



wwPDB EM Validation Summary Report ⓘ

Nov 3, 2024 – 08:58 pm GMT

PDB ID : 8OM4
EMDB ID : EMD-16968
Title : Small subunit of yeast mitochondrial ribosome.
Authors : Itoh, Y.; Chicherin, I.; Kamenski, P.; Amunts, A.
Deposited on : 2023-03-31
Resolution : 2.32 Å(reported)
Based on initial model : 5MRC

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.dev113
Mogul : 1.8.4, CSD as541be (2020)
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) : 2.39

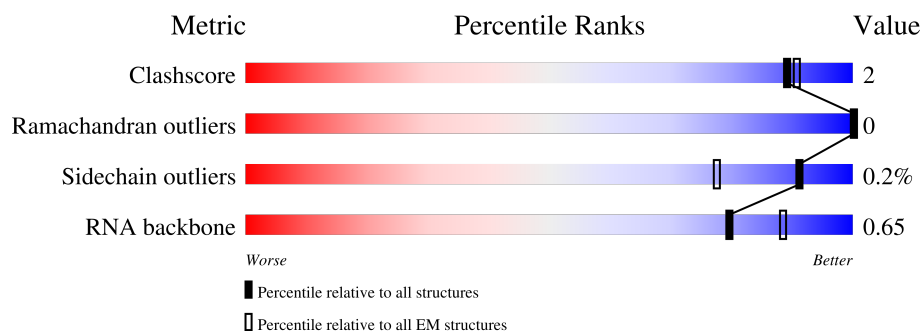
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.32 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)
Clashscore	210492	15764
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	A	344	<div> <div>28%</div> <div>78%</div> <div>10%</div> <div>13%</div> </div>
2	B	394	<div> <div>15%</div> <div>84%</div> <div>13%</div> </div>
3	C	398	<div> <div>19%</div> <div>88%</div> <div>6%</div> <div>7%</div> </div>
4	D	486	<div> <div>8%</div> <div>67%</div> <div>30%</div> </div>
5	E	307	<div> <div>93%</div> </div>
6	F	131	<div> <div>96%</div> </div>
7	G	247	<div> <div>17%</div> <div>76%</div> <div>6%</div> <div>18%</div> </div>

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Mol	Chain	Length	Quality of chain
8	H	155	
9	I	278	
10	J	203	
11	K	217	
12	L	153	
13	M	143	
14	N	115	
15	O	286	
16	P	121	
17	Q	237	
18	R	138	
19	S	91	
20	T	177	
21	U	264	
22	V	318	
23	W	450	
24	X	110	
25	Y	319	
26	Z	95	
27	1	111	
28	2	130	
29	3	266	
30	4	321	
31	5	339	
32	6	345	

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Mol	Chain	Length	Quality of chain
33	8	500	<div><div></div><div>18%</div><div></div><div>89%</div><div></div><div>7%</div></div>
34	r	1647	<div><div></div><div></div><div>80%</div><div>10%</div><div>10%</div></div>

2 Entry composition [i](#)

There are 39 unique types of molecules in this entry. The entry contains 166964 atoms, of which 74046 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 37S ribosomal protein MRP51, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	300	Total	C	H	N	O	S	1	0
			4908	1552	2481	427	441	7		

- Molecule 2 is a protein called 37S ribosomal protein MRP4, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	B	342	Total	C	H	N	O	S	0	0
			5436	1709	2722	467	535	3		

- Molecule 3 is a protein called Ribosomal protein VAR1, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	C	372	Total	C	H	N	O	S	0	0
			6181	1930	3091	553	574	33		

- Molecule 4 is a protein called 37S ribosomal protein NAM9, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	D	341	Total	C	H	N	O	S	0	0
			5729	1842	2896	499	487	5		

- Molecule 5 is a protein called 37S ribosomal protein S5, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	E	294	Total	C	H	N	O	S	0	0
			4708	1494	2360	418	428	8		

- Molecule 6 is a protein called 37S ribosomal protein MRP17, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	F	131	Total	C	H	N	O	S	0	0
			2184	671	1129	189	191	4		

- Molecule 7 is a protein called 37S ribosomal protein S7, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	G	203	Total	C	H	N	O	S	0	0
			3272	1019	1660	289	299	5		

- Molecule 8 is a protein called 37S ribosomal protein S8, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	H	155	Total	C	H	N	O	S	1	0
			2509	774	1286	219	221	9		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	1	ACE	-	acetylation	UNP Q03799

- Molecule 9 is a protein called 37S ribosomal protein S9, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	I	231	Total	C	H	N	O	S	1	0
			3783	1181	1925	334	338	5		

- Molecule 10 is a protein called 37S ribosomal protein S10, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	J	162	Total	C	H	N	O	S	0	0
			2655	853	1334	227	237	4		

- Molecule 11 is a protein called 37S ribosomal protein S18, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	K	151	Total	C	H	N	O	S	1	0
			2475	775	1266	213	215	6		

- Molecule 12 is a protein called 37S ribosomal protein S12, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	L	123	Total	C	H	N	O	S	0	0
			1932	579	993	192	164	4		

- Molecule 13 is a protein called 37S ribosomal protein SWS2, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	M	119	Total	C	H	N	O	S	0	0
			1937	591	1002	178	160	6		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	41	LEU	PHE	variant	UNP P53937

- Molecule 14 is a protein called 37S ribosomal protein MRP2, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
14	N	113	Total	C	H	N	O	S	0	0
			1917	596	986	179	152	4		

- Molecule 15 is a protein called 37S ribosomal protein S28, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
15	O	223	Total	C	H	N	O	S	0	0
			3668	1134	1853	334	339	8		

- Molecule 16 is a protein called 37S ribosomal protein S16, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
16	P	120	Total	C	H	N	O	S	0	0
			1963	604	1011	178	168	2		

- Molecule 17 is a protein called 37S ribosomal protein S17, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
17	Q	235	Total	C	H	N	O	S	1	0
			3944	1208	2014	356	361	5		

- Molecule 18 is a protein called 37S ribosomal protein RSM18, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
18	R	101	Total	C	H	N	O	S	0	0
			1671	507	853	162	145	4		

- Molecule 19 is a protein called 37S ribosomal protein S19, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
19	S	79	Total	C	H	N	O	S	0	0
			1277	404	648	114	109	2		

- Molecule 20 is a protein called 37S ribosomal protein MRP21, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
20	T	92	Total	C	H	N	O	S	1	0
			1569	483	800	150	131	5		

- Molecule 21 is a protein called 37S ribosomal protein S25, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
21	U	237	Total	C	H	N	O	S	0	0
			3868	1228	1929	339	365	7		

- Molecule 22 is a protein called 37S ribosomal protein PET123, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
22	V	286	Total	C	H	N	O	S	0	0
			4692	1450	2398	406	434	4		

- Molecule 23 is a protein called 37S ribosomal protein S23, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
23	W	402	Total	C	H	N	O	S	0	0
			6555	2078	3329	542	598	8		

- Molecule 24 is a protein called Mitochondrial 37S ribosomal protein S27.

Mol	Chain	Residues	Atoms						AltConf	Trace
24	X	98	Total	C	H	N	O	S	0	0
			1619	503	832	142	139	3		

- Molecule 25 is a protein called 37S ribosomal protein S24, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
25	Y	272	Total	C	H	N	O	S	0	0
			4514	1436	2241	408	425	4		

- Molecule 26 is a protein called 37S ribosomal protein MRP10, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
26	Z	92	Total	C	H	N	O	S	0	0
			1487	459	758	137	127	6		

- Molecule 27 is a protein called Mitochondrial mRNA-processing protein COX24.

Mol	Chain	Residues	Atoms						AltConf	Trace
27	1	31	Total	C	H	N	O	S	0	0
			613	170	334	68	39	2		

- Molecule 28 is a protein called Protein FYV4, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
28	2	102	Total	C	H	N	O	S	0	0
			1724	544	866	161	152	1		

- Molecule 29 is a protein called 37S ribosomal protein S26, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
29	3	257	Total	C	H	N	O	S	0	0
			4103	1326	2040	349	383	5		

- Molecule 30 is a protein called 37S ribosomal protein MRP1, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
30	4	303	Total	C	H	N	O	S	0	0
			4859	1538	2423	422	466	10		

- Molecule 31 is a protein called 37S ribosomal protein MRP13, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
31	5	291	Total	C	H	N	O	S	0	0
			4770	1524	2409	404	429	4		

- Molecule 32 is a protein called 37S ribosomal protein S35, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
32	6	319	Total	C	H	N	O	S	0	0
			5208	1646	2615	467	474	6		

- Molecule 33 is a protein called 3-hydroxyisobutyryl-CoA hydrolase, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
33	8	467	Total	C	H	N	O	S	0	0
			7371	2341	3681	621	708	20		

- Molecule 34 is a RNA chain called 15S mitochondrial rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
34	r	1487	Total	C	H	N	O	P	1	0
			47450	14212	15844	5580	10326	1488		

- Molecule 35 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
35	B	1	Total	Mg	0
			1	1	
35	K	1	Total	Mg	0
			1	1	
35	W	1	Total	Mg	0
			1	1	
35	r	86	Total	Mg	0
			86	86	

- Molecule 36 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
36	D	1	Total	K	0
			1	1	
36	M	1	Total	K	0
			1	1	
36	r	35	Total	K	0
			35	35	

- Molecule 37 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: C₂₄H₄₆O₁₁).



Mol	Chain	Residues	Atoms				AltConf
37	O	1	Total	C	H	O	0
			38	12	25	1	

- Molecule 38 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $\text{C}_{10}\text{H}_{16}\text{N}_5\text{O}_{13}\text{P}_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
38	W	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	

- Molecule 39 is water.

Mol	Chain	Residues	Atoms		AltConf
39	A	58	Total 58	O 58	0
39	B	148	Total 148	O 148	0
39	C	19	Total 19	O 19	0
39	D	112	Total 112	O 112	0
39	E	144	Total 144	O 144	0
39	F	18	Total 18	O 18	0
39	G	24	Total 24	O 24	0
39	H	83	Total 83	O 83	0
39	I	58	Total 58	O 58	0
39	J	42	Total 42	O 42	0
39	K	11	Total 11	O 11	0
39	L	38	Total 38	O 38	0
39	M	12	Total 12	O 12	0
39	N	39	Total 39	O 39	0
39	O	55	Total 55	O 55	0
39	P	70	Total 70	O 70	0
39	Q	20	Total 20	O 20	0
39	R	15	Total 15	O 15	0
39	S	8	Total 8	O 8	0
39	T	44	Total 44	O 44	0
39	U	87	Total 87	O 87	0
39	V	34	Total 34	O 34	0

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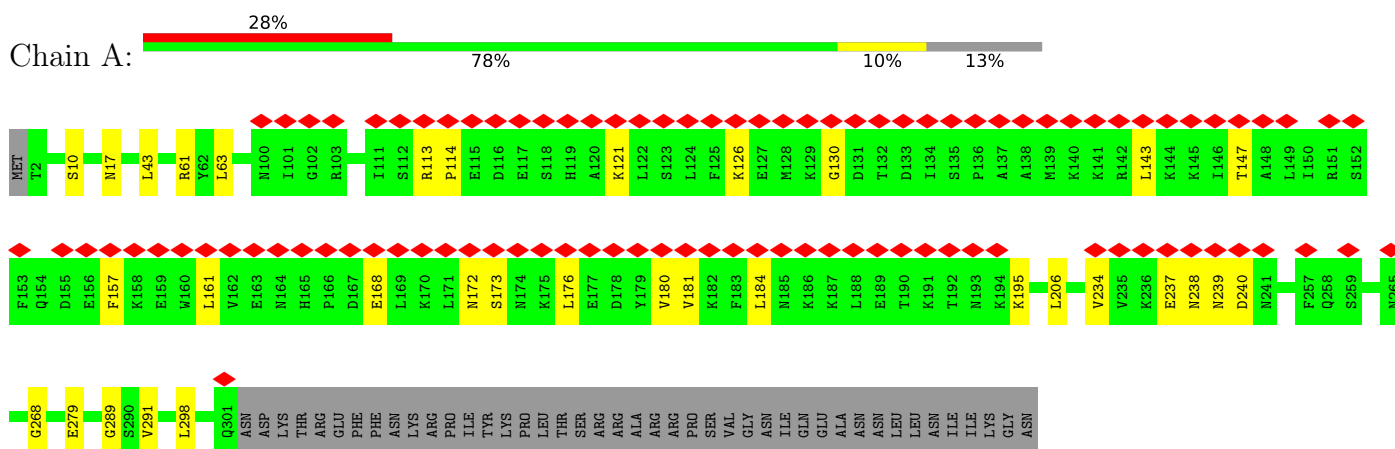
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Mol	Chain	Residues	Atoms		AltConf
39	W	93	Total 93	O 93	0
39	X	9	Total 9	O 9	0
39	Y	46	Total 46	O 46	0
39	Z	25	Total 25	O 25	0
39	1	14	Total 14	O 14	0
39	2	22	Total 22	O 22	0
39	3	31	Total 31	O 31	0
39	4	3	Total 3	O 3	0
39	5	3	Total 3	O 3	0
39	6	69	Total 69	O 69	0
39	8	41	Total 41	O 41	0
39	r	2711	Total 2711	O 2711	0

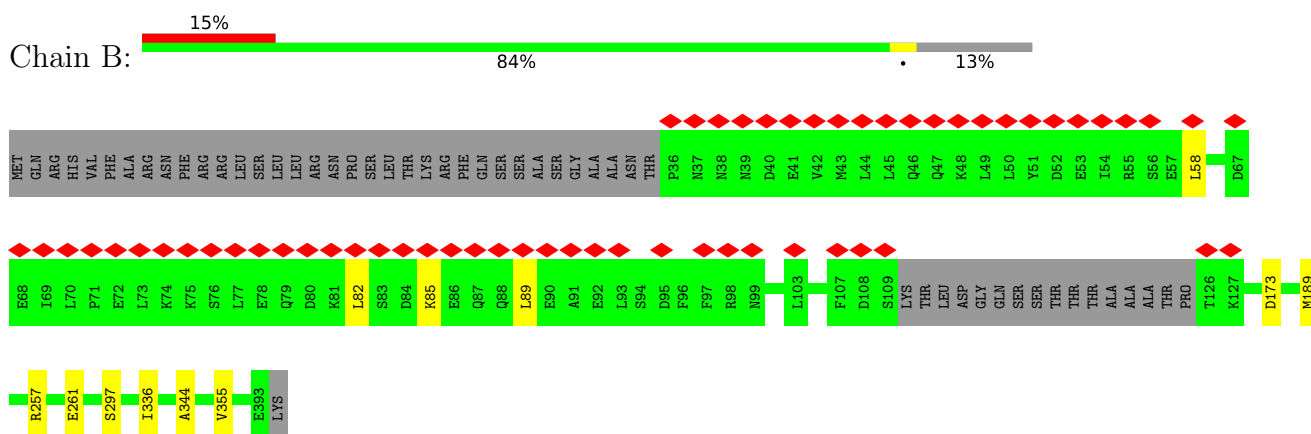
3 Residue-property plots

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.

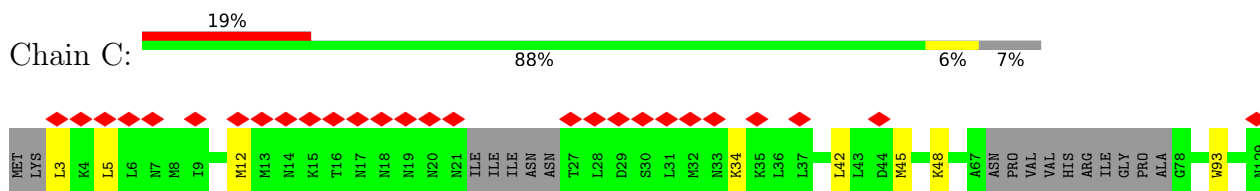
- Molecule 1: 37S ribosomal protein MRP51, mitochondrial

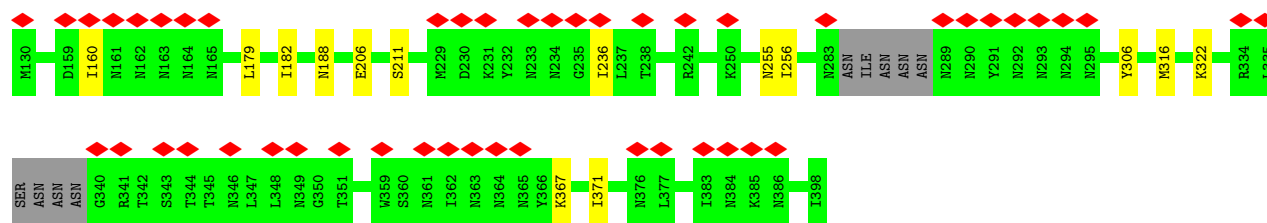


- Molecule 2: 37S ribosomal protein MRP4, mitochondrial

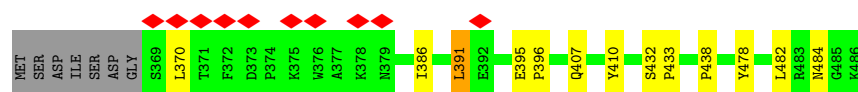
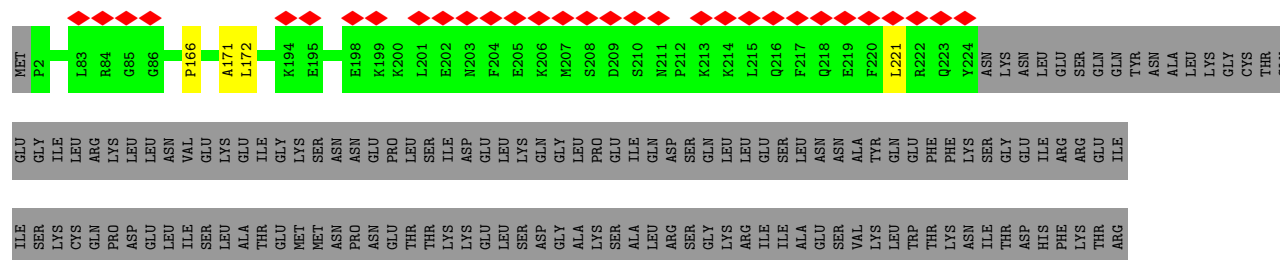


- Molecule 3: Ribosomal protein VAR1, mitochondrial

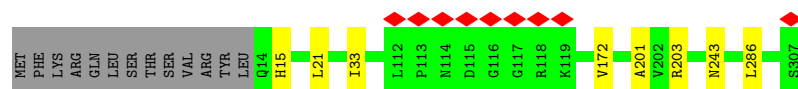




- Molecule 4: 37S ribosomal protein NAM9, mitochondrial



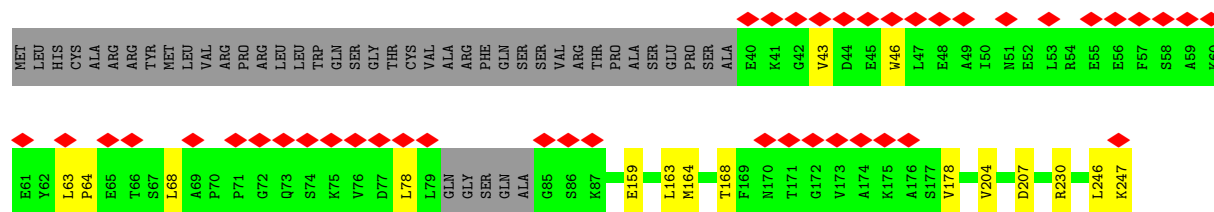
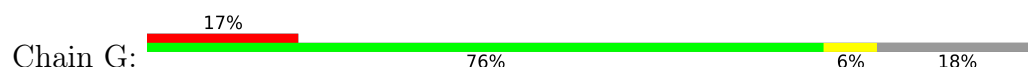
- Molecule 5: 37S ribosomal protein S5, mitochondrial



- Molecule 6: 37S ribosomal protein MRP17, mitochondrial

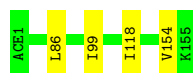


- Molecule 7: 37S ribosomal protein S7, mitochondrial



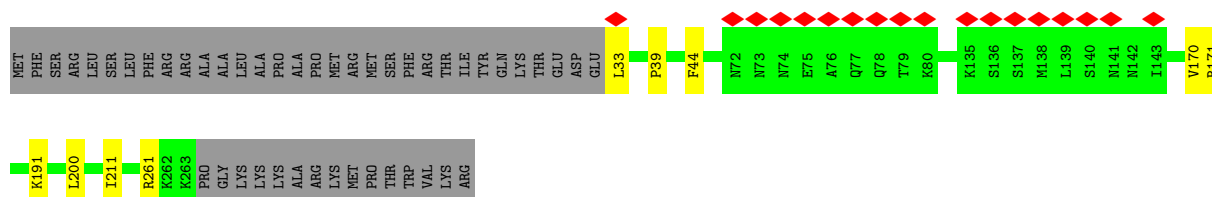
- Molecule 8: 37S ribosomal protein S8, mitochondrial

Chain H:  97%




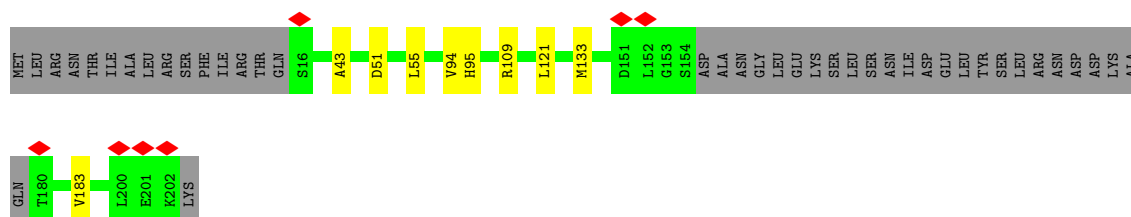
- Molecule 9: 37S ribosomal protein S9, mitochondrial

Chain I:  6% 80% 17%



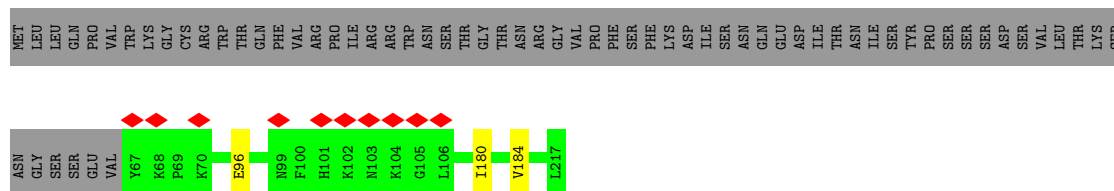
- Molecule 10: 37S ribosomal protein S10, mitochondrial

Chain J:  75% 20%




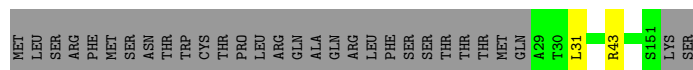
- Molecule 11: 37S ribosomal protein S18, mitochondrial

Chain K:  5% 68% 30%




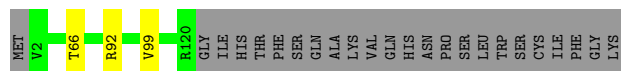
- Molecule 12: 37S ribosomal protein S12, mitochondrial

Chain L:  79% 20%



- Molecule 13: 37S ribosomal protein SWS2, mitochondrial

Chain M:  81% 17%



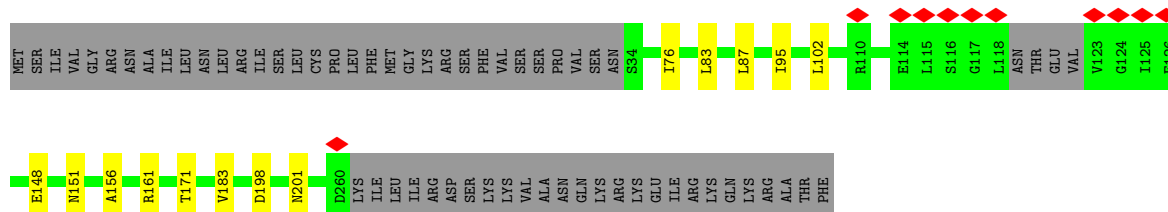
- Molecule 14: 37S ribosomal protein MRP2, mitochondrial

Chain N:  96%



- Molecule 15: 37S ribosomal protein S28, mitochondrial

Chain O:  73% 5% 22%




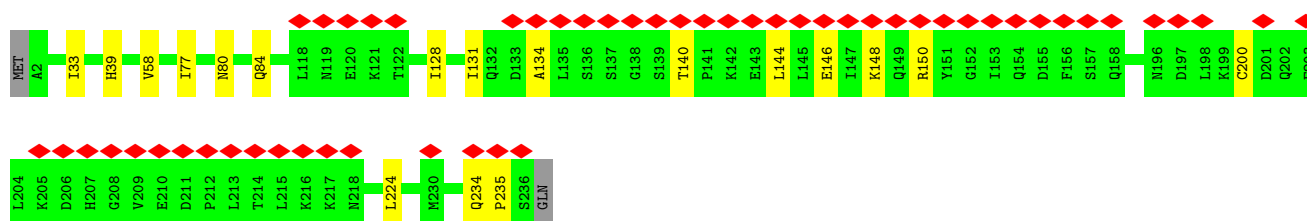
- Molecule 16: 37S ribosomal protein S16, mitochondrial

Chain P:  97%



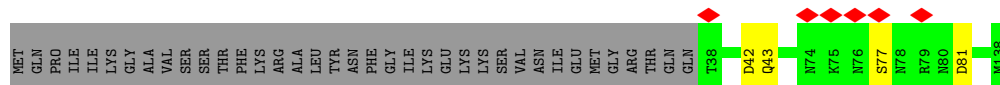
- Molecule 17: 37S ribosomal protein S17, mitochondrial

Chain Q:  23% 92% 8%




- Molecule 18: 37S ribosomal protein RSM18, mitochondrial

Chain R:  70% 27%

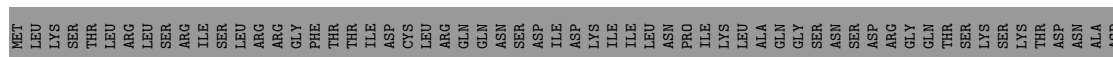


- Molecule 19: 37S ribosomal protein S19, mitochondrial

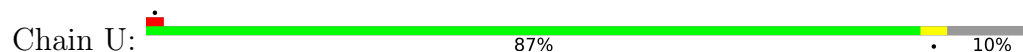
Chain S:  82% 13%



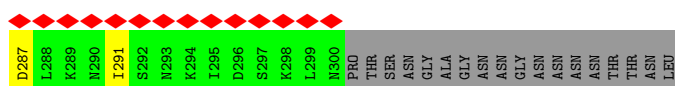
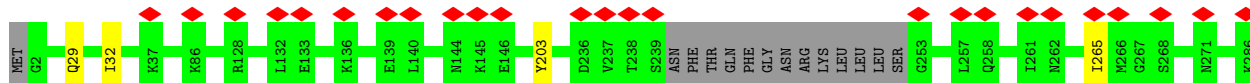
- Molecule 20: 37S ribosomal protein MRP21, mitochondrial



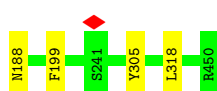
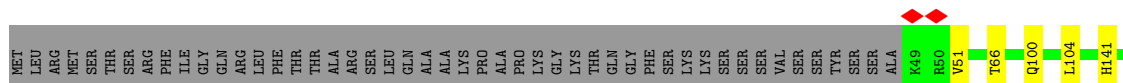
- Molecule 21: 37S ribosomal protein S25, mitochondrial



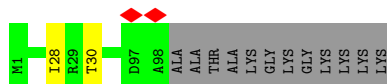
- Molecule 22: 37S ribosomal protein PET123, mitochondrial



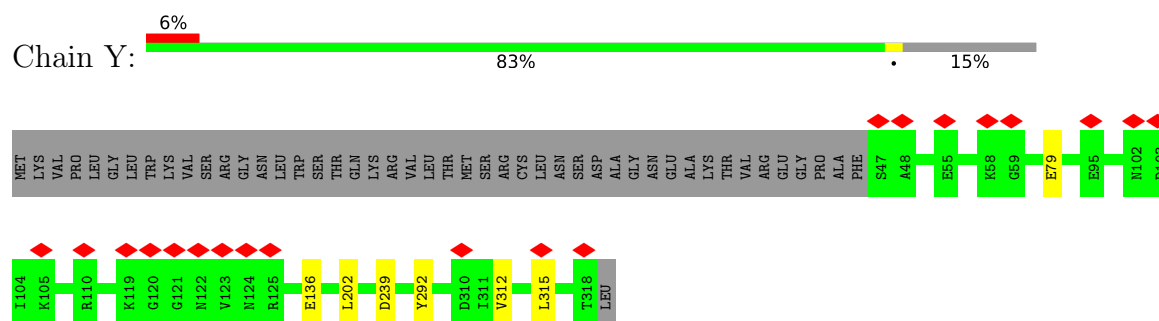
- Molecule 23: 37S ribosomal protein S23, mitochondrial



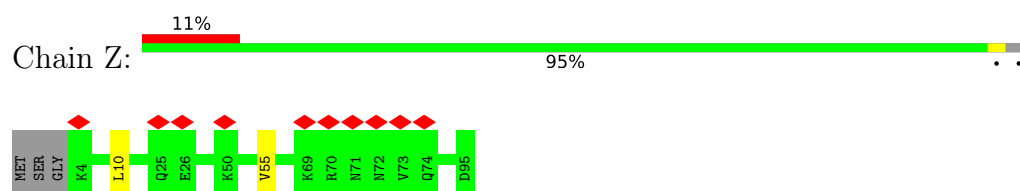
- Molecule 24: Mitochondrial 37S ribosomal protein S27



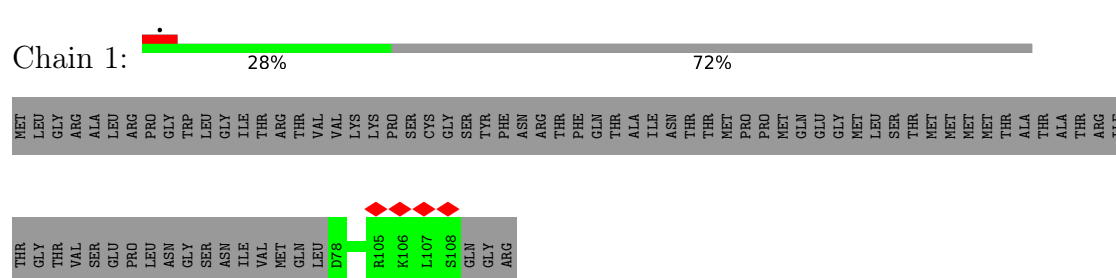
- Molecule 25: 37S ribosomal protein S24, mitochondrial



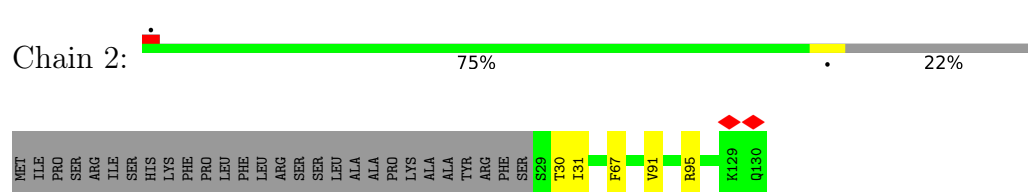
- Molecule 26: 37S ribosomal protein MRP10, mitochondrial



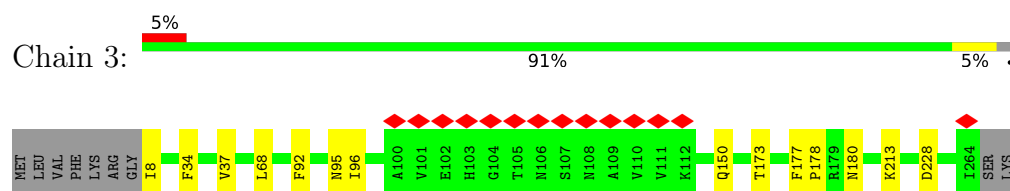
- Molecule 27: Mitochondrial mRNA-processing protein COX24



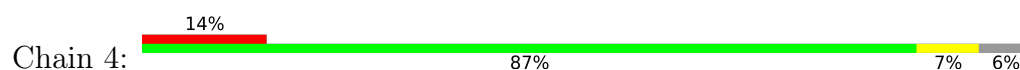
- Molecule 28: Protein FYV4, mitochondrial

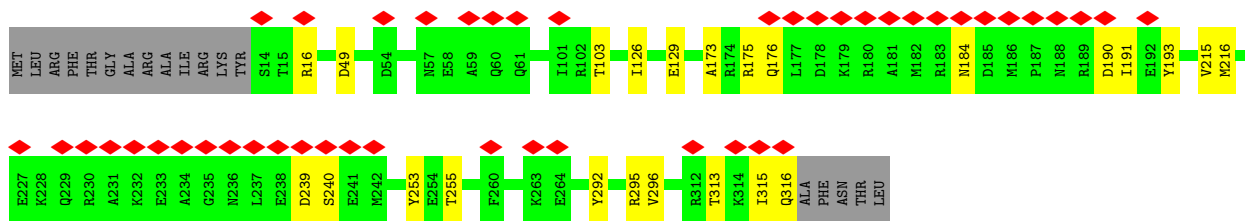


- Molecule 29: 37S ribosomal protein S26, mitochondrial

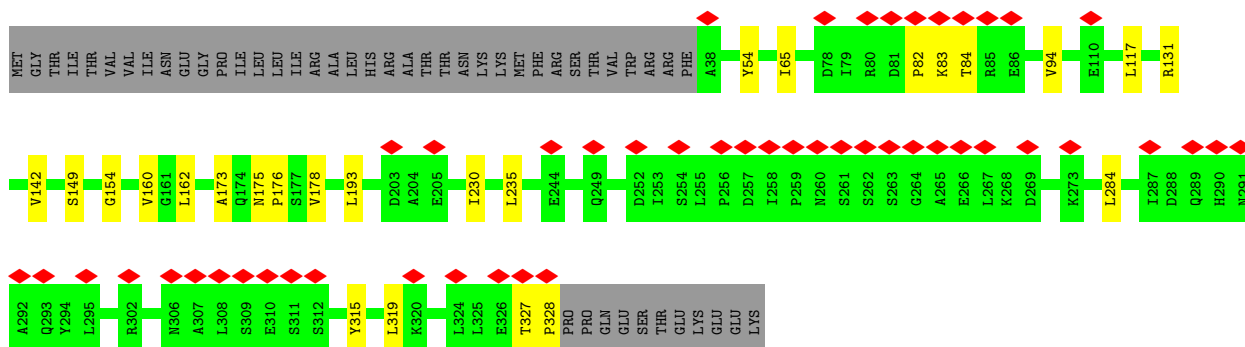
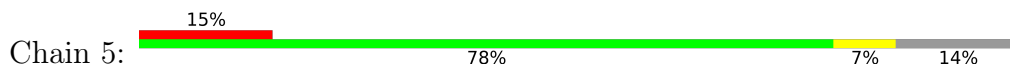


- Molecule 30: 37S ribosomal protein MRP1, mitochondrial

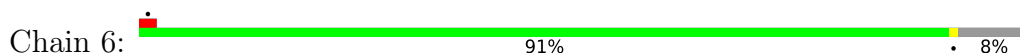




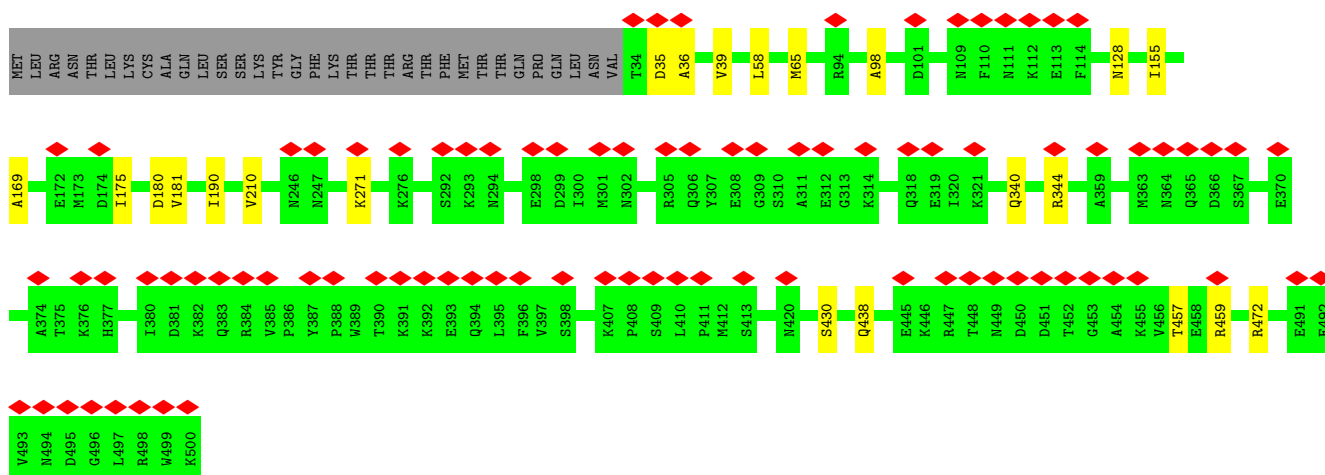
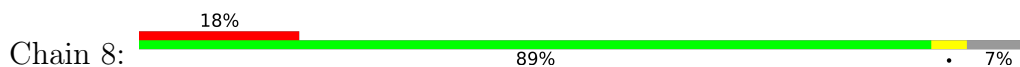
- Molecule 31: 37S ribosomal protein MRP13, mitochondrial



- Molecule 32: 37S ribosomal protein S35, mitochondrial

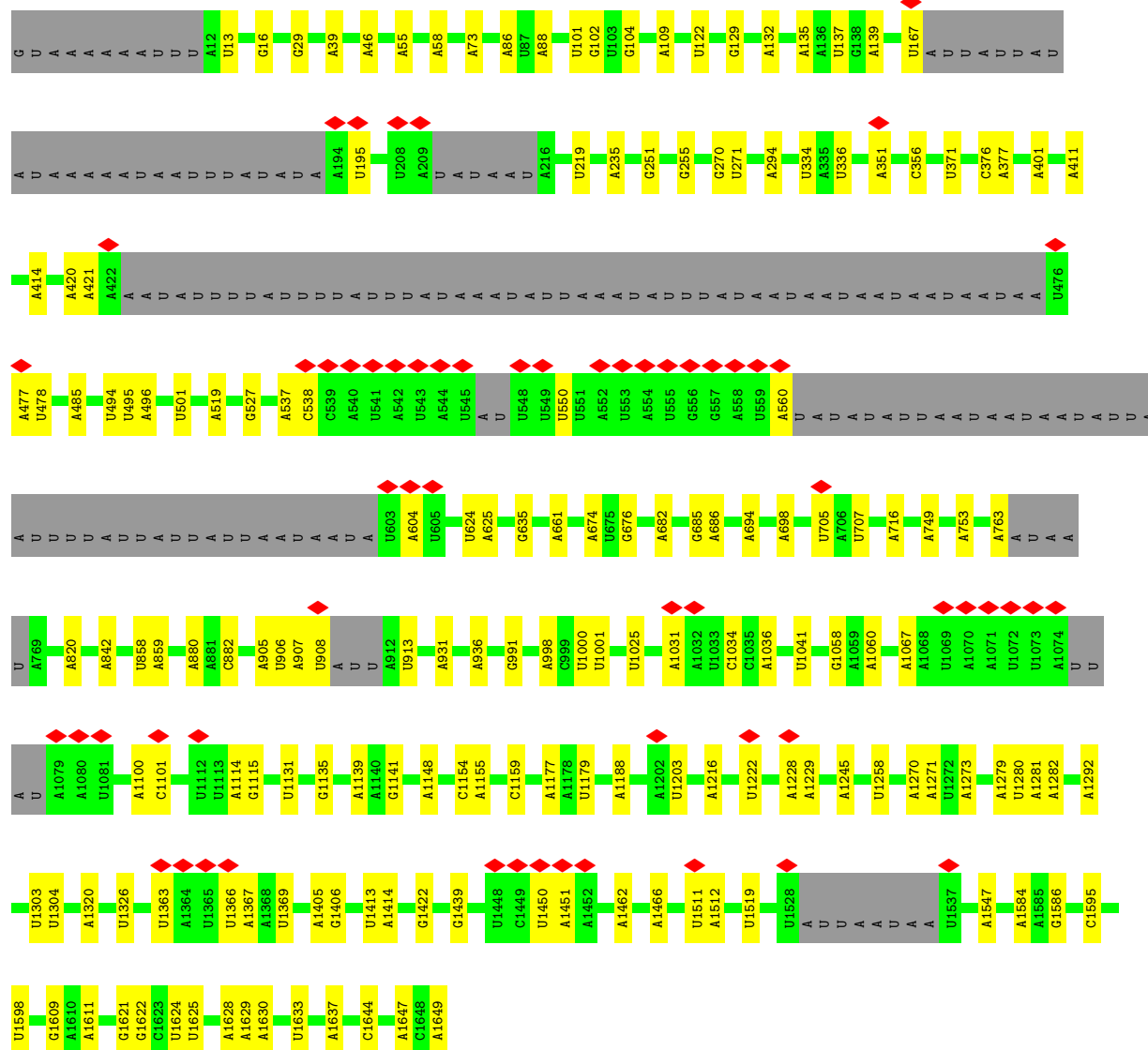


- Molecule 33: 3-hydroxyisobutyryl-CoA hydrolase, mitochondrial



- Molecule 34: 15S mitochondrial rRNA

Frequency	Percentage
Daily	80%
Weekly	10%
Monthly	10%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	778978	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 ($e^-/\text{\AA}^2$)	32	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2800	Depositor
Magnification	165000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.124	Depositor
Minimum map value	-0.125	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.016	Depositor
Recommended contour level	0.05	Depositor
Map size (Å)	398.3976, 398.3976, 398.3976	wwPDB
Map dimensions	720, 720, 720	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.55333, 0.55333, 0.55333	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ATP, K, LMT, ACE, 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	A	0.24	0/2483	0.46	0/3345
2	B	0.24	0/2764	0.45	0/3746
3	C	0.24	0/3133	0.41	0/4215
4	D	0.25	0/2913	0.46	0/3923
5	E	0.25	0/2403	0.47	0/3237
6	F	0.24	0/1068	0.48	0/1430
7	G	0.23	0/1641	0.45	0/2216
8	H	0.24	0/1244	0.46	0/1677
9	I	0.24	0/1895	0.46	0/2552
10	J	0.24	0/1355	0.46	0/1834
11	K	0.25	0/1232	0.47	0/1642
12	L	0.24	0/954	0.55	0/1281
13	M	0.24	0/949	0.50	0/1267
14	N	0.26	0/948	0.52	0/1267
15	O	0.24	0/1837	0.48	0/2457
16	P	0.25	0/968	0.55	0/1307
17	Q	0.24	0/1953	0.48	0/2609
18	R	0.24	0/830	0.52	0/1106
19	S	0.26	0/645	0.50	0/872
20	T	0.25	0/784	0.50	0/1035
21	U	0.24	0/1982	0.46	0/2679
22	V	0.24	0/2325	0.43	0/3112
23	W	0.24	0/3292	0.42	0/4449
24	X	0.25	0/801	0.46	0/1070
25	Y	0.23	0/2329	0.46	0/3142
26	Z	0.23	0/745	0.45	0/1004
27	1	0.23	0/279	0.62	0/355
28	2	0.24	0/877	0.45	0/1173
29	3	0.25	0/2114	0.44	0/2872
30	4	0.24	0/2485	0.46	0/3354
31	5	0.24	0/2417	0.43	0/3275
32	6	0.25	0/2655	0.47	0/3583

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	8	0.24	0/3766	0.45	0/5099
34	r	0.23	0/35392	0.68	0/55064
All	All	0.24	0/93458	0.56	0/133249

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	A	2427	2481	2480	24	0
2	B	2714	2722	2721	12	0
3	C	3090	3091	3085	19	0
4	D	2833	2896	2895	11	0
5	E	2348	2360	2359	5	0
6	F	1055	1129	1129	3	0
7	G	1612	1660	1658	16	0
8	H	1223	1286	1288	2	0
9	I	1858	1925	1925	6	0
10	J	1321	1334	1332	6	0
11	K	1209	1266	1266	2	0
12	L	939	993	992	2	0
13	M	935	1002	1000	2	0
14	N	931	986	985	2	0
15	O	1815	1853	1851	8	0
16	P	952	1011	1010	2	0
17	Q	1930	2014	2014	12	0
18	R	818	853	852	2	0
19	S	629	648	647	2	0
20	T	769	800	800	5	0
21	U	1939	1929	1929	8	0
22	V	2294	2398	2396	5	0
23	W	3226	3329	3327	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	X	787	832	832	1	0
25	Y	2273	2241	2240	8	0
26	Z	729	758	757	2	0
27	1	279	334	333	0	0
28	2	858	866	865	3	0
29	3	2063	2040	2039	7	0
30	4	2436	2423	2422	12	0
31	5	2361	2409	2408	14	0
32	6	2593	2615	2613	4	0
33	8	3690	3681	3680	14	0
34	r	31606	15844	15848	0	0
35	B	1	0	0	0	0
35	K	1	0	0	0	0
35	W	1	0	0	0	0
35	r	86	0	0	0	0
36	D	1	0	0	0	0
36	M	1	0	0	0	0
36	r	35	0	0	0	0
37	O	13	25	25	2	0
38	W	31	12	12	0	0
39	1	14	0	0	0	0
39	2	22	0	0	0	0
39	3	31	0	0	1	0
39	4	3	0	0	0	0
39	5	3	0	0	0	0
39	6	69	0	0	0	0
39	8	41	0	0	1	0
39	A	58	0	0	2	0
39	B	148	0	0	1	0
39	C	19	0	0	1	0
39	D	112	0	0	1	0
39	E	144	0	0	2	0
39	F	18	0	0	1	0
39	G	24	0	0	1	0
39	H	83	0	0	0	0
39	I	58	0	0	1	0
39	J	42	0	0	2	0
39	K	11	0	0	0	0
39	L	38	0	0	1	0
39	M	12	0	0	0	0
39	N	39	0	0	0	0
39	O	55	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
39	P	70	0	0	0	0
39	Q	20	0	0	0	0
39	R	15	0	0	0	0
39	S	8	0	0	0	0
39	T	44	0	0	0	0
39	U	87	0	0	2	0
39	V	34	0	0	0	0
39	W	93	0	0	0	0
39	X	9	0	0	0	0
39	Y	46	0	0	1	0
39	Z	25	0	0	0	0
39	r	2711	0	0	0	0
All	All	92918	74046	74015	193	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 2.

The worst 5 of 193 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)
9:I:200:LEU:HD11	9:I:211:ILE:HD11	1.77	0.67
1:A:289:GLY:O	39:A:401:HOH:O	2.13	0.66
10:J:133:MET:O	39:J:301:HOH:O	2.13	0.66
3:C:255:ASN:OD1	3:C:256:ILE:N	2.30	0.64
16:P:71:ARG:HG2	32:6:314:VAL:HG21	1.80	0.64

There are no symmetry-related clashes.

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	A	299/344 (87%)	286 (96%)	13 (4%)	0	100	100
2	B	338/394 (86%)	329 (97%)	9 (3%)	0	100	100
3	C	362/398 (91%)	353 (98%)	9 (2%)	0	100	100
4	D	337/486 (69%)	334 (99%)	3 (1%)	0	100	100
5	E	292/307 (95%)	285 (98%)	7 (2%)	0	100	100
6	F	129/131 (98%)	127 (98%)	2 (2%)	0	100	100
7	G	199/247 (81%)	196 (98%)	3 (2%)	0	100	100
8	H	154/155 (99%)	152 (99%)	2 (1%)	0	100	100
9	I	230/278 (83%)	226 (98%)	4 (2%)	0	100	100
10	J	158/203 (78%)	152 (96%)	6 (4%)	0	100	100
11	K	150/217 (69%)	148 (99%)	2 (1%)	0	100	100
12	L	121/153 (79%)	120 (99%)	1 (1%)	0	100	100
13	M	117/143 (82%)	115 (98%)	2 (2%)	0	100	100
14	N	111/115 (96%)	111 (100%)	0	0	100	100
15	O	219/286 (77%)	217 (99%)	2 (1%)	0	100	100
16	P	118/121 (98%)	115 (98%)	3 (2%)	0	100	100
17	Q	234/237 (99%)	232 (99%)	2 (1%)	0	100	100
18	R	99/138 (72%)	98 (99%)	1 (1%)	0	100	100
19	S	77/91 (85%)	74 (96%)	3 (4%)	0	100	100
20	T	91/177 (51%)	90 (99%)	1 (1%)	0	100	100
21	U	235/264 (89%)	230 (98%)	5 (2%)	0	100	100
22	V	282/318 (89%)	278 (99%)	4 (1%)	0	100	100
23	W	400/450 (89%)	390 (98%)	10 (2%)	0	100	100
24	X	96/110 (87%)	96 (100%)	0	0	100	100
25	Y	270/319 (85%)	267 (99%)	3 (1%)	0	100	100
26	Z	90/95 (95%)	87 (97%)	3 (3%)	0	100	100
27	1	29/111 (26%)	29 (100%)	0	0	100	100
28	2	100/130 (77%)	98 (98%)	2 (2%)	0	100	100
29	3	255/266 (96%)	246 (96%)	9 (4%)	0	100	100
30	4	301/321 (94%)	289 (96%)	12 (4%)	0	100	100
31	5	289/339 (85%)	281 (97%)	8 (3%)	0	100	100
32	6	317/345 (92%)	310 (98%)	7 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
33	8	465/500 (93%)	451 (97%)	14 (3%)	0	100	100
All	All	6964/8189 (85%)	6812 (98%)	152 (2%)	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	A	270/309 (87%)	270 (100%)	0	100	100
2	B	307/350 (88%)	307 (100%)	0	100	100
3	C	361/385 (94%)	361 (100%)	0	100	100
4	D	306/437 (70%)	304 (99%)	2 (1%)	81	90
5	E	253/266 (95%)	252 (100%)	1 (0%)	89	94
6	F	120/120 (100%)	120 (100%)	0	100	100
7	G	174/211 (82%)	173 (99%)	1 (1%)	84	92
8	H	142/141 (101%)	142 (100%)	0	100	100
9	I	205/245 (84%)	204 (100%)	1 (0%)	86	93
10	J	146/183 (80%)	146 (100%)	0	100	100
11	K	131/192 (68%)	131 (100%)	0	100	100
12	L	102/131 (78%)	102 (100%)	0	100	100
13	M	100/121 (83%)	100 (100%)	0	100	100
14	N	101/103 (98%)	100 (99%)	1 (1%)	73	84
15	O	192/250 (77%)	192 (100%)	0	100	100
16	P	105/106 (99%)	105 (100%)	0	100	100
17	Q	217/218 (100%)	215 (99%)	2 (1%)	75	86
18	R	89/121 (74%)	89 (100%)	0	100	100
19	S	68/78 (87%)	68 (100%)	0	100	100
20	T	82/159 (52%)	82 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	U	212/236 (90%)	212 (100%)	0	100	100
22	V	260/287 (91%)	260 (100%)	0	100	100
23	W	369/409 (90%)	368 (100%)	1 (0%)	91	95
24	X	85/92 (92%)	85 (100%)	0	100	100
25	Y	249/289 (86%)	248 (100%)	1 (0%)	89	94
26	Z	83/85 (98%)	83 (100%)	0	100	100
27	1	30/98 (31%)	30 (100%)	0	100	100
28	2	93/117 (80%)	93 (100%)	0	100	100
29	3	232/240 (97%)	231 (100%)	1 (0%)	89	94
30	4	267/281 (95%)	266 (100%)	1 (0%)	89	94
31	5	259/303 (86%)	259 (100%)	0	100	100
32	6	289/312 (93%)	289 (100%)	0	100	100
33	8	413/444 (93%)	412 (100%)	1 (0%)	92	96
All	All	6312/7319 (86%)	6299 (100%)	13 (0%)	91	96

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
17	Q	39[B]	HIS
23	W	141	HIS
33	8	472	ARG
29	3	95	ASN
30	4	253	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
30	4	69	HIS
31	5	143	GLN
33	8	128	ASN
32	6	169	GLN
23	W	449	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
34	r	1476/1647 (89%)	167 (11%)	0

5 of 167 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
34	r	13	U
34	r	16	G
34	r	29	G
34	r	39	A
34	r	46	A

There are no RNA pucker outliers to report.

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 [i](#)

Of 128 ligands modelled in this entry, 126 are monoatomic - leaving 2 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	$\# Z > 2$
37	LMT	O	301	-	12,12,36	0.15	0	11,11,47	0.20	0
38	ATP	W	501	35	26,33,33	0.75	0	31,52,52	0.67	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
37	LMT	O	301	-	-	0/10/10/61	-
38	ATP	W	501	35	-	0/18/38/38	0/3/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

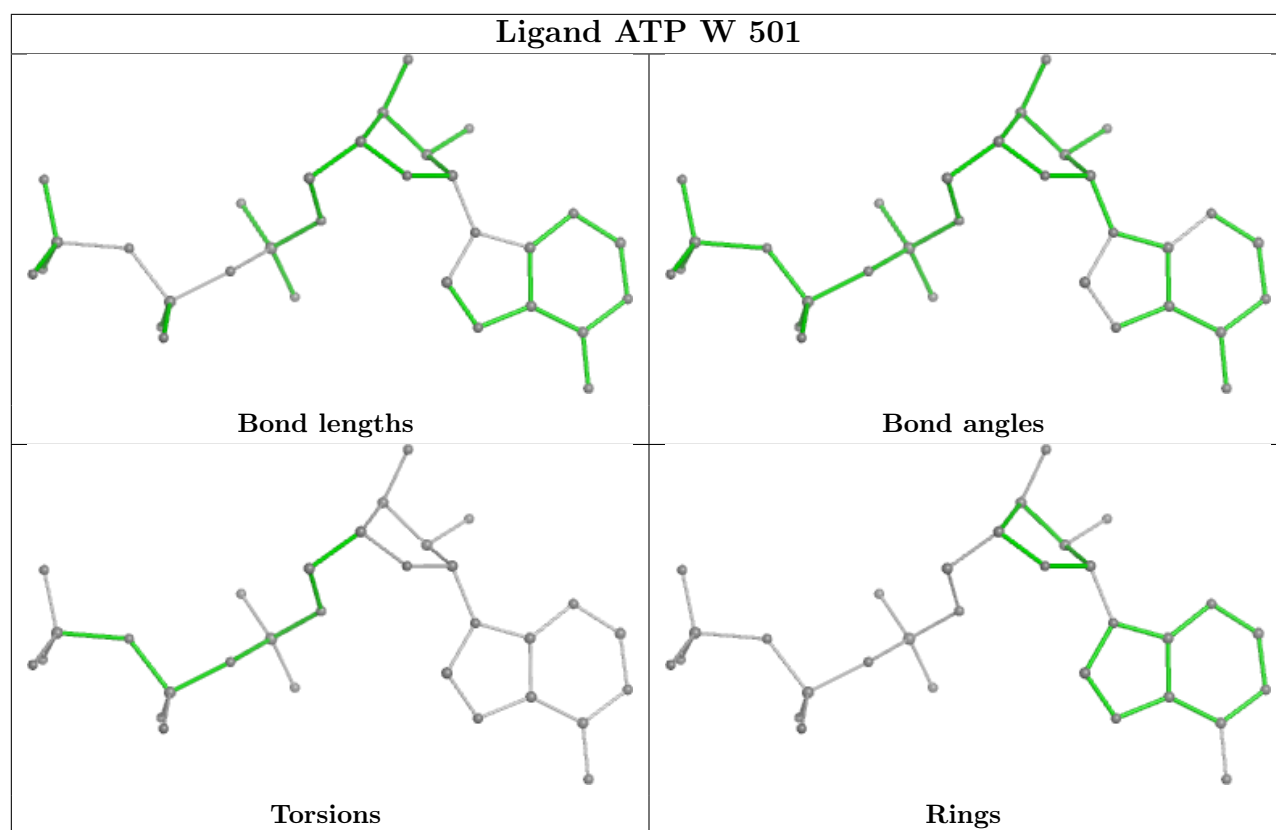
There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
37	O	301	LMT	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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

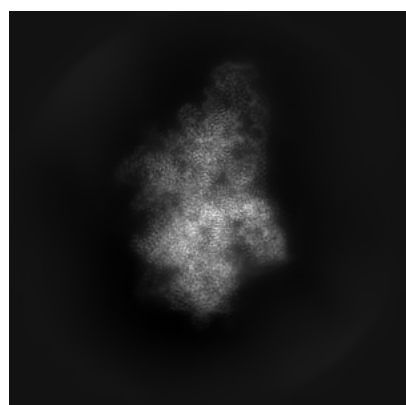
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-16968. These allow visual inspection of the internal detail of the map and identification of artifacts.

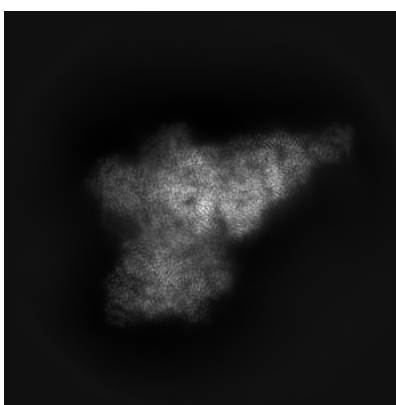
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

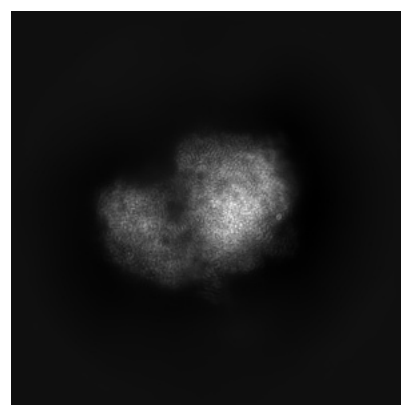
6.1.1 Primary map



X



Y



Z

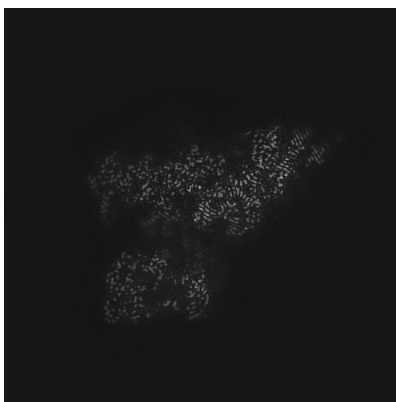
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

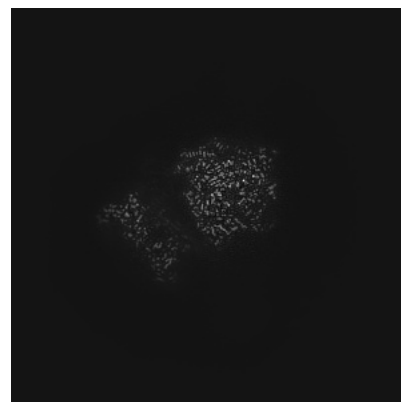
6.2.1 Primary map



X Index: 360



Y Index: 360

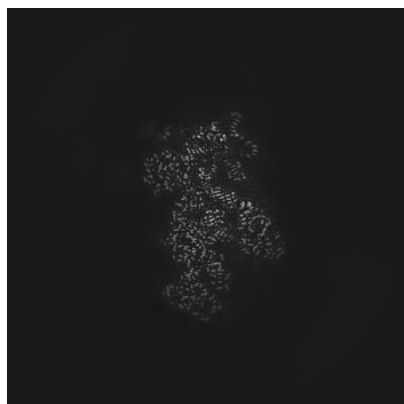


Z Index: 360

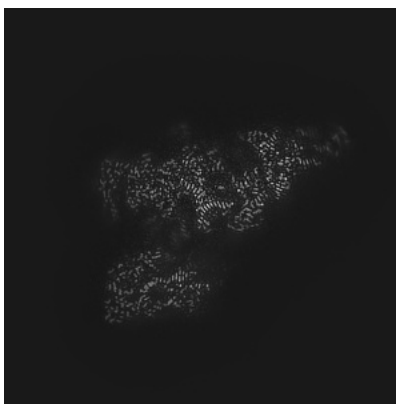
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

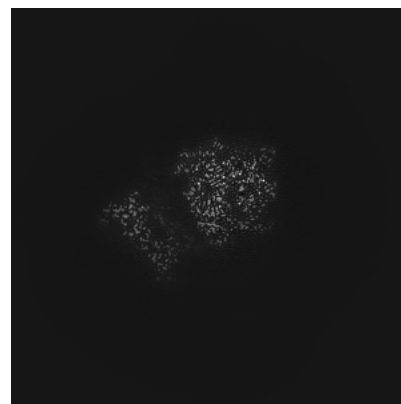
6.3.1 Primary map



X Index: 396



Y Index: 369

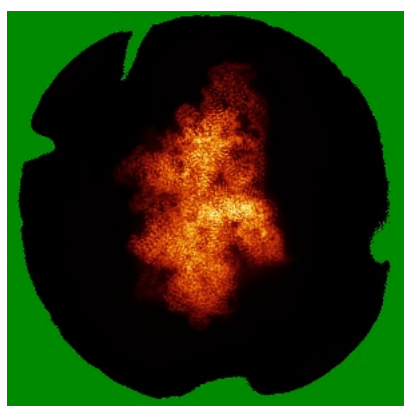


Z Index: 358

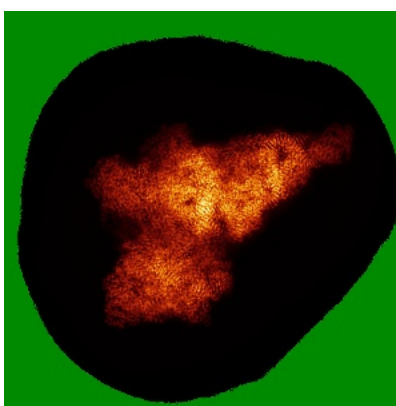
The images above show the largest variance slices of the map in three orthogonal directions.

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

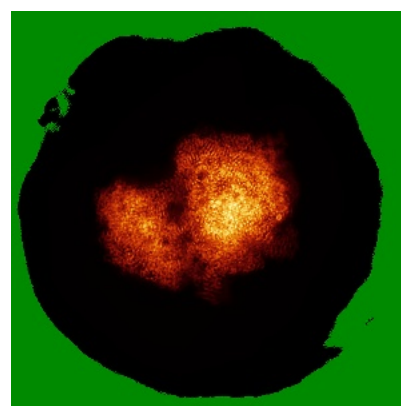
6.4.1 Primary map



X



Y

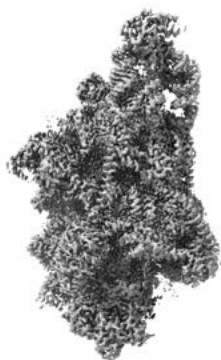


Z

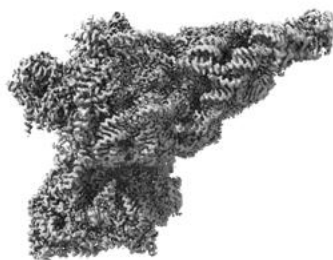
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

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 0.05. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

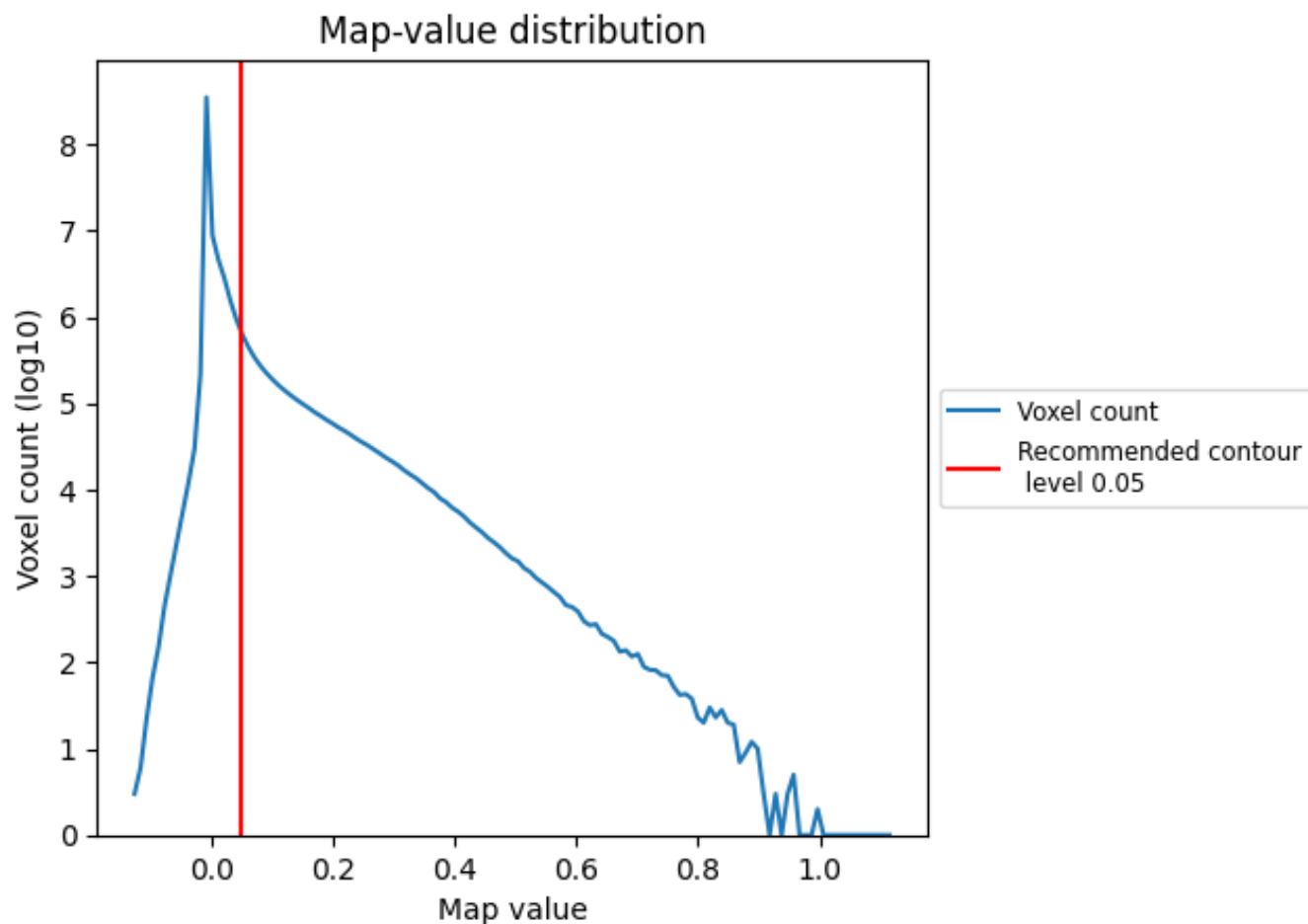
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

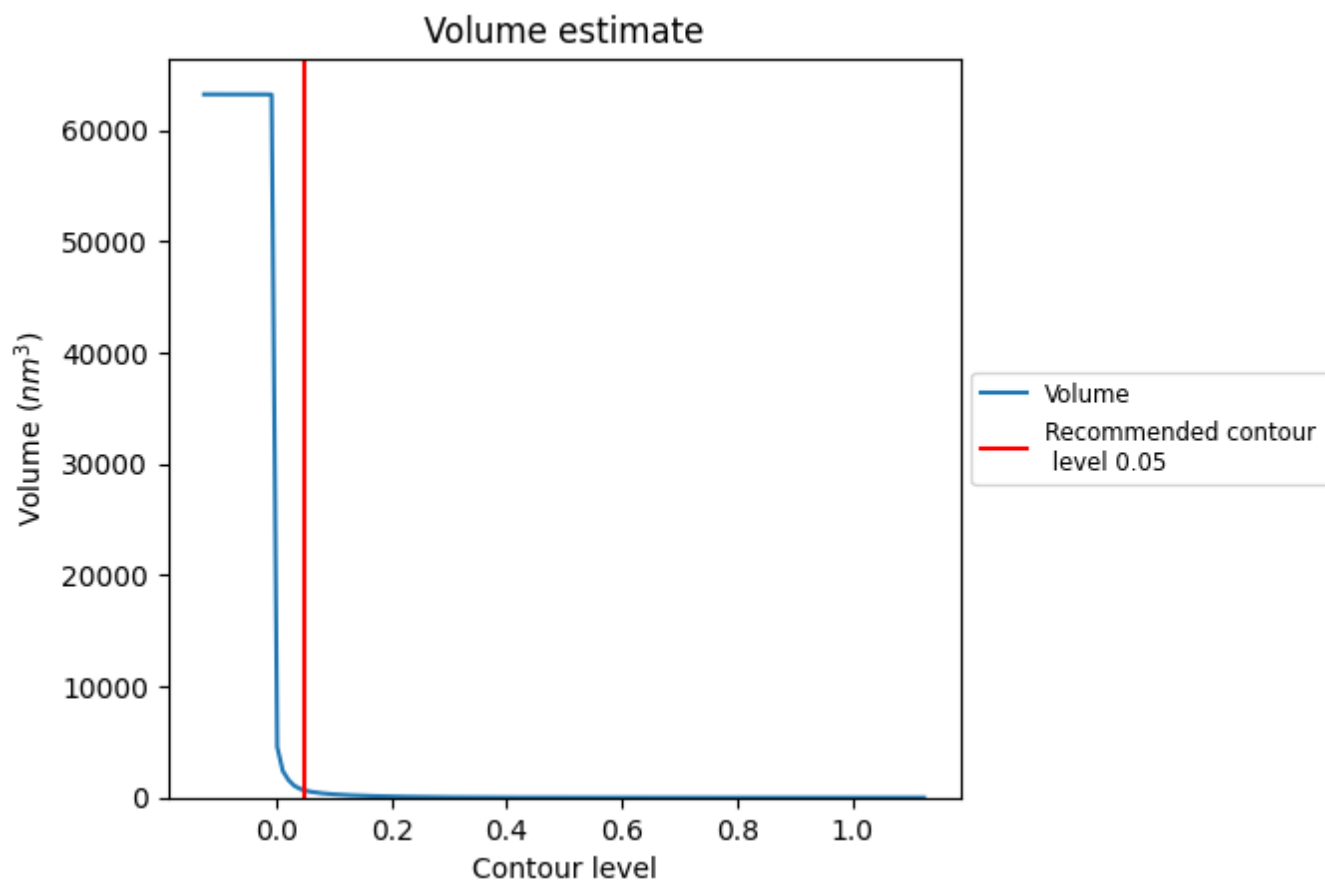
This section contains the results of statistical analysis of the map.

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.

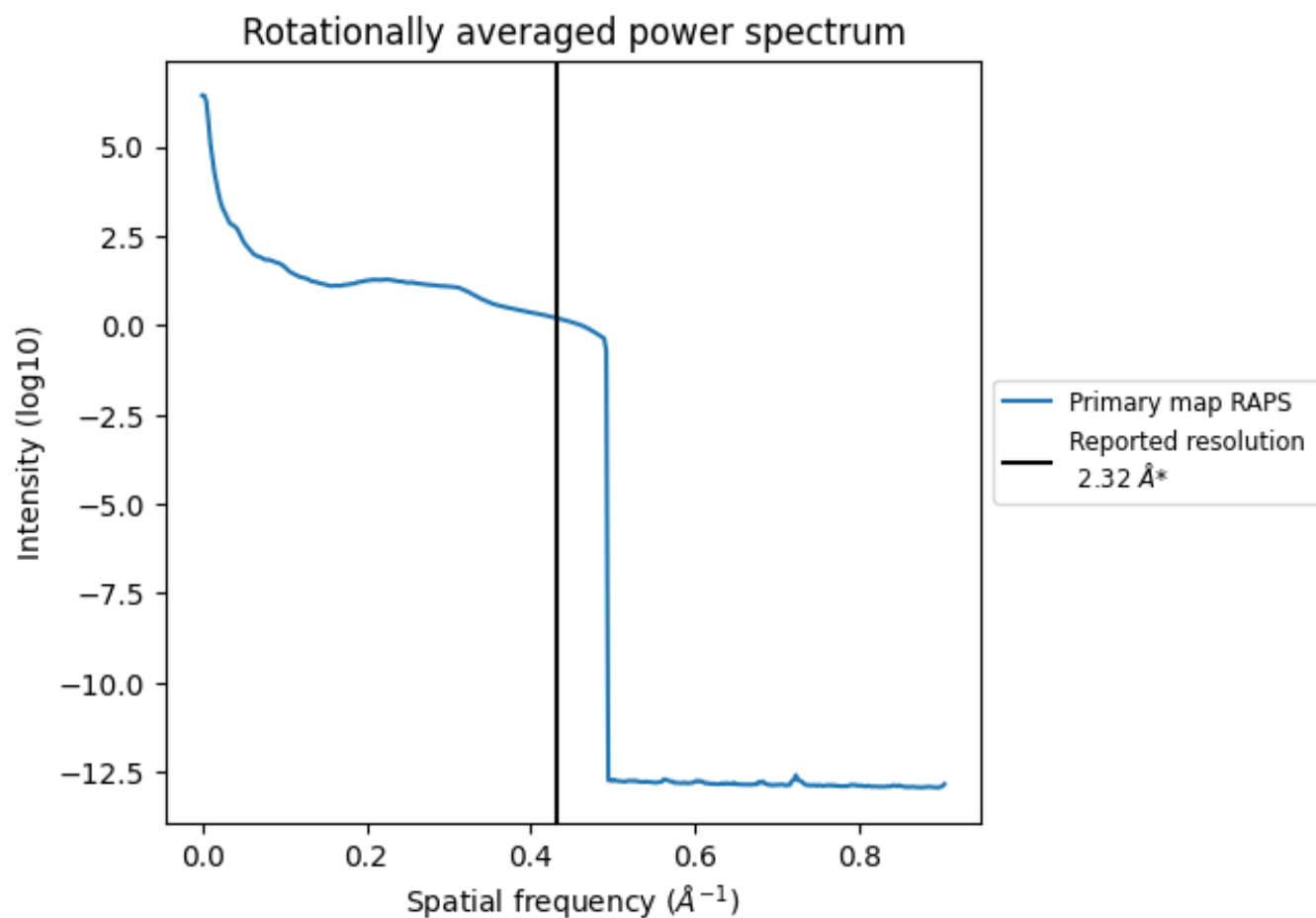
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 643 nm³; this corresponds to an approximate mass of 581 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 0.431 \AA^{-1}

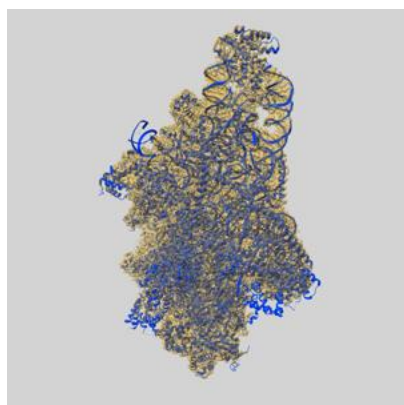
8 Fourier-Shell correlation

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

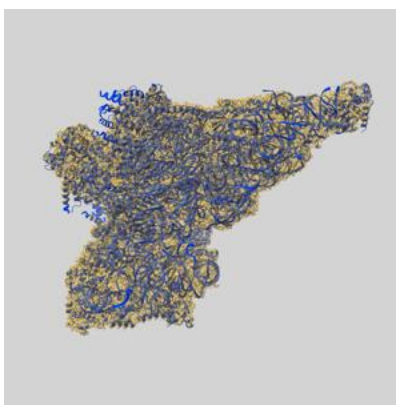
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-16968 and PDB model 8OM4. Per-residue inclusion information can be found in section [3](#) on page [14](#).

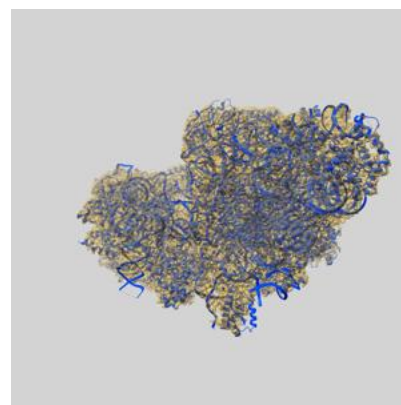
9.1 Map-model overlay [i](#)



X



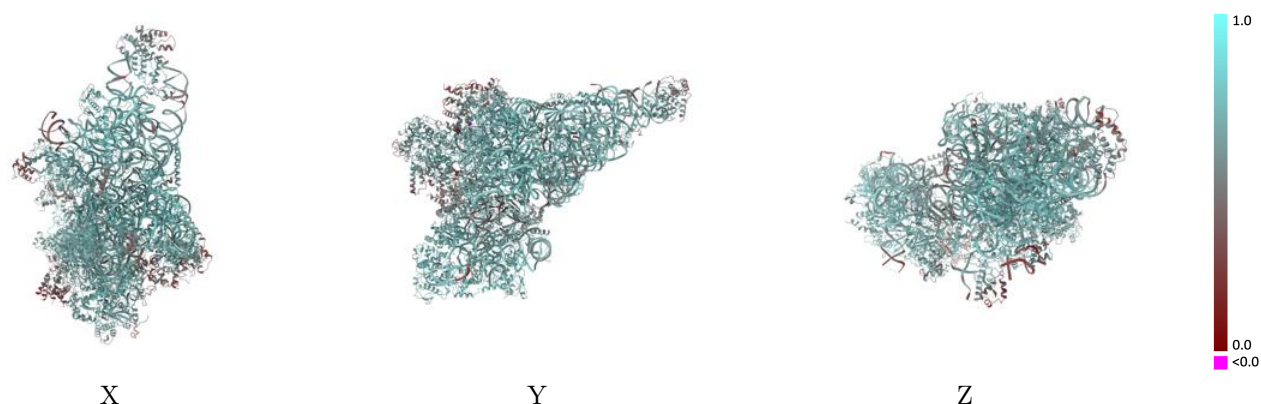
Y



Z

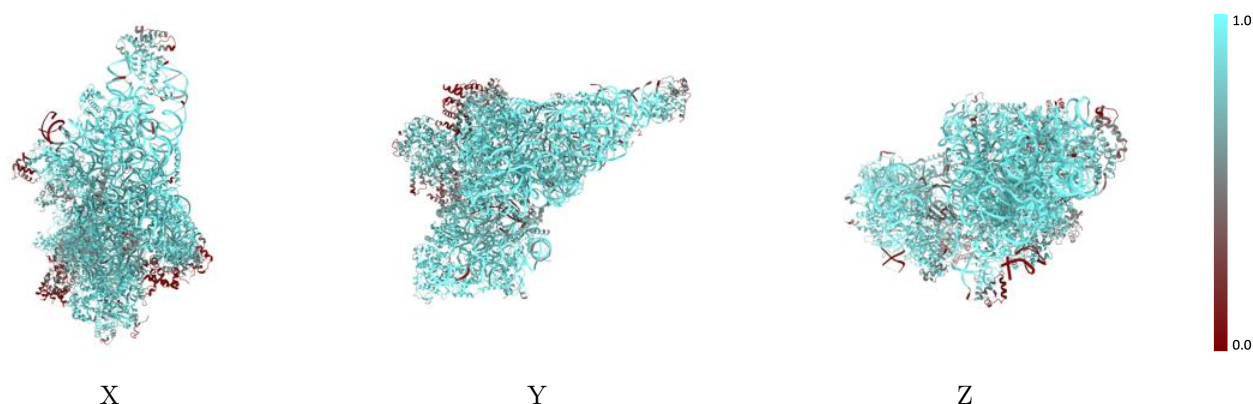
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



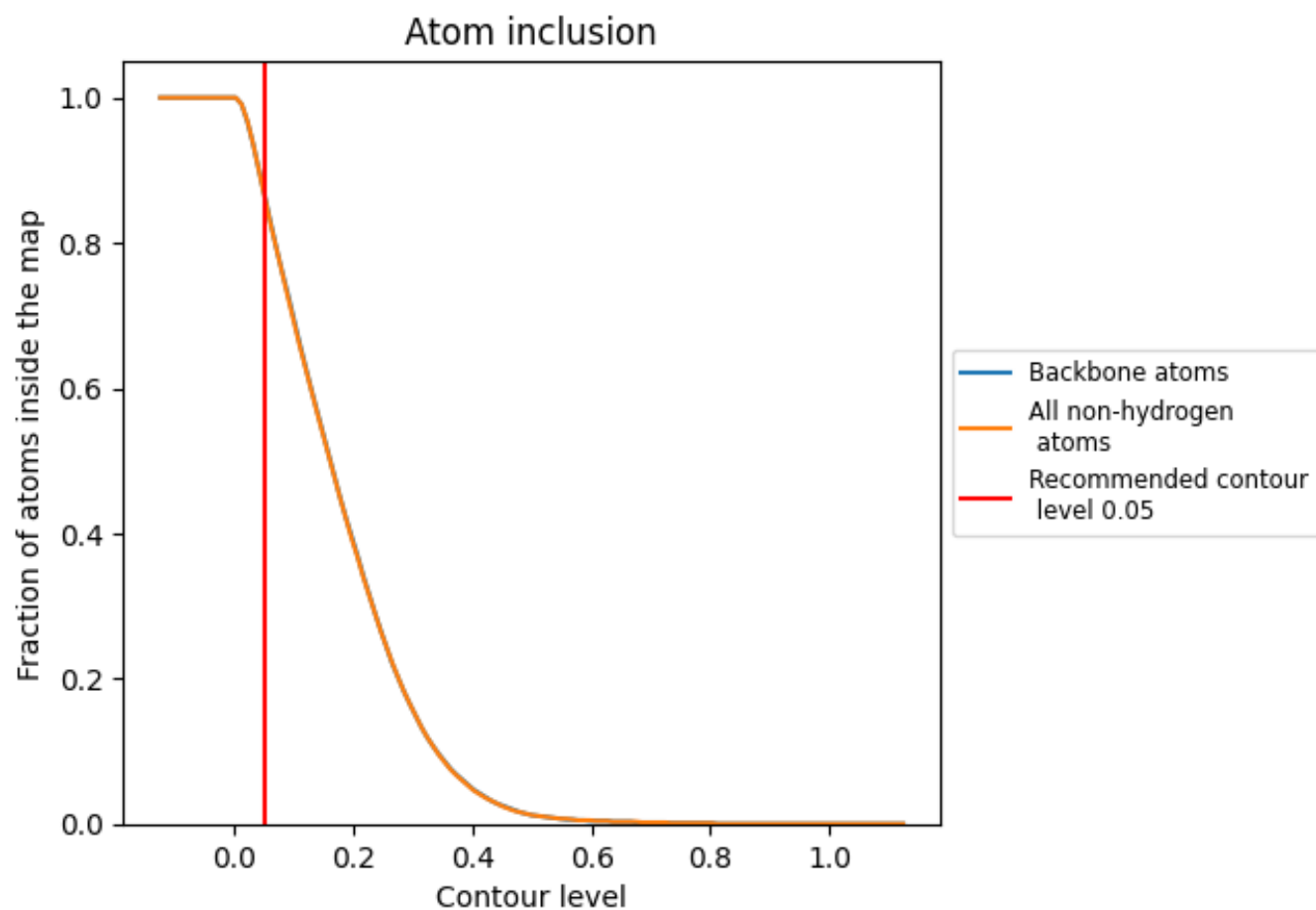
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.05).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 86% 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 (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8650	 0.6540
1	 0.8440	 0.6710
2	 0.9240	 0.6840
3	 0.8870	 0.6630
4	 0.7350	 0.5700
5	 0.7020	 0.5420
6	 0.9040	 0.6740
8	 0.6950	 0.6370
A	 0.6350	 0.5690
B	 0.7950	 0.6580
C	 0.7170	 0.5860
D	 0.8290	 0.6520
E	 0.9350	 0.7060
F	 0.9010	 0.6680
G	 0.7440	 0.6060
H	 0.9790	 0.7530
I	 0.9000	 0.6840
J	 0.9080	 0.7040
K	 0.8560	 0.6370
L	 0.9780	 0.7230
M	 0.9440	 0.6990
N	 0.9670	 0.7300
O	 0.8990	 0.6970
P	 0.9440	 0.7150
Q	 0.6910	 0.5710
R	 0.8940	 0.6750
S	 0.8920	 0.6660
T	 0.8470	 0.6420
U	 0.9310	 0.7010
V	 0.7770	 0.6240
W	 0.9300	 0.6990
X	 0.9020	 0.6650
Y	 0.8400	 0.6450
Z	 0.7920	 0.6070
r	 0.9330	 0.6610

