



Full wwPDB EM Validation Report ⓘ

Apr 17, 2025 – 10:48 AM EDT

PDB ID : 9CN3 / pdb_00009cn3
EMDB ID : EMD-45757
Title : Human 39S mitoribosome in complex with antibiotic Linezolid
Authors : Raskar, T.; Bibel, B.; Galonic Fujimori, D.; Fraser, J.
Deposited on : 2024-07-15
Resolution : 2.62 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The 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:

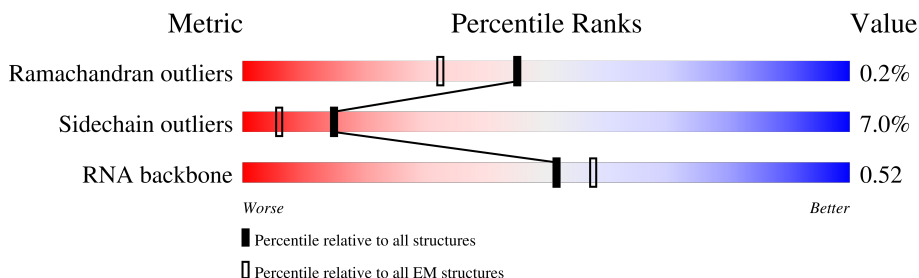
EMDB validation analysis : 0.0.1.dev117
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.42

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.62 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	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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

Mol	Chain	Length	Quality of chain
1	0	188	
2	1	65	
3	2	92	
4	3	188	
5	4	103	
6	5	423	
7	6	380	
8	7	338	











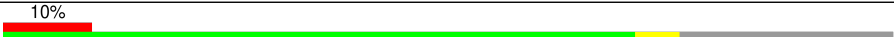


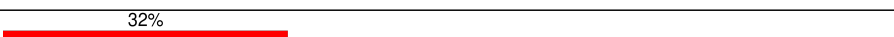
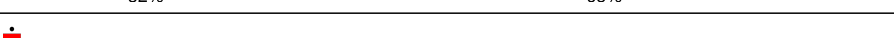
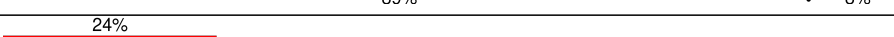

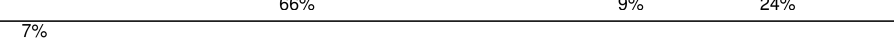

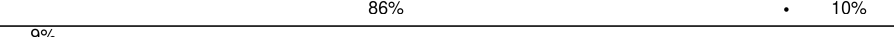



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Mol	Chain	Length	Quality of chain
9	8	206	
10	9	137	
11	A	1559	
12	B	72	
13	D	305	
14	E	348	
15	F	311	
16	H	267	
17	I	261	
18	J	192	
19	K	178	
20	L	145	
21	M	296	
22	N	251	
23	O	175	
24	P	179	
25	Q	292	
26	R	149	
27	S	205	
28	T	212	
29	U	153	
30	V	216	
31	W	148	
32	X	256	
33	Y	250	

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Mol	Chain	Length	Quality of chain
34	Z	161	
35	a	142	
36	b	155	
37	c	332	
38	d	306	
39	e	279	
40	f	194	
41	g	166	
42	h	158	
43	i	128	
44	j	123	
45	k	112	
46	l	138	
47	m	128	
48	o	102	
49	p	206	
50	q	222	
51	r	196	
52	s	439	
53	u	710	
54	TA	198	
54	TB	198	
54	TC	198	

2 Entry composition

There are 58 unique types of molecules in this entry. The entry contains 107417 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called 39S ribosomal protein L32, mitochondrial.

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	46	Total	C	N	O	S	0	0
			376	233	83	59	1		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	4	38	Total	C	N	O	S	0	0
			342	217	72	49	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	5	393	Total	C	N	O	S	0	0
			3205	2070	559	565	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	6	354	Total	C	N	O	S	0	0
			2948	1881	525	533	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	7	297	Total	C	N	O	S	0	0
			2410	1540	409	443	18		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	8	99	Total	C	N	O	S	0	0
			836	535	144	155	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	9	124	Total	C	N	O	S	0	0
			997	644	170	181	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	A	1527	Total	C	N	O	P	0	0
			32395	14536	5844	10488	1527		

- Molecule 12 is a RNA chain called tRNA.

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

- Molecule 13 is a protein called 39S ribosomal protein L2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	D	239	Total	C	N	O	S	0	0
			1866	1162	377	318	9		

- Molecule 14 is a protein called 39S ribosomal protein L3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	E	306	Total	C	N	O	S	0	0
			2410	1547	419	433	11		

- Molecule 15 is a protein called 39S ribosomal protein L4, mitochondrial.

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

- Molecule 16 is a protein called 39S ribosomal protein L9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	H	98	Total	C	N	O		0	0
			806	510	156	140			

- Molecule 17 is a protein called 39S ribosomal protein L10, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	I	179	Total	C	N	O	S	0	0
			1435	925	258	242	10		

- Molecule 18 is a protein called 39S ribosomal protein L11, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	J	175	Total	C	N	O	S	0	0
			1330	847	237	244	2		

- Molecule 19 is a protein called 39S ribosomal protein L13, mitochondrial.

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

- Molecule 20 is a protein called 39S ribosomal protein L14, mitochondrial.

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

- Molecule 21 is a protein called 39S ribosomal protein L15, mitochondrial.

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

- Molecule 22 is a protein called 39S ribosomal protein L16, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	N	222	Total	C	N	O	S	0	0
			1786	1143	326	307	10		

- Molecule 23 is a protein called 39S ribosomal protein L17, mitochondrial.

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

- Molecule 24 is a protein called Mitochondrial ribosomal protein L18, isoform CRA_b.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	P	143	Total	C	N	O	S	0	0
			1165	729	223	208	5		

- Molecule 25 is a protein called 39S ribosomal protein L19, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Q	220	Total	C	N	O	S	0	0
			1834	1174	326	325	9		

- Molecule 26 is a protein called 39S ribosomal protein L20, mitochondrial.

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

- Molecule 27 is a protein called 39S ribosomal protein L21, mitochondrial.

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

- Molecule 28 is a protein called 39S ribosomal protein L22, mitochondrial.

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

- Molecule 29 is a protein called 39S ribosomal protein L23, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	U	152	Total	C	N	O	S	0	0
			1222	773	233	213	3		

- Molecule 30 is a protein called 39S ribosomal protein L24, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	V	206	Total	C	N	O	S	0	0
			1682	1071	299	304	8		

- Molecule 31 is a protein called 39S ribosomal protein L27, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	W	111	Total	C	N	O	S	0	0
			871	558	164	146	3		

- Molecule 32 is a protein called 39S ribosomal protein L28, mitochondrial.

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

- Molecule 33 is a protein called 39S ribosomal protein L47, mitochondrial.

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

- Molecule 34 is a protein called 39S ribosomal protein L30, mitochondrial.

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

- Molecule 35 is a protein called 39S ribosomal protein L42, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	a	108	Total	C	N	O	S	0	0
			896	560	162	169	5		

- Molecule 36 is a protein called 39S ribosomal protein L43, mitochondrial.

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

- Molecule 37 is a protein called 39S ribosomal protein L44, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	c	289	Total	C	N	O	S	0	0
			2322	1483	400	430	9		

- Molecule 38 is a protein called 39S ribosomal protein L45, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	d	257	Total	C	N	O	S	0	0
			2075	1326	363	372	14		

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

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

- Molecule 40 is a protein called 39S ribosomal protein L48, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	f	146	Total	C	N	O	S	0	0
			1126	714	186	222	4		

- Molecule 41 is a protein called 39S ribosomal protein L49, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	g	132	Total	C	N	O	S	0	0
			1096	709	191	194	2		

- Molecule 42 is a protein called 39S ribosomal protein L50, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	h	110	Total	C	N	O	S	0	0
			894	568	156	167	3		

- Molecule 43 is a protein called 39S ribosomal protein L51, mitochondrial.

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

- Molecule 44 is a protein called cDNA FLJ76418, highly similar to Homo sapiens mitochondrial ribosomal protein L52 (MRPL52), transcript variant 1, mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	j	93	Total	C	N	O	S	0	0
			740	460	143	135	2		

- Molecule 45 is a protein called 39S ribosomal protein L53, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	k	96	Total	C	N	O	S	0	0
			743	462	143	133	5		

- Molecule 46 is a protein called 39S ribosomal protein L54, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	l	72	Total	C	N	O	S	0	0
			619	394	112	111	2		

- Molecule 47 is a protein called 39S ribosomal protein L55, mitochondrial.

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

- Molecule 48 is a protein called Ribosomal protein 63, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	o	94	Total	C	N	O	S	0	0
			797	501	165	128	3		

- Molecule 49 is a protein called Peptidyl-tRNA hydrolase ICT1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	p	152	Total	C	N	O	S	0	0
			1227	762	232	229	4		

- Molecule 50 is a protein called Growth arrest and DNA damage-inducible proteins-interacting protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	q	168	Total	C	N	O	S	0	0
			1294	801	255	233	5		

- Molecule 51 is a protein called 39S ribosomal protein S18a, mitochondrial.

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

- Molecule 52 is a protein called 39S ribosomal protein S30, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	s	393	Total	C	N	O	S	0	0
			3178	2036	565	563	14		

- Molecule 53 is a protein called P-site finger.

Mol	Chain	Residues	Atoms				AltConf	Trace
53	u	65	Total	C	N	O	0	0
			325	195	65	65		

- Molecule 54 is a protein called 39S ribosomal protein L12, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
54	TA	45	Total	C	N	O	0	0
			345	222	54	69		
54	TB	27	Total	C	N	O	0	0
			213	137	33	43		
54	TC	71	Total	C	N	O	0	0
			352	210	71	71		

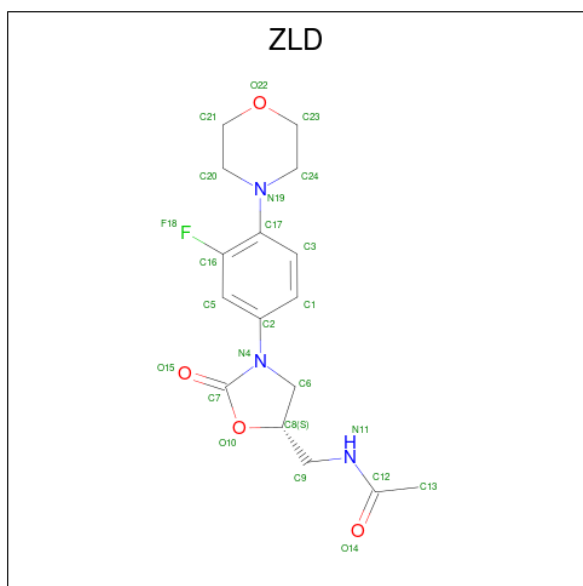
- Molecule 55 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
55	0	1	Total	Zn	0
			1	1	
55	4	1	Total	Zn	0
			1	1	
55	r	1	Total	Zn	0
			1	1	

- Molecule 56 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
56	A	100	Total	Mg	0
			100	100	
56	D	1	Total	Mg	0
			1	1	
56	g	1	Total	Mg	0
			1	1	

- Molecule 57 is N-{[(5S)-3-(3-fluoro-4-morpholin-4-ylphenyl)-2-oxo-1,3-oxazolidin-5-yl]methyl}acetamide (CCD ID: ZLD) (formula: C₁₆H₂₀FN₃O₄).



Mol	Chain	Residues	Atoms					AltConf
57	A	1	Total	C	F	N	O	0
			24	16	1	3	4	

- Molecule 58 is water.

Mol	Chain	Residues	Atoms		AltConf
58	0	16	Total 16	O 16	0
58	1	8	Total 8	O 8	0
58	2	10	Total 10	O 10	0
58	3	15	Total 15	O 15	0
58	4	7	Total 7	O 7	0
58	5	63	Total 63	O 63	0
58	6	99	Total 99	O 99	0
58	7	96	Total 96	O 96	0
58	8	44	Total 44	O 44	0
58	9	23	Total 23	O 23	0
58	A	1975	Total 1975	O 1975	0
58	B	99	Total 99	O 99	0
58	D	31	Total 31	O 31	0
58	E	51	Total 51	O 51	0
58	F	24	Total 24	O 24	0
58	H	29	Total 29	O 29	0
58	I	62	Total 62	O 62	0
58	J	107	Total 107	O 107	0
58	K	28	Total 28	O 28	0
58	L	14	Total 14	O 14	0
58	M	39	Total 39	O 39	0
58	N	49	Total 49	O 49	0

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Mol	Chain	Residues	Atoms		AltConf
58	O	26	Total 26	O 26	0
58	P	34	Total 34	O 34	0
58	Q	50	Total 50	O 50	0
58	R	20	Total 20	O 20	0
58	S	27	Total 27	O 27	0
58	T	29	Total 29	O 29	0
58	U	35	Total 35	O 35	0
58	V	37	Total 37	O 37	0
58	W	19	Total 19	O 19	0
58	X	30	Total 30	O 30	0
58	Y	22	Total 22	O 22	0
58	Z	27	Total 27	O 27	0
58	a	18	Total 18	O 18	0
58	b	34	Total 34	O 34	0
58	c	21	Total 21	O 21	0
58	d	10	Total 10	O 10	0
58	e	196	Total 196	O 196	0
58	f	59	Total 59	O 59	0
58	g	27	Total 27	O 27	0
58	h	36	Total 36	O 36	0
58	i	28	Total 28	O 28	0

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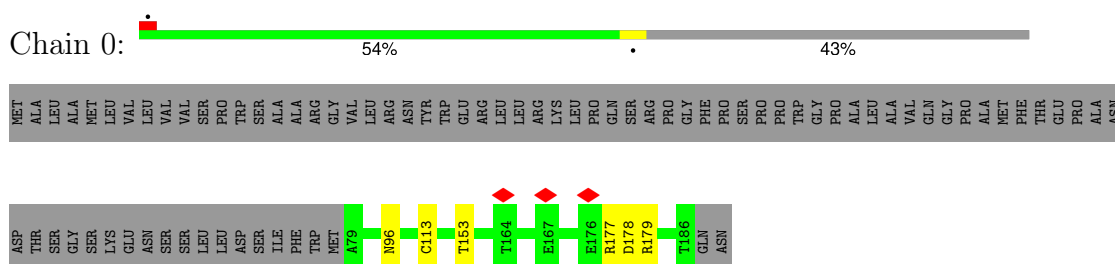
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Mol	Chain	Residues	Atoms		AltConf
58	j	24	Total 24	O 24	0
58	k	32	Total 32	O 32	0
58	l	50	Total 50	O 50	0
58	m	33	Total 33	O 33	0
58	o	18	Total 18	O 18	0
58	p	57	Total 57	O 57	0
58	q	6	Total 6	O 6	0
58	r	44	Total 44	O 44	0
58	s	57	Total 57	O 57	0
58	u	32	Total 32	O 32	0
58	TA	43	Total 43	O 43	0
58	TB	22	Total 22	O 22	0
58	TC	37	Total 37	O 37	0

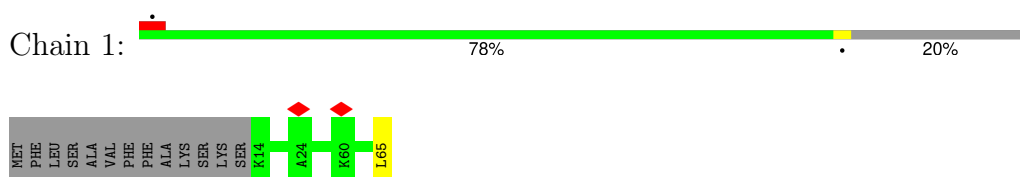
3 Residue-property plots [i](#)

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

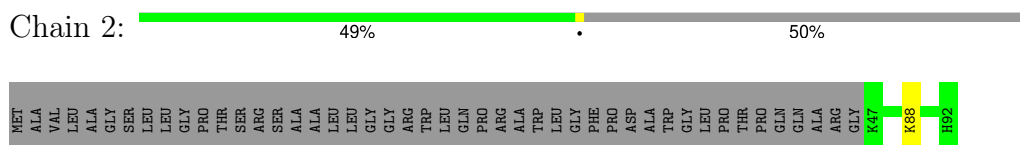
- Molecule 1: 39S ribosomal protein L32, mitochondrial



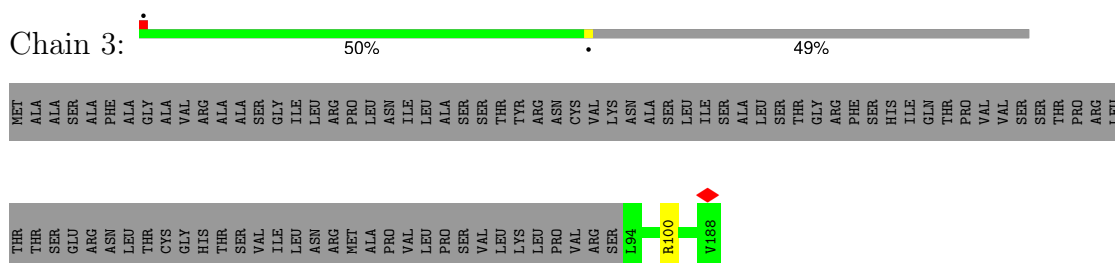
- Molecule 2: 39S ribosomal protein L33, mitochondrial



- Molecule 3: 39S ribosomal protein L34, mitochondrial

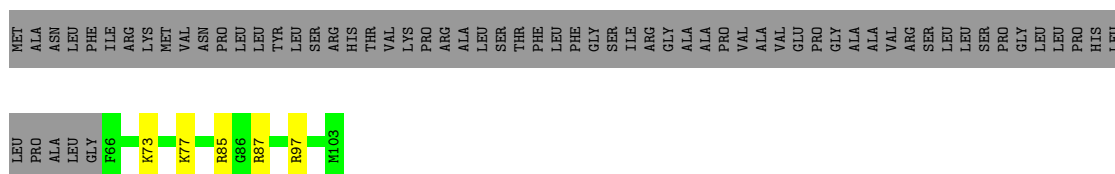


- Molecule 4: 39S ribosomal protein L35, mitochondrial

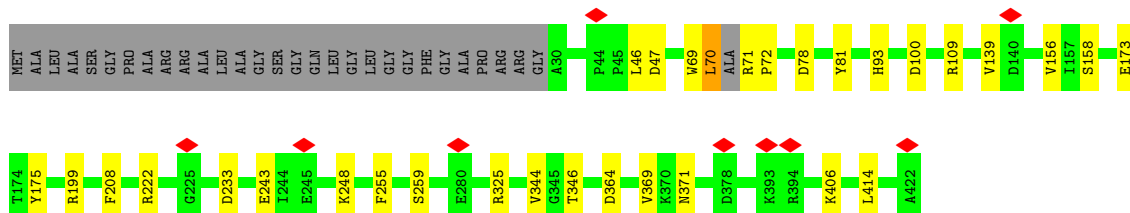
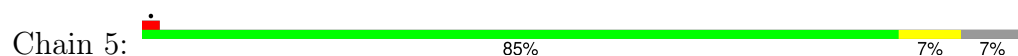


- Molecule 5: 39S ribosomal protein L36, mitochondrial

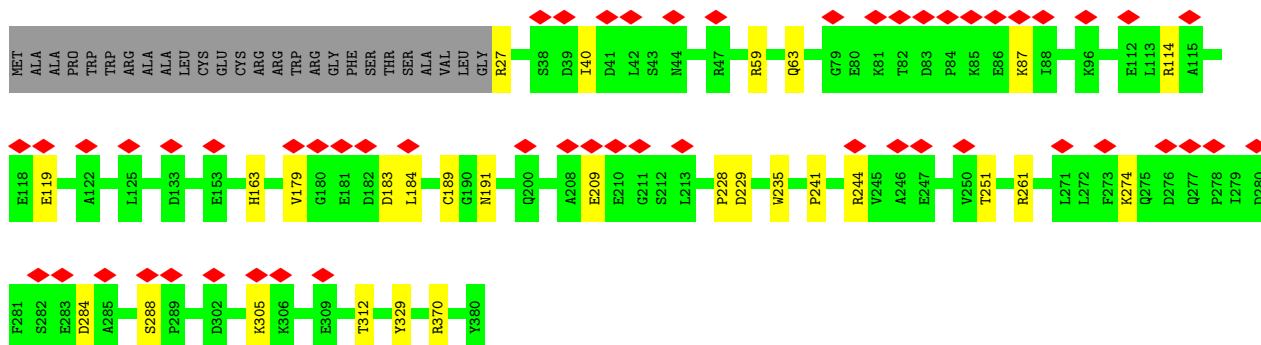
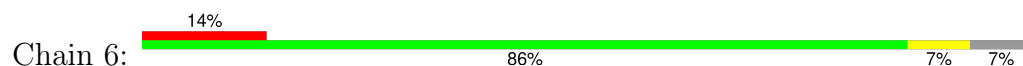




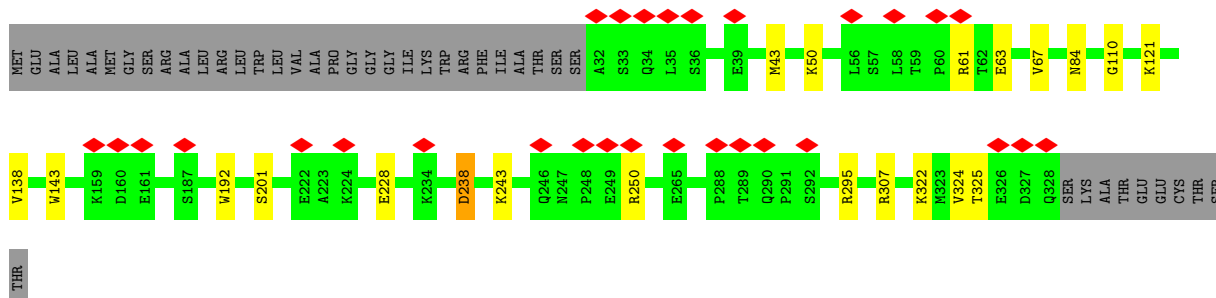
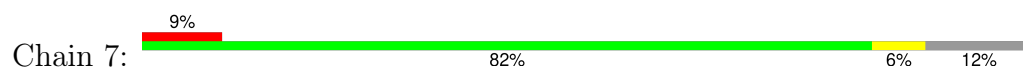
- Molecule 6: 39S ribosomal protein L37, mitochondrial



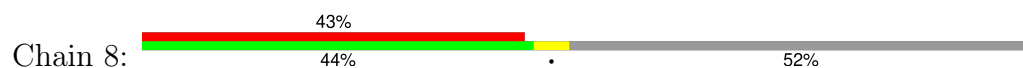
- Molecule 7: 39S ribosomal protein L38, mitochondrial

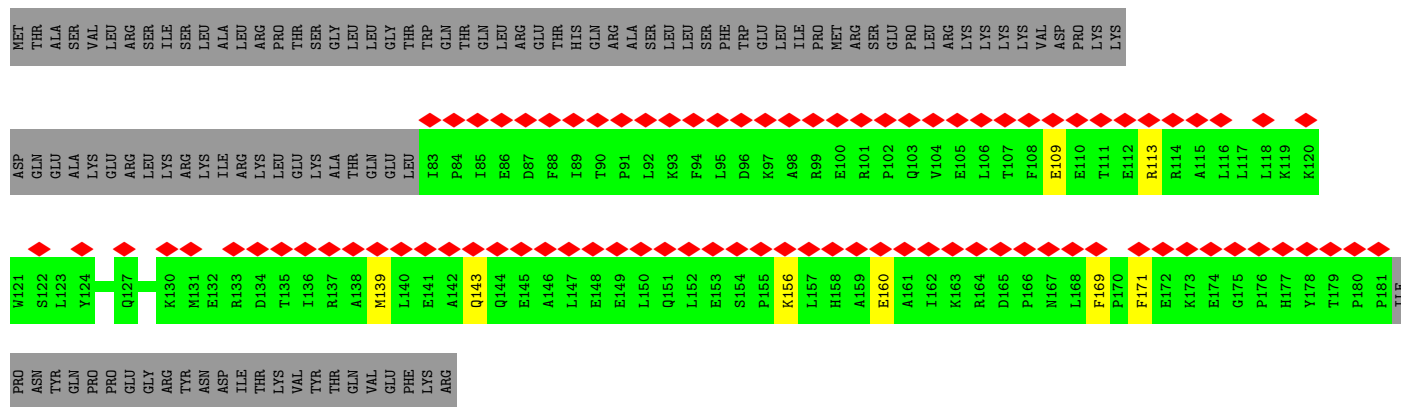


- Molecule 8: 39S ribosomal protein L39, mitochondrial

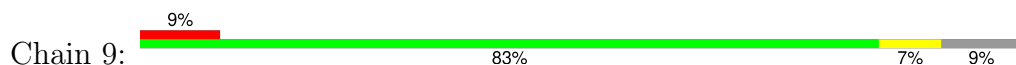


- Molecule 9: 39S ribosomal protein L40, mitochondrial

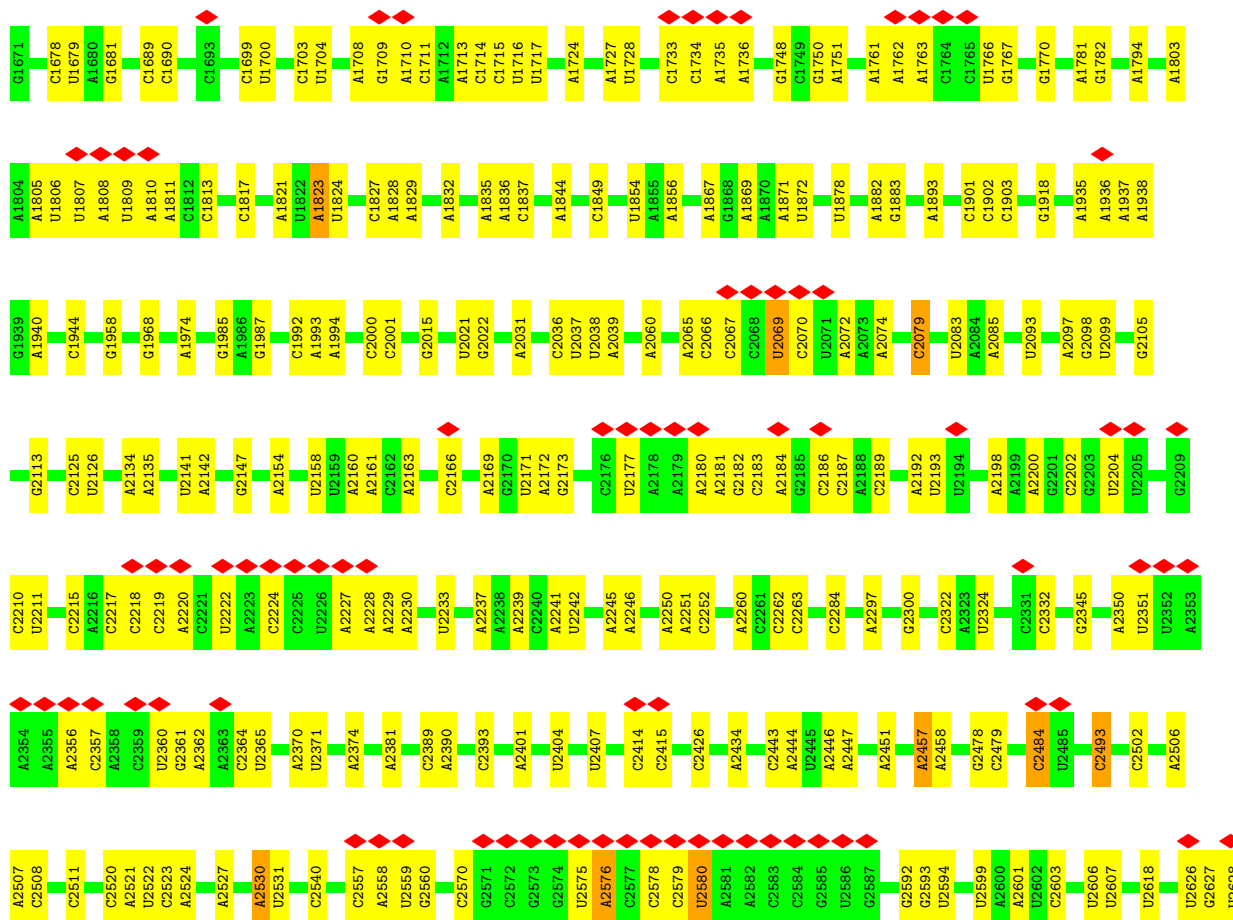


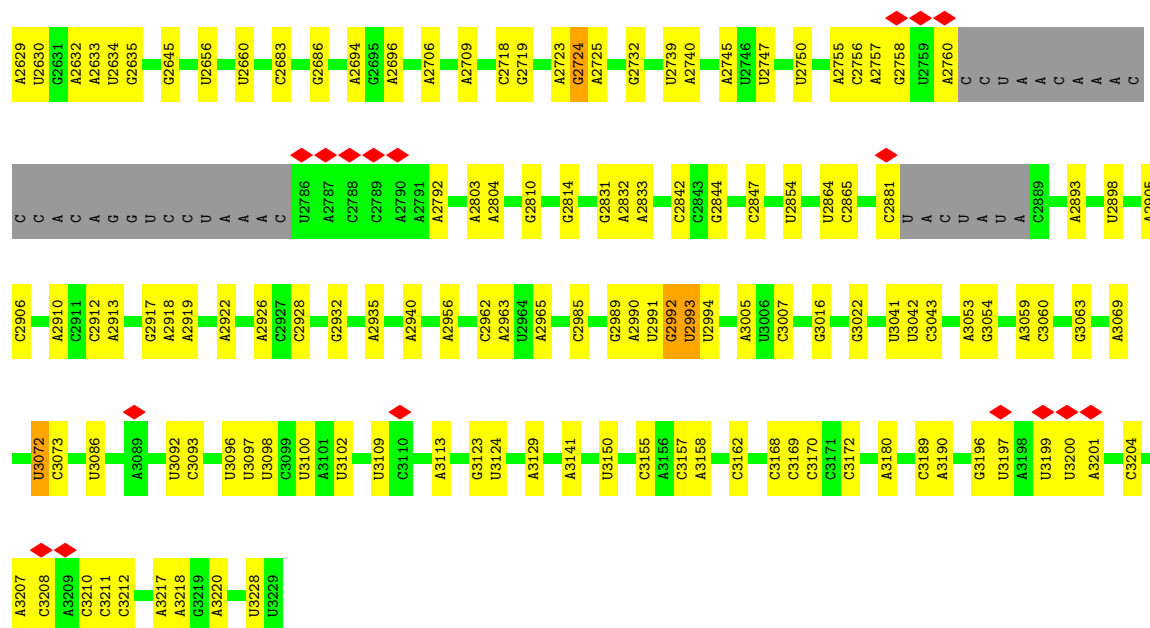


- Molecule 10: 39S ribosomal protein L41, mitochondrial

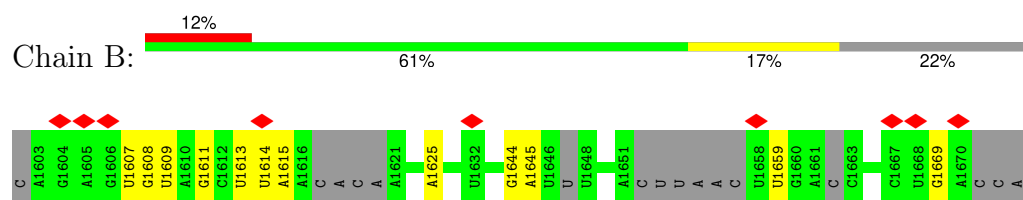


- Molecule 11: 16S rRNA

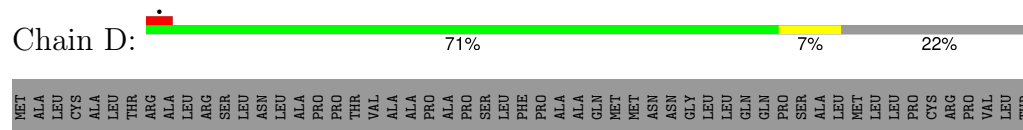




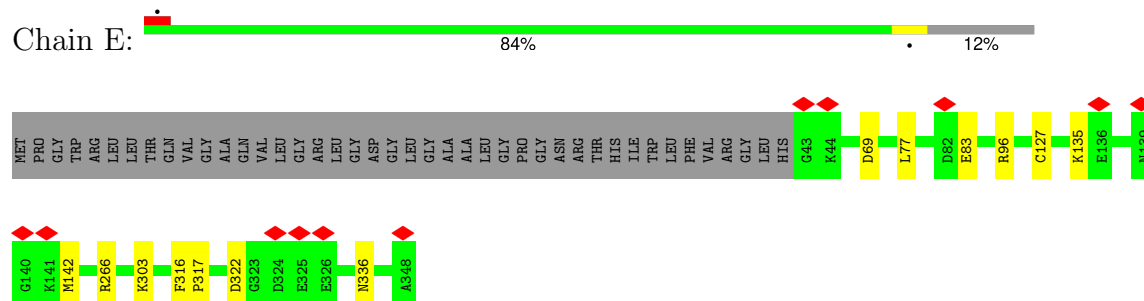
- Molecule 12: tRNA




- Molecule 13: 39S ribosomal protein L2, mitochondrial

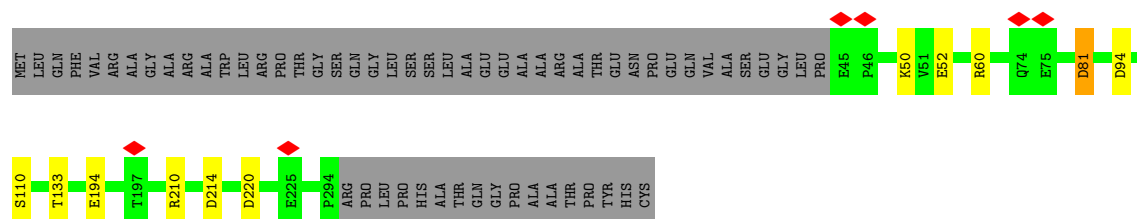


- Molecule 14: 39S ribosomal protein L3, mitochondrial



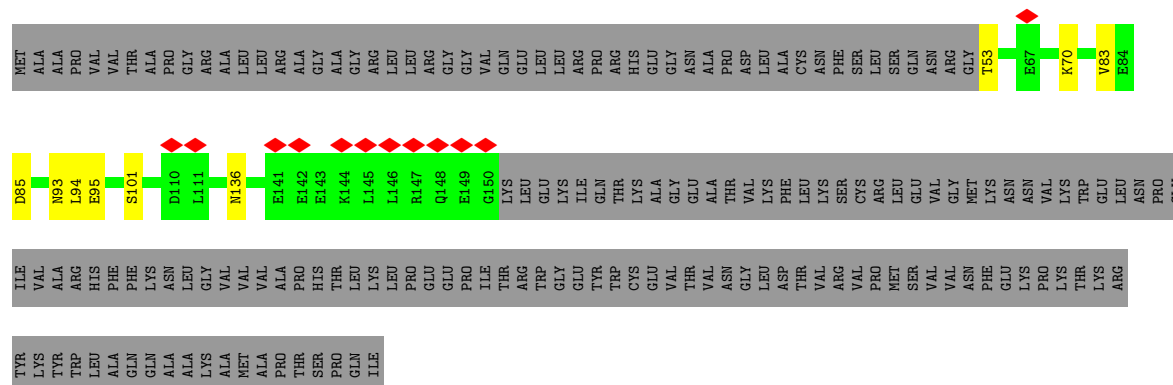
- Molecule 15: 39S ribosomal protein L4, mitochondrial

Chain F: 



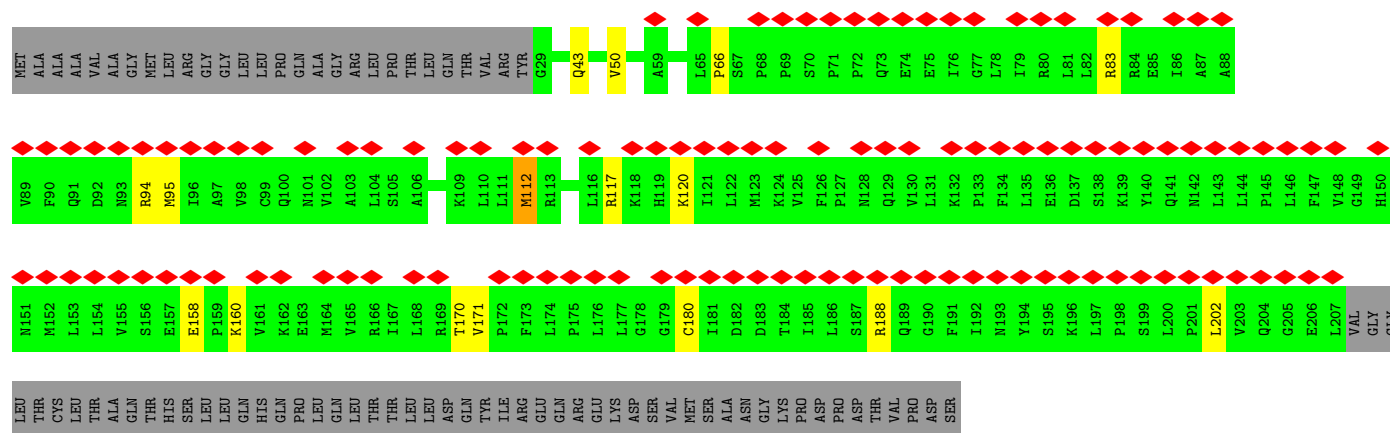
- Molecule 16: 39S ribosomal protein L9, mitochondrial

Chain H: 




- Molecule 17: 39S ribosomal protein L10, mitochondrial

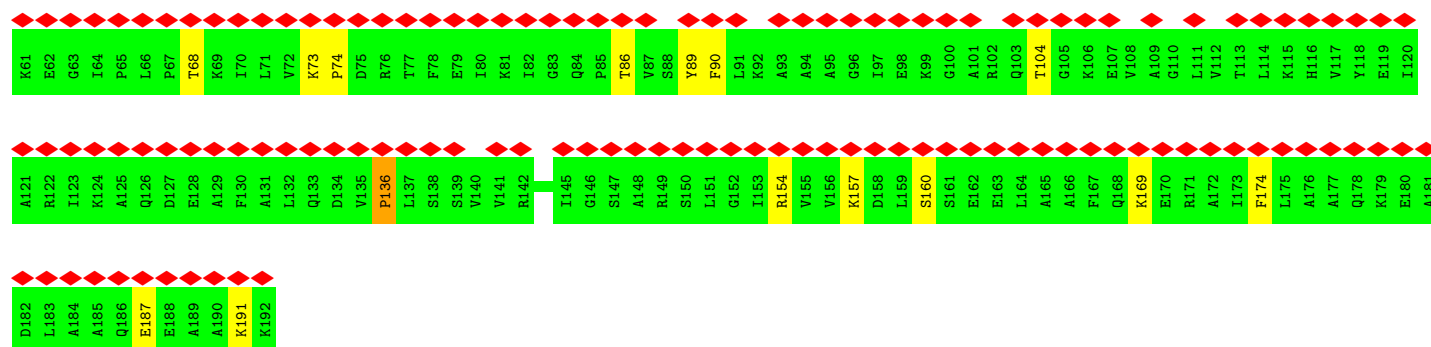
Chain I: 



- Molecule 18: 39S ribosomal protein L11, mitochondrial

Chain J: 





- Molecule 19: 39S ribosomal protein L13, mitochondrial

Chain K: 96%



- Molecule 20: 39S ribosomal protein L14, mitochondrial

Chain L: 71% 8% 21%



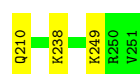
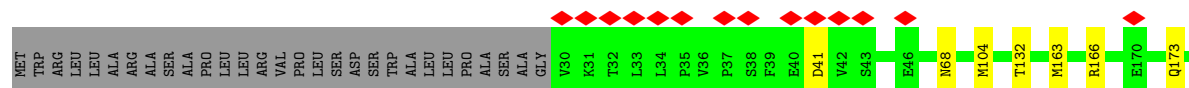
- Molecule 21: 39S ribosomal protein L15, mitochondrial

Chain M: 94%



- Molecule 22: 39S ribosomal protein L16, mitochondrial

Chain N: 6% 84% 12%

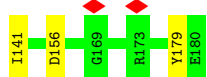
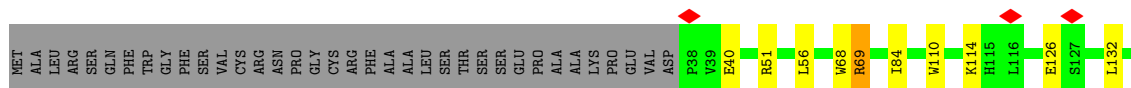


- Molecule 23: 39S ribosomal protein L17, mitochondrial

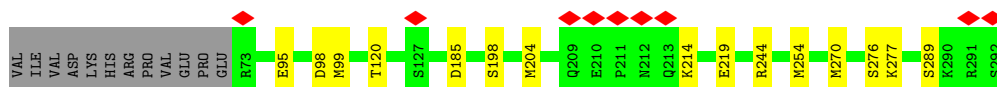
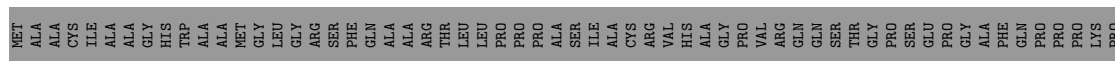
Chain O: 83% 13%



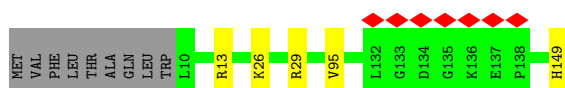
- Molecule 24: Mitochondrial ribosomal protein L18, isoform CRA_b



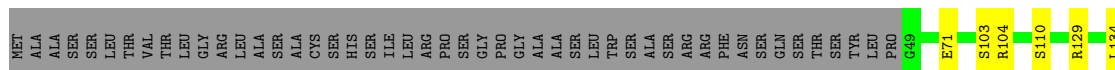
- Molecule 25: 39S ribosomal protein L19, mitochondrial



- Molecule 26: 39S ribosomal protein L20, mitochondrial



- Molecule 27: 39S ribosomal protein L21, mitochondrial

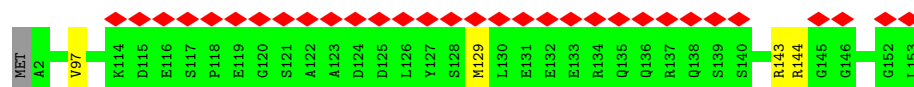


- Molecule 28: 39S ribosomal protein L22, mitochondrial

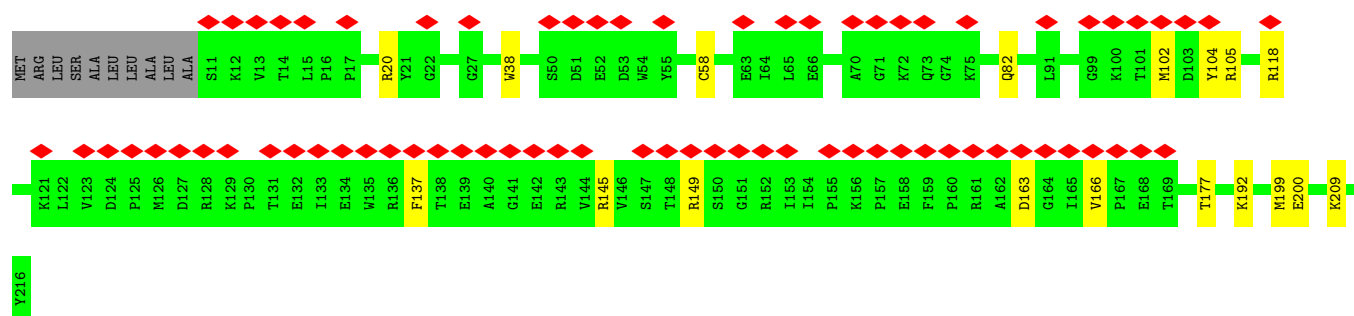
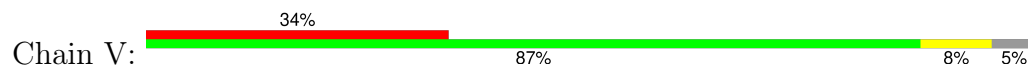




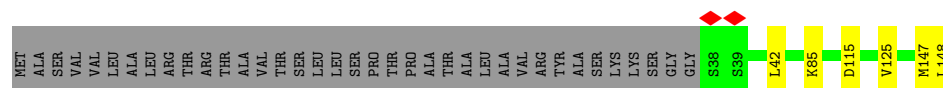
- Molecule 29: 39S ribosomal protein L23, mitochondrial



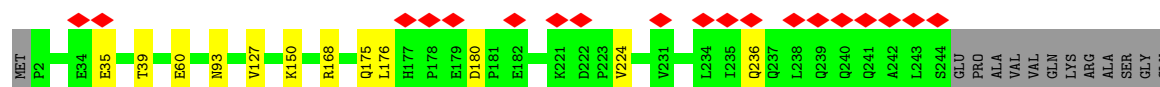
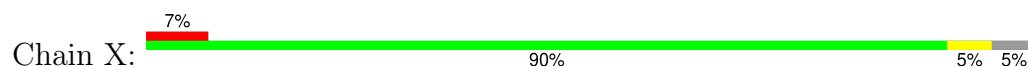
- Molecule 30: 39S ribosomal protein L24, mitochondrial



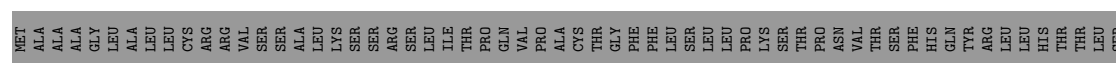
- Molecule 31: 39S ribosomal protein L27, mitochondrial



- Molecule 32: 39S ribosomal protein L28, mitochondrial

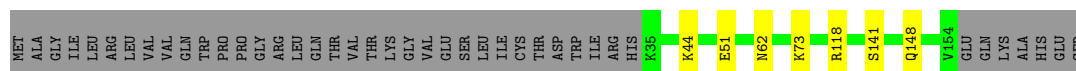


- Molecule 33: 39S ribosomal protein L47, mitochondrial



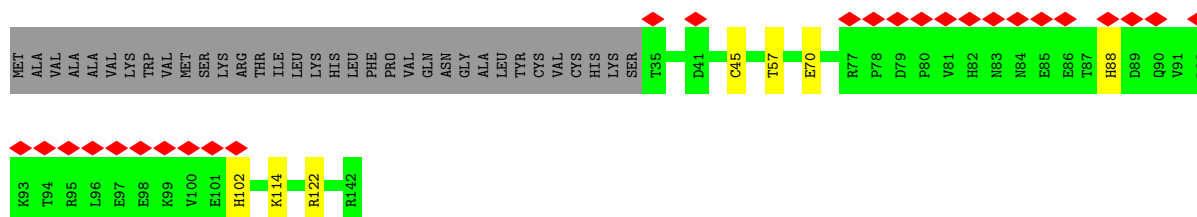
- Molecule 34: 39S ribosomal protein L30, mitochondrial

Chain Z:  70% 25%



- Molecule 35: 39S ribosomal protein L42, mitochondrial

Chain a:  18% 71% 5% 24%




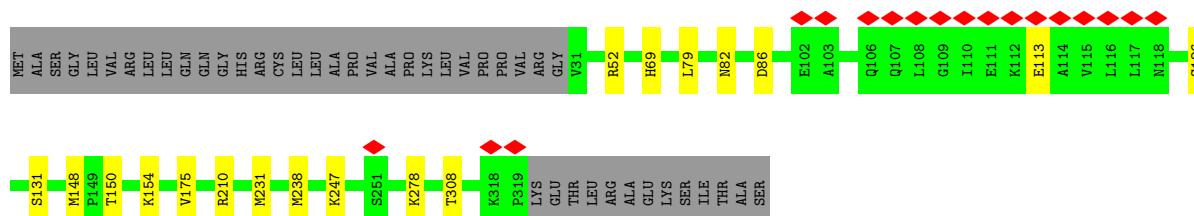
- Molecule 36: 39S ribosomal protein L43, mitochondrial

Chain b:  92% 5%




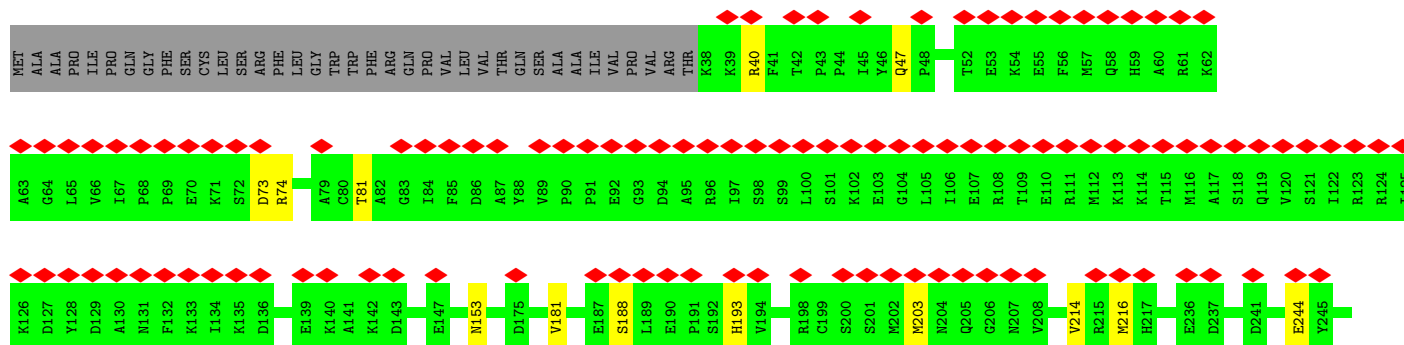
- Molecule 37: 39S ribosomal protein L44, mitochondrial

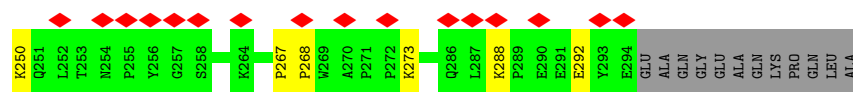
Chain c:  5% 82% 5% 13%



- Molecule 38: 39S ribosomal protein L45, mitochondrial

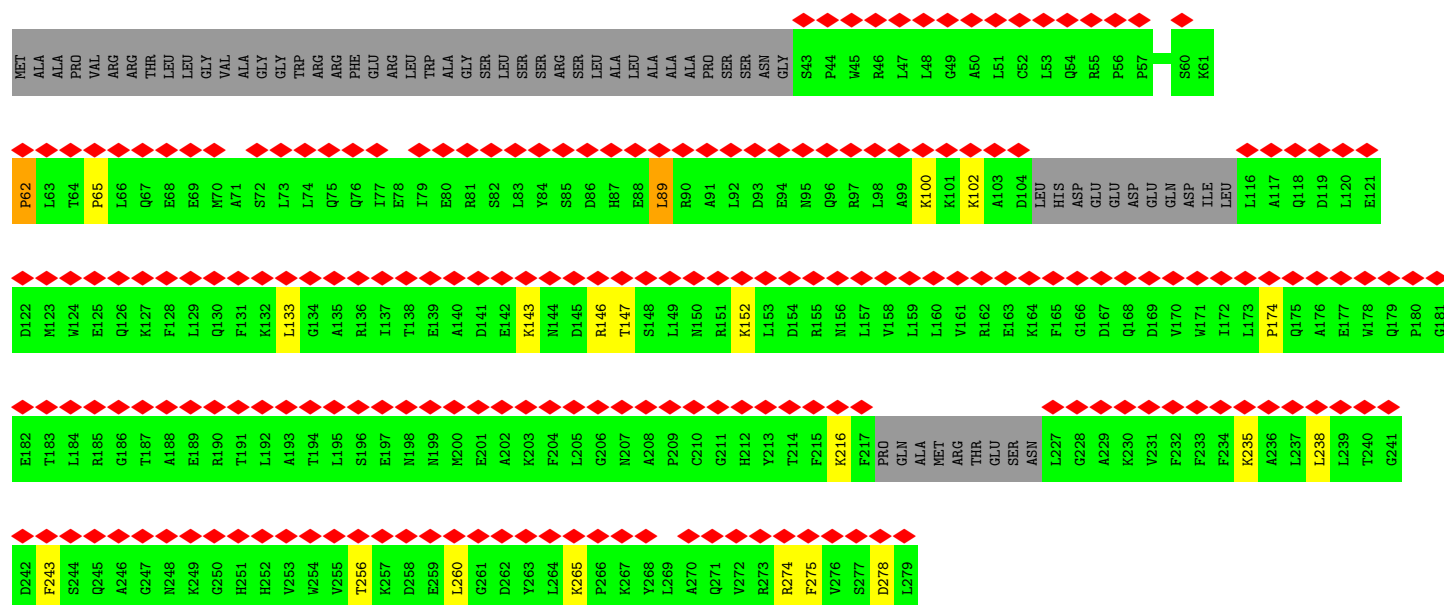
Chain d:  42% 78% 6% 16%





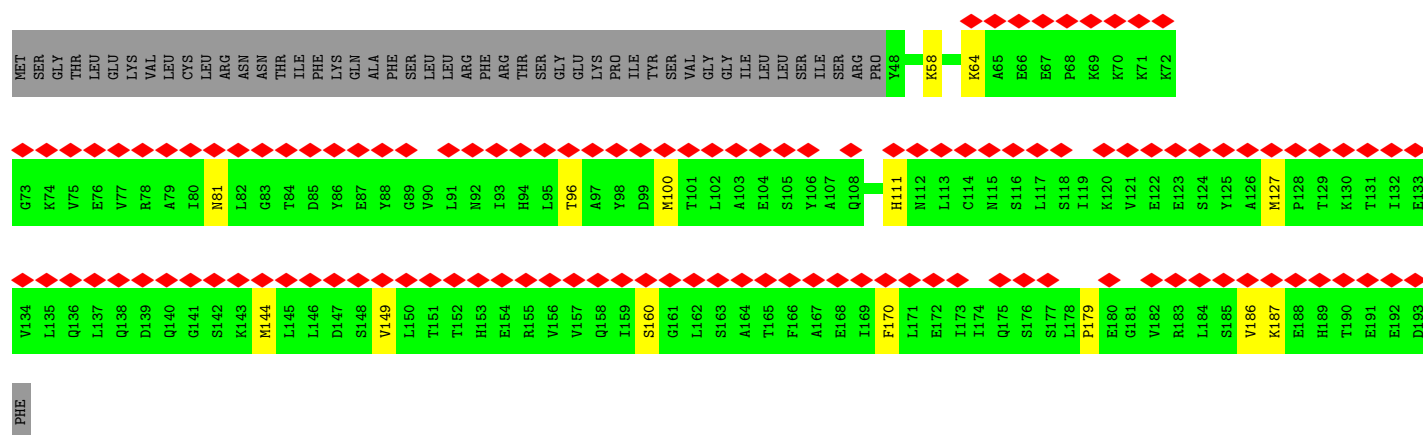
• Molecule 39: 39S ribosomal protein L46, mitochondrial

Chain e:



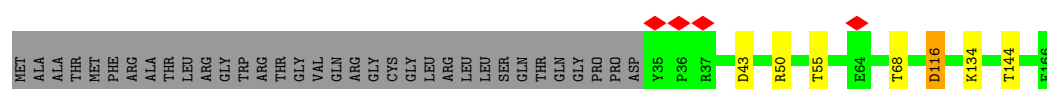
• Molecule 40: 39S ribosomal protein L48, mitochondrial

Chain f:

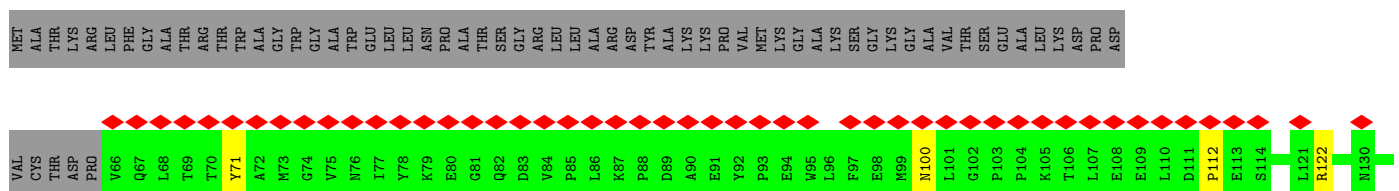
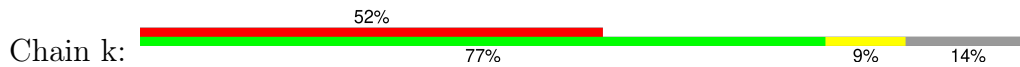


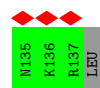
• Molecule 41: 39S ribosomal protein L49, mitochondrial

Chain g:

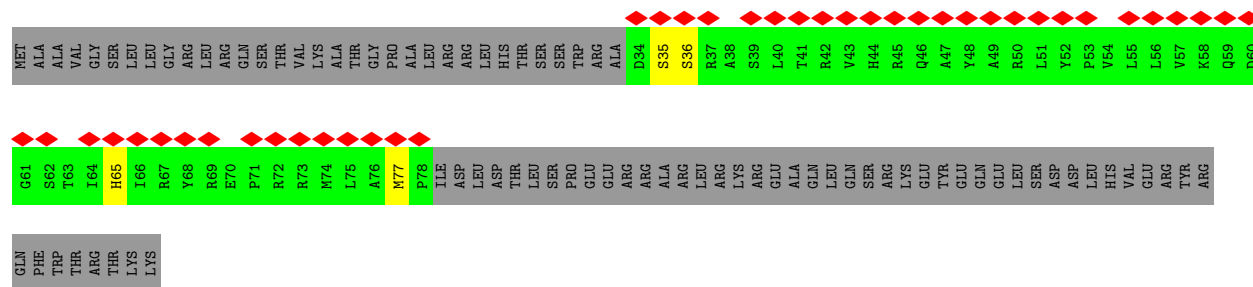


- Chain h: 

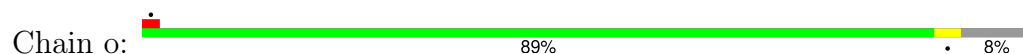




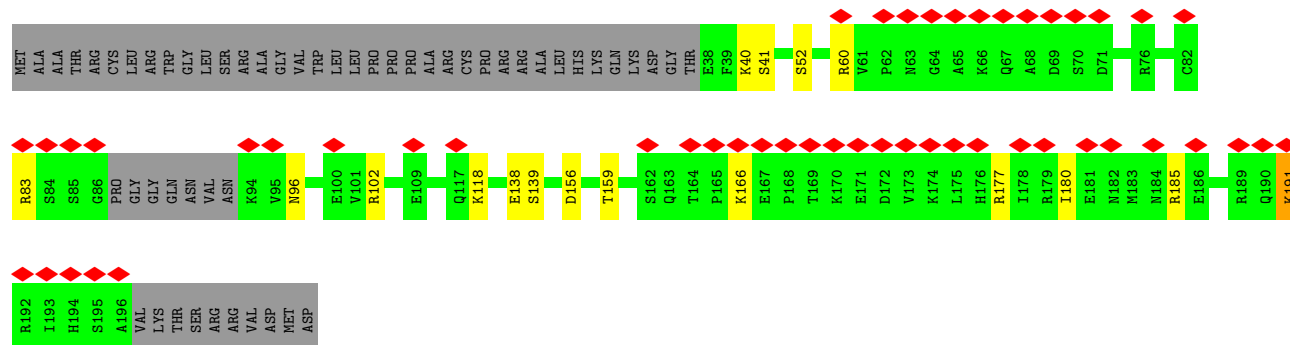
- Molecule 47: 39S ribosomal protein L55, mitochondrial



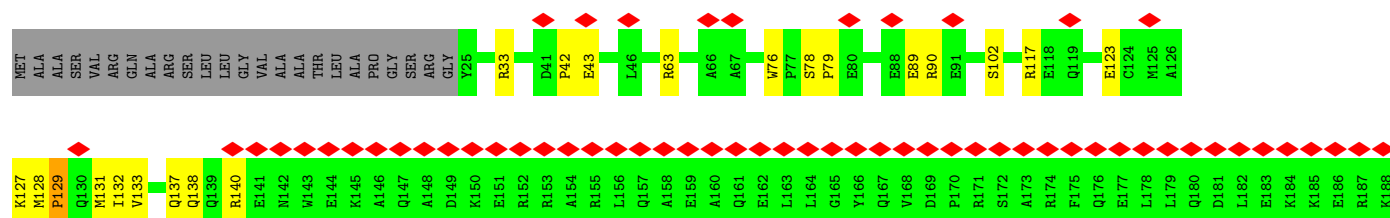
- Molecule 48: Ribosomal protein 63, mitochondrial

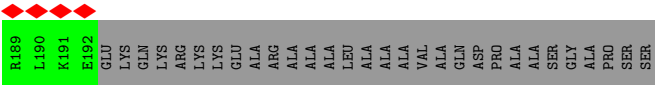


- Molecule 49: Peptidyl-tRNA hydrolase ICT1, mitochondrial

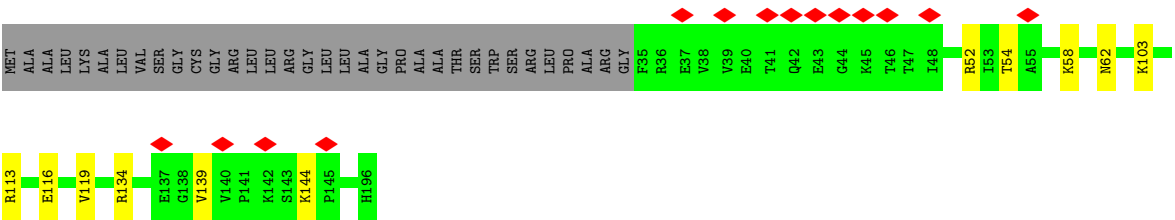
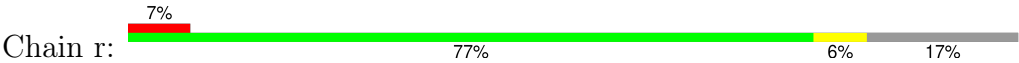


- Molecule 50: Growth arrest and DNA damage-inducible proteins-interacting protein 1

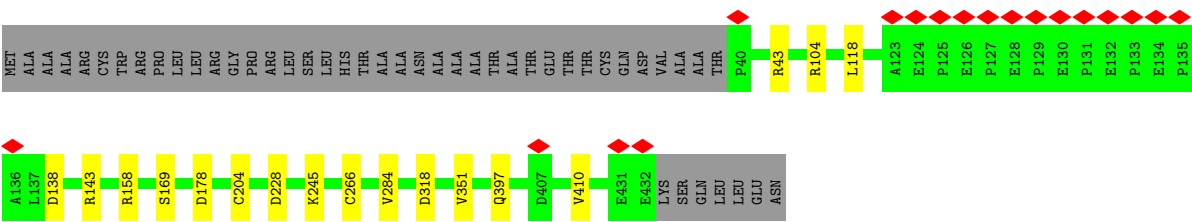
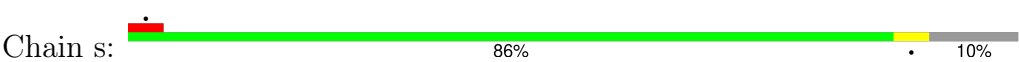




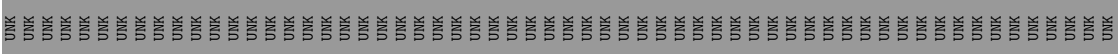
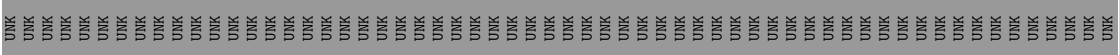
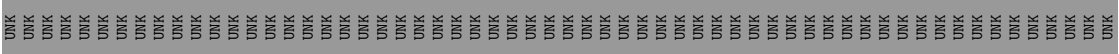
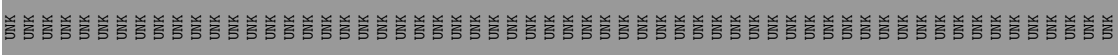
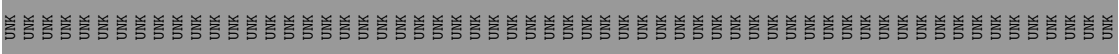
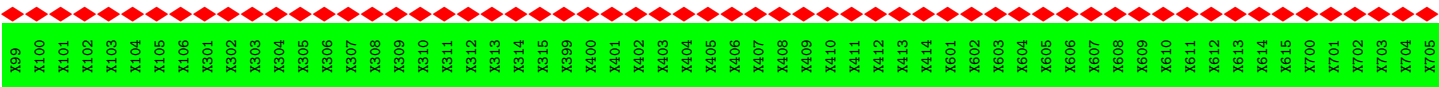
• Molecule 51: 39S ribosomal protein S18a, mitochondrial



• Molecule 52: 39S ribosomal protein S30, mitochondrial



• Molecule 53: P-site finger



[illegible]

- Molecule 54: 39S ribosomal protein L12, mitochondrial

Chain TA: 

ALA	GLU	ILE	P61	MET
LYS	LYS	PRO	P62	LEU
ILE	ALA	ILE	P63	ALA
LYS	LYS	LYS	P64	ALA
ALA	ALA	ARG	P65	ALA
LEU	LEU	THR	P66	PRO
GLU	GLU	HIS	P67	TRP
ALA	ALA	PHE	P68	GLY
VAL	VAL	THR	P69	PRO
GLY	GLY	ARG	D70	CYS
THR	THR	LEU	I71	LEU
VAL	VAL	THR	A72	GLY
VAL	LEU	GLU	S73	LEU
GLU	GLU	ALA	I74	ARG
		PRO	I75	ALA
		LYS	L76	ALA
		ASP	L77	PHE
		LYS	E78	ARG
		VAL	I79	LEU
		LYS	S80	ALA
		ILE	D81	ARG
		LYS	L82	GLN
		GLU	I83	VAL
		ILE	S84	PRO
		LYS	E84	CYS
		ASN	L85	VAL
		TYR	L86	CYS
		ILE	K87	ALA
		GLN	K88	VAL
		GLY	K89	ARG
		ILE	T89	HIS
		ASN	L90	MET
		LEU	LYS	ARG
		VAL	ILE	SER
		GLN	GLN	SER
		ALA	LYS	GLY
		LYS	ASP	HIS
		LYS	VAL	GLN
		LEU	VAL	ARG
		VAL	LEU	GLY
		GLU	VAL	CYS
		SER	VAL	E46
		PRO	PRO	A47
		LEU	MET	L48
		PRO	GLY	A49
		GLN	GLY	D50
		ILE	VAL	MET
		LYS	SER	P52
		ALA	GLY	L53
		ASN	ALA	D54
		VAL	VAL	PRO
		ALA	VAL	N55
		LYS	ALA	A56
		ALA	ALA	P57
		GLU	ALA	K58
			ALA	E59
			GLN	
			GLU	
			ALA	
			VAL	
			GLU	
			ASP	

- Molecule 54: 39S ribosomal protein L12, mitochondrial

Chain TB: 14% 13% 86%

[illegible]

- Molecule 54: 39S ribosomal protein L12, mitochondrial

Chain TC: 

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

WORLDWIDE
PDB
PROTEIN DATA BANK

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	347872	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	21	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	4.661	Depositor
Minimum map value	-2.742	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.096	Depositor
Recommended contour level	0.38	Depositor
Map size (Å)	484.4, 484.4, 484.4	wwPDB
Map dimensions	560, 560, 560	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.865, 0.865, 0.865	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	0	0.29	0/895	0.59	0/1201
2	1	0.26	0/438	0.59	0/583
3	2	0.27	0/382	0.56	0/507
4	3	0.28	0/852	0.54	0/1136
5	4	0.26	0/350	0.58	0/461
6	5	0.29	0/3300	0.54	0/4495
7	6	0.30	0/3043	0.65	4/4140 (0.1%)
8	7	0.26	0/2467	0.50	1/3337 (0.0%)
9	8	0.26	0/855	0.53	0/1152
10	9	0.30	0/1025	0.57	1/1379 (0.1%)
11	A	0.80	9/36246 (0.0%)	0.88	35/56422 (0.1%)
12	B	0.19	0/1328	0.81	0/2056
13	D	0.27	0/1904	0.58	0/2561
14	E	0.27	0/2479	0.50	0/3360
15	F	0.29	0/2071	0.58	2/2817 (0.1%)
16	H	0.29	0/820	0.62	0/1102
17	I	0.53	2/1467 (0.1%)	0.86	5/1984 (0.3%)
18	J	0.89	5/1348 (0.4%)	1.33	11/1813 (0.6%)
19	K	0.27	0/1495	0.55	1/2029 (0.0%)
20	L	0.28	0/904	0.57	0/1218
21	M	0.29	0/2359	0.58	1/3185 (0.0%)
22	N	0.27	0/1833	0.55	1/2468 (0.0%)
23	O	0.28	0/1269	0.55	0/1708
24	P	0.30	0/1191	0.62	1/1611 (0.1%)
25	Q	0.27	0/1875	0.52	0/2523
26	R	0.30	0/1174	0.58	0/1572
27	S	0.27	0/1276	0.56	0/1729
28	T	0.31	0/1402	0.56	1/1886 (0.1%)
29	U	0.29	0/1252	0.58	0/1697
30	V	0.27	0/1727	0.59	1/2341 (0.0%)
31	W	0.29	0/893	0.55	0/1204
32	X	0.28	0/2090	0.51	0/2825

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	Y	0.27	0/1552	0.54	0/2079
34	Z	0.27	0/1003	0.52	0/1354
35	a	0.28	0/923	0.50	0/1254
36	b	0.28	0/1202	0.57	0/1626
37	c	0.27	0/2371	0.50	0/3205
38	d	0.76	3/2132 (0.1%)	0.84	6/2887 (0.2%)
39	e	0.62	3/1797 (0.2%)	1.00	9/2422 (0.4%)
40	f	0.28	0/1144	0.65	2/1551 (0.1%)
41	g	0.30	0/1132	0.57	1/1543 (0.1%)
42	h	0.26	0/917	0.53	0/1249
43	i	0.30	0/849	0.59	0/1135
44	j	0.27	0/755	0.57	0/1016
45	k	0.49	2/754 (0.3%)	0.96	3/1017 (0.3%)
46	l	0.72	1/636 (0.2%)	1.07	4/860 (0.5%)
47	m	0.24	0/379	0.66	0/510
48	o	0.27	0/818	0.59	0/1097
49	p	0.27	0/1246	0.61	1/1675 (0.1%)
50	q	0.34	0/1325	0.62	1/1799 (0.1%)
51	r	0.28	0/1362	0.57	0/1846
52	s	0.29	0/3262	0.54	0/4435
54	TA	1.35	2/349 (0.6%)	1.99	4/475 (0.8%)
54	TB	0.23	0/212	0.50	0/286
54	TC	0.24	0/351	0.42	0/488
All	All	0.55	27/108481 (0.0%)	0.74	96/154311 (0.1%)

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
13	D	0	1
14	E	0	1
19	K	0	1
24	P	0	1
33	Y	0	1
34	Z	0	1
42	h	0	2
49	p	0	1
50	q	0	1
All	All	0	10

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	2576	A	N3-C4	72.27	1.78	1.34
11	A	2576	A	C6-N1	66.72	1.82	1.35
11	A	2576	A	N1-C2	49.44	1.78	1.34
11	A	2576	A	C5-C4	46.90	1.71	1.38
11	A	2576	A	C2-N3	46.81	1.75	1.33
11	A	2576	A	C5-C6	40.59	1.77	1.41
38	d	268	PRO	CG-CD	-30.93	0.48	1.50
18	J	136	PRO	CG-CD	-23.34	0.73	1.50
54	TA	52	PRO	CG-CD	-22.63	0.76	1.50
39	e	62	PRO	CG-CD	-20.40	0.83	1.50
46	l	112	PRO	CG-CD	-15.69	0.98	1.50
17	I	66	PRO	CG-CD	-15.49	0.99	1.50
11	A	2992	G	O3'-P	-14.63	1.43	1.61
18	J	136	PRO	CB-CG	12.54	2.12	1.50
39	e	62	PRO	CB-CG	9.86	1.99	1.50
38	d	268	PRO	CB-CG	9.84	1.99	1.50
18	J	74	PRO	CB-CG	-9.59	1.02	1.50
45	k	62	PRO	CG-CD	-9.38	1.19	1.50
18	J	74	PRO	CG-CD	-8.66	1.22	1.50
54	TA	52	PRO	CB-CG	7.91	1.89	1.50
11	A	2993	U	O3'-P	-7.08	1.52	1.61
11	A	2991	U	O3'-P	-6.86	1.52	1.61
17	I	66	PRO	N-CD	6.57	1.57	1.47
45	k	62	PRO	CB-CG	-6.04	1.19	1.50
38	d	268	PRO	N-CD	5.60	1.55	1.47
18	J	136	PRO	CA-CB	-5.14	1.43	1.53
39	e	62	PRO	CA-CB	-5.13	1.43	1.53

All (96) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	2576	A	N1-C2-N3	-50.48	104.06	129.30
11	A	2576	A	C2-N3-C4	40.06	130.63	110.60
54	TA	52	PRO	N-CD-CG	-32.86	53.91	103.20
38	d	268	PRO	N-CD-CG	-28.97	59.74	103.20
39	e	62	PRO	N-CD-CG	-28.41	60.59	103.20
18	J	136	PRO	N-CD-CG	-25.46	65.00	103.20
11	A	2576	A	C6-N1-C2	21.47	131.48	118.60
39	e	62	PRO	CA-CB-CG	-21.04	64.02	104.00
54	TA	52	PRO	CA-CB-CG	-20.88	64.34	104.00
46	l	112	PRO	N-CD-CG	-19.63	73.76	103.20
17	I	66	PRO	N-CD-CG	-19.29	74.26	103.20
18	J	136	PRO	CA-CB-CG	-19.24	67.44	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	J	74	PRO	N-CD-CG	-18.81	74.98	103.20
18	J	74	PRO	CA-CB-CG	-17.21	71.30	104.00
45	k	62	PRO	N-CD-CG	-16.89	77.86	103.20
18	J	74	PRO	CB-CG-CD	16.65	171.43	106.50
18	J	136	PRO	N-CA-CB	-13.84	86.69	103.30
11	A	2576	A	N7-C8-N9	13.52	120.56	113.80
11	A	2576	A	C4-C5-N7	-13.16	104.12	110.70
18	J	31	PRO	CA-N-CD	-12.66	93.78	111.50
46	l	112	PRO	CA-CB-CG	-12.56	80.13	104.00
17	I	66	PRO	CA-CB-CG	-12.20	80.82	104.00
54	TA	52	PRO	N-CA-CB	-11.85	89.09	103.30
38	d	268	PRO	CA-CB-CG	-11.75	81.67	104.00
45	k	62	PRO	CA-CB-CG	-11.61	81.94	104.00
39	e	62	PRO	N-CA-CB	-11.37	89.66	103.30
46	l	112	PRO	CB-CG-CD	11.20	150.18	106.50
18	J	136	PRO	CB-CG-CD	-11.13	63.08	106.50
11	A	2576	A	N3-C4-N9	10.94	136.15	127.40
38	d	268	PRO	CB-CG-CD	-10.75	64.58	106.50
45	k	62	PRO	CA-N-CD	-10.63	96.62	111.50
7	6	241	PRO	CA-N-CD	-10.48	96.83	111.50
40	f	179	PRO	CA-N-CD	-10.05	97.43	111.50
11	A	2576	A	N3-C4-C5	-9.57	120.10	126.80
18	J	136	PRO	CA-N-CD	-9.53	98.16	111.50
11	A	2579	C	P-O3'-C3'	-9.42	108.40	119.70
17	I	66	PRO	CA-N-CD	-9.31	98.46	111.50
11	A	2580	U	P-O3'-C3'	-9.04	108.85	119.70
17	I	66	PRO	CB-CG-CD	8.90	141.21	106.50
7	6	228	PRO	CA-N-CD	-8.88	99.06	111.50
38	d	268	PRO	N-CA-CB	-8.75	92.80	103.30
7	6	184	LEU	CA-CB-CG	8.52	134.90	115.30
11	A	2576	A	C6-C5-N7	8.13	137.99	132.30
38	d	268	PRO	CA-N-CD	-7.58	100.88	111.50
39	e	62	PRO	CA-N-CD	-7.56	100.91	111.50
18	J	74	PRO	CA-N-CD	-7.23	101.38	111.50
18	J	31	PRO	N-CD-CG	-7.20	92.40	103.20
28	T	67	PRO	CA-N-CD	-7.03	101.65	111.50
39	e	62	PRO	CB-CG-CD	-6.78	80.06	106.50
19	K	175	ASP	CB-CG-OD1	6.78	124.40	118.30
46	l	112	PRO	CA-N-CD	-6.75	102.06	111.50
39	e	89	LEU	CA-CB-CG	6.65	130.59	115.30
39	e	65	PRO	CA-N-CD	-6.49	102.42	111.50
54	TA	52	PRO	CA-N-CD	-6.42	102.51	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	2069	U	C2-N1-C1'	6.35	125.32	117.70
41	g	116	ASP	CB-CG-OD2	6.18	123.86	118.30
50	q	129	PRO	CA-N-CD	-6.13	102.92	111.50
22	N	210	GLN	C-N-CA	-5.98	106.76	121.70
11	A	2484	C	C2-N1-C1'	5.91	125.31	118.80
11	A	2493	C	N1-C2-O2	5.88	122.43	118.90
11	A	2493	C	C2-N1-C1'	5.80	125.18	118.80
10	9	79	PRO	CA-N-CD	-5.73	103.47	111.50
11	A	1835	A	O4'-C1'-N9	5.73	112.78	108.20
11	A	2070	C	C2-N1-C1'	5.72	125.09	118.80
11	A	1837	C	C2-N1-C1'	5.65	125.02	118.80
11	A	2069	U	N1-C2-O2	5.64	126.75	122.80
38	d	267	PRO	C-N-CD	5.50	139.95	128.40
39	e	260	LEU	CA-CB-CG	5.50	127.95	115.30
49	p	191	LYS	CA-CB-CG	5.46	125.40	113.40
11	A	2724	G	P-O3'-C3'	-5.45	113.16	119.70
15	F	94	ASP	CB-CG-OD2	5.44	123.20	118.30
40	f	127	MET	CB-CG-SD	5.44	128.72	112.40
11	A	2069	U	N3-C2-O2	-5.42	118.41	122.20
8	7	238	ASP	CB-CG-OD1	5.41	123.17	118.30
11	A	2576	A	N9-C4-C5	-5.39	103.64	105.80
11	A	2484	C	N1-C2-O2	5.38	122.13	118.90
21	M	287	ASP	CB-CG-OD2	5.38	123.14	118.30
24	P	132	LEU	CA-CB-CG	5.27	127.42	115.30
11	A	2493	C	N3-C2-O2	-5.27	118.21	121.90
11	A	1902	C	C2-N1-C1'	5.26	124.59	118.80
11	A	1823	A	P-O3'-C3'	5.25	126.00	119.70
11	A	2079	C	C2-N1-C1'	5.22	124.55	118.80
11	A	2079	C	C6-N1-C2	-5.22	118.21	120.30
30	V	105	ARG	CG-CD-NE	5.20	122.72	111.80
11	A	1813	C	C2-N1-C1'	5.19	124.50	118.80
11	A	1902	C	N1-C2-O2	5.16	122.00	118.90
17	I	112	MET	CA-CB-CG	5.16	122.07	113.30
11	A	2457	A	P-O3'-C3'	5.15	125.88	119.70
11	A	3072	U	P-O3'-C3'	5.15	125.88	119.70
11	A	3170	C	N1-C2-O2	5.12	121.97	118.90
11	A	2898	U	C2-N1-C1'	5.08	123.80	117.70
39	e	238	LEU	CA-CB-CG	5.07	126.95	115.30
11	A	3170	C	C2-N1-C1'	5.06	124.37	118.80
15	F	81	ASP	CB-CG-OD1	5.04	122.83	118.30
11	A	2530	A	P-O3'-C3'	5.04	125.74	119.70
7	6	229	ASP	CB-CG-OD2	5.03	122.83	118.30

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
13	D	206	TYR	Peptide
14	E	316	PHE	Peptide
19	K	3	SER	Peptide
24	P	68	TRP	Peptide
33	Y	202	LEU	Peptide
34	Z	141	SER	Peptide
42	h	132	VAL	Peptide
42	h	82	LEU	Peptide
49	p	83	ARG	Peptide
50	q	78	SER	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	0	106/188 (56%)	94 (89%)	12 (11%)	0	100	100
2	1	50/65 (77%)	47 (94%)	3 (6%)	0	100	100
3	2	44/92 (48%)	43 (98%)	1 (2%)	0	100	100
4	3	93/188 (50%)	92 (99%)	1 (1%)	0	100	100
5	4	36/103 (35%)	35 (97%)	1 (3%)	0	100	100
6	5	391/423 (92%)	373 (95%)	16 (4%)	2 (0%)	25	45
7	6	352/380 (93%)	324 (92%)	28 (8%)	0	100	100
8	7	295/338 (87%)	279 (95%)	15 (5%)	1 (0%)	37	57
9	8	97/206 (47%)	91 (94%)	6 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	9	122/137 (89%)	116 (95%)	6 (5%)	0	100	100
13	D	237/305 (78%)	225 (95%)	11 (5%)	1 (0%)	30	50
14	E	304/348 (87%)	283 (93%)	20 (7%)	1 (0%)	37	57
15	F	248/311 (80%)	228 (92%)	20 (8%)	0	100	100
16	H	96/267 (36%)	87 (91%)	9 (9%)	0	100	100
17	I	177/261 (68%)	164 (93%)	13 (7%)	0	100	100
18	J	173/192 (90%)	162 (94%)	10 (6%)	1 (1%)	22	40
19	K	175/178 (98%)	157 (90%)	17 (10%)	1 (1%)	22	40
20	L	113/145 (78%)	103 (91%)	10 (9%)	0	100	100
21	M	285/296 (96%)	254 (89%)	30 (10%)	1 (0%)	30	50
22	N	220/251 (88%)	217 (99%)	3 (1%)	0	100	100
23	O	150/175 (86%)	132 (88%)	18 (12%)	0	100	100
24	P	141/179 (79%)	130 (92%)	10 (7%)	1 (1%)	19	36
25	Q	218/292 (75%)	211 (97%)	7 (3%)	0	100	100
26	R	138/149 (93%)	128 (93%)	10 (7%)	0	100	100
27	S	154/205 (75%)	147 (96%)	7 (4%)	0	100	100
28	T	164/212 (77%)	157 (96%)	7 (4%)	0	100	100
29	U	150/153 (98%)	144 (96%)	6 (4%)	0	100	100
30	V	204/216 (94%)	200 (98%)	4 (2%)	0	100	100
31	W	109/148 (74%)	103 (94%)	6 (6%)	0	100	100
32	X	241/256 (94%)	226 (94%)	15 (6%)	0	100	100
33	Y	174/250 (70%)	164 (94%)	10 (6%)	0	100	100
34	Z	118/161 (73%)	109 (92%)	9 (8%)	0	100	100
35	a	106/142 (75%)	103 (97%)	3 (3%)	0	100	100
36	b	146/155 (94%)	139 (95%)	7 (5%)	0	100	100
37	c	287/332 (86%)	265 (92%)	22 (8%)	0	100	100
38	d	255/306 (83%)	241 (94%)	14 (6%)	0	100	100
39	e	211/279 (76%)	194 (92%)	17 (8%)	0	100	100
40	f	144/194 (74%)	136 (94%)	8 (6%)	0	100	100
41	g	130/166 (78%)	121 (93%)	9 (7%)	0	100	100
42	h	108/158 (68%)	99 (92%)	9 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
43	i	95/128 (74%)	91 (96%)	4 (4%)	0	100	100
44	j	91/123 (74%)	87 (96%)	4 (4%)	0	100	100
45	k	94/112 (84%)	90 (96%)	4 (4%)	0	100	100
46	l	70/138 (51%)	62 (89%)	8 (11%)	0	100	100
47	m	43/128 (34%)	39 (91%)	4 (9%)	0	100	100
48	o	92/102 (90%)	86 (94%)	6 (6%)	0	100	100
49	p	148/206 (72%)	134 (90%)	14 (10%)	0	100	100
50	q	166/222 (75%)	154 (93%)	6 (4%)	6 (4%)	3	3
51	r	160/196 (82%)	150 (94%)	10 (6%)	0	100	100
52	s	391/439 (89%)	364 (93%)	27 (7%)	0	100	100
54	TA	43/198 (22%)	39 (91%)	4 (9%)	0	100	100
54	TB	25/198 (13%)	24 (96%)	1 (4%)	0	100	100
54	TC	69/198 (35%)	64 (93%)	5 (7%)	0	100	100
All	All	8449/11190 (76%)	7907 (94%)	527 (6%)	15 (0%)	45	65

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	5	70	LEU
24	P	69	ARG
50	q	43	GLU
50	q	132	ILE
19	K	160	GLN
21	M	288	GLU
14	E	317	PRO
6	5	72	PRO
50	q	42	PRO
50	q	128	MET
50	q	133	VAL
8	7	110	GLY
50	q	79	PRO
13	D	207	ILE
18	J	31	PRO

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	0	97/164 (59%)	91 (94%)	6 (6%)	15	31
2	1	49/60 (82%)	48 (98%)	1 (2%)	50	73
3	2	40/72 (56%)	39 (98%)	1 (2%)	42	67
4	3	88/166 (53%)	87 (99%)	1 (1%)	70	86
5	4	37/89 (42%)	32 (86%)	5 (14%)	3	5
6	5	353/368 (96%)	322 (91%)	31 (9%)	8	16
7	6	313/332 (94%)	289 (92%)	24 (8%)	10	21
8	7	272/303 (90%)	252 (93%)	20 (7%)	11	23
9	8	91/190 (48%)	83 (91%)	8 (9%)	8	16
10	9	104/112 (93%)	95 (91%)	9 (9%)	8	16
13	D	193/245 (79%)	173 (90%)	20 (10%)	5	10
14	E	260/290 (90%)	249 (96%)	11 (4%)	25	48
15	F	217/262 (83%)	207 (95%)	10 (5%)	23	44
16	H	88/228 (39%)	79 (90%)	9 (10%)	6	11
17	I	164/232 (71%)	149 (91%)	15 (9%)	7	15
18	J	138/150 (92%)	121 (88%)	17 (12%)	4	7
19	K	155/156 (99%)	150 (97%)	5 (3%)	34	59
20	L	98/124 (79%)	86 (88%)	12 (12%)	4	7
21	M	245/249 (98%)	238 (97%)	7 (3%)	37	62
22	N	189/211 (90%)	180 (95%)	9 (5%)	21	42
23	O	133/150 (89%)	126 (95%)	7 (5%)	19	38
24	P	125/154 (81%)	114 (91%)	11 (9%)	8	16
25	Q	202/256 (79%)	187 (93%)	15 (7%)	11	23
26	R	118/126 (94%)	113 (96%)	5 (4%)	25	48
27	S	141/180 (78%)	134 (95%)	7 (5%)	20	41
28	T	146/182 (80%)	137 (94%)	9 (6%)	15	31

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
29	U	125/135 (93%)	121 (97%)	4 (3%)	34	59
30	V	184/191 (96%)	167 (91%)	17 (9%)	7	14
31	W	91/119 (76%)	85 (93%)	6 (7%)	14	28
32	X	219/229 (96%)	207 (94%)	12 (6%)	18	37
33	Y	159/223 (71%)	148 (93%)	11 (7%)	13	26
34	Z	111/147 (76%)	105 (95%)	6 (5%)	18	37
35	a	101/133 (76%)	94 (93%)	7 (7%)	13	26
36	b	130/135 (96%)	124 (95%)	6 (5%)	23	44
37	c	253/288 (88%)	235 (93%)	18 (7%)	12	25
38	d	224/274 (82%)	207 (92%)	17 (8%)	11	22
39	e	188/236 (80%)	170 (90%)	18 (10%)	7	13
40	f	122/173 (70%)	110 (90%)	12 (10%)	6	12
41	g	122/148 (82%)	115 (94%)	7 (6%)	17	35
42	h	104/148 (70%)	92 (88%)	12 (12%)	4	8
43	i	86/110 (78%)	83 (96%)	3 (4%)	31	55
44	j	74/97 (76%)	68 (92%)	6 (8%)	9	19
45	k	81/90 (90%)	72 (89%)	9 (11%)	5	9
46	l	67/116 (58%)	64 (96%)	3 (4%)	23	45
47	m	40/113 (35%)	36 (90%)	4 (10%)	6	12
48	o	80/87 (92%)	77 (96%)	3 (4%)	28	52
49	p	134/181 (74%)	118 (88%)	16 (12%)	4	7
50	q	114/178 (64%)	100 (88%)	14 (12%)	4	7
51	r	147/169 (87%)	136 (92%)	11 (8%)	11	22
52	s	336/381 (88%)	319 (95%)	17 (5%)	20	40
54	TA	39/158 (25%)	36 (92%)	3 (8%)	10	21
54	TB	26/158 (16%)	24 (92%)	2 (8%)	10	21
All	All	7413/9468 (78%)	6894 (93%)	519 (7%)	15	25

All (519) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0	96	ASN
1	0	113	CYS

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Mol	Chain	Res	Type
1	0	153	THR
1	0	177	ARG
1	0	178	ASP
1	0	179	ARG
2	1	65	LEU
3	2	88	LYS
4	3	100	ARG
5	4	73	LYS
5	4	77	LYS
5	4	85	ARG
5	4	87	ARG
5	4	97	ARG
6	5	46	LEU
6	5	47	ASP
6	5	69	TRP
6	5	70	LEU
6	5	71	ARG
6	5	78	ASP
6	5	81	TYR
6	5	93	HIS
6	5	100	ASP
6	5	109	ARG
6	5	139	VAL
6	5	156	VAL
6	5	158	SER
6	5	173	GLU
6	5	175	TYR
6	5	199	ARG
6	5	208	PHE
6	5	222	ARG
6	5	233	ASP
6	5	243	GLU
6	5	248	LYS
6	5	255	PHE
6	5	259	SER
6	5	325	ARG
6	5	344	VAL
6	5	346	THR
6	5	364	ASP
6	5	369	VAL
6	5	371	ASN
6	5	406	LYS

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Mol	Chain	Res	Type
6	5	414	LEU
7	6	27	ARG
7	6	40	ILE
7	6	59	ARG
7	6	63	GLN
7	6	87	LYS
7	6	114	ARG
7	6	119	GLU
7	6	163	HIS
7	6	179	VAL
7	6	183	ASP
7	6	189	CYS
7	6	191	ASN
7	6	209	GLU
7	6	235	TRP
7	6	244	ARG
7	6	251	THR
7	6	261	ARG
7	6	274	LYS
7	6	284	ASP
7	6	288	SER
7	6	305	LYS
7	6	312	THR
7	6	329	TYR
7	6	370	ARG
8	7	43	MET
8	7	50	LYS
8	7	61	ARG
8	7	63	GLU
8	7	67	VAL
8	7	84	ASN
8	7	121	LYS
8	7	138	VAL
8	7	143	TRP
8	7	192	TRP
8	7	201	SER
8	7	228	GLU
8	7	238	ASP
8	7	243	LYS
8	7	250	ARG
8	7	295	ARG
8	7	307	ARG

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Mol	Chain	Res	Type
8	7	322	LYS
8	7	324	VAL
8	7	325	THR
9	8	109	GLU
9	8	113	ARG
9	8	139	MET
9	8	143	GLN
9	8	156	LYS
9	8	160	GLU
9	8	169	PHE
9	8	171	PHE
10	9	28	ARG
10	9	29	SER
10	9	31	ARG
10	9	48	TRP
10	9	71	LYS
10	9	87	THR
10	9	104	PHE
10	9	109	PHE
10	9	129	GLN
13	D	69	ARG
13	D	75	THR
13	D	79	MET
13	D	111	ARG
13	D	118	LYS
13	D	123	GLU
13	D	138	ASP
13	D	147	ARG
13	D	155	GLU
13	D	172	MET
13	D	177	ARG
13	D	191	THR
13	D	221	ASN
13	D	232	ARG
13	D	235	GLN
13	D	246	ARG
13	D	253	ASN
13	D	255	ARG
13	D	268	LYS
13	D	294	SER
14	E	69	ASP
14	E	77	LEU

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Mol	Chain	Res	Type
14	E	83	GLU
14	E	96	ARG
14	E	127	CYS
14	E	135	LYS
14	E	142	MET
14	E	266	ARG
14	E	303	LYS
14	E	322	ASP
14	E	336	ASN
15	F	50	LYS
15	F	52	GLU
15	F	60	ARG
15	F	81	ASP
15	F	110	SER
15	F	133	THR
15	F	194	GLU
15	F	210	ARG
15	F	214	ASP
15	F	220	ASP
16	H	53	THR
16	H	70	LYS
16	H	83	VAL
16	H	85	ASP
16	H	93	ASN
16	H	94	LEU
16	H	95	GLU
16	H	101	SER
16	H	136	ASN
17	I	43	GLN
17	I	50	VAL
17	I	83	ARG
17	I	94	ARG
17	I	95	MET
17	I	112	MET
17	I	117	ARG
17	I	120	LYS
17	I	158	GLU
17	I	160	LYS
17	I	170	THR
17	I	171	VAL
17	I	180	CYS
17	I	188	ARG

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Mol	Chain	Res	Type
17	I	202	LEU
18	J	35	LEU
18	J	51	LYS
18	J	54	ASN
18	J	68	THR
18	J	73	LYS
18	J	86	THR
18	J	89	TYR
18	J	90	PHE
18	J	104	THR
18	J	136	PRO
18	J	154	ARG
18	J	157	LYS
18	J	160	SER
18	J	169	LYS
18	J	174	PHE
18	J	187	GLU
18	J	191	LYS
19	K	25	MET
19	K	124	ARG
19	K	155	LEU
19	K	158	TYR
19	K	175	ASP
20	L	35	MET
20	L	38	VAL
20	L	39	ARG
20	L	48	ASN
20	L	51	TYR
20	L	53	ARG
20	L	62	LYS
20	L	101	ASP
20	L	105	VAL
20	L	118	ARG
20	L	125	THR
20	L	129	LYS
21	M	41	ARG
21	M	119	THR
21	M	128	THR
21	M	204	MET
21	M	219	ASN
21	M	222	TYR
21	M	258	THR

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Mol	Chain	Res	Type
22	N	41	ASP
22	N	68	ASN
22	N	104	MET
22	N	132	THR
22	N	163	MET
22	N	166	ARG
22	N	173	GLN
22	N	238	LYS
22	N	249	LYS
23	O	20	LEU
23	O	45	PRO
23	O	84	ASP
23	O	104	TYR
23	O	114	SER
23	O	138	ARG
23	O	144	LEU
24	P	40	GLU
24	P	51	ARG
24	P	56	LEU
24	P	69	ARG
24	P	84	ILE
24	P	110	TRP
24	P	114	LYS
24	P	126	GLU
24	P	141	ILE
24	P	156	ASP
24	P	179	TYR
25	Q	95	GLU
25	Q	98	ASP
25	Q	99	MET
25	Q	120	THR
25	Q	185	ASP
25	Q	198	SER
25	Q	204	MET
25	Q	214	LYS
25	Q	219	GLU
25	Q	244	ARG
25	Q	254	MET
25	Q	270	MET
25	Q	276	SER
25	Q	277	LYS
25	Q	289	SER

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Mol	Chain	Res	Type
26	R	13	ARG
26	R	26	LYS
26	R	29	ARG
26	R	95	VAL
26	R	149	HIS
27	S	71	GLU
27	S	103	SER
27	S	104	ARG
27	S	110	SER
27	S	129	ARG
27	S	134	LEU
27	S	161	ILE
28	T	47	ILE
28	T	72	GLU
28	T	84	LYS
28	T	87	MET
28	T	98	SER
28	T	133	ASN
28	T	157	ARG
28	T	191	THR
28	T	205	SER
29	U	97	VAL
29	U	129	MET
29	U	143	ARG
29	U	144	ARG
30	V	20	ARG
30	V	38	TRP
30	V	58	CYS
30	V	82	GLN
30	V	102	MET
30	V	104	TYR
30	V	118	ARG
30	V	137	PHE
30	V	145	ARG
30	V	149	ARG
30	V	163	ASP
30	V	166	VAL
30	V	177	THR
30	V	192	LYS
30	V	199	MET
30	V	200	GLU
30	V	209	LYS

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Mol	Chain	Res	Type
31	W	42	LEU
31	W	85	LYS
31	W	115	ASP
31	W	125	VAL
31	W	147	MET
31	W	148	LEU
32	X	35	GLU
32	X	39	THR
32	X	60	GLU
32	X	93	ASN
32	X	127	VAL
32	X	150	LYS
32	X	168	ARG
32	X	175	GLN
32	X	176	LEU
32	X	180	ASP
32	X	224	VAL
32	X	236	GLN
33	Y	69	ASP
33	Y	72	LYS
33	Y	78	LYS
33	Y	81	SER
33	Y	123	ARG
33	Y	143	ASP
33	Y	151	ASP
33	Y	169	ARG
33	Y	185	VAL
33	Y	228	ARG
33	Y	235	LEU
34	Z	44	LYS
34	Z	51	GLU
34	Z	62	ASN
34	Z	73	LYS
34	Z	118	ARG
34	Z	148	GLN
35	a	45	CYS
35	a	57	THR
35	a	70	GLU
35	a	88	HIS
35	a	102	HIS
35	a	114	LYS
35	a	122	ARG

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Mol	Chain	Res	Type
36	b	23	VAL
36	b	51	VAL
36	b	68	ARG
36	b	116	ARG
36	b	141	ARG
36	b	147	GLU
37	c	52	ARG
37	c	69	HIS
37	c	79	LEU
37	c	82	ASN
37	c	86	ASP
37	c	113	GLU
37	c	126	SER
37	c	131	SER
37	c	148	MET
37	c	150	THR
37	c	154	LYS
37	c	175	VAL
37	c	210	ARG
37	c	231	MET
37	c	238	MET
37	c	247	LYS
37	c	278	LYS
37	c	308	THR
38	d	40	ARG
38	d	47	GLN
38	d	73	ASP
38	d	74	ARG
38	d	81	THR
38	d	153	ASN
38	d	181	VAL
38	d	188	SER
38	d	193	HIS
38	d	203	MET
38	d	214	VAL
38	d	216	MET
38	d	244	GLU
38	d	250	LYS
38	d	273	LYS
38	d	288	LYS
38	d	292	GLU
39	e	62	PRO

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Mol	Chain	Res	Type
39	e	89	LEU
39	e	100	LYS
39	e	102	LYS
39	e	133	LEU
39	e	143	LYS
39	e	146	ARG
39	e	147	THR
39	e	152	LYS
39	e	174	PRO
39	e	216	LYS
39	e	235	LYS
39	e	243	PHE
39	e	256	THR
39	e	265	LYS
39	e	274	ARG
39	e	275	PHE
39	e	278	ASP
40	f	58	LYS
40	f	64	LYS
40	f	81	ASN
40	f	96	THR
40	f	100	MET
40	f	111	HIS
40	f	144	MET
40	f	149	VAL
40	f	160	SER
40	f	170	PHE
40	f	186	VAL
40	f	187	LYS
41	g	43	ASP
41	g	50	ARG
41	g	55	THR
41	g	68	THR
41	g	116	ASP
41	g	134	LYS
41	g	144	THR
42	h	50	LEU
42	h	58	ARG
42	h	70	LEU
42	h	85	ASN
42	h	92	GLU
42	h	94	SER

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Mol	Chain	Res	Type
42	h	95	ARG
42	h	96	LEU
42	h	115	SER
42	h	118	HIS
42	h	126	VAL
42	h	142	GLU
43	i	63	LEU
43	i	68	LYS
43	i	98	VAL
44	j	40	TYR
44	j	61	LYS
44	j	81	SER
44	j	89	GLN
44	j	102	GLN
44	j	110	LYS
45	k	8	LEU
45	k	18	VAL
45	k	31	ARG
45	k	44	SER
45	k	45	THR
45	k	47	LEU
45	k	68	PHE
45	k	92	SER
45	k	95	ARG
46	l	71	TYR
46	l	100	ASN
46	l	122	ARG
47	m	35	SER
47	m	36	SER
47	m	65	HIS
47	m	77	MET
48	o	15	ARG
48	o	82	PHE
48	o	93	ASP
49	p	40	LYS
49	p	41	SER
49	p	52	SER
49	p	60	ARG
49	p	96	ASN
49	p	102	ARG
49	p	118	LYS
49	p	138	GLU

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Mol	Chain	Res	Type
49	p	139	SER
49	p	156	ASP
49	p	159	THR
49	p	166	LYS
49	p	177	ARG
49	p	180	ILE
49	p	185	ARG
49	p	191	LYS
50	q	33	ARG
50	q	63	ARG
50	q	76	TRP
50	q	89	GLU
50	q	90	ARG
50	q	102	SER
50	q	117	ARG
50	q	123	GLU
50	q	127	LYS
50	q	129	PRO
50	q	131	MET
50	q	137	GLN
50	q	138	GLN
50	q	140	ARG
51	r	52	ARG
51	r	54	THR
51	r	58	LYS
51	r	62	ASN
51	r	103	LYS
51	r	113	ARG
51	r	116	GLU
51	r	119	VAL
51	r	134	ARG
51	r	139	VAL
51	r	144	LYS
52	s	43	ARG
52	s	104	ARG
52	s	118	LEU
52	s	138	ASP
52	s	143	ARG
52	s	158	ARG
52	s	169	SER
52	s	178	ASP
52	s	204	CYS

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Mol	Chain	Res	Type
52	s	228	ASP
52	s	245	LYS
52	s	266	CYS
52	s	284	VAL
52	s	318	ASP
52	s	351	VAL
52	s	397	GLN
52	s	410	VAL
54	TA	46	GLU
54	TA	86	LEU
54	TA	88	LYS
54	TB	67	LEU
54	TB	82	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	0	106	ASN
6	5	190	GLN
7	6	239	ASN
7	6	249	GLN
7	6	295	GLN
7	6	307	HIS
10	9	123	GLN
14	E	52	HIS
15	F	83	HIS
17	I	100	GLN
19	K	26	GLN
23	O	112	ASN
26	R	12	ASN
26	R	79	HIS
35	a	44	ASN
35	a	90	GLN
37	c	192	GLN
39	e	248	ASN
42	h	99	ASN
44	j	102	GLN
45	k	35	GLN
50	q	120	HIS
50	q	142	ASN
51	r	79	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
11	A	1523/1559 (97%)	360 (23%)	24 (1%)
12	B	51/72 (70%)	12 (23%)	1 (1%)
All	All	1574/1631 (96%)	372 (23%)	25 (1%)

All (372) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
11	A	1678	C
11	A	1679	U
11	A	1681	G
11	A	1689	C
11	A	1690	C
11	A	1699	C
11	A	1700	U
11	A	1704	U
11	A	1708	A
11	A	1709	G
11	A	1710	A
11	A	1711	C
11	A	1713	A
11	A	1714	C
11	A	1715	C
11	A	1716	U
11	A	1717	U
11	A	1724	A
11	A	1727	A
11	A	1728	U
11	A	1733	C
11	A	1734	C
11	A	1735	A
11	A	1736	A
11	A	1748	G
11	A	1750	G
11	A	1751	A
11	A	1761	A
11	A	1762	A
11	A	1763	A
11	A	1766	U
11	A	1767	G
11	A	1770	G
11	A	1781	A

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Mol	Chain	Res	Type
11	A	1782	G
11	A	1794	A
11	A	1803	A
11	A	1805	A
11	A	1806	U
11	A	1807	U
11	A	1808	A
11	A	1809	U
11	A	1810	A
11	A	1811	A
11	A	1817	C
11	A	1821	A
11	A	1823	A
11	A	1824	U
11	A	1827	C
11	A	1828	A
11	A	1829	A
11	A	1832	A
11	A	1836	A
11	A	1844	A
11	A	1849	C
11	A	1854	U
11	A	1856	A
11	A	1867	A
11	A	1869	A
11	A	1872	U
11	A	1878	U
11	A	1882	A
11	A	1883	G
11	A	1893	A
11	A	1901	C
11	A	1903	C
11	A	1918	G
11	A	1935	A
11	A	1936	A
11	A	1937	A
11	A	1938	A
11	A	1940	A
11	A	1944	C
11	A	1958	G
11	A	1968	G
11	A	1974	A

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Mol	Chain	Res	Type
11	A	1985	G
11	A	1987	G
11	A	1992	C
11	A	1993	A
11	A	1994	A
11	A	2000	C
11	A	2001	C
11	A	2015	G
11	A	2021	U
11	A	2022	G
11	A	2031	A
11	A	2036	C
11	A	2037	U
11	A	2038	U
11	A	2039	A
11	A	2060	A
11	A	2065	A
11	A	2066	C
11	A	2067	C
11	A	2069	U
11	A	2072	A
11	A	2074	A
11	A	2079	C
11	A	2083	U
11	A	2085	A
11	A	2093	U
11	A	2097	A
11	A	2098	G
11	A	2099	U
11	A	2105	G
11	A	2113	G
11	A	2125	C
11	A	2126	U
11	A	2134	A
11	A	2135	A
11	A	2141	U
11	A	2142	A
11	A	2147	G
11	A	2154	A
11	A	2158	U
11	A	2160	A
11	A	2161	A

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Mol	Chain	Res	Type
11	A	2163	A
11	A	2166	C
11	A	2169	A
11	A	2171	U
11	A	2172	A
11	A	2173	G
11	A	2177	U
11	A	2180	A
11	A	2181	A
11	A	2182	G
11	A	2183	C
11	A	2184	A
11	A	2187	C
11	A	2189	C
11	A	2192	A
11	A	2193	U
11	A	2198	A
11	A	2200	A
11	A	2202	C
11	A	2204	U
11	A	2210	C
11	A	2211	U
11	A	2215	C
11	A	2217	C
11	A	2218	C
11	A	2219	C
11	A	2220	A
11	A	2222	U
11	A	2224	C
11	A	2227	A
11	A	2228	A
11	A	2229	A
11	A	2230	A
11	A	2233	U
11	A	2237	A
11	A	2239	A
11	A	2241	A
11	A	2242	U
11	A	2245	A
11	A	2246	A
11	A	2250	A
11	A	2251	A

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Mol	Chain	Res	Type
11	A	2252	C
11	A	2260	A
11	A	2262	C
11	A	2263	C
11	A	2284	C
11	A	2297	A
11	A	2300	G
11	A	2322	C
11	A	2324	U
11	A	2332	C
11	A	2345	G
11	A	2350	A
11	A	2351	U
11	A	2356	A
11	A	2357	C
11	A	2360	U
11	A	2361	G
11	A	2362	A
11	A	2364	C
11	A	2365	U
11	A	2370	A
11	A	2371	U
11	A	2374	A
11	A	2381	A
11	A	2389	C
11	A	2390	A
11	A	2393	C
11	A	2401	A
11	A	2404	U
11	A	2407	U
11	A	2414	C
11	A	2415	C
11	A	2426	C
11	A	2434	A
11	A	2443	C
11	A	2444	A
11	A	2446	A
11	A	2447	A
11	A	2451	A
11	A	2458	A
11	A	2478	G
11	A	2479	C

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Mol	Chain	Res	Type
11	A	2484	C
11	A	2493	C
11	A	2502	C
11	A	2506	A
11	A	2507	A
11	A	2508	C
11	A	2511	C
11	A	2520	C
11	A	2521	A
11	A	2522	U
11	A	2523	C
11	A	2524	A
11	A	2527	A
11	A	2531	U
11	A	2540	C
11	A	2557	C
11	A	2558	A
11	A	2559	U
11	A	2560	G
11	A	2570	C
11	A	2575	U
11	A	2576	A
11	A	2578	C
11	A	2580	U
11	A	2592	G
11	A	2593	G
11	A	2594	U
11	A	2599	U
11	A	2601	A
11	A	2603	C
11	A	2607	U
11	A	2618	U
11	A	2626	U
11	A	2627	G
11	A	2629	A
11	A	2630	U
11	A	2632	A
11	A	2633	A
11	A	2634	U
11	A	2635	G
11	A	2645	G
11	A	2656	U

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Mol	Chain	Res	Type
11	A	2660	U
11	A	2683	C
11	A	2686	G
11	A	2694	A
11	A	2696	A
11	A	2706	A
11	A	2709	A
11	A	2718	C
11	A	2719	G
11	A	2723	A
11	A	2724	G
11	A	2725	A
11	A	2732	G
11	A	2739	U
11	A	2740	A
11	A	2745	A
11	A	2747	U
11	A	2750	U
11	A	2755	A
11	A	2756	C
11	A	2757	A
11	A	2758	G
11	A	2760	A
11	A	2792	A
11	A	2803	A
11	A	2804	A
11	A	2810	G
11	A	2814	G
11	A	2831	G
11	A	2832	A
11	A	2833	A
11	A	2842	C
11	A	2844	G
11	A	2847	C
11	A	2854	U
11	A	2864	U
11	A	2865	C
11	A	2881	C
11	A	2893	A
11	A	2906	C
11	A	2910	A
11	A	2912	C

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Mol	Chain	Res	Type
11	A	2913	A
11	A	2917	G
11	A	2918	A
11	A	2919	A
11	A	2922	A
11	A	2926	A
11	A	2928	C
11	A	2932	G
11	A	2935	A
11	A	2940	A
11	A	2956	A
11	A	2962	C
11	A	2963	A
11	A	2965	A
11	A	2985	C
11	A	2989	G
11	A	2990	A
11	A	2992	G
11	A	2993	U
11	A	2994	U
11	A	3005	A
11	A	3007	C
11	A	3016	G
11	A	3022	G
11	A	3041	U
11	A	3042	U
11	A	3043	C
11	A	3053	A
11	A	3054	G
11	A	3059	A
11	A	3060	C
11	A	3063	G
11	A	3069	A
11	A	3072	U
11	A	3073	C
11	A	3086	U
11	A	3093	C
11	A	3096	U
11	A	3097	U
11	A	3098	U
11	A	3100	U
11	A	3102	U

Continued on next page...

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Mol	Chain	Res	Type
11	A	3109	U
11	A	3113	A
11	A	3123	G
11	A	3124	U
11	A	3129	A
11	A	3141	A
11	A	3150	U
11	A	3155	C
11	A	3157	C
11	A	3158	A
11	A	3162	C
11	A	3168	C
11	A	3169	C
11	A	3172	C
11	A	3180	A
11	A	3189	C
11	A	3190	A
11	A	3196	G
11	A	3197	U
11	A	3199	U
11	A	3200	U
11	A	3201	A
11	A	3204	C
11	A	3207	A
11	A	3208	C
11	A	3210	C
11	A	3211	C
11	A	3212	C
11	A	3217	A
11	A	3218	A
11	A	3220	A
11	A	3228	U
12	B	1607	U
12	B	1608	G
12	B	1609	U
12	B	1611	G
12	B	1613	U
12	B	1614	U
12	B	1615	A
12	B	1625	A
12	B	1644	G
12	B	1645	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
12	B	1659	U
12	B	1669	G

All (25) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
11	A	1703	C
11	A	1709	G
11	A	1713	A
11	A	1805	A
11	A	1806	U
11	A	1807	U
11	A	1823	A
11	A	1871	A
11	A	2186	C
11	A	2245	A
11	A	2361	G
11	A	2457	A
11	A	2507	A
11	A	2530	A
11	A	2559	U
11	A	2606	U
11	A	2628	U
11	A	2905	A
11	A	2989	G
11	A	3041	U
11	A	3072	U
11	A	3092	U
11	A	3123	G
11	A	3196	G
12	B	1607	U

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 106 ligands modelled in this entry, 105 are monoatomic - leaving 1 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
57	ZLD	A	3400	56	26,26,26	0.88	1 (3%)	36,36,36	1.21	2 (5%)

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
57	ZLD	A	3400	56	-	2/13/33/33	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	A	3400	ZLD	C7-N4	-2.31	1.34	1.36

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	A	3400	ZLD	C6-C8-C9	4.30	118.25	113.38
57	A	3400	ZLD	O10-C7-O15	-2.63	119.32	122.40

There are no chirality outliers.

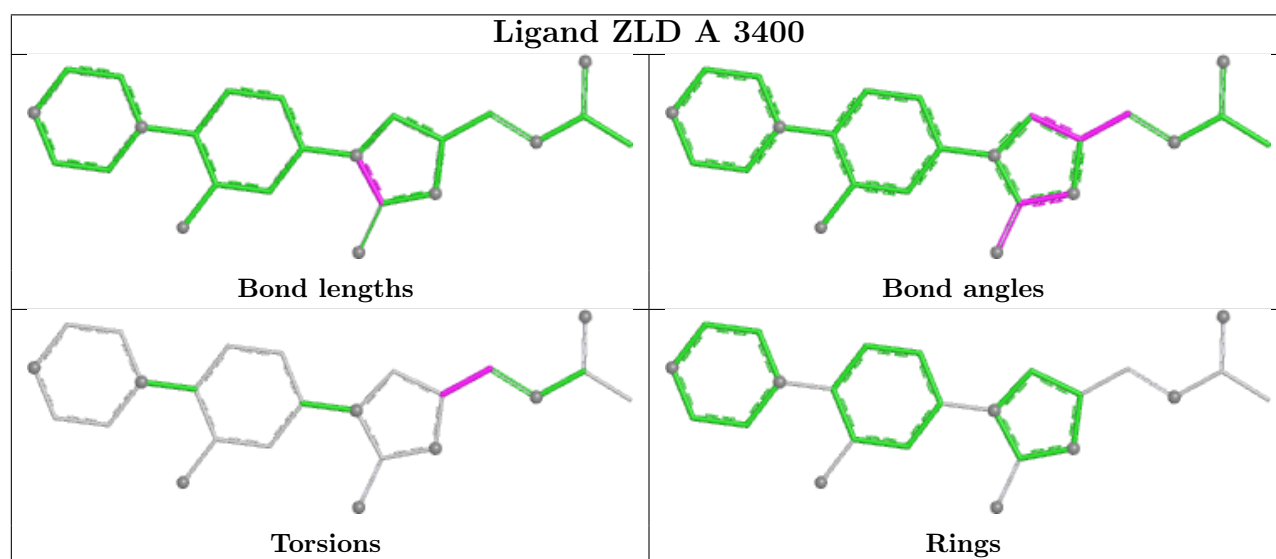
All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
57	A	3400	ZLD	C6-C8-C9-N11
57	A	3400	ZLD	O10-C8-C9-N11

There are no ring outliers.

No monomer is involved in short contacts.

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
53	u	4

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	u	414:UNK	C	601:UNK	N	50.73

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	u	106:UNK	C	301:UNK	N	32.84
1	u	315:UNK	C	399:UNK	N	24.40
1	u	615:UNK	C	700:UNK	N	14.68

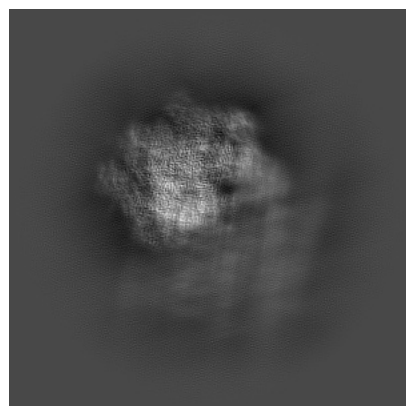
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-45757. These allow visual inspection of the internal detail of the map and identification of artifacts.

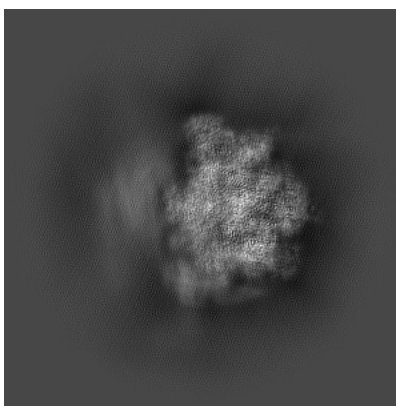
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

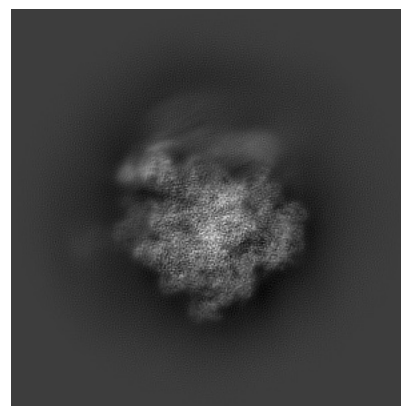
6.1.1 Primary map



X

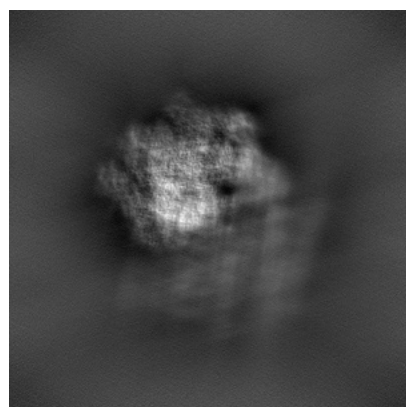


Y

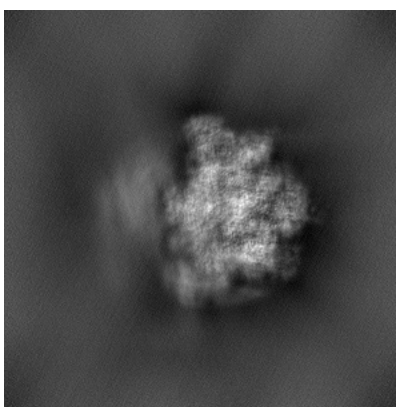


Z

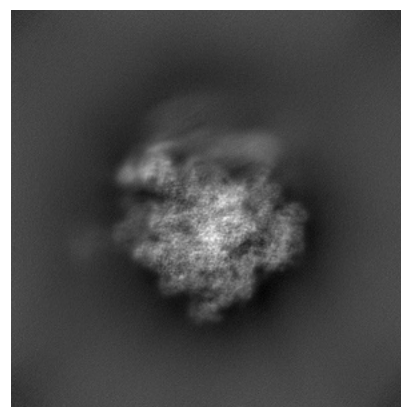
6.1.2 Raw map



X



Y

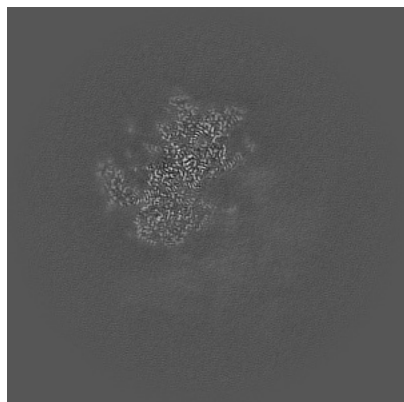


Z

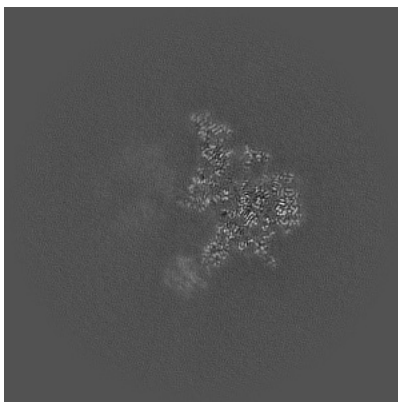
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

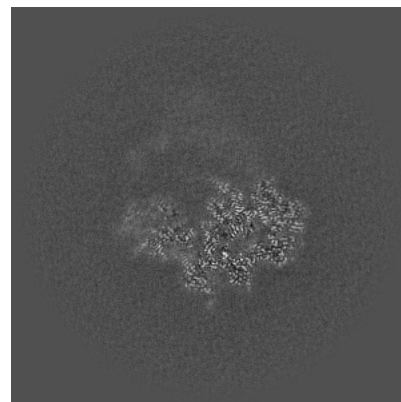
6.2.1 Primary map



X Index: 280

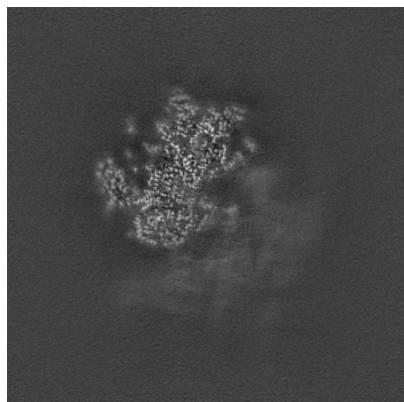


Y Index: 280

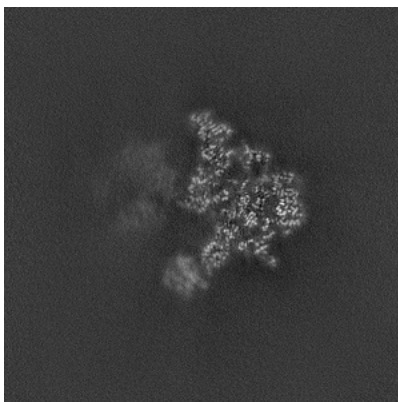


Z Index: 280

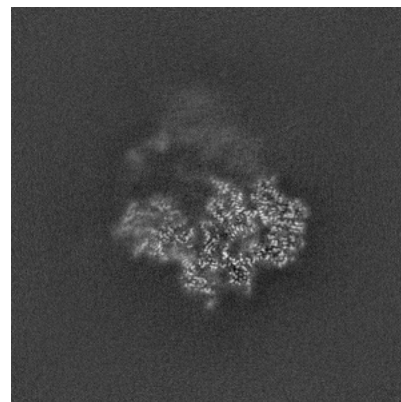
6.2.2 Raw map



X Index: 280



Y Index: 280

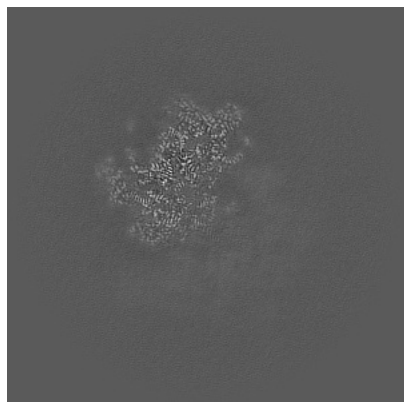


Z Index: 280

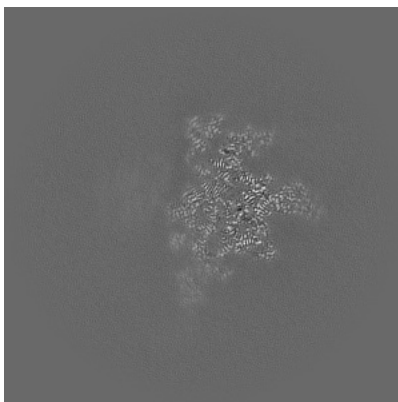
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

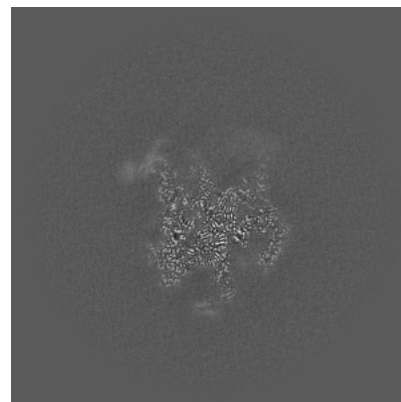
6.3.1 Primary map



X Index: 286

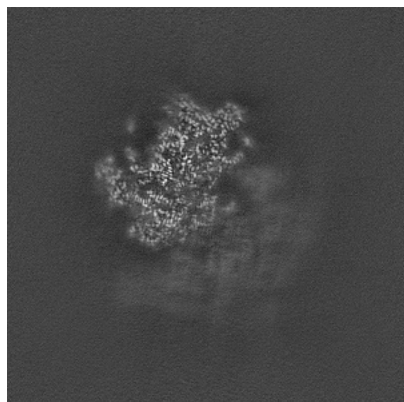


Y Index: 239

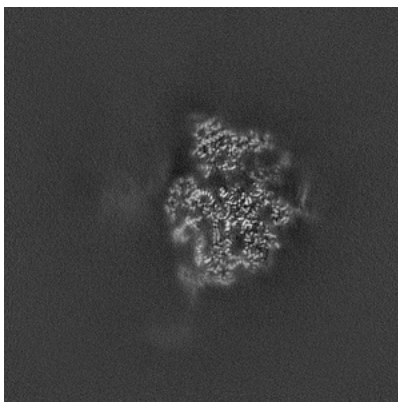


Z Index: 338

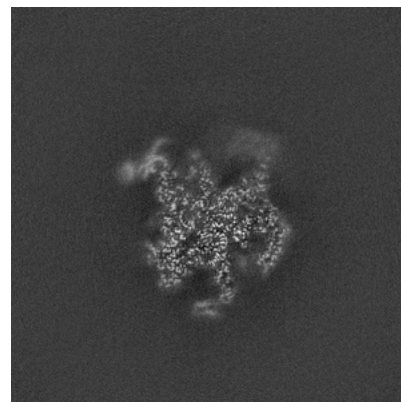
6.3.2 Raw map



X Index: 286



Y Index: 220

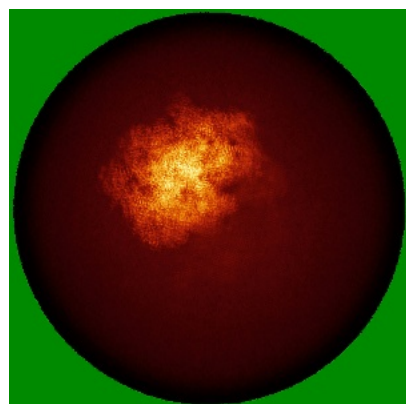


Z Index: 338

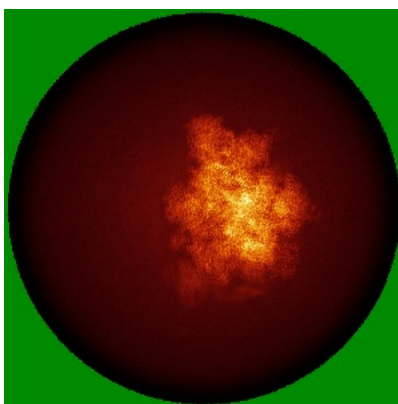
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) ⓘ

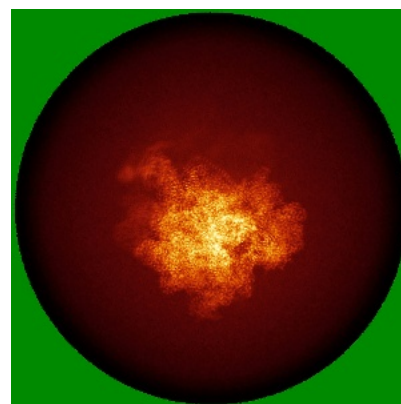
6.4.1 Primary map



X

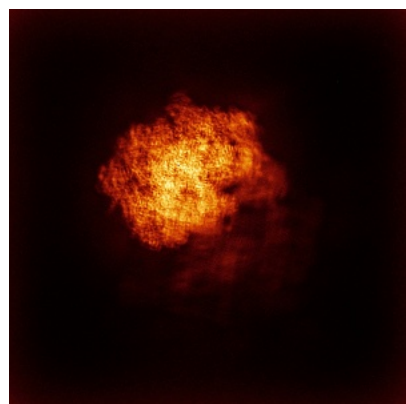


Y

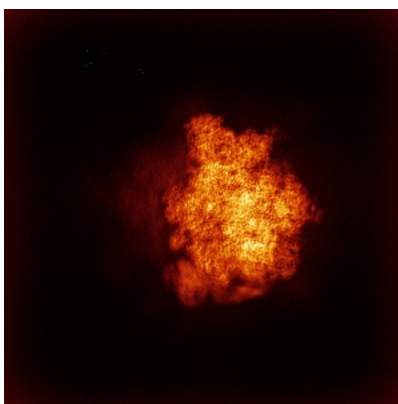


Z

6.4.2 Raw map



X



Y

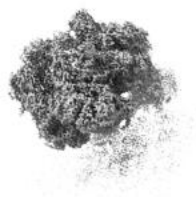


Z

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](#)

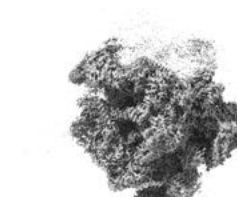
6.5.1 Primary map



X



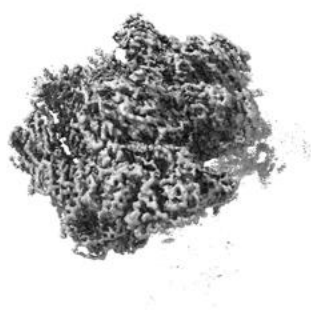
Y



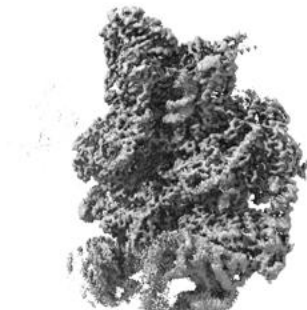
Z

The images above show the 3D surface view of the map at the recommended contour level 0.38. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 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.

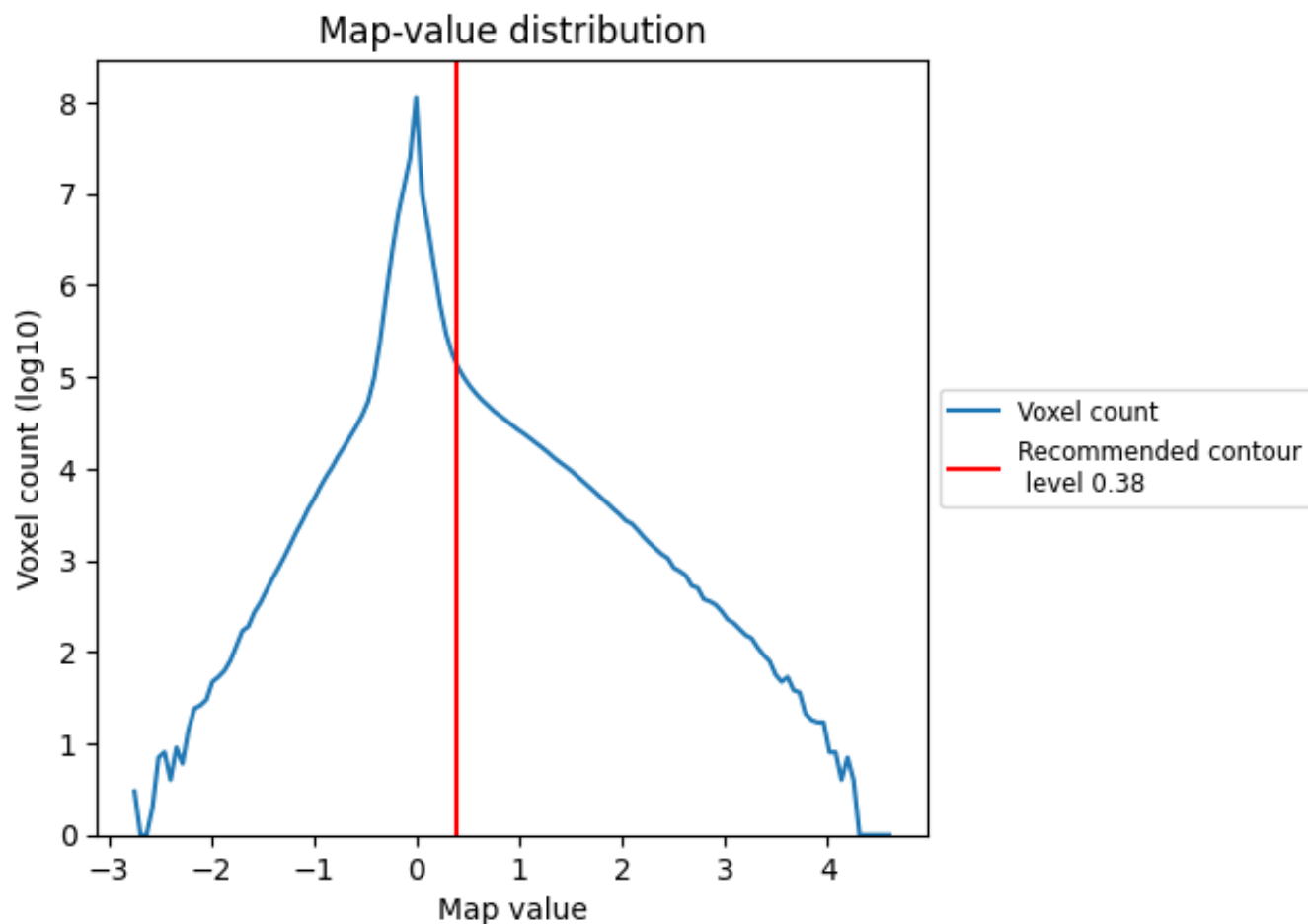
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

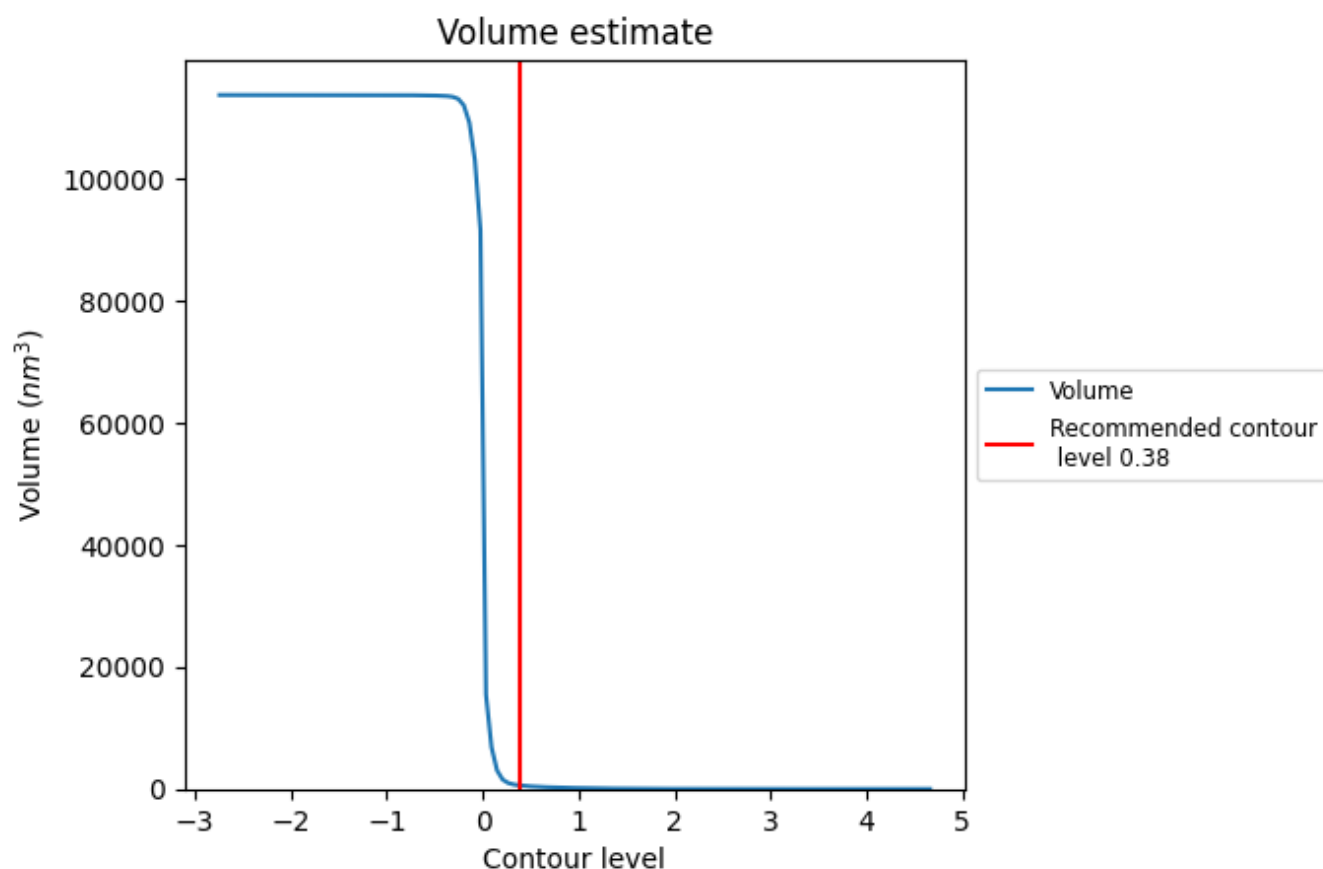
This section contains the results of statistical analysis of the map.

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.

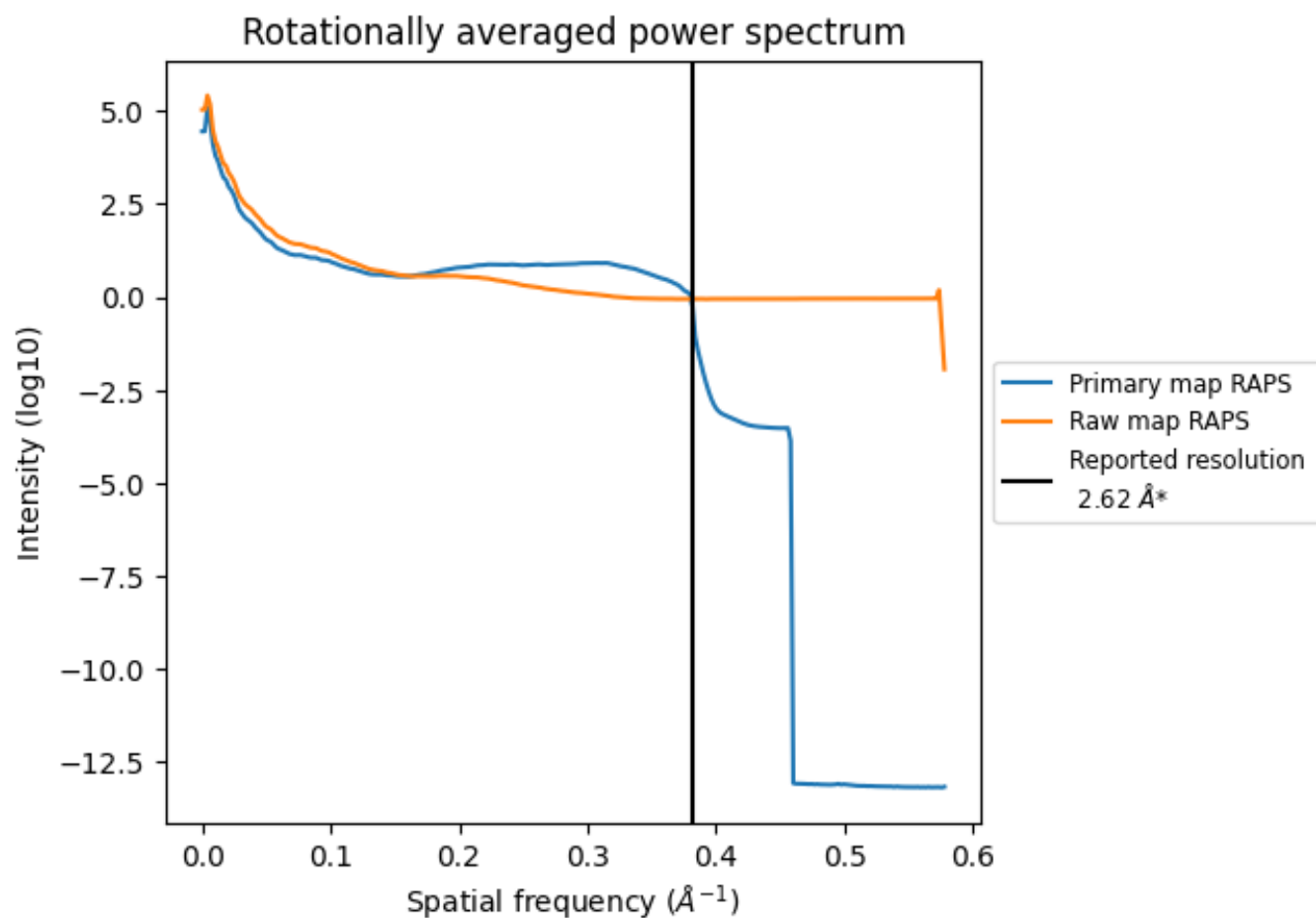
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 592 nm^3 ; this corresponds to an approximate mass of 535 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 ⓘ

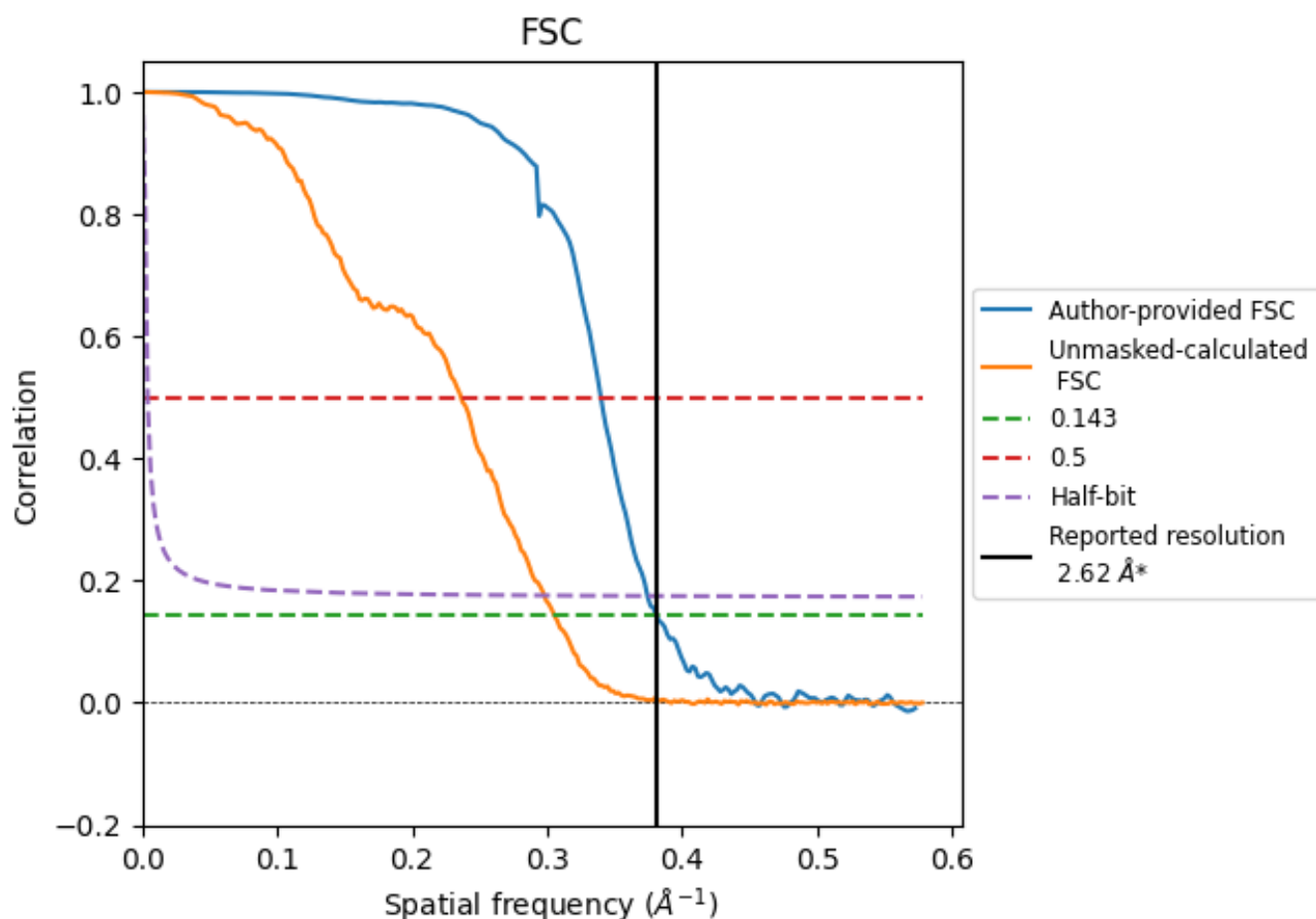


*Reported resolution corresponds to spatial frequency of 0.382 \AA^{-1}

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.382 \AA^{-1}

8.2 Resolution estimates [i](#)

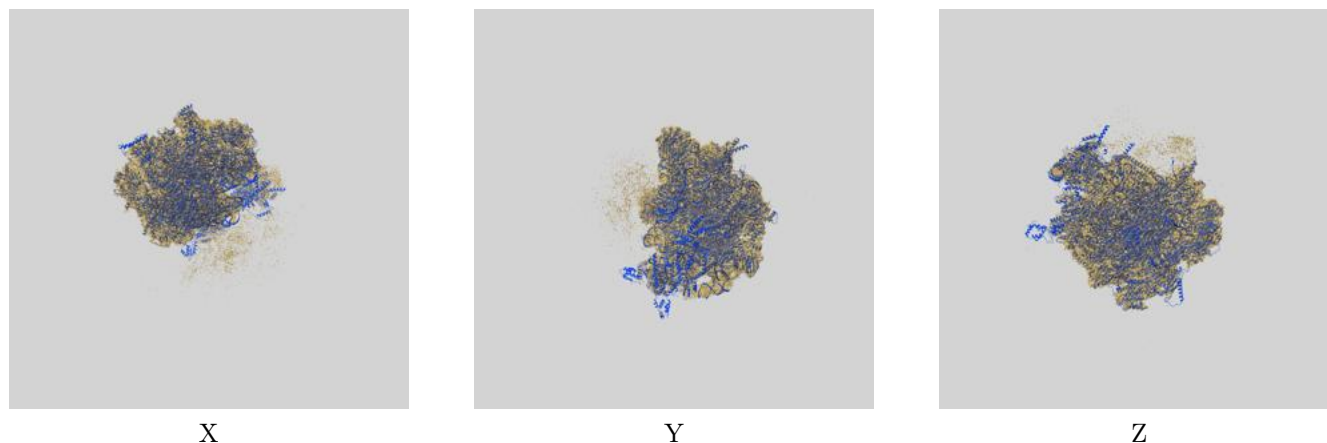
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.62	-	-
Author-provided FSC curve	2.62	2.94	2.67
Unmasked-calculated*	3.27	4.23	3.36

*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 3.27 differs from the reported value 2.62 by more than 10 %

9 Map-model fit [i](#)

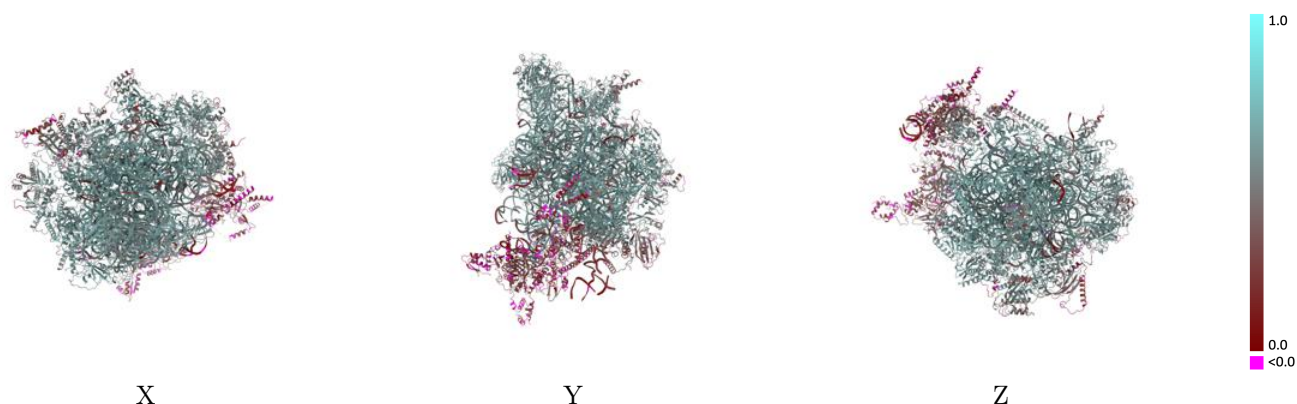
This section contains information regarding the fit between EMDB map EMD-45757 and PDB model 9CN3. Per-residue inclusion information can be found in section [3](#) on page [17](#).

9.1 Map-model overlay [i](#)



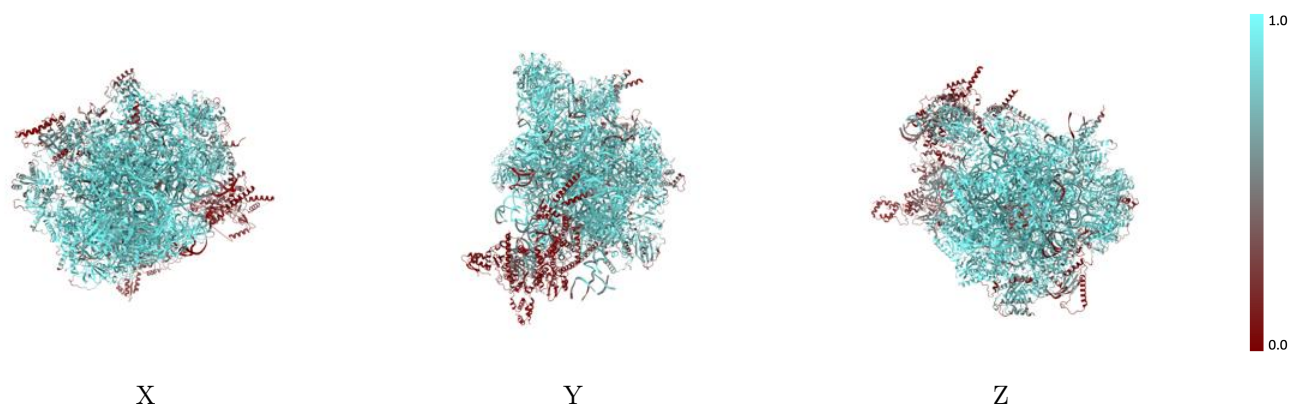
The images above show the 3D surface view of the map at the recommended contour level 0.38 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



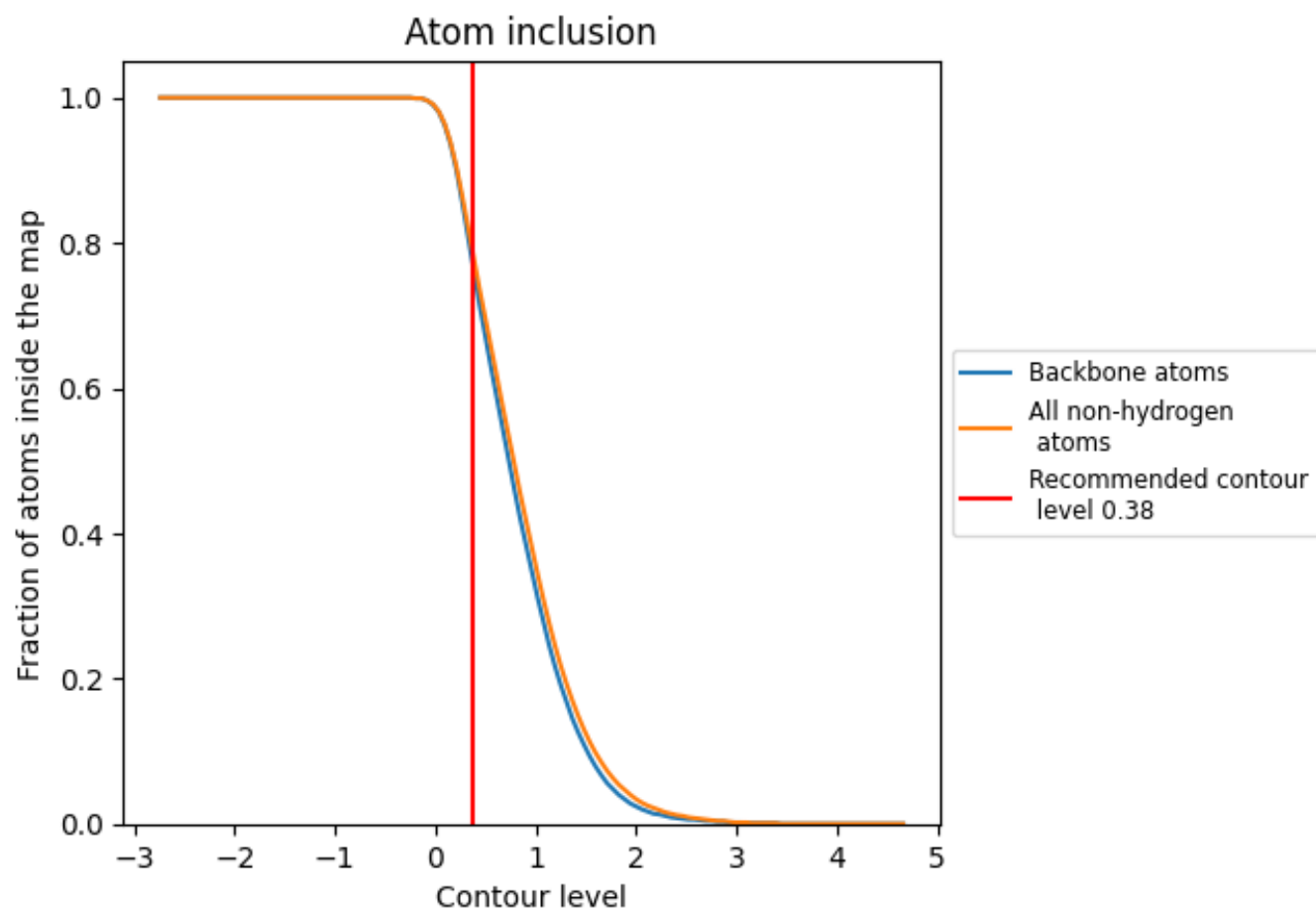
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.38).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 76% of all backbone atoms, 78% 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 (0.38) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7800	 0.5250
0	 0.8840	 0.5860
1	 0.8090	 0.5550
2	 0.9830	 0.6510
3	 0.9640	 0.6510
4	 0.9390	 0.6080
5	 0.8520	 0.5610
6	 0.7050	 0.4490
7	 0.7500	 0.5070
8	 0.1510	 0.1860
9	 0.7750	 0.5410
A	 0.8900	 0.5670
B	 0.6800	 0.2220
D	 0.8750	 0.5870
E	 0.8990	 0.5950
F	 0.9020	 0.6000
H	 0.7490	 0.5100
I	 0.3410	 0.2930
J	 0.1060	 0.1880
K	 0.9370	 0.6170
L	 0.8700	 0.5820
M	 0.8900	 0.5990
N	 0.8590	 0.5830
O	 0.9270	 0.6070
P	 0.8180	 0.5070
Q	 0.8540	 0.5870
R	 0.9320	 0.6180
S	 0.9500	 0.6200
T	 0.9220	 0.6250
TA	 0.0000	 0.1000
TB	 0.0000	 0.0950
TC	 0.0000	 0.0990
U	 0.7970	 0.5530
V	 0.5390	 0.4850
W	 0.9150	 0.6090



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Chain	Atom inclusion	Q-score
X	 0.8270	 0.5680
Y	 0.9100	 0.5990
Z	 0.9450	 0.6270
a	 0.7170	 0.5100
b	 0.9470	 0.6200
c	 0.8330	 0.5610
d	 0.4200	 0.4060
e	 0.0830	 0.1650
f	 0.2070	 0.2670
g	 0.9000	 0.5900
h	 0.5180	 0.4440
i	 0.9430	 0.6320
j	 0.8100	 0.5520
k	 0.3390	 0.2760
l	 0.2530	 0.3000
m	 0.1440	 0.1790
o	 0.9230	 0.6150
p	 0.5740	 0.4420
q	 0.5340	 0.4170
r	 0.8410	 0.5380
s	 0.8790	 0.5800
u	 0.0090	 0.0780