



wwPDB EM Validation Summary Report ⓘ

Aug 27, 2026 – 08:49 am BST

PDB ID : 7ODS / pdb_00007ods
EMDB ID : EMD-12846
Title : State B of the human mitoribosomal large subunit assembly intermediate
Authors : Lenarcic, T.; Jaskolowski, M.; Leibundgut, M.; Scaiola, A.; Schoenhut, T.;
Saurer, M.; Lee, R.G.; Rackham, O.; Filipovska, A.; Ban, N.
Deposited on : 2021-04-30
Resolution : 3.10 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:

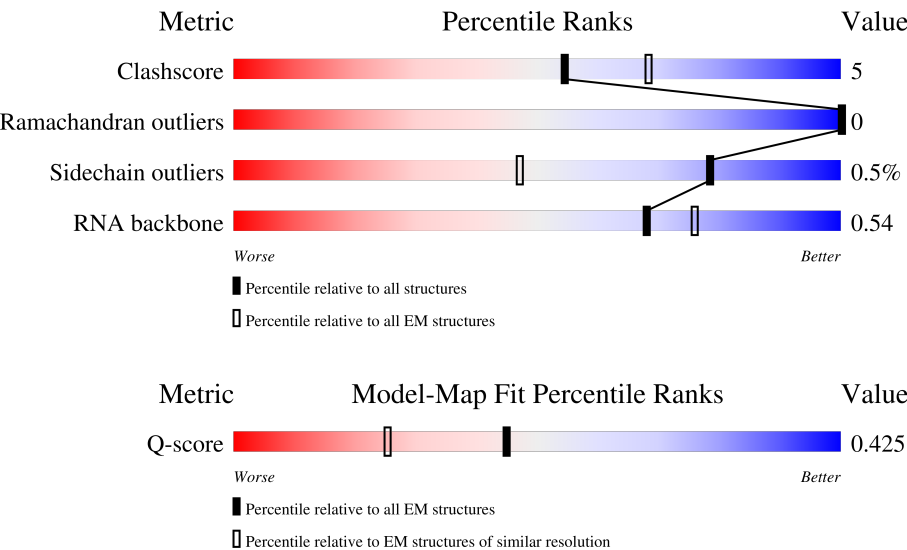
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

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.



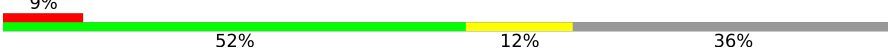
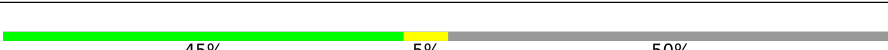
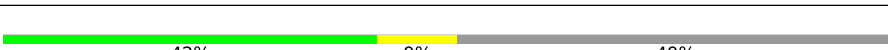
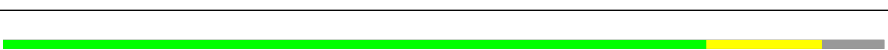
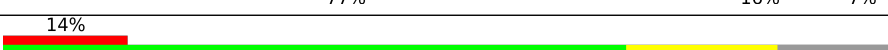
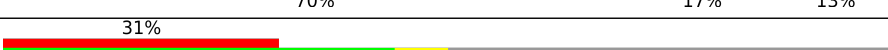
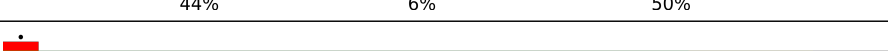
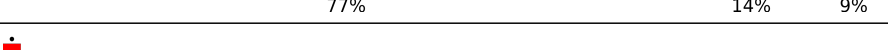
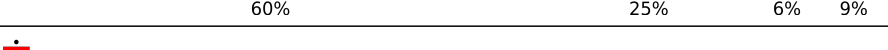
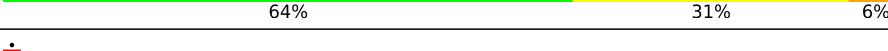
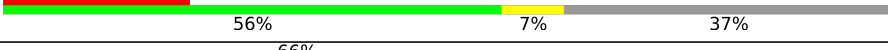
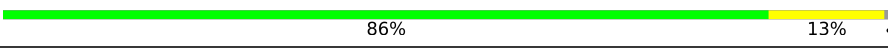
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	14724 (2.60 - 3.60)

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

Mol	Chain	Length	Quality of chain
1	u	234	
2	v	70	
3	w	156	

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Mol	Chain	Length	Quality of chain
4	x	384	
5	y	381	
6	z	246	
7	0	188	
8	1	65	
9	2	92	
10	3	188	
11	4	103	
12	5	423	
13	6	380	
14	7	338	
15	8	206	
16	9	137	
17	A	1589	
18	B	72	
19	D	305	
20	E	348	
21	F	311	
22	H	267	
23	I	261	
24	J	192	
25	K	178	
26	L	145	
27	M	296	
28	N	251	

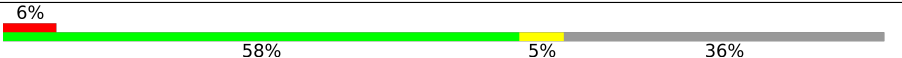
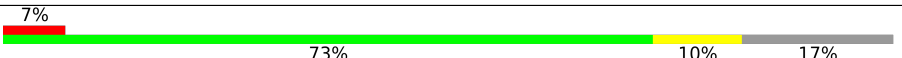
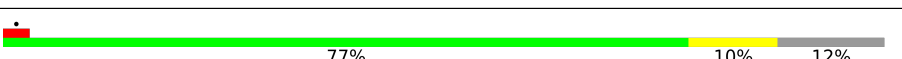
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Mol	Chain	Length	Quality of chain
29	O	175	
30	P	180	
31	Q	292	
32	R	149	
33	S	205	
34	T	206	
35	U	153	
36	V	216	
37	W	148	
38	X	256	
39	Y	250	
40	Z	161	
41	a	142	
42	b	215	
43	c	332	
44	d	306	
45	e	279	
46	f	212	
47	g	166	
48	h	158	
49	i	128	
50	j	123	
51	k	112	
52	l	138	
53	m	128	

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Mol	Chain	Length	Quality of chain
54	o	102	
55	p	206	
56	q	222	
57	r	196	
58	s	439	

2 Entry composition

There are 65 unique types of molecules in this entry. The entry contains 108339 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 assembly of ribosomal large subunit protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	u	110	Total	C	N	O	S	0	0
			919	591	154	164	10		

- Molecule 2 is a protein called MIEF1 upstream open reading frame protein.

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

- Molecule 3 is a protein called Acyl carrier protein, mitochondrial.

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

- Molecule 4 is a protein called 5-methylcytosine rRNA methyltransferase NSUN4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	x	336	Total	C	N	O	S	0	0
			2660	1694	465	484	17		

- Molecule 5 is a protein called Transcription termination factor 4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	y	244	Total	C	N	O	S	0	0
			1980	1264	342	362	12		

- Molecule 6 is a protein called rRNA methyltransferase 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	z	181	Total	C	N	O	S	0	0
			1366	869	238	253	6		

- Molecule 7 is a protein called 39S ribosomal protein L32, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	0	110	Total	C	N	O	S	0	0
			898	554	176	162	6		

- Molecule 8 is a protein called 39S ribosomal protein L33, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	1	55	Total	C	N	O	S	0	0
			455	290	87	76	2		

- Molecule 9 is a protein called 39S ribosomal protein L34, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	2	46	Total	C	N	O	S	0	0
			377	233	83	60	1		

- Molecule 10 is a protein called 39S ribosomal protein L35, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	3	95	Total	C	N	O	S	0	0
			832	539	162	128	3		

- Molecule 11 is a protein called 39S ribosomal protein L36, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	4	38	Total	C	N	O	S	0	0
			342	217	72	49	4		

- Molecule 12 is a protein called 39S ribosomal protein L37, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	5	394	Total	C	N	O	S	0	0
			3210	2073	560	566	11		

- Molecule 13 is a protein called 39S ribosomal protein L38, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	6	354	Total	C	N	O	S	0	0
			2948	1881	525	533	9		

- Molecule 14 is a protein called 39S ribosomal protein L39, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	7	294	Total	C	N	O	S	0	0
			2390	1529	405	438	18		

- Molecule 15 is a protein called 39S ribosomal protein L40, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	8	102	Total	C	N	O	S	0	0
			860	543	152	163	2		

- Molecule 16 is a protein called 39S ribosomal protein L41, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	9	124	Total	C	N	O	S	0	0
			997	644	170	181	2		

- Molecule 17 is a RNA chain called 16S mitochondrial rRNA, DNA (30-MER),16S mitochondrial rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	A	1445	Total	C	N	O	P	0	0
			30407	13635	5434	9893	1445		

- Molecule 18 is a RNA chain called mitochondrial tRNA^{Val}.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	B	72	Total	C	N	O	P	0	0
			1522	683	269	498	72		

- Molecule 19 is a protein called 39S ribosomal protein L2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	D	240	Total	C	N	O	S	0	0
			1872	1165	378	320	9		

- Molecule 20 is a protein called 39S ribosomal protein L3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	E	305	Total	C	N	O	S	0	0
			2406	1545	418	432	11		

- Molecule 21 is a protein called 39S ribosomal protein L4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	F	252	Total	C	N	O	S	0	0
			2031	1305	370	350	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
22	H	97	Total	C	N	O		0	0
			802	508	155	139			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
23	I	164	Total	C	N	O	S	0	0
			1331	858	241	222	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
24	J	175	Total	C	N	O	S	0	0
			1330	847	237	244	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
			1455	936	259	253	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
			890	559	171	155	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
27	M	291	Total	C	N	O	S	0	0
			2327	1483	430	408	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
28	N	209	Total	C	N	O	S	0	0
			1702	1093	307	293	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
29	O	154	Total	C	N	O	S	0	0
			1259	792	241	219	7		

- Molecule 30 is a protein called 39S ribosomal protein L18, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	P	144	Total	C	N	O	S	0	0
			1173	733	224	211	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
31	Q	221	Total	C	N	O	S	0	0
			1843	1179	327	328	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
			1154	732	231	187	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
33	S	161	Total	C	N	O	S	0	0
			1293	835	227	227	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
			1369	875	254	233	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
35	U	152	Total	C	N	O	S	0	0
			1251	788	234	226	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
			1653	1053	294	298	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
37	W	106	Total	C	N	O	S	0	0
			835	536	157	139	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
38	X	244	Total	C	N	O	S	0	0
			2044	1322	352	365	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
39	Y	181	Total	C	N	O	S	0	0
			1556	995	298	259	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
40	Z	122	Total	C	N	O	S	0	0
			996	636	186	171	3		

- Molecule 41 is a protein called 39S ribosomal protein L42, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	a	100	Total	C	N	O	S	0	0
			840	529	152	154	5		

- Molecule 42 is a protein called 39S ribosomal protein L43, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	b	149	Total	C	N	O	S	0	0
			1189	739	230	217	3		

- Molecule 43 is a protein called 39S ribosomal protein L44, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	c	286	Total	C	N	O	S	0	0
			2299	1470	397	423	9		

- Molecule 44 is a protein called 39S ribosomal protein L45, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	d	223	Total	C	N	O	S	0	0
			1824	1160	316	335	13		

- Molecule 45 is a protein called 39S ribosomal protein L46, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	e	228	Total	C	N	O	S	0	0
			1848	1174	326	342	6		

- Molecule 46 is a protein called 39S ribosomal protein L48, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	f	150	Total	C	N	O	S	0	0
			1196	764	197	231	4		

- Molecule 47 is a protein called 39S ribosomal protein L49, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	g	134	Total	C	N	O	S	0	0
			1113	719	193	199	2		

- Molecule 48 is a protein called 39S ribosomal protein L50, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	h	110	Total	C	N	O	S	0	0
			895	568	156	168	3		

- Molecule 49 is a protein called 39S ribosomal protein L51, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	i	97	Total	C	N	O	S	0	0
			828	532	165	127	4		

- Molecule 50 is a protein called 39S ribosomal protein L52, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	j	94	Total	C	N	O	S	0	0
			745	463	144	136	2		

- Molecule 51 is a protein called 39S ribosomal protein L53, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	k	101	Total	C	N	O	S	0	0
			774	479	148	142	5		

- Molecule 52 is a protein called 39S ribosomal protein L54, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	l	82	Total	C	N	O	S	0	0
			688	437	120	128	3		

- Molecule 53 is a protein called 39S ribosomal protein L55, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	m	51	Total	C	N	O	S	0	0
			419	262	82	73	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
54	o	81	Total	C	N	O	S	0	0
			688	432	138	115	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
55	p	147	Total	C	N	O	S	0	0
			1205	748	228	225	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	141	Total	C	N	O	S	0	0
			1177	732	229	211	5		

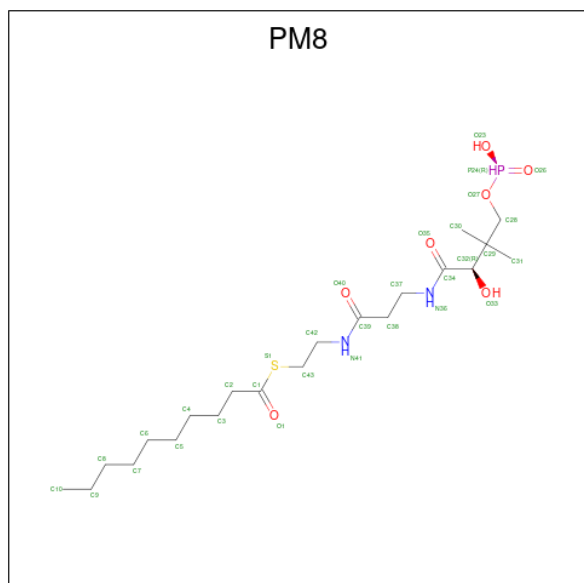
- Molecule 57 is a protein called 39S ribosomal protein S18a, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	r	162	Total	C	N	O	S	0	0
			1322	839	252	223	8		

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

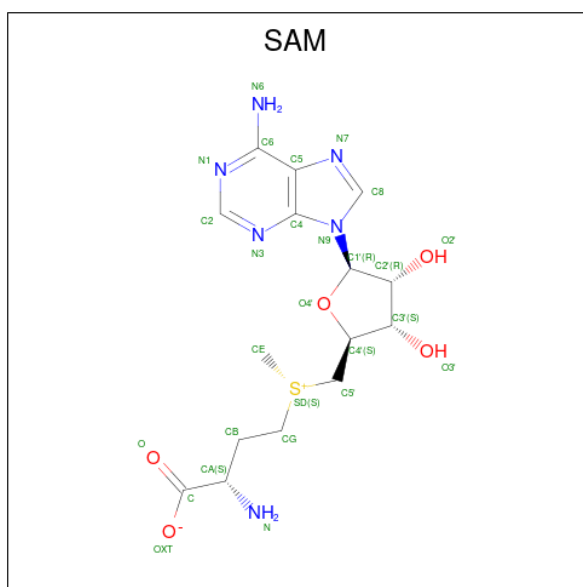
Mol	Chain	Residues	Atoms					AltConf	Trace
58	s	386	Total	C	N	O	S	0	0
			3155	2023	559	559	14		

- Molecule 59 is S-(2-{[N-(2-HYDROXY-4-{[HYDROXY(OXIDO)PHOSPHINO]OXY}-3,3-DIMETHYLBUTANOYL)-BETA-ALANYL]AMINO}ETHYL) DECANETHIOATE (CCD ID: PM8) (formula: C₂₁H₄₁N₂O₇PS).



Mol	Chain	Residues	Atoms						AltConf
59	w	1	Total	C	N	O	P	S	0
			32	21	2	7	1	1	

- Molecule 60 is S-ADENOSYLMETHIONINE (CCD ID: SAM) (formula: C₁₅H₂₂N₆O₅S).



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

- Molecule 61 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
61	0	1	Total	Zn	0
			1	1	
61	4	1	Total	Zn	0
			1	1	

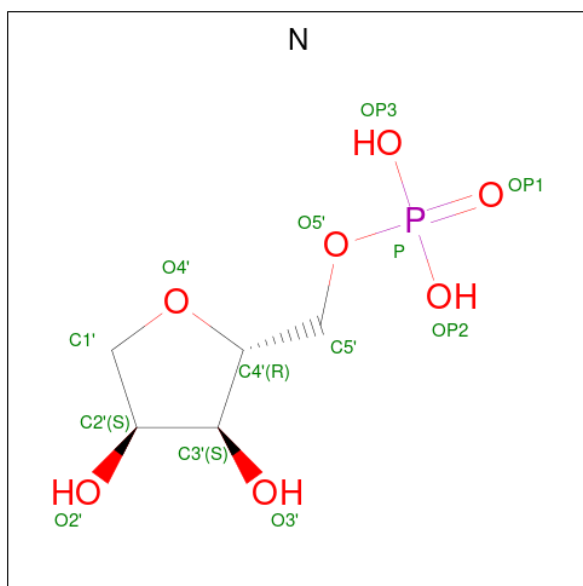
- Molecule 62 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
62	A	85	Total	Mg	0
			85	85	
62	D	1	Total	Mg	0
			1	1	
62	E	1	Total	Mg	0
			1	1	
62	O	1	Total	Mg	0
			1	1	

- Molecule 63 is POTASSIUM ION (CCD ID: K) (formula: K).

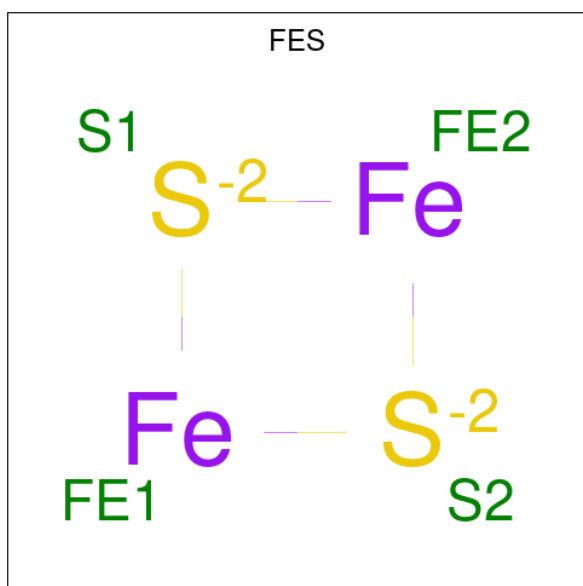
Mol	Chain	Residues	Atoms		AltConf
63	A	8	Total	K	0
			8	8	

- Molecule 64 is ANY 5'-MONOPHOSPHATE NUCLEOTIDE (CCD ID: N) (formula: $C_5H_{11}O_7P$).



Mol	Chain	Residues	Atoms				AltConf
64	A	1	Total	C	O	P	0
			12	5	6	1	

- Molecule 65 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).

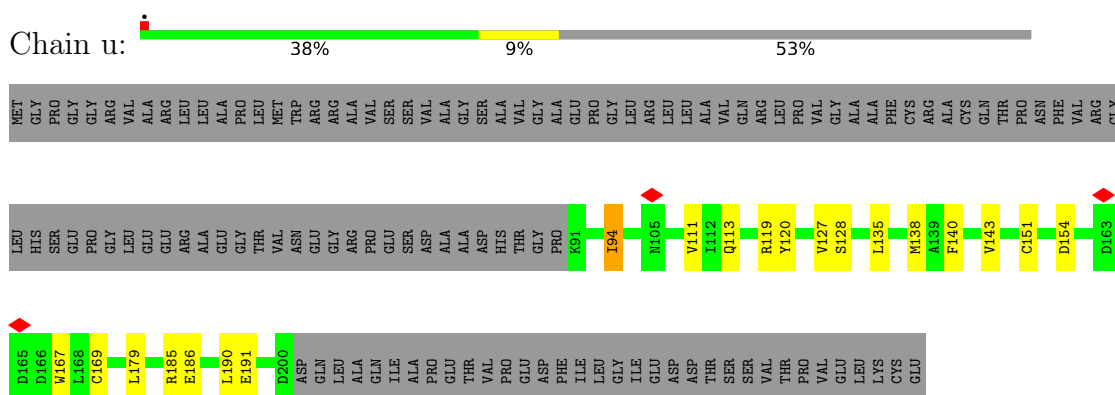


Mol	Chain	Residues	Atoms			AltConf
65	r	1	Total	Fe	S	0
			4	2	2	

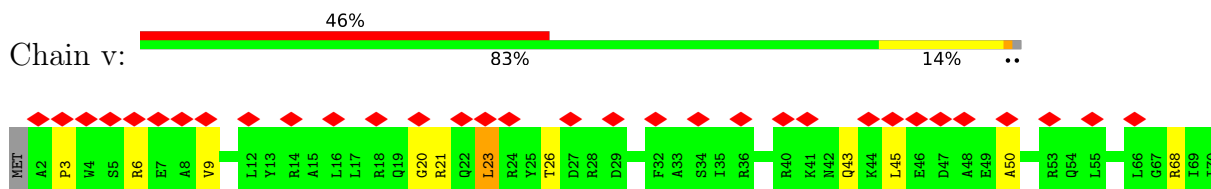
3 Residue-property plots

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.

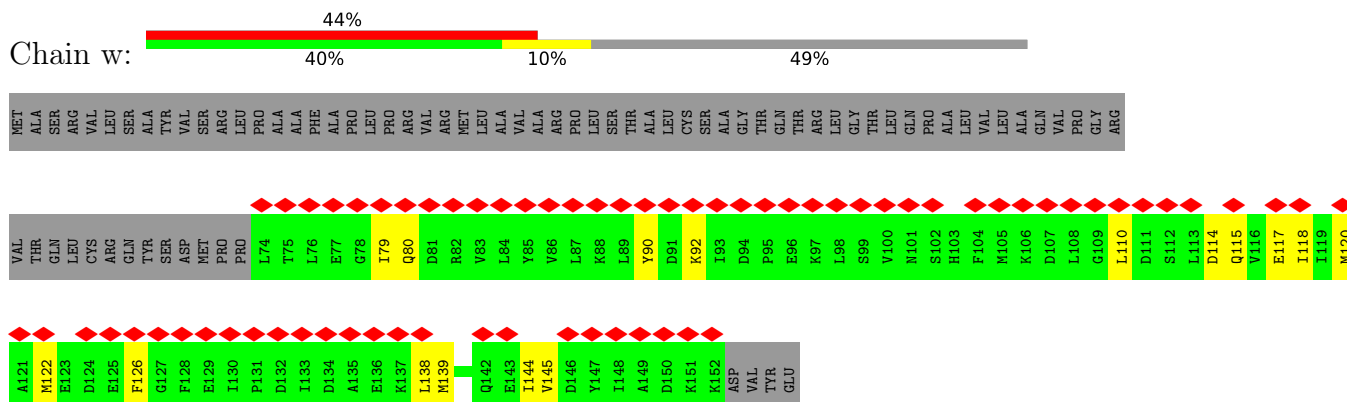
- Molecule 1: Mitochondrial assembly of ribosomal large subunit protein 1



- Molecule 2: MIEF1 upstream open reading frame protein



- Molecule 3: Acyl carrier protein, mitochondrial



- Molecule 4: 5-methylcytosine rRNA methyltransferase NSUN4

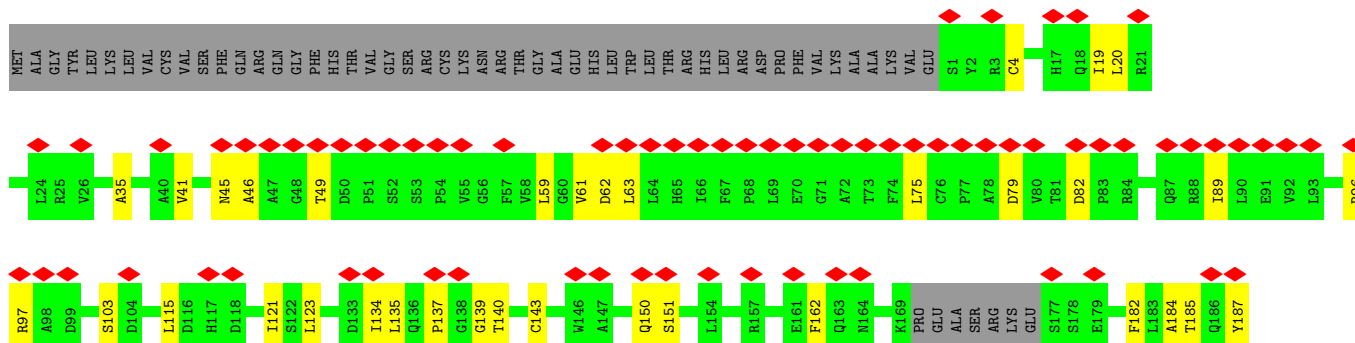
Frequency	Percentage
Daily	70%
Weekly	17%
Monthly	12%



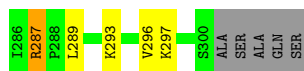
Frequency	Percentage
Never	9%
Often	52%
Sometimes	12%
Not sure	36%



Response	Percentage
Current government is the best	30%
A different government is the best	59%
No government is the best	14%
No answer	26%

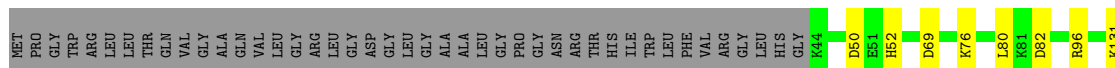






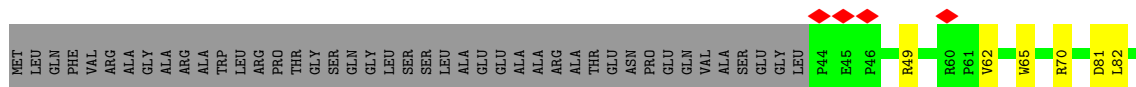
- Molecule 20: 39S ribosomal protein L3, mitochondrial

Chain E: 76% 12% 12%



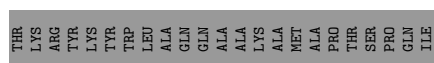
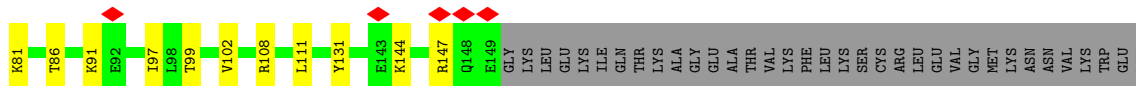
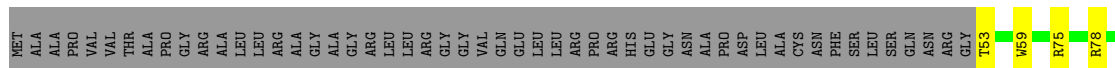
- Molecule 21: 39S ribosomal protein L4, mitochondrial

Chain F: 66% 15% 19%



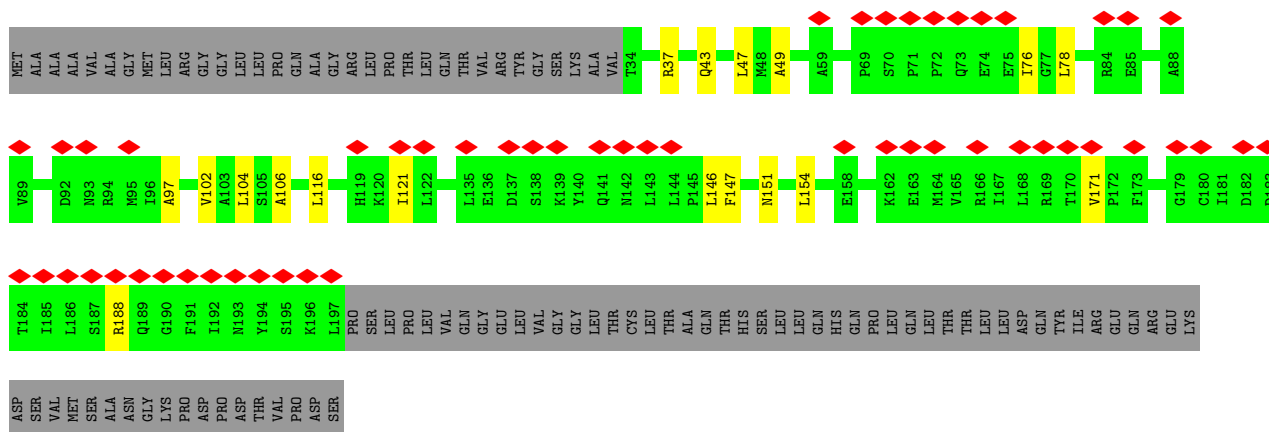
- Molecule 22: 39S ribosomal protein L9, mitochondrial

Chain H: 31% 6% 64%

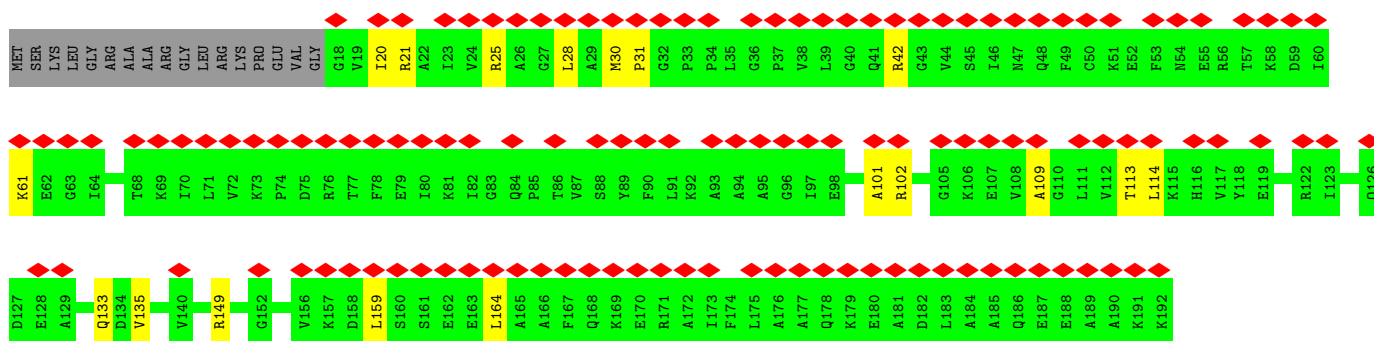
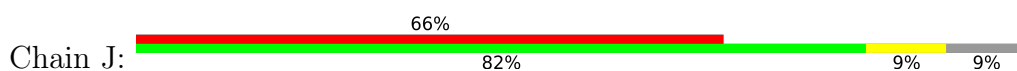


- Molecule 23: 39S ribosomal protein L10, mitochondrial

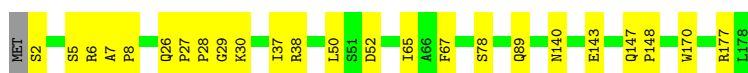
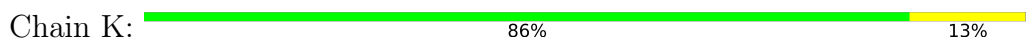
Chain I: 21% 56% 7% 37%



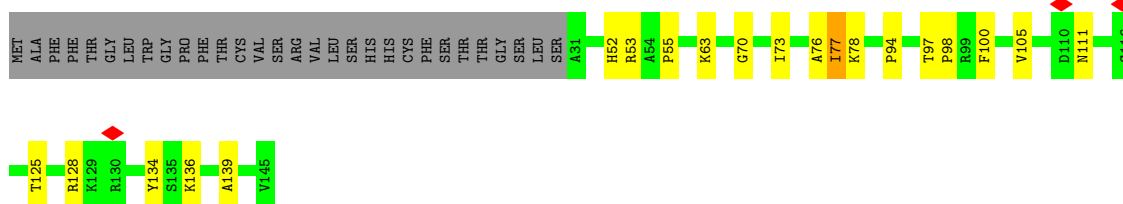
• Molecule 24: 39S ribosomal protein L11, mitochondrial



• Molecule 25: 39S ribosomal protein L13, mitochondrial

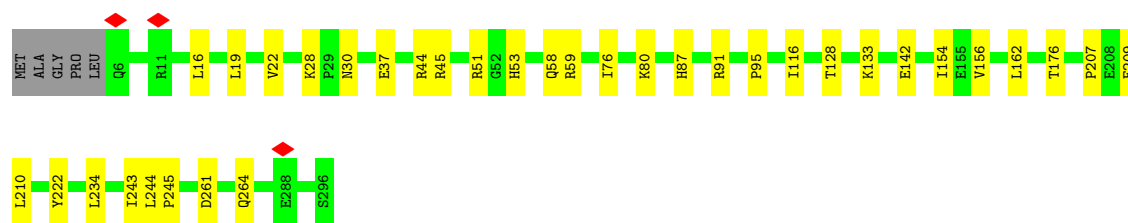


• Molecule 26: 39S ribosomal protein L14, mitochondrial



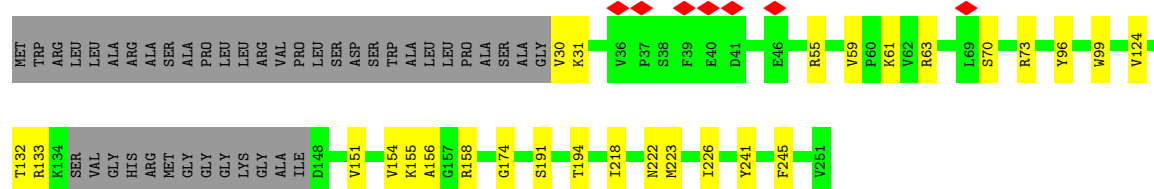
• Molecule 27: 39S ribosomal protein L15, mitochondrial





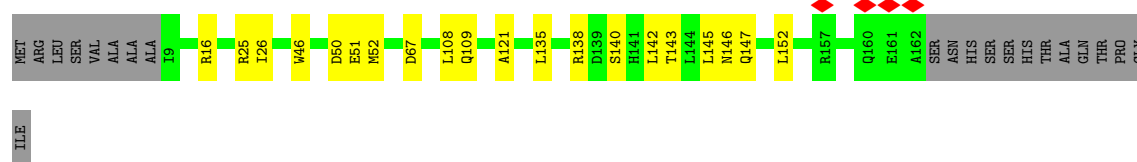
- Molecule 28: 39S ribosomal protein L16, mitochondrial

Chain N: 73% 11% 17%



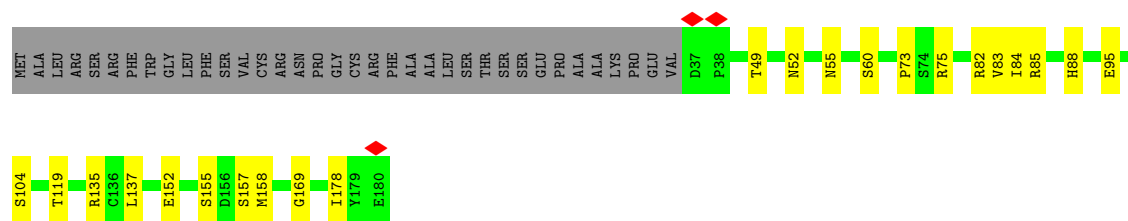
- Molecule 29: 39S ribosomal protein L17, mitochondrial

Chain O: 77% 11% 12%



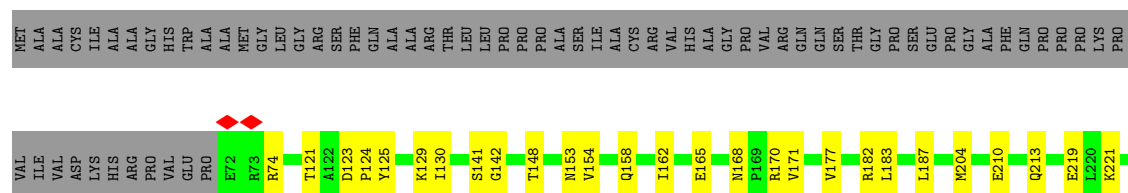
- Molecule 30: 39S ribosomal protein L18, mitochondrial

Chain P: 68% 12% 20%



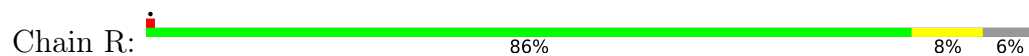
- Molecule 31: 39S ribosomal protein L19, mitochondrial

Chain Q: 64% 11% 24%

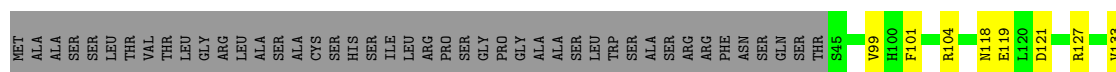




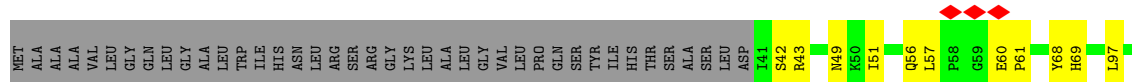
- Molecule 32: 39S ribosomal protein L20, mitochondrial



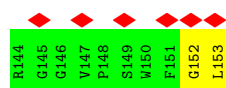
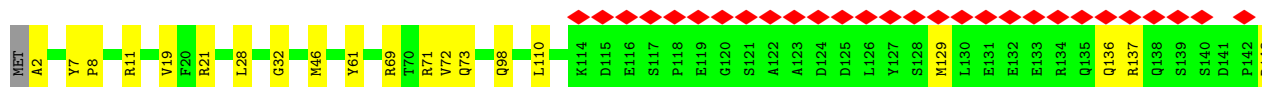
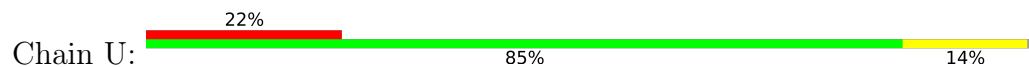
- Molecule 33: 39S ribosomal protein L21, mitochondrial



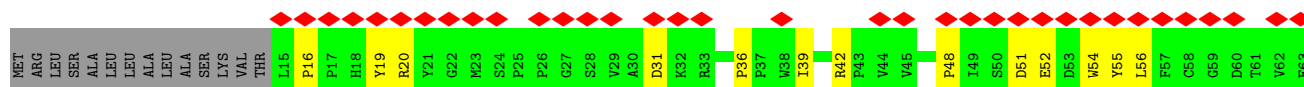
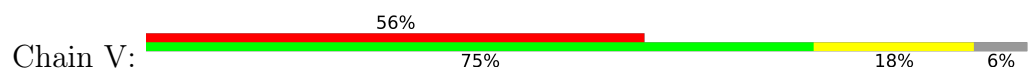
- Molecule 34: 39S ribosomal protein L22, mitochondrial

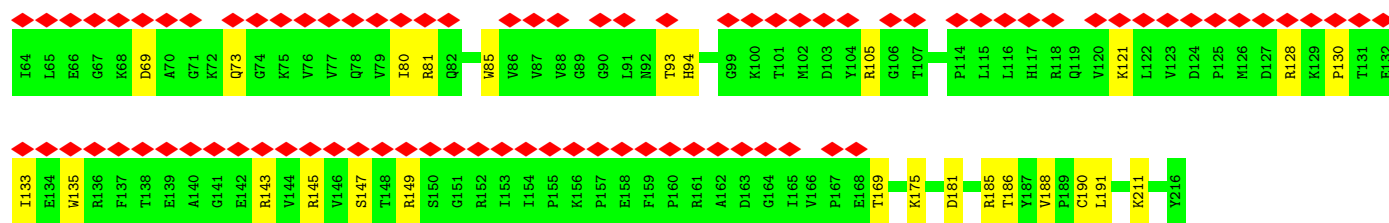


- Molecule 35: 39S ribosomal protein L23, mitochondrial



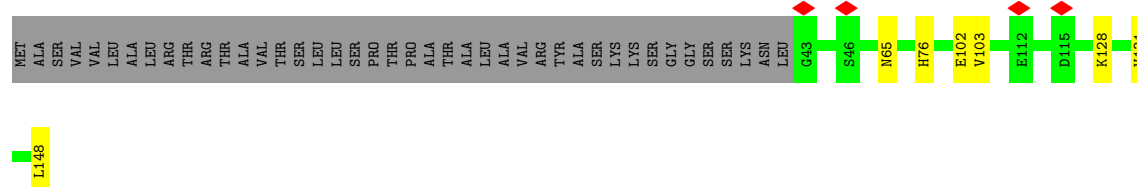
- Molecule 36: 39S ribosomal protein L24, mitochondrial





- Molecule 37: 39S ribosomal protein L27, mitochondrial

Chain W: 67% 5% 28%



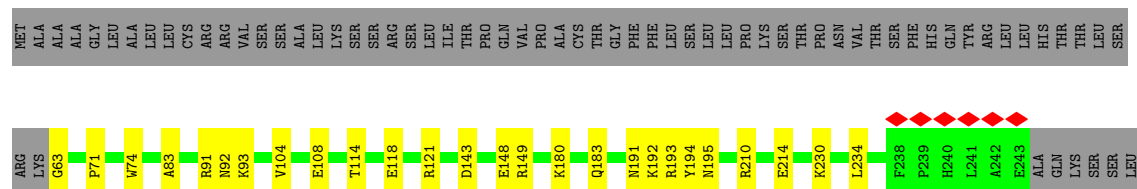
- Molecule 38: 39S ribosomal protein L28, mitochondrial

Chain X: 85% 11% 5%



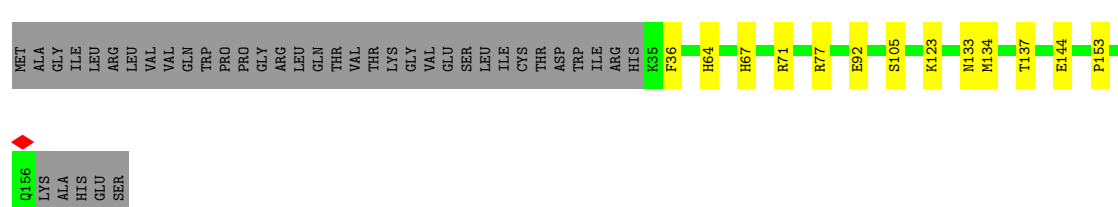
- Molecule 39: 39S ribosomal protein L47, mitochondrial

Chain Y: 62% 10% 28%

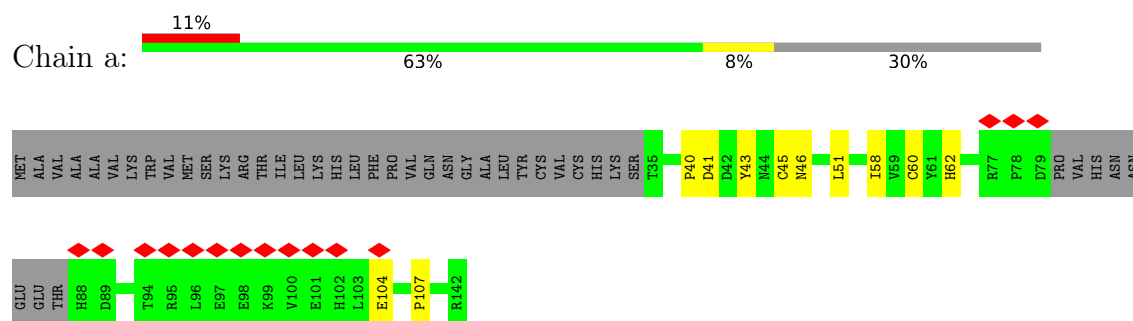


- Molecule 40: 39S ribosomal protein L30, mitochondrial

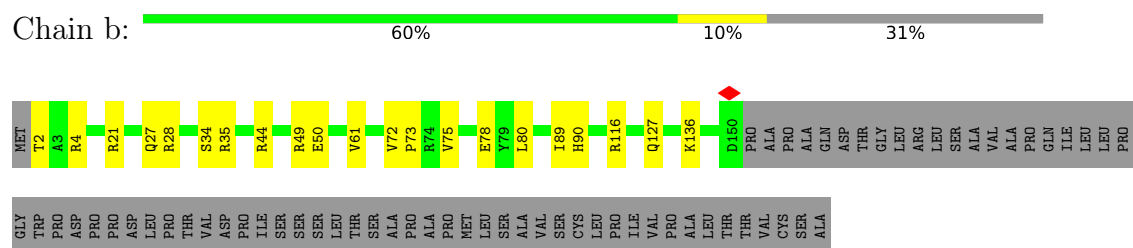
Chain Z: 68% 8% 24%



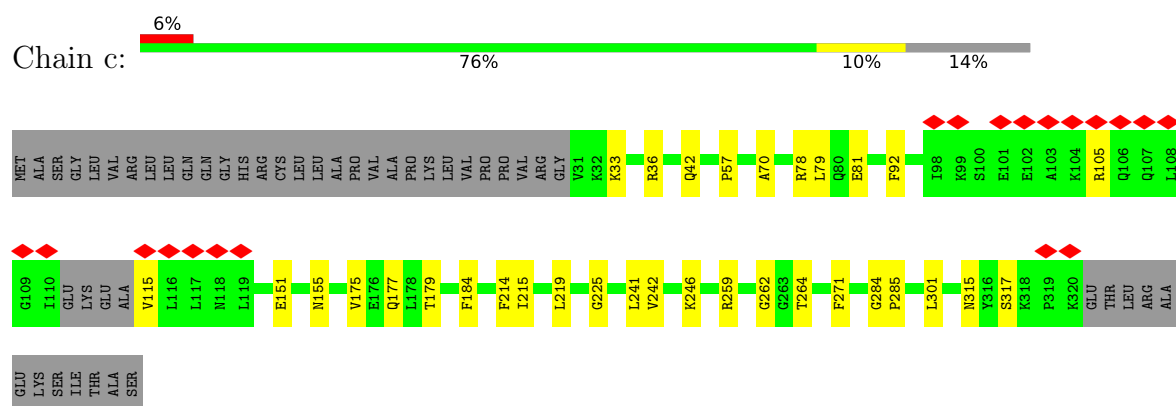
- Molecule 41: 39S ribosomal protein L42, mitochondrial



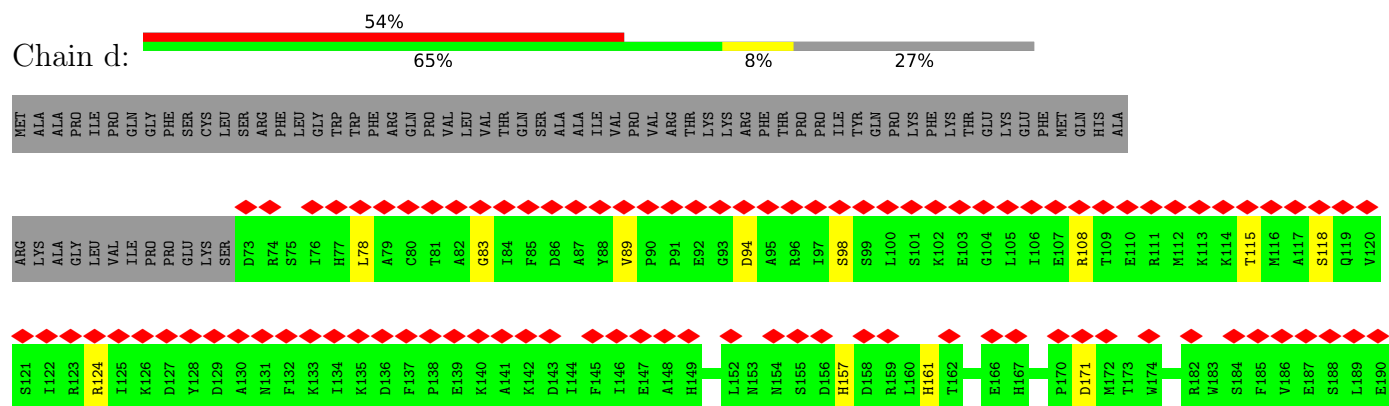
- Molecule 42: 39S ribosomal protein L43, mitochondrial

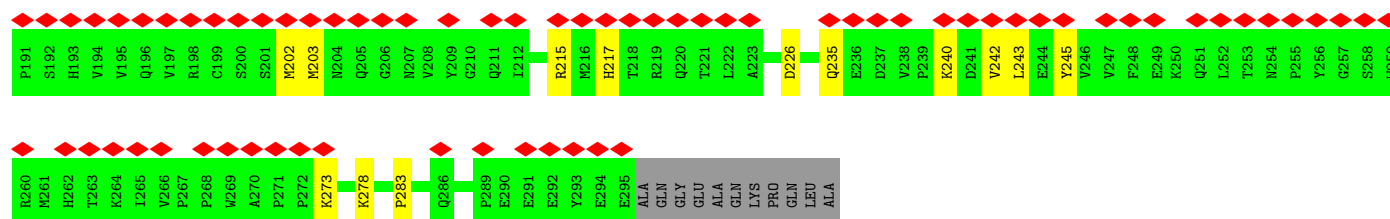


- Molecule 43: 39S ribosomal protein L44, mitochondrial

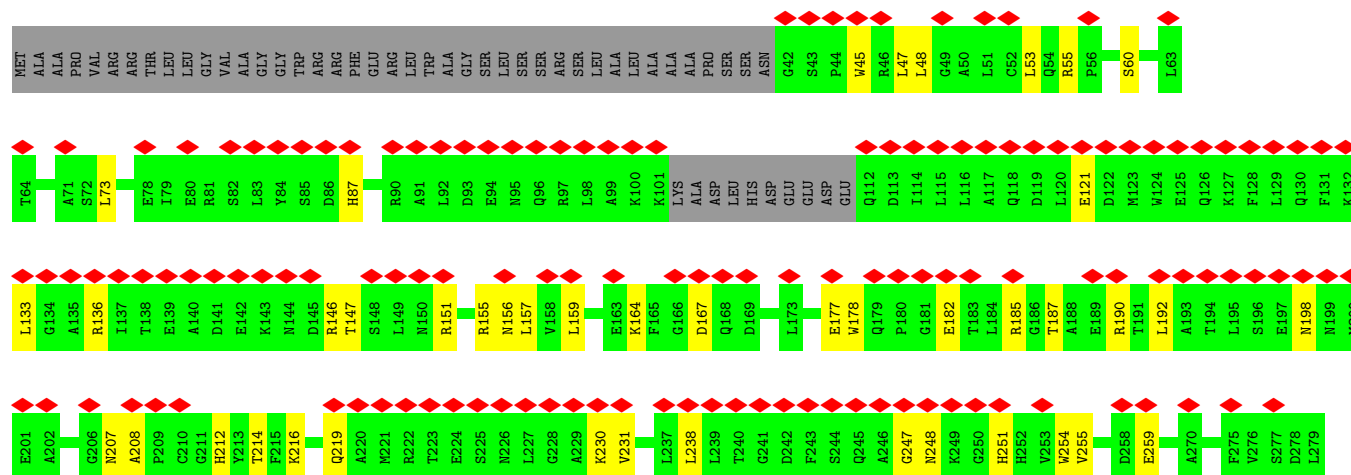


- Molecule 44: 39S ribosomal protein L45, mitochondrial

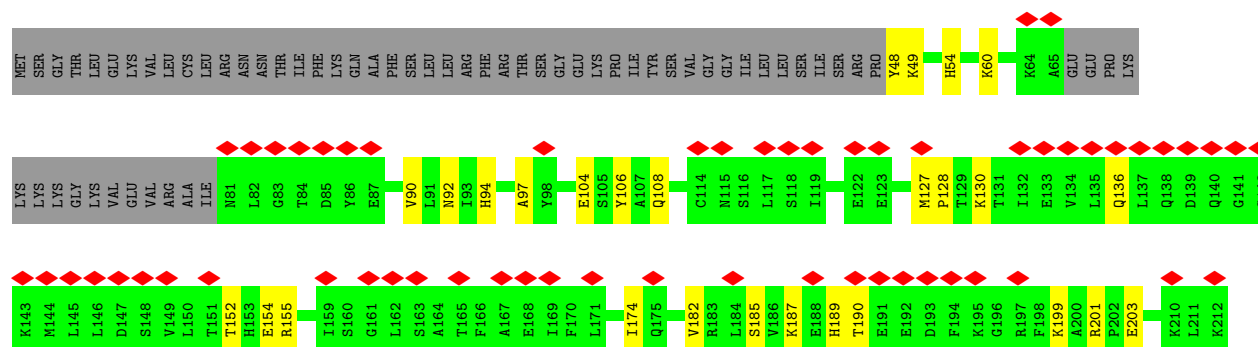




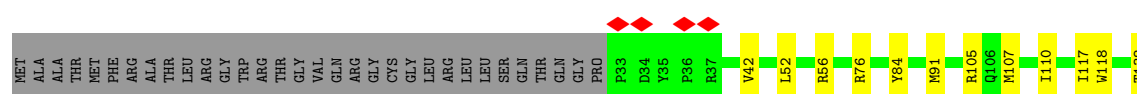
• Molecule 45: 39S ribosomal protein L46, mitochondrial

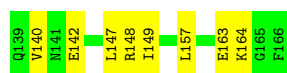


• Molecule 46: 39S ribosomal protein L48, mitochondrial

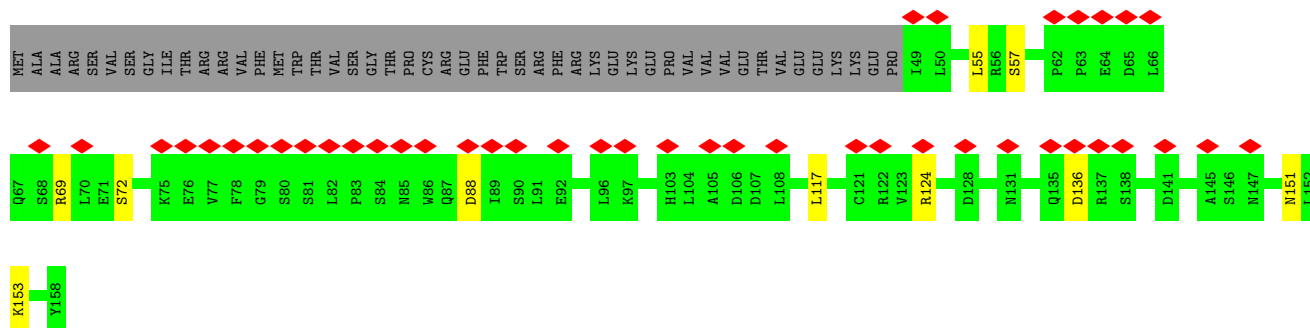


• Molecule 47: 39S ribosomal protein L49, mitochondrial

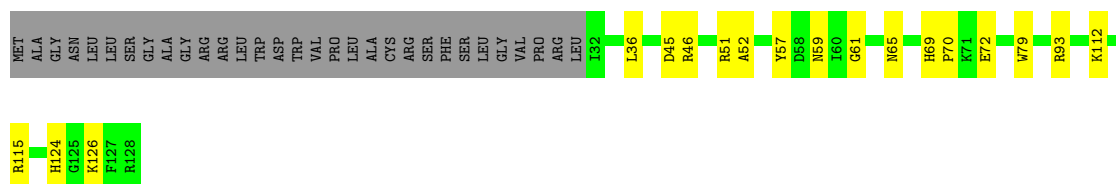




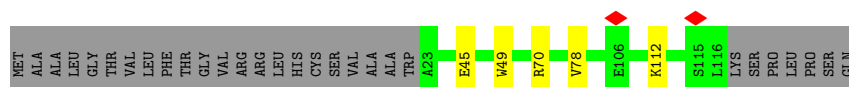
- Molecule 48: 39S ribosomal protein L50, mitochondrial



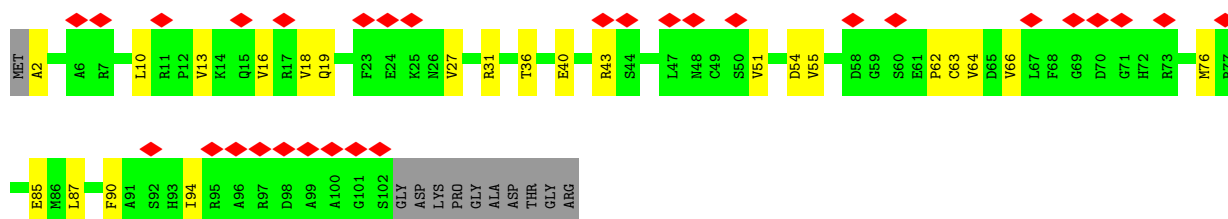
- Molecule 49: 39S ribosomal protein L51, mitochondrial



- Molecule 50: 39S ribosomal protein L52, mitochondrial



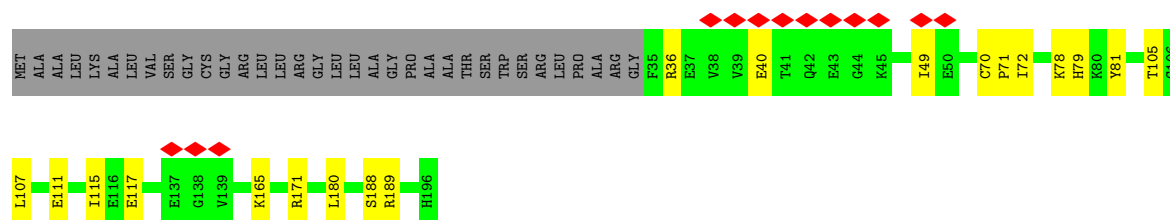
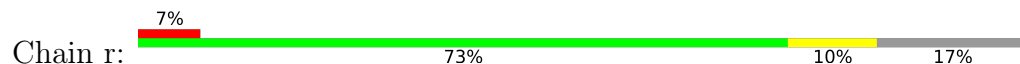
- Molecule 51: 39S ribosomal protein L53, mitochondrial



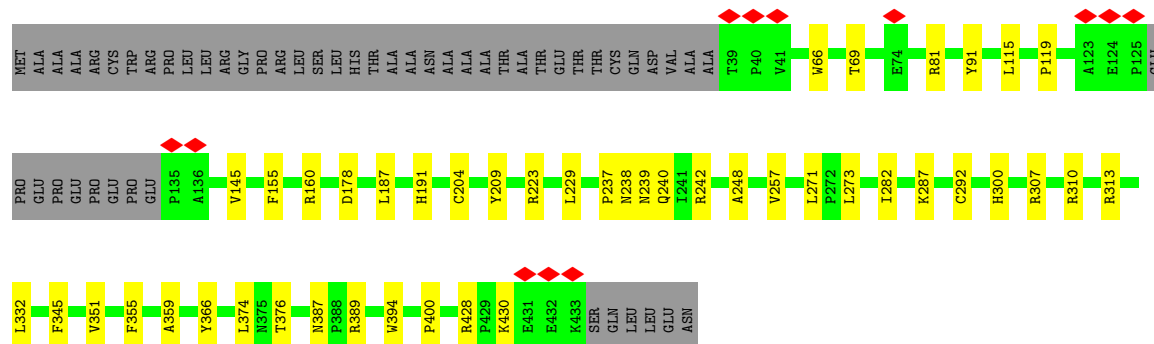
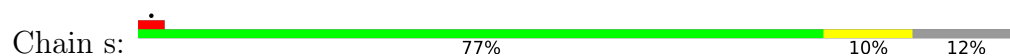
- Molecule 52: 39S ribosomal protein L54, mitochondrial



- Molecule 57: 39S ribosomal protein S18a, mitochondrial



- Molecule 58: 39S ribosomal protein S30, mitochondrial



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	114557	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	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	5.839	Depositor
Minimum map value	-1.970	Depositor
Average map value	-0.002	Depositor
Map value standard deviation	0.190	Depositor
Recommended contour level	0.7	Depositor
Map size (Å)	486.976, 486.976, 486.976	wwPDB
Map dimensions	448, 448, 448	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.087, 1.087, 1.087	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: MG, PM8, ZN, K, SAC, THC, AYA, FES, OMU, SAM

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	u	0.10	0/941	0.27	0/1270
2	v	0.12	0/597	0.26	0/796
3	w	0.10	0/647	0.28	0/871
4	x	0.10	0/2721	0.28	0/3691
5	y	0.08	0/2011	0.23	0/2702
6	z	0.15	0/1394	0.30	0/1901
7	0	0.09	0/913	0.23	0/1224
8	1	0.09	0/460	0.25	0/610
9	2	0.10	0/383	0.23	0/507
10	3	0.10	0/853	0.24	0/1136
11	4	0.10	0/350	0.25	0/461
12	5	0.10	0/3305	0.27	0/4502
13	6	0.10	0/3043	0.26	0/4140
14	7	0.08	0/2447	0.23	0/3310
15	8	0.09	0/880	0.23	0/1188
16	9	0.11	0/1025	0.26	0/1379
17	A	0.08	0/33594	0.15	0/52281
18	B	0.05	0/1700	0.09	0/2641
19	D	0.10	0/1910	0.26	0/2569
20	E	0.10	0/2475	0.26	0/3355
21	F	0.10	0/2090	0.27	0/2842
22	H	0.09	0/816	0.25	0/1097
23	I	0.12	0/1361	0.31	0/1839
24	J	0.10	0/1348	0.28	0/1813
25	K	0.10	0/1490	0.26	0/2021
26	L	0.11	0/905	0.34	0/1218
27	M	0.10	0/2381	0.25	0/3212
28	N	0.09	0/1747	0.23	0/2354
29	O	0.10	0/1283	0.26	0/1727
30	P	0.09	0/1199	0.28	0/1623
31	Q	0.09	0/1884	0.26	0/2535
32	R	0.09	0/1175	0.22	0/1572

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	S	0.12	0/1320	0.29	0/1789
34	T	0.09	0/1403	0.24	0/1886
35	U	0.09	0/1274	0.25	0/1723
36	V	0.10	0/1698	0.24	0/2302
37	W	0.10	0/857	0.26	0/1155
38	X	0.09	0/2099	0.23	0/2837
39	Y	0.09	0/1593	0.23	0/2136
40	Z	0.11	0/1021	0.26	0/1378
41	a	0.10	0/866	0.27	0/1174
42	b	0.10	0/1203	0.29	0/1627
43	c	0.09	0/2347	0.24	0/3171
44	d	0.09	0/1871	0.25	0/2533
45	e	0.08	0/1885	0.24	0/2542
46	f	0.09	0/1216	0.24	0/1638
47	g	0.11	0/1151	0.28	0/1569
48	h	0.09	0/918	0.24	0/1249
49	i	0.10	0/850	0.23	0/1135
50	j	0.09	0/760	0.23	0/1023
51	k	0.08	0/777	0.23	0/1048
52	l	0.10	0/707	0.26	0/960
53	m	0.09	0/426	0.24	0/575
54	o	0.08	0/705	0.23	0/945
55	p	0.08	0/1223	0.26	0/1641
56	q	0.08	0/1208	0.21	0/1633
57	r	0.12	0/1362	0.29	0/1846
58	s	0.10	0/3239	0.25	0/4400
All	All	0.09	0/113307	0.23	0/160302

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	u	919	0	917	15	0
2	v	588	0	604	11	0
3	w	638	0	636	9	0
4	x	2660	0	2640	44	0
5	y	1980	0	2066	27	0
6	z	1366	0	1350	17	0
7	0	898	0	916	11	0
8	1	455	0	498	7	0
9	2	377	0	406	5	0
10	3	832	0	883	11	0
11	4	342	0	361	7	0
12	5	3210	0	3206	39	0
13	6	2948	0	2841	46	0
14	7	2390	0	2397	38	0
15	8	860	0	852	12	0
16	9	997	0	987	16	0
17	A	30407	0	15508	255	0
18	B	1522	0	776	13	0
19	D	1872	0	1932	24	0
20	E	2406	0	2415	26	0
21	F	2031	0	2065	37	0
22	H	802	0	846	10	0
23	I	1331	0	1407	15	0
24	J	1330	0	1407	14	0
25	K	1455	0	1452	19	0
26	L	890	0	941	15	0
27	M	2327	0	2395	25	0
28	N	1702	0	1729	19	0
29	O	1259	0	1294	15	0
30	P	1173	0	1165	14	0
31	Q	1843	0	1878	21	0
32	R	1154	0	1214	12	0
33	S	1293	0	1365	15	0
34	T	1369	0	1410	16	0
35	U	1251	0	1232	20	0
36	V	1653	0	1658	26	0
37	W	835	0	858	5	0
38	X	2044	0	2060	20	0
39	Y	1556	0	1597	25	0
40	Z	996	0	1044	10	0
41	a	840	0	810	10	0
42	b	1189	0	1183	16	0
43	c	2299	0	2320	23	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	d	1824	0	1806	18	0
45	e	1848	0	1849	28	0
46	f	1196	0	1212	19	0
47	g	1113	0	1097	13	0
48	h	895	0	881	8	0
49	i	828	0	857	18	0
50	j	745	0	746	4	0
51	k	774	0	784	16	0
52	l	688	0	674	8	0
53	m	419	0	435	11	0
54	o	688	0	689	9	0
55	p	1205	0	1223	14	0
56	q	1177	0	1154	8	0
57	r	1322	0	1348	14	0
58	s	3155	0	3139	30	0
59	w	32	0	39	8	0
60	x	27	0	22	2	0
61	0	1	0	0	0	0
61	4	1	0	0	0	0
62	A	85	0	0	0	0
62	D	1	0	0	0	0
62	E	1	0	0	0	0
62	O	1	0	0	0	0
63	A	8	0	0	0	0
64	A	12	0	9	0	0
65	r	4	0	0	0	0
All	All	108339	0	93485	975	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

The worst 5 of 975 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:H:53:THR:N	22:H:86:THR:HG1	1.81	0.79
17:A:2499:U:OP2	17:A:2504:A:N6	2.18	0.75
35:U:11:ARG:HE	36:V:211:LYS:HB3	1.51	0.75
17:A:1777:A:N6	17:A:1780:U:OP2	2.20	0.74
1:u:135:LEU:HD22	1:u:179:LEU:HB3	1.69	0.74

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	u	108/234 (46%)	106 (98%)	2 (2%)	0	100	100
2	v	67/70 (96%)	67 (100%)	0	0	100	100
3	w	77/156 (49%)	72 (94%)	5 (6%)	0	100	100
4	x	332/384 (86%)	329 (99%)	3 (1%)	0	100	100
5	y	242/381 (64%)	241 (100%)	1 (0%)	0	100	100
6	z	177/246 (72%)	176 (99%)	1 (1%)	0	100	100
7	0	108/188 (57%)	107 (99%)	1 (1%)	0	100	100
8	1	53/65 (82%)	53 (100%)	0	0	100	100
9	2	44/92 (48%)	43 (98%)	1 (2%)	0	100	100
10	3	93/188 (50%)	92 (99%)	1 (1%)	0	100	100
11	4	36/103 (35%)	36 (100%)	0	0	100	100
12	5	392/423 (93%)	384 (98%)	8 (2%)	0	100	100
13	6	352/380 (93%)	345 (98%)	7 (2%)	0	100	100
14	7	292/338 (86%)	286 (98%)	6 (2%)	0	100	100
15	8	100/206 (48%)	100 (100%)	0	0	100	100
16	9	122/137 (89%)	121 (99%)	1 (1%)	0	100	100
19	D	238/305 (78%)	234 (98%)	4 (2%)	0	100	100
20	E	303/348 (87%)	296 (98%)	7 (2%)	0	100	100
21	F	250/311 (80%)	248 (99%)	2 (1%)	0	100	100
22	H	95/267 (36%)	95 (100%)	0	0	100	100
23	I	162/261 (62%)	160 (99%)	2 (1%)	0	100	100
24	J	173/192 (90%)	173 (100%)	0	0	100	100
25	K	175/178 (98%)	174 (99%)	1 (1%)	0	100	100
26	L	113/145 (78%)	113 (100%)	0	0	100	100
27	M	289/296 (98%)	283 (98%)	6 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	N	205/251 (82%)	204 (100%)	1 (0%)	0	100	100
29	O	152/175 (87%)	150 (99%)	2 (1%)	0	100	100
30	P	142/180 (79%)	139 (98%)	3 (2%)	0	100	100
31	Q	219/292 (75%)	218 (100%)	1 (0%)	0	100	100
32	R	138/149 (93%)	138 (100%)	0	0	100	100
33	S	159/205 (78%)	159 (100%)	0	0	100	100
34	T	164/206 (80%)	162 (99%)	2 (1%)	0	100	100
35	U	150/153 (98%)	149 (99%)	1 (1%)	0	100	100
36	V	200/216 (93%)	198 (99%)	2 (1%)	0	100	100
37	W	104/148 (70%)	102 (98%)	2 (2%)	0	100	100
38	X	242/256 (94%)	240 (99%)	2 (1%)	0	100	100
39	Y	179/250 (72%)	178 (99%)	1 (1%)	0	100	100
40	Z	120/161 (74%)	119 (99%)	1 (1%)	0	100	100
41	a	96/142 (68%)	95 (99%)	1 (1%)	0	100	100
42	b	147/215 (68%)	144 (98%)	3 (2%)	0	100	100
43	c	282/332 (85%)	278 (99%)	4 (1%)	0	100	100
44	d	221/306 (72%)	219 (99%)	2 (1%)	0	100	100
45	e	224/279 (80%)	219 (98%)	5 (2%)	0	100	100
46	f	146/212 (69%)	142 (97%)	4 (3%)	0	100	100
47	g	132/166 (80%)	131 (99%)	1 (1%)	0	100	100
48	h	108/158 (68%)	106 (98%)	2 (2%)	0	100	100
49	i	95/128 (74%)	95 (100%)	0	0	100	100
50	j	92/123 (75%)	90 (98%)	2 (2%)	0	100	100
51	k	99/112 (88%)	98 (99%)	1 (1%)	0	100	100
52	l	80/138 (58%)	80 (100%)	0	0	100	100
53	m	49/128 (38%)	49 (100%)	0	0	100	100
54	o	79/102 (78%)	79 (100%)	0	0	100	100
55	p	141/206 (68%)	139 (99%)	2 (1%)	0	100	100
56	q	139/222 (63%)	139 (100%)	0	0	100	100
57	r	160/196 (82%)	159 (99%)	1 (1%)	0	100	100
58	s	382/439 (87%)	376 (98%)	6 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	9239/12140 (76%)	9128 (99%)	111 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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	u	104/200 (52%)	101 (97%)	3 (3%)	37	66
2	v	59/60 (98%)	58 (98%)	1 (2%)	53	74
3	w	73/136 (54%)	73 (100%)	0	100	100
4	x	291/328 (89%)	288 (99%)	3 (1%)	68	79
5	y	226/350 (65%)	225 (100%)	1 (0%)	84	86
6	z	146/209 (70%)	144 (99%)	2 (1%)	59	76
7	0	99/164 (60%)	98 (99%)	1 (1%)	68	79
8	1	52/60 (87%)	52 (100%)	0	100	100
9	2	40/72 (56%)	40 (100%)	0	100	100
10	3	88/166 (53%)	87 (99%)	1 (1%)	65	78
11	4	37/89 (42%)	37 (100%)	0	100	100
12	5	353/368 (96%)	352 (100%)	1 (0%)	86	87
13	6	313/332 (94%)	311 (99%)	2 (1%)	78	83
14	7	270/303 (89%)	269 (100%)	1 (0%)	84	86
15	8	93/190 (49%)	93 (100%)	0	100	100
16	9	104/112 (93%)	104 (100%)	0	100	100
19	D	194/245 (79%)	193 (100%)	1 (0%)	81	85
20	E	260/290 (90%)	260 (100%)	0	100	100
21	F	219/262 (84%)	218 (100%)	1 (0%)	81	85
22	H	88/228 (39%)	87 (99%)	1 (1%)	65	78
23	I	152/232 (66%)	151 (99%)	1 (1%)	76	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
24	J	138/150 (92%)	138 (100%)	0	100	100
25	K	154/155 (99%)	153 (99%)	1 (1%)	78	83
26	L	98/124 (79%)	97 (99%)	1 (1%)	68	79
27	M	246/249 (99%)	244 (99%)	2 (1%)	73	81
28	N	182/211 (86%)	180 (99%)	2 (1%)	65	78
29	O	134/150 (89%)	134 (100%)	0	100	100
30	P	126/155 (81%)	126 (100%)	0	100	100
31	Q	203/256 (79%)	200 (98%)	3 (2%)	57	75
32	R	118/126 (94%)	118 (100%)	0	100	100
33	S	146/180 (81%)	146 (100%)	0	100	100
34	T	146/176 (83%)	145 (99%)	1 (1%)	76	82
35	U	134/135 (99%)	133 (99%)	1 (1%)	76	82
36	V	180/191 (94%)	176 (98%)	4 (2%)	45	71
37	W	86/119 (72%)	85 (99%)	1 (1%)	63	78
38	X	220/229 (96%)	220 (100%)	0	100	100
39	Y	163/223 (73%)	163 (100%)	0	100	100
40	Z	113/147 (77%)	113 (100%)	0	100	100
41	a	96/133 (72%)	96 (100%)	0	100	100
42	b	130/185 (70%)	129 (99%)	1 (1%)	73	81
43	c	251/288 (87%)	251 (100%)	0	100	100
44	d	204/274 (74%)	203 (100%)	1 (0%)	81	85
45	e	198/236 (84%)	198 (100%)	0	100	100
46	f	133/188 (71%)	133 (100%)	0	100	100
47	g	124/148 (84%)	123 (99%)	1 (1%)	73	81
48	h	104/148 (70%)	104 (100%)	0	100	100
49	i	86/110 (78%)	86 (100%)	0	100	100
50	j	74/97 (76%)	74 (100%)	0	100	100
51	k	83/90 (92%)	83 (100%)	0	100	100
52	l	76/116 (66%)	75 (99%)	1 (1%)	61	77
53	m	46/113 (41%)	45 (98%)	1 (2%)	45	71
54	o	70/87 (80%)	70 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
55	p	135/181 (75%)	134 (99%)	1 (1%)	76	82
56	q	119/178 (67%)	119 (100%)	0	100	100
57	r	147/169 (87%)	147 (100%)	0	100	100
58	s	340/381 (89%)	340 (100%)	0	100	100
All	All	8264/10494 (79%)	8222 (100%)	42 (0%)	78	85

5 of 42 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
31	Q	130	ILE
37	W	131	VAL
34	T	51	ILE
36	V	169	THR
44	d	89	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 109 such sidechains are listed below:

Mol	Chain	Res	Type
26	L	52	HIS
36	V	73	GLN
52	l	82	GLN
27	M	102	GLN
34	T	69	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
17	A	1406/1589 (88%)	262 (18%)	8 (0%)
18	B	71/72 (98%)	13 (18%)	0
All	All	1477/1661 (88%)	275 (18%)	8 (0%)

5 of 275 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
17	A	1689	C
17	A	1694	U
17	A	1699	C
17	A	1700	U
17	A	1704	U

5 of 8 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
17	A	3040	G
17	A	2905	A
17	A	2457	A
17	A	2245	A
17	A	2530	A

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
42	THC	b	2	42	8,9,10	1.06	1 (12%)	9,11,13	0.66	0
35	AYA	U	2	35	6,7,8	1.27	1 (16%)	5,8,10	1.24	1 (20%)
25	SAC	K	2	25	7,8,9	1.03	0	8,9,11	0.83	1 (12%)
51	AYA	k	2	51	6,7,8	1.26	1 (16%)	5,8,10	1.31	1 (20%)
17	OMU	A	3039	17	19,22,23	1.23	3 (15%)	26,31,34	1.71	5 (19%)

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
42	THC	b	2	42	-	0/8/10/12	-
35	AYA	U	2	35	-	1/4/6/8	-
25	SAC	K	2	25	-	2/7/8/10	-
51	AYA	k	2	51	-	0/4/6/8	-
17	OMU	A	3039	17	-	4/9/27/28	0/2/2/2

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	U	2	AYA	CA-N	-2.43	1.44	1.46
17	A	3039	OMU	C4-N3	-2.41	1.34	1.38
51	k	2	AYA	CA-N	-2.37	1.44	1.46
17	A	3039	OMU	C2-N1	2.27	1.42	1.38
42	b	2	THC	CA-N1	-2.07	1.43	1.46

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	A	3039	OMU	C4-N3-C2	-4.33	120.86	126.58
17	A	3039	OMU	N3-C2-N1	3.93	120.11	114.89
17	A	3039	OMU	C5-C4-N3	3.56	120.17	114.84
17	A	3039	OMU	O4-C4-C5	-3.05	119.80	125.16
51	k	2	AYA	CB-CA-N	2.72	112.63	109.61

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
25	K	2	SAC	N-CA-CB-OG
25	K	2	SAC	C-CA-CB-OG
17	A	3039	OMU	O4'-C4'-C5'-O5'
17	A	3039	OMU	C3'-C4'-C5'-O5'
17	A	3039	OMU	C4'-C5'-O5'-P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 102 ligands modelled in this entry, 98 are monoatomic - leaving 4 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	PM8	w	200	3	25,31,31	0.22	0	30,38,38	0.41	0
65	FES	r	201	23,57	0,4,4	-	-	-	-	-
60	SAM	x	401	-	27,29,29	1.08	4 (14%)	36,42,42	2.01	9 (25%)
64	N	A	3394	17	9,12,13	0.66	0	10,16,19	0.65	0

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	PM8	w	200	3	-	13/36/38/38	-
65	FES	r	201	23,57	-	-	0/1/1/1
60	SAM	x	401	-	-	6/16/33/33	0/3/3/3
64	N	A	3394	17	-	0/3/18/19	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
60	x	401	SAM	C2-N3	2.49	1.38	1.33
60	x	401	SAM	C2-N1	2.44	1.38	1.33
60	x	401	SAM	C8-N7	2.15	1.35	1.31
60	x	401	SAM	OXT-C	-2.14	1.23	1.30

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
60	x	401	SAM	N3-C2-N1	-5.33	120.26	128.60
60	x	401	SAM	C5-C4-N3	-4.88	120.38	126.75
60	x	401	SAM	N9-C8-N7	-3.94	108.53	113.91
60	x	401	SAM	C5-N7-C8	3.68	108.74	103.51
60	x	401	SAM	C2-N3-C4	3.59	120.22	111.75

There are no chirality outliers.

5 of 19 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
59	w	200	PM8	O27-C28-C29-C32

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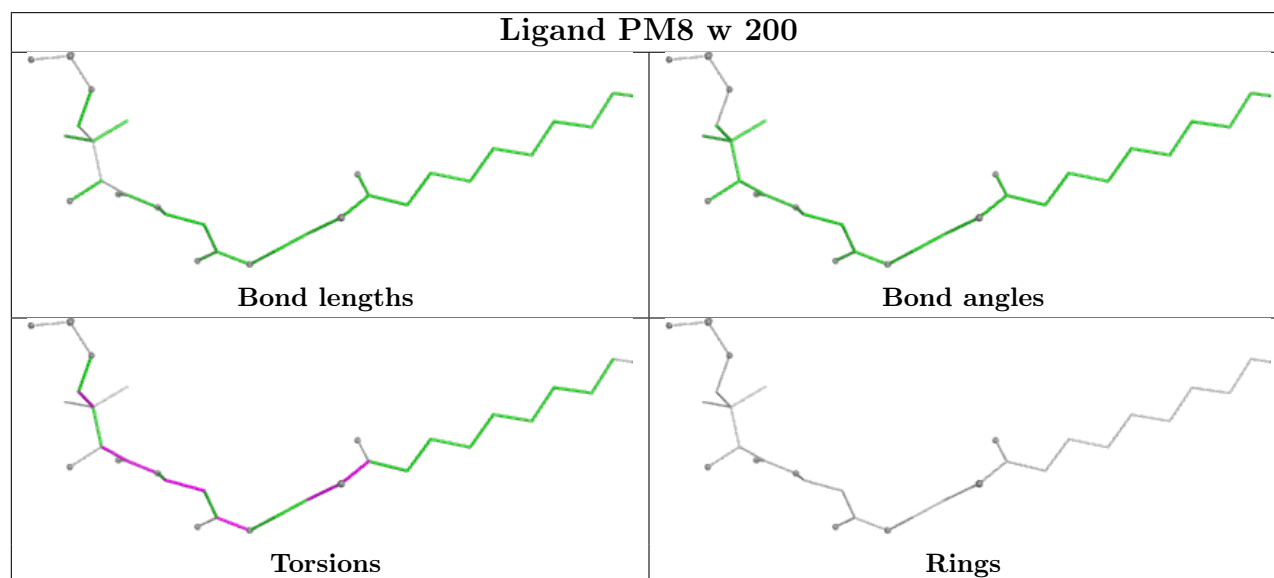
Mol	Chain	Res	Type	Atoms
59	w	200	PM8	C32-C34-N36-C37
59	w	200	PM8	O1-C1-S1-C43
59	w	200	PM8	C2-C1-S1-C43
60	x	401	SAM	N-CA-CB-CG

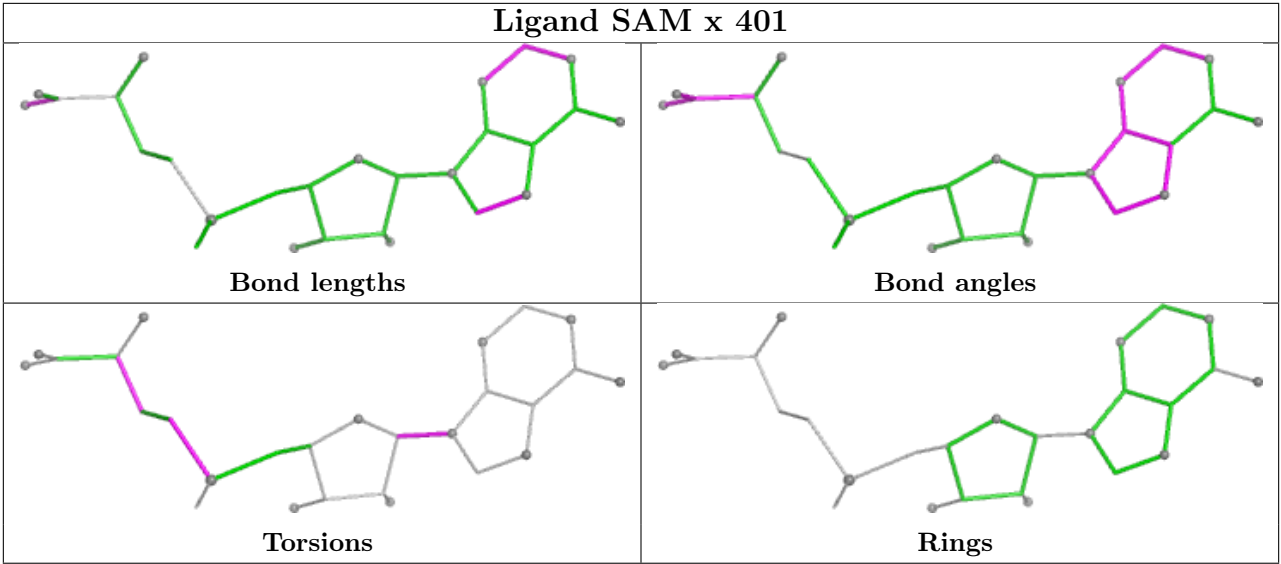
There are no ring outliers.

2 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
59	w	200	PM8	8	0
60	x	401	SAM	2	0

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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
17	A	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	3250:N	O3'	3251:N	P	17.38
1	A	3235:N	O3'	3236:N	P	13.89

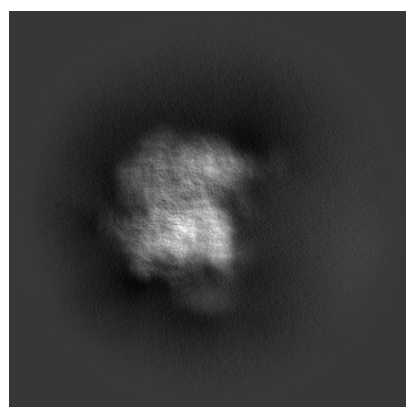
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-12846. These allow visual inspection of the internal detail of the map and identification of artifacts.

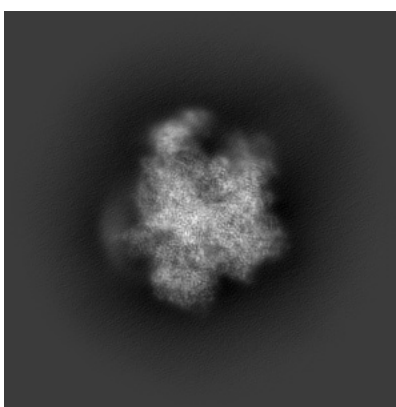
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

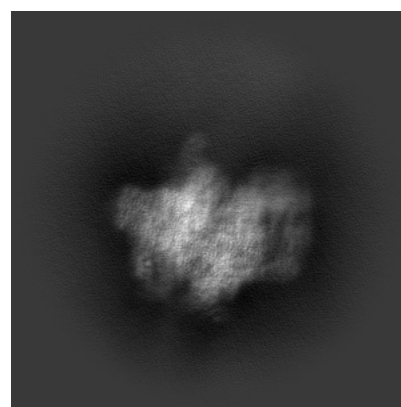
6.1.1 Primary map



X



Y

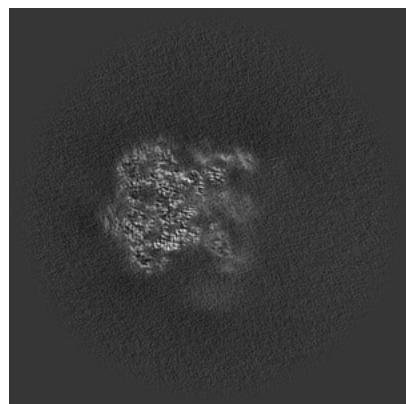


Z

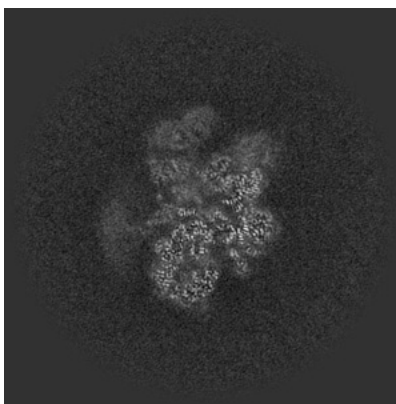
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

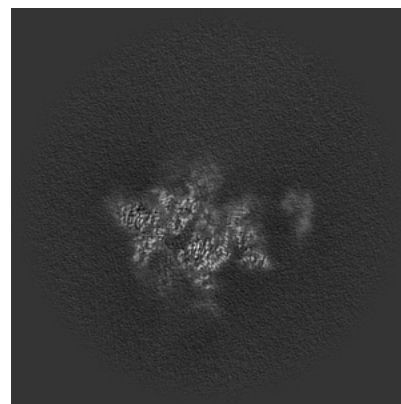
6.2.1 Primary map



X Index: 224



Y Index: 224

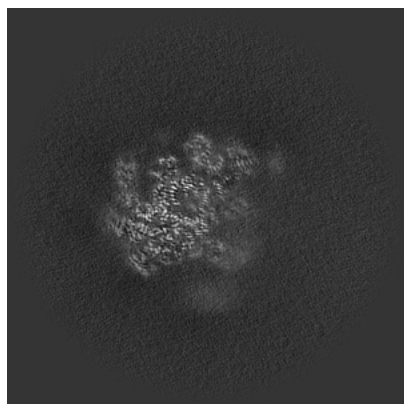


Z Index: 224

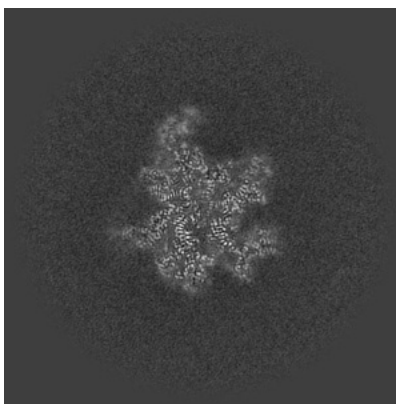
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

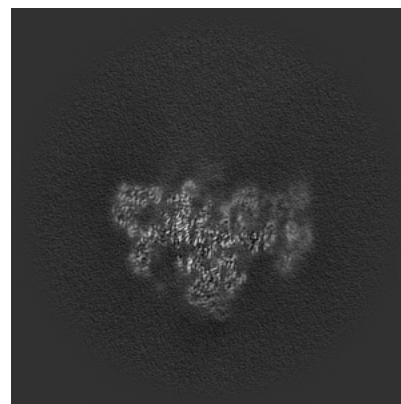
6.3.1 Primary map



X Index: 215



Y Index: 193

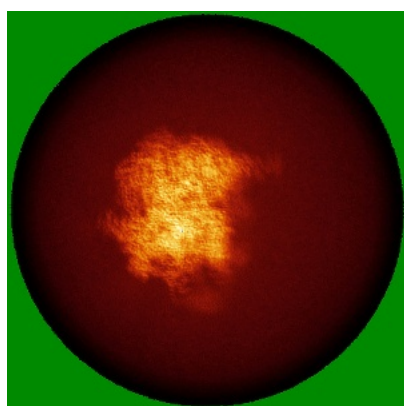


Z Index: 203

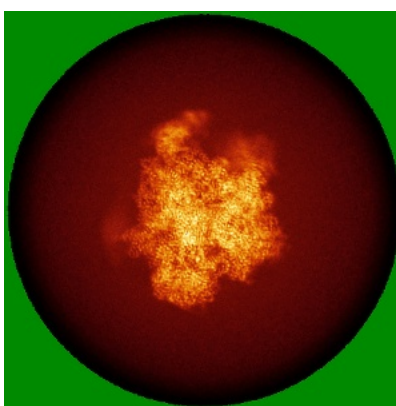
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

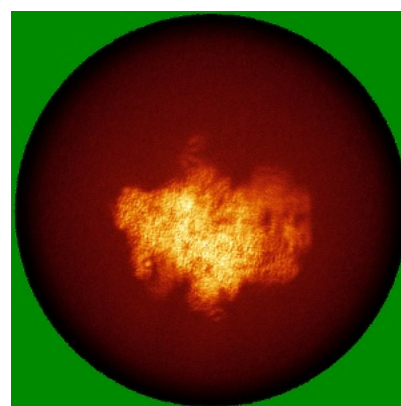
6.4.1 Primary map



X



Y



Z

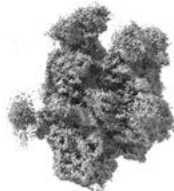
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.7. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

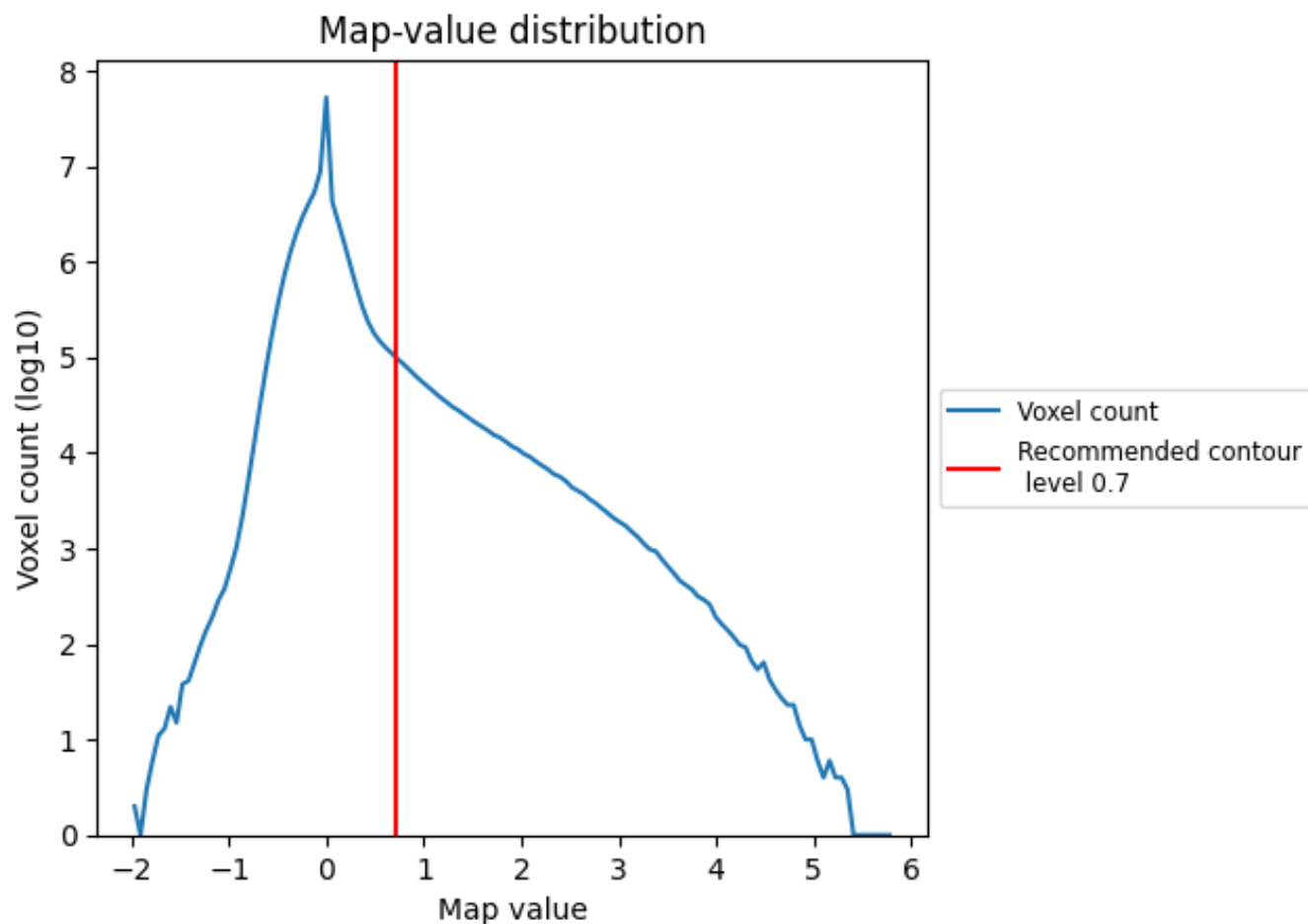
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

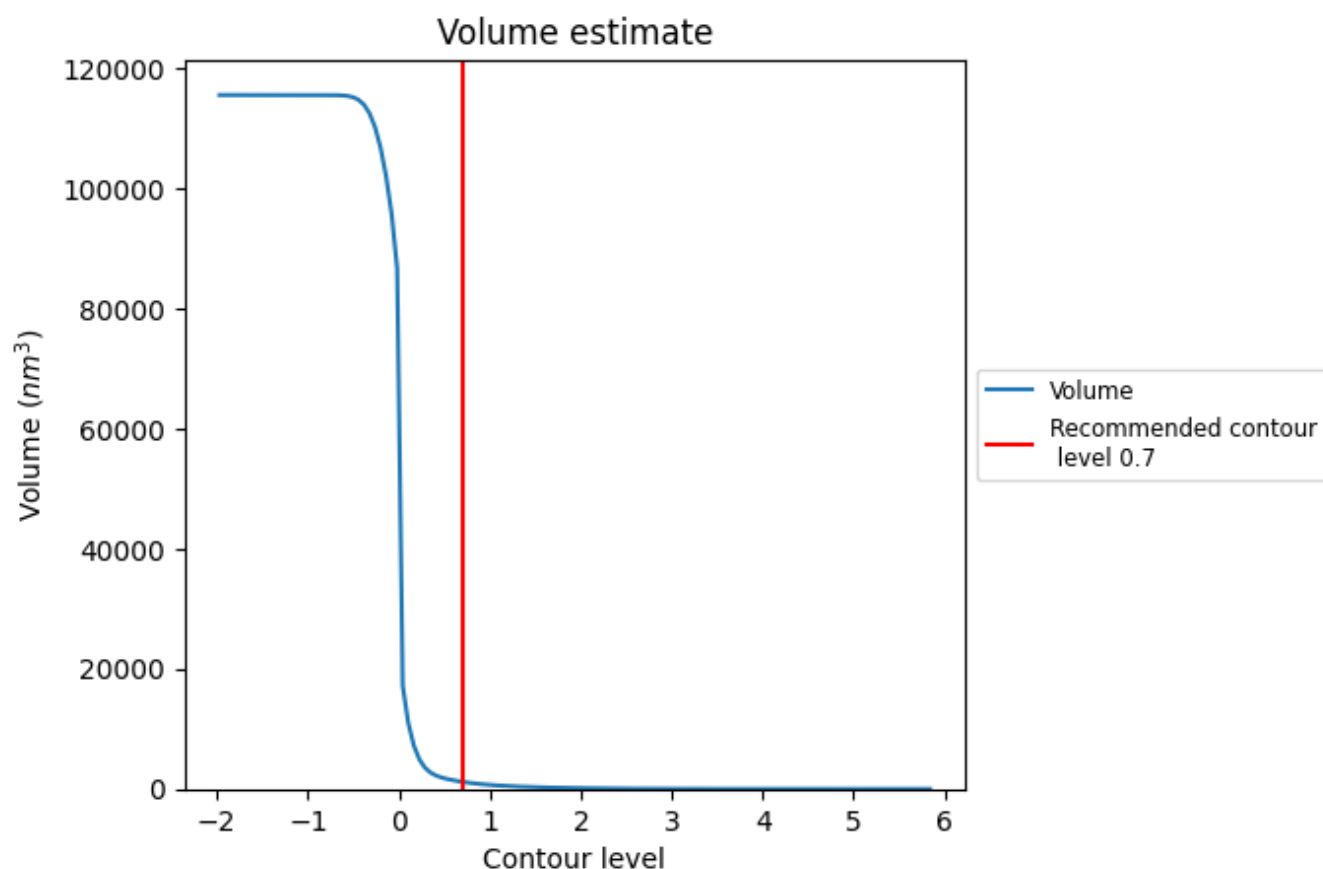
This section contains the results of statistical analysis of the map.

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.

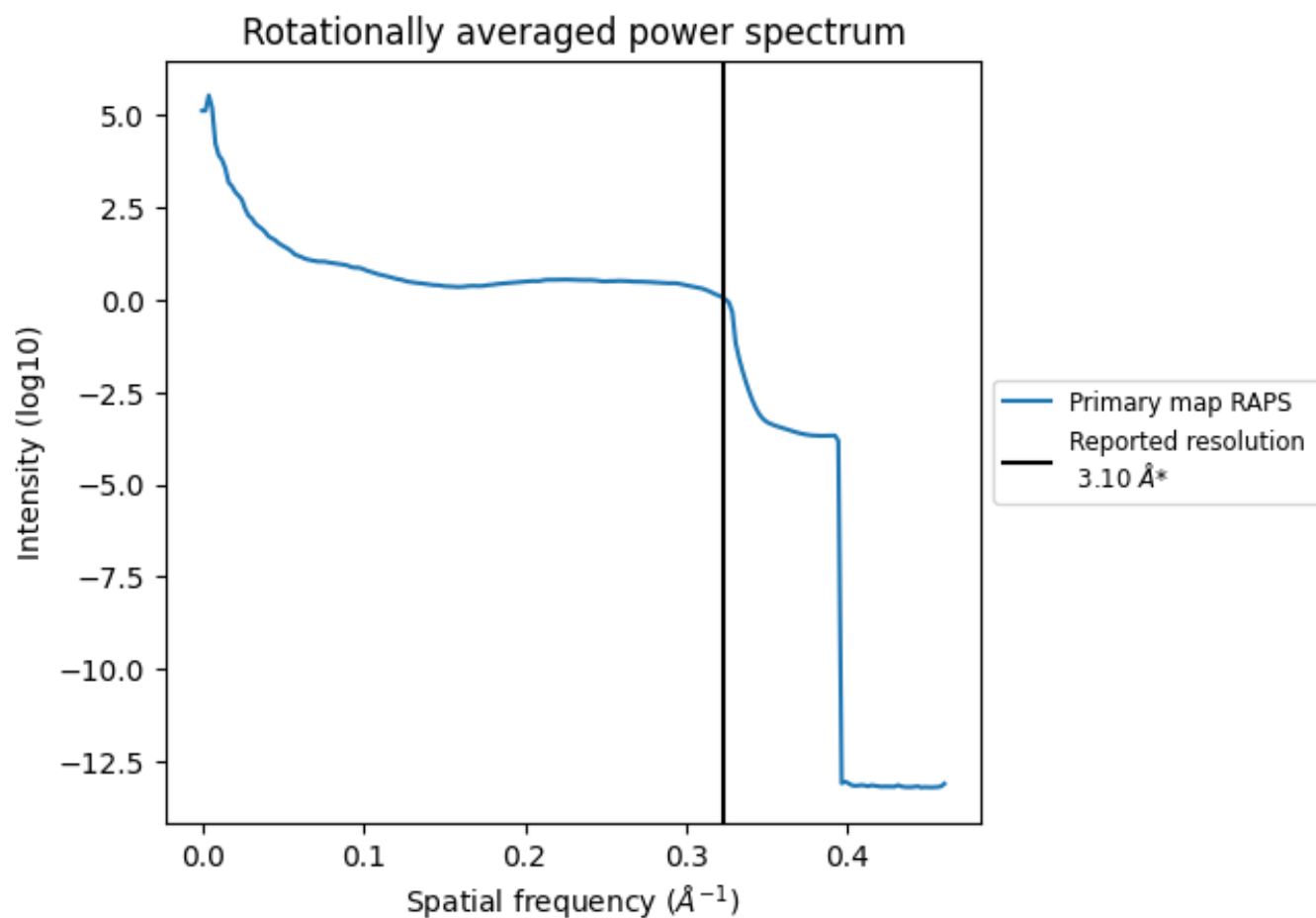
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1183 nm³; this corresponds to an approximate mass of 1069 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 ⓘ



*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

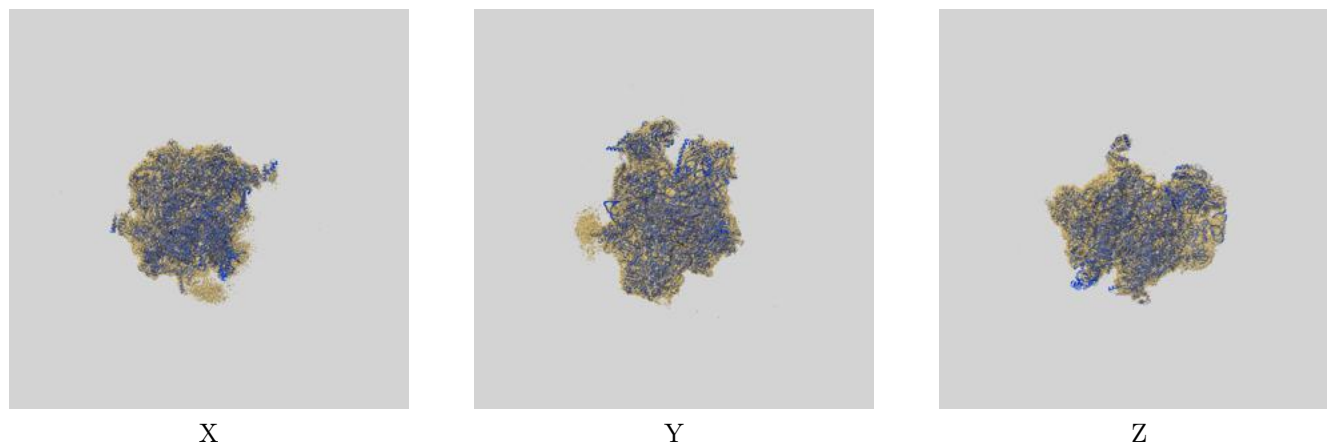
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

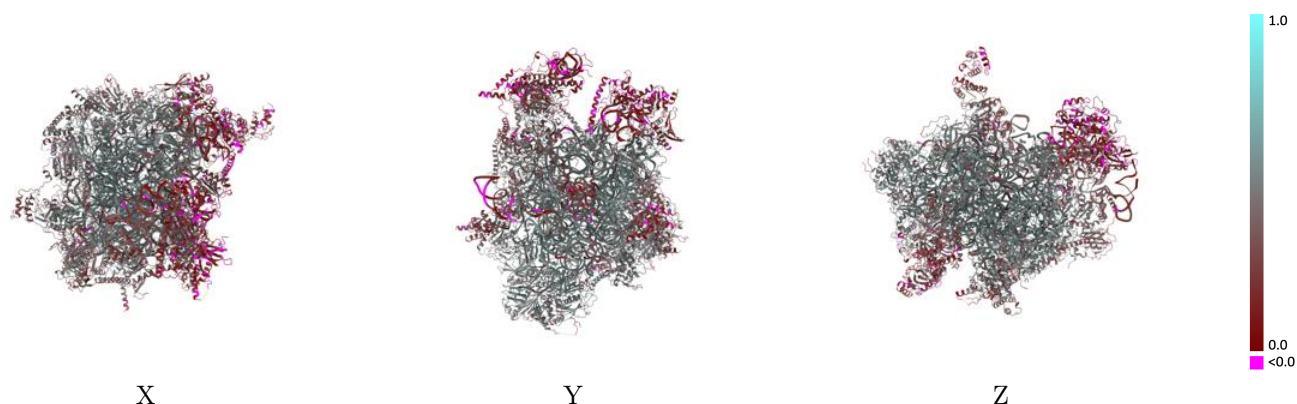
This section contains information regarding the fit between EMDB map EMD-12846 and PDB model 7ODS. Per-residue inclusion information can be found in section [3](#) on page [18](#).

9.1 Map-model overlay [i](#)



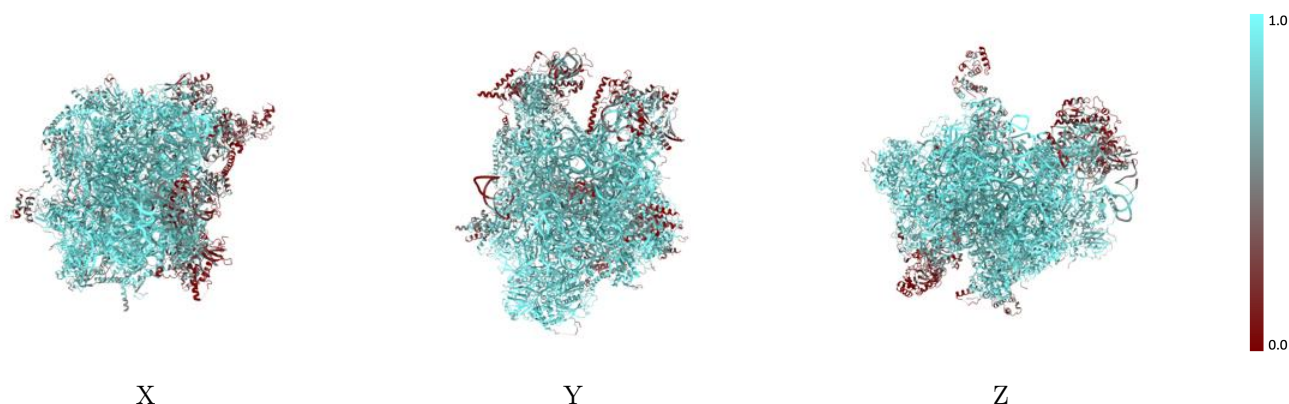
The images above show the 3D surface view of the map at the recommended contour level 0.7 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



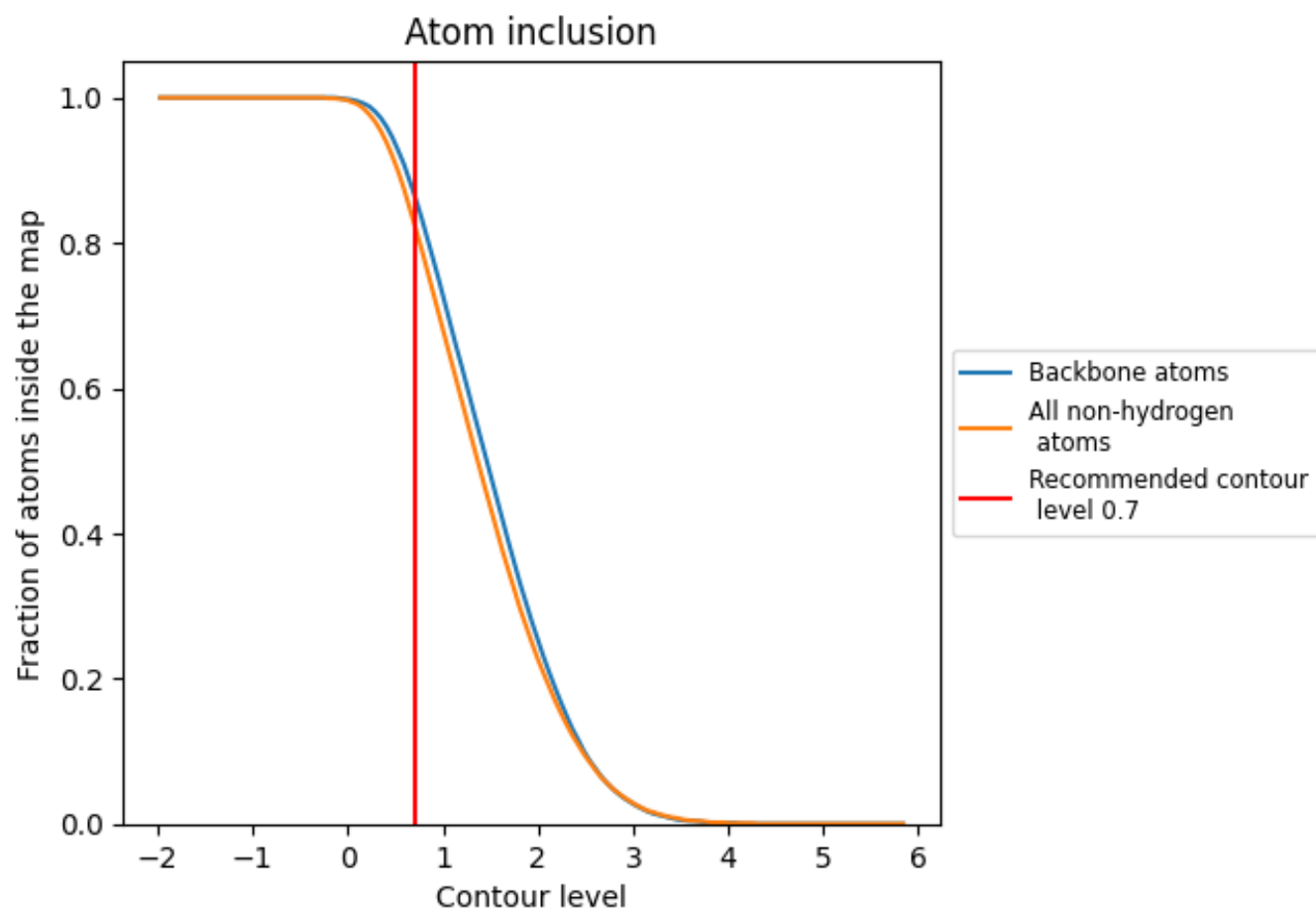
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 [i](#)



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 (0.7).

9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 83% 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 (0.7) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8260	 0.4250
0	 0.8980	 0.4730
1	 0.8800	 0.4400
2	 0.9560	 0.5630
3	 0.9710	 0.5520
4	 0.9730	 0.5070
5	 0.9290	 0.4860
6	 0.8760	 0.3820
7	 0.7210	 0.3360
8	 0.3610	 0.1730
9	 0.8510	 0.4510
A	 0.9590	 0.4870
B	 0.8440	 0.2570
D	 0.9130	 0.4860
E	 0.9350	 0.4920
F	 0.8850	 0.4690
H	 0.8070	 0.4300
I	 0.5680	 0.2290
J	 0.2660	 0.1280
K	 0.9510	 0.5080
L	 0.8450	 0.4760
M	 0.9020	 0.4870
N	 0.8410	 0.4270
O	 0.9310	 0.4910
P	 0.9280	 0.4350
Q	 0.9000	 0.4760
R	 0.9500	 0.5190
S	 0.9330	 0.4810
T	 0.9030	 0.4930
U	 0.7560	 0.4270
V	 0.3800	 0.3220
W	 0.9010	 0.5140
X	 0.8570	 0.4700
Y	 0.8800	 0.4730
Z	 0.9010	 0.5010



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Chain	Atom inclusion	Q-score
a	 0.7890	 0.4410
b	 0.9290	 0.4860
c	 0.8070	 0.4080
d	 0.2490	 0.2550
e	 0.3400	 0.1250
f	 0.5020	 0.2330
g	 0.8870	 0.4620
h	 0.5050	 0.3360
i	 0.9320	 0.5090
j	 0.8850	 0.4490
k	 0.5810	 0.2670
l	 0.3860	 0.1860
m	 0.2780	 0.1200
o	 0.9230	 0.5000
p	 0.6820	 0.3690
q	 0.7470	 0.3820
r	 0.8780	 0.4580
s	 0.9100	 0.4920
u	 0.7690	 0.3810
v	 0.4800	 0.2570
w	 0.1930	 0.1380
x	 0.8290	 0.3700
y	 0.7010	 0.3350
z	 0.4720	 0.2380