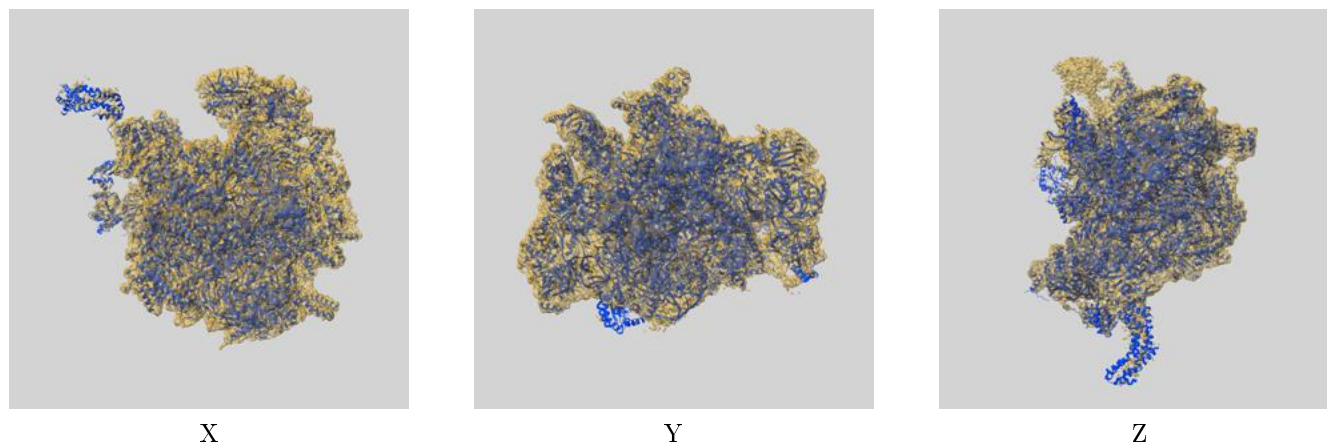
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.11	3.91	3.14
Calculated*	3.34	6.43	3.50

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

## 9 Map-model fit [i](#)

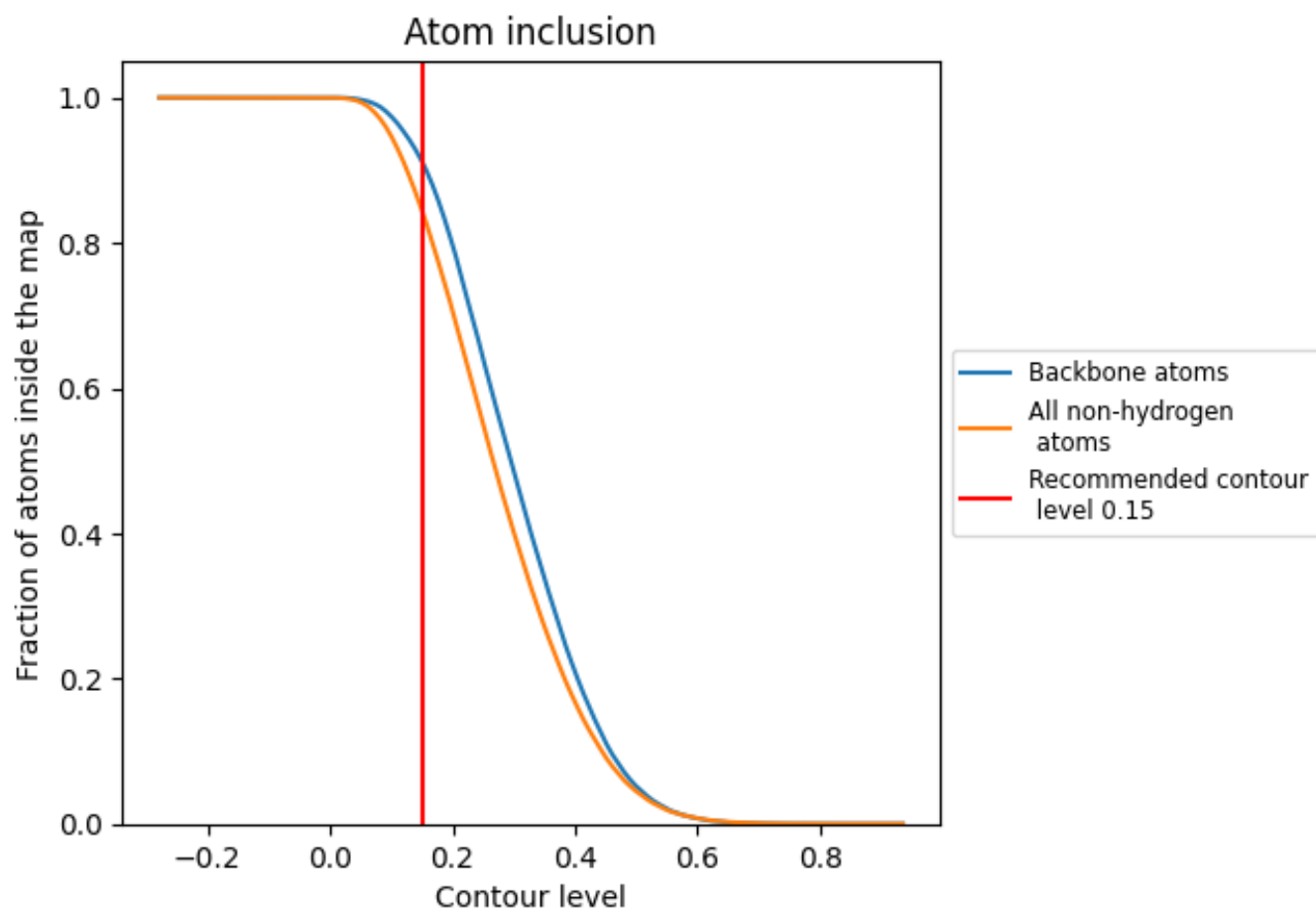
This section contains information regarding the fit between EMDB map EMD-12763 and PDB model 7O9K. Per-residue inclusion information can be found in section 3 on page 19.

### 9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 9.2 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 84% of all non-hydrogen atoms, are inside the map.