



## wwPDB EM Validation Summary Report ⓘ

Dec 12, 2022 – 10:10 am GMT

PDB ID : 6YWV  
EMDB ID : EMD-10977  
Title : The structure of the Atp25 bound assembly intermediate of the mitoribosome from *Neurospora crassa*  
Authors : Amunts, A.; Itoh, Y.; Naschberger, A.  
Deposited on : 2020-04-30  
Resolution : 3.03 Å (reported)

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

We welcome your comments at [validation@mail.wwpdb.org](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:

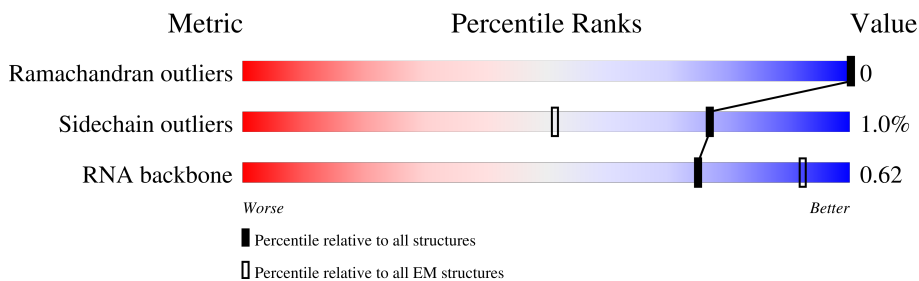
EMDB validation analysis : 0.0.1.dev43  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry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

# 1 Overall quality at a glance i

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

The reported resolution of this entry is 3.03 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	A	3464	
2	B	383	
3	C	384	
4	D	325	
5	E	352	
6	F	255	
7	f	347	
8	g	158	

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Mol	Chain	Length	Quality of chain
9	H	183	100%
10	I	131	88% 9%
11	J	312	77% 22%
12	K	249	63% 37%
13	L	193	98%
14	M	258	74% 25%
15	N	217	61% 39%
16	O	364	74% 25%
17	P	228	79% 21%
18	Q	396	89% 11%
19	R	447	51% 48%
20	S	274	65% 35%
21	T	263	65% 35%
22	U	161	86% 14%
23	V	219	25% 74%
24	W	129	46% 54%
25	X	59	81% 19%
26	Y	140	32% 67%
27	0	124	37% 63%
28	1	449	81% 18%
29	2	370	33% 67%
30	3	103	90% 8%
31	4	138	99%
32	5	439	79% 20%
33	6	368	73% 26%

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Mol	Chain	Length	Quality of chain
34	7	165	50% 49%
35	8	443	9% 74% 25%
36	h	98	96% 96%
37	i	218	53% 56% 44%
38	9	267	77% 23%
39	a	225	71% 28%
40	b	162	6% 99%
41	c	110	88% 11%
42	d	292	80% 20%
43	n	699	26% 73%

## 2 Entry composition [i](#)

There are 48 unique types of molecules in this entry. The entry contains 207611 atoms, of which 91129 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 RNA chain called 23 S rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
1	A	2529	81042	24198	27083	9701	17531	2529	0	0

- Molecule 2 is a protein called 60S ribosomal protein L2.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
2	B	317	4997	1541	2519	497	425	15	0	0

- Molecule 3 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
3	C	307	4759	1468	2423	447	413	8	0	0

- Molecule 4 is a protein called 60S ribosomal protein L4, variant.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
4	D	254	4068	1280	2040	372	371	5	0	0

- Molecule 5 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
5	E	309	4910	1558	2461	436	443	12	0	0

- Molecule 6 is a protein called 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
6	F	201	3253	1022	1645	290	288	8	0	0

- Molecule 7 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
7	f	245	3801	1202	1925	325	346	3	0	0

- Molecule 8 is a protein called 60S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
8	g	147	2257	700	1154	203	196	4	0	0

- Molecule 9 is a protein called Ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
9	H	183	2885	899	1459	268	251	8	0	0

- Molecule 10 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
10	I	119	1898	564	985	182	159	8	0	0

- Molecule 11 is a protein called 50S ribosomal subunit protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
11	J	243	3827	1198	1939	346	343	1	0	0

- Molecule 12 is a protein called 60S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
12	K	157	2591	805	1319	246	217	4	0	0

- Molecule 13 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
13	L	192	3135	960	1590	294	285	6	0	0

- Molecule 14 is a protein called Mitochondrial ribosomal protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
14	M	194	3164	981	1628	292	253	10	0	0

- Molecule 15 is a protein called Aconitate hydratase.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
15	N	133	2176	673	1120	195	182	6	0	0

- Molecule 16 is a protein called Mitochondrial large ribosomal subunit.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
16	O	272	4532	1392	2323	424	387	6	0	0

- Molecule 17 is a protein called Mitochondrial ribosomal protein subunit L23.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
17	P	180	2975	953	1494	270	254	4	0	0

- Molecule 18 is a protein called KOW domain-containing protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
18	Q	353	5829	1786	2961	547	524	11	0	0

- Molecule 19 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
19	R	231	3851	1184	1968	372	323	4	0	0

- Molecule 20 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
20	S	179	2979	937	1507	281	252	2	0	0

- Molecule 21 is a protein called 54S ribosomal protein L4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
21	T	171	Total	C	H	N	O	S	0	0
			2782	886	1366	260	267	3		

- Molecule 22 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace	
22	U	138	Total	C	H	N	O	S	0	0
			2263	698	1164	213	185	3		

- Molecule 23 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms					AltConf	Trace	
23	V	56	Total	C	H	N	O	S	0	0
			921	291	462	85	82	1		

- Molecule 24 is a protein called Mitochondrial ribosomal protein subunit L32.

Mol	Chain	Residues	Atoms					AltConf	Trace	
24	W	59	Total	C	H	N	O	S	0	0
			950	282	490	98	72	8		

- Molecule 25 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms					AltConf	Trace	
25	X	48	Total	C	H	N	O	S	0	0
			836	263	433	71	65	4		

- Molecule 26 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms					AltConf	Trace	
26	Y	46	Total	C	H	N	O	S	0	0
			777	224	412	84	56	1		

- Molecule 27 is a protein called Ribosomal protein.

Mol	Chain	Residues	Atoms					AltConf	Trace	
27	0	46	Total	C	H	N	O	S	0	0
			797	240	409	86	58	4		

- Molecule 28 is a protein called Mitochondrial large ribosomal subunit YmL35.



Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
28	1	367	6014	1899	3029	547	531	8	0	0

- Molecule 29 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
29	2	123	2101	660	1055	211	171	4	0	0

- Molecule 30 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
30	3	95	1536	489	773	135	137	2	0	0

- Molecule 31 is a protein called Mitochondrial ribosomal protein L43.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
31	4	137	2139	671	1087	192	183	6	0	0

- Molecule 32 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
32	5	350	5429	1740	2710	477	493	9	0	0

- Molecule 33 is a protein called 50S ribosomal subunit L30.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
33	6	273	4474	1418	2248	399	401	8	0	0

- Molecule 34 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			
34	7	84	1383	431	709	130	113		0	0

- Molecule 35 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
35	8	331	5374	1683	2714	480	489	8	0	0

- Molecule 36 is a protein called Mitochondrial ribosomal protein L44.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
36	h	94	1525	474	774	134	139	4	0	0

- Molecule 37 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
37	i	121	1949	599	995	177	174	4	0	0

- Molecule 38 is a protein called RNase III domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
38	9	206	3341	1051	1698	295	290	7	0	0

- Molecule 39 is a protein called 60S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
39	a	161	2671	837	1340	253	235	6	0	0

- Molecule 40 is a protein called Mitochondrial 60S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
40	b	161	2693	840	1379	249	221	4	0	0

- Molecule 41 is a protein called 54S ribosomal protein L31, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
41	c	98	1700	528	873	162	134	3	0	0

- Molecule 42 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
42	d	235	3797	1180	1909	363	339	6	0	0

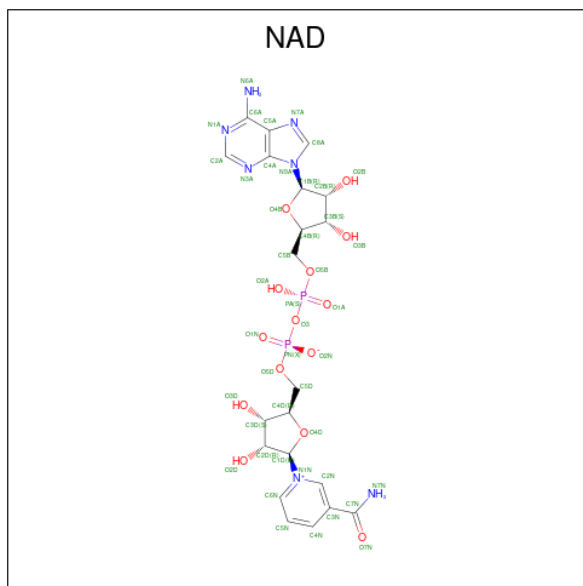
- Molecule 43 is a protein called ATPase synthesis protein 25, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
43	n	186	2951	913	1505	261	265	7	0	0

- Molecule 44 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

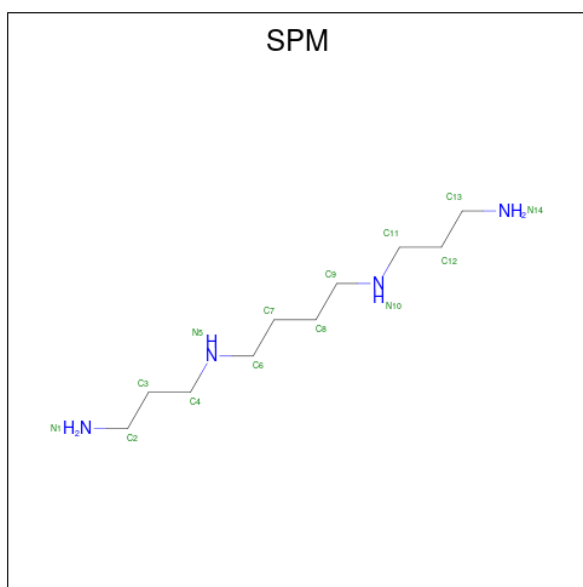
Mol	Chain	Residues	Atoms		AltConf
44	A	142	Total	Mg	0
			142	142	
44	K	1	Total	Mg	0
			1	1	
44	c	1	Total	Mg	0
			1	1	

- Molecule 45 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: C<sub>21</sub>H<sub>27</sub>N<sub>7</sub>O<sub>14</sub>P<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
			Total	C	H	N	O	P	
45	A	1	70	21	26	7	14	2	0

- Molecule 46 is SPERMINE (three-letter code: SPM) (formula: C<sub>10</sub>H<sub>26</sub>N<sub>4</sub>).



Mol	Chain	Residues	Atoms			AltConf	
			Total	C	H		N
46	A	1	40	10	26	4	0

- Molecule 47 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
			Total	K	
47	A	23	23	23	0

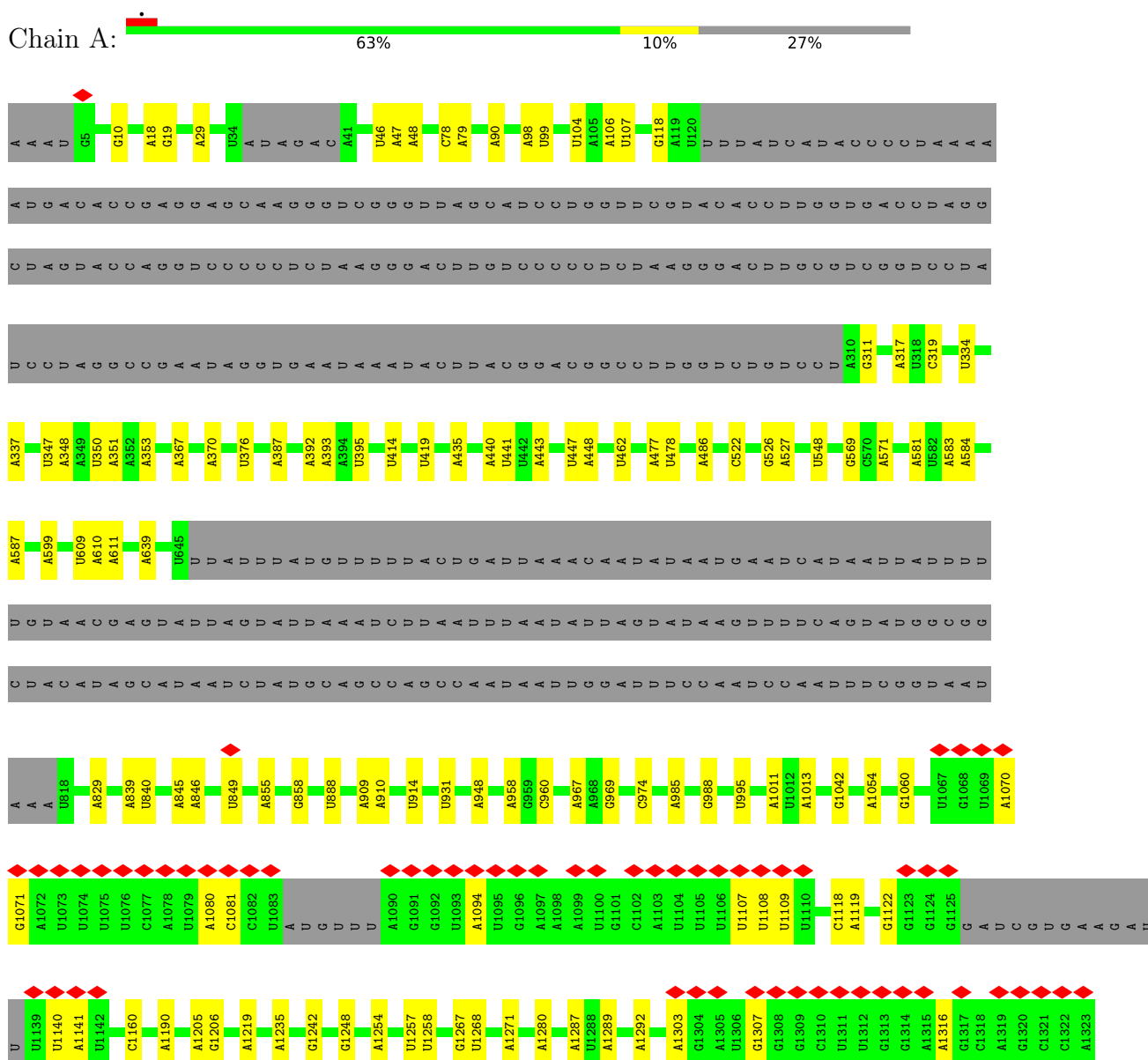
- Molecule 48 is ZINC ION (three-letter code: ZN) (formula: Zn).

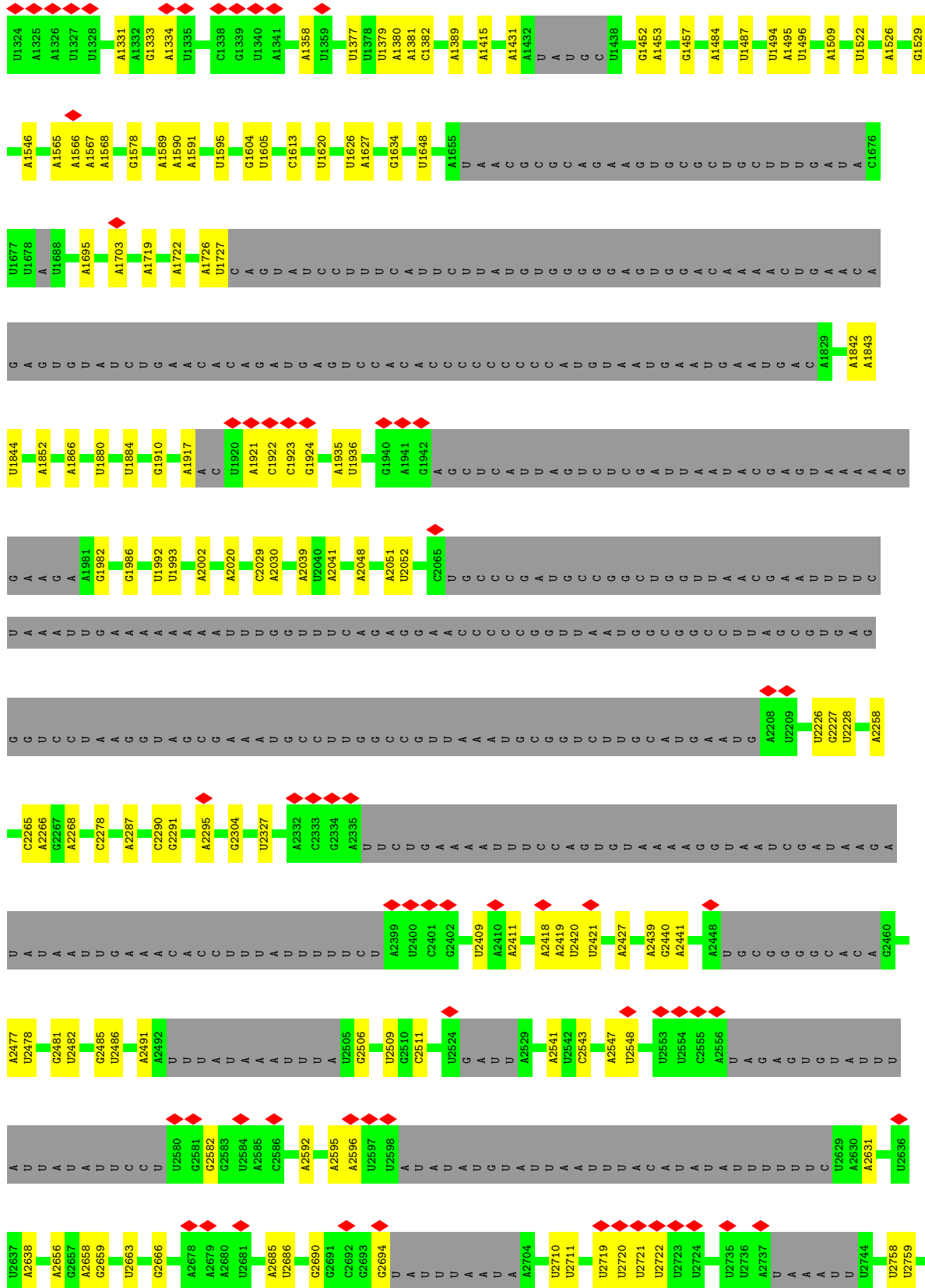
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
48	W	1	1	1	0
48	0	1	1	1	0

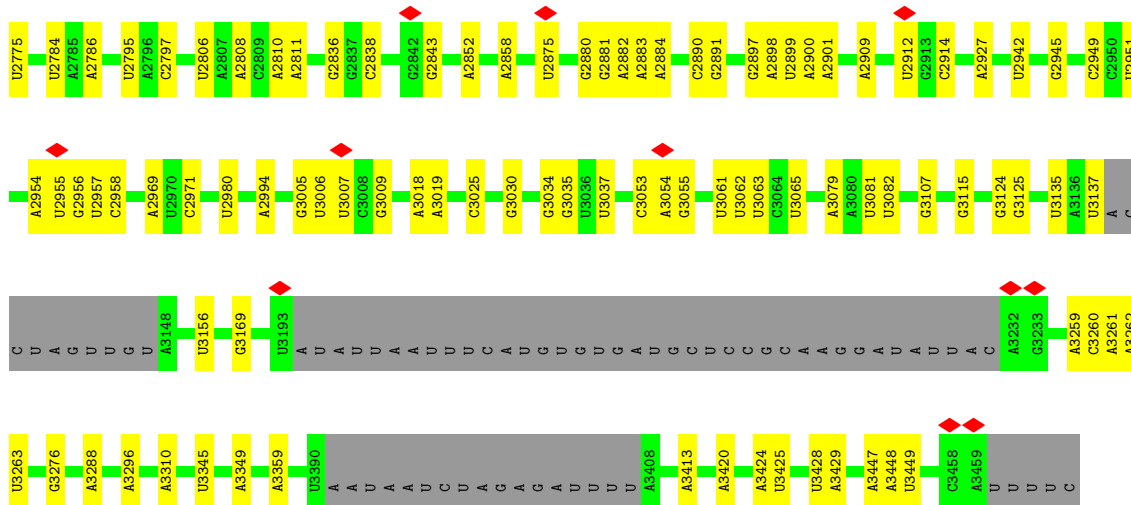
### 3 Residue-property plots [i](#)

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

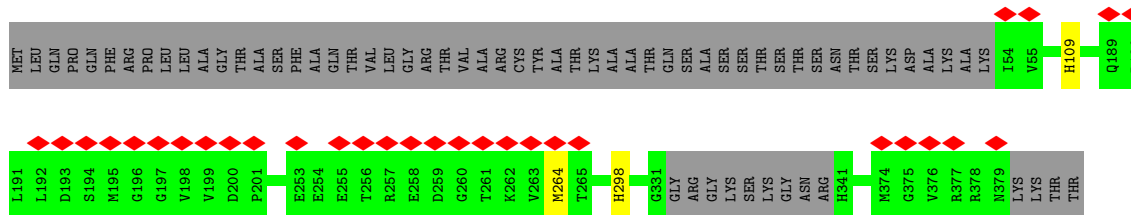
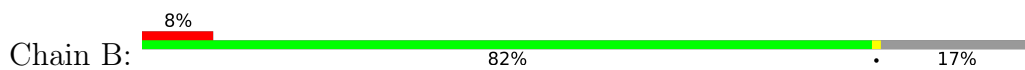
#### • Molecule 1: 23 S rRNA



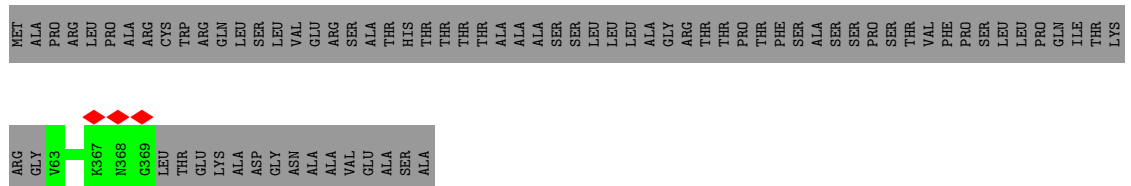
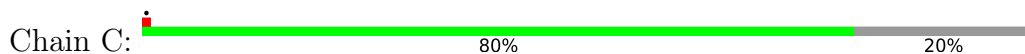




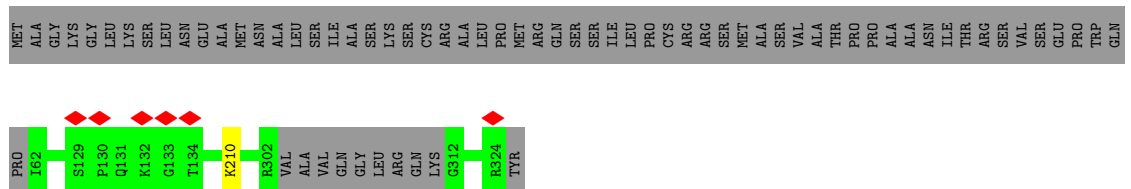
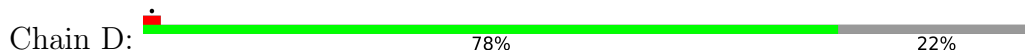
• Molecule 2: 60S ribosomal protein L2



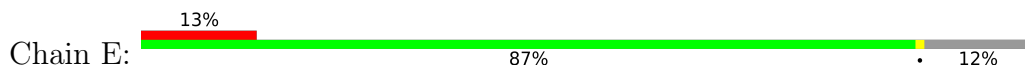
• Molecule 3: 60S ribosomal protein L3

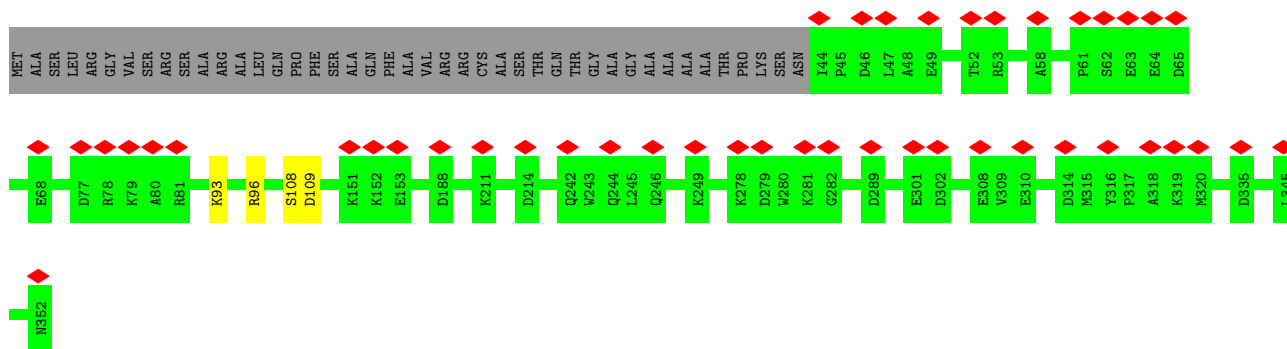


• Molecule 4: 60S ribosomal protein L4, variant

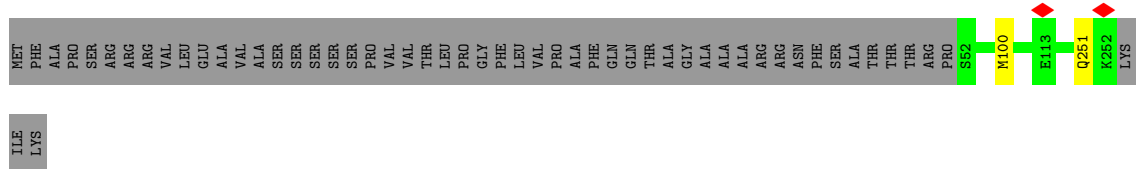
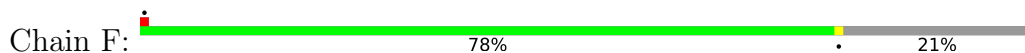


• Molecule 5: 50S ribosomal protein L5

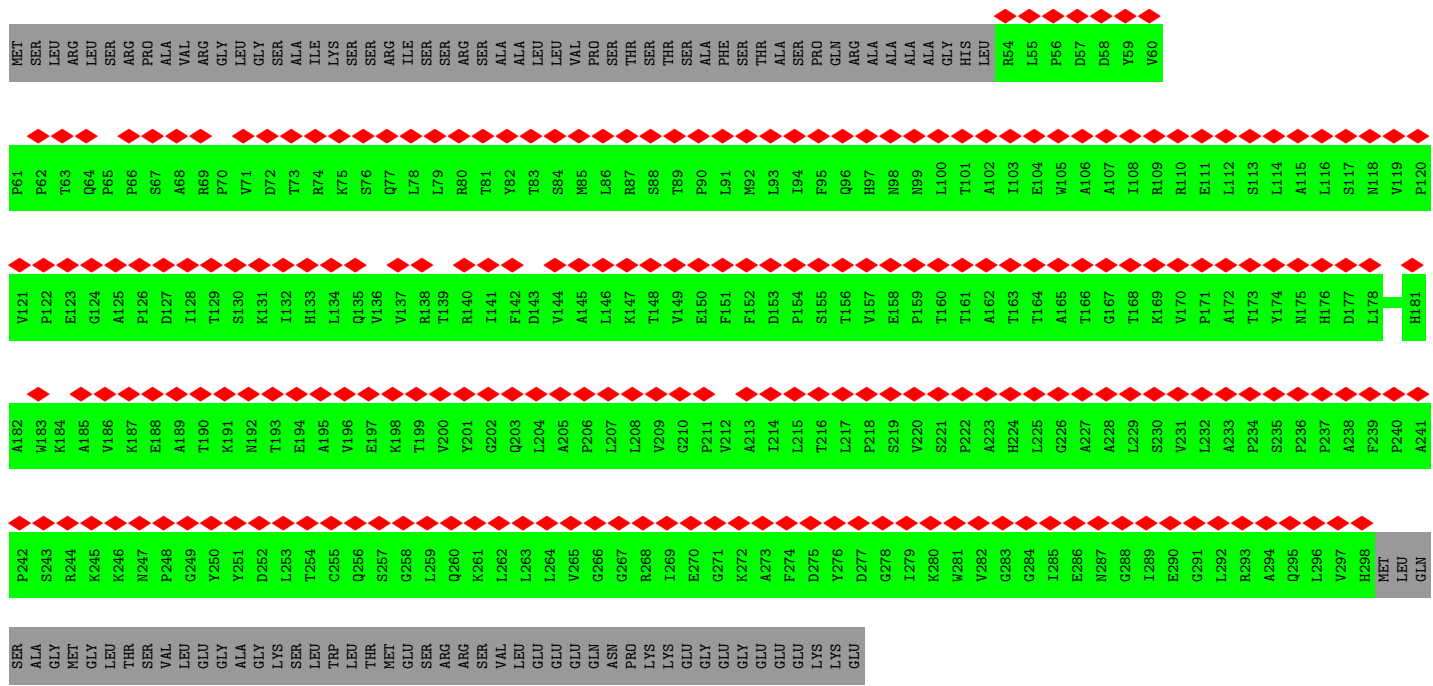




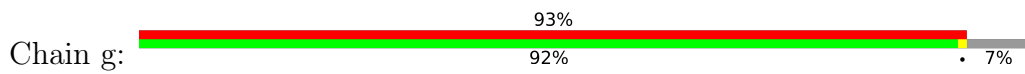
• Molecule 6: 60S ribosomal protein L6



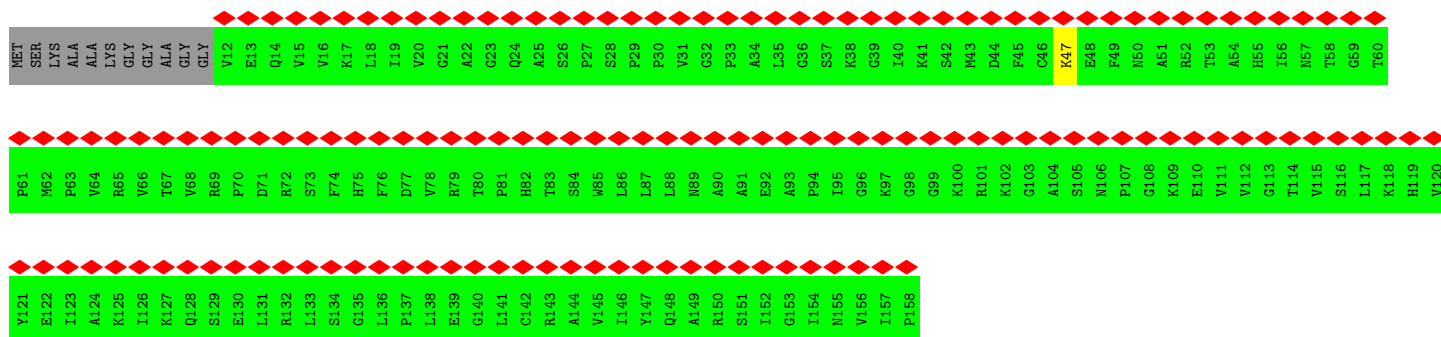
• Molecule 7: Uncharacterized protein



• Molecule 8: 60S ribosomal protein L19



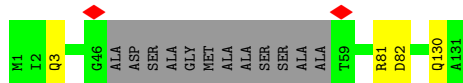
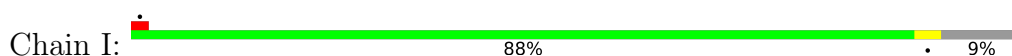




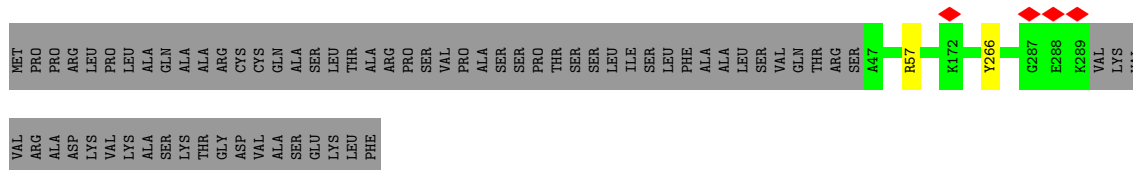
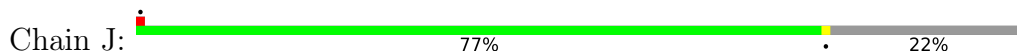
• Molecule 9: Ribosomal protein L13



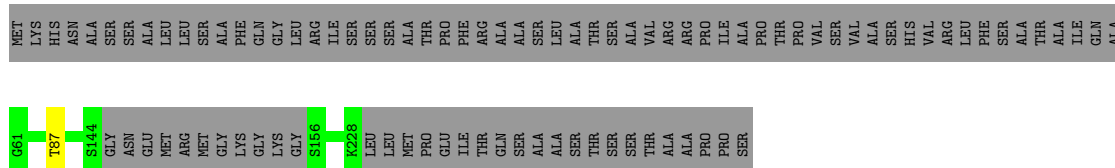
• Molecule 10: 50S ribosomal protein L14



• Molecule 11: 50S ribosomal subunit protein L15



• Molecule 12: 60S ribosomal protein L16

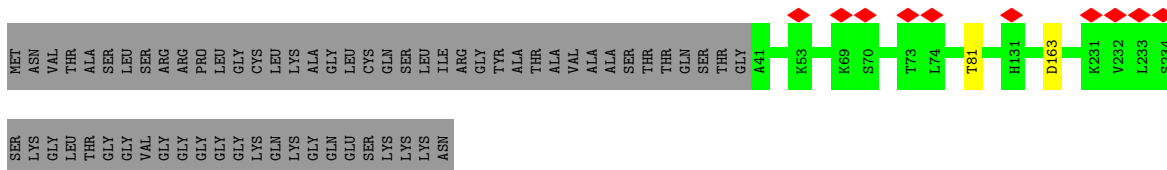
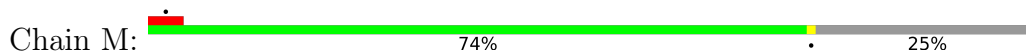


• Molecule 13: 50S ribosomal protein L17

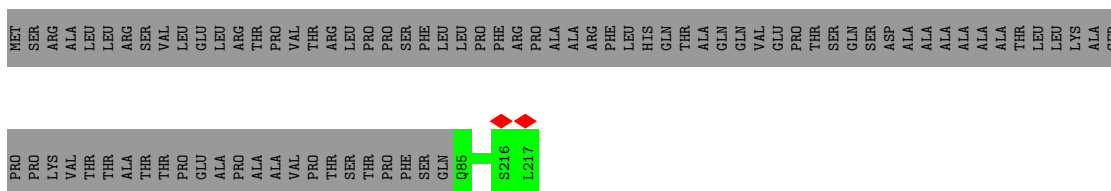




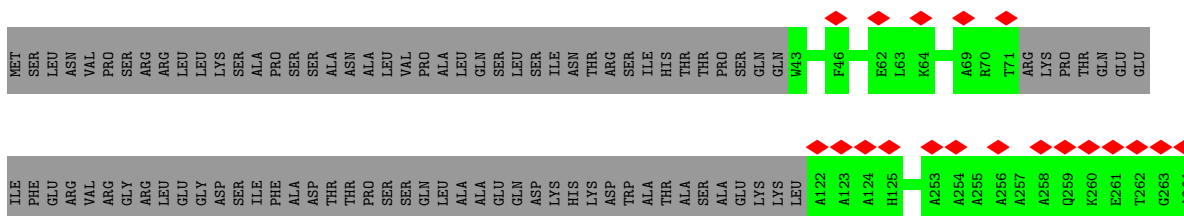
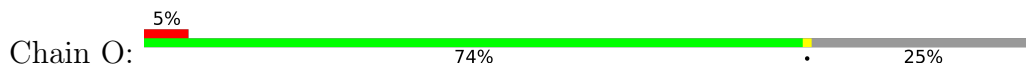
• Molecule 14: Mitochondrial ribosomal protein



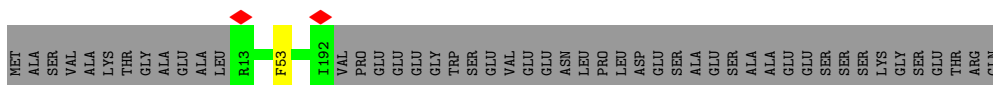
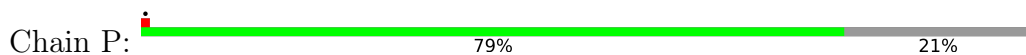
• Molecule 15: Aconitate hydratase



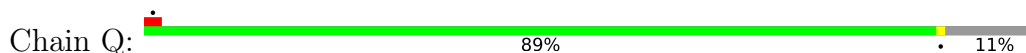
• Molecule 16: Mitochondrial large ribosomal subunit



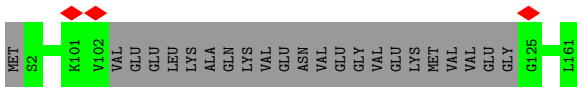
• Molecule 17: Mitochondrial ribosomal protein subunit L23



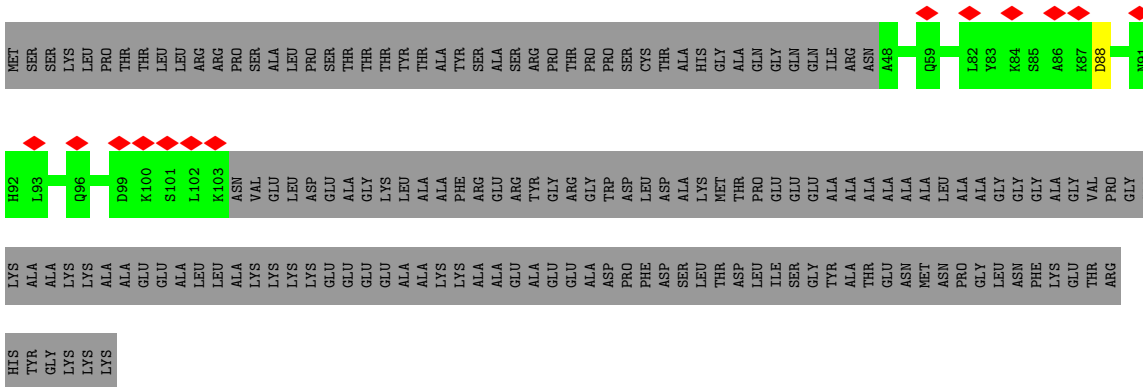
• Molecule 18: KOW domain-containing protein



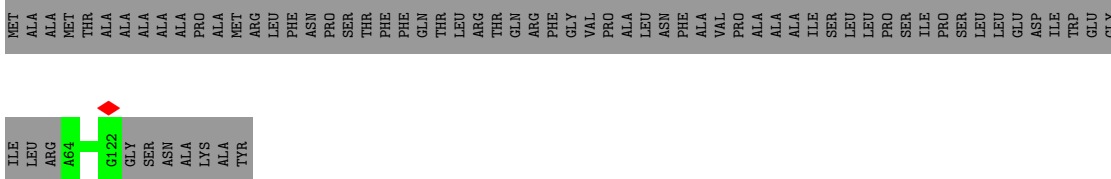




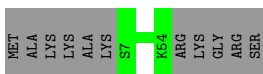
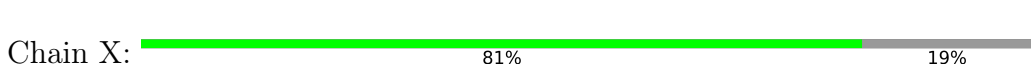
• Molecule 23: Uncharacterized protein



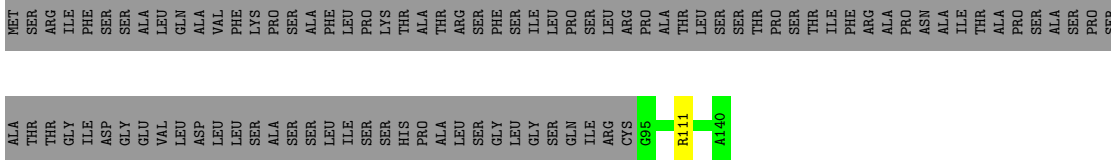
• Molecule 24: Mitochondrial ribosomal protein subunit L32



• Molecule 25: Uncharacterized protein



• Molecule 26: Uncharacterized protein

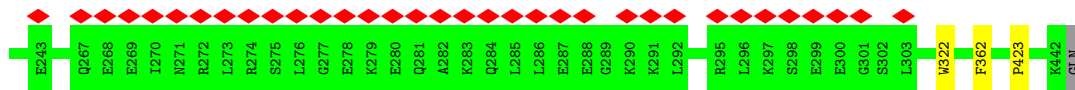


• Molecule 27: Ribosomal protein

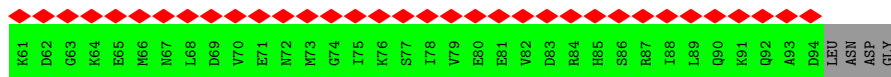
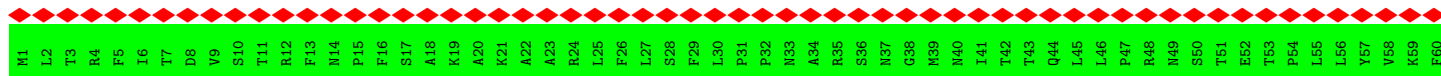




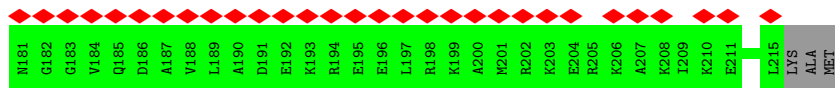




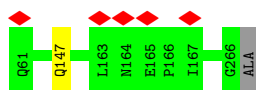
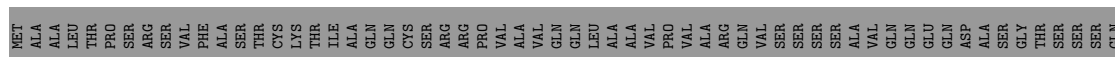
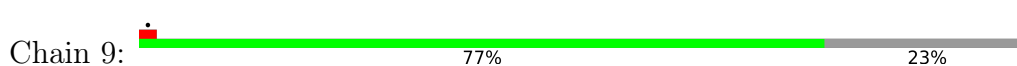
• Molecule 36: Mitochondrial ribosomal protein L44



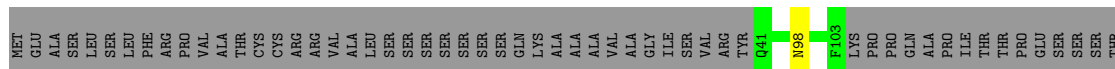
• Molecule 37: Uncharacterized protein

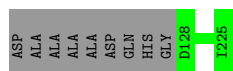


• Molecule 38: RNase III domain-containing protein

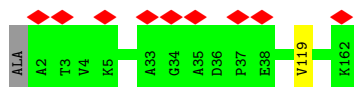


• Molecule 39: 60S ribosomal protein L20

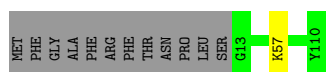
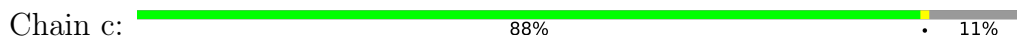




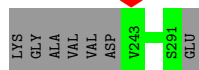
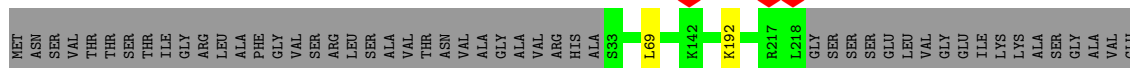
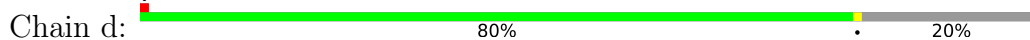
- Molecule 40: Mitochondrial 60S ribosomal protein L25



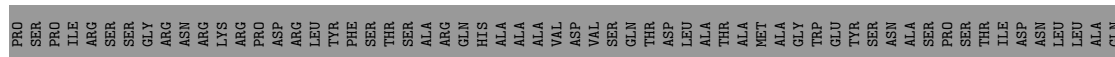
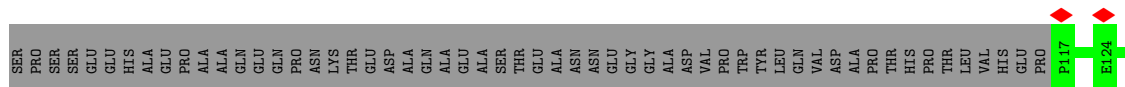
- Molecule 41: 54S ribosomal protein L31, mitochondrial



- Molecule 42: Uncharacterized protein



- Molecule 43: ATPase synthesis protein 25, mitochondrial





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LEU  
SER  
MET  
ASP  
VAL  
ILE  
ASP  
MET  
LEU  
PHE  
SER  
ARG  
GLY  
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ALA  
TRP  
GLY  
ALA

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	24142	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 ( $e^-/\text{\AA}^2$ )	35	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.486	Depositor
Minimum map value	-0.282	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.011	Depositor
Recommended contour level	0.0292	Depositor
Map size ( $\text{\AA}$ )	423.99997, 423.99997, 423.99997	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.06, 1.06, 1.06	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: SPM, MG, NAD, K, ZN

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	0.22	0/60430	0.67	0/94085
2	B	0.24	0/2536	0.45	0/3421
3	C	0.25	0/2380	0.46	0/3209
4	D	0.23	0/2072	0.42	0/2794
5	E	0.24	0/2518	0.40	0/3427
6	F	0.24	0/1644	0.41	0/2218
7	f	0.24	0/1923	0.41	0/2631
8	g	0.24	0/1126	0.41	0/1525
9	H	0.25	0/1460	0.42	0/1975
10	I	0.25	0/918	0.48	0/1225
11	J	0.24	0/1931	0.43	0/2597
12	K	0.24	0/1297	0.41	0/1740
13	L	0.24	0/1569	0.40	0/2106
14	M	0.24	0/1572	0.43	0/2117
15	N	0.25	0/1077	0.44	0/1452
16	O	0.24	0/2248	0.42	0/3015
17	P	0.24	0/1523	0.39	0/2058
18	Q	0.23	0/2916	0.41	0/3927
19	R	0.24	0/1918	0.42	0/2573
20	S	0.24	0/1510	0.41	0/2042
21	T	0.22	0/1454	0.39	0/1974
22	U	0.24	0/1117	0.43	0/1496
23	V	0.24	0/471	0.41	0/638
24	W	0.24	0/467	0.43	0/616
25	X	0.24	0/411	0.42	0/551
26	Y	0.23	0/368	0.42	0/485
27	0	0.25	0/395	0.45	0/523
28	1	0.24	0/3053	0.40	0/4108
29	2	0.23	0/1074	0.39	0/1449
30	3	0.26	0/783	0.44	0/1056
31	4	0.25	0/1077	0.43	0/1453
32	5	0.25	0/2790	0.42	0/3794

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
33	6	0.24	0/2274	0.40	0/3062
34	7	0.24	0/686	0.42	0/919
35	8	0.24	0/2714	0.39	0/3657
36	h	0.25	0/763	0.40	0/1027
37	i	0.24	0/967	0.41	0/1296
38	9	0.24	0/1678	0.40	0/2267
39	a	0.24	0/1364	0.40	0/1842
40	b	0.23	0/1348	0.37	0/1816
41	c	0.23	0/846	0.40	0/1134
42	d	0.23	0/1930	0.41	0/2597
43	n	0.23	0/1470	0.40	0/1980
All	All	0.23	0/124068	0.56	0/179877

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 [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	313/383 (82%)	310 (99%)	3 (1%)	0	100	100
3	C	305/384 (79%)	298 (98%)	7 (2%)	0	100	100
4	D	250/325 (77%)	246 (98%)	4 (2%)	0	100	100
5	E	307/352 (87%)	306 (100%)	1 (0%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	F	199/255 (78%)	196 (98%)	3 (2%)	0	100	100
7	f	243/347 (70%)	238 (98%)	5 (2%)	0	100	100
8	g	145/158 (92%)	142 (98%)	3 (2%)	0	100	100
9	H	181/183 (99%)	178 (98%)	3 (2%)	0	100	100
10	I	115/131 (88%)	111 (96%)	4 (4%)	0	100	100
11	J	241/312 (77%)	235 (98%)	6 (2%)	0	100	100
12	K	153/249 (61%)	151 (99%)	2 (1%)	0	100	100
13	L	190/193 (98%)	189 (100%)	1 (0%)	0	100	100
14	M	192/258 (74%)	187 (97%)	5 (3%)	0	100	100
15	N	131/217 (60%)	126 (96%)	5 (4%)	0	100	100
16	O	268/364 (74%)	262 (98%)	6 (2%)	0	100	100
17	P	178/228 (78%)	178 (100%)	0	0	100	100
18	Q	351/396 (89%)	349 (99%)	2 (1%)	0	100	100
19	R	227/447 (51%)	223 (98%)	4 (2%)	0	100	100
20	S	175/274 (64%)	172 (98%)	3 (2%)	0	100	100
21	T	169/263 (64%)	167 (99%)	2 (1%)	0	100	100
22	U	134/161 (83%)	134 (100%)	0	0	100	100
23	V	54/219 (25%)	54 (100%)	0	0	100	100
24	W	57/129 (44%)	55 (96%)	2 (4%)	0	100	100
25	X	46/59 (78%)	46 (100%)	0	0	100	100
26	Y	44/140 (31%)	44 (100%)	0	0	100	100
27	0	44/124 (36%)	44 (100%)	0	0	100	100
28	1	365/449 (81%)	360 (99%)	5 (1%)	0	100	100
29	2	121/370 (33%)	120 (99%)	1 (1%)	0	100	100
30	3	93/103 (90%)	90 (97%)	3 (3%)	0	100	100
31	4	135/138 (98%)	133 (98%)	2 (2%)	0	100	100
32	5	346/439 (79%)	343 (99%)	3 (1%)	0	100	100
33	6	267/368 (73%)	263 (98%)	4 (2%)	0	100	100
34	7	82/165 (50%)	80 (98%)	2 (2%)	0	100	100
35	8	329/443 (74%)	325 (99%)	4 (1%)	0	100	100
36	h	92/98 (94%)	91 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
37	i	117/218 (54%)	111 (95%)	6 (5%)	0	100	100
38	9	204/267 (76%)	199 (98%)	5 (2%)	0	100	100
39	a	157/225 (70%)	156 (99%)	1 (1%)	0	100	100
40	b	159/162 (98%)	157 (99%)	2 (1%)	0	100	100
41	c	96/110 (87%)	94 (98%)	2 (2%)	0	100	100
42	d	231/292 (79%)	230 (100%)	1 (0%)	0	100	100
43	n	182/699 (26%)	175 (96%)	7 (4%)	0	100	100
All	All	7688/11097 (69%)	7568 (98%)	120 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	261/312 (84%)	258 (99%)	3 (1%)	73	90
3	C	242/303 (80%)	242 (100%)	0	100	100
4	D	216/274 (79%)	215 (100%)	1 (0%)	88	95
5	E	267/296 (90%)	263 (98%)	4 (2%)	65	86
6	F	173/216 (80%)	171 (99%)	2 (1%)	71	89
7	f	206/287 (72%)	206 (100%)	0	100	100
8	g	120/124 (97%)	119 (99%)	1 (1%)	81	92
9	H	149/149 (100%)	149 (100%)	0	100	100
10	I	100/105 (95%)	96 (96%)	4 (4%)	31	66
11	J	198/255 (78%)	196 (99%)	2 (1%)	76	91
12	K	135/205 (66%)	134 (99%)	1 (1%)	84	93
13	L	164/165 (99%)	162 (99%)	2 (1%)	71	89
14	M	164/209 (78%)	162 (99%)	2 (1%)	71	89
15	N	119/188 (63%)	119 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	O	235/315 (75%)	232 (99%)	3 (1%)	69	88
17	P	158/196 (81%)	157 (99%)	1 (1%)	86	94
18	Q	312/347 (90%)	310 (99%)	2 (1%)	86	94
19	R	196/359 (55%)	192 (98%)	4 (2%)	55	81
20	S	159/242 (66%)	158 (99%)	1 (1%)	86	94
21	T	153/224 (68%)	153 (100%)	0	100	100
22	U	118/138 (86%)	118 (100%)	0	100	100
23	V	52/170 (31%)	51 (98%)	1 (2%)	57	82
24	W	50/102 (49%)	50 (100%)	0	100	100
25	X	46/54 (85%)	46 (100%)	0	100	100
26	Y	38/116 (33%)	37 (97%)	1 (3%)	46	76
27	0	41/108 (38%)	41 (100%)	0	100	100
28	1	316/384 (82%)	313 (99%)	3 (1%)	78	91
29	2	109/317 (34%)	108 (99%)	1 (1%)	78	91
30	3	83/91 (91%)	81 (98%)	2 (2%)	49	78
31	4	113/114 (99%)	113 (100%)	0	100	100
32	5	279/351 (80%)	276 (99%)	3 (1%)	73	90
33	6	238/310 (77%)	233 (98%)	5 (2%)	53	80
34	7	69/136 (51%)	67 (97%)	2 (3%)	42	74
35	8	285/378 (75%)	281 (99%)	4 (1%)	67	86
36	h	85/88 (97%)	85 (100%)	0	100	100
37	i	99/162 (61%)	99 (100%)	0	100	100
38	9	176/225 (78%)	175 (99%)	1 (1%)	86	94
39	a	146/196 (74%)	145 (99%)	1 (1%)	84	93
40	b	141/141 (100%)	140 (99%)	1 (1%)	84	93
41	c	86/96 (90%)	85 (99%)	1 (1%)	71	89
42	d	201/243 (83%)	199 (99%)	2 (1%)	76	91
43	n	157/590 (27%)	154 (98%)	3 (2%)	57	82
All	All	6655/9281 (72%)	6591 (99%)	64 (1%)	77	91

5 of 64 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
40	b	119	VAL
42	d	69	LEU
16	O	357	SER
16	O	356	THR
42	d	192	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
10	I	30	HIS

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2505/3464 (72%)	349 (13%)	12 (0%)

5 of 349 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	10	G
1	A	18	A
1	A	19	G
1	A	29	A
1	A	46	U

5 of 12 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	2758	U
1	A	2883	A
1	A	2957	U
1	A	2890	C
1	A	1567	A

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

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



## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 171 ligands modelled in this entry, 169 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
45	NAD	A	3607	-	42,48,48	0.73	1 (2%)	50,73,73	0.76	1 (2%)
46	SPM	A	3644	-	13,13,13	0.35	0	12,12,12	0.76	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
45	NAD	A	3607	-	-	3/26/62/62	0/5/5/5
46	SPM	A	3644	-	-	4/11/11/11	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	A	3607	NAD	C2N-N1N	-2.00	1.32	1.35

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	A	3607	NAD	N3A-C2A-N1A	-2.63	124.56	128.68

There are no chirality outliers.

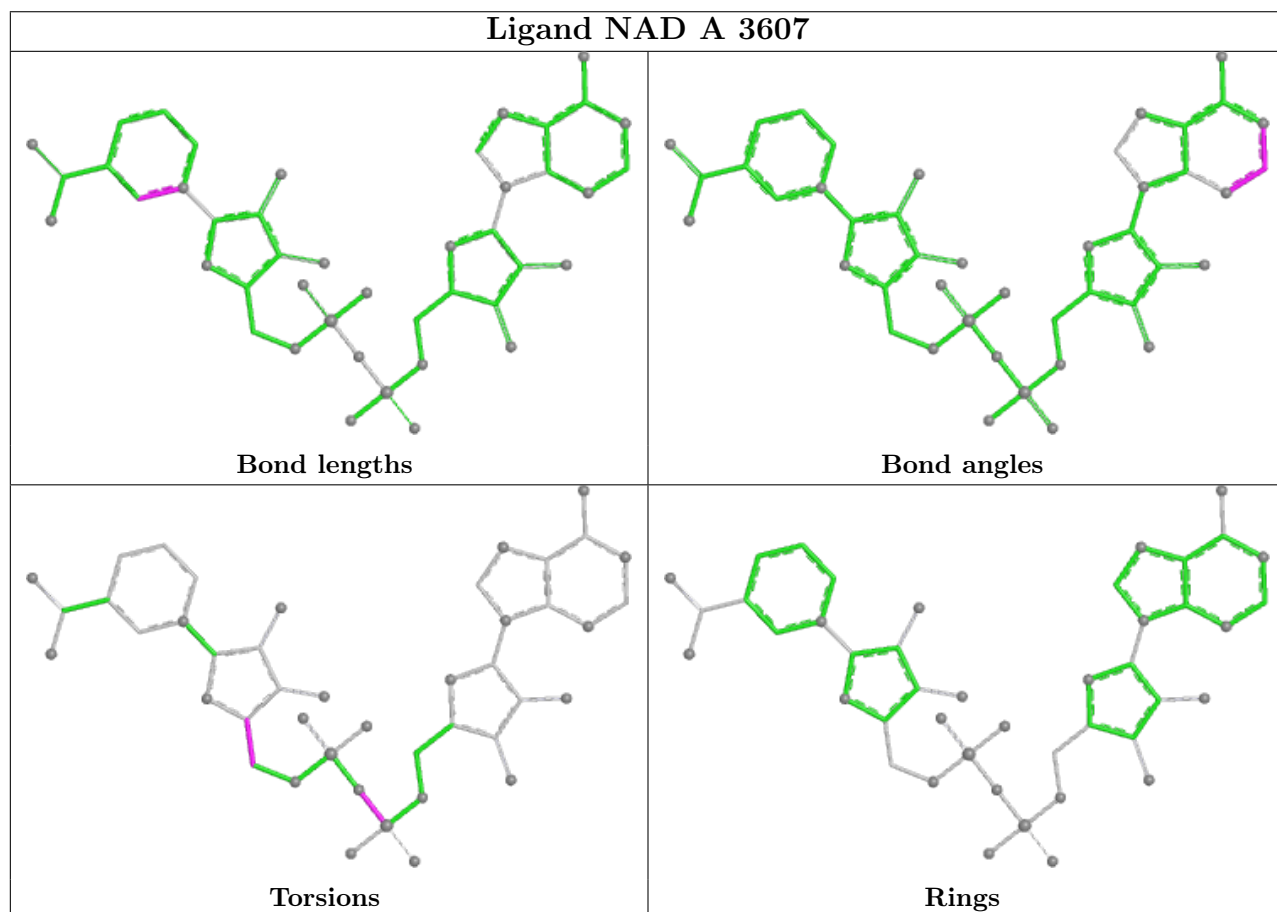
5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
46	A	3644	SPM	C7-C8-C9-N10
45	A	3607	NAD	O4D-C4D-C5D-O5D
46	A	3644	SPM	C2-C3-C4-N5
45	A	3607	NAD	C3D-C4D-C5D-O5D
46	A	3644	SPM	C7-C6-N5-C4

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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.

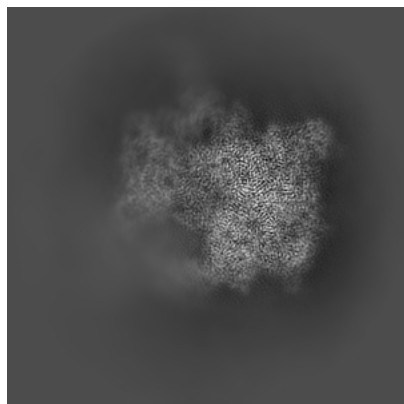
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10977. These allow visual inspection of the internal detail of the map and identification of artifacts.

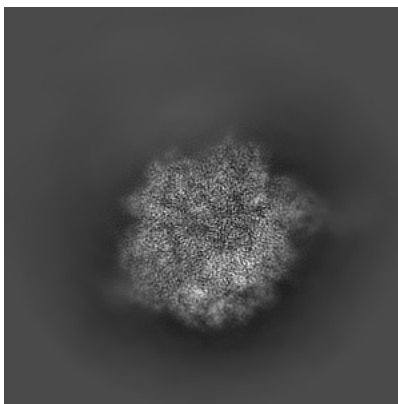
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

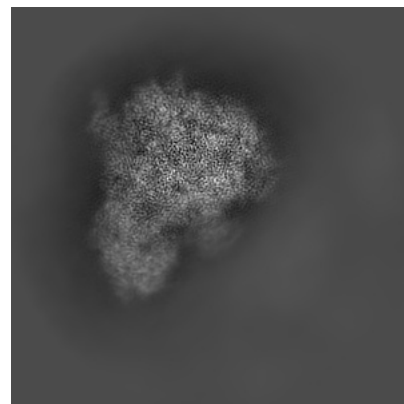
#### 6.1.1 Primary map



X

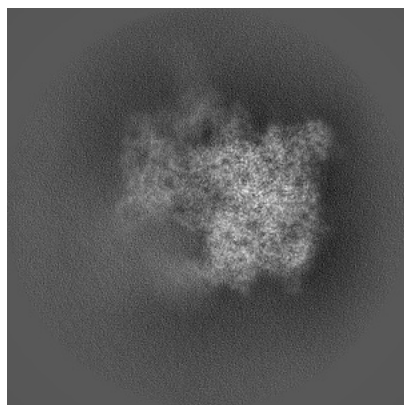


Y

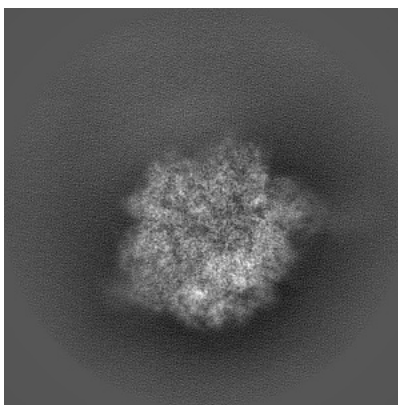


Z

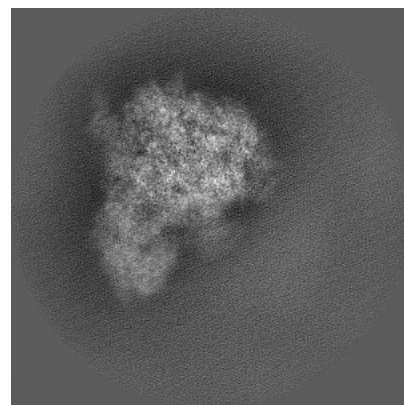
#### 6.1.2 Raw map



X



Y

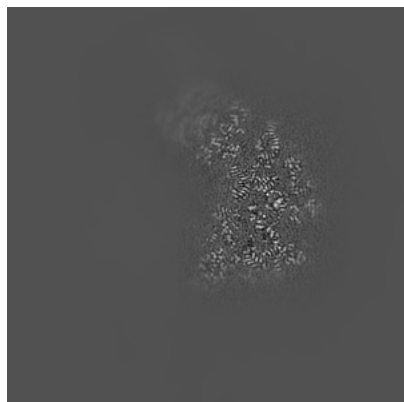


Z

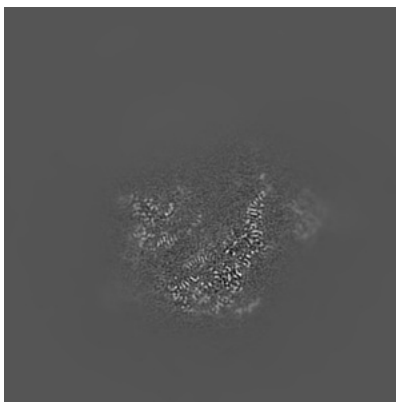
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

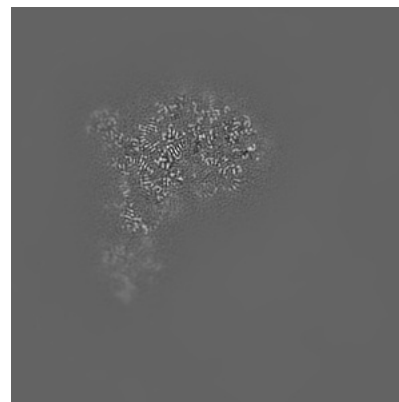
### 6.2.1 Primary map



X Index: 200

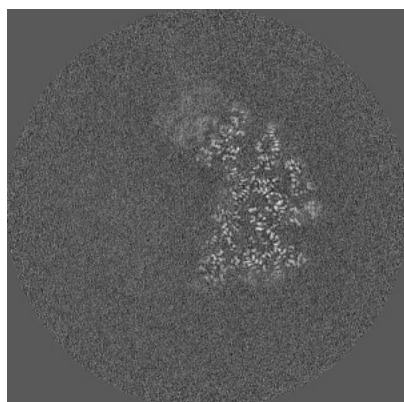


Y Index: 200

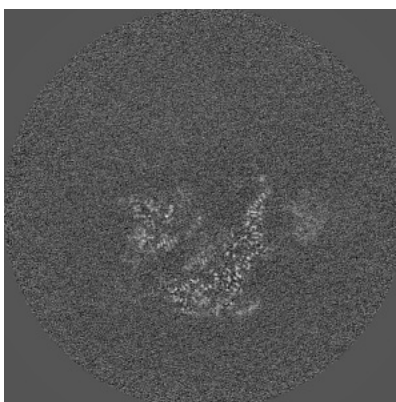


Z Index: 200

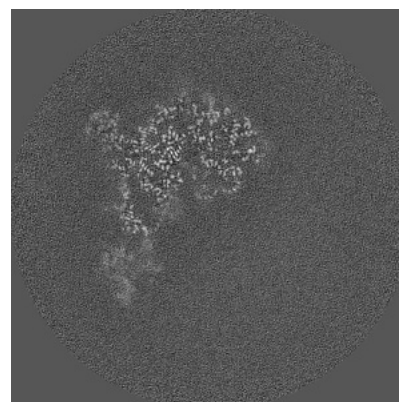
### 6.2.2 Raw map



X Index: 200



Y Index: 200

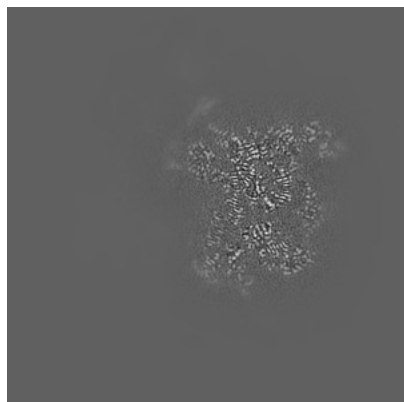


Z Index: 200

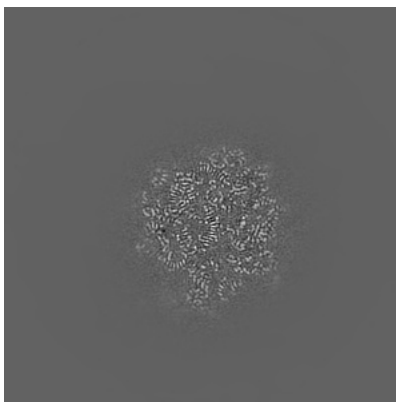
The images above show central slices of the map in three orthogonal directions.

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

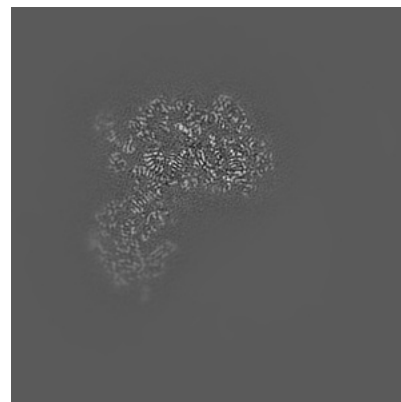
### 6.3.1 Primary map



X Index: 171

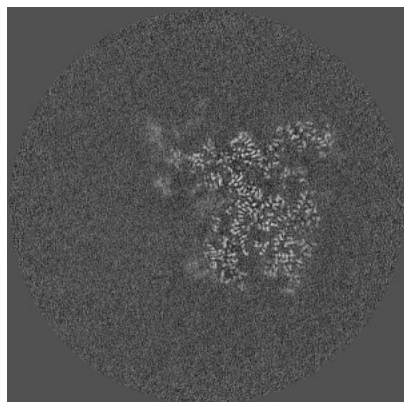


Y Index: 259

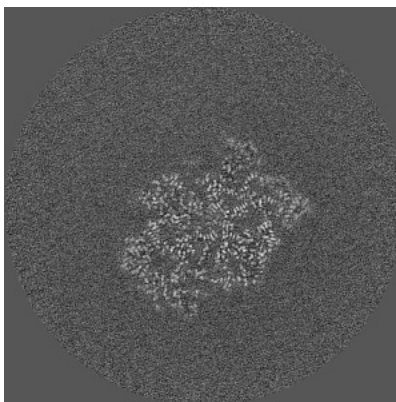


Z Index: 215

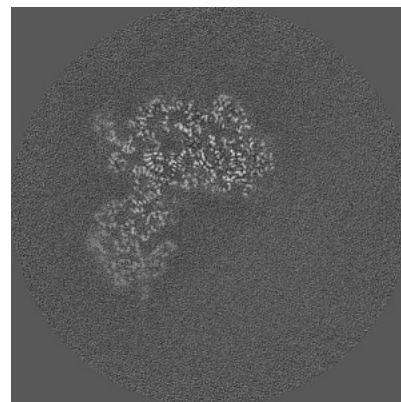
### 6.3.2 Raw map



X Index: 161



Y Index: 228



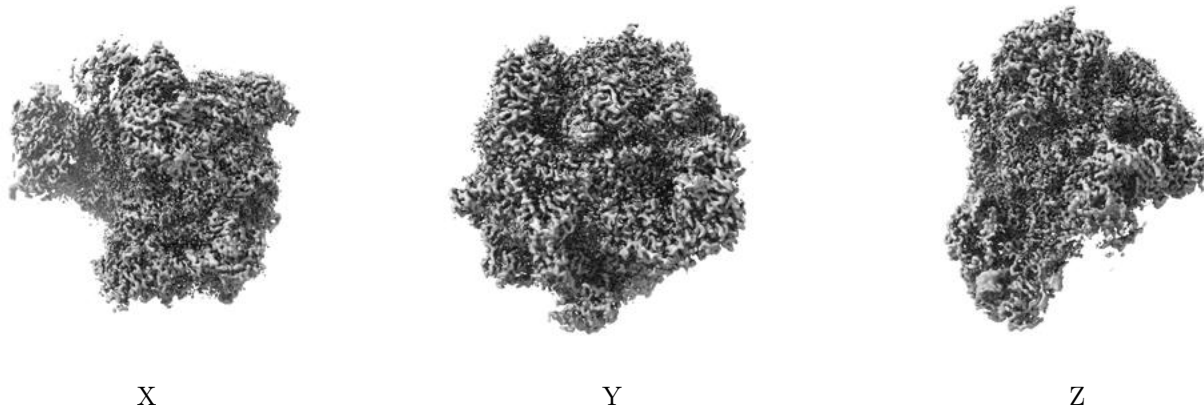
Z Index: 215

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



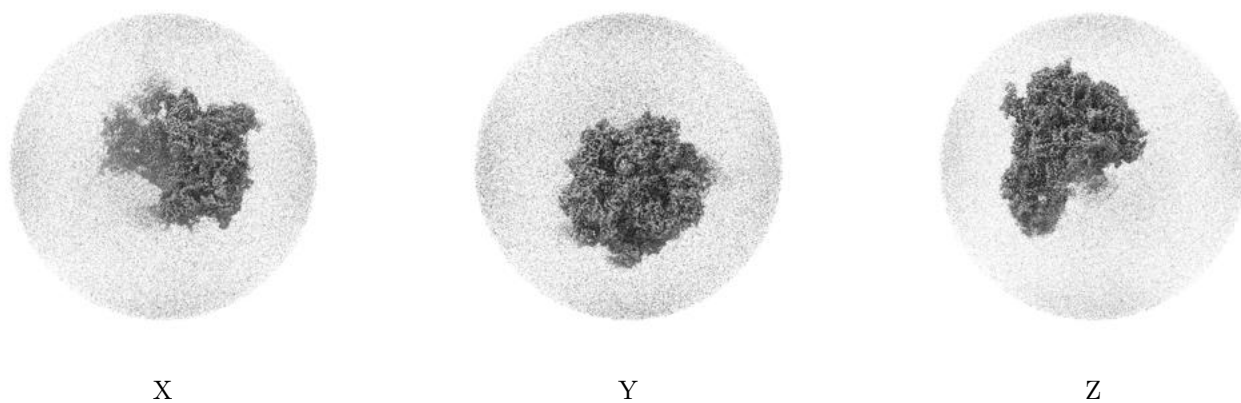
## 6.4 Orthogonal surface views [i](#)

### 6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0292. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.4.2 Raw map



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

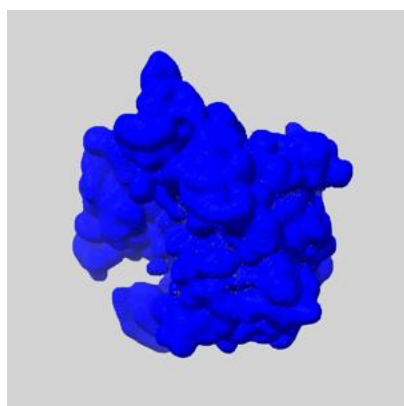
## 6.5 Mask visualisation [i](#)

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

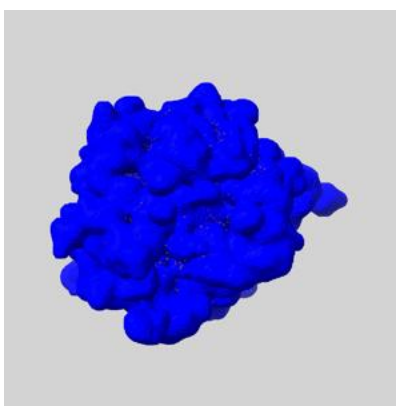
A mask typically either:

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

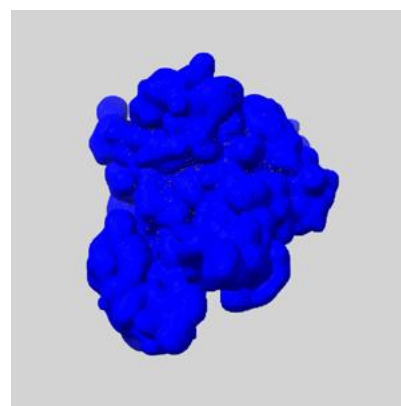
### 6.5.1 emd\_10977\_msk\_1.map [i](#)



X



Y



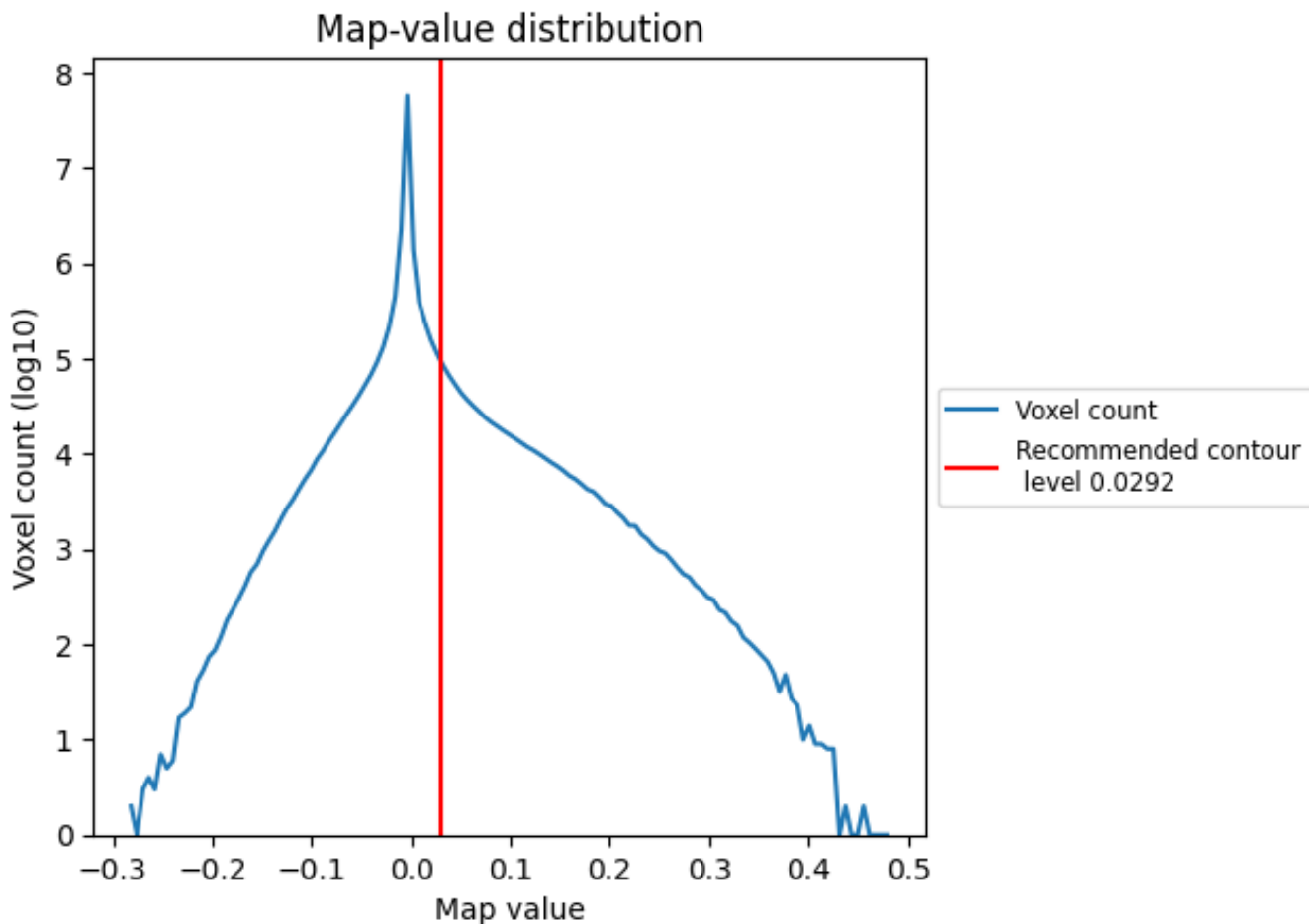
Z



## 7 Map analysis [i](#)

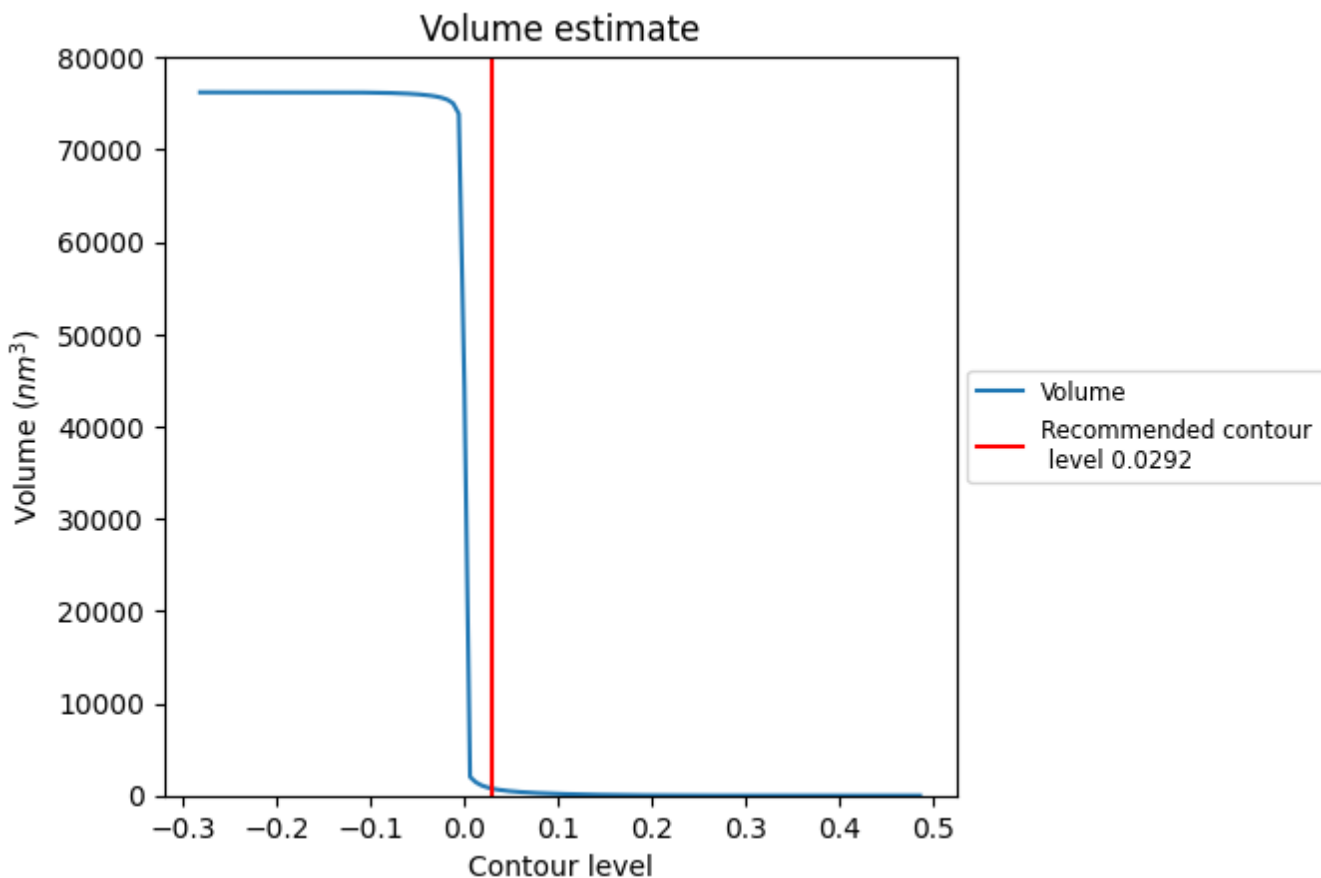
This section contains the results of statistical analysis of the map.

### 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.

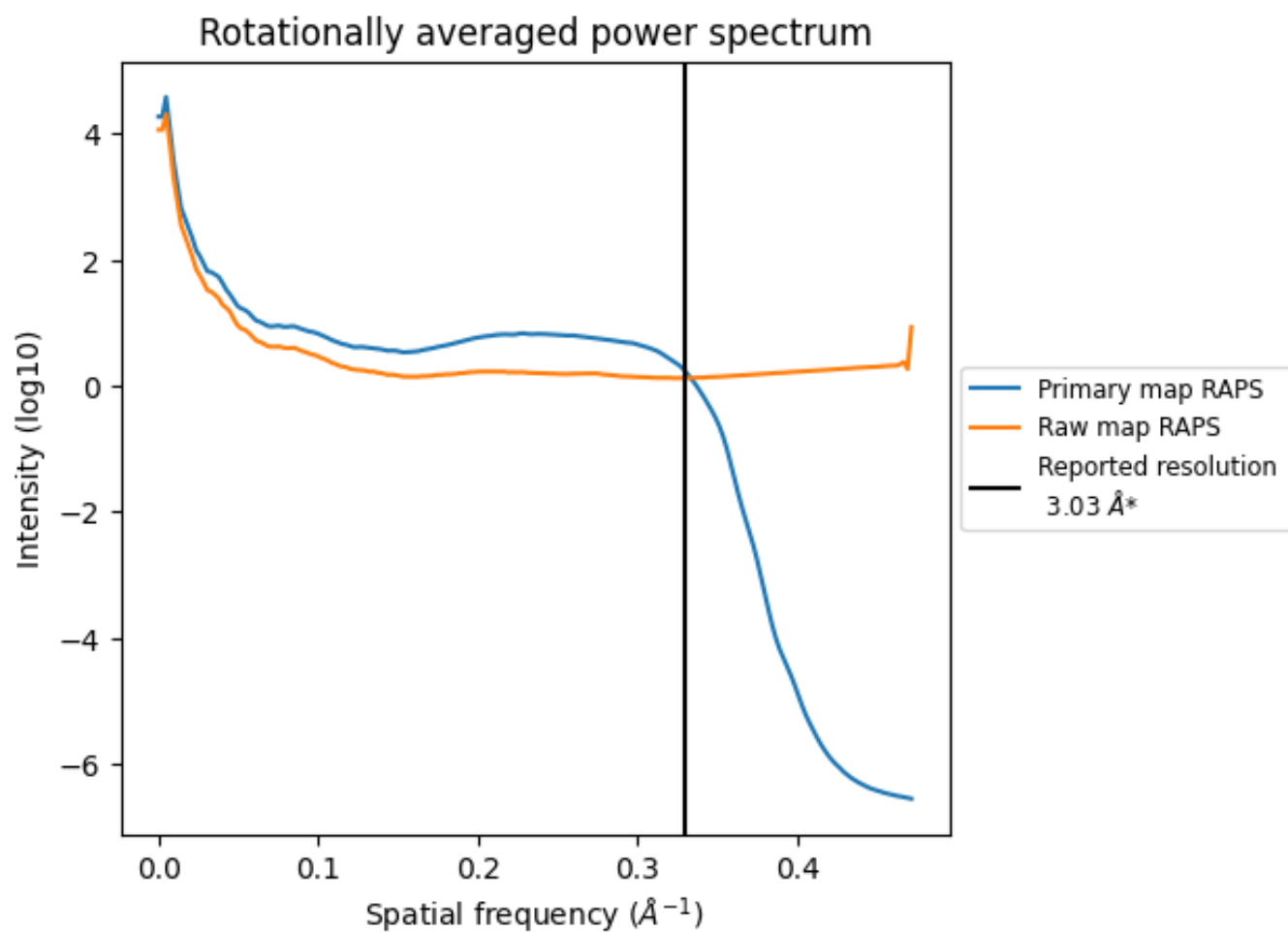
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 766 nm<sup>3</sup>; this corresponds to an approximate mass of 692 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum i

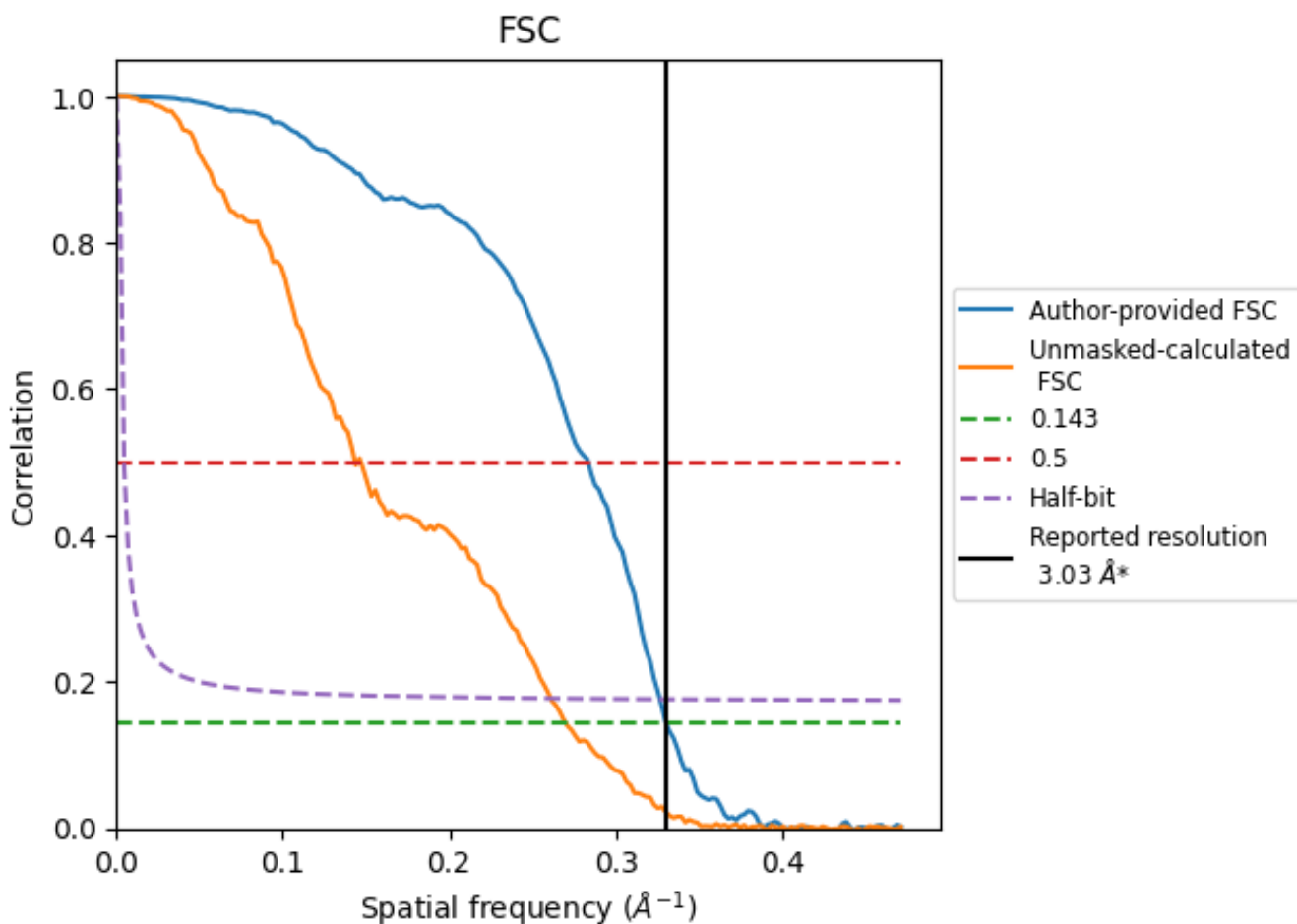


\*Reported resolution corresponds to spatial frequency of 0.330 Å<sup>-1</sup>

## 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 0.330 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

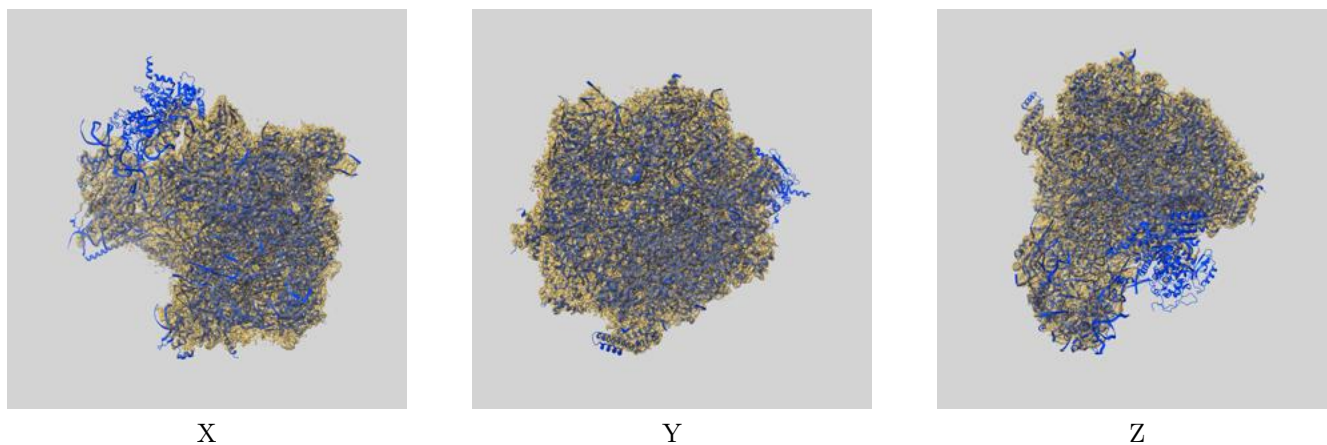
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.03	-	-
Author-provided FSC curve	3.03	3.53	3.06
Unmasked-calculated*	3.70	6.97	3.83

\*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 3.70 differs from the reported value 3.03 by more than 10 %

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

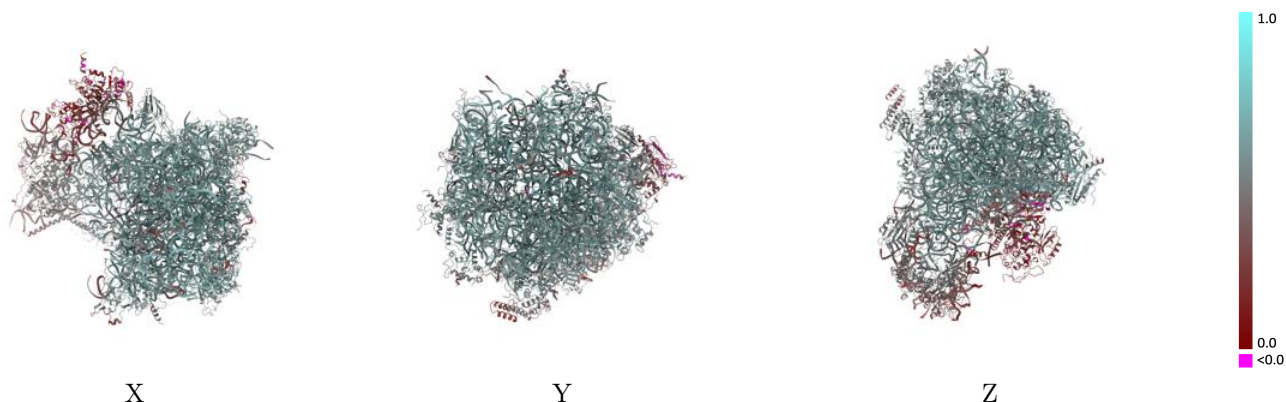
This section contains information regarding the fit between EMDB map EMD-10977 and PDB model 6YWV. Per-residue inclusion information can be found in section 3 on page 13.

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



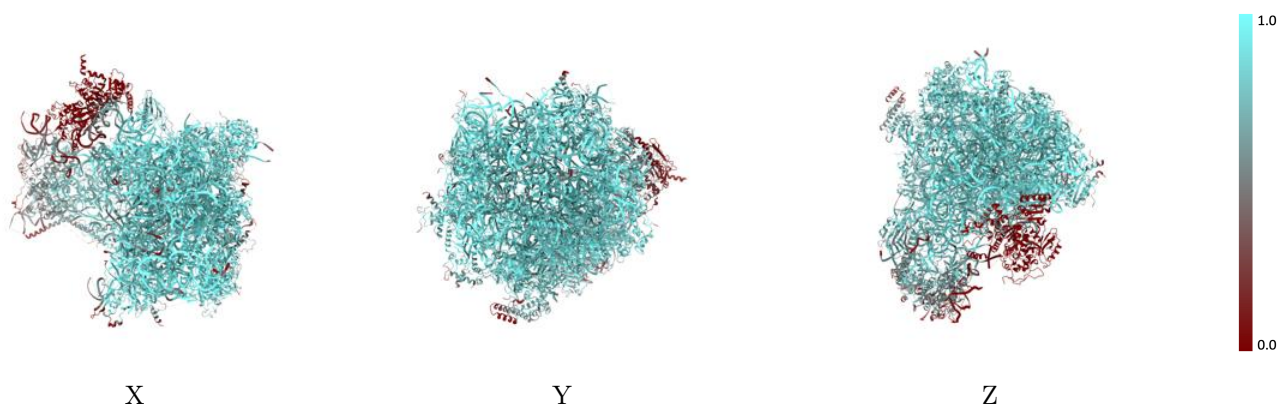
The images above show the 3D surface view of the map at the recommended contour level 0.0292 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



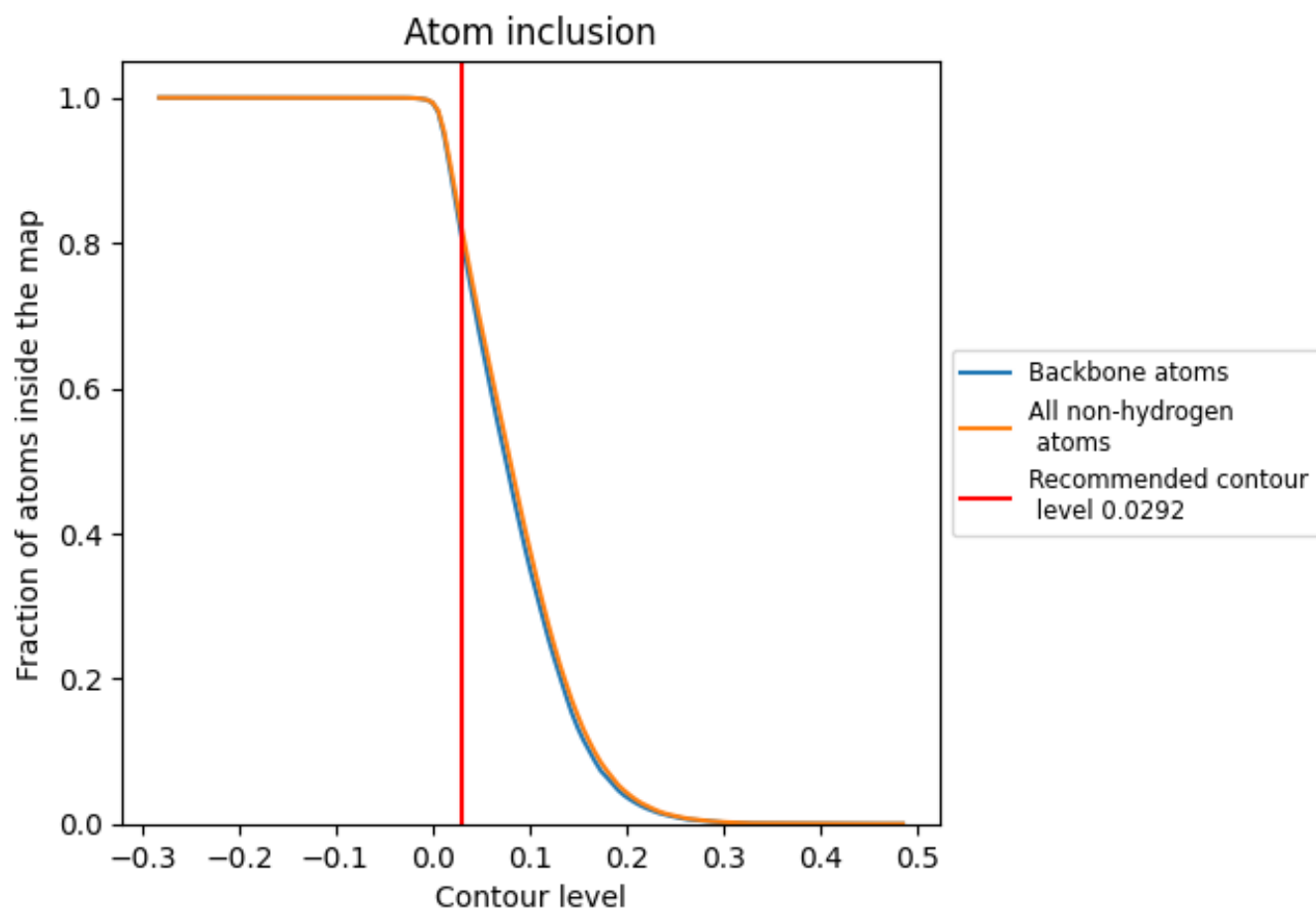
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0292).

## 9.4 Atom inclusion [i](#)









































































At the recommended contour level, 81% of all backbone atoms, 83% of all non-hydrogen atoms, are inside the map.



## 9.5 Map-model fit summary



















The table lists the average atom inclusion at the recommended contour level (0.0292) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8276	 0.5440
0	 0.9704	 0.6220
1	 0.7335	 0.5000
2	 0.6156	 0.4440
3	 0.9031	 0.5780
4	 0.9400	 0.6120
5	 0.8811	 0.5710
6	 0.4598	 0.3880
7	 0.8855	 0.5760
8	 0.6837	 0.4810
9	 0.8064	 0.5320
A	 0.9009	 0.5690
B	 0.8028	 0.5510
C	 0.9325	 0.6080
D	 0.8648	 0.5660
E	 0.6242	 0.4630
F	 0.8163	 0.5350
H	 0.9502	 0.6160
I	 0.9045	 0.5910
J	 0.8715	 0.5730
K	 0.8743	 0.5800
L	 0.9131	 0.5920
M	 0.8487	 0.5580
N	 0.9031	 0.5910
O	 0.8585	 0.5750
P	 0.9136	 0.5880
Q	 0.8417	 0.5530
R	 0.7138	 0.5000
S	 0.8582	 0.5630
T	 0.8791	 0.5750
U	 0.8818	 0.5790
V	 0.5471	 0.4340
W	 0.9490	 0.6040
X	 0.8943	 0.5700
Y	 0.9654	 0.6270



*Continued on next page...*

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Chain	Atom inclusion	Q-score
a	 0.8695	 0.5570
b	 0.8109	 0.5370
c	 0.9497	 0.6170
d	 0.8810	 0.5810
f	 0.0673	 0.2410
g	 0.0065	 0.1910
h	 0.0000	 0.1860
i	 0.0462	 0.2230
n	 0.7305	 0.5220