



## wwPDB EM Validation Summary Report ⓘ

Nov 4, 2024 – 06:06 AM EST

PDB ID : 8D8K  
EMDB ID : EMD-27250  
Title : Yeast mitochondrial small subunit assembly intermediate (State 2)  
Authors : Burnside, C.; Harper, N.J.; Klinge, S.  
Deposited on : 2022-06-08  
Resolution : 3.13 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.dev113  
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) : 2.39

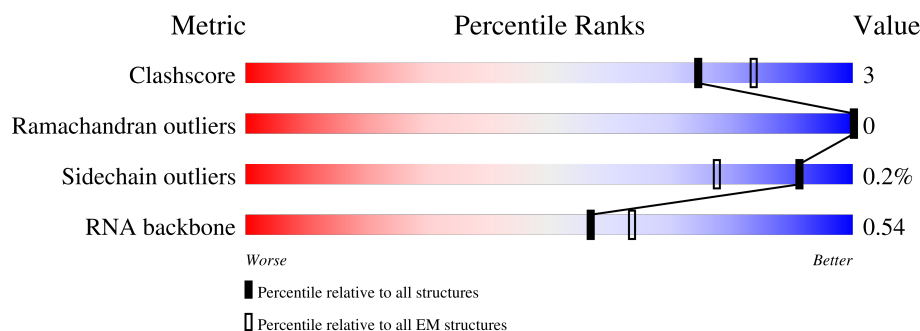
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.13 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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	0	628	<div> <div>42%</div> <div>58%</div> <div>10%</div> <div>32%</div> </div>
2	5	339	<div> <div>75%</div> <div>70%</div> <div>9%</div> <div>20%</div> </div>
3	C	398	<div> <div>10%</div> <div>51%</div> <div>9%</div> <div>40%</div> </div>
4	d	864	<div> <div>33%</div> <div>76%</div> <div>24%</div> </div>
5	M	143	<div> <div>11%</div> <div>55%</div> <div>42%</div> </div>
6	N	115	<div> <div>97%</div> </div>
7	O	286	<div> <div>11%</div> <div>71%</div> <div>27%</div> </div>

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Mol	Chain	Length	Quality of chain
8	P	121	
9	Q	237	
10	R	138	
11	S	91	
12	T	177	
13	U	264	
14	V	318	
15	W	450	
16	X	110	
17	Y	319	
18	Z	95	
19	A	344	
20	B	394	
21	2	130	
22	3	266	
23	D	486	
24	4	321	
25	E	307	
26	F	131	
27	6	345	
28	G	247	
29	H	155	
30	I	278	
31	a	1713	
32	J	203	

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Mol	Chain	Length	Quality of chain
33	K	217	<div><div></div><div>24%</div><div>59%</div><div>6%</div><div>35%</div></div>
34	c	94	<div><div></div><div>89%</div><div>100%</div></div>
35	L	153	<div><div></div><div>9%</div><div>78%</div><div>•</div><div>21%</div></div>

## 2 Entry composition

There are 39 unique types of molecules in this entry. The entry contains 88977 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 Probable S-adenosyl-L-methionine-dependent RNA methyltransferase RSM22, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	429	Total	C	N	O	S	0	0
			3471	2204	626	629	12		

- Molecule 2 is a protein called 37S ribosomal protein MRP13, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	5	270	Total	C	N	O	S	0	0
			2199	1426	375	394	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	239	Total	C	N	O	S	0	0
			2014	1275	348	364	27		

- Molecule 4 is a protein called Mitochondrial group I intron splicing factor CCM1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	d	660	Total	C	N	O	S	0	0
			5497	3530	934	999	34		

- Molecule 5 is a protein called 37S ribosomal protein SWS2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	M	83	Total	C	N	O	S	0	0
			645	417	111	112	5		

- Molecule 6 is a protein called 37S ribosomal protein MRP2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	N	113	Total	C	N	O	S	0	0
			931	596	179	152	4		

- Molecule 7 is a protein called 37S ribosomal protein S28, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	O	210	Total	C	N	O	S	0	0
			1724	1079	318	319	8		

- Molecule 8 is a protein called 37S ribosomal protein S16, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	P	116	Total	C	N	O	S	0	0
			919	586	172	159	2		

- Molecule 9 is a protein called 37S ribosomal protein S17, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	Q	205	Total	C	N	O	S	0	0
			1690	1059	316	310	5		

- Molecule 10 is a protein called 37S ribosomal protein RSM18, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	R	91	Total	C	N	O	S	0	0
			738	463	143	128	4		

- Molecule 11 is a protein called 37S ribosomal protein S19, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	S	75	Total	C	N	O	S	0	0
			595	383	109	101	2		

- Molecule 12 is a protein called 37S ribosomal protein MRP21, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	T	92	Total	C	N	O	S	0	0
			760	475	150	130	5		

- Molecule 13 is a protein called 37S ribosomal protein S25, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	U	233	Total	C	N	O	S	0	0
			1907	1211	331	358	7		

- Molecule 14 is a protein called 37S ribosomal protein PET123, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	V	233	Total	C	N	O	S	0	0
			1872	1189	338	342	3		

- Molecule 15 is a protein called 37S ribosomal protein S23, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	W	395	Total	C	N	O	S	0	0
			3174	2047	531	588	8		

- Molecule 16 is a protein called Mitochondrial 37S ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	X	96	Total	C	N	O	S	0	0
			774	496	140	135	3		

- Molecule 17 is a protein called 37S ribosomal protein S24, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Y	263	Total	C	N	O	S	0	0
			2208	1400	393	411	4		

- Molecule 18 is a protein called 37S ribosomal protein MRP10, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	Z	84	Total	C	N	O	S	0	0
			660	418	121	115	6		

- Molecule 19 is a protein called 37S ribosomal protein MRP51, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	A	199	Total	C	N	O	S	0	0
			1585	1023	278	279	5		

- Molecule 20 is a protein called 37S ribosomal protein MRP4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	B	266	Total	C	N	O	S	0	0
			2085	1313	366	404	2		

- Molecule 21 is a protein called Protein FYV4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	2	99	Total	C	N	O	S	0	0
			833	530	156	146	1		

- Molecule 22 is a protein called 37S ribosomal protein S26, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	3	244	Total	C	N	O	S	0	0
			1953	1261	328	359	5		

- Molecule 23 is a protein called 37S ribosomal protein NAM9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	D	308	Total	C	N	O	S	0	0
			2567	1677	452	434	4		

- Molecule 24 is a protein called 37S ribosomal protein MRP1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	4	271	Total	C	N	O	S	0	0
			2182	1390	373	412	7		

- Molecule 25 is a protein called 37S ribosomal protein S5, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	E	291	Total	C	N	O	S	0	0
			2321	1479	411	423	8		

- Molecule 26 is a protein called 37S ribosomal protein MRP17, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	F	131	Total	C	N	O	S	0	0
			1054	671	189	190	4		

- Molecule 27 is a protein called 37S ribosomal protein S35, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	6	251	Total	C	N	O	S	0	0
			2071	1322	375	368	6		

- Molecule 28 is a protein called 37S ribosomal protein S7, mitochondrial.



Mol	Chain	Residues	Atoms					AltConf	Trace
28	G	148	Total	C	N	O	S	0	0
			1185	749	220	211	5		

- Molecule 29 is a protein called 37S ribosomal protein S8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	H	155	Total	C	N	O	S	0	0
			1221	772	218	221	10		

- Molecule 30 is a protein called 37S ribosomal protein S9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	I	208	Total	C	N	O	S	0	0
			1667	1067	299	297	4		

- Molecule 31 is a RNA chain called 15S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	a	1538	Total	C	N	O	P	0	0
			32666	14691	5767	10670	1538		

- Molecule 32 is a protein called 37S ribosomal protein S10, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	J	144	Total	C	N	O	S	0	0
			1186	768	204	210	4		

- Molecule 33 is a protein called 37S ribosomal protein S18, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	K	141	Total	C	N	O	S	0	0
			1113	711	194	202	6		

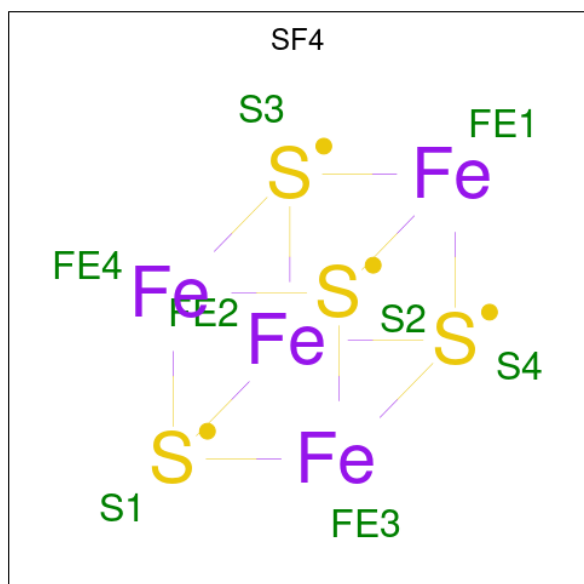
- Molecule 34 is a protein called unknown protein sequence.

Mol	Chain	Residues	Atoms				AltConf	Trace
34	c	94	Total	C	N	O	0	0
			470	282	94	94		

- Molecule 35 is a protein called MRPS12 isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	L	121	Total	C	N	O	S	0	0
			926	571	190	161	4		

- Molecule 36 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula:  $\text{Fe}_4\text{S}_4$ ) (labeled as "Ligand of Interest" by depositor).

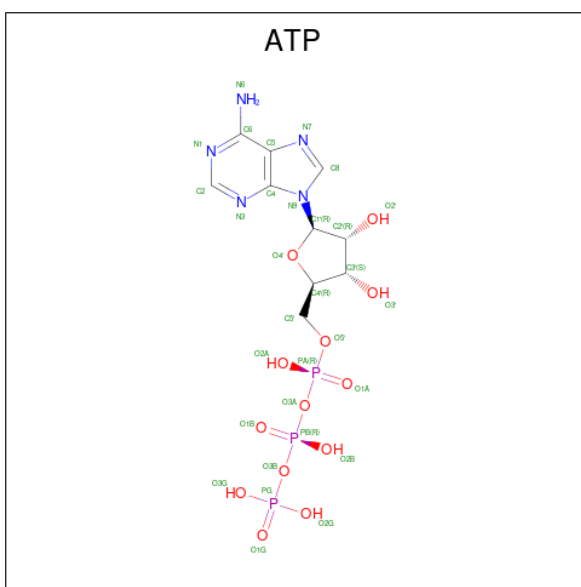


Mol	Chain	Residues	Atoms			AltConf
36	0	1	Total	Fe	S	0
			8	4	4	

- Molecule 37 is MAGNESIUM ION (three-letter code: MG) (formula:  $\text{Mg}$ ) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
37	Q	1	Total	Mg	0
			1	1	
37	W	1	Total	Mg	0
			1	1	
37	B	1	Total	Mg	0
			1	1	
37	a	69	Total	Mg	0
			69	69	

- 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	N	O	P	0
			31	10	5	13	3	

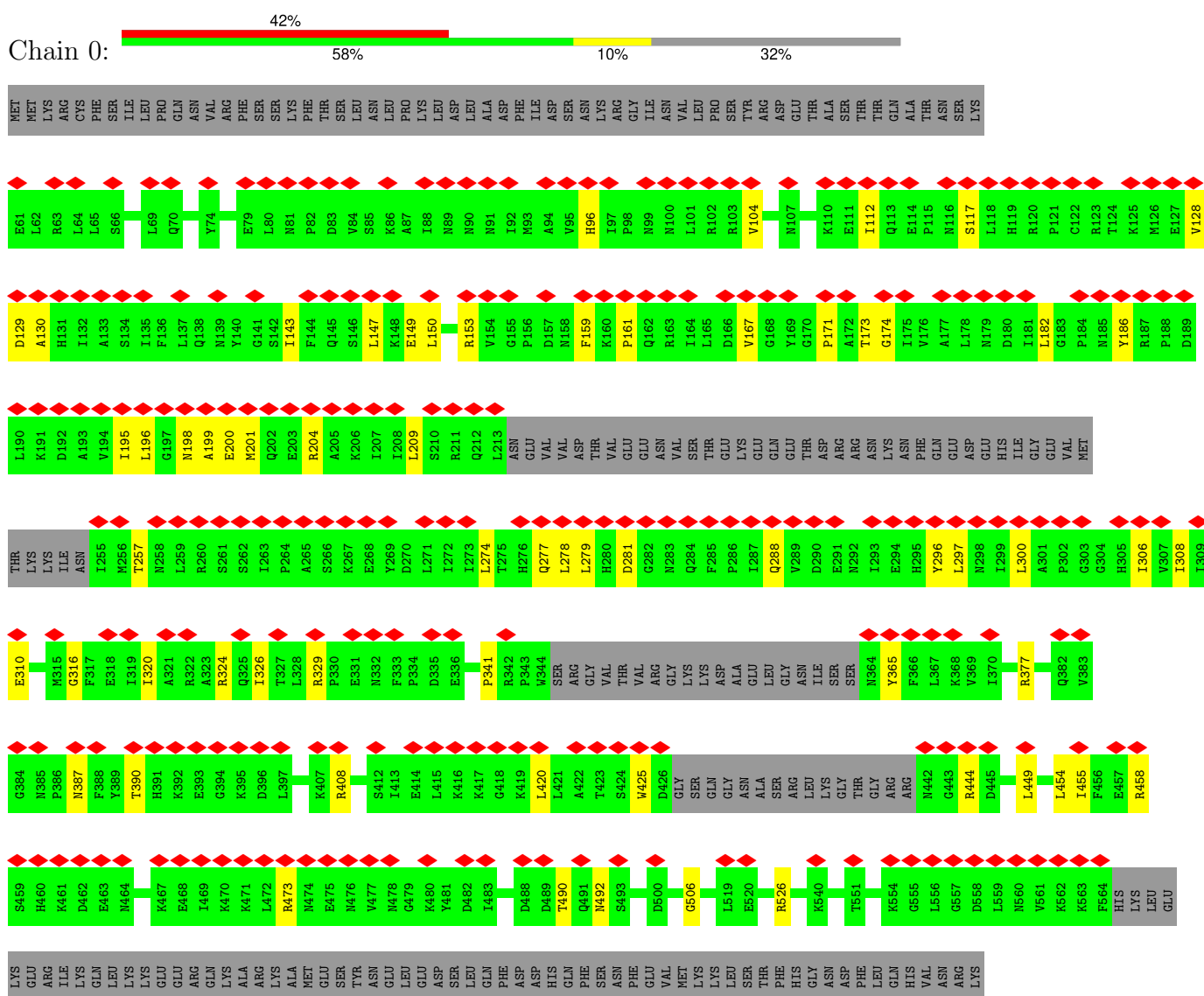
- Molecule 39 is water.

Mol	Chain	Residues	Atoms	AltConf
39	W	3	Total O 3 3	0

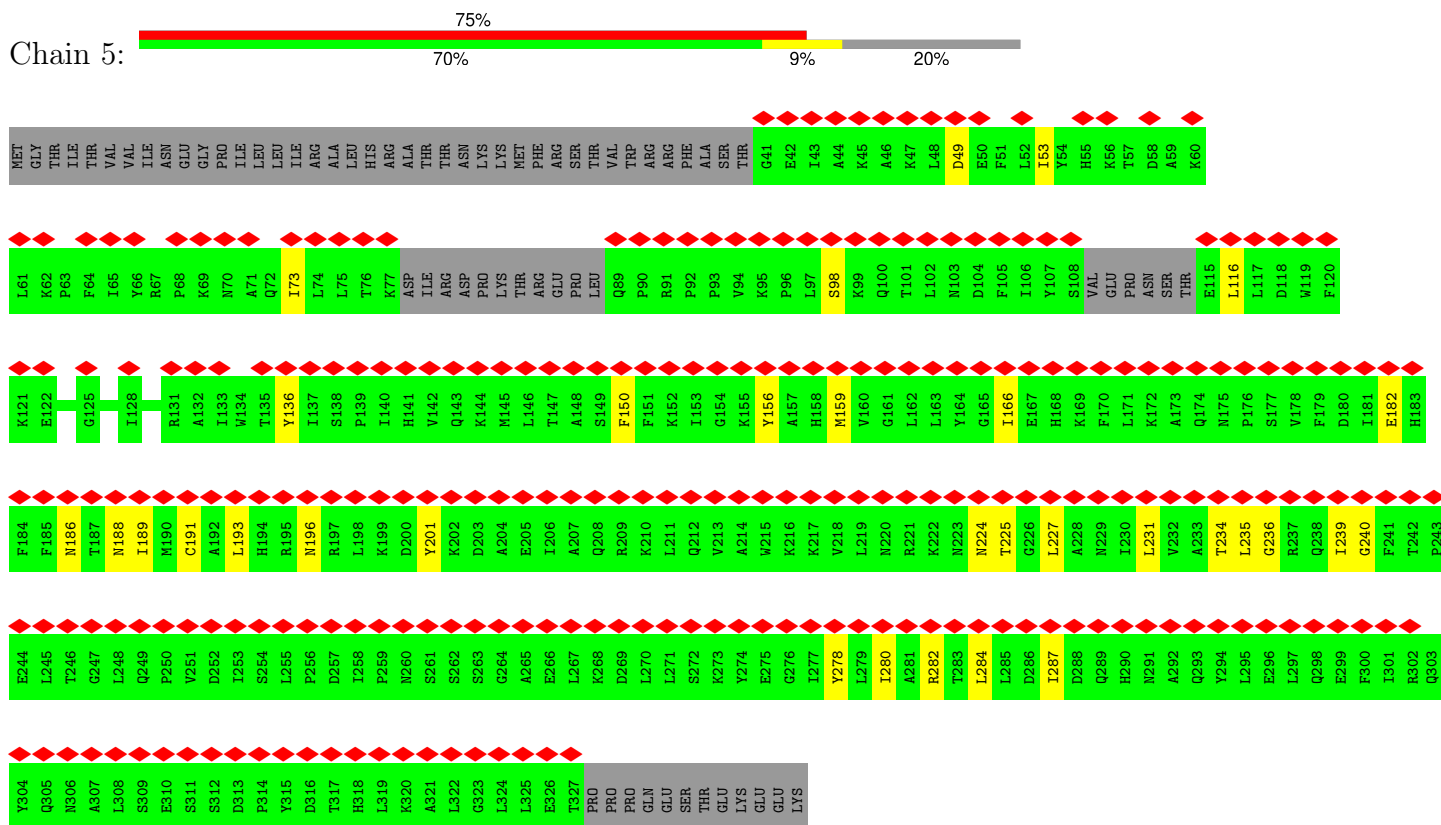
### 3 Residue-property plots

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.

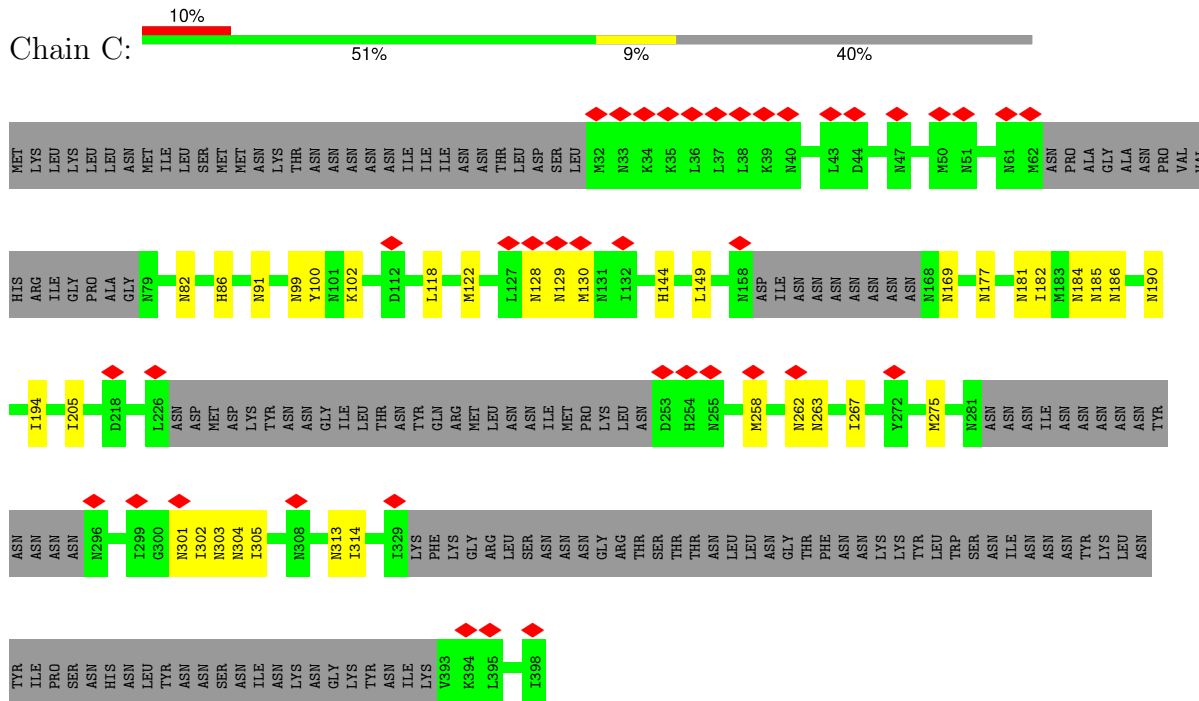
- Molecule 1: Probable S-adenosyl-L-methionine-dependent RNA methyltransferase RSM22, mitochondrial



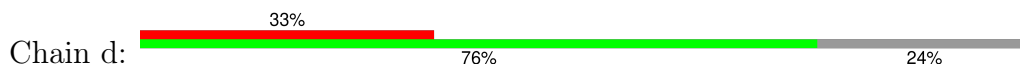
- Molecule 2: 37S ribosomal protein MRP13, mitochondrial



- Molecule 3: Ribosomal protein VAR1, mitochondrial

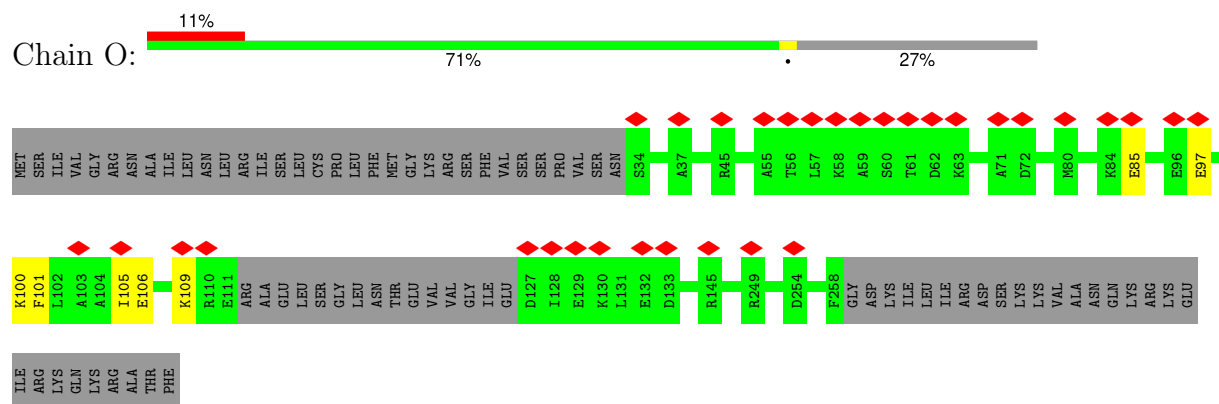


- Molecule 4: Mitochondrial group I intron splicing factor CCM1

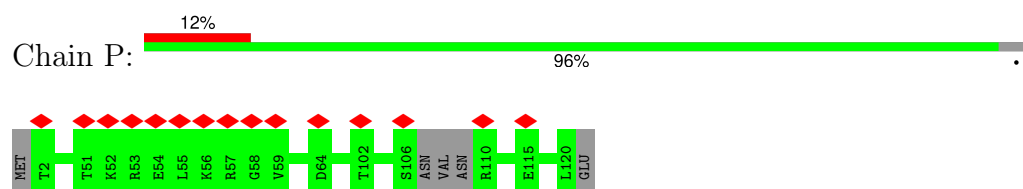




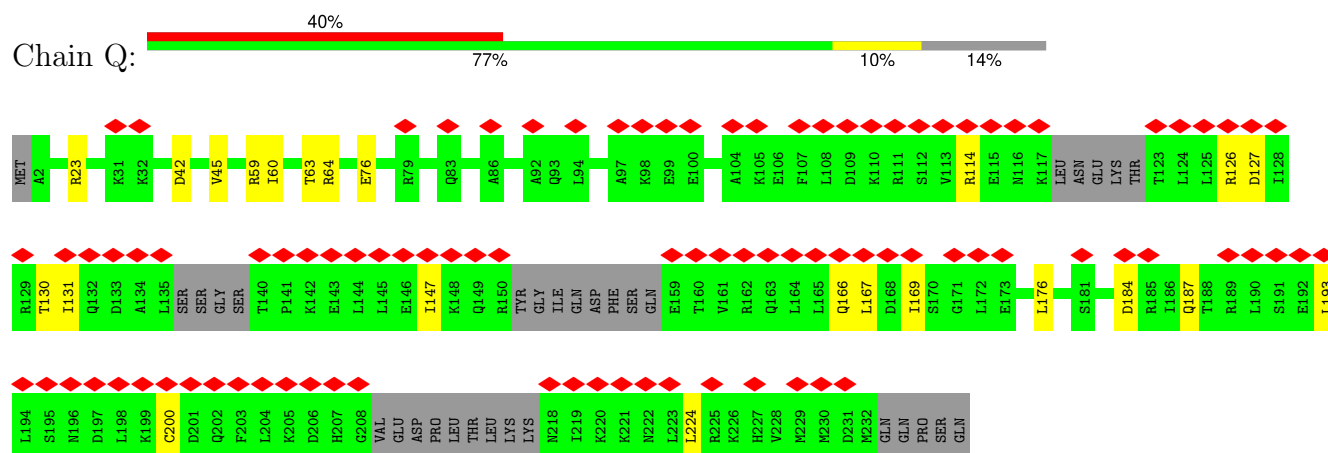
- Molecule 7: 37S ribosomal protein S28, mitochondrial



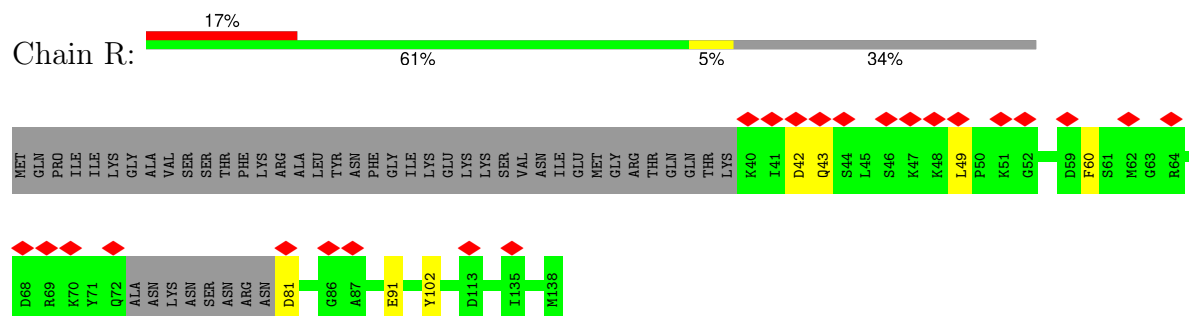
- Molecule 8: 37S ribosomal protein S16, mitochondrial



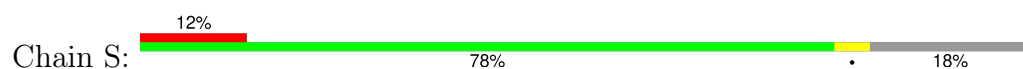
- Molecule 9: 37S ribosomal protein S17, mitochondrial

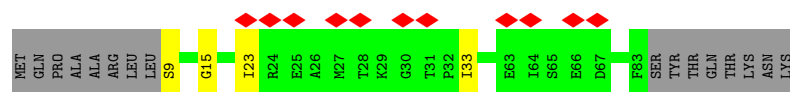


- Molecule 10: 37S ribosomal protein RSM18, mitochondrial

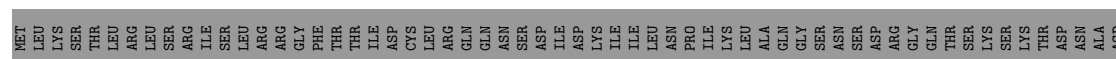


- Molecule 11: 37S ribosomal protein S19, mitochondrial

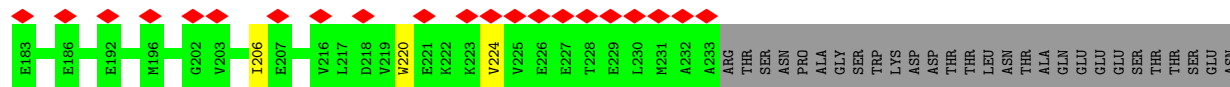
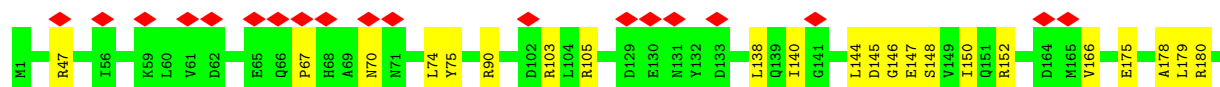
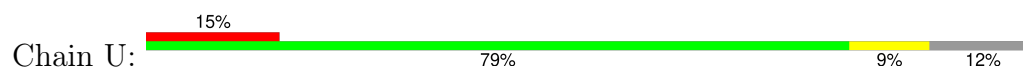




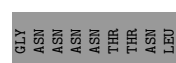
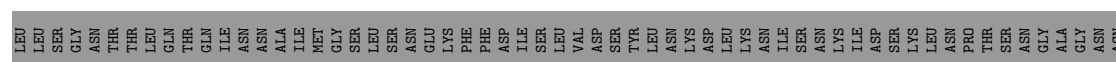
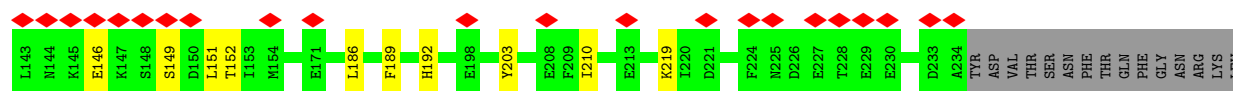
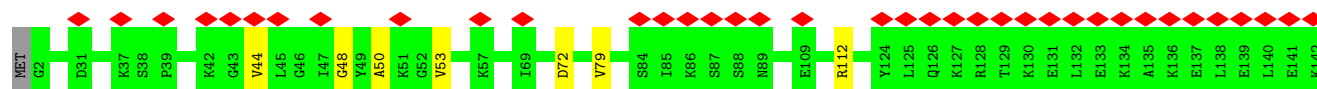
- Molecule 12: 37S ribosomal protein MRP21, mitochondrial



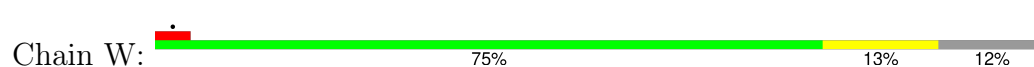
- Molecule 13: 37S ribosomal protein S25, mitochondrial



- Molecule 14: 37S ribosomal protein PET123, mitochondrial

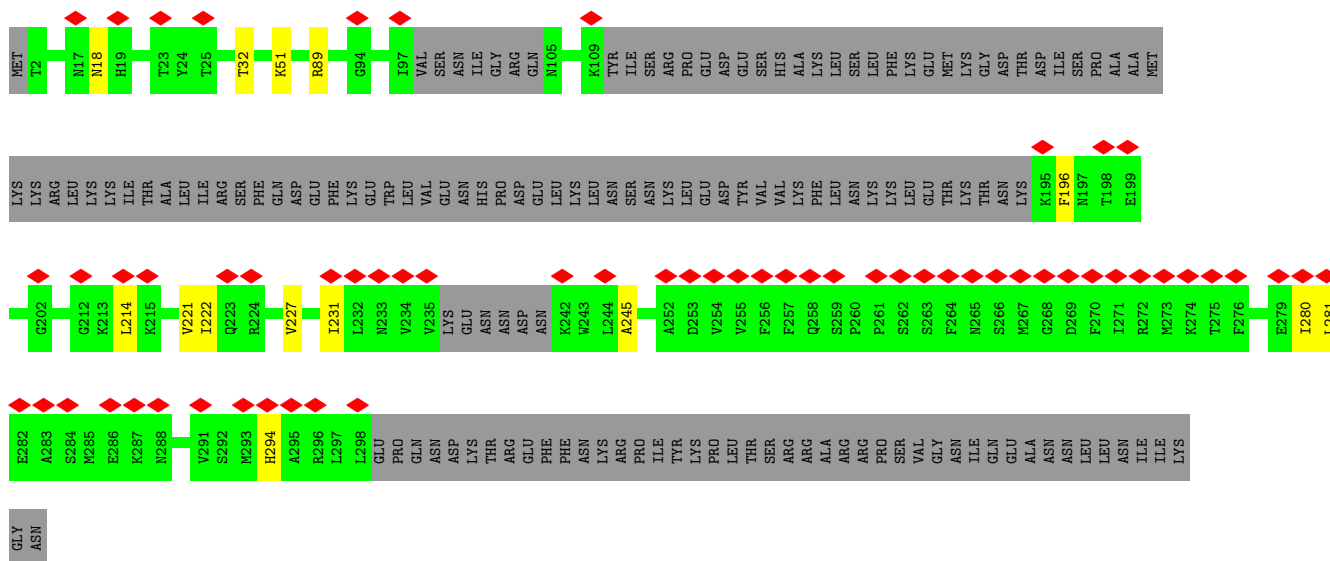


- Molecule 15: 37S ribosomal protein S23, mitochondrial

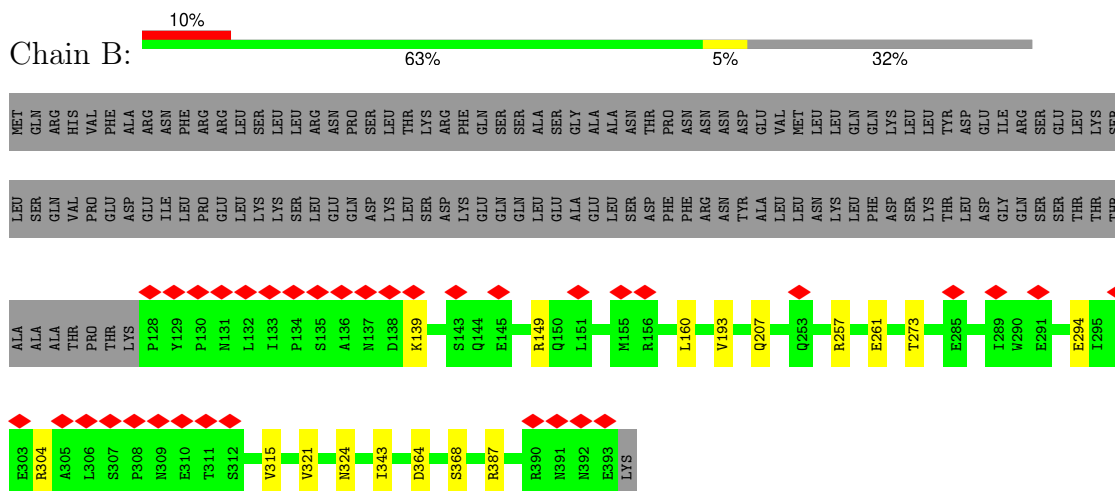




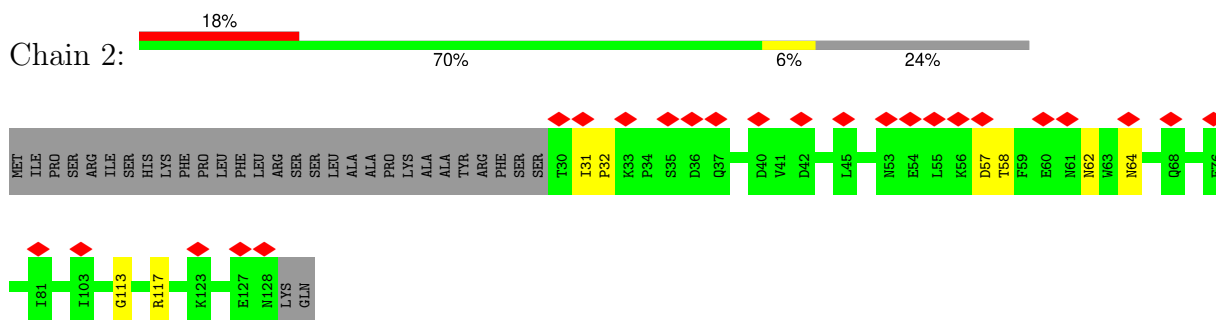




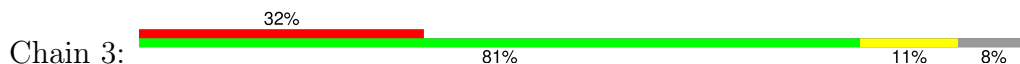
- Molecule 20: 37S ribosomal protein MRP4, mitochondrial



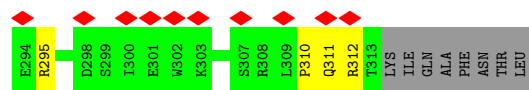
- Molecule 21: Protein FYV4, mitochondrial



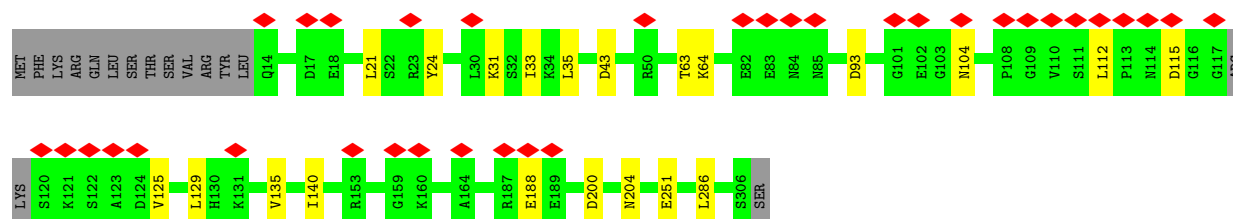
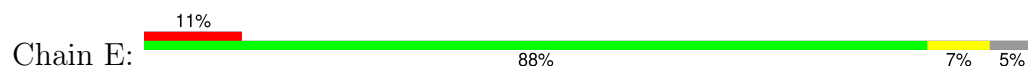
- Molecule 22: 37S ribosomal protein S26, mitochondrial



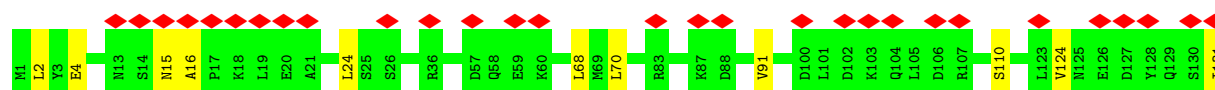
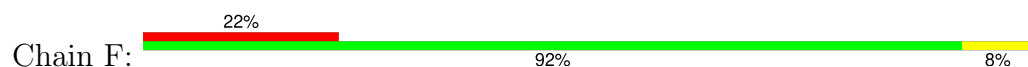




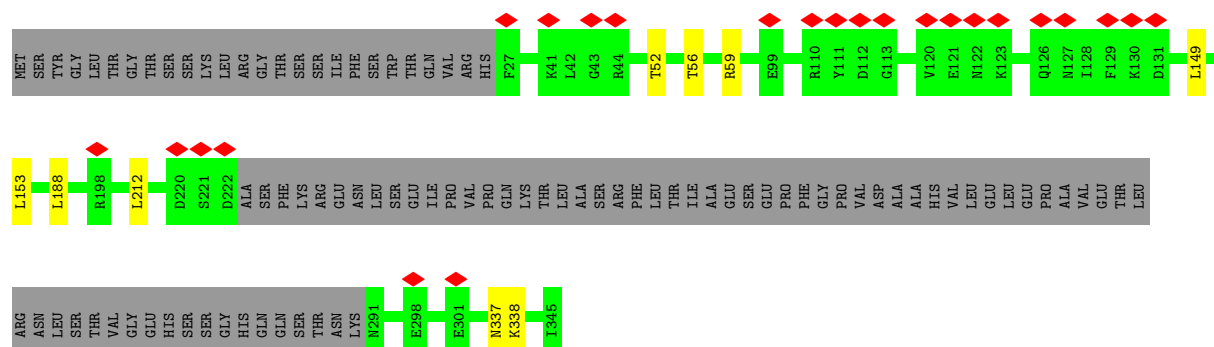
- Molecule 25: 37S ribosomal protein S5, mitochondrial



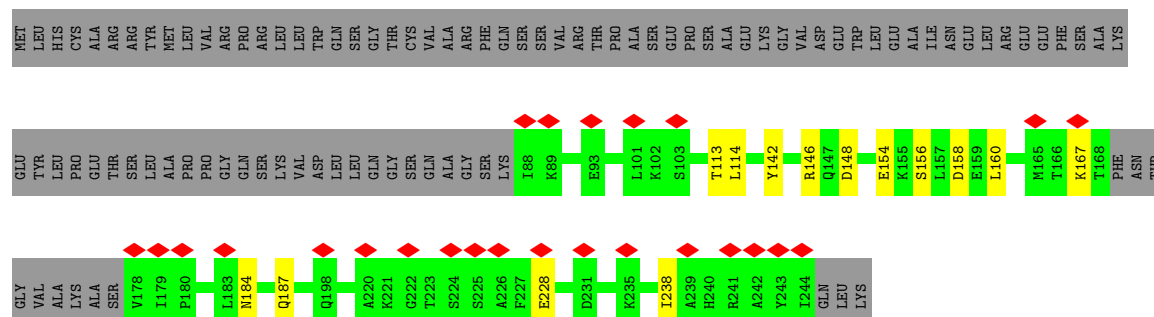
- Molecule 26: 37S ribosomal protein MRP17, mitochondrial



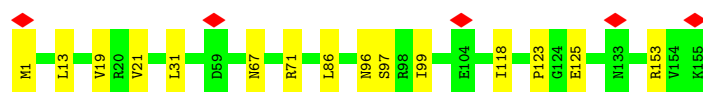
- Molecule 27: 37S ribosomal protein S35, mitochondrial



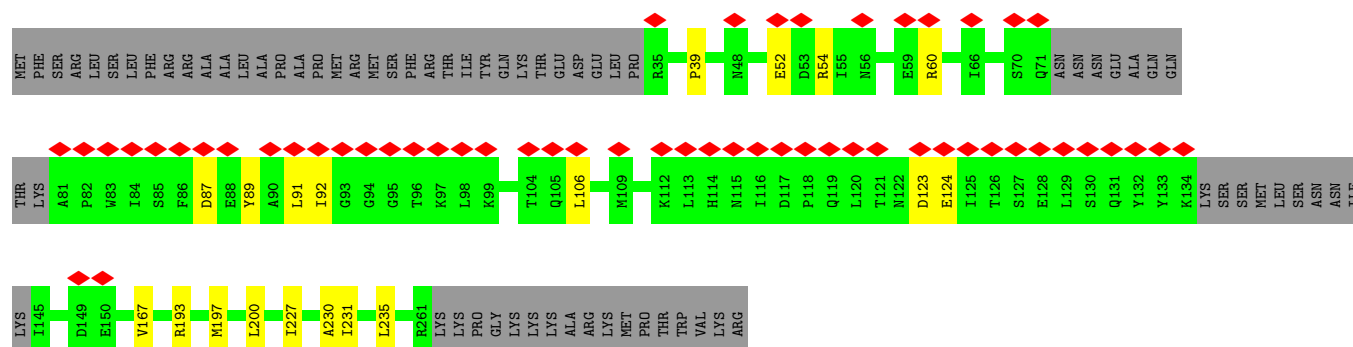
- Molecule 28: 37S ribosomal protein S7, mitochondrial



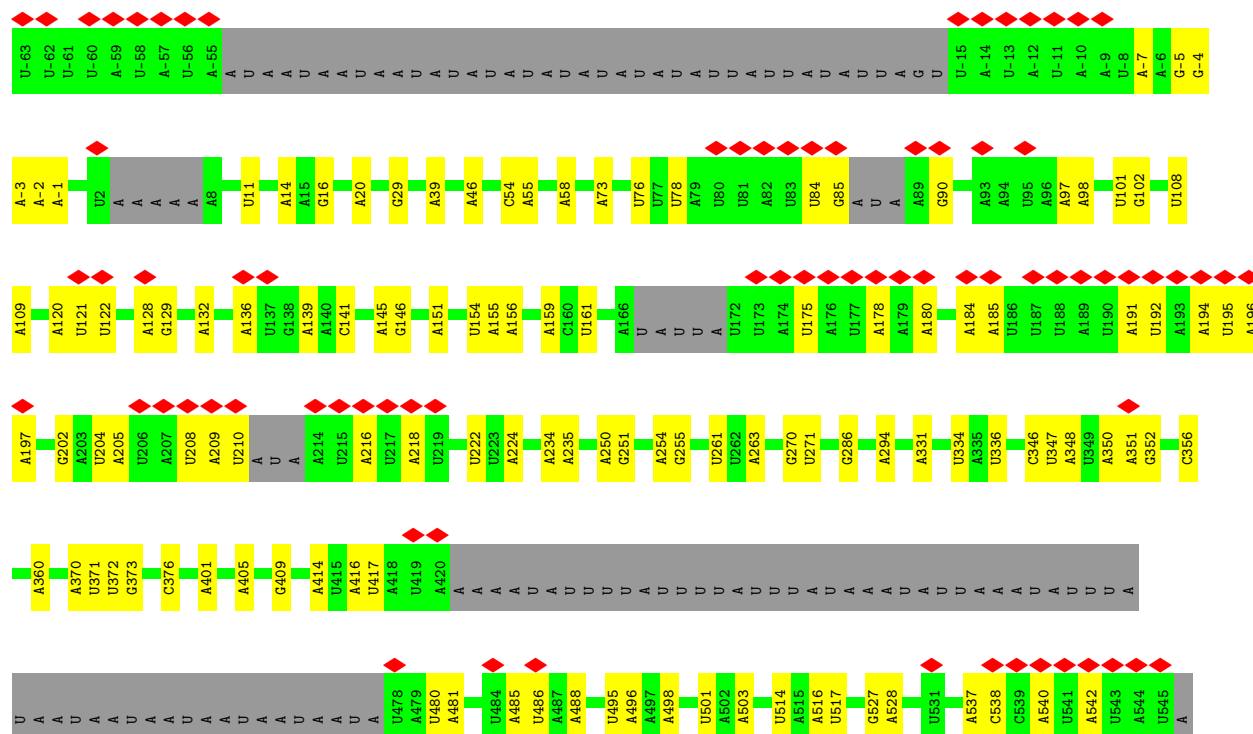
- Chain H:  90% 10%



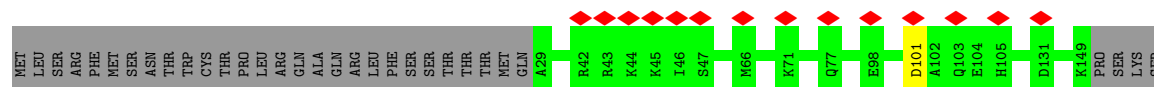
- Chain I:  20% 68% 7% 25%



- Chain a: 







## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	54519	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 ( $e^-/\text{\AA}^2$ )	61.73	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	64000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	24.070	Depositor
Minimum map value	-11.921	Depositor
Average map value	0.010	Depositor
Map value standard deviation	1.048	Depositor
Recommended contour level	4.5	Depositor
Map size (Å)	422.80002, 422.80002, 422.80002	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.057, 1.057, 1.057	Depositor



## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ATP, SF4

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	0.27	0/3544	0.55	0/4778
2	5	0.27	0/2249	0.52	0/3040
3	C	0.26	0/2040	0.46	0/2735
4	d	0.27	0/5612	0.51	0/7552
5	M	0.25	0/655	0.49	0/874
6	N	0.26	0/948	0.56	0/1267
7	O	0.25	0/1746	0.54	0/2335
8	P	0.26	0/934	0.60	0/1260
9	Q	0.27	0/1701	0.58	0/2262
10	R	0.25	0/749	0.58	0/998
11	S	0.26	0/610	0.55	0/824
12	T	0.26	0/771	0.56	0/1019
13	U	0.26	0/1950	0.51	0/2636
14	V	0.28	0/1900	0.53	0/2540
15	W	0.26	0/3239	0.49	1/4379 (0.0%)
16	X	0.27	0/788	0.53	0/1052
17	Y	0.27	0/2263	0.55	0/3053
18	Z	0.26	0/674	0.49	0/908
19	A	0.26	0/1621	0.55	0/2186
20	B	0.24	0/2128	0.51	0/2892
21	2	0.26	0/852	0.48	0/1142
22	3	0.26	0/2002	0.48	0/2721
23	D	0.26	0/2642	0.51	0/3561
24	4	0.40	2/2228 (0.1%)	0.63	3/3009 (0.1%)
25	E	0.25	0/2375	0.52	0/3201
26	F	0.26	0/1067	0.55	0/1430
27	6	0.26	0/2121	0.52	0/2856
28	G	0.25	0/1206	0.51	0/1630
29	H	0.25	0/1240	0.52	0/1670
30	I	0.25	0/1698	0.54	0/2287
31	a	0.22	0/36577	0.79	2/56897 (0.0%)
32	J	0.26	0/1216	0.52	0/1646

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
33	K	0.26	0/1128	0.56	0/1504
35	L	0.24	0/940	0.61	0/1261
All	All	0.25	2/93414 (0.0%)	0.66	6/133405 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	0	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	4	310	PRO	CG-CD	-12.78	1.08	1.50
24	4	310	PRO	N-CD	5.91	1.56	1.47

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	4	310	PRO	N-CD-CG	-13.95	82.27	103.20
24	4	310	PRO	CA-N-CD	-9.38	98.37	111.50
24	4	310	PRO	CA-CB-CG	-7.73	89.32	104.00
31	a	999	C	C6-N1-C2	-6.31	117.78	120.30
15	W	237	PRO	CA-N-CD	-6.10	102.95	111.50

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	310	GLU	Peptide

## 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	0	3471	0	3510	40	0
2	5	2199	0	2246	19	0
3	C	2014	0	2038	23	0
4	d	5497	0	5513	0	0
5	M	645	0	691	3	0
6	N	931	0	985	1	0
7	O	1724	0	1761	6	0
8	P	919	0	982	0	0
9	Q	1690	0	1776	23	0
10	R	738	0	771	4	0
11	S	595	0	618	2	0
12	T	760	0	791	4	0
13	U	1907	0	1898	16	0
14	V	1872	0	1978	14	0
15	W	3174	0	3270	38	0
16	X	774	0	823	14	0
17	Y	2208	0	2177	30	0
18	Z	660	0	684	3	0
19	A	1585	0	1618	11	0
20	B	2085	0	2094	13	0
21	2	833	0	839	4	0
22	3	1953	0	1913	18	0
23	D	2567	0	2630	12	0
24	4	2182	0	2172	11	0
25	E	2321	0	2327	15	0
26	F	1054	0	1129	8	0
27	6	2071	0	2099	6	0
28	G	1185	0	1234	10	0
29	H	1221	0	1289	10	0
30	I	1667	0	1719	11	0
31	a	32666	0	16387	0	0
32	J	1186	0	1193	7	0
33	K	1113	0	1161	9	0
34	c	470	0	103	0	0
35	L	926	0	980	1	0
36	0	8	0	0	0	0
37	B	1	0	0	0	0
37	Q	1	0	0	0	0
37	W	1	0	0	0	0
37	a	69	0	0	0	0
38	W	31	0	12	1	0
39	W	3	0	0	1	0
All	All	88977	0	73411	330	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 3.

The worst 5 of 330 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)
1:0:149:GLU:OE2	1:0:153:ARG:NH1	2.02	0.91
1:0:300:LEU:O	1:0:458:ARG:NH1	2.09	0.85
24:4:125:THR:O	24:4:153:ARG:NH2	2.10	0.85
13:U:145:ASP:O	13:U:148:SER:OG	1.98	0.81
15:W:350:ARG:NH1	15:W:352:ASN:OD1	2.17	0.77

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	0	421/628 (67%)	405 (96%)	16 (4%)	0	100	100
2	5	264/339 (78%)	260 (98%)	4 (2%)	0	100	100
3	C	227/398 (57%)	224 (99%)	3 (1%)	0	100	100
4	d	652/864 (76%)	639 (98%)	13 (2%)	0	100	100
5	M	81/143 (57%)	81 (100%)	0	0	100	100
6	N	111/115 (96%)	111 (100%)	0	0	100	100
7	O	206/286 (72%)	205 (100%)	1 (0%)	0	100	100
8	P	112/121 (93%)	110 (98%)	2 (2%)	0	100	100
9	Q	195/237 (82%)	195 (100%)	0	0	100	100
10	R	87/138 (63%)	85 (98%)	2 (2%)	0	100	100
11	S	73/91 (80%)	72 (99%)	1 (1%)	0	100	100
12	T	90/177 (51%)	88 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	U	231/264 (88%)	229 (99%)	2 (1%)	0	100	100
14	V	231/318 (73%)	228 (99%)	3 (1%)	0	100	100
15	W	393/450 (87%)	386 (98%)	7 (2%)	0	100	100
16	X	94/110 (86%)	94 (100%)	0	0	100	100
17	Y	259/319 (81%)	252 (97%)	7 (3%)	0	100	100
18	Z	80/95 (84%)	79 (99%)	1 (1%)	0	100	100
19	A	191/344 (56%)	189 (99%)	2 (1%)	0	100	100
20	B	264/394 (67%)	260 (98%)	4 (2%)	0	100	100
21	2	97/130 (75%)	97 (100%)	0	0	100	100
22	3	240/266 (90%)	234 (98%)	6 (2%)	0	100	100
23	D	302/486 (62%)	298 (99%)	4 (1%)	0	100	100
24	4	265/321 (83%)	256 (97%)	9 (3%)	0	100	100
25	E	287/307 (94%)	279 (97%)	8 (3%)	0	100	100
26	F	129/131 (98%)	124 (96%)	5 (4%)	0	100	100
27	6	247/345 (72%)	243 (98%)	4 (2%)	0	100	100
28	G	144/247 (58%)	143 (99%)	1 (1%)	0	100	100
29	H	153/155 (99%)	152 (99%)	1 (1%)	0	100	100
30	I	202/278 (73%)	200 (99%)	2 (1%)	0	100	100
32	J	138/203 (68%)	133 (96%)	5 (4%)	0	100	100
33	K	137/217 (63%)	135 (98%)	2 (2%)	0	100	100
35	L	119/153 (78%)	119 (100%)	0	0	100	100
All	All	6722/9070 (74%)	6605 (98%)	117 (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	0	382/564 (68%)	382 (100%)	0	100	100
2	5	239/303 (79%)	239 (100%)	0	100	100
3	C	237/385 (62%)	237 (100%)	0	100	100
4	d	610/803 (76%)	609 (100%)	1 (0%)	92	96
5	M	69/121 (57%)	69 (100%)	0	100	100
6	N	101/103 (98%)	101 (100%)	0	100	100
7	O	183/250 (73%)	183 (100%)	0	100	100
8	P	101/106 (95%)	101 (100%)	0	100	100
9	Q	188/218 (86%)	188 (100%)	0	100	100
10	R	80/121 (66%)	80 (100%)	0	100	100
11	S	64/78 (82%)	64 (100%)	0	100	100
12	T	81/159 (51%)	80 (99%)	1 (1%)	67	81
13	U	208/236 (88%)	206 (99%)	2 (1%)	73	85
14	V	208/287 (72%)	208 (100%)	0	100	100
15	W	363/409 (89%)	362 (100%)	1 (0%)	91	95
16	X	84/92 (91%)	81 (96%)	3 (4%)	30	57
17	Y	242/289 (84%)	242 (100%)	0	100	100
18	Z	75/85 (88%)	75 (100%)	0	100	100
19	A	174/309 (56%)	174 (100%)	0	100	100
20	B	233/350 (67%)	233 (100%)	0	100	100
21	2	90/117 (77%)	90 (100%)	0	100	100
22	3	216/240 (90%)	216 (100%)	0	100	100
23	D	277/437 (63%)	277 (100%)	0	100	100
24	4	239/281 (85%)	238 (100%)	1 (0%)	89	94
25	E	250/266 (94%)	250 (100%)	0	100	100
26	F	120/120 (100%)	120 (100%)	0	100	100
27	6	230/312 (74%)	230 (100%)	0	100	100
28	G	128/211 (61%)	127 (99%)	1 (1%)	79	88
29	H	142/142 (100%)	142 (100%)	0	100	100
30	I	180/245 (74%)	179 (99%)	1 (1%)	84	91
32	J	130/183 (71%)	130 (100%)	0	100	100
33	K	121/192 (63%)	121 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
35	L	100/131 (76%)	100 (100%)	0	100	100
All	All	6145/8145 (75%)	6134 (100%)	11 (0%)	91	96

5 of 11 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
16	X	92	LYS
24	4	16	ARG
30	I	60	ARG
28	G	167	LYS
15	W	273	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
29	H	67	ASN
25	E	198	HIS
17	Y	113	GLN
24	4	21	HIS
15	W	188	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
31	a	1524/1713 (88%)	365 (23%)	0

5 of 365 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
31	a	-7	A
31	a	-5	G
31	a	-4	G
31	a	-3	A
31	a	-2	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 74 ligands modelled in this entry, 72 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	$\# Z  > 2$
36	SF4	0	701	1	0,12,12	-	-	-		
38	ATP	W	501	37	28,33,33	0.65	0	34,52,52	0.93	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
36	SF4	0	701	1	-	-	0/6/5/5
38	ATP	W	501	37	-	2/18/38/38	0/3/3/3

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	W	501	ATP	C5-C6-N6	2.31	123.83	120.31
38	W	501	ATP	O3'-C3'-C4'	-2.08	105.10	111.08

There are no chirality outliers.



All (2) torsion outliers are listed below:

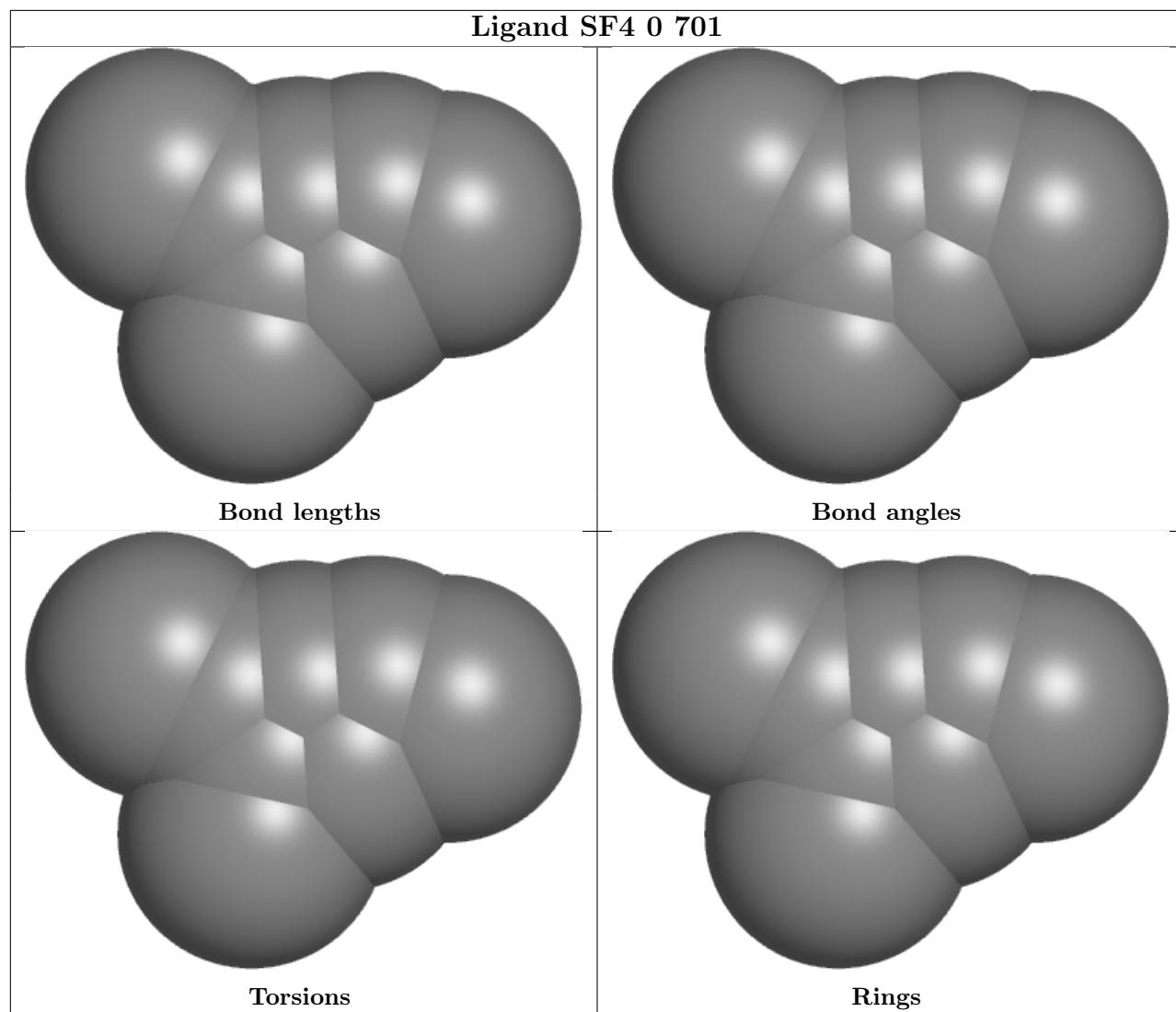
Mol	Chain	Res	Type	Atoms
38	W	501	ATP	O4'-C4'-C5'-O5'
38	W	501	ATP	C3'-C4'-C5'-O5'

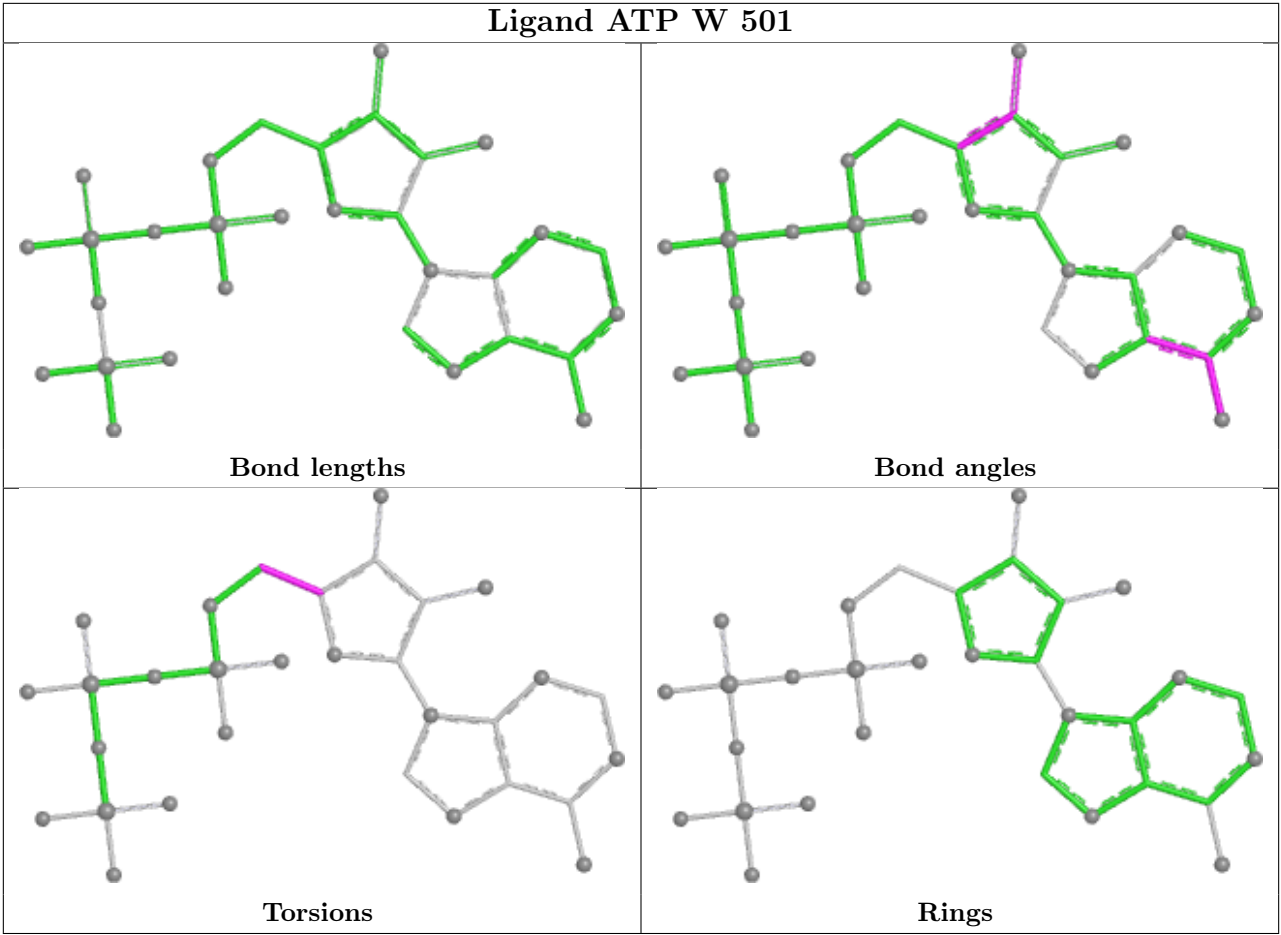
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
38	W	501	ATP	1	0

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





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
34	c	3

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	c	59:UNK	C	76:UNK	N	23.27
1	c	93:UNK	C	105:UNK	N	20.76
1	c	37:UNK	C	40:UNK	N	10.25

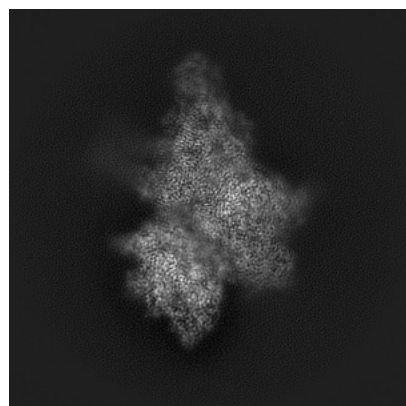
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-27250. These allow visual inspection of the internal detail of the map and identification of artifacts.

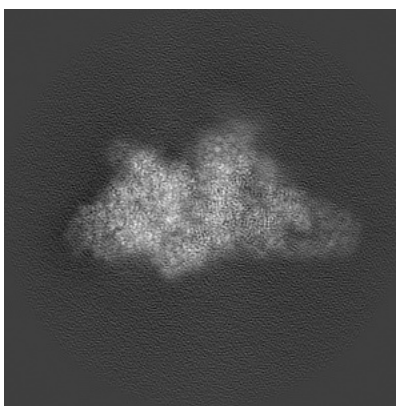
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

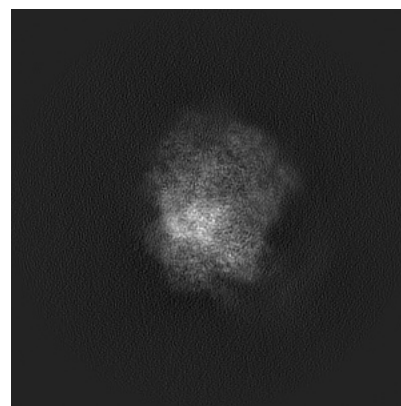
#### 6.1.1 Primary map



X

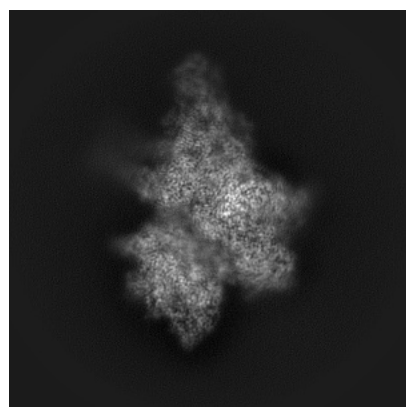


Y

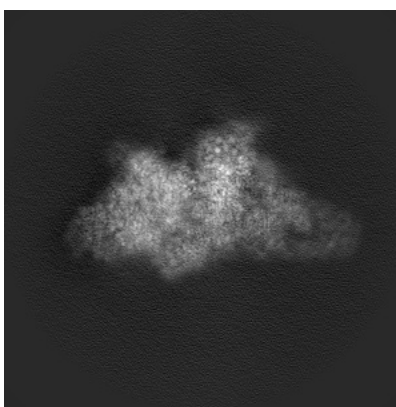


Z

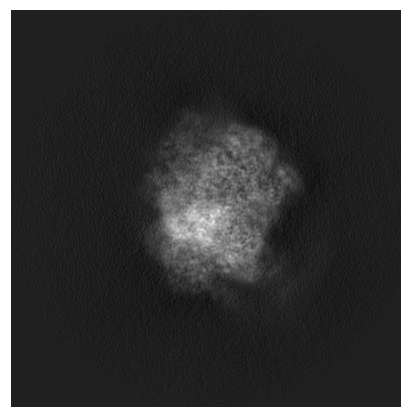
#### 6.1.2 Raw map



X



Y

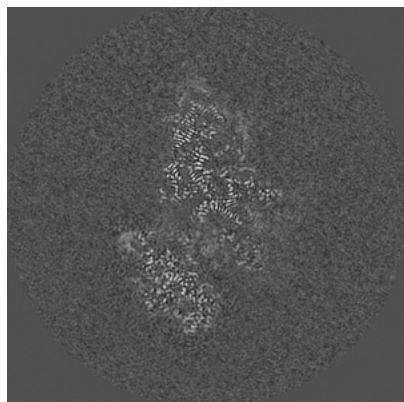


Z

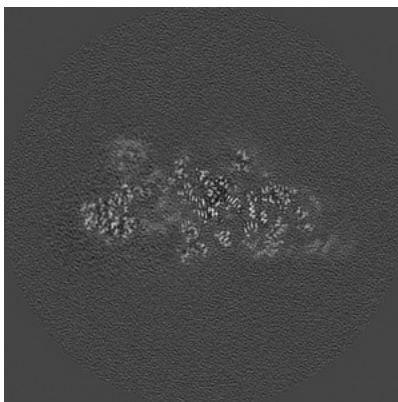
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

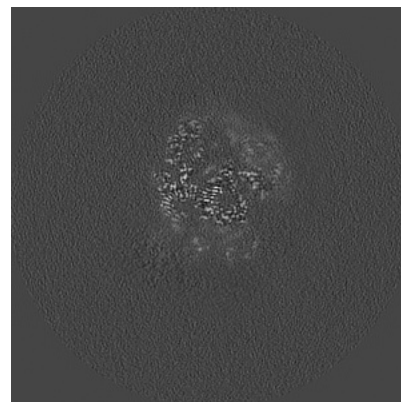
### 6.2.1 Primary map



X Index: 200

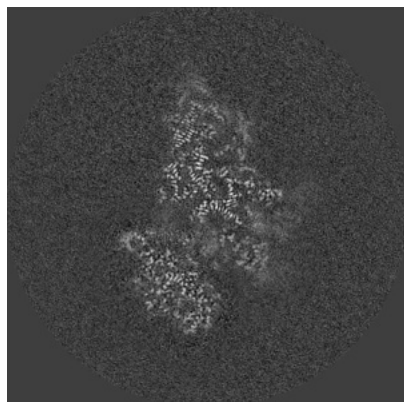


Y Index: 200

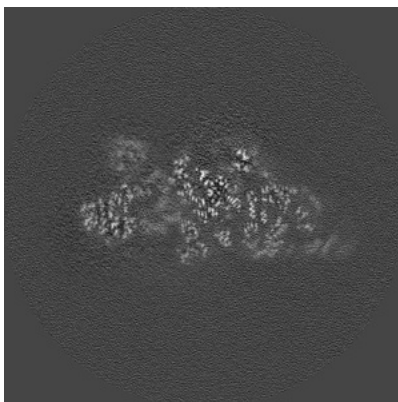


Z Index: 200

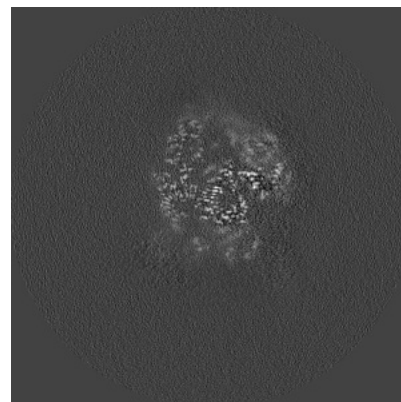
### 6.2.2 Raw map



X Index: 200



Y Index: 200

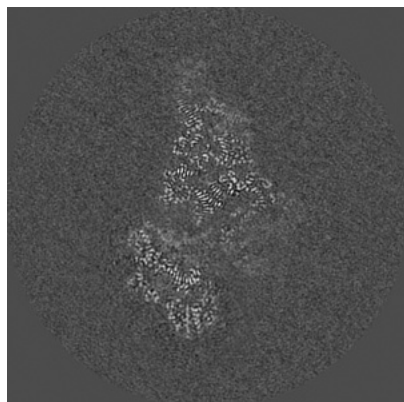


Z Index: 200

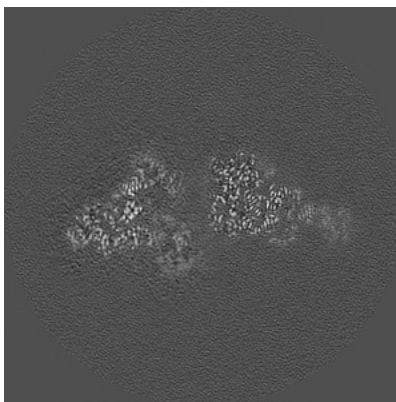
The images above show central slices of the map in three orthogonal directions.

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

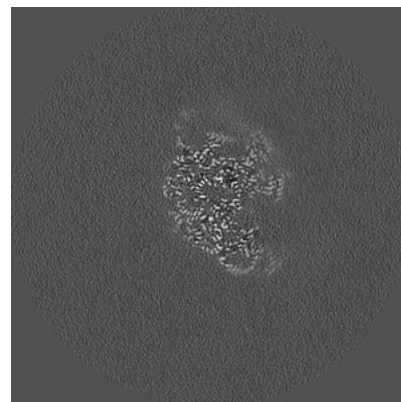
### 6.3.1 Primary map



X Index: 191

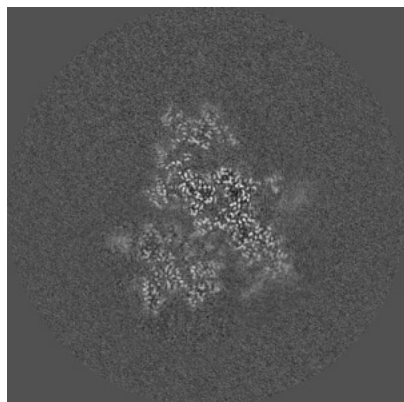


Y Index: 173

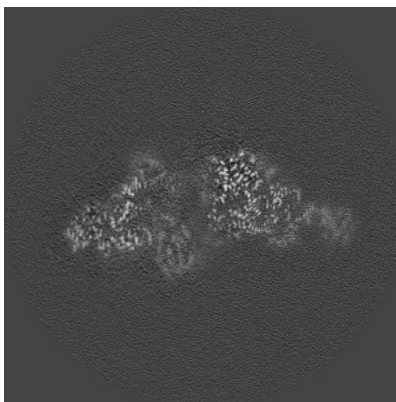


Z Index: 215

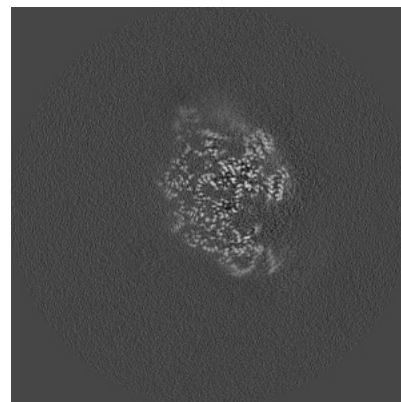
### 6.3.2 Raw map



X Index: 216



Y Index: 174



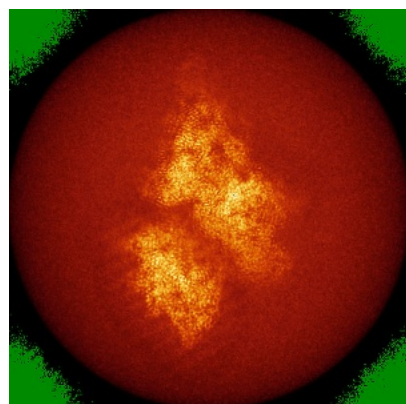
Z Index: 213

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

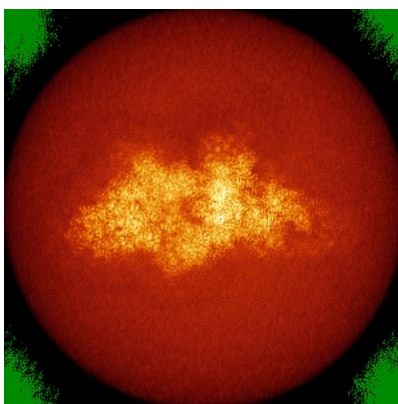


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

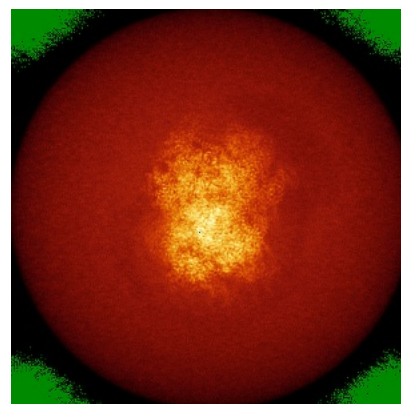
### 6.4.1 Primary map



X

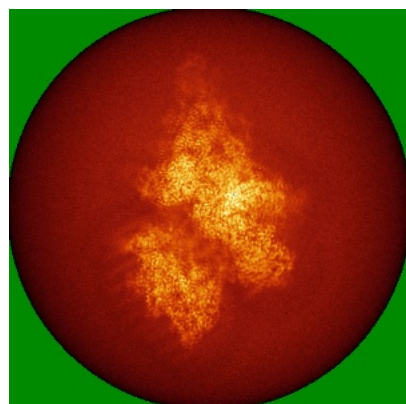


Y

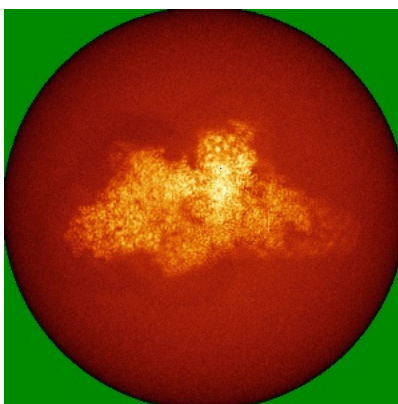


Z

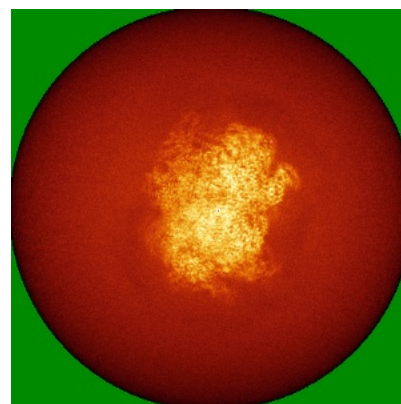
### 6.4.2 Raw map



X



Y

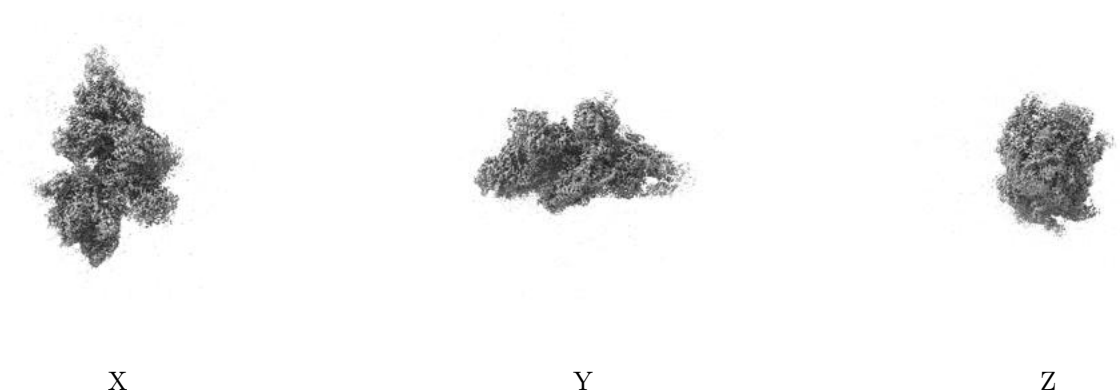


Z

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



The images above show the 3D surface view of the map at the recommended contour level 4.5. 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



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.



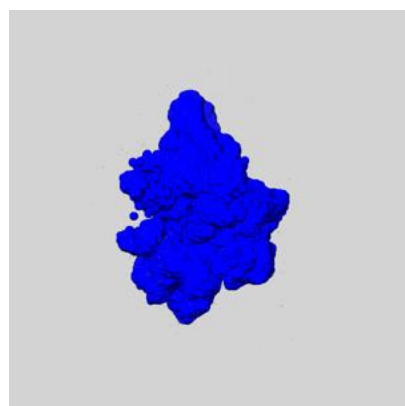
## 6.6 Mask visualisation [i](#)

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

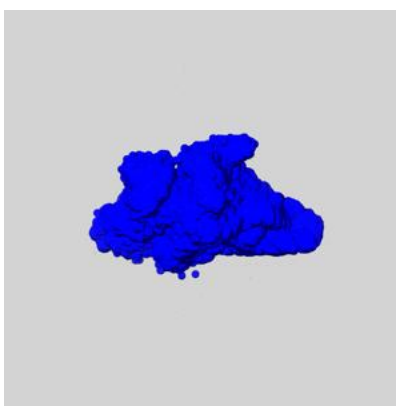
A mask typically either:

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

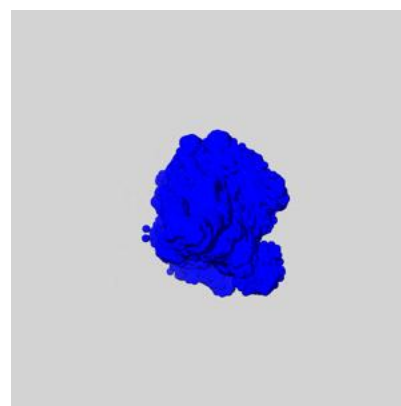
### 6.6.1 emd\_27250\_msk\_1.map [i](#)



X



Y

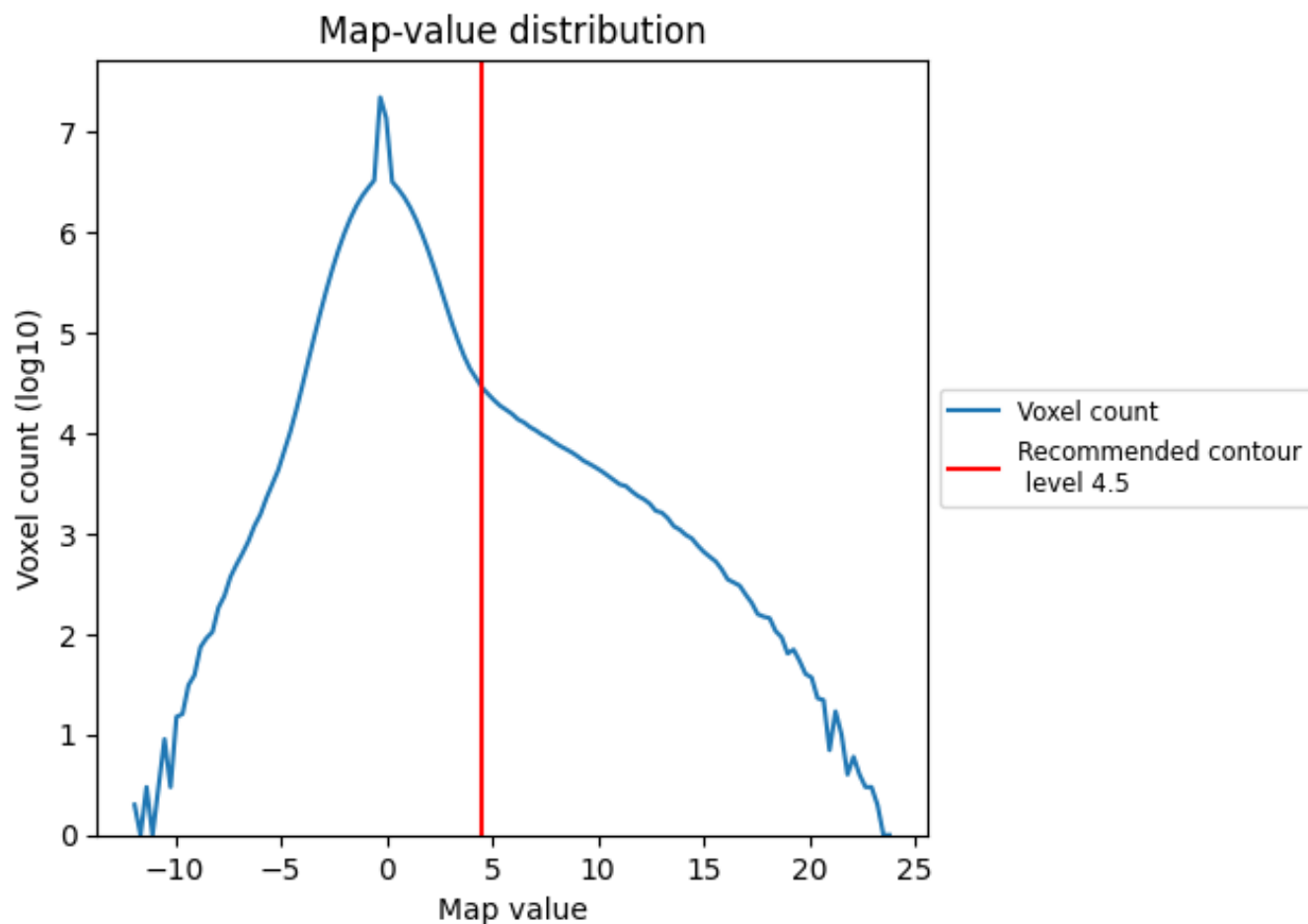


Z

## 7 Map analysis [i](#)

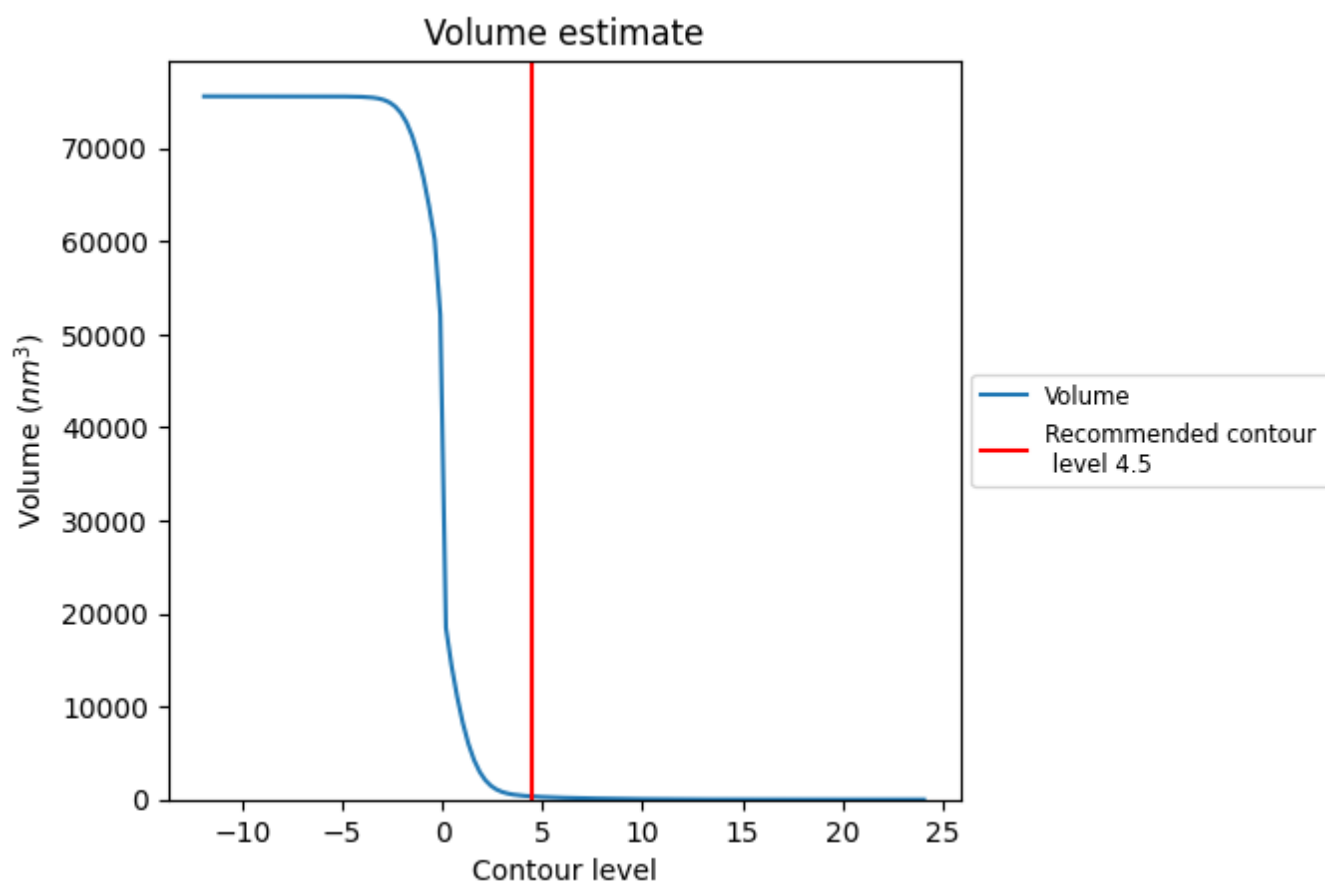
This section contains the results of statistical analysis of the map.

### 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.

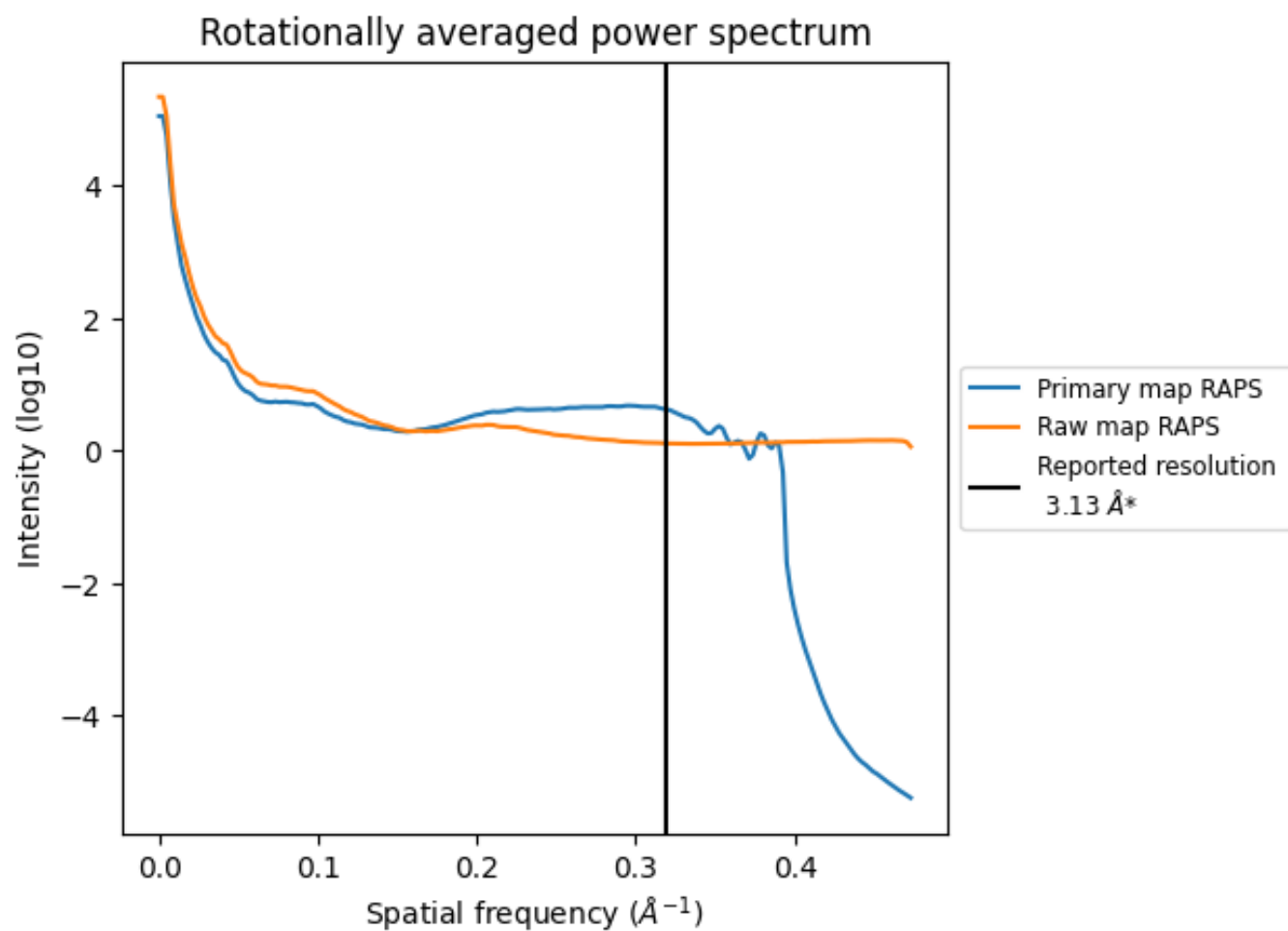
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 337 nm<sup>3</sup>; this corresponds to an approximate mass of 305 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 ⓘ

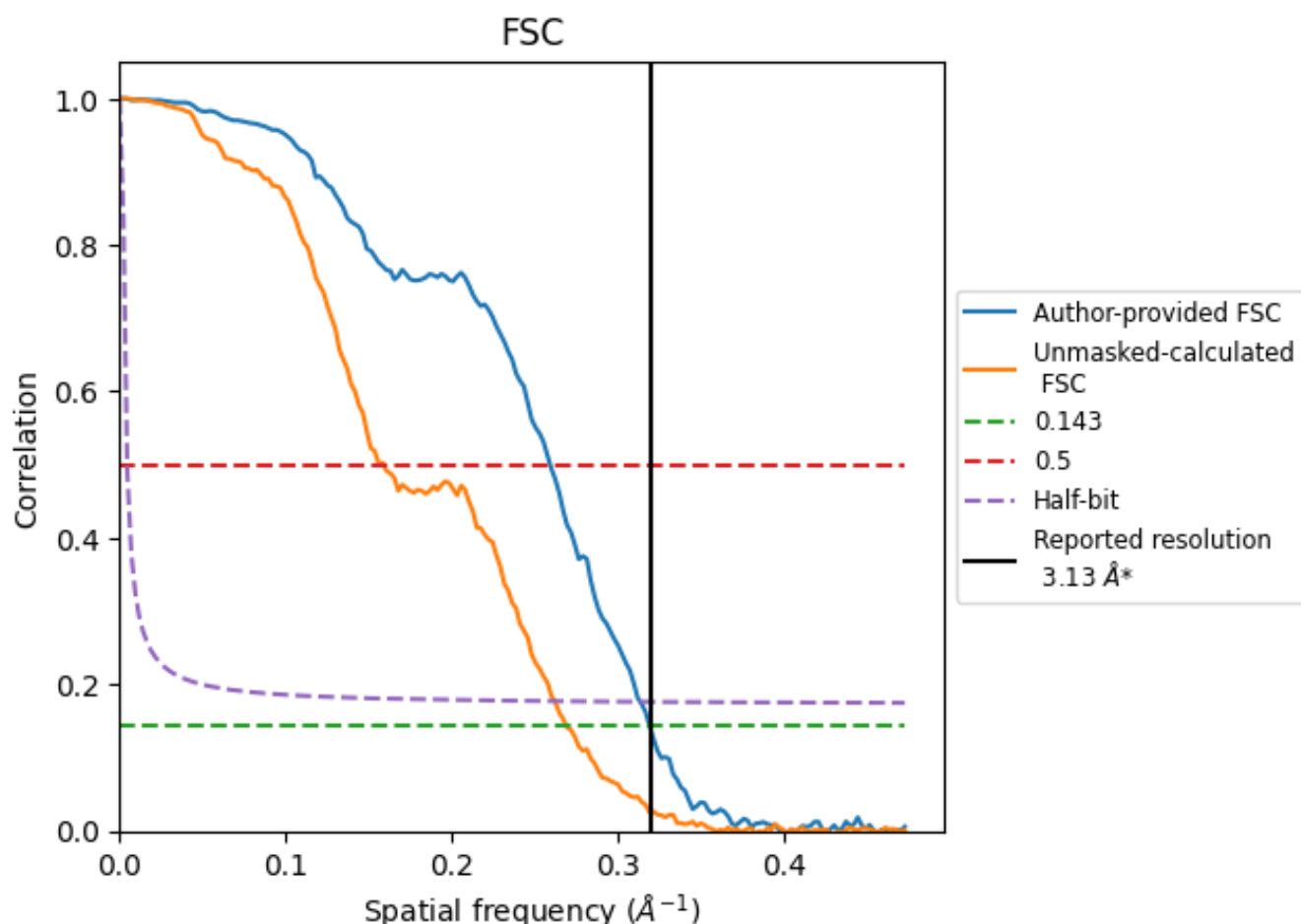


\*Reported resolution corresponds to spatial frequency of 0.319 Å<sup>-1</sup>

## 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 0.319 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

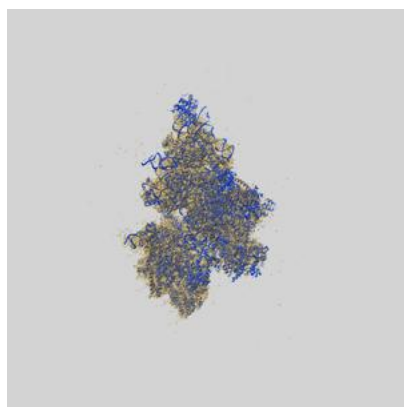
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.13	-	-
Author-provided FSC curve	3.13	3.86	3.19
Unmasked-calculated*	3.71	6.29	3.81

\*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 3.71 differs from the reported value 3.13 by more than 10 %

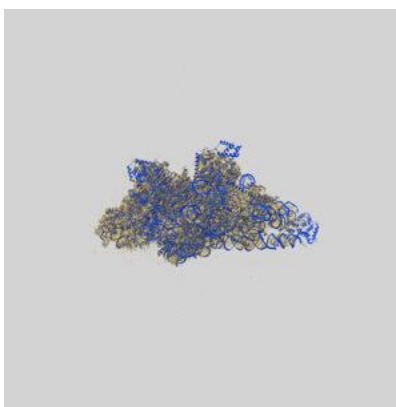
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-27250 and PDB model 8D8K. Per-residue inclusion information can be found in [section 3](#) on [page 12](#).

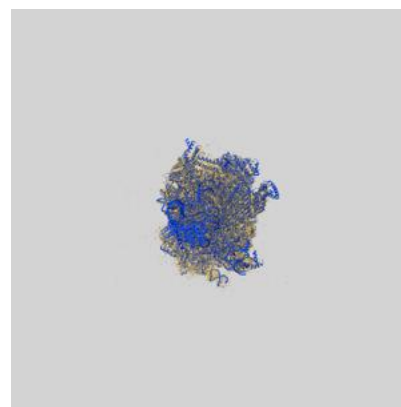
### 9.1 Map-model overlay [i](#)



X



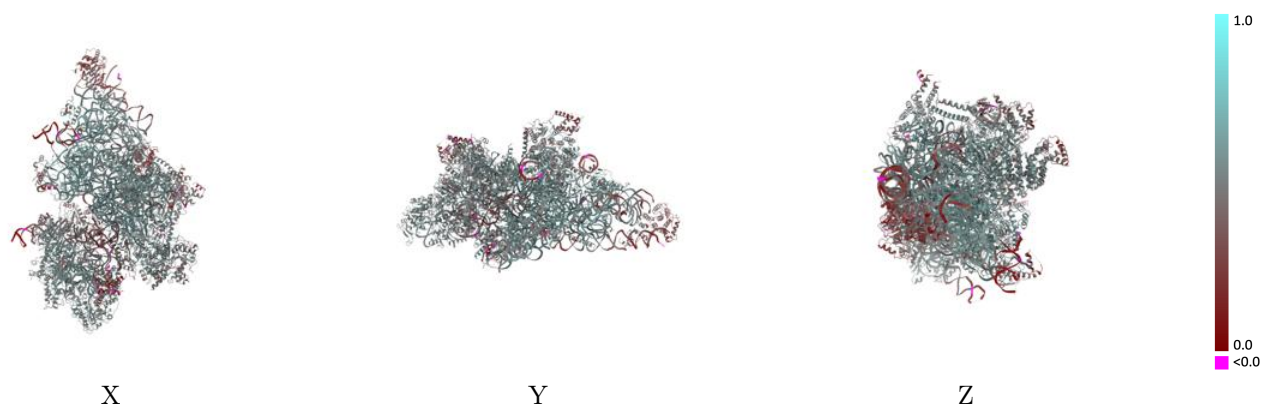
Y



Z

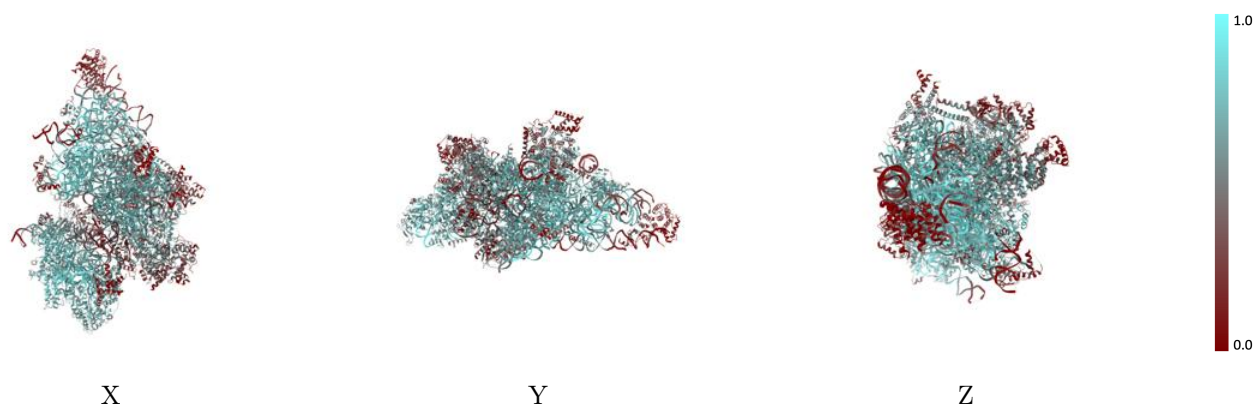
The images above show the 3D surface view of the map at the recommended contour level 4.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 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.

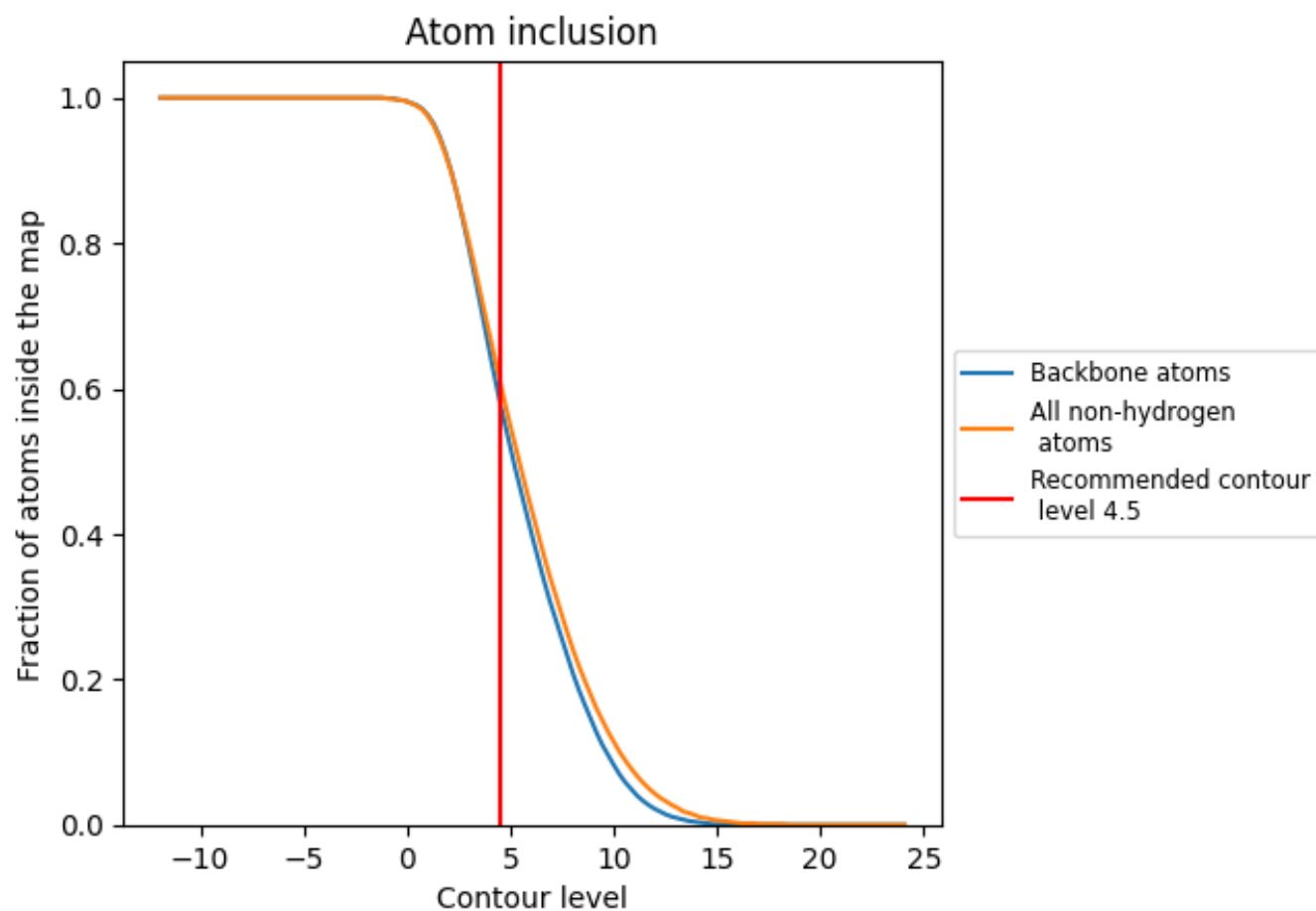
## 9.3 Atom inclusion mapped to coordinate model [i](#)



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 (4.5).











































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 58% of all backbone atoms, 61% 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 (4.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6100	 0.5080
0	 0.3570	 0.3560
2	 0.5740	 0.5350
3	 0.5140	 0.5260
4	 0.3280	 0.4690
5	 0.1050	 0.3390
6	 0.7170	 0.5790
A	 0.5470	 0.5460
B	 0.6880	 0.5710
C	 0.6320	 0.4980
D	 0.6830	 0.5500
E	 0.6960	 0.5620
F	 0.5660	 0.5390
G	 0.6230	 0.4990
H	 0.8140	 0.6110
I	 0.6030	 0.5200
J	 0.7730	 0.5460
K	 0.4730	 0.5230
L	 0.6730	 0.5730
M	 0.6240	 0.4930
N	 0.7780	 0.5440
O	 0.6520	 0.5670
P	 0.6920	 0.5750
Q	 0.4580	 0.4940
R	 0.6100	 0.5700
S	 0.6830	 0.4950
T	 0.5120	 0.4950
U	 0.6270	 0.5560
V	 0.5520	 0.5290
W	 0.7060	 0.5360
X	 0.6800	 0.5080
Y	 0.6520	 0.4930
Z	 0.3430	 0.5010
a	 0.7000	 0.5060
c	 0.2040	 0.2480
d	 0.4440	 0.4920

