Full wwPDB EM Validation Report (i)

Apr 29, 2024 – 04:56 pm BST

PDB ID	:	4V1A
EMDB ID	:	EMD-2787
Title	:	Structure of the large subunit of the mammalian mitoribosome, part 2 of 2
Authors	:	Greber, B.J.; Boehringer, D.; Leibundgut, M.; Bieri, P.; Leitner, A.; Schmitz, N.; Aebersold, R.; Ban, N.
Deposited on	:	2014-09-25
Resolution	:	3.40 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

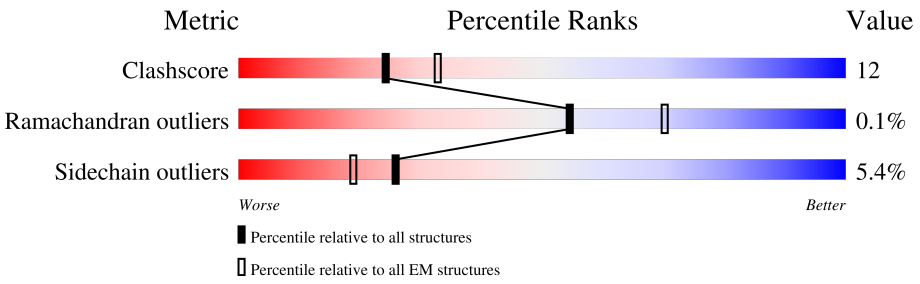
EMDB validation analysis	:	0.0.1.dev92
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 3.40 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	423	• 89% • 7%
2	b	380	9% 89% • 7%
3	c	334	8% 85% • 12%
4	d	206	25% 45% • 52%
5	e	135	8% 85% • 10%
6	f	142	19% 70% 6% 24%
7	g	159	• 84% 9% 7%
8	h	332	8% 82% 5% 13%

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Mol	Chain	Length	Quality of chain
9	i	312	38% 75% 22%
10	j	279	39% 73% 5% 22%
11	k	212	23% 60% 38%
12	l	166	76% 20%
13	m	159	13% 67% 31%
14	n	128	70% 6% 24%
15	o	124	6% 71% 5% 24%
16	p	112	44% 86% 13%
17	q	138	8% 27% 73%
18	t	102	84% 8% 8%
19	u	205	36% 71% 26%
20	v	222	27% 58% 41%
21	w	433	5% 84% 6% 11%
22	x	196	11% 77% 6% 17%
23	z	47	96% 100%

2 Entry composition (i)

There are 24 unique types of molecules in this entry. The entry contains 31917 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 MITORIBOSOMAL PROTEIN ML37, MRPL37.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	a	393	3173	2040	556	565	12	0	0

- Molecule 2 is a protein called MITORIBOSOMAL PROTEIN ML38, MRPL38.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	b	354	2952	1876	542	525	9	0	0

- Molecule 3 is a protein called MITORIBOSOMAL PROTEIN ML39, MRPL39.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	c	295	2408	1541	410	441	16	0	0

- Molecule 4 is a protein called MITORIBOSOMAL PROTEIN ML40, MRPL40.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	d	99	832	528	148	155	1	0	0

- Molecule 5 is a protein called MITORIBOSOMAL PROTEIN ML41, MRPL41.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	e	121	968	626	167	172	3	0	0

- Molecule 6 is a protein called MITORIBOSOMAL PROTEIN ML42, MRPL42.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	f	108	852	544	154	150	4	0	0

- Molecule 7 is a protein called MITORIBOSOMAL PROTEIN ML43, MRPL43.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	g	148	1167	727	225	212	3	0	0

- Molecule 8 is a protein called MITORIBOSOMAL PROTEIN ML44, MRPL44.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	h	289	2319	1486	399	426	8	0	0

- Molecule 9 is a protein called MITORIBOSOMAL PROTEIN ML45, MRPL45.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	i	242	1979	1266	352	351	10	0	0

- Molecule 10 is a protein called MITORIBOSOMAL PROTEIN ML46, MRPL46.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	j	217	1775	1137	311	321	6	0	0

- Molecule 11 is a protein called MITORIBOSOMAL PROTEIN ML48, MRPL48.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	k	131	1050	671	178	196	5	0	0

- Molecule 12 is a protein called MITORIBOSOMAL PROTEIN ML49, MRPL49.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	l	133	1097	709	192	194	2	0	0

- Molecule 13 is a protein called MITORIBOSOMAL PROTEIN ML50, MRPL50.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	m	109	893	568	160	162	3	0	0

- Molecule 14 is a protein called MITORIBOSOMAL PROTEIN ML51, MRPL51.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	n	97	837	539	166	128	4	0	0

- Molecule 15 is a protein called MITORIBOSOMAL PROTEIN ML52, MRPL52.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	o	94	747	466	143	136	2	0	0

- Molecule 16 is a protein called MITORIBOSOMAL PROTEIN ML53, MRPL53.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	p	97	742	459	143	134	6	0	0

- Molecule 17 is a protein called MITORIBOSOMAL PROTEIN ML54, MRPL54.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
17	q	37	336	214	69	53	0	0

- Molecule 18 is a protein called MITORIBOSOMAL PROTEIN ML63, MRPL57, MRP63.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	t	94	780	485	168	126	1	0	0

- Molecule 19 is a protein called MITORIBOSOMAL PROTEIN ML62, MRPL58, ICT1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	u	151	1208	748	233	222	5	0	0

- Molecule 20 is a protein called MITORIBOSOMAL PROTEIN ML64, MRPL59, CRIF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	v	131	1068	662	206	195	5	0	0

- Molecule 21 is a protein called MITORIBOSOMAL PROTEIN ML65, MRPS30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	w	387	3126	2011	548	555	12	0	0

- Molecule 22 is a protein called MITORIBOSOMAL PROTEIN ML66, MRPS18A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	x	162	1325	845	249	224	7	0	0

- Molecule 23 is a protein called UNASSIGNED SECONDARY STRUCTURE ELEMENTS.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
23	z	47	282	188	47	47	0	0

- Molecule 24 is ZINC ION (three-letter code: ZN) (formula: Zn).

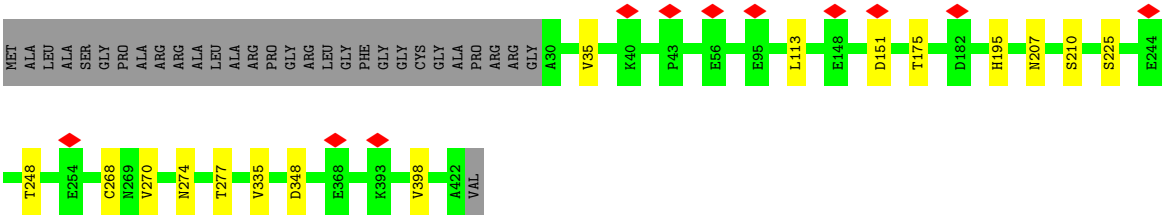
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
24	x	1	1	1	0

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.

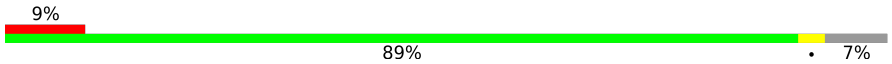
• Molecule 1: MITORIBOSOMAL PROTEIN ML37, MRPL37

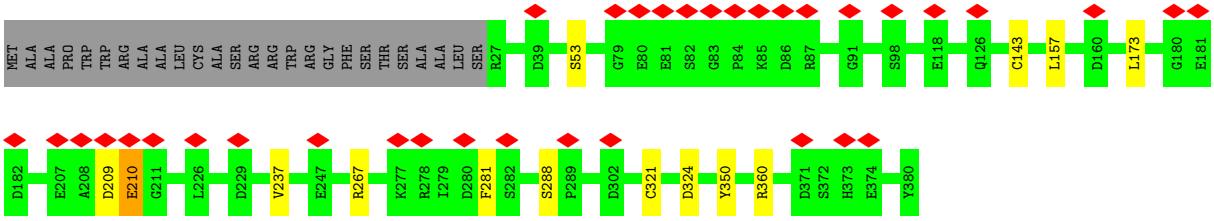
Chain a:



• Molecule 2: MITORIBOSOMAL PROTEIN ML38, MRPL38

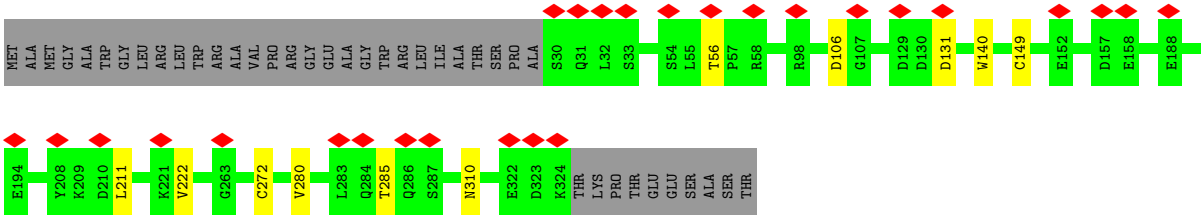
Chain b:





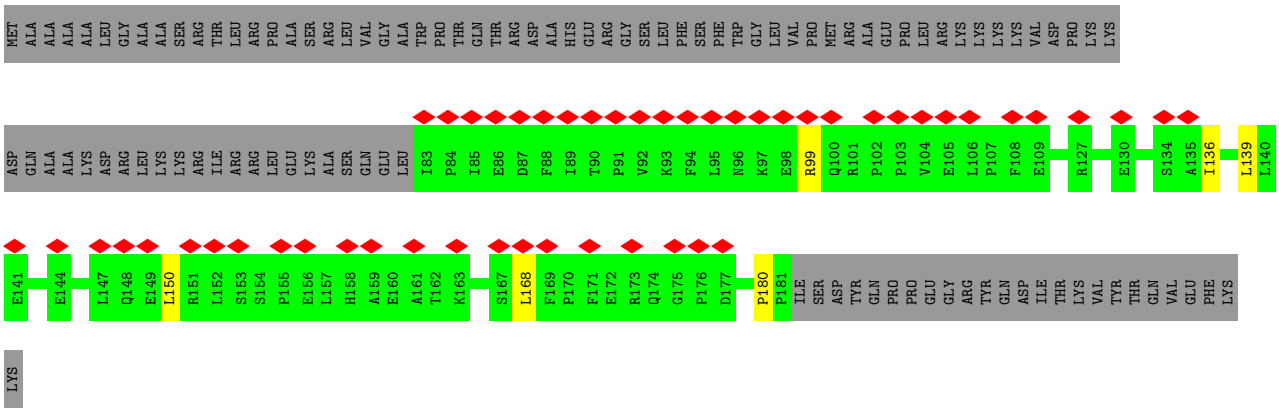
• Molecule 3: MITORIBOSOMAL PROTEIN ML39, MRPL39

Chain c:



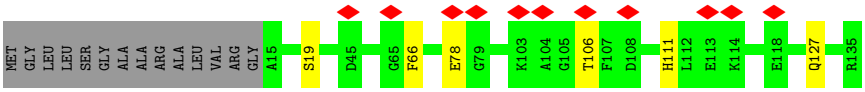
• Molecule 4: MITORIBOSOMAL PROTEIN ML40, MRPL40

Chain d:



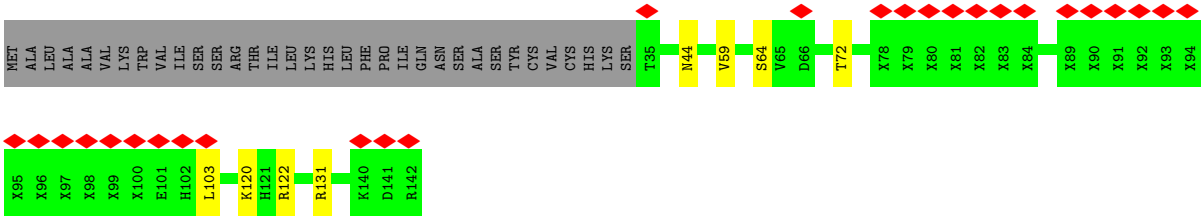
- Molecule 5: MITORIBOSOMAL PROTEIN ML41, MRPL41

Chain e:



- Molecule 6: MITORIBOSOMAL PROTEIN ML42, MRPL42

Chain f:

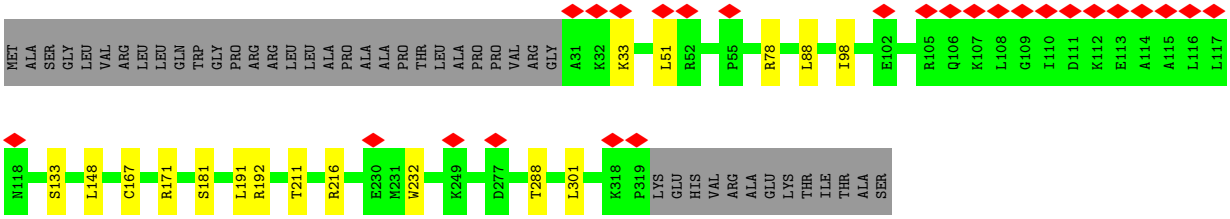


- Molecule 7: MITORIBOSOMAL PROTEIN ML43, MRPL43

Chain g:

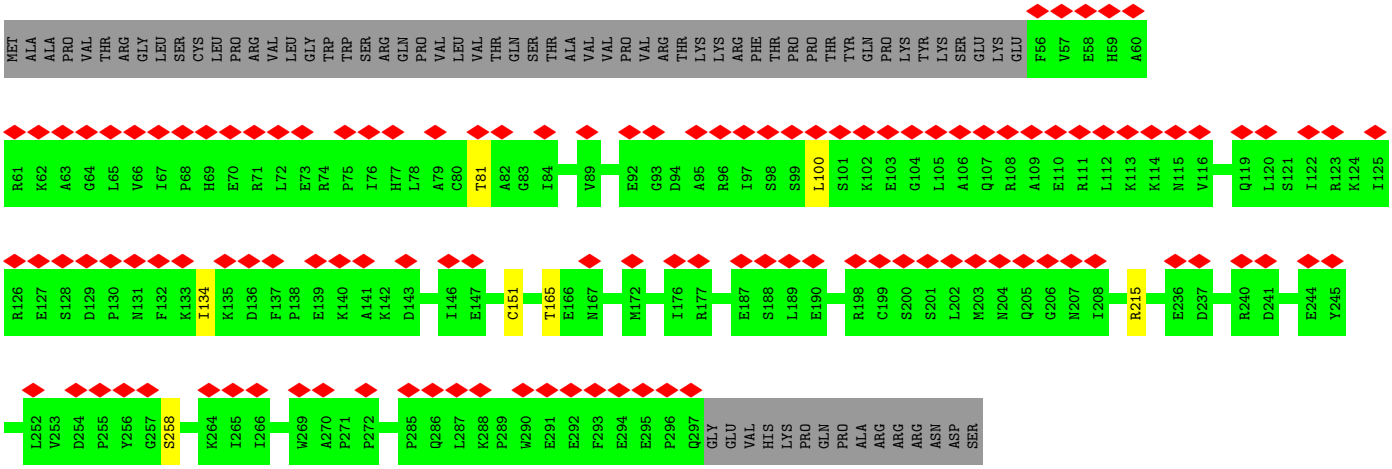
- Molecule 8: MITORIBOSOMAL PROTEIN ML44, MRPL44

Chain h:



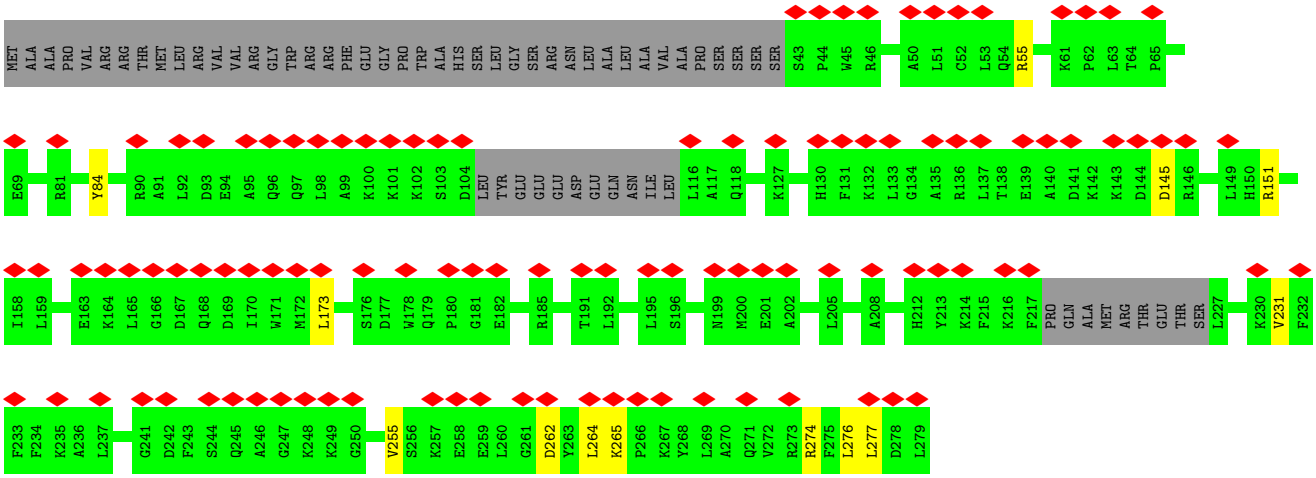
- Molecule 9: MITORIBOSOMAL PROTEIN ML45, MRPL45

Chain i:



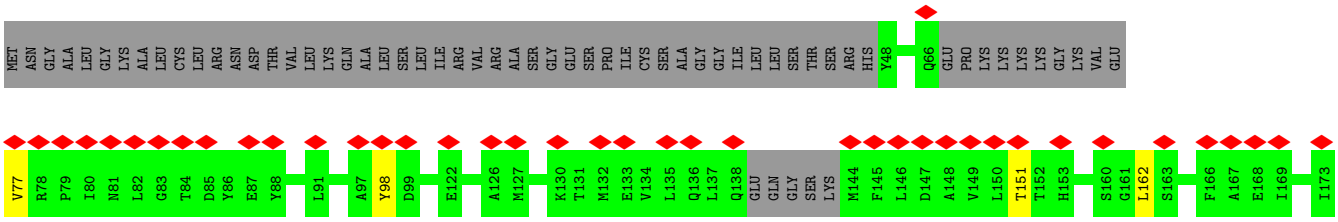
- Molecule 10: MITORIBOSOMAL PROTEIN ML46, MRPL46

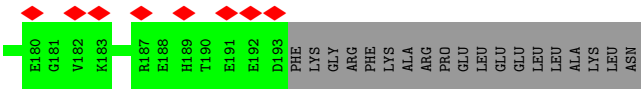
Chain j:



- Molecule 11: MITORIBOSOMAL PROTEIN ML48, MRPL48

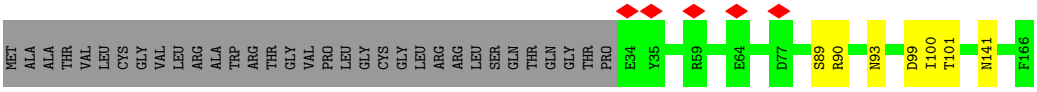
Chain k:





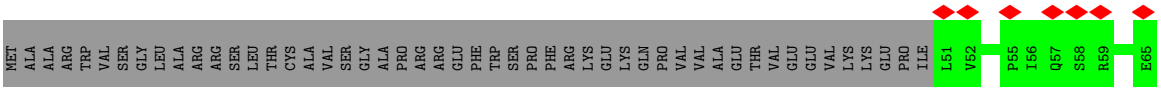
• Molecule 12: MITORIBOSOMAL PROTEIN ML49, MRPL49

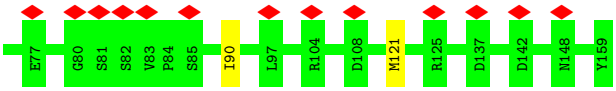
Chain l:



• Molecule 13: MITORIBOSOMAL PROTEIN ML50, MRPL50

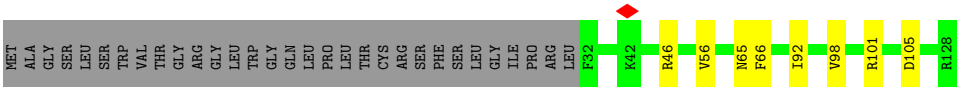
Chain m:





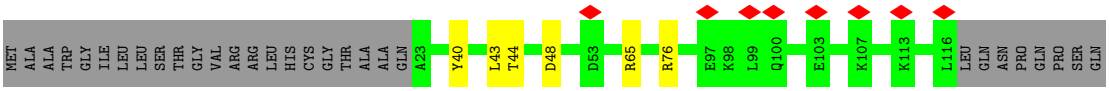
• Molecule 14: MITORIBOSOMAL PROTEIN ML51, MRPL51

Chain n:



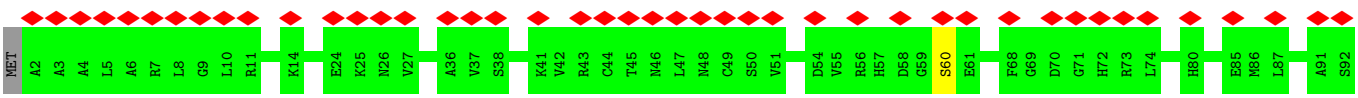
• Molecule 15: MITORIBOSOMAL PROTEIN ML52, MRPL52

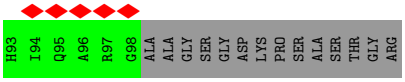
Chain o:



• Molecule 16: MITORIBOSOMAL PROTEIN ML53, MRPL53

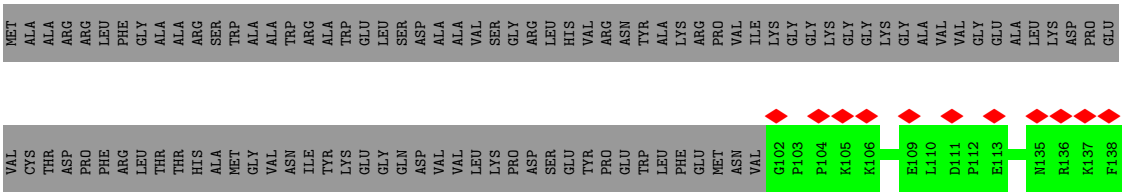
Chain p:





• Molecule 17: MITORIBOSOMAL PROTEIN ML54, MRPL54

Chain q:

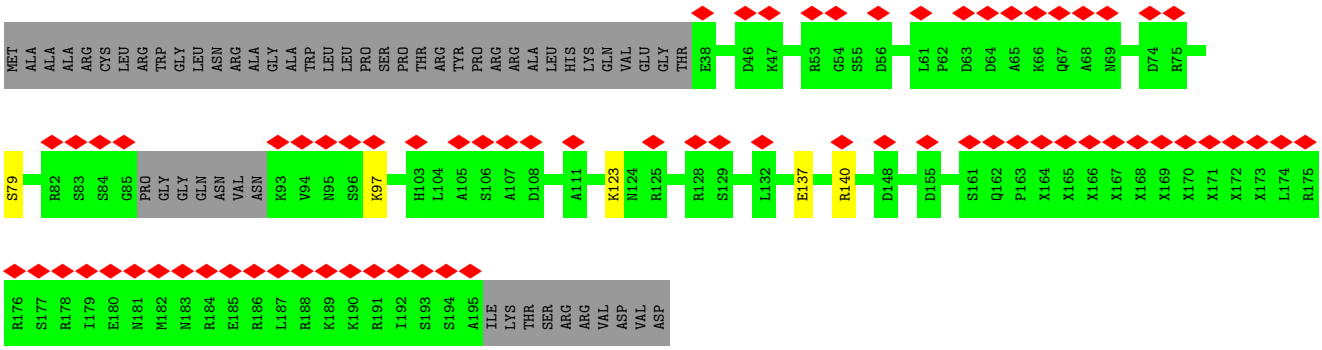


- Molecule 18: MITORIBOSOMAL PROTEIN ML63, MRPL57, MRP63

Chain t:

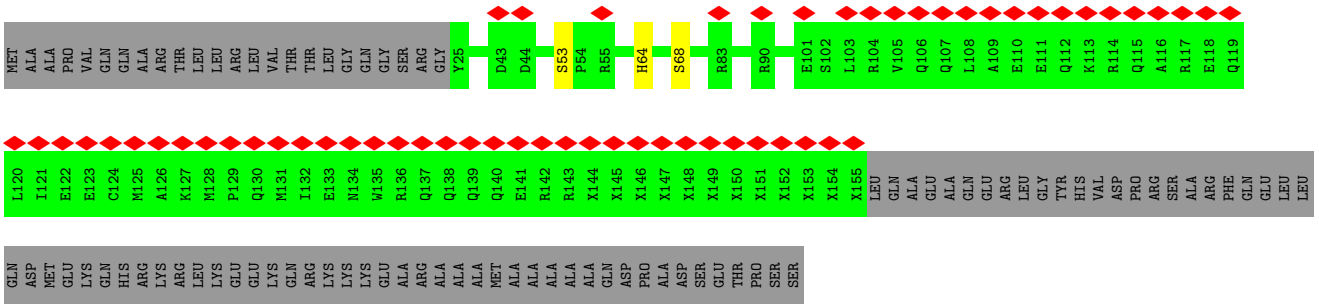
- Molecule 19: MITORIBOSOMAL PROTEIN ML62, MRPL58, ICT1

Chain u:



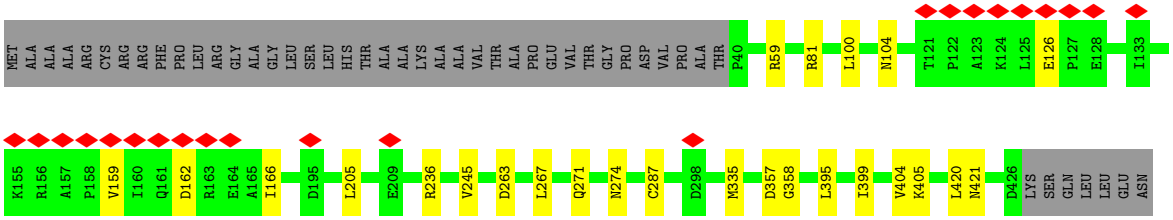
- Molecule 20: MITORIBOSOMAL PROTEIN ML64, MRPL59, CRIF1

Chain v:



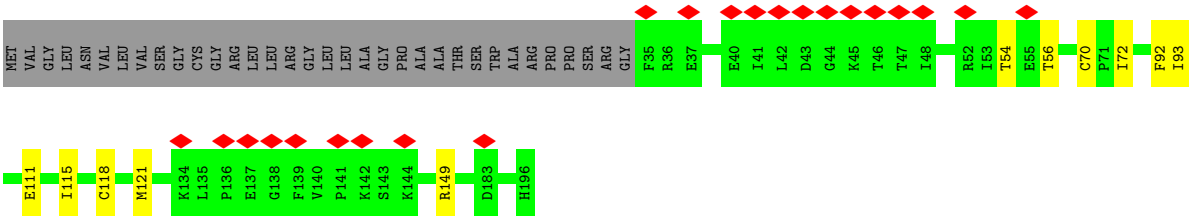
- Molecule 21: MITORIBOSOMAL PROTEIN ML65, MRPS30

Chain w:



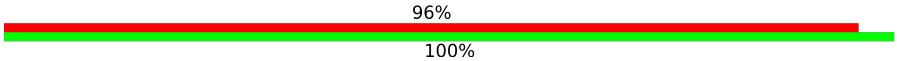
• Molecule 22: MITORIBOSOMAL PROTEIN ML66, MRPS18A

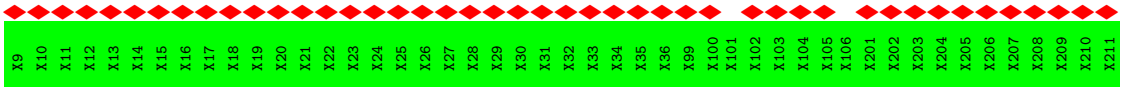
Chain x:



• Molecule 23: UNASSIGNED SECONDARY STRUCTURE ELEMENTS

Chain z:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	141675	Depositor
Resolution determination method	Not provided	
CTF correction method	PER DETECTOR FRAME	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	20	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	100000	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.560	Depositor
Minimum map value	-0.257	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.025	Depositor
Recommended contour level	0.07	Depositor
Map size (Å)	302.4, 302.4, 302.4	wwPDB
Map dimensions	216, 216, 216	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.4, 1.4, 1.4	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: 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	0.34	0/3267	0.53	0/4455
2	b	0.36	0/3047	0.55	0/4139
3	c	0.33	0/2464	0.50	0/3330
4	d	0.38	0/853	0.56	1/1153 (0.1%)
5	e	0.37	0/996	0.56	0/1340
6	f	0.38	0/731	0.54	0/990
7	g	0.38	0/1191	0.58	0/1614
8	h	0.35	0/2372	0.53	0/3211
9	i	0.32	0/2034	0.52	0/2759
10	j	0.34	0/1811	0.56	0/2436
11	k	0.35	0/1070	0.55	0/1448
12	l	0.38	0/1135	0.53	0/1549
13	m	0.30	0/917	0.49	0/1248
14	n	0.44	0/860	0.60	0/1150
15	o	0.39	0/762	0.52	0/1022
16	p	0.34	0/752	0.53	0/1013
17	q	0.29	0/346	0.47	0/463
18	t	0.41	0/798	0.61	0/1073
19	u	0.31	0/1163	0.49	0/1557
20	v	0.33	0/1022	0.44	0/1382
21	w	0.39	0/3206	0.55	0/4354
22	x	0.36	0/1364	0.62	0/1849
All	All	0.36	0/32161	0.54	1/43535 (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
2	b	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
10	j	0	1
14	n	0	1
21	w	0	1
All	All	0	4

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	d	180	PRO	C-N-CD	-5.25	109.05	120.60

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	b	210	GLU	Peptide
10	j	173	LEU	Peptide
14	n	65	ASN	Peptide
21	w	357	ASP	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	a	3173	0	3153	0	0
2	b	2952	0	2840	0	0
3	c	2408	0	2415	0	0
4	d	832	0	828	0	0
5	e	968	0	968	0	0
6	f	852	0	834	0	0
7	g	1167	0	1173	0	0
8	h	2319	0	2332	0	0
9	i	1979	0	1974	0	0
10	j	1775	0	1797	0	0
11	k	1050	0	1044	0	0
12	l	1097	0	1080	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	m	893	0	878	0	0
14	n	837	0	860	0	0
15	o	747	0	748	0	0
16	p	742	0	749	0	0
17	q	336	0	342	0	0
18	t	780	0	792	0	0
19	u	1208	0	1227	0	0
20	v	1068	0	1034	0	0
21	w	3126	0	3153	0	0
22	x	1325	0	1354	0	0
23	z	282	0	294	0	0
24	x	1	0	0	0	0
All	All	31917	0	31869	0	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 12.

There are no clashes within the asymmetric unit.

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	a	391/423 (92%)	375 (96%)	16 (4%)	0	100	100
2	b	352/380 (93%)	329 (94%)	23 (6%)	0	100	100
3	c	293/334 (88%)	279 (95%)	14 (5%)	0	100	100
4	d	97/206 (47%)	92 (95%)	5 (5%)	0	100	100
5	e	119/135 (88%)	115 (97%)	4 (3%)	0	100	100
6	f	82/142 (58%)	81 (99%)	1 (1%)	0	100	100
7	g	146/159 (92%)	141 (97%)	5 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	h	287/332 (86%)	270 (94%)	17 (6%)	0	100	100
9	i	240/312 (77%)	230 (96%)	10 (4%)	0	100	100
10	j	211/279 (76%)	200 (95%)	9 (4%)	2 (1%)	17	49
11	k	125/212 (59%)	119 (95%)	6 (5%)	0	100	100
12	l	131/166 (79%)	127 (97%)	4 (3%)	0	100	100
13	m	107/159 (67%)	101 (94%)	6 (6%)	0	100	100
14	n	95/128 (74%)	91 (96%)	4 (4%)	0	100	100
15	o	92/124 (74%)	87 (95%)	5 (5%)	0	100	100
16	p	95/112 (85%)	90 (95%)	5 (5%)	0	100	100
17	q	35/138 (25%)	33 (94%)	2 (6%)	0	100	100
18	t	92/102 (90%)	88 (96%)	4 (4%)	0	100	100
19	u	137/205 (67%)	130 (95%)	7 (5%)	0	100	100
20	v	118/222 (53%)	116 (98%)	2 (2%)	0	100	100
21	w	385/433 (89%)	363 (94%)	20 (5%)	2 (0%)	29	61
22	x	160/196 (82%)	155 (97%)	4 (2%)	1 (1%)	25	57
All	All	3790/4899 (77%)	3612 (95%)	173 (5%)	5 (0%)	54	82

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
21	w	159	VAL
22	x	93	ILE
10	j	84	TYR
10	j	151	ARG
21	w	358	GLY

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	
1	a	348/365 (95%)	332 (95%)	16 (5%)	27	57
2	b	310/328 (94%)	296 (96%)	14 (4%)	27	58
3	c	271/299 (91%)	260 (96%)	11 (4%)	30	59
4	d	92/181 (51%)	87 (95%)	5 (5%)	22	52
5	e	100/108 (93%)	94 (94%)	6 (6%)	19	49
6	f	80/110 (73%)	72 (90%)	8 (10%)	7	27
7	g	128/136 (94%)	113 (88%)	15 (12%)	5	20
8	h	251/284 (88%)	234 (93%)	17 (7%)	16	45
9	i	218/281 (78%)	211 (97%)	7 (3%)	39	67
10	j	190/242 (78%)	180 (95%)	10 (5%)	22	52
11	k	115/181 (64%)	111 (96%)	4 (4%)	36	65
12	l	122/147 (83%)	115 (94%)	7 (6%)	20	50
13	m	103/145 (71%)	101 (98%)	2 (2%)	57	78
14	n	88/113 (78%)	81 (92%)	7 (8%)	12	38
15	o	74/97 (76%)	68 (92%)	6 (8%)	11	38
16	p	79/88 (90%)	78 (99%)	1 (1%)	69	84
17	q	36/114 (32%)	36 (100%)	0	100	100
18	t	75/82 (92%)	67 (89%)	8 (11%)	6	24
19	u	126/169 (75%)	121 (96%)	5 (4%)	31	60
20	v	102/173 (59%)	99 (97%)	3 (3%)	42	69
21	w	340/373 (91%)	318 (94%)	22 (6%)	17	46
22	x	149/173 (86%)	139 (93%)	10 (7%)	16	46
All	All	3397/4189 (81%)	3213 (95%)	184 (5%)	26	52

All (184) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	a	35	VAL
1	a	113	LEU
1	a	151	ASP
1	a	175	THR
1	a	195	HIS
1	a	207	ASN
1	a	210	SER
1	a	225	SER

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Mol	Chain	Res	Type
1	a	248	THR
1	a	268	CYS
1	a	270	VAL
1	a	274	ASN
1	a	277	THR
1	a	335	VAL
1	a	348	ASP
1	a	398	VAL
2	b	53	SER
2	b	143	CYS
2	b	157	LEU
2	b	173	LEU
2	b	209	ASP
2	b	210	GLU
2	b	237	VAL
2	b	267	ARG
2	b	281	PHE
2	b	288	SER
2	b	321	CYS
2	b	324	ASP
2	b	350	TYR
2	b	360	ARG
3	c	56	THR
3	c	106	ASP
3	c	131	ASP
3	c	140	TRP
3	c	149	CYS
3	c	211	LEU
3	c	222	VAL
3	c	272	CYS
3	c	280	VAL
3	c	285	THR
3	c	310	ASN
4	d	99	ARG
4	d	136	ILE
4	d	139	LEU
4	d	150	LEU
4	d	168	LEU
5	e	19	SER
5	e	66	PHE
5	e	78	GLU
5	e	106	THR

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Mol	Chain	Res	Type
5	e	111	HIS
5	e	127	GLN
6	f	44	ASN
6	f	59	VAL
6	f	64	SER
6	f	72	THR
6	f	103	LEU
6	f	120	LYS
6	f	122	ARG
6	f	131	ARG
7	g	6	THR
7	g	9	ARG
7	g	14	VAL
7	g	21	ARG
7	g	28	ARG
7	g	33	LEU
7	g	34	SER
7	g	39	SER
7	g	70	CYS
7	g	94	VAL
7	g	108	SER
7	g	112	VAL
7	g	114	ARG
7	g	126	ILE
7	g	138	THR
8	h	33	LYS
8	h	51	LEU
8	h	78	ARG
8	h	88	LEU
8	h	98	ILE
8	h	133	SER
8	h	148	LEU
8	h	167	CYS
8	h	171	ARG
8	h	181	SER
8	h	191	LEU
8	h	192	ARG
8	h	211	THR
8	h	216	ARG
8	h	232	TRP
8	h	288	THR
8	h	301	LEU

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Mol	Chain	Res	Type
9	i	81	THR
9	i	100	LEU
9	i	134	ILE
9	i	151	CYS
9	i	165	THR
9	i	215	ARG
9	i	258	SER
10	j	55	ARG
10	j	145	ASP
10	j	231	VAL
10	j	255	VAL
10	j	262	ASP
10	j	264	LEU
10	j	265	LYS
10	j	274	ARG
10	j	276	LEU
10	j	277	LEU
11	k	77	VAL
11	k	98	TYR
11	k	151	THR
11	k	162	LEU
12	l	89	SER
12	l	90	ARG
12	l	93	ASN
12	l	99	ASP
12	l	100	ILE
12	l	101	THR
12	l	141	ASN
13	m	90	ILE
13	m	121	MET
14	n	46	ARG
14	n	56	VAL
14	n	66	PHE
14	n	92	ILE
14	n	98	VAL
14	n	101	ARG
14	n	105	ASP
15	o	40	TYR
15	o	43	LEU
15	o	44	THR
15	o	48	ASP
15	o	65	ARG

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Mol	Chain	Res	Type
15	o	76	ARG
16	p	60	SER
18	t	9	ARG
18	t	25	ARG
18	t	45	ASN
18	t	49	LEU
18	t	51	ARG
18	t	82	PHE
18	t	86	ARG
18	t	101	TRP
19	u	79	SER
19	u	97	LYS
19	u	123	LYS
19	u	137	GLU
19	u	140	ARG
20	v	53	SER
20	v	64	HIS
20	v	68	SER
21	w	59	ARG
21	w	81	ARG
21	w	100	LEU
21	w	104	ASN
21	w	126	GLU
21	w	162	ASP
21	w	166	ILE
21	w	205	LEU
21	w	236	ARG
21	w	245	VAL
21	w	263	ASP
21	w	267	LEU
21	w	271	GLN
21	w	274	ASN
21	w	287	CYS
21	w	335	MET
21	w	395	LEU
21	w	399	ILE
21	w	404	VAL
21	w	405	LYS
21	w	420	LEU
21	w	421	ASN
22	x	54	THR
22	x	56	THR

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Mol	Chain	Res	Type
22	x	70	CYS
22	x	72	ILE
22	x	92	PHE
22	x	111	GLU
22	x	115	ILE
22	x	118	CYS
22	x	121	MET
22	x	149	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (59) such sidechains are listed below:

Mol	Chain	Res	Type
1	a	96	HIS
1	a	108	HIS
1	a	156	ASN
1	a	223	HIS
1	a	274	ASN
1	a	289	HIS
1	a	343	GLN
1	a	360	ASN
1	a	420	HIS
2	b	220	ASN
2	b	224	HIS
2	b	266	HIS
2	b	308	GLN
2	b	320	GLN
3	c	281	HIS
3	c	294	GLN
3	c	305	HIS
3	c	310	ASN
6	f	44	ASN
6	f	121	HIS
6	f	130	HIS
7	g	17	ASN
7	g	120	HIS
7	g	131	HIS
8	h	94	ASN
8	h	177	GLN
8	h	260	GLN
9	i	115	ASN
9	i	157	HIS
9	i	193	GLN

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Mol	Chain	Res	Type
9	i	196	GLN
9	i	217	HIS
9	i	274	GLN
11	k	61	HIS
11	k	177	ASN
12	l	93	ASN
12	l	141	ASN
13	m	107	ASN
14	n	69	HIS
14	n	122	ASN
14	n	124	HIS
15	o	63	GLN
16	p	72	HIS
16	p	93	HIS
18	t	34	ASN
18	t	45	ASN
18	t	85	HIS
19	u	103	HIS
19	u	145	ASN
21	w	101	ASN
21	w	104	ASN
21	w	173	GLN
21	w	228	ASN
21	w	233	ASN
21	w	234	GLN
21	w	367	GLN
21	w	385	ASN
22	x	164	ASN
22	x	184	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
23	z	5
20	v	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	z	36:UNK	C	99:UNK	N	57.05
1	z	106:UNK	C	201:UNK	N	13.00
1	z	105:UNK	C	106:UNK	N	3.37
1	v	154:UNK	C	155:UNK	N	3.12
1	z	35:UNK	C	36:UNK	N	3.12
1	z	210:UNK	C	211:UNK	N	3.12

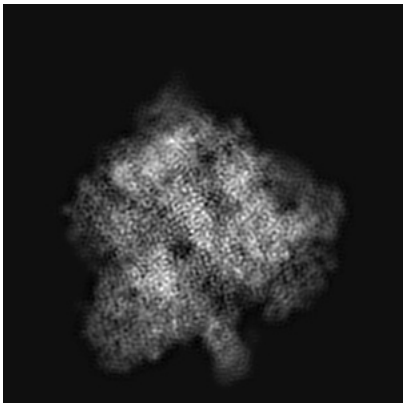
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-2787. These allow visual inspection of the internal detail of the map and identification of artifacts.

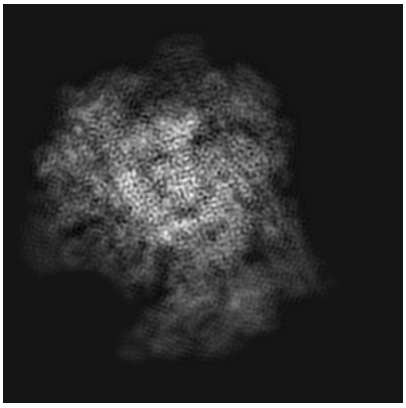
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

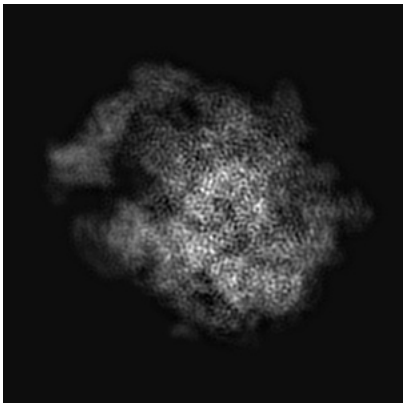
6.1.1 Primary map



X



Y

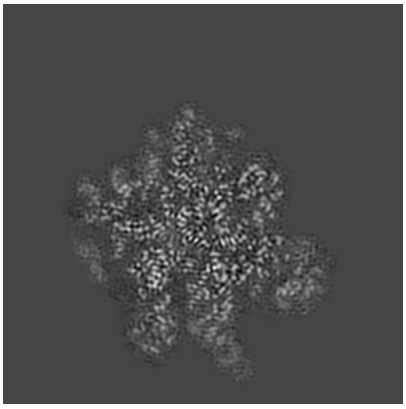


Z

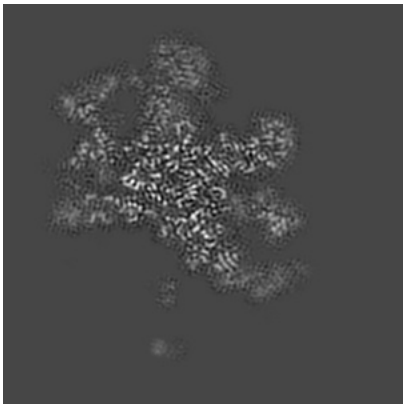
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

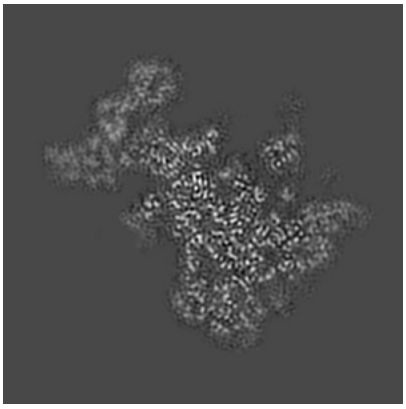
6.2.1 Primary map



X Index: 108



Y Index: 108

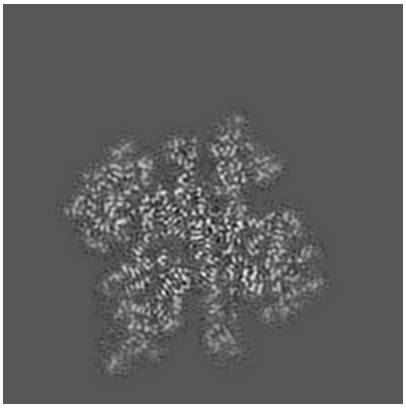


Z Index: 108

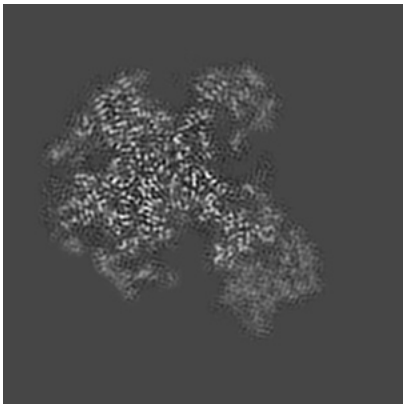
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

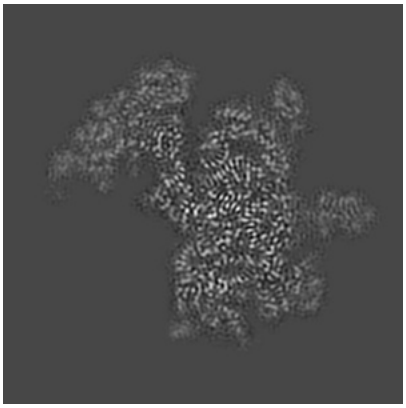
6.3.1 Primary map



X Index: 120



Y Index: 86

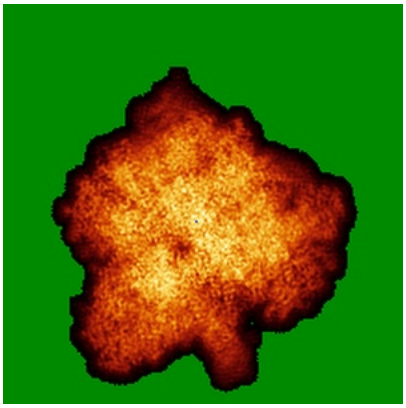


Z Index: 98

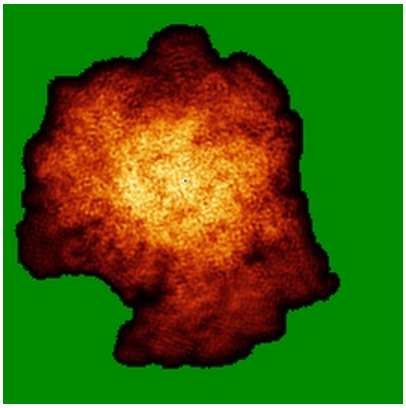
The images above show the largest variance slices of the map in three orthogonal directions.

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

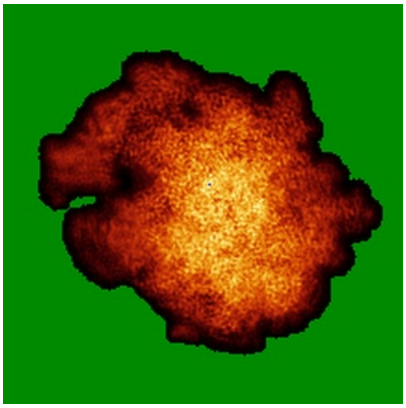
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.07. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

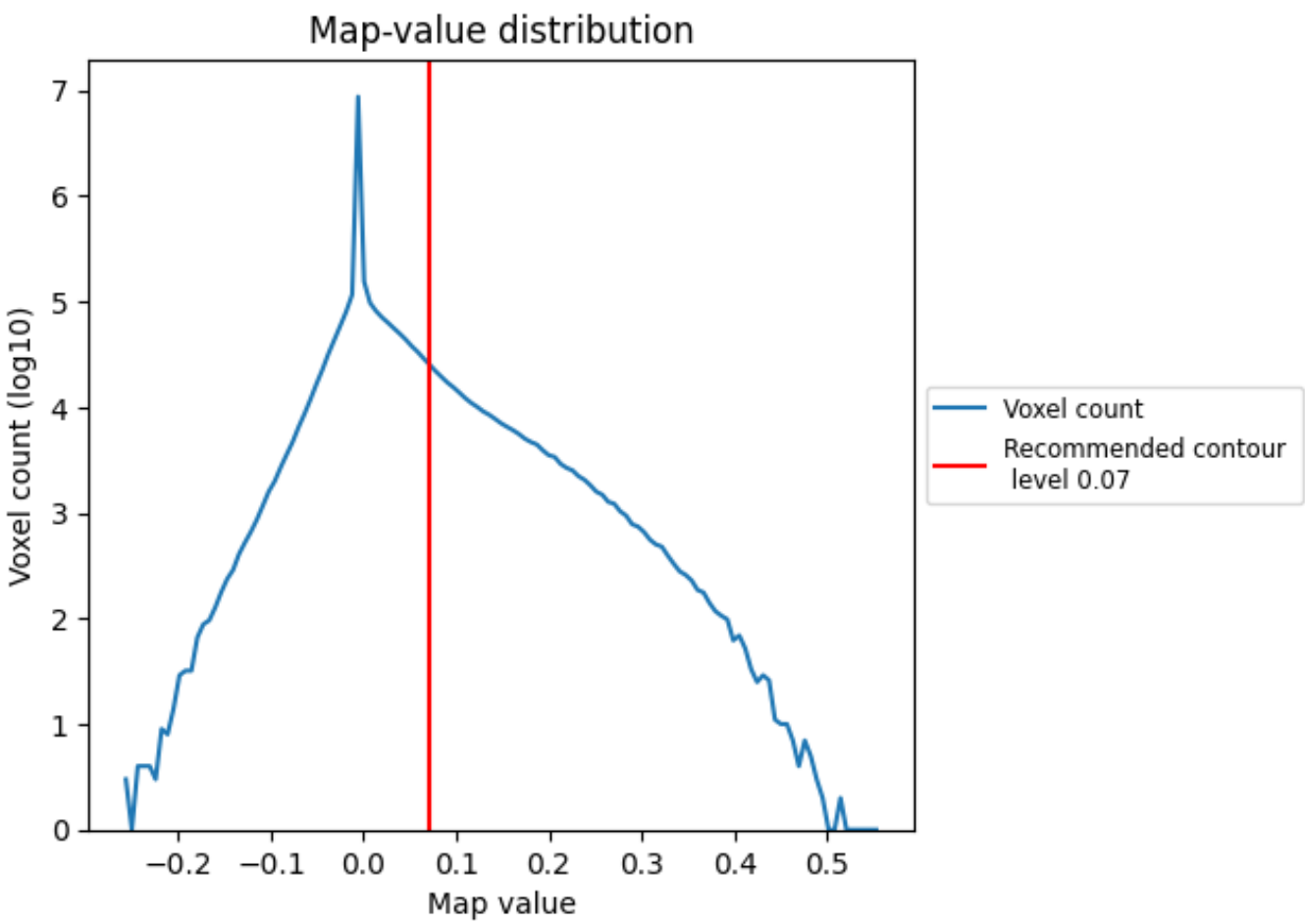
6.6 Mask visualisation (i)

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

7 Map analysis (i)

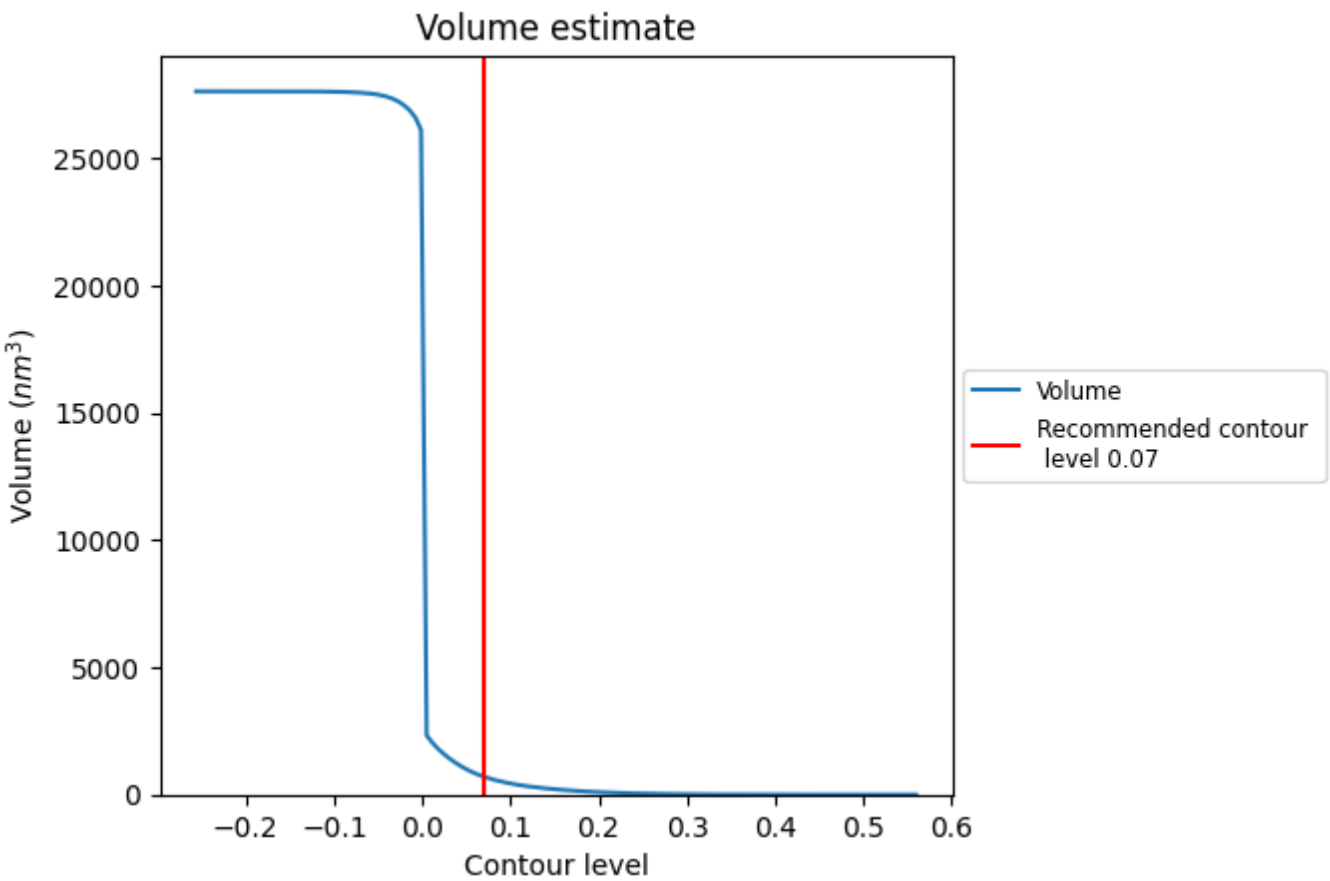
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

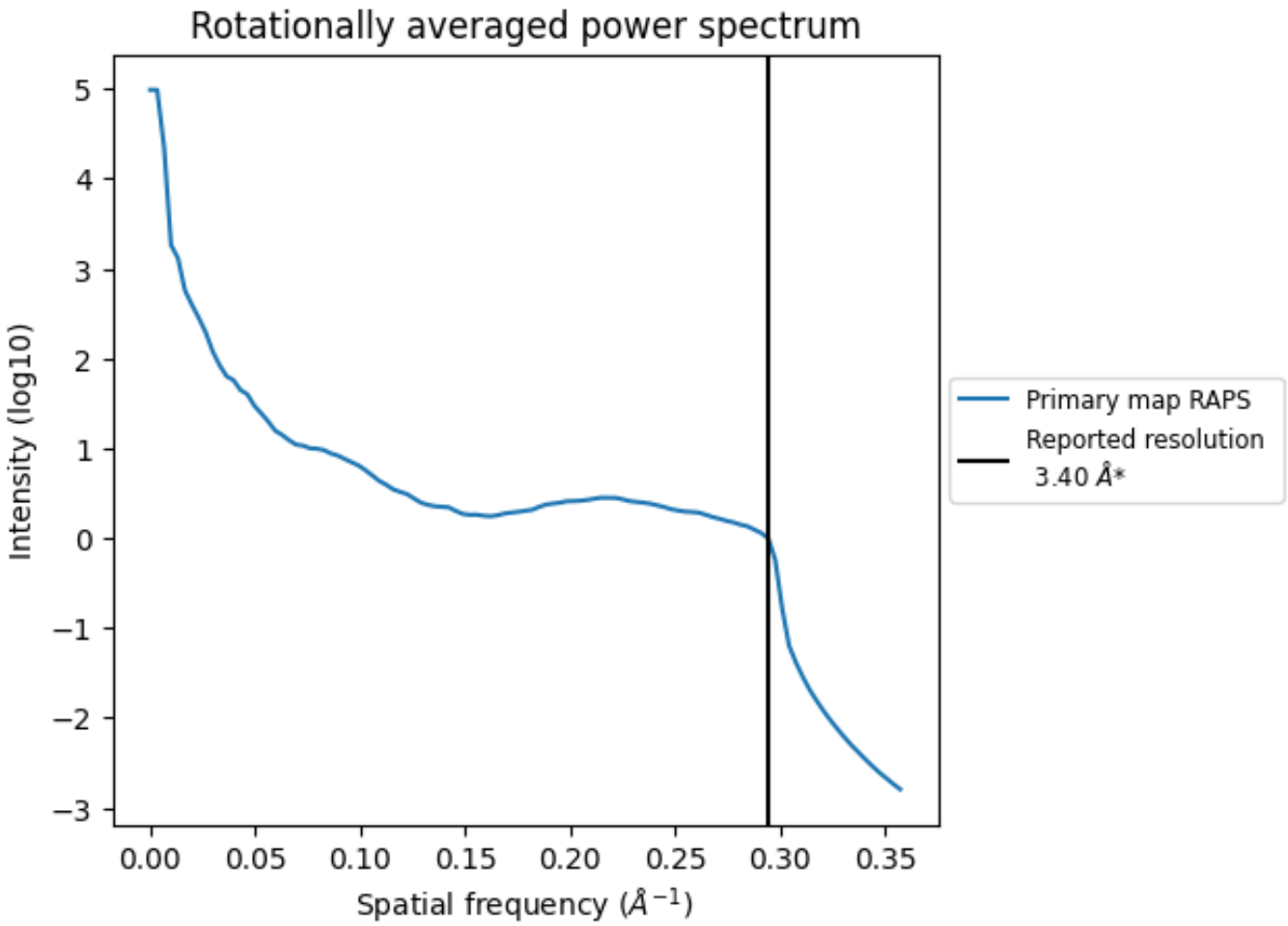
7.2 Volume estimate (i)



The volume at the recommended contour level is 700 nm^3; this corresponds to an approximate mass of 632 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 0.294 Å^{-1}

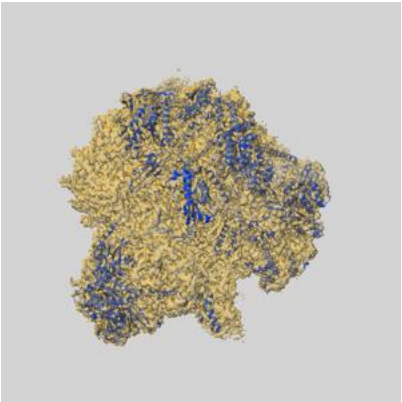
8 Fourier-Shell correlation (i)

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

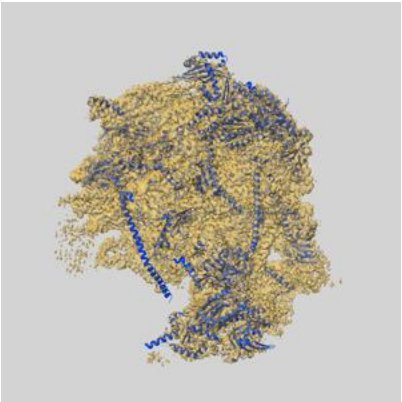
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-2787 and PDB model 4V1A. Per-residue inclusion information can be found in section 3 on page 8.

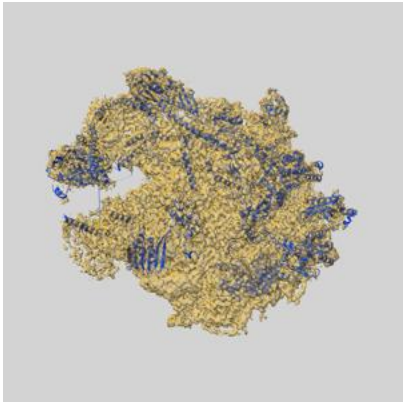
9.1 Map-model overlay (i)



X



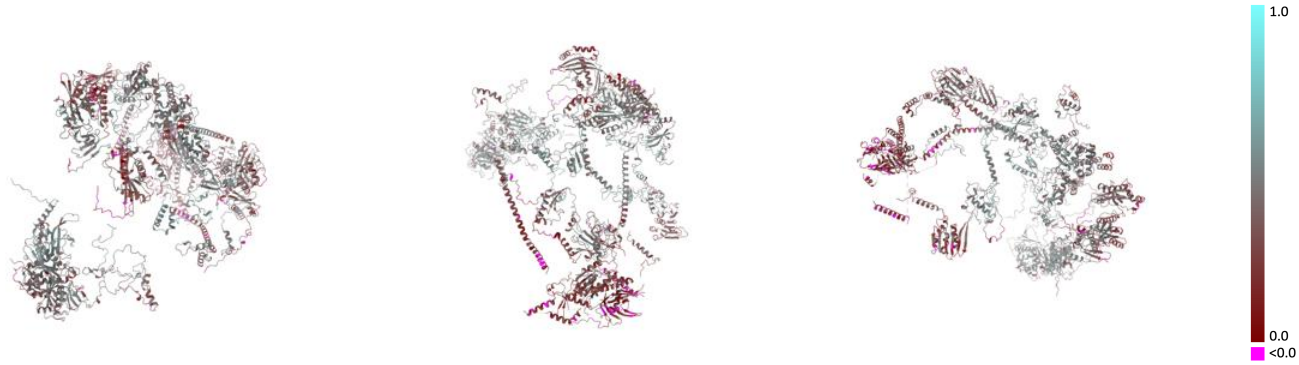
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.07 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.

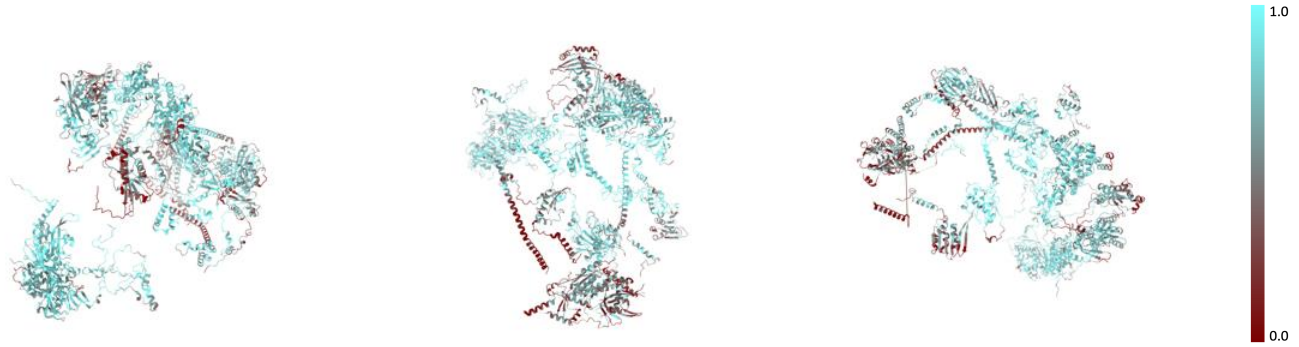
9.2 Q-score mapped to coordinate model (i)



X Y Z

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.

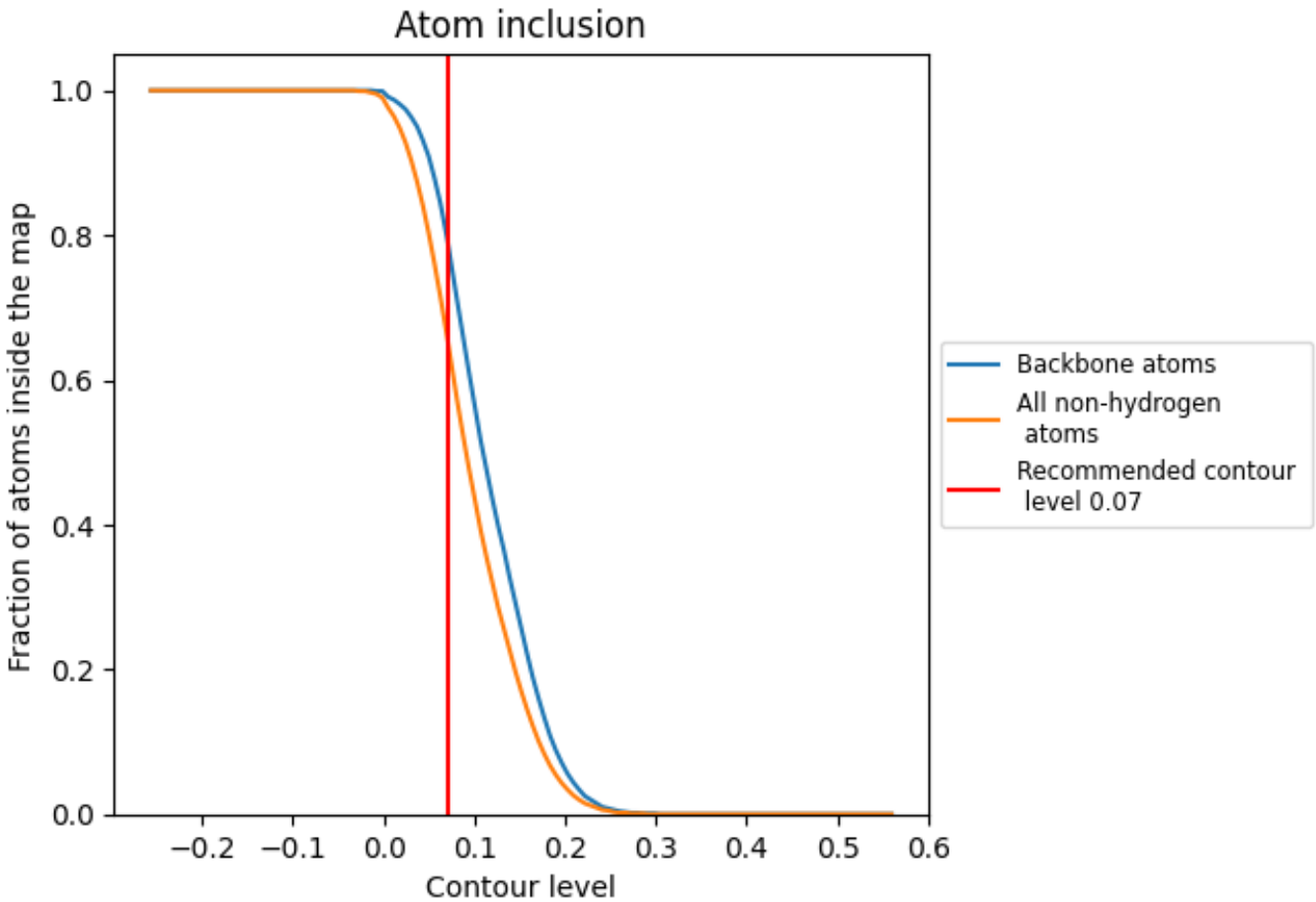
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.07).

9.4 Atom inclusion (i)



At the recommended contour level, 80% of all backbone atoms, 66% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.07) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6590	0.3880
a	0.7830	0.4530
b	0.7240	0.3930
c	0.6960	0.3920
d	0.4400	0.2390
e	0.7290	0.4160
f	0.6830	0.4250
g	0.8320	0.5020
h	0.7240	0.4250
i	0.4170	0.3120
j	0.4130	0.1810
k	0.4980	0.2970
l	0.8170	0.4700
m	0.6160	0.3680
n	0.8570	0.5090
o	0.7600	0.4480
p	0.4210	0.2680
q	0.5110	0.2740
t	0.8510	0.5140
u	0.4020	0.2990
v	0.4530	0.3110
w	0.7940	0.4580
x	0.7540	0.4420
z	0.1210	0.1570