wwPDB EM Validation Summary Report

Dec 19, 2022 – 06:31 am GMT

PDB ID	:	7NSH
EMDB ID	:	EMD-12567
Title	:	39S mammalian mitochondrial large ribosomal subunit with mtRRF (post) and mtEFG2
Authors	:	Kummer, E.; Schubert, K.; Ban, N.
Deposited on	:	2021-03-07
Resolution	:	3.20 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

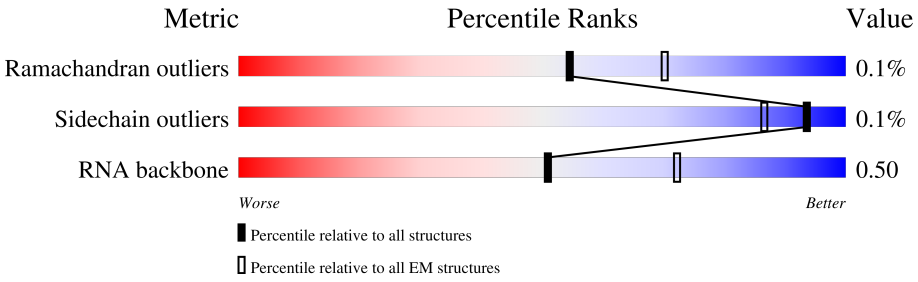
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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 3.20 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 <=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	B0	148	74% 26%
2	BY	216	11% 94% 5%
3	Ba	423	93% 7%
4	B8	188	51% 49%
5	Bb	380	93% 7%
6	Bc	334	88% 12%
7	Bd	206	50% 68% 32%
8	Be	135	90% 10%

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Mol	Chain	Length	Quality of chain
9	Bf	142	13% 74% 24%
10	Bg	159	93% 7%
11	Bh	332	87% 13%
12	Bi	306	20% 85% 15%
13	Bj	279	63% 77% 22%
14	Bk	269	33% 58% 42%
15	Bl	166	80% 20%
16	Bm	198	16% 55% 45%
17	Bn	128	75% 24%
18	Bo	124	78% 22%
19	Bp	112	9% 87% 13%
20	Bq	138	9% 57% 42%
21	Bt	102	92% 8%
22	Bu	205	13% 73% 26%
23	Bv	222	8% 61% 39%
24	Bw	433	89% 11%
25	Bx	196	83% 17%
26	CL	198	21% 23% 77%
26	DL	198	13% 13% 86%
26	EL	198	14% 14% 86%
26	FL	198	14% 14% 86%
26	GL	198	14% 14% 86%
26	HL	198	13% 13% 87%
26	LL	198	35% 35% 65%
27	B1	256	95% 5%

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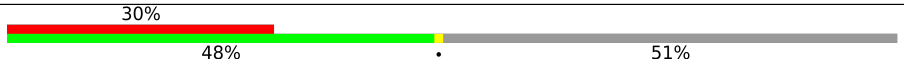
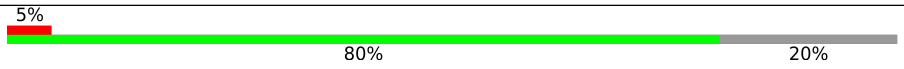
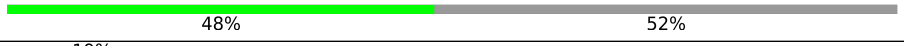
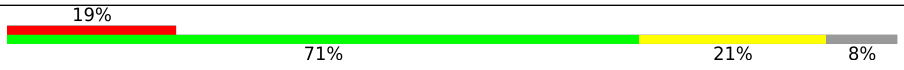
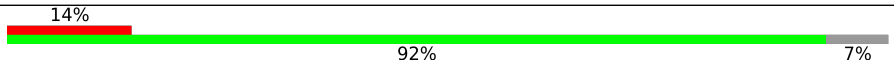
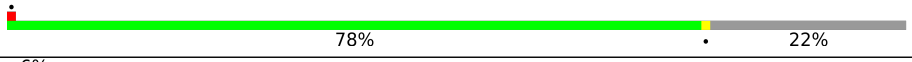
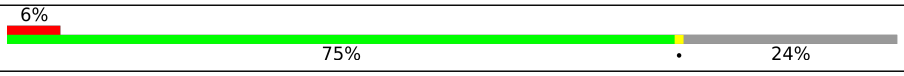
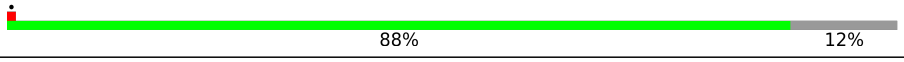
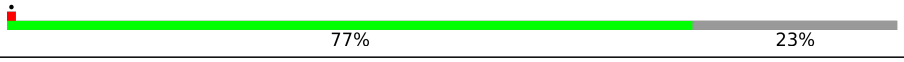
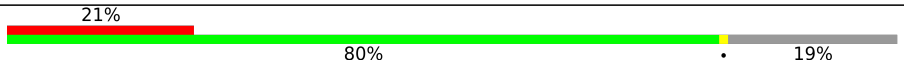
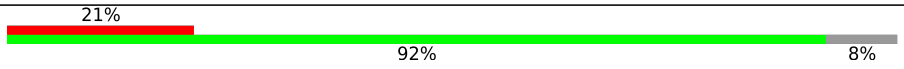
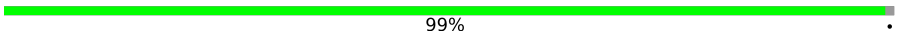
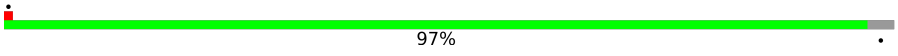
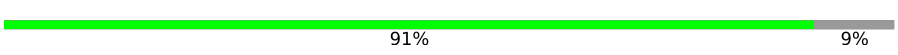
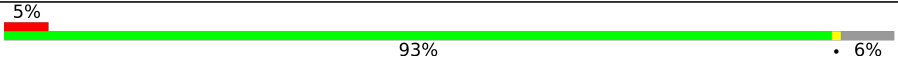
Mol	Chain	Length	Quality of chain
28	B9	100	
29	BA	1571	
30	B2	252	
31	B3	161	
32	B4	126	
33	B5	188	
34	B6	65	
35	B7	95	
36	BB	73	
37	BC	755	
38	BD	306	
39	BG	257	
40	BQ	251	
41	BE	399	
42	BF	294	
43	BI	268	
44	BJ	262	
45	BK	192	
46	BN	178	
47	BO	145	
48	BP	296	
49	BR	169	
50	BS	180	
51	BT	292	
52	BU	149	

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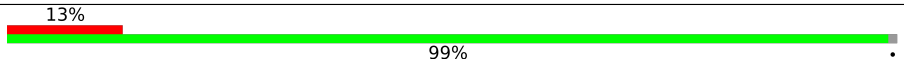
Mol	Chain	Length	Quality of chain
53	BV	209	
54	BW	210	
55	BX	150	

2 Entry composition (i)

There are 61 unique types of molecules in this entry. The entry contains 112448 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 Mitochondrial ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	B0	110	857	553	156	145	3	0	0

- Molecule 2 is a protein called uL24m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	BY	206	1678	1056	308	309	5	0	0

- Molecule 3 is a protein called Mitochondrial ribosomal protein L37.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	Ba	393	3173	2040	556	565	12	0	0

- Molecule 4 is a protein called Mitochondrial ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	B8	95	833	539	163	129	2	0	0

- Molecule 5 is a protein called Mitochondrial ribosomal protein L38.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	Bb	354	2952	1876	542	525	9	0	0

- Molecule 6 is a protein called Mitochondrial ribosomal protein L39.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	Bc	295	2408	1541	410	441	16	0	0

- Molecule 7 is a protein called Mitochondrial ribosomal protein L40.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	Bd	140	Total	C	N	O	S	0	0
			1177	742	213	221	1		

- Molecule 8 is a protein called Mitochondrial ribosomal protein L41.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	Be	122	Total	C	N	O	S	0	0
			972	628	168	173	3		

- Molecule 9 is a protein called mL42.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	Bf	108	Total	C	N	O	S	0	0
			827	519	154	150	4		

- Molecule 10 is a protein called Mitochondrial ribosomal protein L43.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	Bg	148	Total	C	N	O	S	0	0
			1167	727	225	212	3		

- Molecule 11 is a protein called mL44.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	Bh	289	Total	C	N	O	S	0	0
			2319	1486	399	426	8		

- Molecule 12 is a protein called Mitochondrial ribosomal protein L45.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	Bi	260	Total	C	N	O	S	0	0
			2138	1370	379	379	10		

- Molecule 13 is a protein called Mitochondrial ribosomal protein L46.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	Bj	217	Total	C	N	O	S	0	0
			1775	1137	311	321	6		

- Molecule 14 is a protein called 39S ribosomal protein L48, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	Bk	155	Total	C	N	O	S	0	0
			1246	796	214	231	5		

- Molecule 15 is a protein called Mrpl34.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	Bl	133	Total	C	N	O	S	0	0
			1097	709	192	194	2		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Bl	59	ARG	LYS	conflict	UNP A0A0R4J8D6

- Molecule 16 is a protein called Mitochondrial ribosomal protein L50.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Bm	109	Total	C	N	O	S	0	0
			893	568	160	162	3		

- Molecule 17 is a protein called Mitochondrial ribosomal protein L51.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Bn	97	Total	C	N	O	S	0	0
			837	539	166	128	4		

- Molecule 18 is a protein called mL52.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	Bo	97	Total	C	N	O	S	0	0
			772	481	148	141	2		

- Molecule 19 is a protein called mL53.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	Bp	97	Total	C	N	O	S	0	0
			742	459	143	134	6		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Bp	12	ALA	SER	conflict	UNP A0A341D604

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Chain	Residue	Modelled	Actual	Comment	Reference
Bp	107	SER	GLY	conflict	UNP A0A341D604

- Molecule 20 is a protein called mL54.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	Bq	80	Total	C	N	O	S	0	0
			672	431	123	116	2		

- Molecule 21 is a protein called Mitochondrial ribosomal protein L57.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	Bt	94	Total	C	N	O	S	0	0
			780	485	168	126	1		

- Molecule 22 is a protein called mL62 (ICT1).

Mol	Chain	Residues	Atoms					AltConf	Trace
22	Bu	151	Total	C	N	O	S	0	0
			1198	738	233	222	5		

- Molecule 23 is a protein called mL64.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Bv	135	Total	C	N	O	S	0	0
			1131	692	223	211	5		

- Molecule 24 is a protein called 39S ribosomal protein S30, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Bw	387	Total	C	N	O	S	0	0
			3126	2011	548	555	12		

- Molecule 25 is a protein called Mitochondrial ribosomal protein S18A.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Bx	162	Total	C	N	O	S	0	0
			1325	845	249	224	7		

- Molecule 26 is a protein called Mitochondrial ribosomal protein L12.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	CL	45	Total	C	N	O	0	0
			317	203	52	62		
26	DL	27	Total	C	N	O	0	0
			213	137	33	43		
26	EL	28	Total	C	N	O	0	0
			222	143	35	44		
26	FL	27	Total	C	N	O	0	0
			213	137	33	43		
26	GL	27	Total	C	N	O	0	0
			213	137	33	43		
26	HL	26	Total	C	N	O	0	0
			205	131	32	42		
26	LL	70	Total	C	N	O	0	0
			537	346	93	98		

- Molecule 27 is a protein called Mitochondrial ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	B1	244	Total	C	N	O	S	0	0
			2036	1315	363	353	5		

- Molecule 28 is a protein called Ribosomal protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	B9	38	Total	C	N	O	S	0	0
			335	214	70	47	4		

- Molecule 29 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	BA	1544	Total	C	N	O	P	0	0
			32844	14750	5972	10578	1544		

- Molecule 30 is a protein called Mitochondrial ribosomal protein L47.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	B2	179	Total	C	N	O	S	0	0
			1548	992	290	260	6		

- Molecule 31 is a protein called uL30m.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	B3	118	Total	C	N	O	S	0	0
			968	622	178	165	3		

- Molecule 32 is a protein called bL31m.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	B4	62	Total	C	N	O	S	0	0
			474	296	94	81	3		

- Molecule 33 is a protein called bL32m.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	B5	110	Total	C	N	O	S	0	0
			902	553	181	162	6		

- Molecule 34 is a protein called bL33m.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	B6	52	Total	C	N	O	S	0	0
			425	274	78	71	2		

- Molecule 35 is a protein called Mitochondrial ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	B7	46	Total	C	N	O	S	0	0
			387	239	89	58	1		

- Molecule 36 is a RNA chain called CP tRNAPhe.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	BB	67	Total	C	N	O	P	0	0
			1427	640	261	459	67		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BB	71	C	-	insertion	GB 76262549

- Molecule 37 is a protein called Ribosome-releasing factor 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	BC	700	Total	C	N	O	S	0	0
			5434	3428	936	1045	25		

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BC	25	MET	-	initiating methionine	UNP Q969S9
BC	26	HIS	-	expression tag	UNP Q969S9
BC	27	HIS	-	expression tag	UNP Q969S9
BC	28	HIS	-	expression tag	UNP Q969S9
BC	29	HIS	-	expression tag	UNP Q969S9
BC	30	HIS	-	expression tag	UNP Q969S9
BC	31	HIS	-	expression tag	UNP Q969S9
BC	32	GLU	-	expression tag	UNP Q969S9
BC	33	ASN	-	expression tag	UNP Q969S9
BC	34	LEU	-	expression tag	UNP Q969S9
BC	35	TYR	-	expression tag	UNP Q969S9
BC	36	PHE	-	expression tag	UNP Q969S9
BC	37	GLN	-	expression tag	UNP Q969S9
BC	38	SER	-	expression tag	UNP Q969S9
BC	39	GLY	-	expression tag	UNP Q969S9
BC	40	GLY	-	expression tag	UNP Q969S9
BC	41	SER	-	expression tag	UNP Q969S9
BC	42	GLY	-	expression tag	UNP Q969S9
BC	43	SER	-	expression tag	UNP Q969S9
BC	44	GLY	-	expression tag	UNP Q969S9

- Molecule 38 is a protein called uL2m.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	BD	240	Total	C	N	O	S	0	0
			1860	1160	371	319	10		

- Molecule 39 is a protein called Ribosome-recycling factor, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	BG	196	Total	C	N	O	S	0	0
			1520	940	273	299	8		

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BG	6	MET	-	initiating methionine	UNP Q96E11

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Chain	Residue	Modelled	Actual	Comment	Reference
BG	7	HIS	-	expression tag	UNP Q96E11
BG	8	HIS	-	expression tag	UNP Q96E11
BG	9	HIS	-	expression tag	UNP Q96E11
BG	10	HIS	-	expression tag	UNP Q96E11
BG	11	HIS	-	expression tag	UNP Q96E11
BG	12	HIS	-	expression tag	UNP Q96E11
BG	13	GLU	-	expression tag	UNP Q96E11
BG	14	ASN	-	expression tag	UNP Q96E11
BG	15	LEU	-	expression tag	UNP Q96E11
BG	16	TYR	-	expression tag	UNP Q96E11
BG	17	PHE	-	expression tag	UNP Q96E11
BG	18	GLN	-	expression tag	UNP Q96E11
BG	19	SER	-	expression tag	UNP Q96E11
BG	20	GLY	-	expression tag	UNP Q96E11
BG	21	GLY	-	expression tag	UNP Q96E11
BG	22	SER	-	expression tag	UNP Q96E11
BG	23	GLY	-	expression tag	UNP Q96E11
BG	24	SER	-	expression tag	UNP Q96E11
BG	25	GLY	-	expression tag	UNP Q96E11

- Molecule 40 is a protein called uL16m.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	BQ	222	Total	C	N	O	S	0	0
			1803	1156	331	306	10		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BQ	237	HIS	TYR	conflict	UNP F1RI89

- Molecule 41 is a protein called ICT1.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	BE	307	Total	C	N	O	S	0	0
			2420	1554	426	430	10		

- Molecule 42 is a protein called Mitochondrial ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	BF	250	Total	C	N	O	S	0	0
			2011	1294	367	344	6		

- Molecule 43 is a protein called Mitochondrial ribosomal protein L9.

Mol	Chain	Residues	Atoms				AltConf	Trace
43	BI	98	Total	C	N	O	0	0
			805	509	155	141		

- Molecule 44 is a protein called Mitochondrial ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	BJ	212	Total	C	N	O	S	0	0
			1705	1100	306	290	9		

- Molecule 45 is a protein called Mitochondrial ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	BK	176	Total	C	N	O	S	0	0
			1339	851	243	243	2		

- Molecule 46 is a protein called uL13m.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	BN	177	Total	C	N	O	S	0	0
			1444	926	258	253	7		

- Molecule 47 is a protein called uL14m.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	BO	115	Total	C	N	O	S	0	0
			896	562	176	154	4		

- Molecule 48 is a protein called uL15m.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	BP	288	Total	C	N	O	S	0	0
			2312	1473	430	403	6		

- Molecule 49 is a protein called bL17m.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	BR	153	Total	C	N	O	S	0	0
			1240	777	236	222	5		

- Molecule 50 is a protein called Mitochondrial ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	BS	143	Total	C	N	O	S	0	0
			1168	733	227	204	4		

- Molecule 51 is a protein called Mitochondrial ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	BT	223	Total	C	N	O	S	0	0
			1851	1184	322	336	9		

- Molecule 52 is a protein called Mitochondrial ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	BU	140	Total	C	N	O	S	0	0
			1159	732	239	185	3		

- Molecule 53 is a protein called Mitochondrial ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	BV	155	Total	C	N	O	S	0	0
			1231	789	219	219	4		

- Molecule 54 is a protein called uL22m.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	BW	166	Total	C	N	O	S	0	0
			1374	876	258	234	6		

- Molecule 55 is a protein called uL23m.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	BX	149	Total	C	N	O	S	0	0
			1181	752	227	200	2		

- Molecule 56 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
56	B0	1	Total	Mg	0
			1	1	
56	Bb	1	Total	Mg	0
			1	1	
56	Be	1	Total	Mg	0
			1	1	

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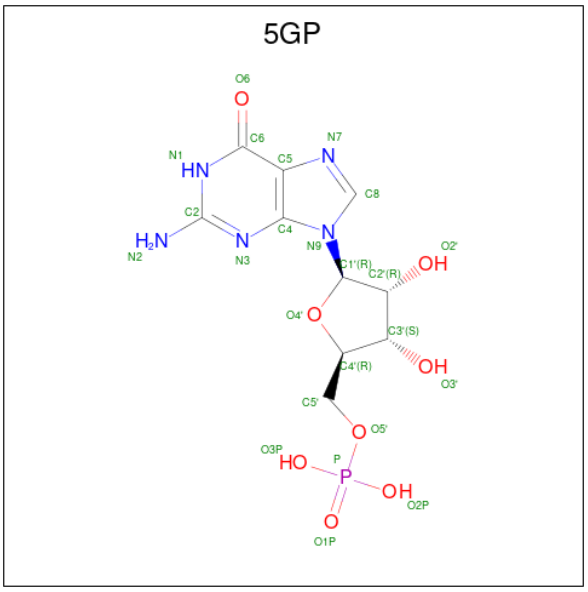
Mol	Chain	Residues	Atoms	AltConf
56	Bl	1	Total Mg 1 1	0
56	Bt	1	Total Mg 1 1	0
56	BA	205	Total Mg 205 205	0
56	B3	1	Total Mg 1 1	0
56	BC	1	Total Mg 1 1	0
56	BD	3	Total Mg 3 3	0
56	BQ	1	Total Mg 1 1	0
56	BE	1	Total Mg 1 1	0
56	BJ	1	Total Mg 1 1	0
56	BP	2	Total Mg 2 2	0
56	BR	1	Total Mg 1 1	0

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

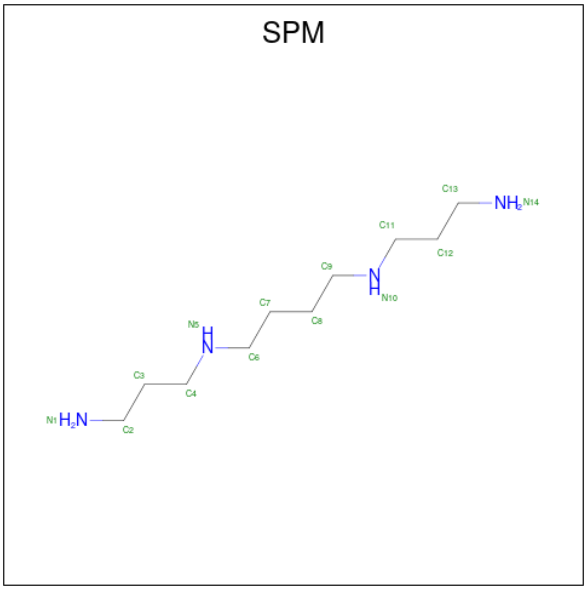
Mol	Chain	Residues	Atoms	AltConf
57	Bx	1	Total Zn 1 1	0
57	B9	1	Total Zn 1 1	0
57	B5	1	Total Zn 1 1	0

- Molecule 58 is GUANOSINE-5'-MONOPHOSPHATE (three-letter code: 5GP) (formula: $C_{10}H_{14}N_5O_8P$).



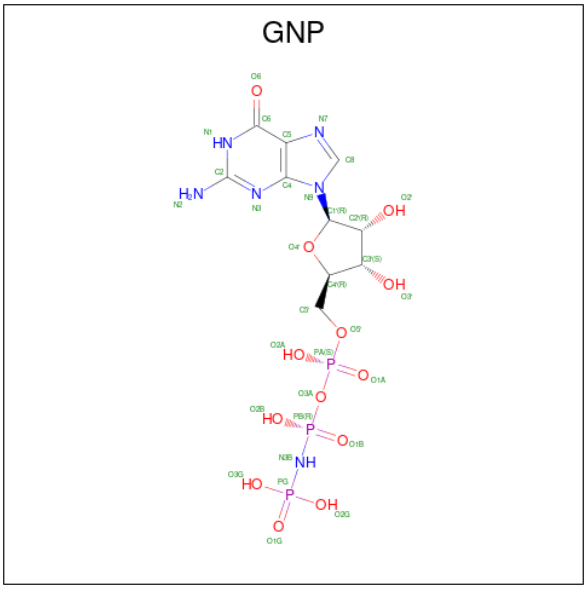
Mol	Chain	Residues	Atoms					AltConf
58	BA	1	Total	C	N	O	P	0
			48	20	10	16	2	
58	BA	1	Total	C	N	O	P	0
			48	20	10	16	2	

- Molecule 59 is SPERMINE (three-letter code: SPM) (formula: $C_{10}H_{26}N_4$).



Mol	Chain	Residues	Atoms			AltConf
59	BA	1	Total	C	N	0
			28	20	8	
59	BA	1	Total	C	N	0
			28	20	8	

- Molecule 60 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (three-letter code: GNP) (formula: $C_{10}H_{17}N_6O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
60	BC	1	Total	C	N	O	P	0
			32	10	6	13	3	

- Molecule 61 is water.

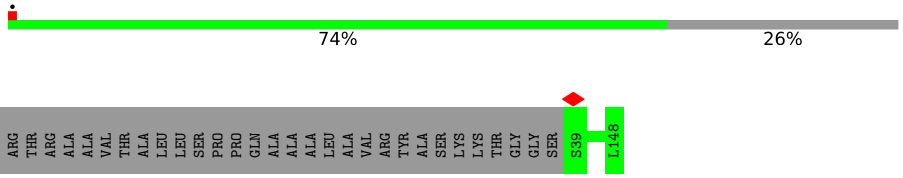
Mol	Chain	Residues	Atoms		AltConf
61	BC	2	Total	O	0
			2	2	

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.

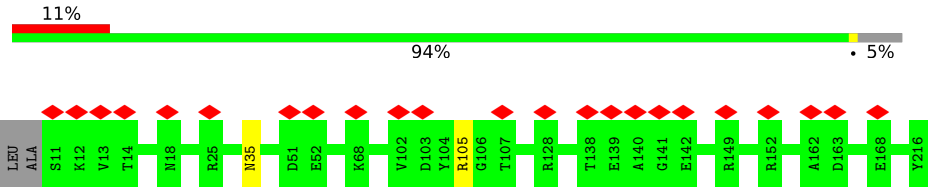
• Molecule 1: Mitochondrial ribosomal protein L27

Chain B0:



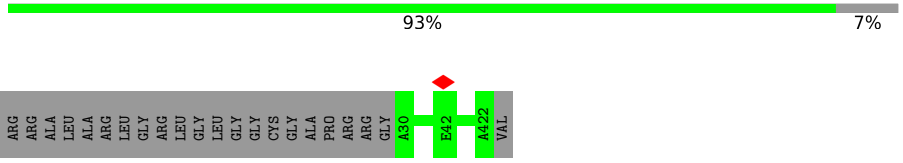
• Molecule 2: uL24m

Chain BY:



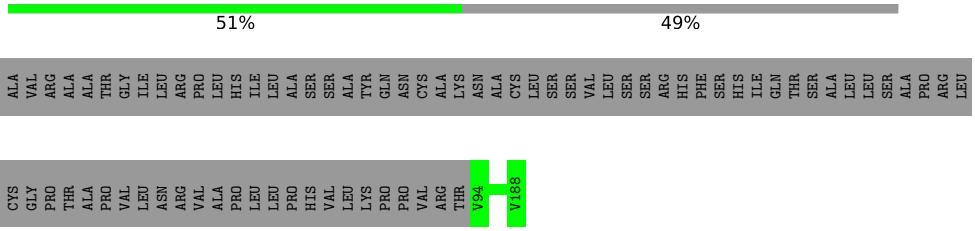
• Molecule 3: Mitochondrial ribosomal protein L37

Chain Ba:



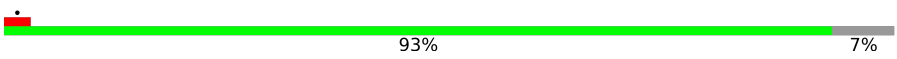
• Molecule 4: Mitochondrial ribosomal protein L35

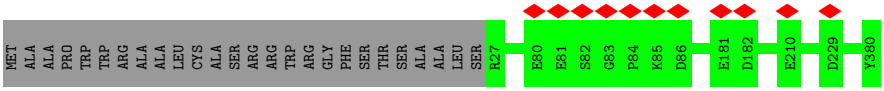
Chain B8:



• Molecule 5: Mitochondrial ribosomal protein L38

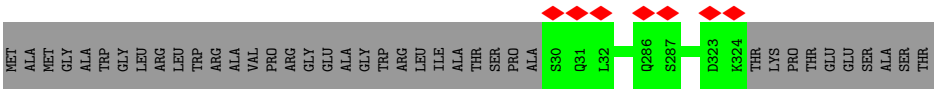
Chain Bb:





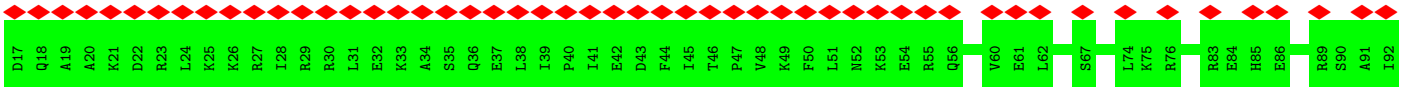
• Molecule 6: Mitochondrial ribosomal protein L39

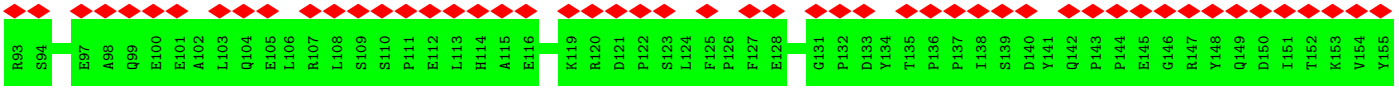
Chain Bc:

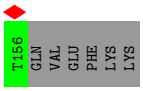


• Molecule 7: Mitochondrial ribosomal protein L40

Chain Bd:

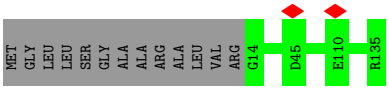






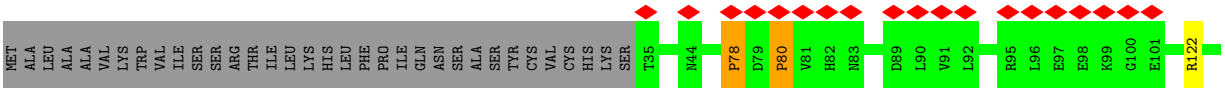
• Molecule 8: Mitochondrial ribosomal protein L41

Chain Be:



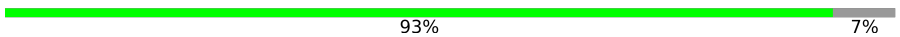
• Molecule 9: mL42

Chain Bf:



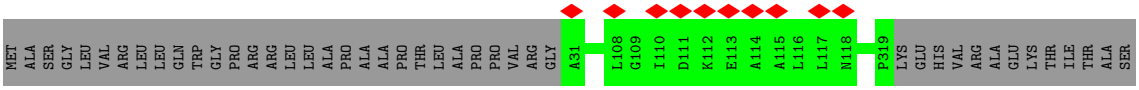
• Molecule 10: Mitochondrial ribosomal protein L43

Chain Bg:



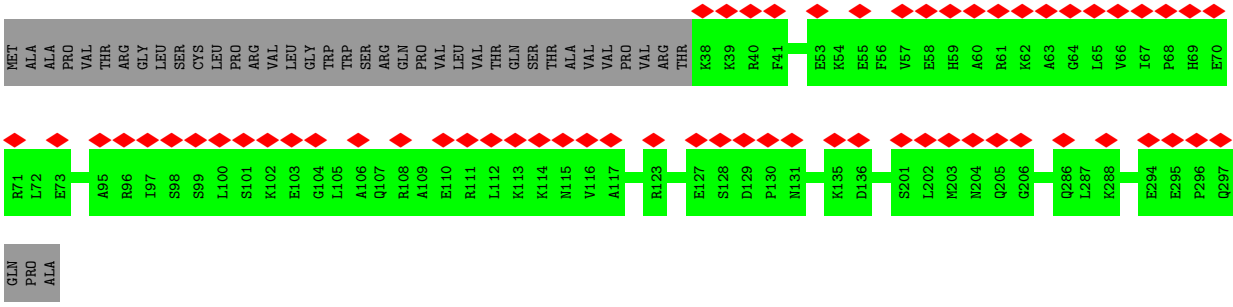
• Molecule 11: mL44

Chain Bh:



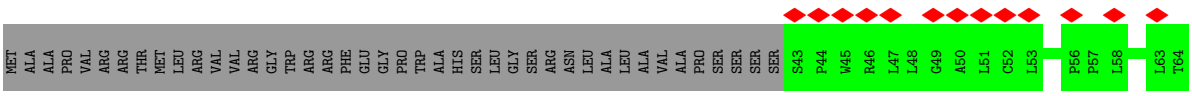
• Molecule 12: Mitochondrial ribosomal protein L45

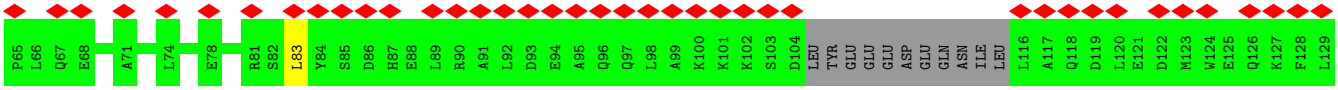
Chain Bi:

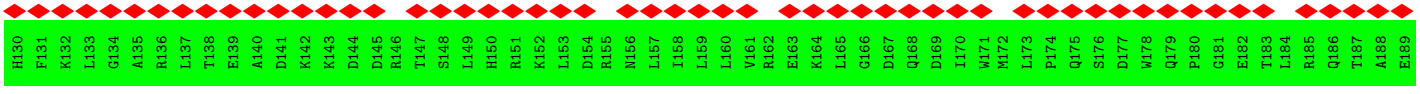


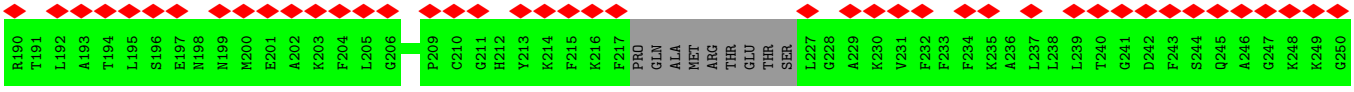
• Molecule 13: Mitochondrial ribosomal protein L46

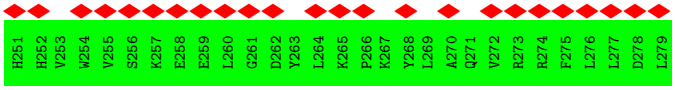
Chain Bj:





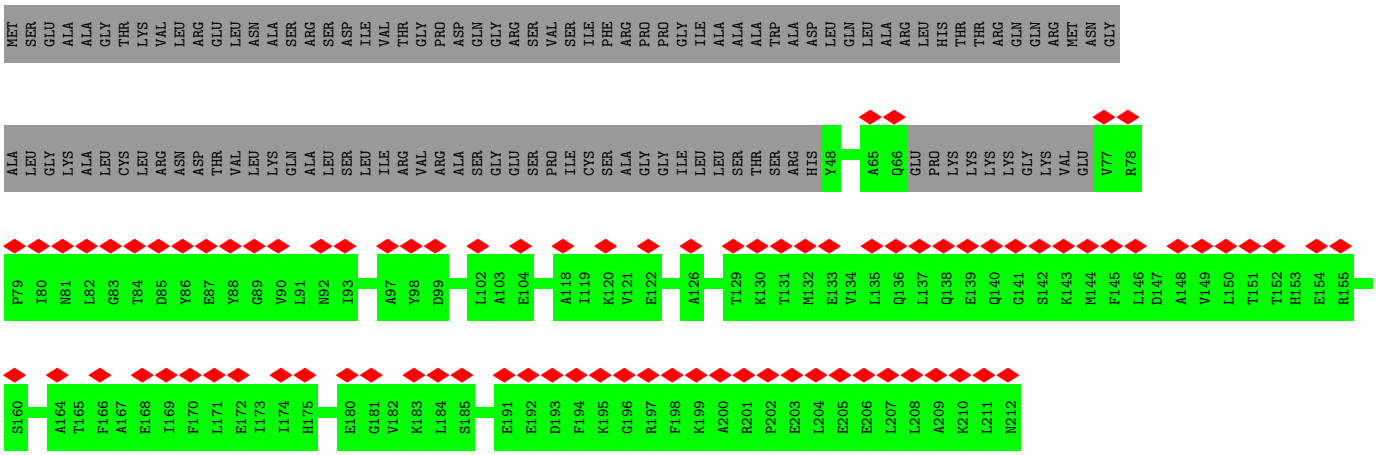






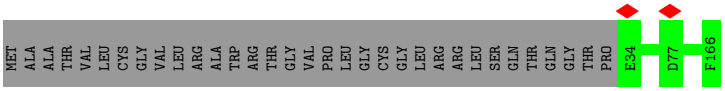
• Molecule 14: 39S ribosomal protein L48, mitochondrial

Chain Bk:



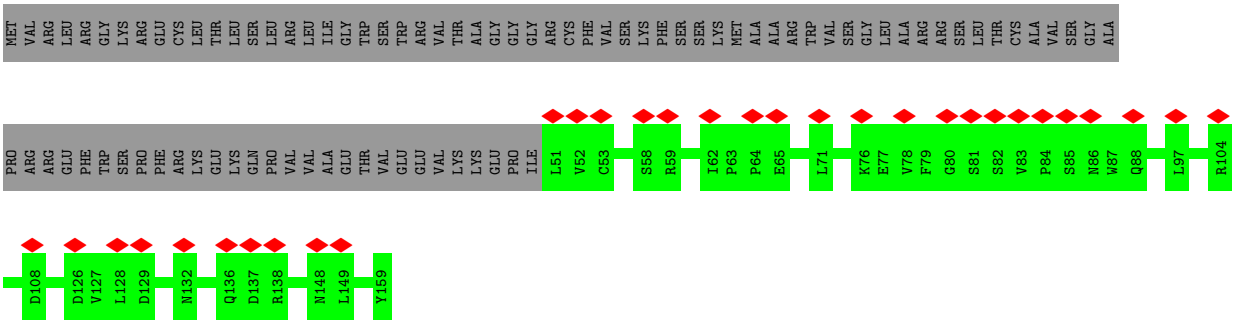
• Molecule 15: Mrpl34

Chain Bl:



• Molecule 16: Mitochondrial ribosomal protein L50

Chain Bm:

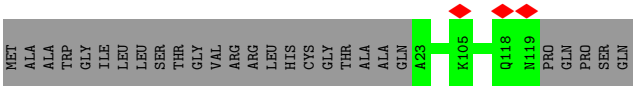


• Molecule 17: Mitochondrial ribosomal protein L51

Chain Bn:

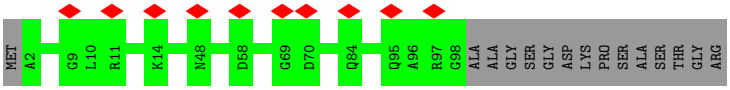
• Molecule 18: mL52

Chain Bo:



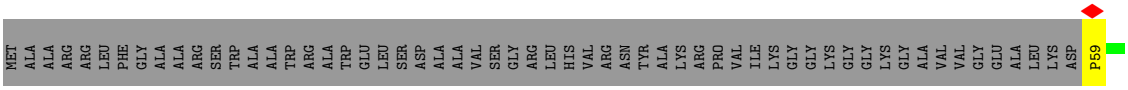
• Molecule 19: mL53

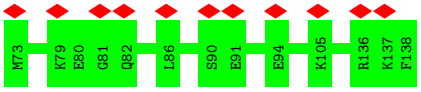
Chain Bp:



• Molecule 20: mL54

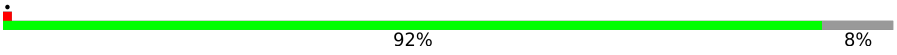
Chain Bq:

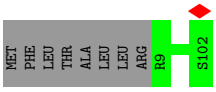




• Molecule 21: Mitochondrial ribosomal protein L57

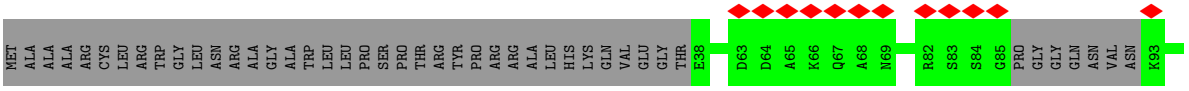
Chain Bt:

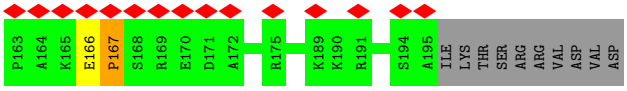




• Molecule 22: mL62 (ICT1)

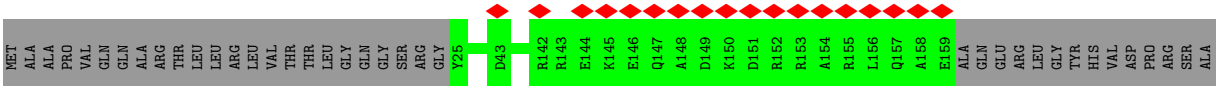
Chain Bu:

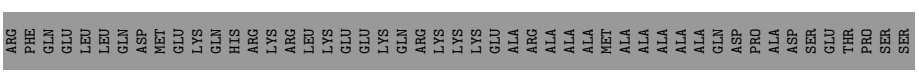




• Molecule 23: mL64

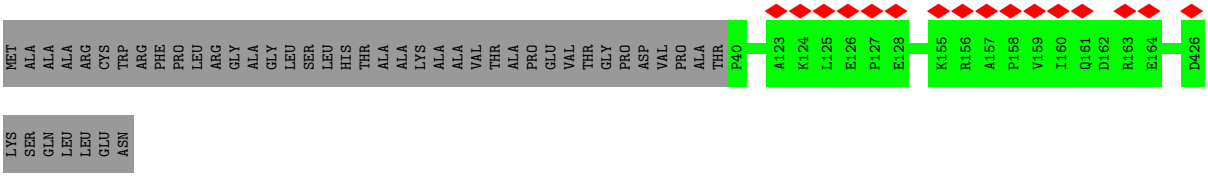
Chain Bv:





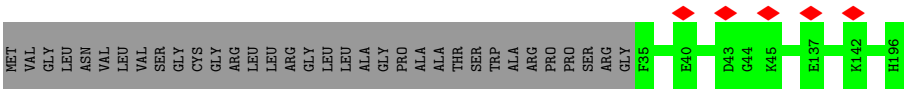
• Molecule 24: 39S ribosomal protein S30, mitochondrial

Chain Bw:



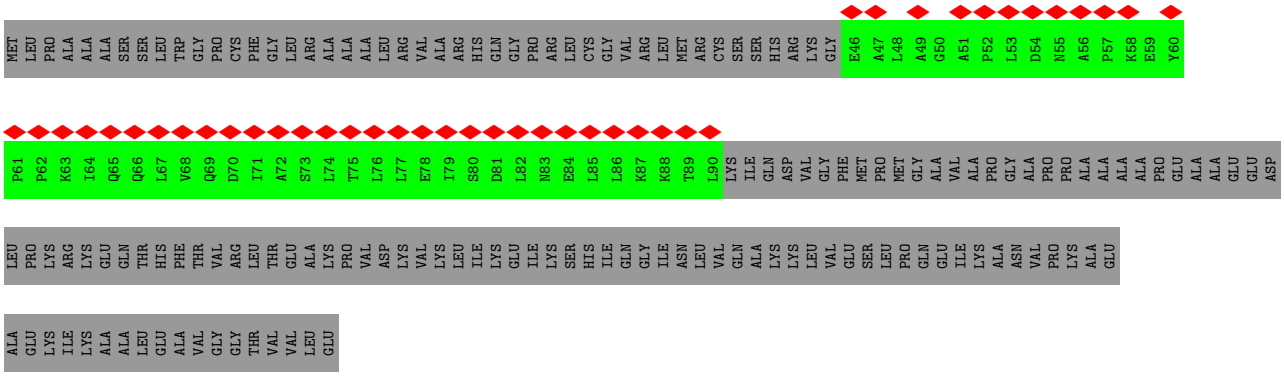
• Molecule 25: Mitochondrial ribosomal protein S18A

Chain Bx:



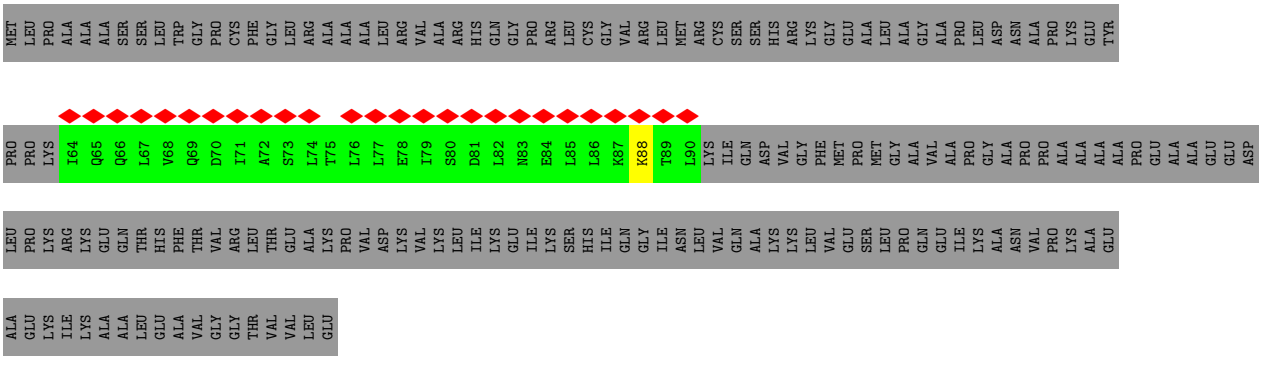
• Molecule 26: Mitochondrial ribosomal protein L12

Chain CL:



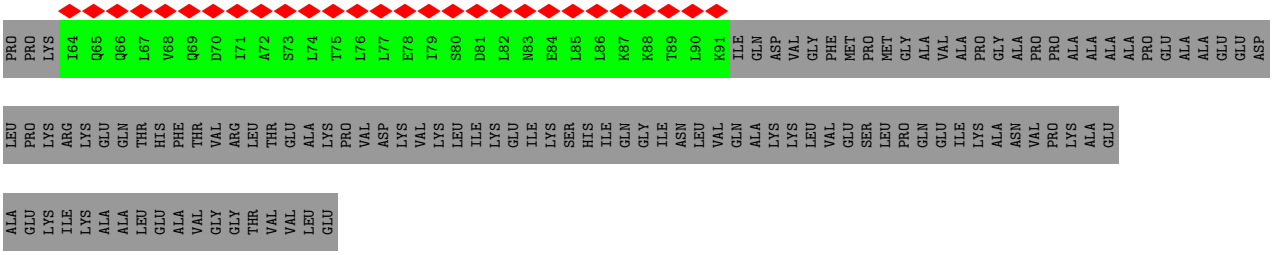
• Molecule 26: Mitochondrial ribosomal protein L12

Chain DL:

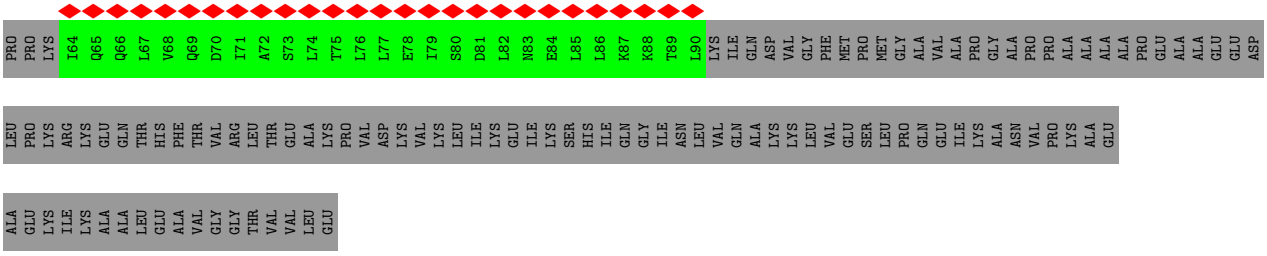


• Molecule 26: Mitochondrial ribosomal protein L12

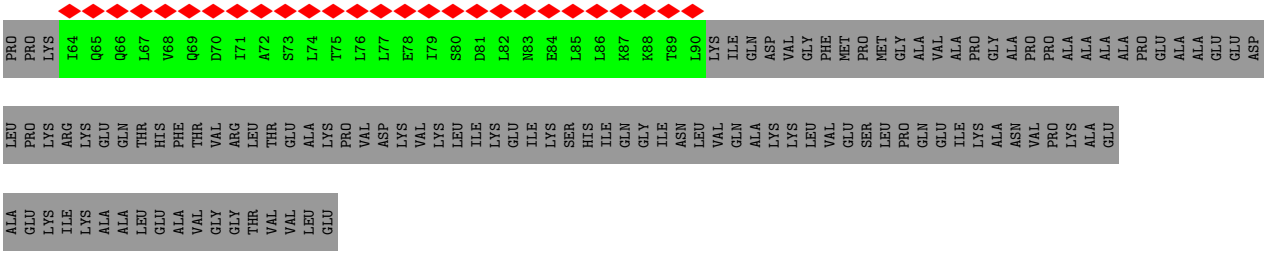
Chain EL:



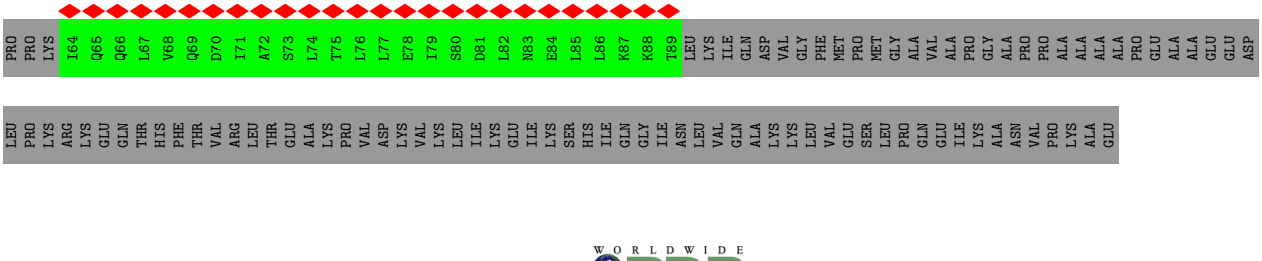
• Molecule 26: Mitochondrial ribosomal protein L12

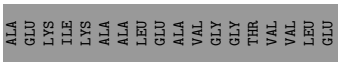


• Molecule 26: Mitochondrial ribosomal protein L12



• Molecule 26: Mitochondrial ribosomal protein L12



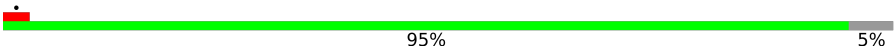


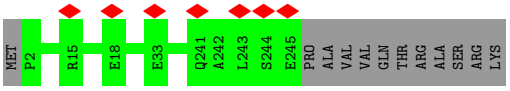
• Molecule 26: Mitochondrial ribosomal protein L12

Chain LL:

• Molecule 27: Mitochondrial ribosomal protein L28

Chain B1:



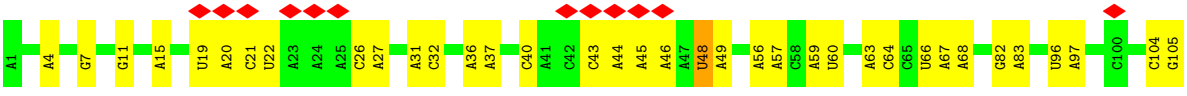


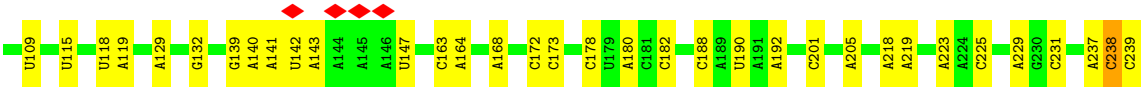
• Molecule 28: Ribosomal protein

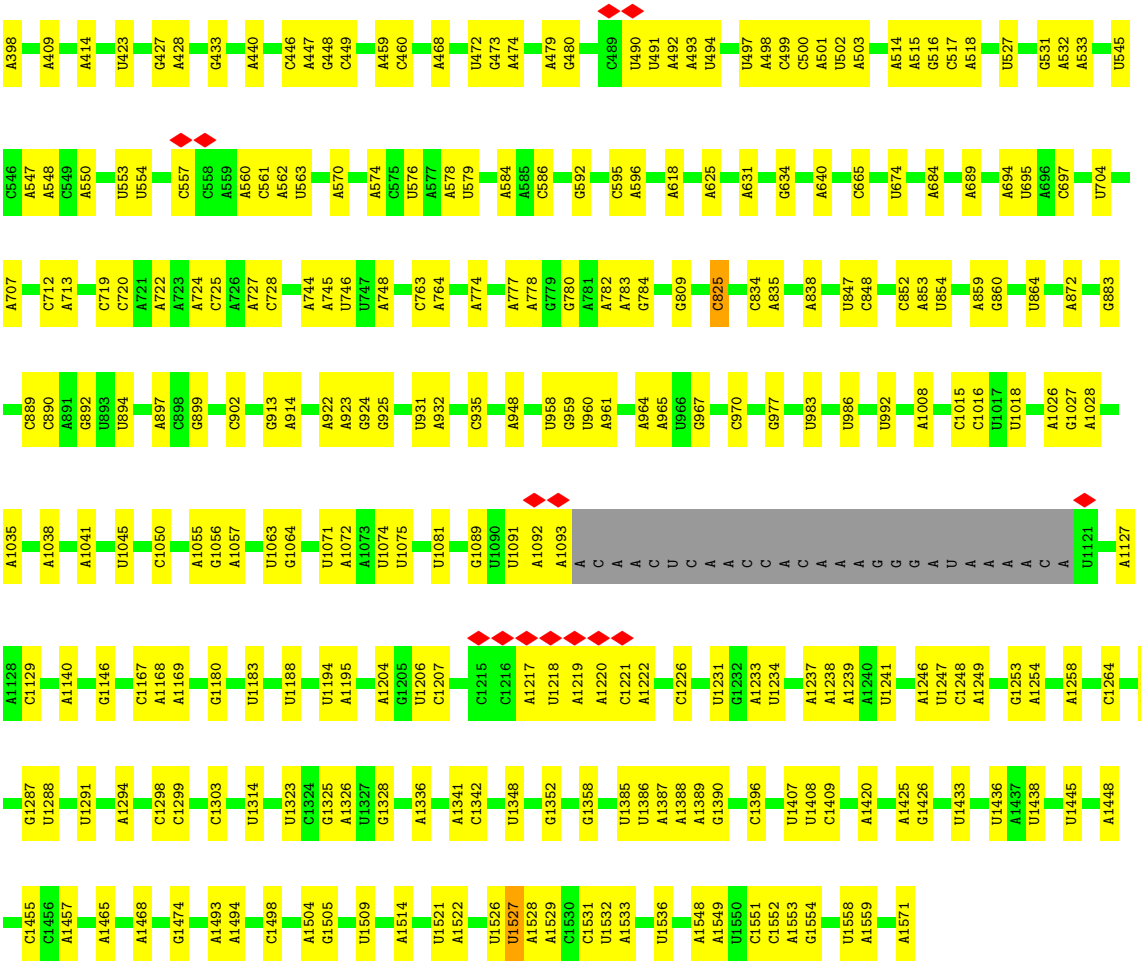
Chain B9:

• Molecule 29: 16S rRNA

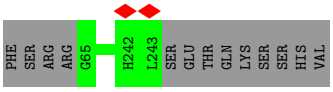
Chain BA:



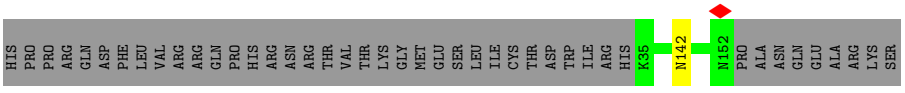




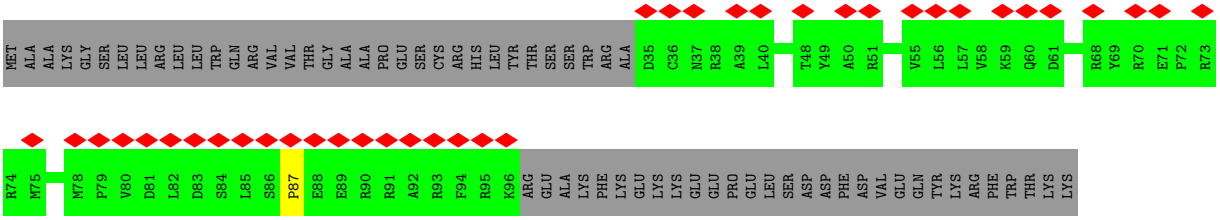
• Molecule 30: Mitochondrial ribosomal protein L47



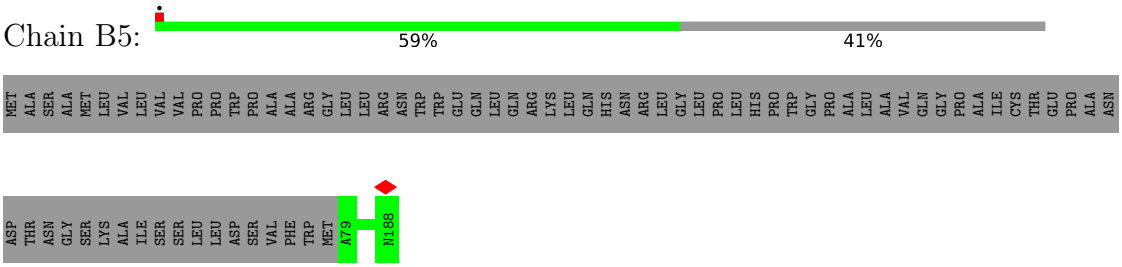
• Molecule 31: uL30m



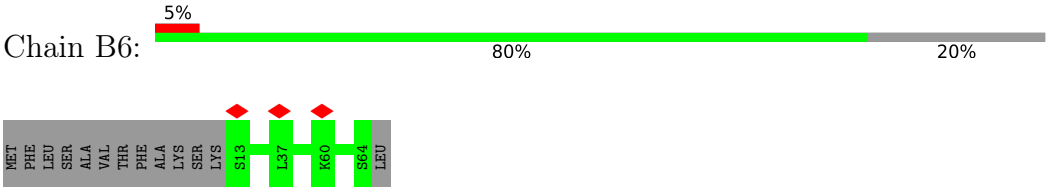
• Molecule 32: bL31m



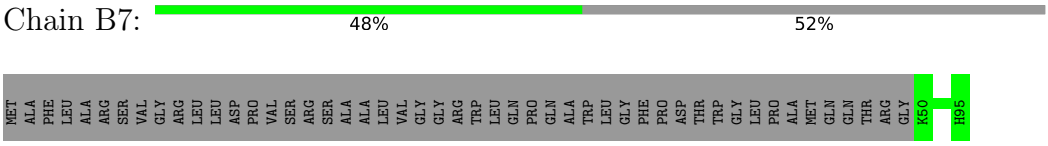
• Molecule 33: bL32m



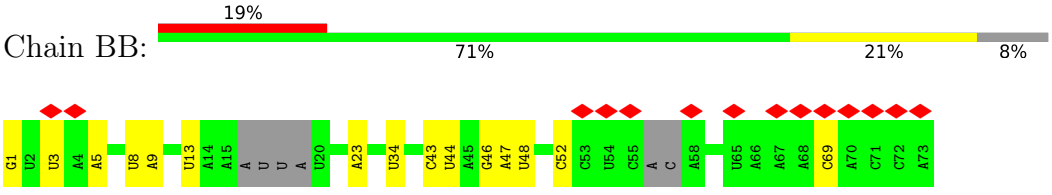
• Molecule 34: bL33m



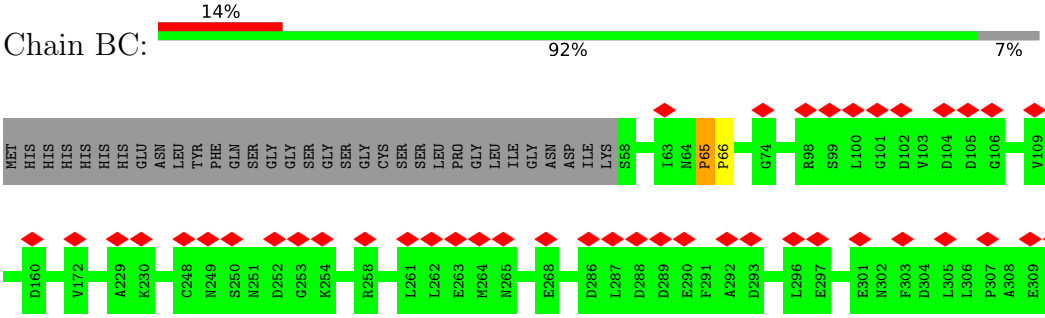
• Molecule 35: Mitochondrial ribosomal protein L34

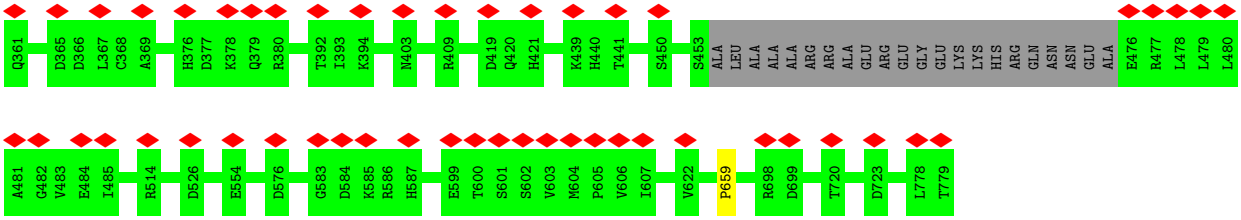


• Molecule 36: CP tRNAPhe

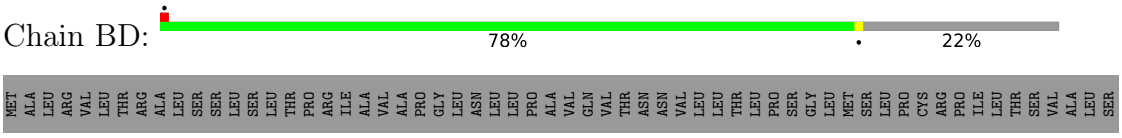


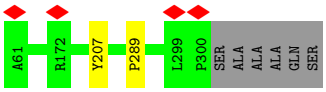
• Molecule 37: Ribosome-releasing factor 2, mitochondrial



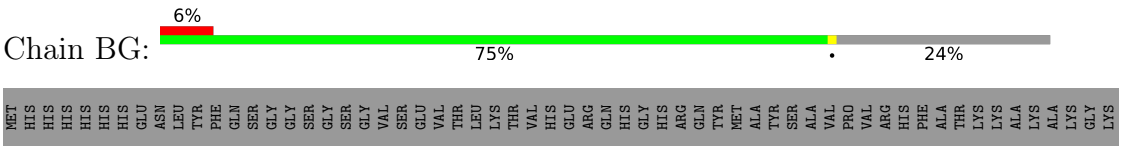


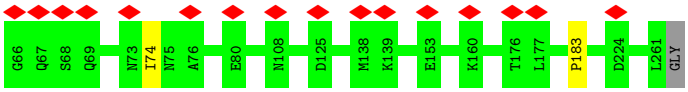
• Molecule 38: uL2m



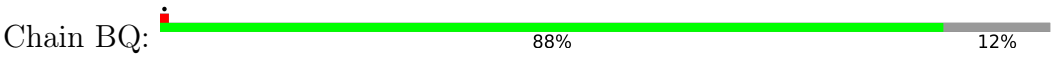


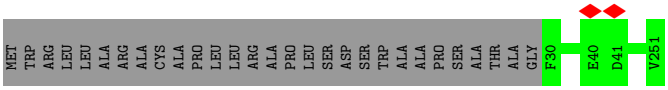
• Molecule 39: Ribosome-recycling factor, mitochondrial



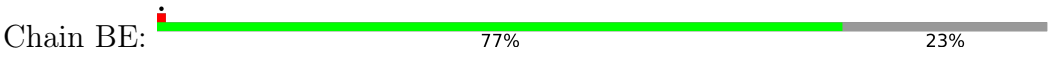


• Molecule 40: uL16m

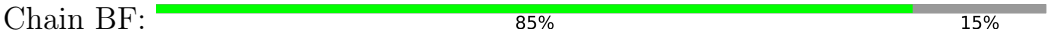


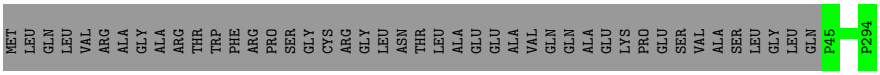


• Molecule 41: ICT1



• Molecule 42: Mitochondrial ribosomal protein L4



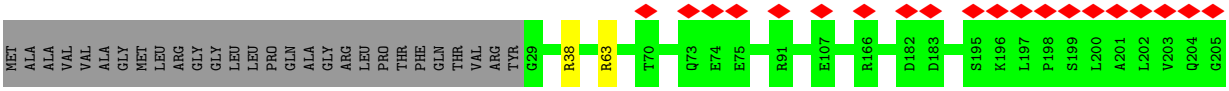


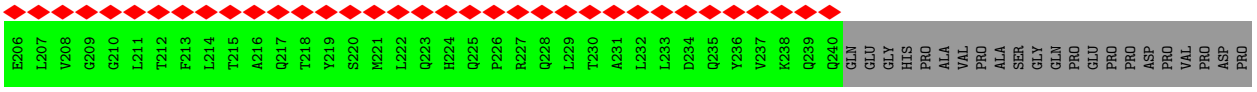
• Molecule 43: Mitochondrial ribosomal protein L9

Chain BI:

• Molecule 44: Mitochondrial ribosomal protein L10

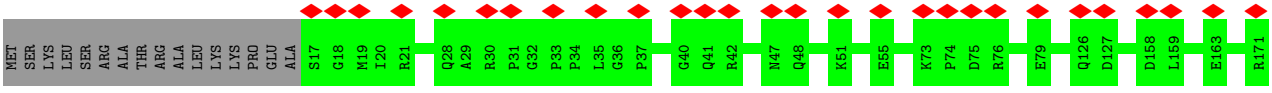
Chain BJ:

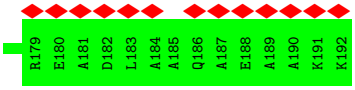




• Molecule 45: Mitochondrial ribosomal protein L11

Chain BK:



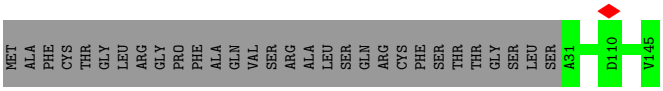


• Molecule 46: uL13m

Chain BN:

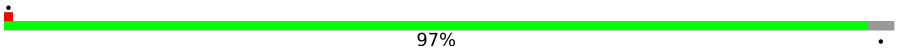
• Molecule 47: uL14m

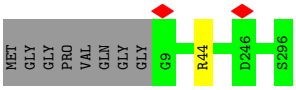
Chain BO:



• Molecule 48: uL15m

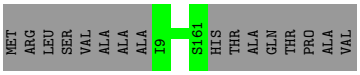
Chain BP:





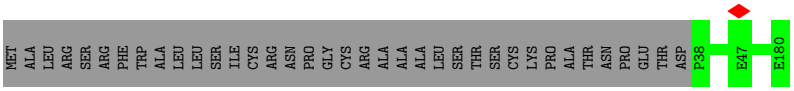
• Molecule 49: bL17m

Chain BR:



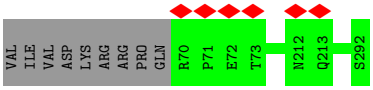
• Molecule 50: Mitochondrial ribosomal protein L18

Chain BS:



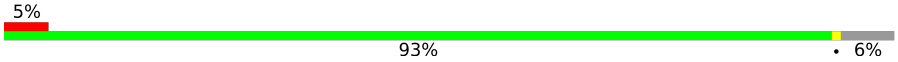
• Molecule 51: Mitochondrial ribosomal protein L19

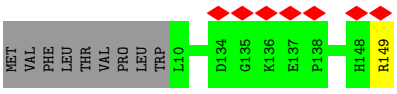
Chain BT:



• Molecule 52: Mitochondrial ribosomal protein L20

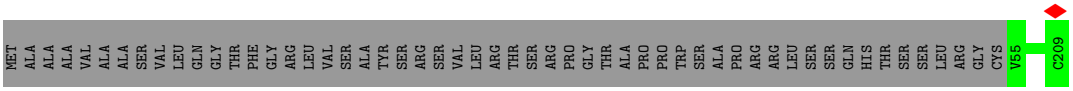
Chain BU:





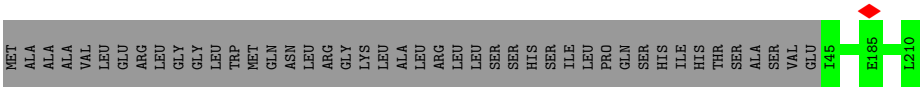
• Molecule 53: Mitochondrial ribosomal protein L21

Chain BV:



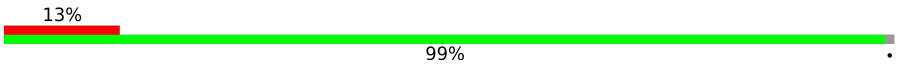
• Molecule 54: uL22m

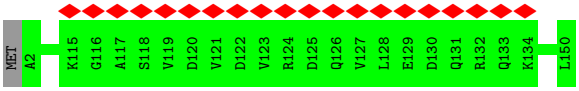
Chain BW:



• Molecule 55: uL23m

Chain BX:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	224731	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 ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.284	Depositor
Minimum map value	-0.144	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.028	Depositor
Map size (Å)	521.76, 521.76, 521.76	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.087, 1.087, 1.087	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GNP, MG, ZN, 5GP, SPM

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	B0	0.27	0/880	0.41	0/1189
2	BY	0.24	0/1719	0.42	0/2329
3	Ba	0.25	0/3267	0.43	0/4455
4	B8	0.24	0/853	0.38	0/1136
5	Bb	0.26	0/3047	0.41	0/4139
6	Bc	0.25	0/2464	0.42	0/3330
7	Bd	0.24	0/1203	0.38	0/1622
8	Be	0.26	0/1000	0.43	0/1345
9	Bf	0.25	0/851	0.52	2/1159 (0.2%)
10	Bg	0.25	0/1191	0.43	0/1614
11	Bh	0.25	0/2372	0.42	0/3211
12	Bi	0.25	0/2199	0.41	0/2980
13	Bj	0.24	0/1811	0.49	1/2436 (0.0%)
14	Bk	0.24	0/1270	0.43	0/1714
15	Bl	0.25	0/1135	0.42	0/1549
16	Bm	0.23	0/917	0.36	0/1248
17	Bn	0.25	0/860	0.42	0/1150
18	Bo	0.24	0/787	0.37	0/1056
19	Bp	0.24	0/752	0.42	0/1013
20	Bq	0.23	0/692	0.42	1/936 (0.1%)
21	Bt	0.24	0/798	0.39	0/1073
22	Bu	0.24	0/1214	0.46	1/1630 (0.1%)
23	Bv	0.23	0/1157	0.35	0/1560
24	Bw	0.25	0/3206	0.42	0/4354
25	Bx	0.26	0/1364	0.43	0/1849
26	CL	0.23	0/319	0.42	0/435
26	DL	0.21	0/212	0.43	0/286
26	EL	0.22	0/221	0.40	0/297
26	FL	0.43	0/212	0.45	0/286
26	GL	0.22	0/212	0.44	0/286
26	HL	0.22	0/204	0.39	0/275
26	LL	0.23	0/542	0.42	0/729

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
27	B1	0.24	0/2093	0.38	0/2835
28	B9	0.24	0/342	0.42	0/450
29	BA	0.24	0/36784	0.78	15/57270 (0.0%)
30	B2	0.24	0/1586	0.39	0/2123
31	B3	0.25	0/993	0.43	0/1341
32	B4	0.23	0/481	0.53	1/653 (0.2%)
33	B5	0.24	0/917	0.40	0/1227
34	B6	0.24	0/430	0.41	0/570
35	B7	0.23	0/395	0.37	0/524
36	BB	0.31	1/1595 (0.1%)	0.74	0/2475
37	BC	0.26	1/5523 (0.0%)	0.49	3/7495 (0.0%)
38	BD	0.26	0/1898	0.46	1/2555 (0.0%)
39	BG	0.24	0/1529	0.42	0/2058
40	BQ	0.25	0/1850	0.42	0/2491
41	BE	0.26	0/2493	0.43	0/3387
42	BF	0.25	0/2069	0.42	0/2816
43	BI	0.23	0/819	0.44	0/1101
44	BJ	0.24	0/1742	0.44	0/2358
45	BK	0.25	0/1359	0.43	0/1828
46	BN	0.24	0/1487	0.38	0/2017
47	BO	0.24	0/912	0.43	0/1231
48	BP	0.26	0/2368	0.42	0/3198
49	BR	0.24	0/1262	0.41	0/1700
50	BS	0.24	0/1197	0.45	0/1624
51	BT	0.25	0/1894	0.42	0/2555
52	BU	0.24	0/1179	0.37	0/1578
53	BV	0.24	0/1256	0.44	0/1706
54	BW	0.26	0/1407	0.41	0/1891
55	BX	0.26	0/1211	0.40	0/1646
All	All	0.25	2/118002 (0.0%)	0.58	25/167374 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
17	Bn	0	1
26	FL	1	0
38	BD	0	1
All	All	1	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	BB	1	G	OP3-P	-10.59	1.48	1.61
37	BC	659	PRO	CG-CD	-5.65	1.32	1.50

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	BC	659	PRO	N-CD-CG	-8.85	89.93	103.20
29	BA	1527	U	C2-N1-C1'	7.12	126.24	117.70
9	Bf	80	PRO	N-CA-CB	6.61	111.23	103.30
22	Bu	167	PRO	N-CA-CB	6.54	111.15	103.30
9	Bf	78	PRO	N-CA-CB	6.53	111.14	103.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
26	FL	89	THR	CB

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
38	BD	207	TYR	Peptide
17	Bn	65	ASN	Peptide

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	B0	108/148 (73%)	106 (98%)	2 (2%)	0	100	100
2	BY	204/216 (94%)	199 (98%)	5 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	Ba	391/423 (92%)	371 (95%)	20 (5%)	0	100	100
4	B8	93/188 (50%)	91 (98%)	2 (2%)	0	100	100
5	Bb	352/380 (93%)	334 (95%)	18 (5%)	0	100	100
6	Bc	293/334 (88%)	278 (95%)	15 (5%)	0	100	100
7	Bd	138/206 (67%)	131 (95%)	7 (5%)	0	100	100
8	Be	120/135 (89%)	114 (95%)	6 (5%)	0	100	100
9	Bf	106/142 (75%)	100 (94%)	4 (4%)	2 (2%)	8	39
10	Bg	146/159 (92%)	136 (93%)	10 (7%)	0	100	100
11	Bh	287/332 (86%)	272 (95%)	15 (5%)	0	100	100
12	Bi	258/306 (84%)	245 (95%)	13 (5%)	0	100	100
13	Bj	211/279 (76%)	203 (96%)	8 (4%)	0	100	100
14	Bk	151/269 (56%)	146 (97%)	5 (3%)	0	100	100
15	Bl	131/166 (79%)	128 (98%)	3 (2%)	0	100	100
16	Bm	107/198 (54%)	103 (96%)	4 (4%)	0	100	100
17	Bn	95/128 (74%)	92 (97%)	3 (3%)	0	100	100
18	Bo	95/124 (77%)	93 (98%)	2 (2%)	0	100	100
19	Bp	95/112 (85%)	88 (93%)	7 (7%)	0	100	100
20	Bq	78/138 (56%)	72 (92%)	6 (8%)	0	100	100
21	Bt	92/102 (90%)	88 (96%)	4 (4%)	0	100	100
22	Bu	147/205 (72%)	141 (96%)	4 (3%)	2 (1%)	11	46
23	Bv	133/222 (60%)	133 (100%)	0	0	100	100
24	Bw	385/433 (89%)	367 (95%)	18 (5%)	0	100	100
25	Bx	160/196 (82%)	153 (96%)	7 (4%)	0	100	100
26	CL	43/198 (22%)	40 (93%)	3 (7%)	0	100	100
26	DL	25/198 (13%)	25 (100%)	0	0	100	100
26	EL	26/198 (13%)	26 (100%)	0	0	100	100
26	FL	25/198 (13%)	25 (100%)	0	0	100	100
26	GL	25/198 (13%)	25 (100%)	0	0	100	100
26	HL	24/198 (12%)	24 (100%)	0	0	100	100
26	LL	68/198 (34%)	67 (98%)	1 (2%)	0	100	100
27	B1	242/256 (94%)	240 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	B9	36/100 (36%)	36 (100%)	0	0	100	100
30	B2	177/252 (70%)	174 (98%)	3 (2%)	0	100	100
31	B3	116/161 (72%)	114 (98%)	2 (2%)	0	100	100
32	B4	60/126 (48%)	52 (87%)	8 (13%)	0	100	100
33	B5	108/188 (57%)	108 (100%)	0	0	100	100
34	B6	50/65 (77%)	49 (98%)	1 (2%)	0	100	100
35	B7	44/95 (46%)	43 (98%)	1 (2%)	0	100	100
37	BC	696/755 (92%)	637 (92%)	58 (8%)	1 (0%)	51	83
38	BD	238/306 (78%)	226 (95%)	12 (5%)	0	100	100
39	BG	194/257 (76%)	178 (92%)	14 (7%)	2 (1%)	15	54
40	BQ	220/251 (88%)	215 (98%)	5 (2%)	0	100	100
41	BE	305/399 (76%)	289 (95%)	16 (5%)	0	100	100
42	BF	248/294 (84%)	241 (97%)	7 (3%)	0	100	100
43	BI	96/268 (36%)	94 (98%)	2 (2%)	0	100	100
44	BJ	210/262 (80%)	199 (95%)	11 (5%)	0	100	100
45	BK	174/192 (91%)	164 (94%)	10 (6%)	0	100	100
46	BN	175/178 (98%)	171 (98%)	4 (2%)	0	100	100
47	BO	113/145 (78%)	111 (98%)	2 (2%)	0	100	100
48	BP	286/296 (97%)	275 (96%)	11 (4%)	0	100	100
49	BR	151/169 (89%)	143 (95%)	8 (5%)	0	100	100
50	BS	141/180 (78%)	133 (94%)	8 (6%)	0	100	100
51	BT	221/292 (76%)	218 (99%)	3 (1%)	0	100	100
52	BU	138/149 (93%)	137 (99%)	1 (1%)	0	100	100
53	BV	153/209 (73%)	147 (96%)	6 (4%)	0	100	100
54	BW	164/210 (78%)	158 (96%)	6 (4%)	0	100	100
55	BX	147/150 (98%)	143 (97%)	4 (3%)	0	100	100
All	All	9515/13132 (72%)	9111 (96%)	397 (4%)	7 (0%)	54	83

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	Bf	80	PRO
22	Bu	167	PRO

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Mol	Chain	Res	Type
9	Bf	78	PRO
37	BC	65	PRO
22	Bu	166	GLU

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	B0	90/115 (78%)	90 (100%)	0	100	100
2	BY	185/192 (96%)	183 (99%)	2 (1%)	73	88
3	Ba	348/365 (95%)	348 (100%)	0	100	100
4	B8	87/162 (54%)	87 (100%)	0	100	100
5	Bb	310/328 (94%)	310 (100%)	0	100	100
6	Bc	271/299 (91%)	271 (100%)	0	100	100
7	Bd	129/181 (71%)	129 (100%)	0	100	100
8	Be	100/108 (93%)	100 (100%)	0	100	100
9	Bf	80/133 (60%)	79 (99%)	1 (1%)	69	87
10	Bg	128/136 (94%)	128 (100%)	0	100	100
11	Bh	251/284 (88%)	251 (100%)	0	100	100
12	Bi	236/275 (86%)	236 (100%)	0	100	100
13	Bj	190/242 (78%)	190 (100%)	0	100	100
14	Bk	135/226 (60%)	135 (100%)	0	100	100
15	Bl	122/147 (83%)	122 (100%)	0	100	100
16	Bm	103/178 (58%)	103 (100%)	0	100	100
17	Bn	88/113 (78%)	88 (100%)	0	100	100
18	Bo	77/97 (79%)	77 (100%)	0	100	100
19	Bp	79/88 (90%)	79 (100%)	0	100	100
20	Bq	70/114 (61%)	70 (100%)	0	100	100
21	Bt	75/82 (92%)	75 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
22	Bu	126/177 (71%)	126 (100%)	0	100	100
23	Bv	115/183 (63%)	115 (100%)	0	100	100
24	Bw	340/373 (91%)	340 (100%)	0	100	100
25	Bx	149/173 (86%)	149 (100%)	0	100	100
26	CL	30/157 (19%)	30 (100%)	0	100	100
26	DL	26/157 (17%)	25 (96%)	1 (4%)	33	67
26	EL	27/157 (17%)	27 (100%)	0	100	100
26	FL	26/157 (17%)	26 (100%)	0	100	100
26	GL	26/157 (17%)	26 (100%)	0	100	100
26	HL	25/157 (16%)	25 (100%)	0	100	100
26	LL	59/157 (38%)	59 (100%)	0	100	100
27	B1	219/229 (96%)	219 (100%)	0	100	100
28	B9	36/77 (47%)	36 (100%)	0	100	100
30	B2	164/228 (72%)	164 (100%)	0	100	100
31	B3	110/150 (73%)	109 (99%)	1 (1%)	78	91
32	B4	45/114 (40%)	45 (100%)	0	100	100
33	B5	99/163 (61%)	99 (100%)	0	100	100
34	B6	49/60 (82%)	49 (100%)	0	100	100
35	B7	41/78 (53%)	41 (100%)	0	100	100
37	BC	600/651 (92%)	599 (100%)	1 (0%)	93	98
38	BD	193/248 (78%)	193 (100%)	0	100	100
39	BG	175/224 (78%)	175 (100%)	0	100	100
40	BQ	190/210 (90%)	190 (100%)	0	100	100
41	BE	263/320 (82%)	263 (100%)	0	100	100
42	BF	217/251 (86%)	217 (100%)	0	100	100
43	BI	88/228 (39%)	88 (100%)	0	100	100
44	BJ	192/230 (84%)	190 (99%)	2 (1%)	76	90
45	BK	138/151 (91%)	138 (100%)	0	100	100
46	BN	156/157 (99%)	156 (100%)	0	100	100
47	BO	99/123 (80%)	99 (100%)	0	100	100
48	BP	245/249 (98%)	244 (100%)	1 (0%)	91	95

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
49	BR	132/143 (92%)	132 (100%)	0	100 100
50	BS	123/153 (80%)	123 (100%)	0	100 100
51	BT	205/258 (80%)	205 (100%)	0	100 100
52	BU	118/127 (93%)	117 (99%)	1 (1%)	81 93
53	BV	136/178 (76%)	136 (100%)	0	100 100
54	BW	144/180 (80%)	144 (100%)	0	100 100
55	BX	116/134 (87%)	116 (100%)	0	100 100
All	All	8396/11184 (75%)	8386 (100%)	10 (0%)	93 98

5 of 10 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
44	BJ	63	ARG
48	BP	44	ARG
52	BU	149	ARG
26	DL	88	LYS
31	B3	142	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
32	B4	60	GLN
40	BQ	98	HIS
37	BC	637	GLN
41	BE	69	ASN
12	Bi	251	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
29	BA	1542/1571 (98%)	373 (24%)	1 (0%)
36	BB	64/73 (87%)	14 (21%)	0
All	All	1606/1644 (97%)	387 (24%)	1 (0%)

5 of 387 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
29	BA	4	A
29	BA	7	G
29	BA	11	G
29	BA	15	A
29	BA	19	U

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
29	BA	48	U

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 229 ligands modelled in this entry, 224 are monoatomic - leaving 5 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
59	SPM	BA	3208	-	13,13,13	0.31	0	12,12,12	0.79	0
59	SPM	BA	3209	-	13,13,13	0.34	0	12,12,12	0.75	0
58	5GP	BA	3206	-	22,26,26	1.23	2 (9%)	26,40,40	1.27	4 (15%)
60	GNP	BC	1000	56	29,34,34	1.61	7 (24%)	33,54,54	2.13	6 (18%)
58	5GP	BA	3207	56	22,26,26	1.25	2 (9%)	26,40,40	1.25	4 (15%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
59	SPM	BA	3208	-	-	2/11/11/11	-
59	SPM	BA	3209	-	-	2/11/11/11	-
58	5GP	BA	3206	-	-	1/6/26/26	0/3/3/3
60	GNP	BC	1000	56	-	2/14/38/38	0/3/3/3
58	5GP	BA	3207	56	-	0/6/26/26	0/3/3/3

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
60	BC	1000	GNP	PB-O3A	4.37	1.64	1.59
58	BA	3207	5GP	C5-C6	-4.15	1.39	1.47
58	BA	3206	5GP	C5-C6	-4.02	1.39	1.47
60	BC	1000	GNP	C6-N1	3.12	1.38	1.33
60	BC	1000	GNP	PB-O1B	3.06	1.51	1.46

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
60	BC	1000	GNP	C5-C6-N1	-8.39	111.96	123.43
60	BC	1000	GNP	C2-N1-C6	5.84	125.21	115.93
58	BA	3206	5GP	C5-C6-N1	3.21	119.62	113.95
58	BA	3207	5GP	C5-C6-N1	3.13	119.47	113.95
60	BC	1000	GNP	N3-C2-N1	-2.80	123.49	127.22

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
60	BC	1000	GNP	PG-N3B-PB-O1B
60	BC	1000	GNP	PG-N3B-PB-O3A
59	BA	3208	SPM	C7-C8-C9-N10
59	BA	3209	SPM	C7-C8-C9-N10
59	BA	3208	SPM	C7-C6-N5-C4

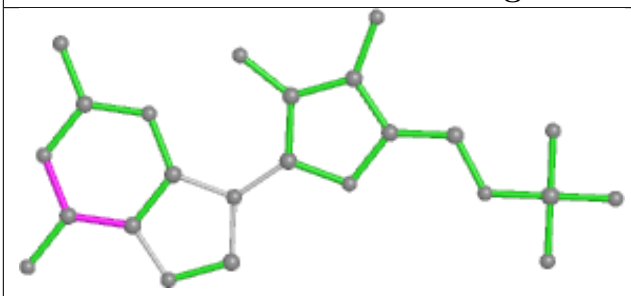
There are no ring outliers.

No monomer is involved in short contacts.

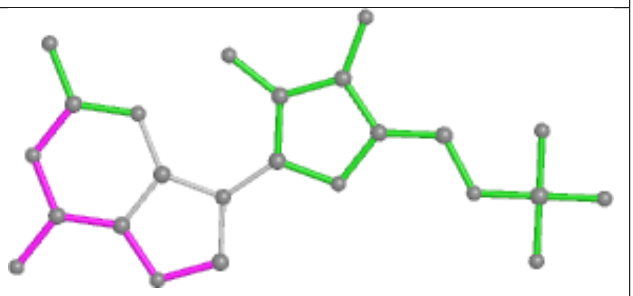
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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

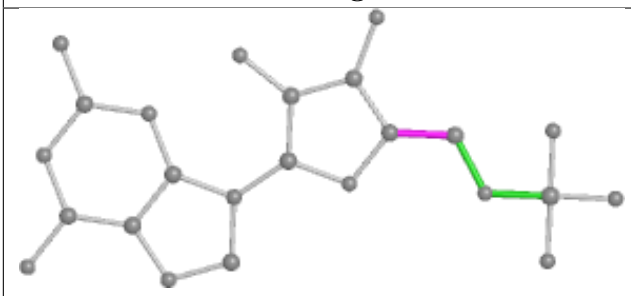
Ligand 5GP BA 3206



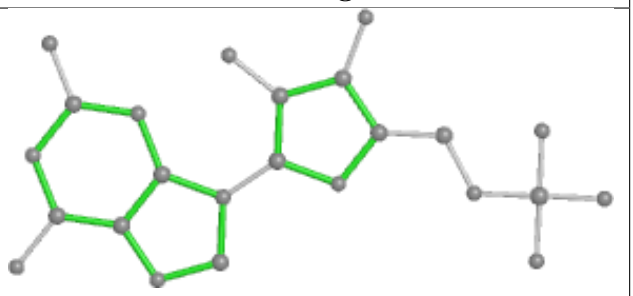
Bond lengths



Bond angles

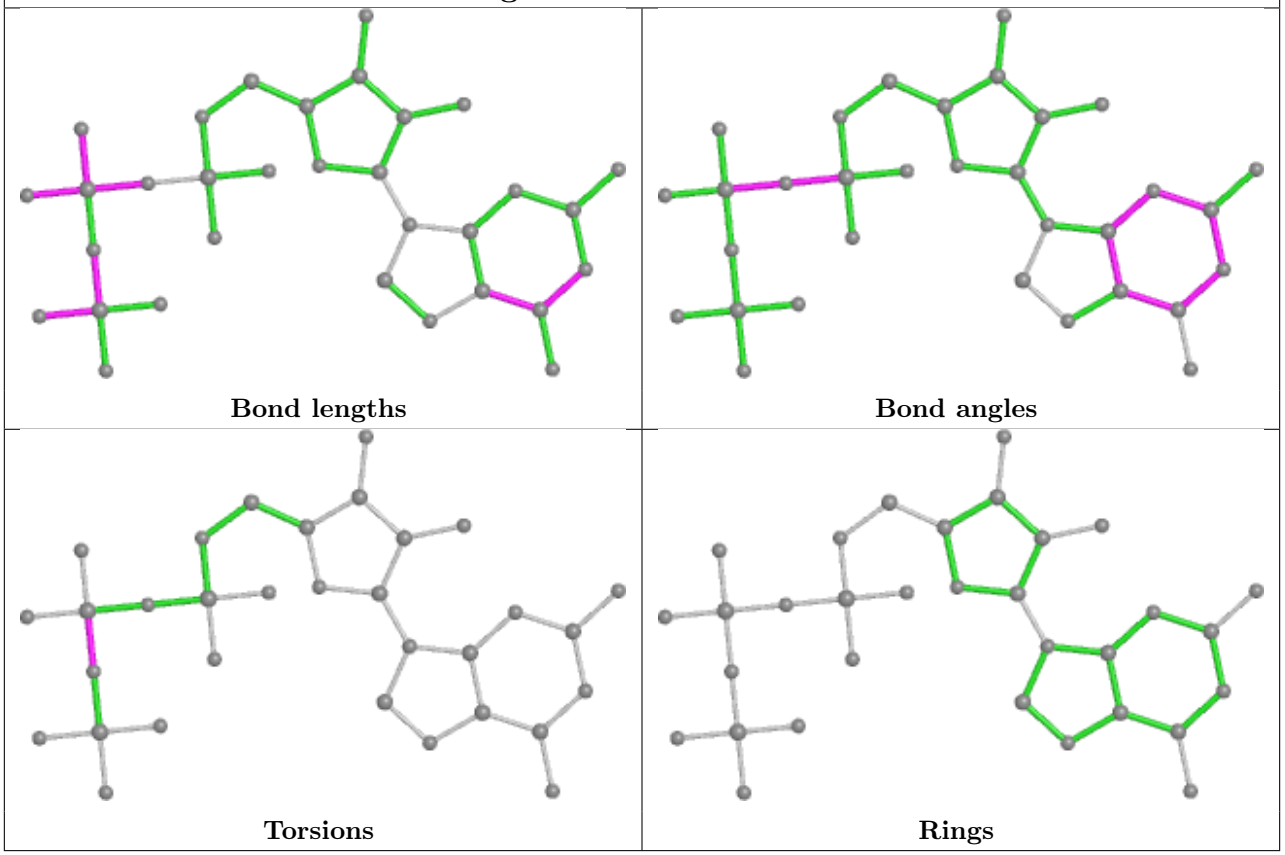


Torsions

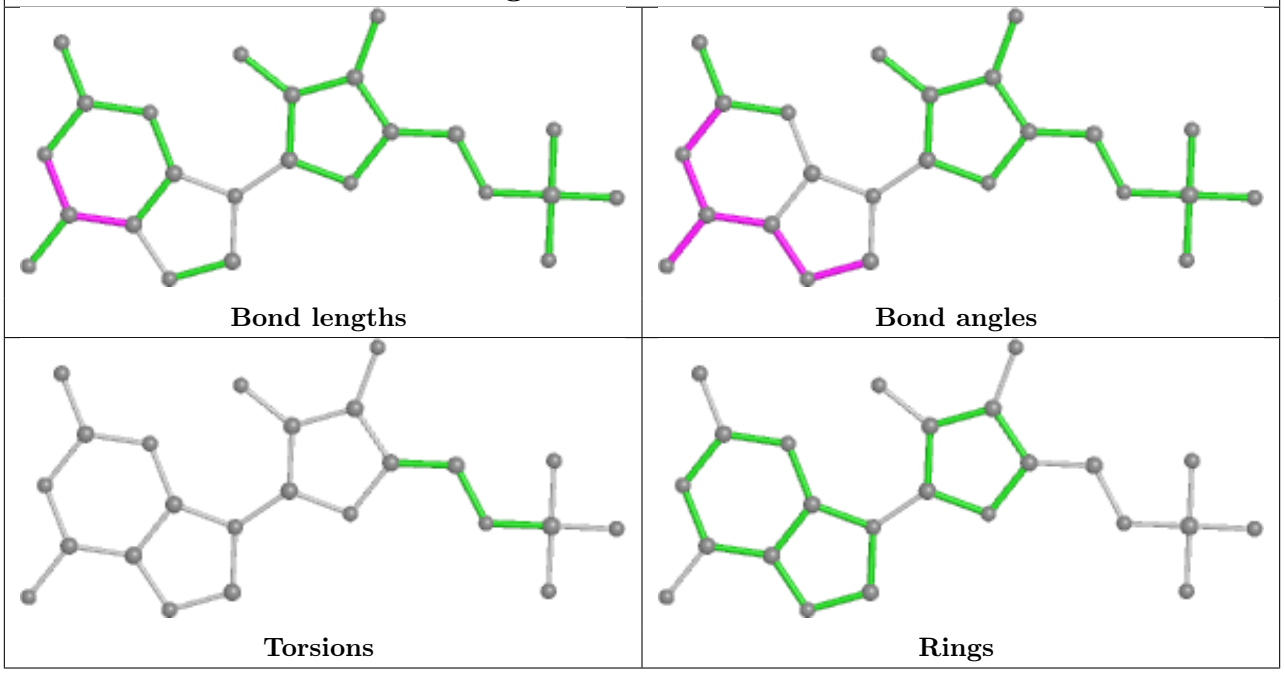


Rings

Ligand GNP BC 1000



Ligand 5GP BA 3207



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.

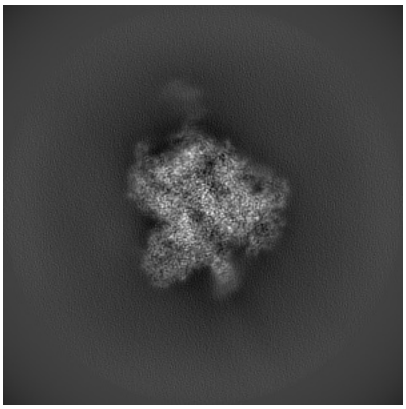
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-12567. These allow visual inspection of the internal detail of the map and identification of artifacts.

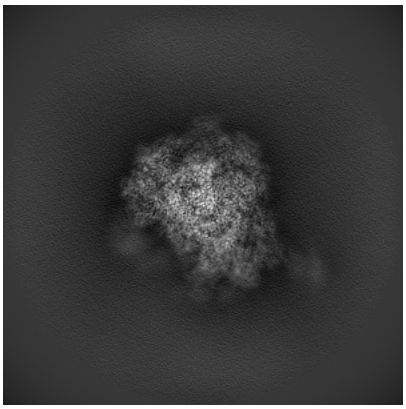
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

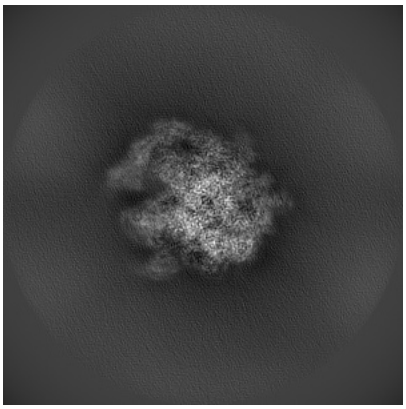
6.1.1 Primary map



X

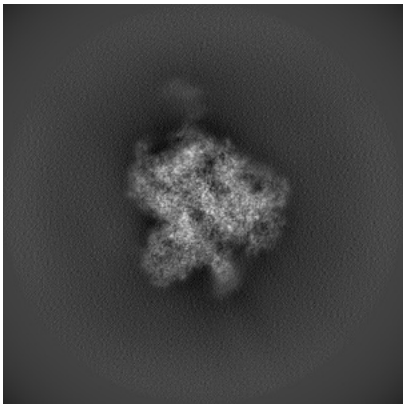


Y

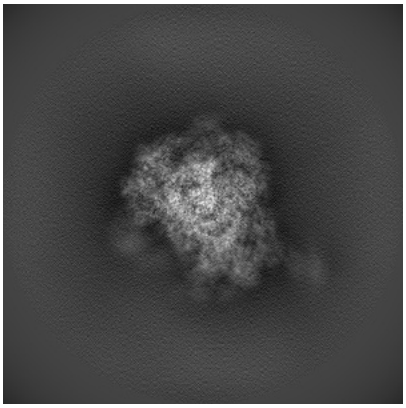


Z

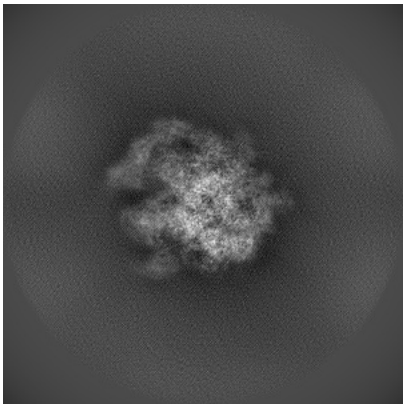
6.1.2 Raw map



X



Y

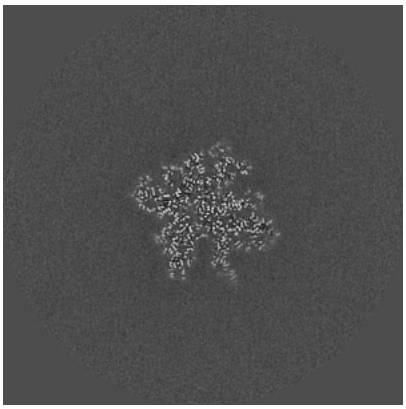


Z

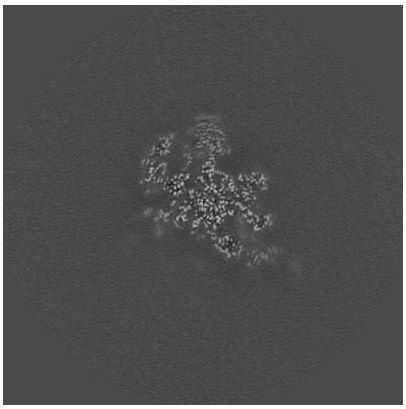
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

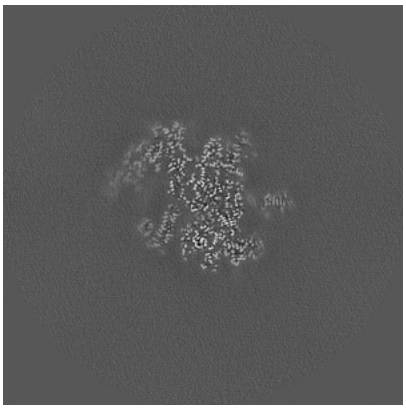
6.2.1 Primary map



X Index: 240

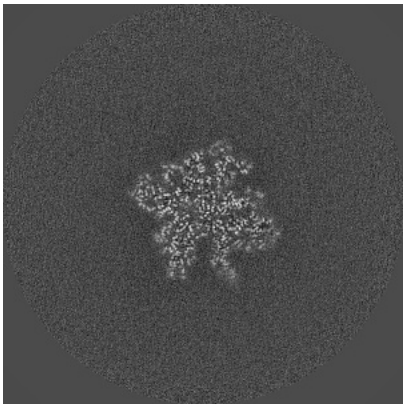


Y Index: 240

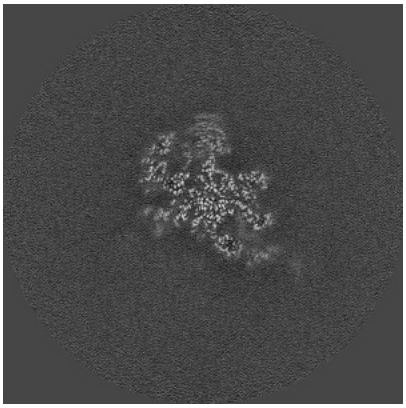


Z Index: 240

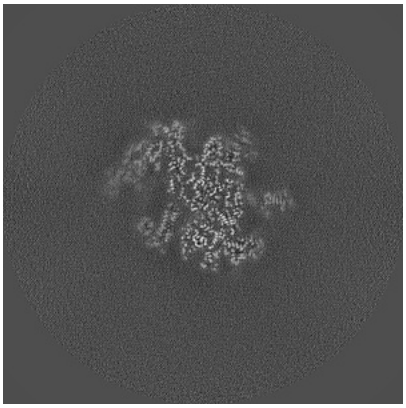
6.2.2 Raw map



X Index: 240



Y Index: 240

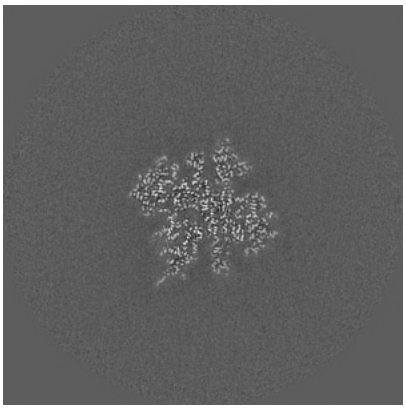


Z Index: 240

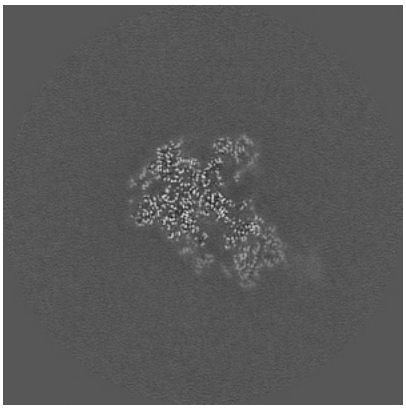
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

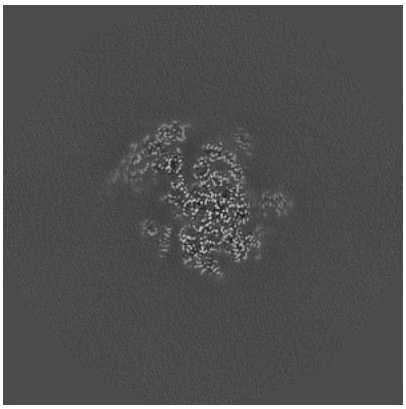
6.3.1 Primary map



X Index: 246

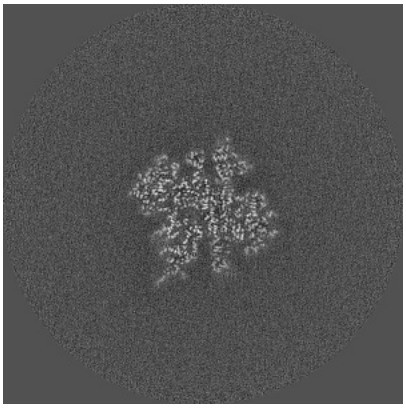


Y Index: 219

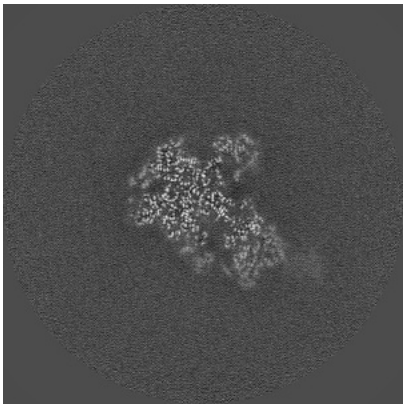


Z Index: 247

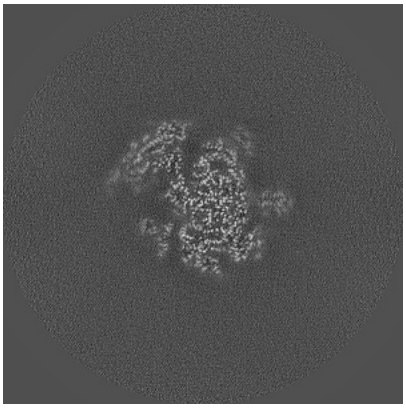
6.3.2 Raw map



X Index: 246



Y Index: 219



Z Index: 246

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

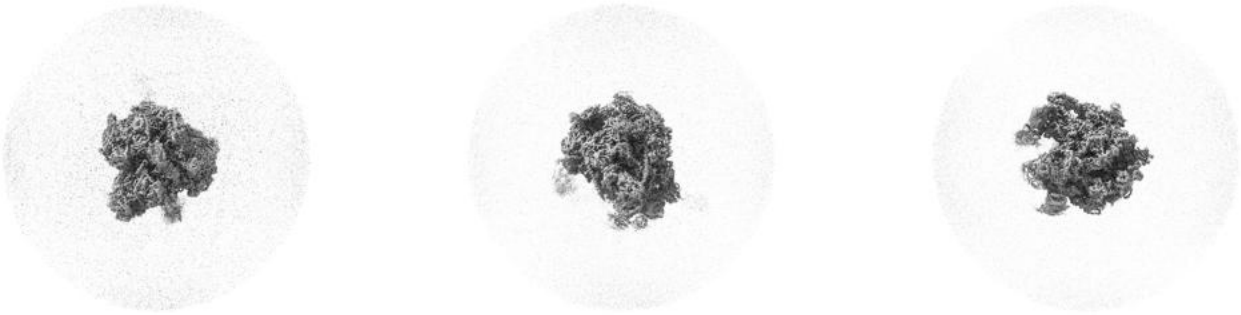
6.4 Orthogonal surface views (i)

6.4.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.028. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map



X Y Z

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

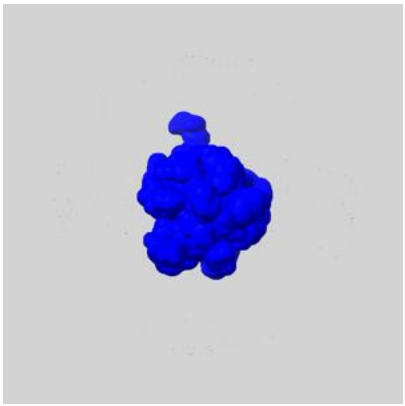
6.5 Mask visualisation (i)

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

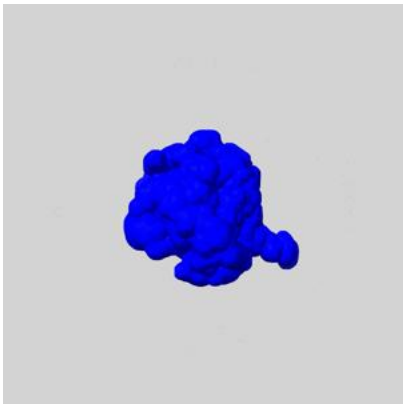
A mask typically either:

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

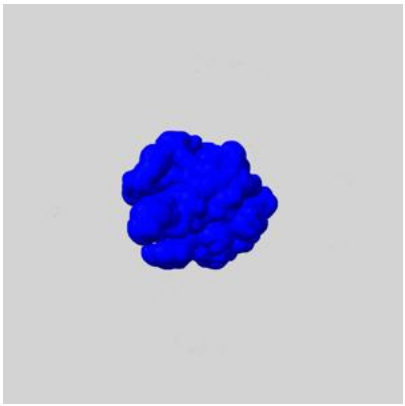
6.5.1 emd_12567_msk_1.map (i)



X



Y

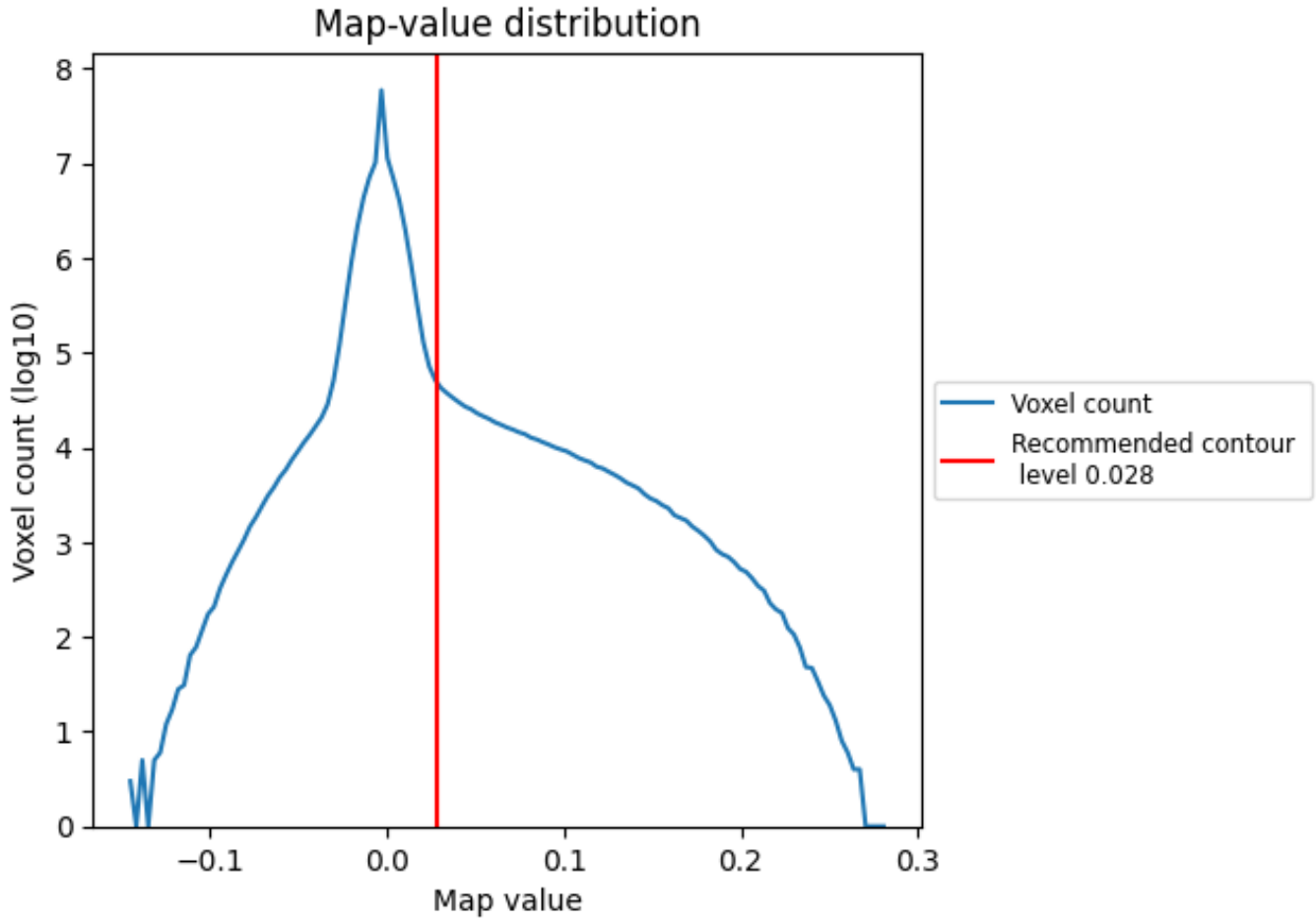


Z

7 Map analysis

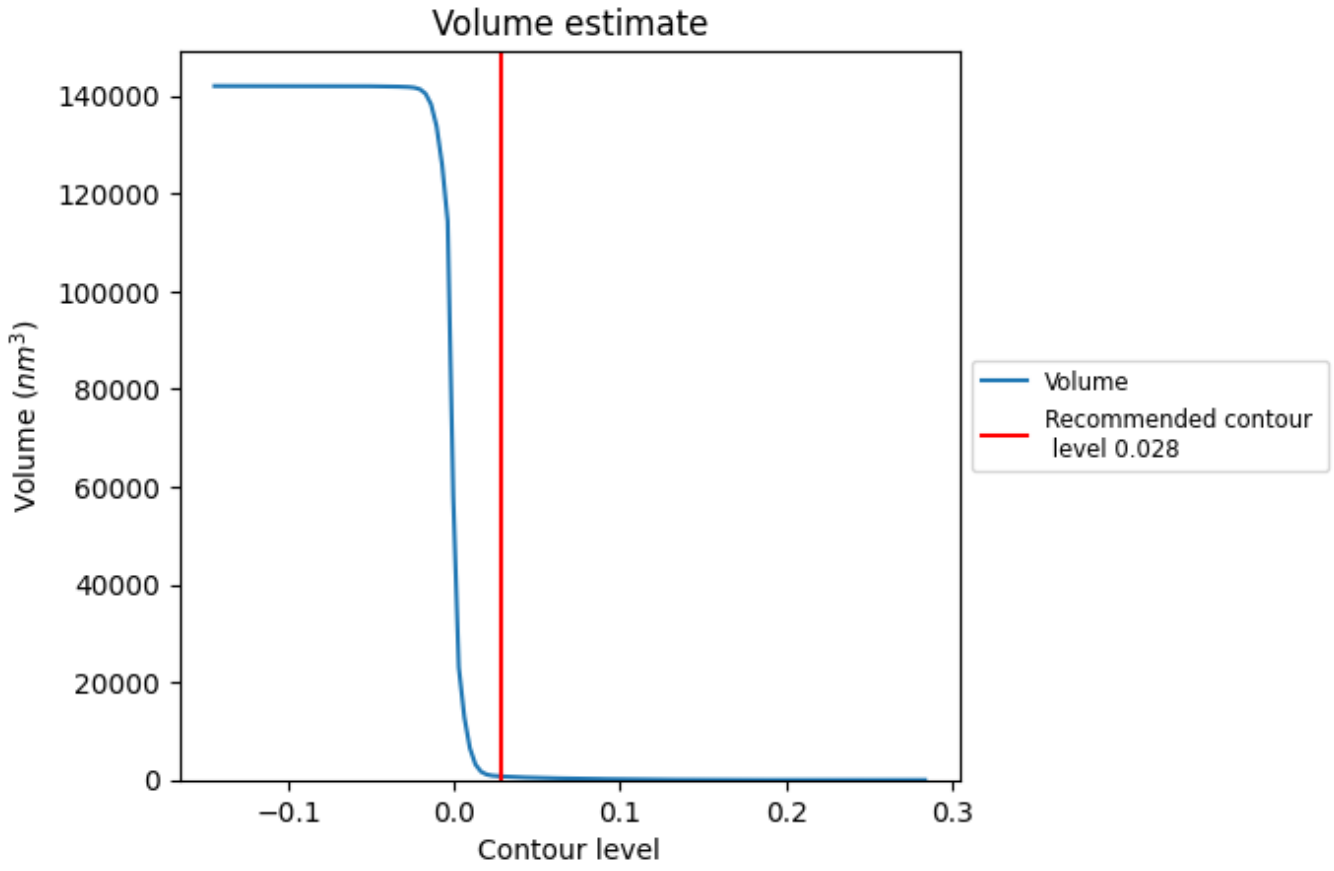
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

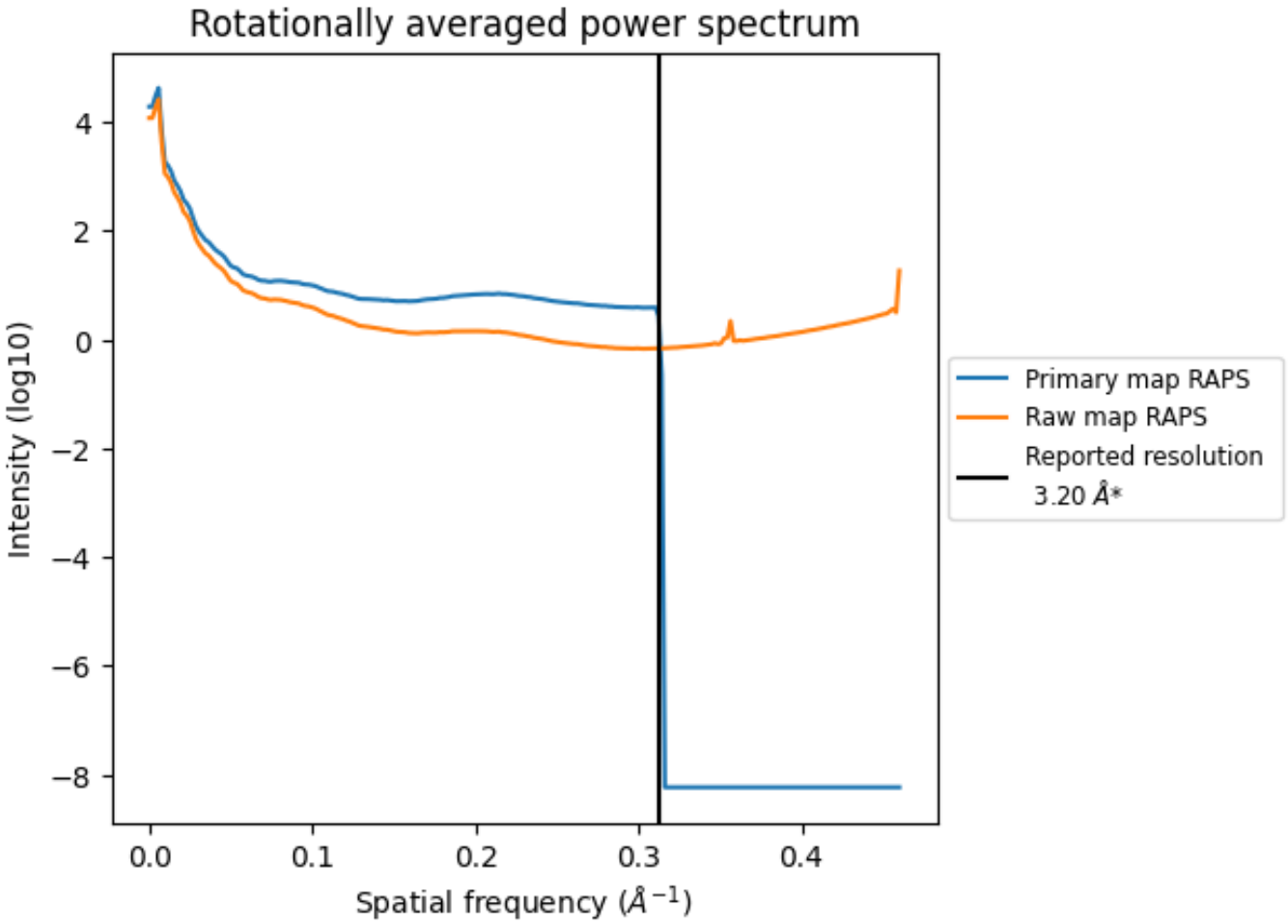
7.2 Volume estimate (i)



The volume at the recommended contour level is 742 nm^3; this corresponds to an approximate mass of 670 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)

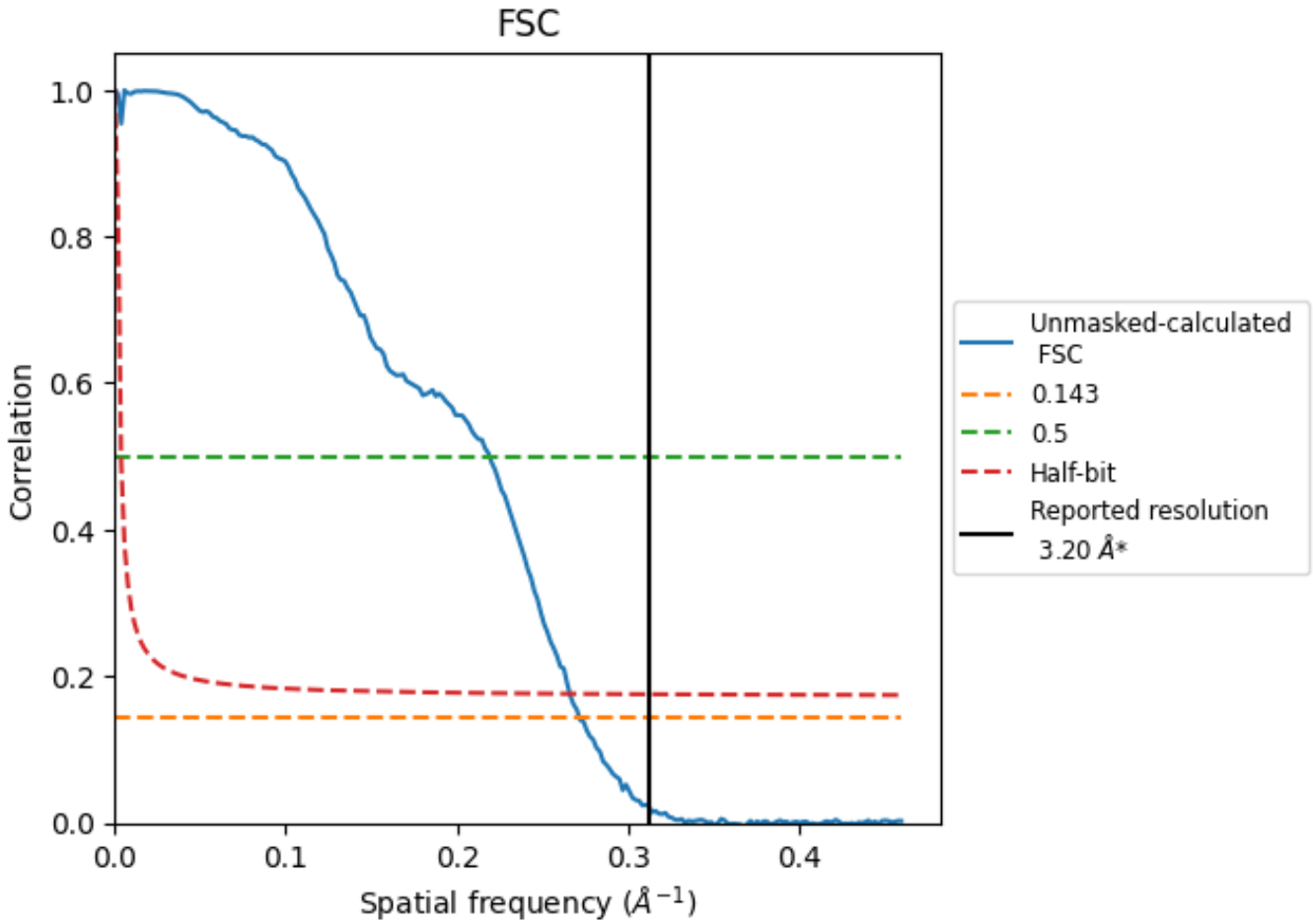


*Reported resolution corresponds to spatial frequency of 0.312 $Å^{-1}$

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.312 Å^{-1}

8.2 Resolution estimates (i)

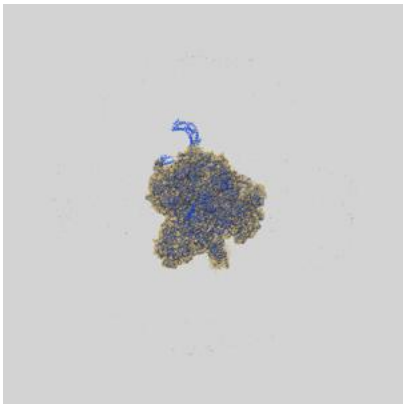
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.68	4.56	3.76

*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 3.68 differs from the reported value 3.2 by more than 10 %

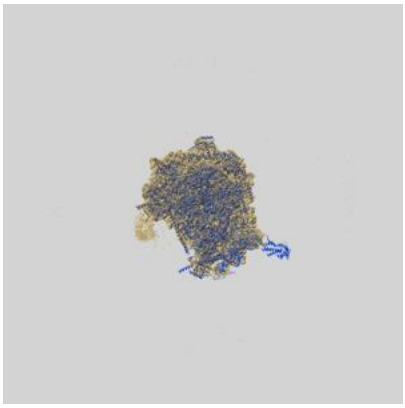
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-12567 and PDB model 7NSH. Per-residue inclusion information can be found in section 3 on page 19.

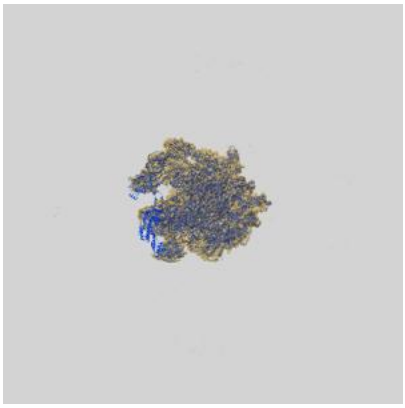
9.1 Map-model overlay



X



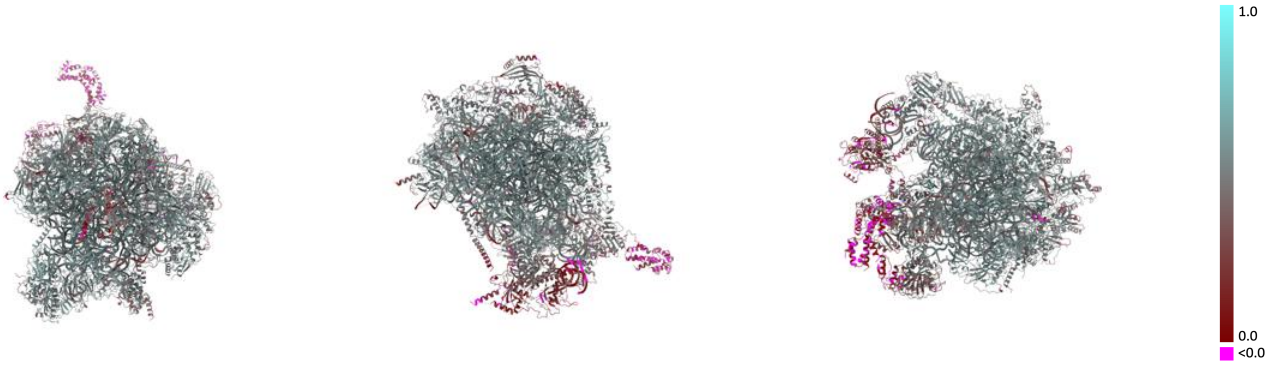
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.028 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.

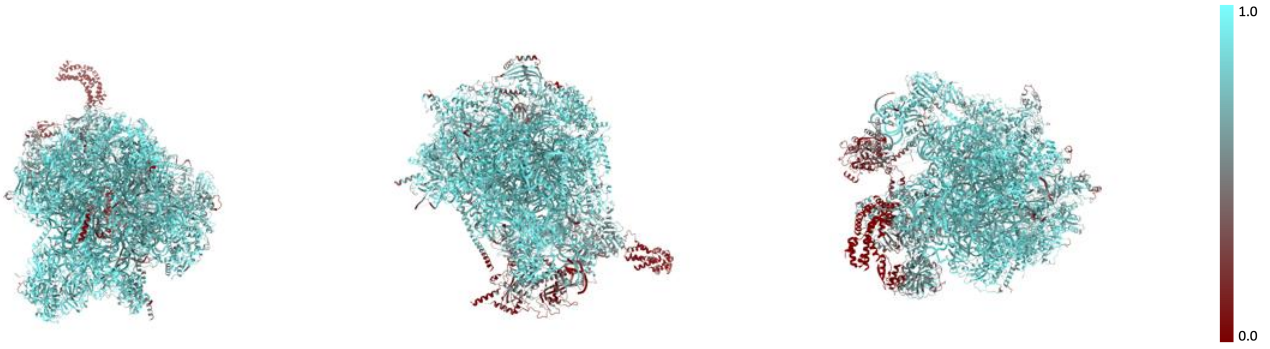
9.2 Q-score mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

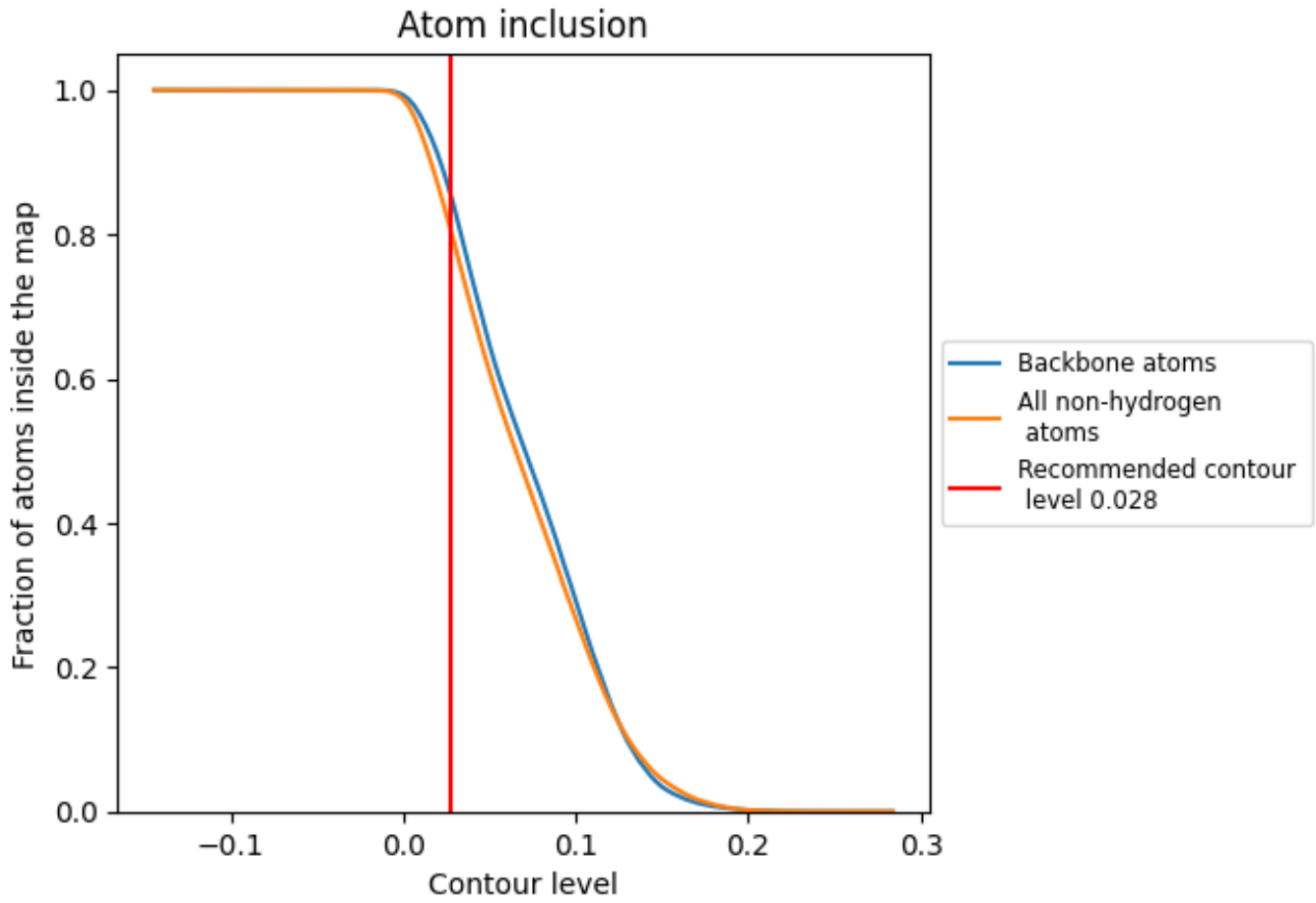
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.028).

9.4 Atom inclusion (i)



At the recommended contour level, 85% of all backbone atoms, 80% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.028) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8019	0.4900
B0	0.9133	0.5640
B1	0.8251	0.5160
B2	0.8651	0.5270
B3	0.8632	0.5440
B4	0.3604	0.2400
B5	0.8622	0.5290
B6	0.7692	0.4910
B7	0.9268	0.5790
B8	0.9009	0.5690
B9	0.9283	0.5790
BA	0.9288	0.5330
BB	0.6762	0.2790
BC	0.6051	0.4180
BD	0.8979	0.5540
BE	0.8935	0.5450
BF	0.8848	0.5470
BG	0.6687	0.4700
BI	0.7792	0.4800
BJ	0.5607	0.3680
BK	0.5484	0.3740
BN	0.9001	0.5560
BO	0.9000	0.5560
BP	0.8887	0.5430
BQ	0.8738	0.5390
BR	0.8926	0.5440
BS	0.8686	0.5200
BT	0.8664	0.5260
BU	0.8726	0.5390
BV	0.8731	0.5380
BW	0.8849	0.5500
BX	0.8311	0.5150
BY	0.7049	0.4750
Ba	0.8817	0.5320
Bb	0.8464	0.4930

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Chain	Atom inclusion	Q-score
Bc	0.8086	0.4770
Bd	0.2537	0.2300
Be	0.8396	0.4990
Bf	0.7910	0.4800
Bg	0.8990	0.5490
Bh	0.8469	0.5030
Bi	0.6122	0.4210
Bj	0.2092	0.1820
Bk	0.3775	0.3010
Bl	0.8821	0.5320
Bm	0.5505	0.4460
Bn	0.8821	0.5480
Bo	0.8389	0.5200
Bp	0.6630	0.4130
Bq	0.6580	0.4240
Bt	0.8779	0.5540
Bu	0.6964	0.4440
Bv	0.7300	0.4450
Bw	0.8611	0.5240
Bx	0.8547	0.5120
CL	0.0443	0.1680
DL	0.0282	0.0720
EL	0.0000	0.0540
FL	0.0000	0.0730
GL	0.0000	0.0210
HL	0.0000	0.0750
LL	0.0000	0.0820