



wwPDB EM Validation Summary Report ⓘ

Dec 30, 2024 – 09:04 AM EST

PDB ID : 8B0X
EMDB ID : EMD-15793
Title : Translating 70S ribosome in the unrotated state (P and E, tRNAs)
Authors : Fromm, S.A.; O'Connor, K.M.; Purdy, M.; Bhatt, P.R.; Loughran, G.; Atkins, J.F.; Jomaa, A.; Mattei, S.
Deposited on : 2022-09-08
Resolution : 1.55 Å(reported)
Based on initial model : 7K00

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev113
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.40

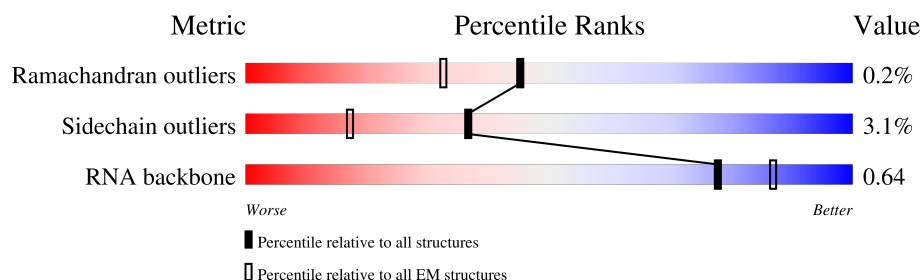
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 1.55 Å.

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





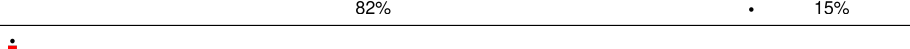
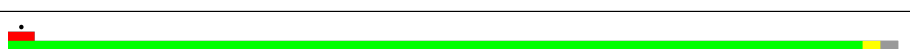


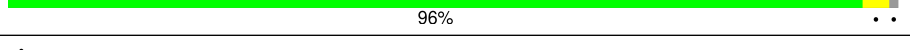
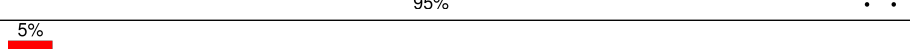
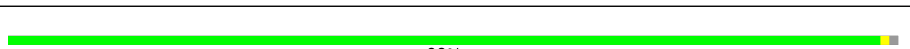
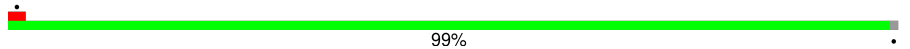

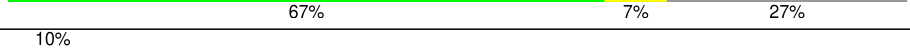

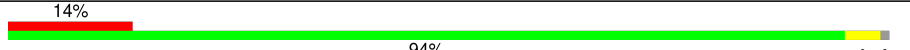
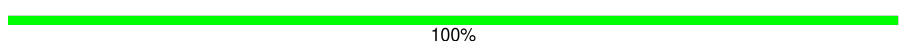

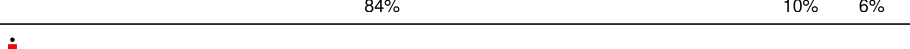

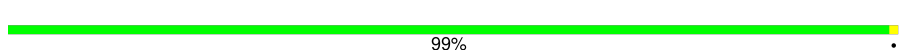
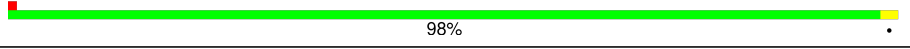
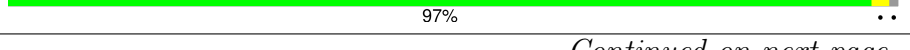



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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

Mol	Chain	Length	Quality of chain
1	0	55	89% 7%
2	1	46	98% .
3	2	65	97% ..
4	3	38	97% .
5	A	1554	10% 85% 12% .
6	B	241	10% 88% 5% 7%
7	C	233	6% 85% . 12%
8	D	206	95% .


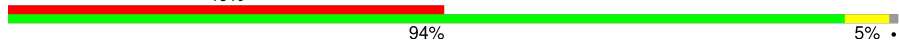
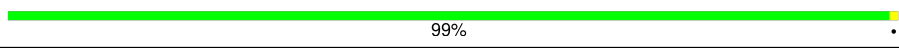
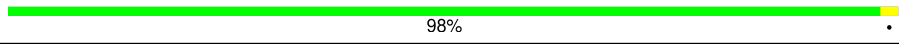
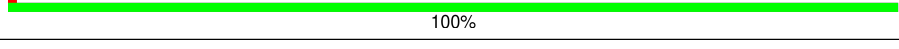
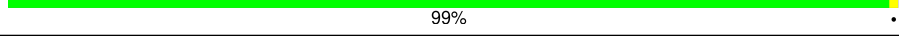
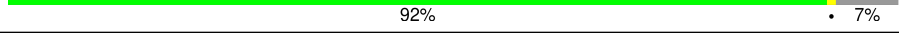
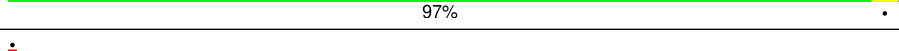
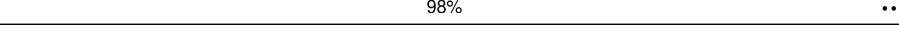
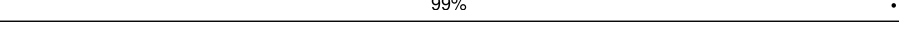
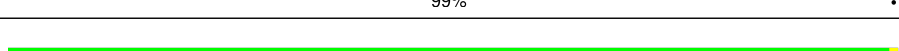
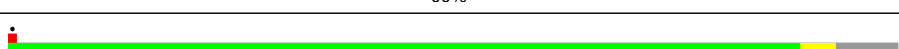

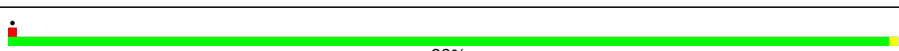
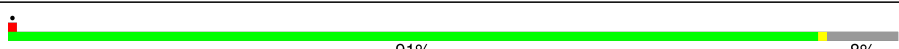
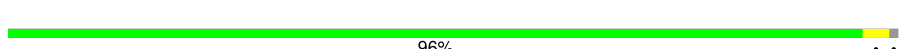
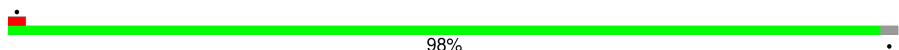
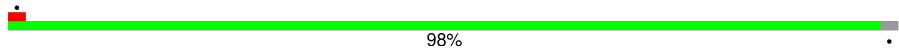
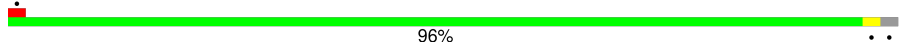

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Mol	Chain	Length	Quality of chain
9	E	167	
10	F	135	
11	G	179	
12	H	130	
13	I	130	
14	J	103	
15	K	129	
16	L	124	
17	M	118	
18	N	101	
19	O	89	
20	P	82	
21	Q	84	
22	R	75	
23	S	92	
24	T	87	
25	U	71	
26	X	6	
27	Z	77	
28	a	2925	
29	b	119	
30	c	273	
31	d	209	
32	e	201	
33	f	179	

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Mol	Chain	Length	Quality of chain
34	g	177	
35	h	149	
36	i	142	
37	j	123	
38	k	144	
39	l	136	
40	m	127	
41	n	117	
42	o	115	
43	p	118	
44	q	103	
45	r	110	
46	s	100	
47	t	104	
48	u	94	
49	v	85	
50	w	78	
51	x	63	
52	y	59	
53	z	57	

2 Entry composition

There are 57 unique types of molecules in this entry. The entry contains 151507 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 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	0	51	Total	C	N	O	0	0
			417	269	76	72		

- Molecule 2 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 3 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 4 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	3	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 5 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	A	1500	Total	C	N	O	P	0	0
			32211	14373	5920	10418	1500		

- Molecule 6 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	B	224	Total	C	N	O	S	0	0
			1753	1109	315	321	8		

- Molecule 7 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	C	206	Total	C	N	O	S	0	0
			1624	1028	305	288	3		

- Molecule 8 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	D	205	Total	C	N	O	S	0	0
			1643	1026	315	298	4		

- Molecule 9 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	E	156	Total	C	N	O	S	0	0
			1152	717	217	212	6		

- Molecule 10 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	F	103	Total	C	N	O	S	0	0
			839	530	151	151	7		

- Molecule 11 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	G	153	Total	C	N	O	S	0	0
			1203	750	231	218	4		

- Molecule 12 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	H	129	Total	C	N	O	S	0	0
			979	616	173	184	6		

- Molecule 13 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	I	127	Total	C	N	O	S	0	0
			1022	634	206	179	3		

- Molecule 14 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	J	98	Total	C	N	O	S	0	0
			786	493	150	142	1		

- Molecule 15 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	K	117	Total	C	N	O	S	0	0
			877	540	173	161	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	119	IAS	ASN	modified residue	UNP P0A7R9

- Molecule 16 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	L	123	Total	C	N	O	S	0	0
			957	591	196	165	5		

- Molecule 17 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	M	115	Total	C	N	O	S	0	0
			891	552	179	157	3		

- Molecule 18 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	N	100	Total	C	N	O	S	0	0
			805	499	164	139	3		

- Molecule 19 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	O	88	Total	C	N	O	S	0	0
			714	439	144	130	1		

- Molecule 20 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	P	81	Total	C	N	O	S	0	0
			643	403	127	112	1		

- Molecule 21 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	Q	79	Total	C	N	O	S	0	0
			641	406	120	112	3		

- Molecule 22 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	R	55	Total	C	N	O	0	0
			455	288	86	81		

- Molecule 23 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	S	84	Total	C	N	O	S	0	0
			668	427	127	112	2		

- Molecule 24 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	T	86	Total	C	N	O	S	0	0
			670	414	138	115	3		

- Molecule 25 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	U	70	Total	C	N	O	S	0	0
			589	366	125	97	1		

- Molecule 26 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	X	6	Total	C	N	O	P	0	0
			131	59	27	39	6		

- Molecule 27 is a RNA chain called P-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	Z	75	Total	C	N	O	P	0	0
			1603	714	292	522	75		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Z	34	U	C	conflict	GB 1804121330
Z	36	C	U	conflict	GB 1804121330

- Molecule 28 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	a	2748	Total	C	N	O	P	0	0
			59025	26336	10876	19065	2748		

- Molecule 29 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	b	119	Total	C	N	O	P	0	0
			2549	1135	466	829	119		

- Molecule 30 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	c	271	Total	C	N	O	S	0	0
			2082	1288	423	364	7		

- Molecule 31 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	d	209	Total	C	N	O	S	0	0
			1566	980	288	294	4		

- Molecule 32 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	e	201	Total	C	N	O	S	0	0
			1552	974	283	290	5		

- Molecule 33 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	f	177	Total	C	N	O	S	0	0
			1410	899	249	256	6		

- Molecule 34 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	g	176	Total	C	N	O	S	0	0
			1323	832	243	246	2		

- Molecule 35 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	h	148	Total	C	N	O	S	0	0
			1101	694	196	210	1		

- Molecule 36 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	i	142	Total	C	N	O	S	0	0
			1129	714	212	199	4		

- Molecule 37 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	j	123	Total	C	N	O	S	0	0
			946	593	181	166	6		

- Molecule 38 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	k	144	Total	C	N	O	S	0	0
			1053	654	207	190	2		

- Molecule 39 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	l	136	Total	C	N	O	S	0	0
			1075	686	205	177	7		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	82	MS6	MET	modified residue	UNP P0ADY7

- Molecule 40 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	m	118	Total	C	N	O	S	0	0
			945	585	194	161	5		

- Molecule 41 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	n	116	Total	C	N	O		0	0
			892	552	178	162			

- Molecule 42 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	o	114	Total	C	N	O	S	0	0
			917	574	179	163	1		

- Molecule 43 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	p	117	Total	C	N	O		0	0
			947	604	192	151			

- Molecule 44 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	q	103	Total	C	N	O	S	0	0
			816	516	153	145	2		

- Molecule 45 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	r	110	Total	C	N	O	S	0	0
			857	532	166	156	3		

- Molecule 46 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	s	93	Total	C	N	O	S	0	0
			738	466	139	131	2		

- Molecule 47 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	t	102	Total	C	N	O	S	0	0
			779	492	146	141			

- Molecule 48 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	u	94	Total	C	N	O	S	0	0
			753	479	137	134	3		

- Molecule 49 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	v	78	Total	C	N	O	S	0	0
			586	362	116	107	1		

- Molecule 50 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	w	77	Total	C	N	O	S	0	0
			625	388	129	106	2		

- Molecule 51 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	x	62	Total	C	N	O	S	0	0
			501	308	98	94	1		

- Molecule 52 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	y	58	Total	C	N	O	S	0	0
			449	281	87	79	2		

- Molecule 53 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	z	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

- Molecule 54 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
54	3	1	Total	Zn	0
			1	1	

- Molecule 55 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
55	A	48	Total	K	0
			48	48	
55	a	112	Total	K	0
			112	112	
55	b	1	Total	K	0
			1	1	
55	c	4	Total	K	0
			4	4	
55	d	1	Total	K	0
			1	1	
55	e	1	Total	K	0
			1	1	
55	f	1	Total	K	0
			1	1	

- Molecule 56 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
56	A	97	Total	Mg	0
			97	97	
56	X	1	Total	Mg	0
			1	1	
56	a	254	Total	Mg	0
			254	254	
56	b	5	Total	Mg	0
			5	5	
56	c	2	Total	Mg	0
			2	2	
56	d	1	Total	Mg	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
56	z	1	Total 1	Mg 1	0

- Molecule 57 is water.

Mol	Chain	Residues	Atoms		AltConf
57	0	5	Total 5	O 5	0
57	1	51	Total 51	O 51	0
57	2	45	Total 45	O 45	0
57	3	13	Total 13	O 13	0
57	A	2886	Total 2886	O 2886	0
57	B	7	Total 7	O 7	0
57	C	16	Total 16	O 16	0
57	D	14	Total 14	O 14	0
57	E	38	Total 38	O 38	0
57	F	5	Total 5	O 5	0
57	G	4	Total 4	O 4	0
57	H	45	Total 45	O 45	0
57	I	11	Total 11	O 11	0
57	J	15	Total 15	O 15	0
57	K	22	Total 22	O 22	0
57	L	35	Total 35	O 35	0
57	M	2	Total 2	O 2	0
57	N	8	Total 8	O 8	0

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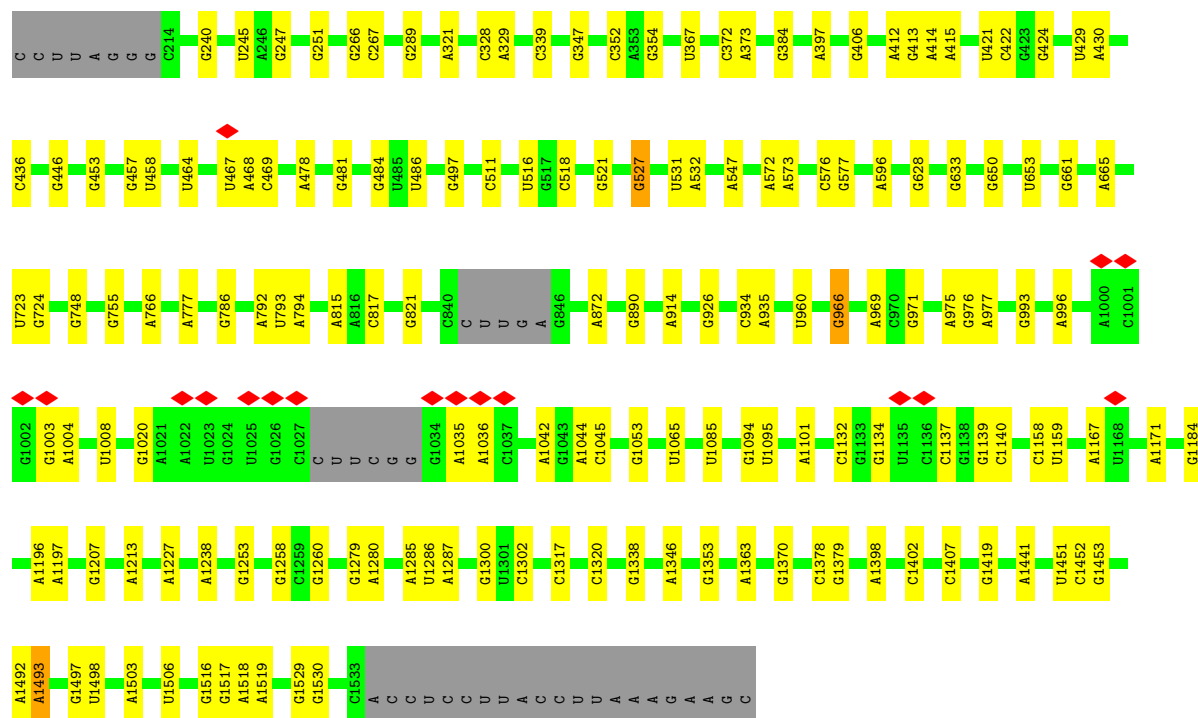
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Mol	Chain	Residues	Atoms		AltConf
57	O	29	Total 29	O 29	0
57	P	22	Total 22	O 22	0
57	Q	9	Total 9	O 9	0
57	R	13	Total 13	O 13	0
57	T	18	Total 18	O 18	0
57	U	17	Total 17	O 17	0
57	X	19	Total 19	O 19	0
57	Z	20	Total 20	O 20	0
57	a	6905	Total 6905	O 6905	0
57	b	81	Total 81	O 81	0
57	c	195	Total 195	O 195	0
57	d	107	Total 107	O 107	0
57	e	80	Total 80	O 80	0
57	h	1	Total 1	O 1	0
57	i	70	Total 70	O 70	0
57	j	58	Total 58	O 58	0
57	k	72	Total 72	O 72	0
57	l	57	Total 57	O 57	0
57	m	61	Total 61	O 61	0
57	n	3	Total 3	O 3	0
57	o	71	Total 71	O 71	0

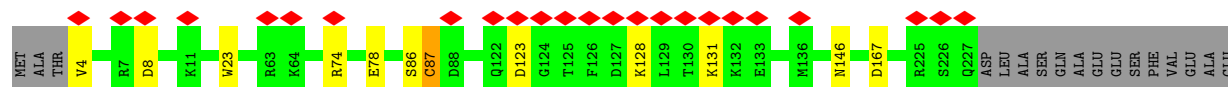
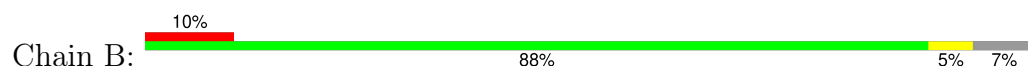
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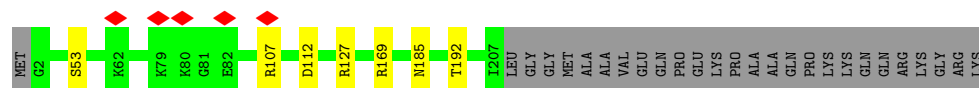
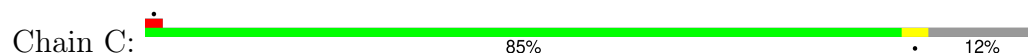
Mol	Chain	Residues	Atoms		AltConf
57	p	66	Total 66	O 66	0
57	q	37	Total 37	O 37	0
57	r	58	Total 58	O 58	0
57	s	24	Total 24	O 24	0
57	t	8	Total 8	O 8	0
57	u	5	Total 5	O 5	0
57	v	33	Total 33	O 33	0
57	w	28	Total 28	O 28	0
57	x	2	Total 2	O 2	0
57	y	16	Total 16	O 16	0
57	z	54	Total 54	O 54	0



• Molecule 6: 30S ribosomal protein S2



• Molecule 7: 30S ribosomal protein S3

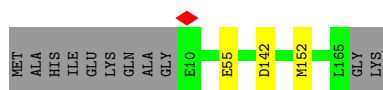


• Molecule 8: 30S ribosomal protein S4



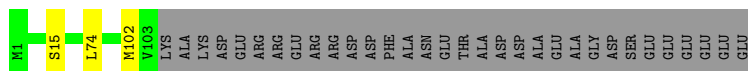
• Molecule 9: 30S ribosomal protein S5





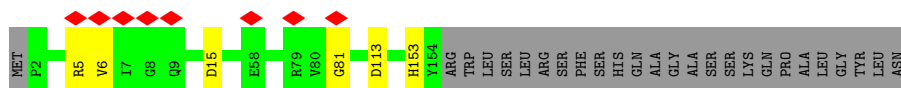
- Molecule 10: 30S ribosomal protein S6

Chain F: 74% 24%



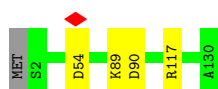
- Molecule 11: 30S ribosomal protein S7

Chain G: 82% 15%



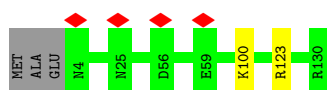
- Molecule 12: 30S ribosomal protein S8

Chain H: 96% 2%



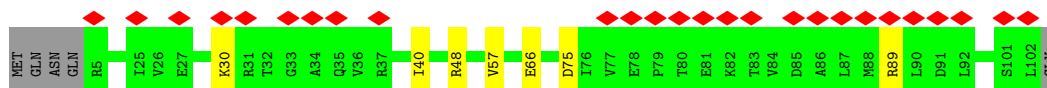
- Molecule 13: 30S ribosomal protein S9

Chain I: 96% 2%



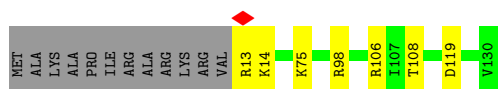
- Molecule 14: 30S ribosomal protein S10

Chain J: 25% 88% 7% 5%



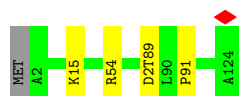
- Molecule 15: 30S ribosomal protein S11

Chain K: 85% 5% 9%



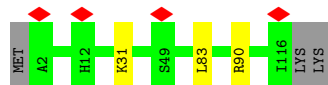
- Molecule 16: 30S ribosomal protein S12

Chain L:  96%



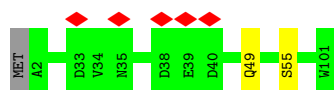
- Molecule 17: 30S ribosomal protein S13

Chain M:  95%



- Molecule 18: 30S ribosomal protein S14

Chain N:  5% 97%



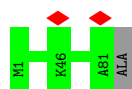
- Molecule 19: 30S ribosomal protein S15

Chain O:  98%




- Molecule 20: 30S ribosomal protein S16

Chain P:  99%



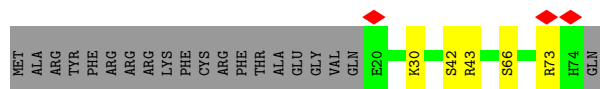
- Molecule 21: 30S ribosomal protein S17

Chain Q:  89% 5% 6%

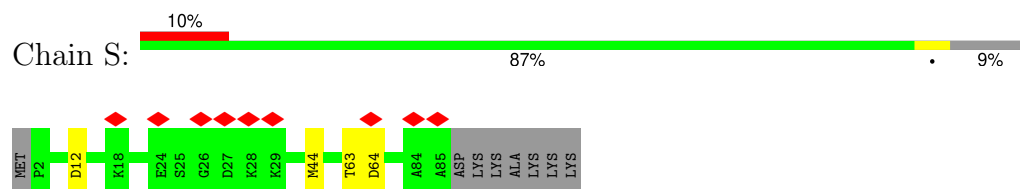


- Molecule 22: 30S ribosomal protein S18

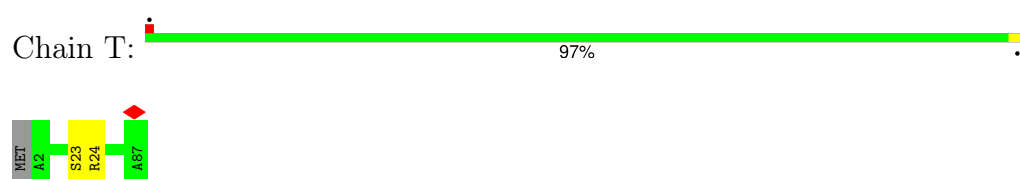
Chain R:  67% 7% 27%



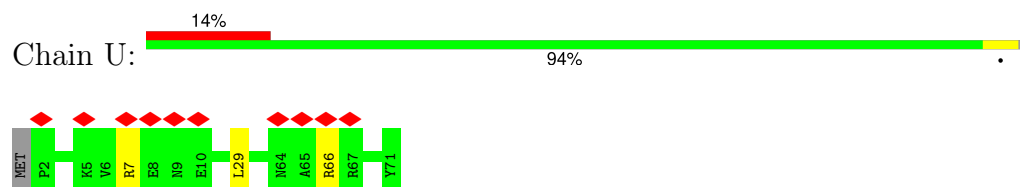
- Molecule 23: 30S ribosomal protein S19



- Molecule 24: 30S ribosomal protein S20



- Molecule 25: 30S ribosomal protein S21

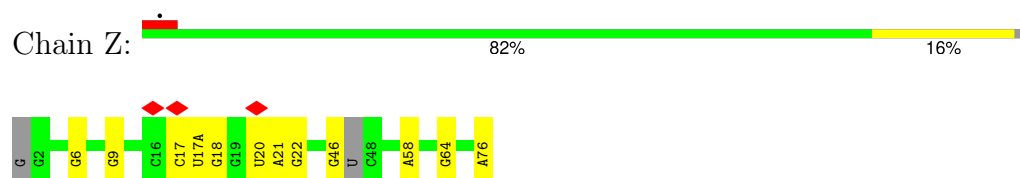


- Molecule 26: mRNA

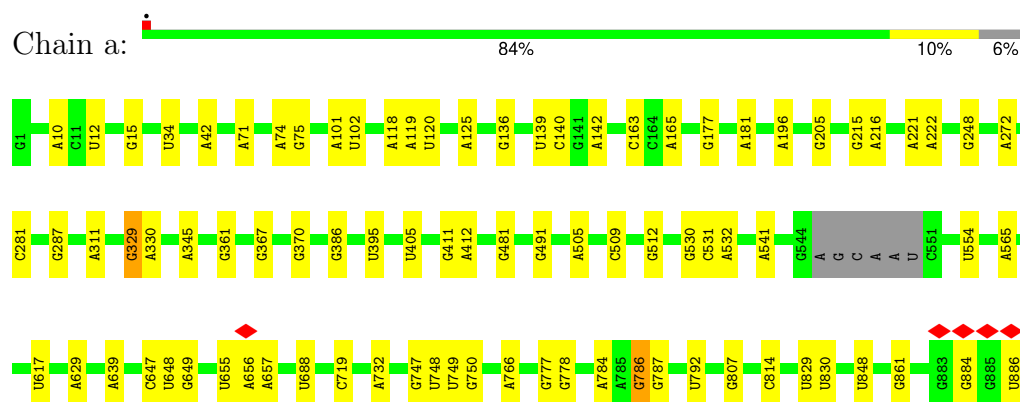


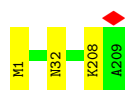
There are no outlier residues recorded for this chain.

- Molecule 27: P-site tRNA



- Molecule 28: 23S rRNA

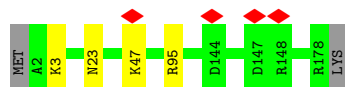




- Molecule 32: 50S ribosomal protein L4



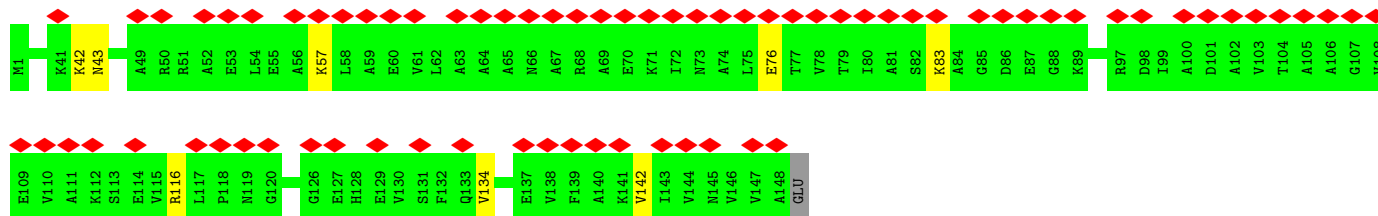
- Molecule 33: 50S ribosomal protein L5



- Molecule 34: 50S ribosomal protein L6



- Molecule 35: 50S ribosomal protein L9



- Molecule 36: 50S ribosomal protein L13



- Molecule 37: 50S ribosomal protein L14





- Molecule 38: 50S ribosomal protein L15

Chain k: 100%



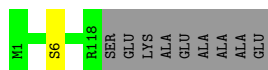
- Molecule 39: 50S ribosomal protein L16

Chain l: 99%



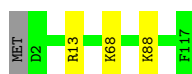
- Molecule 40: 50S ribosomal protein L17

Chain m: 92%



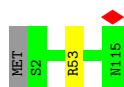
- Molecule 41: 50S ribosomal protein L18

Chain n: 97%



- Molecule 42: 50S ribosomal protein L19

Chain o: 98%



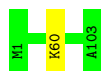
- Molecule 43: 50S ribosomal protein L20

Chain p: 99%



- Molecule 44: 50S ribosomal protein L21

Chain q: 99%



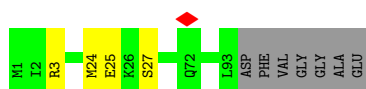
- Molecule 45: 50S ribosomal protein L22

Chain r: 99%



- Molecule 46: 50S ribosomal protein L23

Chain s: 89% 7%



- Molecule 47: 50S ribosomal protein L24

Chain t: 94%



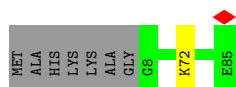
- Molecule 48: 50S ribosomal protein L25

Chain u: 99%



- Molecule 49: 50S ribosomal protein L27

Chain v: 91% 8%



- Molecule 50: 50S ribosomal protein L28

Chain w: 96%



- Molecule 51: 50S ribosomal protein L29

Chain x:  98% .



- Molecule 52: 50S ribosomal protein L30

Chain y:  98% .



- Molecule 53: 50S ribosomal protein L32

Chain z:  96% . .



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	506020	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; per-particle CTF correction	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	165000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	7.947	Depositor
Minimum map value	-2.498	Depositor
Average map value	0.008	Depositor
Map value standard deviation	0.093	Depositor
Recommended contour level	0.2	Depositor
Map size (Å)	409.36002, 409.36002, 409.36002	wwPDB
Map dimensions	560, 560, 560	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.731, 0.731, 0.731	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: PSU, 2MG, IAS, G7M, K, 5MC, MA6, 3TD, 5MU, D2T, 4D4, 1MG, UR3, 6MZ, MG, MS6, OMU, ZN, H2U, MEQ, OMC, 2MA, 4OC, OMG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	0	0.37	0/424	0.55	0/565
2	1	0.37	0/380	0.70	0/498
3	2	0.37	0/513	0.56	0/676
4	3	0.37	0/303	0.59	0/397
5	A	0.70	0/35787	0.78	6/55816 (0.0%)
6	B	0.29	0/1784	0.51	0/2403
7	C	0.32	0/1651	0.53	0/2225
8	D	0.30	0/1665	0.54	0/2227
9	E	0.35	0/1165	0.54	0/1568
10	F	0.34	0/858	0.54	0/1160
11	G	0.29	0/1219	0.53	0/1635
12	H	0.34	0/989	0.50	0/1326
13	I	0.31	0/1034	0.59	0/1375
14	J	0.31	0/796	0.57	0/1077
15	K	0.35	0/884	0.57	0/1191
16	L	0.35	0/960	0.62	0/1286
17	M	0.28	0/900	0.56	0/1204
18	N	0.30	0/817	0.57	0/1088
19	O	0.30	0/722	0.53	0/964
20	P	0.35	0/653	0.57	0/877
21	Q	0.36	0/650	0.55	0/871
22	R	0.37	0/462	0.59	0/621
23	S	0.29	0/685	0.53	0/922
24	T	0.28	0/676	0.50	0/895
25	U	0.30	0/597	0.58	0/792
26	X	0.60	0/147	0.65	0/227
27	Z	0.50	0/1790	0.79	0/2787
28	a	0.97	1/65531 (0.0%)	0.91	27/102222 (0.0%)
29	b	0.79	0/2850	0.77	0/4444
30	c	0.40	0/2121	0.61	0/2852
31	d	0.38	0/1576	0.56	0/2119

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	e	0.37	0/1571	0.53	0/2113
33	f	0.33	0/1434	0.52	0/1926
34	g	0.36	0/1343	0.53	0/1816
35	h	0.32	0/1112	0.53	0/1503
36	i	0.40	0/1152	0.54	0/1551
37	j	0.39	0/955	0.61	0/1279
38	k	0.37	0/1062	0.62	0/1413
39	l	0.38	0/1073	0.58	0/1433
40	m	0.37	0/958	0.60	0/1281
41	n	0.35	0/902	0.57	0/1209
42	o	0.40	0/929	0.56	0/1242
43	p	0.39	0/960	0.57	0/1278
44	q	0.41	0/829	0.57	0/1107
45	r	0.35	0/864	0.55	0/1156
46	s	0.38	0/744	0.54	0/994
47	t	0.36	0/787	0.54	0/1051
48	u	0.39	0/766	0.52	0/1025
49	v	0.38	0/593	0.56	0/785
50	w	0.37	0/635	0.60	0/848
51	x	0.30	0/502	0.50	0/667
52	y	0.33	0/453	0.59	0/605
53	z	0.40	0/450	0.65	0/599
All	All	0.76	1/150663 (0.0%)	0.79	33/225191 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	a	541	A	N9-C4	-5.01	1.34	1.37

The worst 5 of 33 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1492	A	P-O3'-C3'	-8.16	109.91	119.70
28	a	2433	G	P-O3'-C3'	-8.14	109.93	119.70
28	a	12	U	N3-C2-O2	-8.11	116.52	122.20
28	a	512	G	O4'-C1'-N9	7.43	114.14	108.20
28	a	986	A	O4'-C1'-N9	6.75	113.60	108.20

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	49/55 (89%)	49 (100%)	0	0	100	100
2	1	44/46 (96%)	44 (100%)	0	0	100	100
3	2	62/65 (95%)	60 (97%)	2 (3%)	0	100	100
4	3	36/38 (95%)	36 (100%)	0	0	100	100
6	B	222/241 (92%)	210 (95%)	9 (4%)	3 (1%)	9	1
7	C	204/233 (88%)	193 (95%)	11 (5%)	0	100	100
8	D	203/206 (98%)	197 (97%)	6 (3%)	0	100	100
9	E	154/167 (92%)	150 (97%)	4 (3%)	0	100	100
10	F	101/135 (75%)	99 (98%)	2 (2%)	0	100	100
11	G	151/179 (84%)	136 (90%)	13 (9%)	2 (1%)	10	1
12	H	127/130 (98%)	122 (96%)	5 (4%)	0	100	100
13	I	125/130 (96%)	120 (96%)	5 (4%)	0	100	100
14	J	96/103 (93%)	88 (92%)	7 (7%)	1 (1%)	13	3
15	K	113/129 (88%)	108 (96%)	5 (4%)	0	100	100
16	L	120/124 (97%)	116 (97%)	3 (2%)	1 (1%)	16	4
17	M	113/118 (96%)	109 (96%)	4 (4%)	0	100	100
18	N	98/101 (97%)	95 (97%)	3 (3%)	0	100	100
19	O	86/89 (97%)	84 (98%)	2 (2%)	0	100	100
20	P	79/82 (96%)	77 (98%)	2 (2%)	0	100	100
21	Q	77/84 (92%)	70 (91%)	7 (9%)	0	100	100
22	R	53/75 (71%)	51 (96%)	1 (2%)	1 (2%)	6	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
23	S	82/92 (89%)	74 (90%)	8 (10%)	0	100	100
24	T	84/87 (97%)	84 (100%)	0	0	100	100
25	U	68/71 (96%)	67 (98%)	1 (2%)	0	100	100
30	c	269/273 (98%)	259 (96%)	10 (4%)	0	100	100
31	d	206/209 (99%)	200 (97%)	6 (3%)	0	100	100
32	e	199/201 (99%)	194 (98%)	5 (2%)	0	100	100
33	f	175/179 (98%)	165 (94%)	10 (6%)	0	100	100
34	g	174/177 (98%)	160 (92%)	13 (8%)	1 (1%)	22	6
35	h	146/149 (98%)	134 (92%)	10 (7%)	2 (1%)	9	1
36	i	140/142 (99%)	140 (100%)	0	0	100	100
37	j	121/123 (98%)	118 (98%)	3 (2%)	0	100	100
38	k	142/144 (99%)	138 (97%)	4 (3%)	0	100	100
39	l	132/136 (97%)	127 (96%)	5 (4%)	0	100	100
40	m	116/127 (91%)	112 (97%)	4 (3%)	0	100	100
41	n	114/117 (97%)	113 (99%)	1 (1%)	0	100	100
42	o	112/115 (97%)	110 (98%)	2 (2%)	0	100	100
43	p	115/118 (98%)	114 (99%)	1 (1%)	0	100	100
44	q	101/103 (98%)	100 (99%)	1 (1%)	0	100	100
45	r	108/110 (98%)	106 (98%)	2 (2%)	0	100	100
46	s	91/100 (91%)	90 (99%)	1 (1%)	0	100	100
47	t	100/104 (96%)	96 (96%)	3 (3%)	1 (1%)	13	3
48	u	92/94 (98%)	90 (98%)	2 (2%)	0	100	100
49	v	76/85 (89%)	75 (99%)	1 (1%)	0	100	100
50	w	75/78 (96%)	75 (100%)	0	0	100	100
51	x	60/63 (95%)	60 (100%)	0	0	100	100
52	y	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
53	z	54/57 (95%)	53 (98%)	1 (2%)	0	100	100
All	All	5521/5843 (94%)	5323 (96%)	186 (3%)	12 (0%)	45	24

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	B	87	CYS

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Mol	Chain	Res	Type
6	B	131	LYS
11	G	81	GLY
14	J	57	VAL
34	g	126	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	0	46/49 (94%)	44 (96%)	2 (4%)	25 3
2	1	38/38 (100%)	37 (97%)	1 (3%)	41 13
3	2	51/52 (98%)	50 (98%)	1 (2%)	50 22
4	3	34/34 (100%)	33 (97%)	1 (3%)	37 10
6	B	186/199 (94%)	176 (95%)	10 (5%)	18 2
7	C	170/190 (90%)	163 (96%)	7 (4%)	26 4
8	D	172/173 (99%)	163 (95%)	9 (5%)	19 2
9	E	119/126 (94%)	116 (98%)	3 (2%)	42 14
10	F	90/116 (78%)	87 (97%)	3 (3%)	33 8
11	G	126/147 (86%)	122 (97%)	4 (3%)	34 8
12	H	104/105 (99%)	100 (96%)	4 (4%)	28 5
13	I	105/107 (98%)	103 (98%)	2 (2%)	52 24
14	J	86/90 (96%)	80 (93%)	6 (7%)	12 1
15	K	89/98 (91%)	83 (93%)	6 (7%)	13 1
16	L	102/103 (99%)	100 (98%)	2 (2%)	50 22
17	M	93/96 (97%)	90 (97%)	3 (3%)	34 8
18	N	83/84 (99%)	81 (98%)	2 (2%)	44 16
19	O	76/77 (99%)	75 (99%)	1 (1%)	65 41
20	P	65/65 (100%)	65 (100%)	0	100 100
21	Q	73/78 (94%)	69 (94%)	4 (6%)	18 2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
22	R	48/65 (74%)	44 (92%)	4 (8%)	9	0
23	S	72/79 (91%)	68 (94%)	4 (6%)	17	2
24	T	65/66 (98%)	63 (97%)	2 (3%)	35	9
25	U	60/61 (98%)	57 (95%)	3 (5%)	20	2
30	c	216/218 (99%)	214 (99%)	2 (1%)	75	58
31	d	163/163 (100%)	160 (98%)	3 (2%)	54	27
32	e	165/165 (100%)	160 (97%)	5 (3%)	36	9
33	f	148/150 (99%)	144 (97%)	4 (3%)	40	12
34	g	137/138 (99%)	123 (90%)	14 (10%)	6	0
35	h	113/114 (99%)	107 (95%)	6 (5%)	19	2
36	i	116/116 (100%)	114 (98%)	2 (2%)	56	29
37	j	104/104 (100%)	102 (98%)	2 (2%)	52	24
38	k	103/103 (100%)	103 (100%)	0	100	100
39	l	107/107 (100%)	106 (99%)	1 (1%)	75	58
40	m	98/103 (95%)	97 (99%)	1 (1%)	73	53
41	n	86/87 (99%)	83 (96%)	3 (4%)	31	7
42	o	99/100 (99%)	98 (99%)	1 (1%)	73	53
43	p	89/90 (99%)	89 (100%)	0	100	100
44	q	84/84 (100%)	83 (99%)	1 (1%)	67	45
45	r	93/93 (100%)	92 (99%)	1 (1%)	70	49
46	s	80/84 (95%)	76 (95%)	4 (5%)	20	2
47	t	83/85 (98%)	80 (96%)	3 (4%)	30	6
48	u	78/78 (100%)	77 (99%)	1 (1%)	65	41
49	v	58/63 (92%)	57 (98%)	1 (2%)	56	29
50	w	67/68 (98%)	65 (97%)	2 (3%)	36	9
51	x	54/55 (98%)	54 (100%)	0	100	100
52	y	48/49 (98%)	48 (100%)	0	100	100
53	z	47/48 (98%)	46 (98%)	1 (2%)	48	20
All	All	4589/4763 (96%)	4447 (97%)	142 (3%)	37	9

5 of 142 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
35	h	116	ARG
36	i	96	ARG
46	s	3	ARG
14	J	40	ILE
14	J	30	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
35	h	66	ASN
47	t	54	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
26	X	5/6 (83%)	0	0
27	Z	73/77 (94%)	11 (15%)	1 (1%)
28	a	2738/2925 (93%)	257 (9%)	0
29	b	118/119 (99%)	10 (8%)	0
5	A	1492/1554 (96%)	172 (11%)	6 (0%)
All	All	4426/4681 (94%)	450 (10%)	7 (0%)

5 of 450 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
5	A	4	U
5	A	5	U
5	A	9	G
5	A	22	G
5	A	32	A

5 of 7 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
5	A	766	A
5	A	786	G
27	Z	17(A)	U
5	A	1035	A
5	A	467	U

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

39 non-standard protein/DNA/RNA residues are modelled in this entry.

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
5	UR3	A	1498	5	19,22,23	2.60	7 (36%)	26,32,35	1.68	4 (15%)
5	2MG	A	966	5	18,26,27	1.30	3 (16%)	16,38,41	0.80	0
15	IAS	K	119	15	6,7,8	0.98	1 (16%)	3,8,10	1.29	1 (33%)
28	OMG	a	2255	27,28,55	19,26,27	1.34	3 (15%)	21,38,41	0.79	1 (4%)
5	5MC	A	1407	5	19,22,23	0.83	1 (5%)	26,32,35	0.59	0
16	D2T	L	89	16	8,9,10	1.38	1 (12%)	6,11,13	1.82	2 (33%)
28	3TD	a	1919	28	19,22,23	4.11	7 (36%)	23,32,35	1.91	3 (13%)
28	G7M	a	2073	28,55	20,26,27	2.43	7 (35%)	16,39,42	1.15	2 (12%)
28	5MU	a	749	28	19,22,23	0.68	0	27,32,35	0.54	0
28	5MU	a	1943	28,55	19,22,23	0.78	0	27,32,35	0.46	0
28	PSU	a	2461	28	18,21,22	1.14	2 (11%)	21,30,33	1.98	4 (19%)
28	PSU	a	957	28	18,21,22	1.11	1 (5%)	21,30,33	1.90	2 (9%)
5	5MC	A	967	5	19,22,23	0.70	0	26,32,35	0.63	0
31	MEQ	d	150	31	8,9,10	0.83	0	5,10,12	0.76	0
28	5MC	a	1966	28,55	19,22,23	0.80	1 (5%)	26,32,35	0.54	0
28	H2U	a	2453	28	18,21,22	0.64	0	19,30,33	1.01	2 (10%)
5	4OC	A	1402	5	20,23,24	3.00	8 (40%)	25,32,35	0.95	1 (4%)
5	MA6	A	1519	5	19,26,27	1.58	2 (10%)	18,38,41	2.99	4 (22%)
5	PSU	A	516	5,56	18,21,22	1.10	1 (5%)	21,30,33	2.07	6 (28%)
5	2MG	A	1207	5,55	18,26,27	1.24	3 (16%)	16,38,41	0.90	1 (6%)
28	1MG	a	747	28	19,26,27	2.79	6 (31%)	18,39,42	1.32	2 (11%)
5	2MG	A	1516	5	18,26,27	1.37	3 (16%)	16,38,41	0.91	1 (6%)
28	2MG	a	2449	28	18,26,27	1.48	3 (16%)	16,38,41	0.67	0
5	MA6	A	1518	5	19,26,27	1.58	2 (10%)	18,38,41	2.87	4 (22%)
28	PSU	a	748	56,28	18,21,22	1.13	2 (11%)	21,30,33	1.73	3 (14%)
39	4D4	l	81	39	9,11,12	0.56	0	7,13,15	0.90	1 (14%)
28	PSU	a	2584	28	18,21,22	1.12	3 (16%)	21,30,33	1.89	3 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	6MZ	a	1620	28	17,25,26	1.77	3 (17%)	15,36,39	2.63	5 (33%)
28	OMC	a	2502	56,28	19,22,23	0.79	1 (5%)	25,31,34	0.66	0
28	2MA	a	2507	56,28,55	17,25,26	2.35	6 (35%)	16,37,40	2.22	5 (31%)
28	OMU	a	2556	56,28,55	19,22,23	3.11	7 (36%)	25,31,34	1.78	4 (16%)
5	G7M	A	527	5,55	20,26,27	2.63	7 (35%)	16,39,42	1.12	1 (6%)
28	6MZ	a	2034	28	17,25,26	1.75	5 (29%)	15,36,39	2.60	5 (33%)
28	PSU	a	2608	28	18,21,22	1.08	2 (11%)	21,30,33	2.00	5 (23%)
28	2MG	a	1837	28	18,26,27	1.39	3 (16%)	16,38,41	0.81	1 (6%)
28	PSU	a	1921	28	18,21,22	1.06	1 (5%)	21,30,33	1.97	5 (23%)
28	PSU	a	2609	28	18,21,22	1.07	1 (5%)	21,30,33	2.07	5 (23%)
28	PSU	a	1915	28	18,21,22	1.05	1 (5%)	21,30,33	1.90	4 (19%)
28	PSU	a	2508	28,55	18,21,22	1.05	1 (5%)	21,30,33	2.02	4 (19%)

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
5	UR3	A	1498	5	-	0/7/25/26	0/2/2/2
5	2MG	A	966	5	-	0/5/27/28	0/3/3/3
15	IAS	K	119	15	-	0/7/7/8	-
28	OMG	a	2255	27,28,55	-	1/5/27/28	0/3/3/3
5	5MC	A	1407	5	-	0/7/25/26	0/2/2/2
16	D2T	L	89	16	-	4/7/12/14	-
28	3TD	a	1919	28	-	2/7/25/26	0/2/2/2
28	G7M	a	2073	28,55	-	1/3/25/26	0/3/3/3
28	5MU	a	749	28	-	0/7/25/26	0/2/2/2
28	5MU	a	1943	28,55	-	0/7/25/26	0/2/2/2
28	PSU	a	2461	28	-	0/7/25/26	0/2/2/2
28	PSU	a	957	28	-	0/7/25/26	0/2/2/2
5	5MC	A	967	5	-	0/7/25/26	0/2/2/2
31	MEQ	d	150	31	-	2/8/9/11	-
28	5MC	a	1966	28,55	-	0/7/25/26	0/2/2/2
28	H2U	a	2453	28	-	0/7/38/39	0/2/2/2
5	4OC	A	1402	5	-	0/9/29/30	0/2/2/2
5	MA6	A	1519	5	-	3/7/29/30	0/3/3/3
5	PSU	A	516	5,56	-	0/7/25/26	0/2/2/2
5	2MG	A	1207	5,55	-	0/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	1MG	a	747	28	-	0/3/25/26	0/3/3/3
5	2MG	A	1516	5	-	0/5/27/28	0/3/3/3
28	2MG	a	2449	28	-	0/5/27/28	0/3/3/3
5	MA6	A	1518	5	-	0/7/29/30	0/3/3/3
28	PSU	a	748	56,28	-	2/7/25/26	0/2/2/2
39	4D4	l	81	39	-	7/11/12/14	-
28	PSU	a	2584	28	-	0/7/25/26	0/2/2/2
28	6MZ	a	1620	28	-	0/5/27/28	0/3/3/3
28	OMC	a	2502	56,28	-	0/9/27/28	0/2/2/2
28	2MA	a	2507	56,28,55	-	1/3/25/26	0/3/3/3
28	OMU	a	2556	56,28,55	-	0/9/27/28	0/2/2/2
5	G7M	A	527	5,55	-	3/3/25/26	0/3/3/3
28	6MZ	a	2034	28	-	2/5/27/28	0/3/3/3
28	PSU	a	2608	28	-	0/7/25/26	0/2/2/2
28	2MG	a	1837	28	-	0/5/27/28	0/3/3/3
28	PSU	a	1921	28	-	0/7/25/26	0/2/2/2
28	PSU	a	2609	28	-	0/7/25/26	0/2/2/2
28	PSU	a	1915	28	-	0/7/25/26	0/2/2/2
28	PSU	a	2508	28,55	-	0/7/25/26	0/2/2/2

The worst 5 of 105 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	a	1919	3TD	C6-C5	12.86	1.49	1.35
28	a	1919	3TD	C2-N1	9.07	1.48	1.37
28	a	747	1MG	C2-N3	7.67	1.45	1.33
5	A	1402	4OC	C4-N3	6.53	1.43	1.32
5	A	1498	UR3	C2-N1	6.53	1.47	1.38

The worst 5 of 91 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1519	MA6	N1-C6-N6	-8.67	106.81	116.83
5	A	1518	MA6	N1-C6-N6	-8.17	107.40	116.83
5	A	1519	MA6	N3-C2-N1	-6.89	119.32	128.67
5	A	1518	MA6	N3-C2-N1	-6.79	119.45	128.67
28	a	1919	3TD	N1-C2-N3	6.41	120.79	116.13

There are no chirality outliers.

5 of 28 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1519	MA6	C5-C6-N6-C9
39	l	81	4D4	NH2-CZ-NE-CD
39	l	81	4D4	NH1-CZ-NE-CD
28	a	2255	OMG	C1'-C2'-O2'-CM2
31	d	150	MEQ	OE1-CD-CG-CB

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 530 ligands modelled in this entry, 530 are 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](#)

There are no chain breaks in this entry.

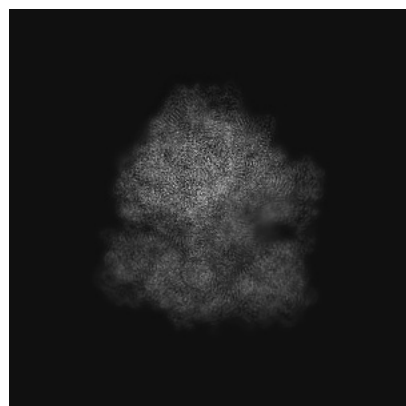
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-15793. These allow visual inspection of the internal detail of the map and identification of artifacts.

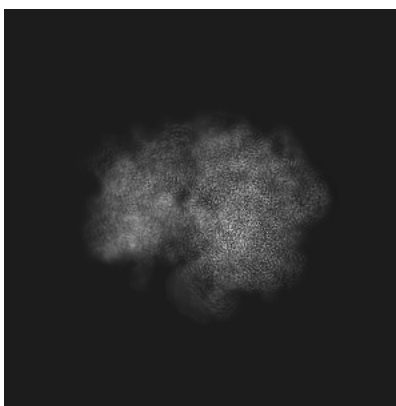
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

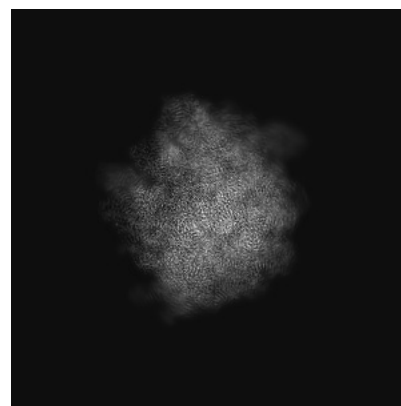
6.1.1 Primary map



X

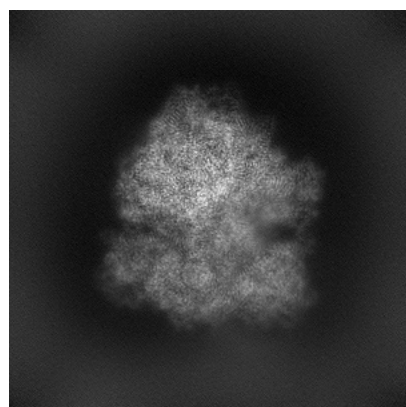


Y

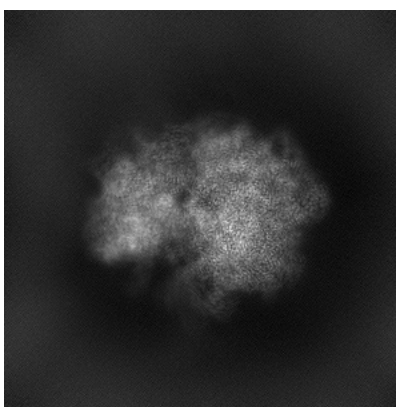


Z

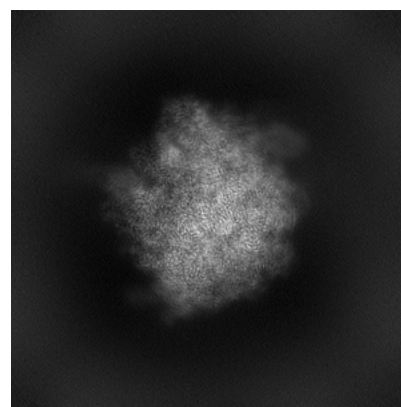
6.1.2 Raw map



X



Y



Z

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

6.2 Central slices [i](#)

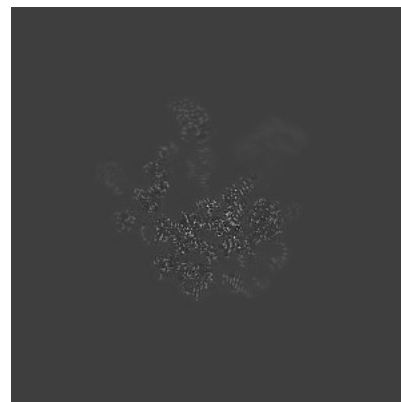
6.2.1 Primary map



X Index: 280

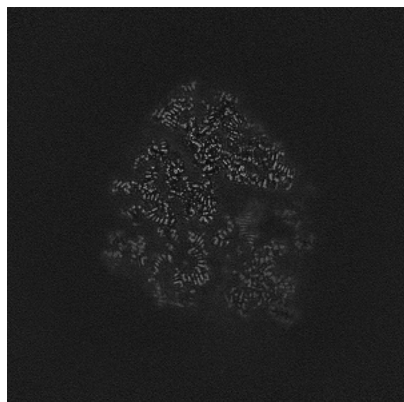


Y Index: 280

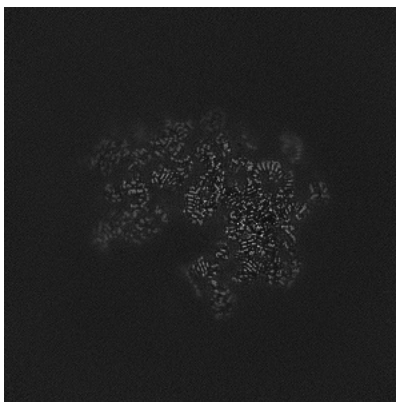


Z Index: 280

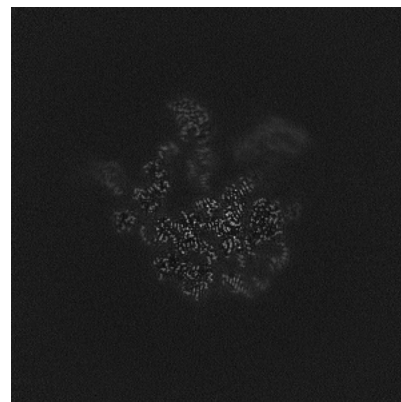
6.2.2 Raw map



X Index: 280



Y Index: 280

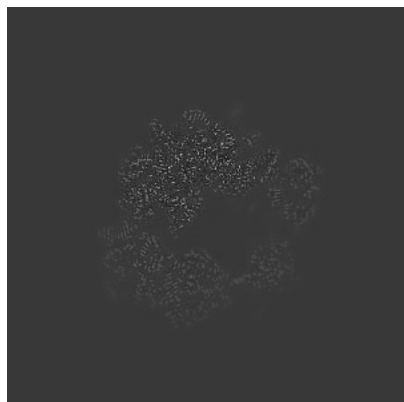


Z Index: 280

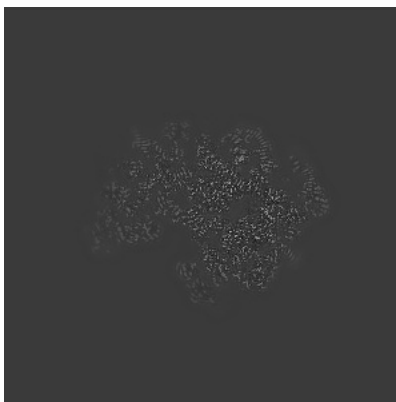
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

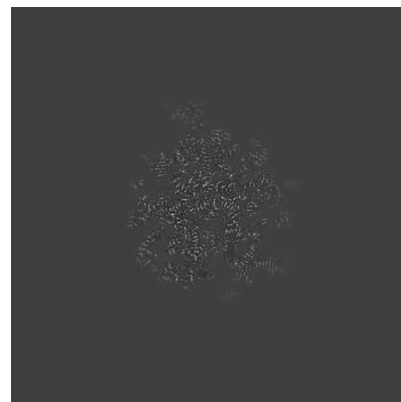
6.3.1 Primary map



X Index: 246

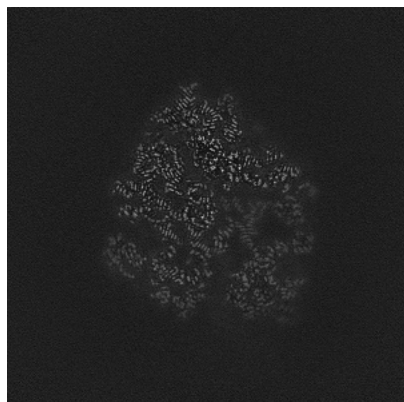


Y Index: 260

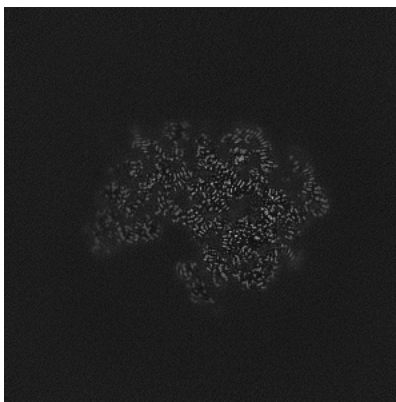


Z Index: 342

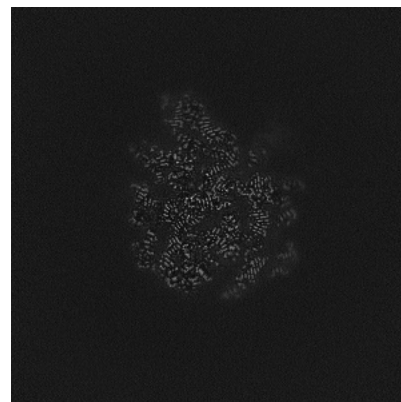
6.3.2 Raw map



X Index: 274



Y Index: 260

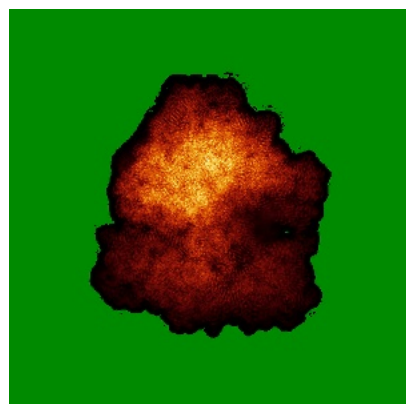


Z Index: 334

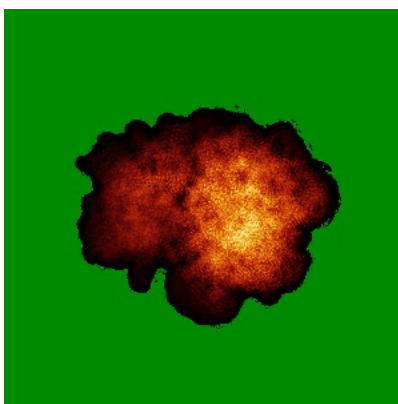
The images above show the largest variance slices of the map in three orthogonal directions.

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

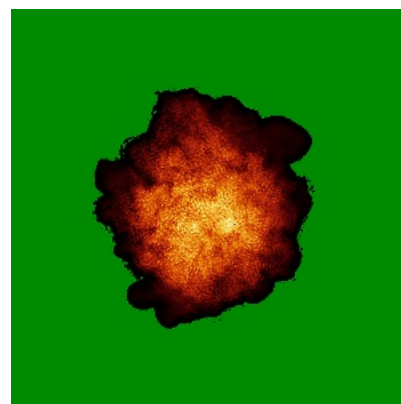
6.4.1 Primary map



X

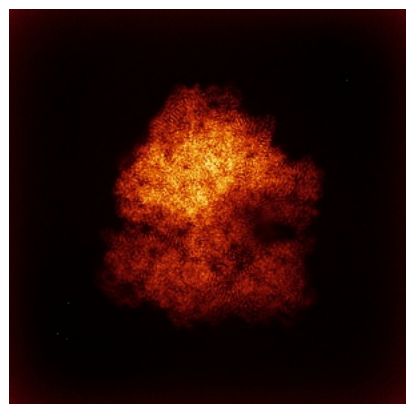


Y

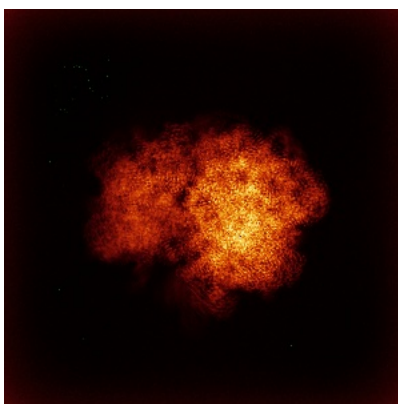


Z

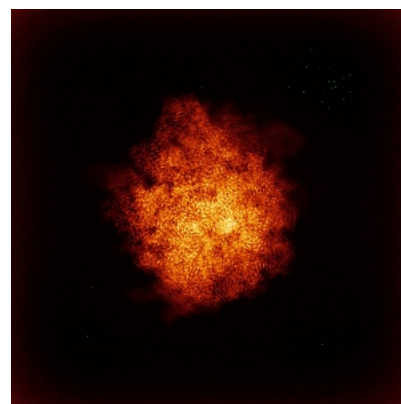
6.4.2 Raw map



X



Y

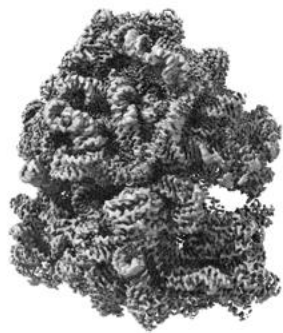


Z

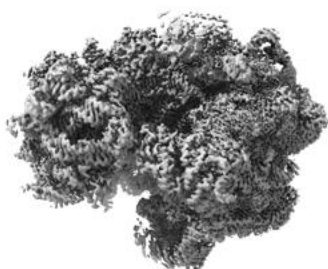
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

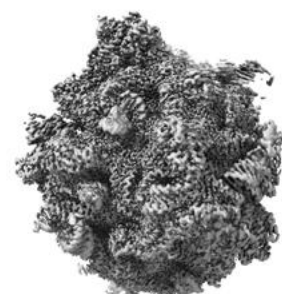
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.2. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X



Y



Z

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

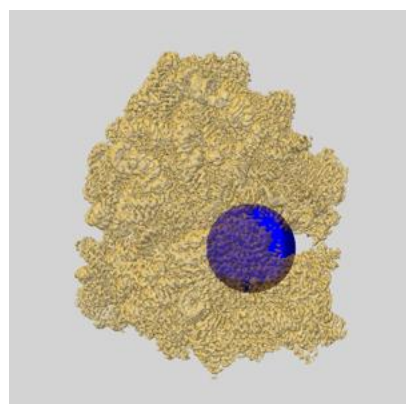
6.6 Mask visualisation [i](#)

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

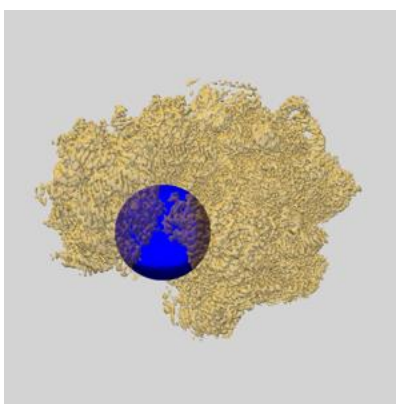
A mask typically either:

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

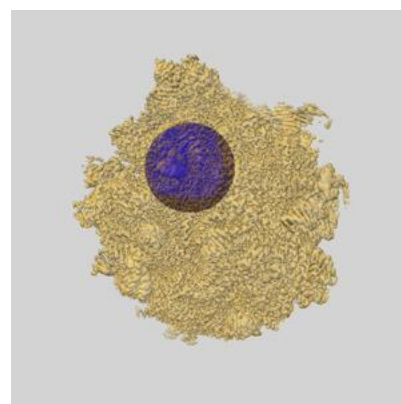
6.6.1 emd_15793_msk_1.map [i](#)



X

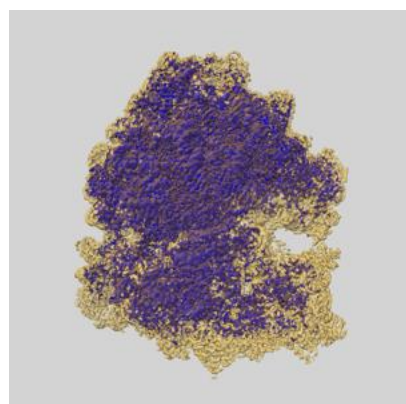


Y

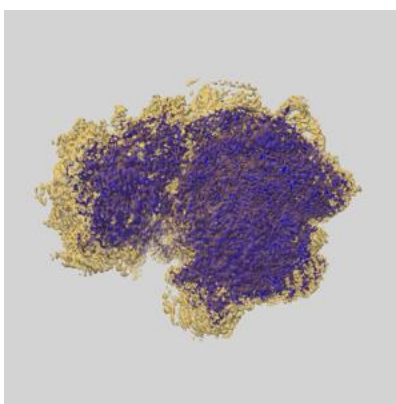


Z

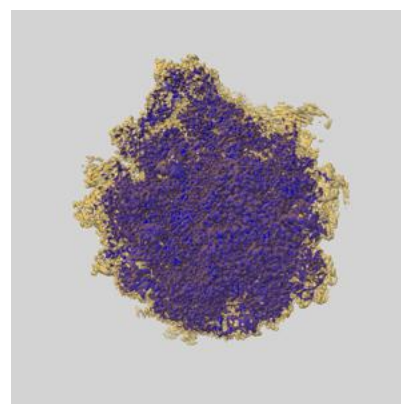
6.6.2 emd_15793_msk_2.map [i](#)



X



Y

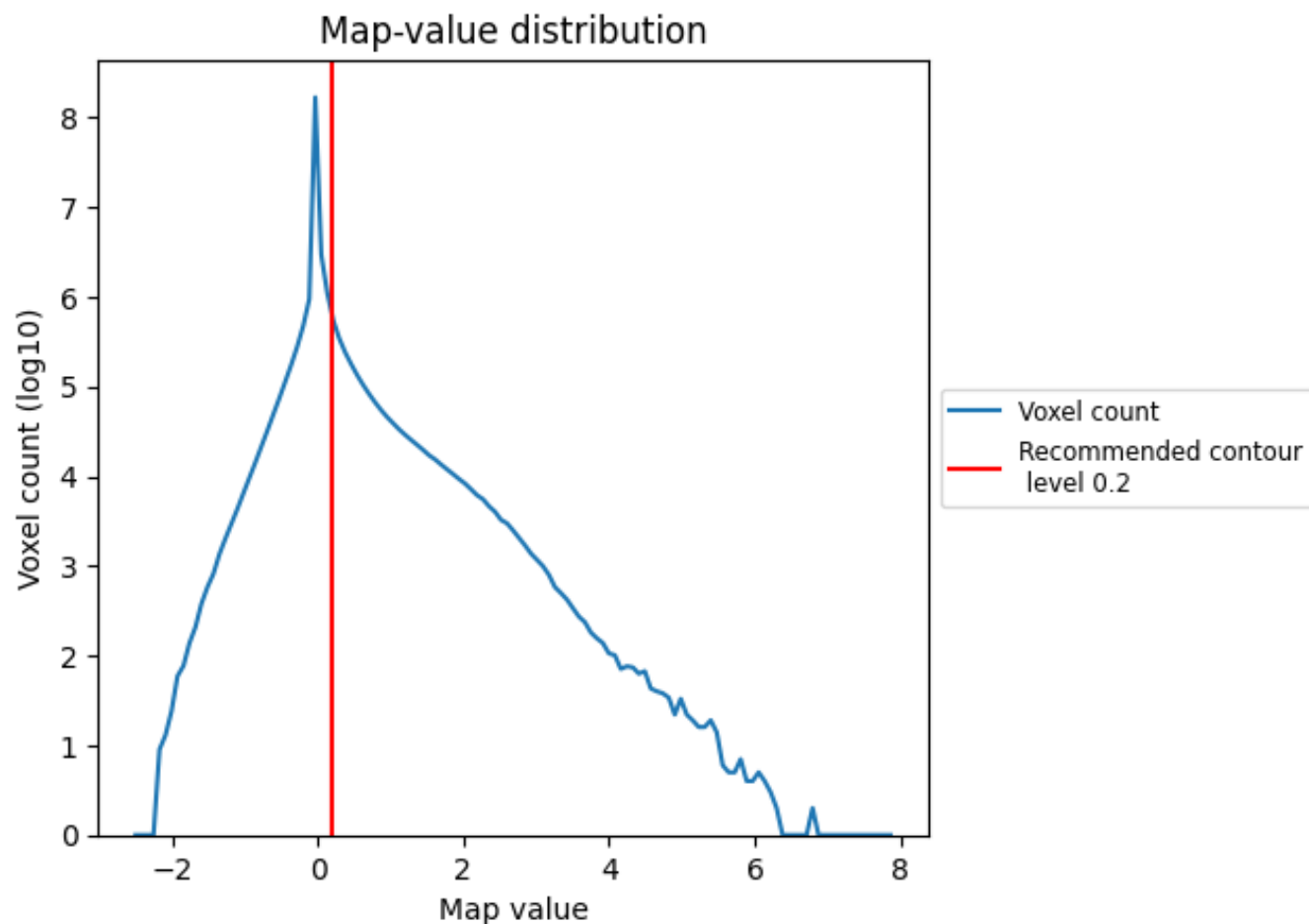


Z

7 Map analysis [i](#)

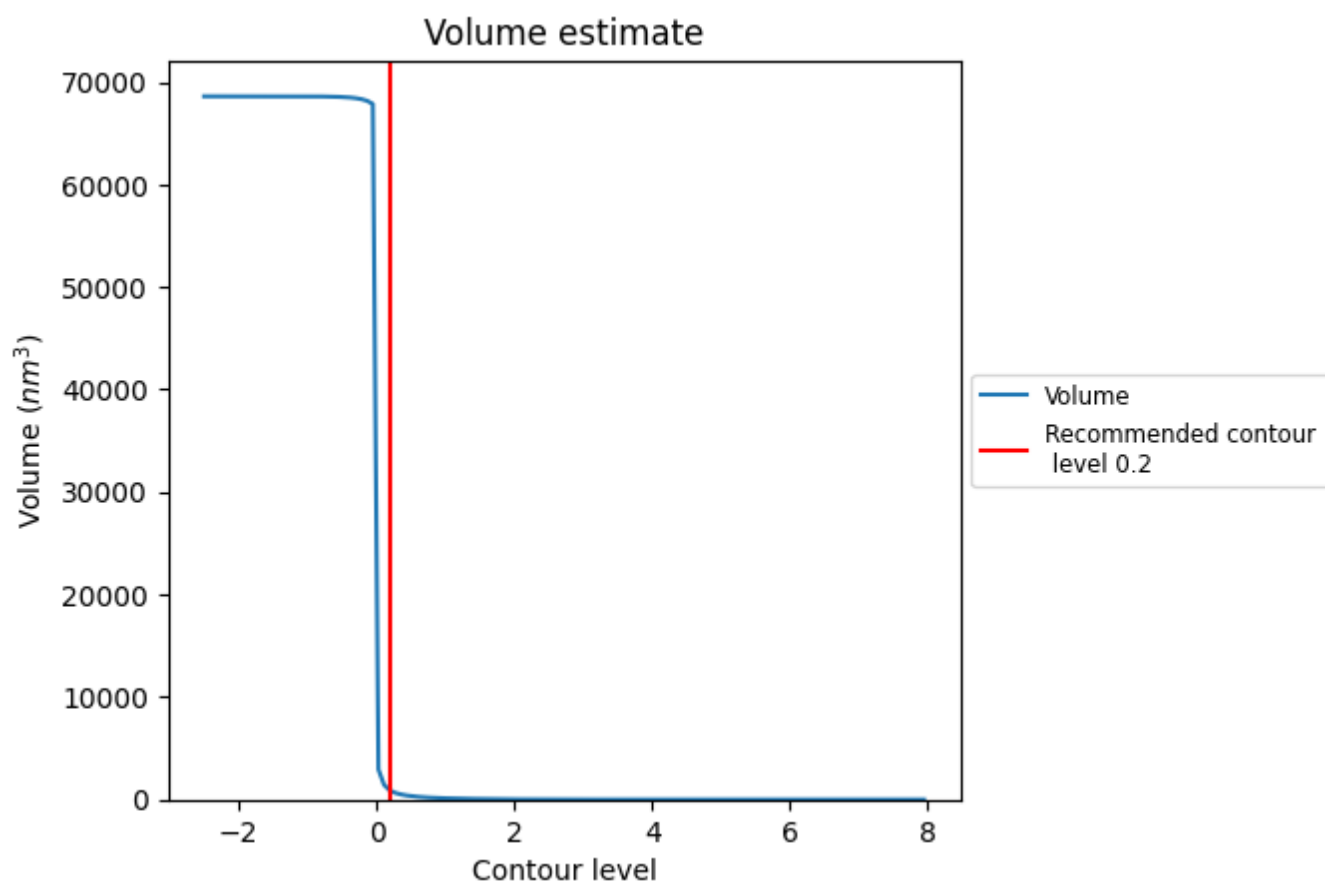
This section contains the results of statistical analysis of the map.

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.

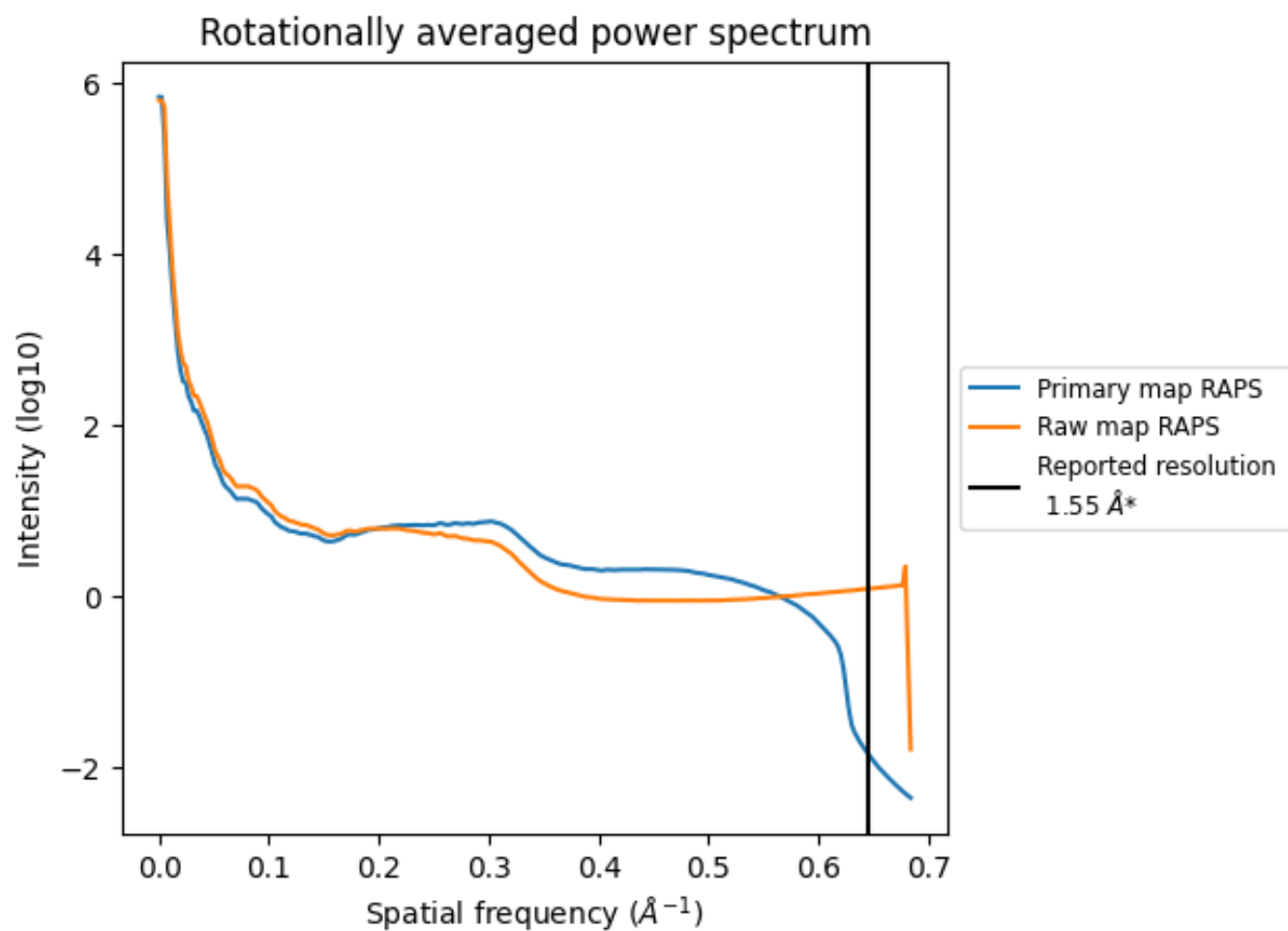
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 882 nm^3 ; this corresponds to an approximate mass of 797 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

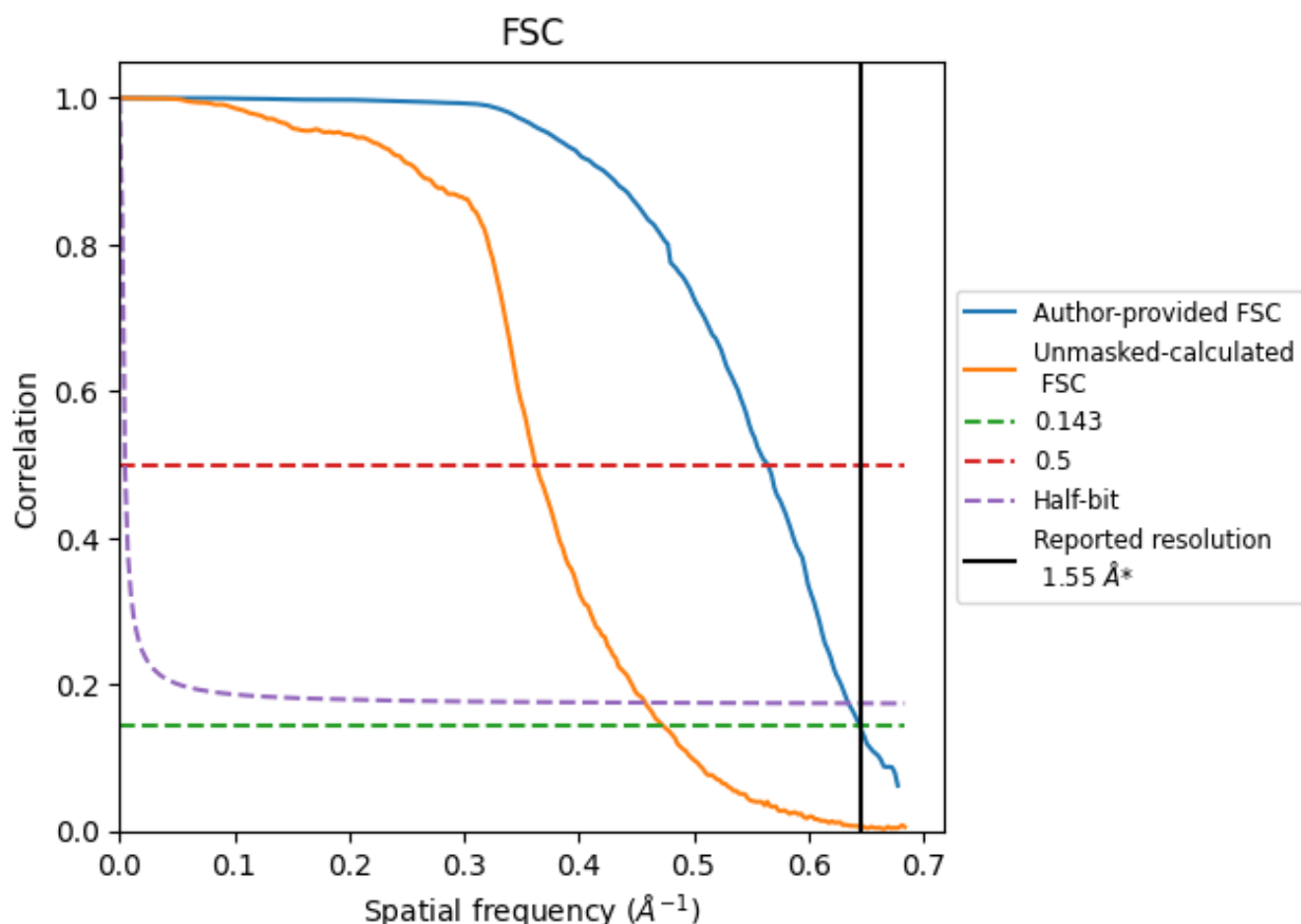


*Reported resolution corresponds to spatial frequency of 0.645 \AA^{-1}

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.645 \AA^{-1}

8.2 Resolution estimates [i](#)

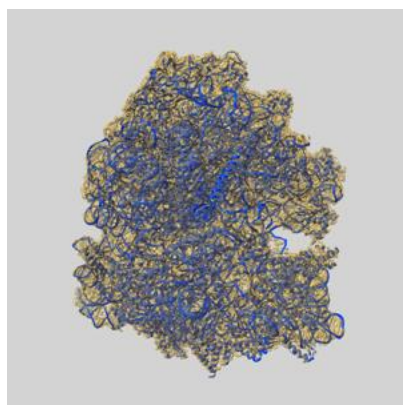
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	1.55	-	-
Author-provided FSC curve	1.55	1.77	1.57
Unmasked-calculated*	2.11	2.76	2.18

*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 2.11 differs from the reported value 1.55 by more than 10 %

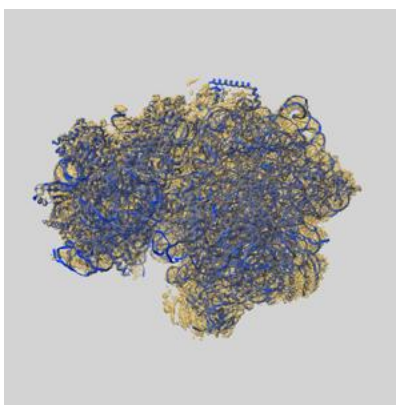
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-15793 and PDB model 8B0X. Per-residue inclusion information can be found in section [3](#) on page [17](#).

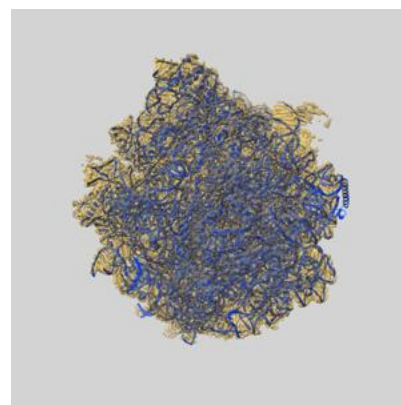
9.1 Map-model overlay [i](#)



X



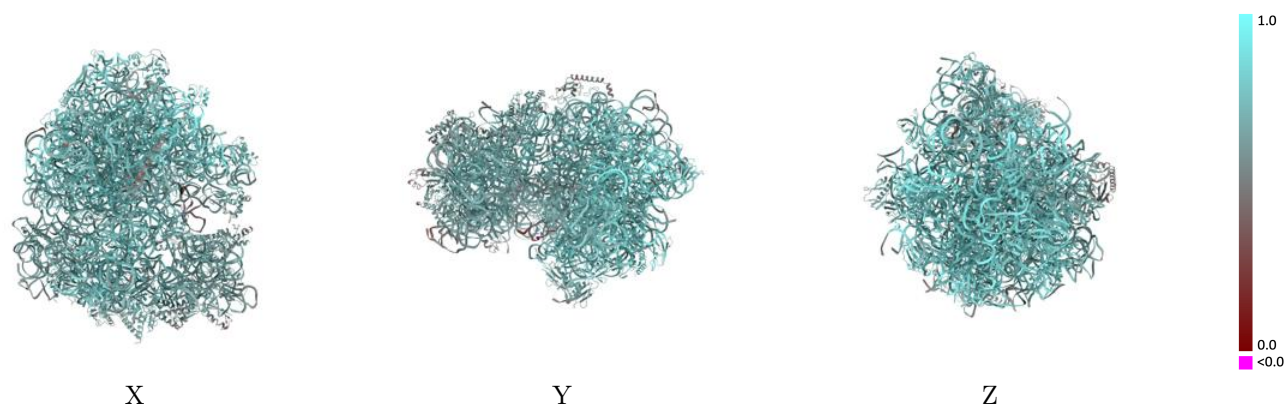
Y



Z

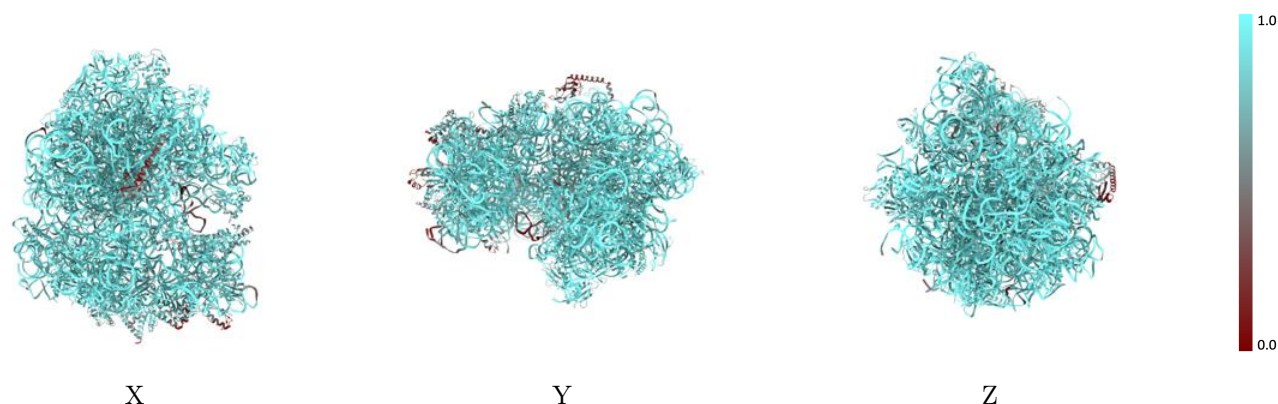
The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



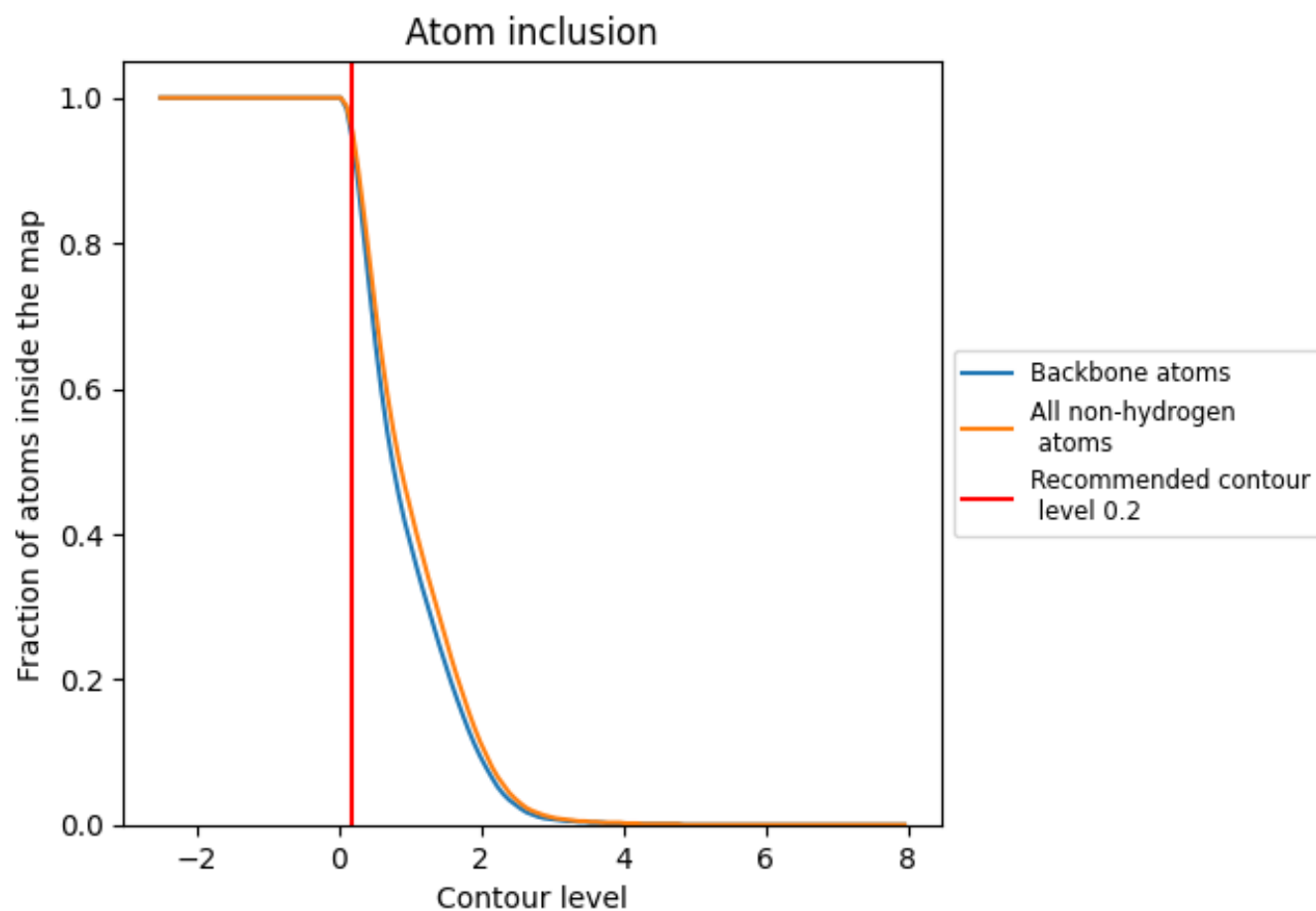
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.2).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 95% 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 (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9520	 0.7670
0	 0.9660	 0.7960
1	 0.9890	 0.8720
2	 0.9960	 0.8680
3	 0.9760	 0.8180
A	 0.9670	 0.7190
B	 0.7510	 0.6360
C	 0.8730	 0.6750
D	 0.8490	 0.6700
E	 0.9500	 0.7590
F	 0.8970	 0.6690
G	 0.8030	 0.6290
H	 0.9460	 0.7570
I	 0.8410	 0.6420
J	 0.6610	 0.5890
K	 0.9300	 0.7010
L	 0.9450	 0.7400
M	 0.8060	 0.6250
N	 0.8770	 0.6570
O	 0.9380	 0.7380
P	 0.9400	 0.7110
Q	 0.8910	 0.6720
R	 0.9110	 0.7090
S	 0.7590	 0.5930
T	 0.9240	 0.7140
U	 0.6890	 0.6250
X	 0.9550	 0.7130
Z	 0.8790	 0.6240
a	 0.9830	 0.8160
b	 0.9820	 0.7330
c	 0.9910	 0.8530
d	 0.9770	 0.8440
e	 0.9460	 0.7990
f	 0.8600	 0.6460
g	 0.8880	 0.6690



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Chain	Atom inclusion	Q-score
h	 0.4910	 0.5610
i	 0.9860	 0.8440
j	 0.9780	 0.8380
k	 0.9780	 0.8330
l	 0.9850	 0.8240
m	 0.9990	 0.8690
n	 0.9470	 0.7390
o	 0.9640	 0.8300
p	 0.9970	 0.8660
q	 0.9550	 0.8090
r	 0.9810	 0.8460
s	 0.9380	 0.7810
t	 0.9230	 0.7540
u	 0.9310	 0.7500
v	 0.9720	 0.8250
w	 0.9770	 0.8260
x	 0.9240	 0.7440
y	 0.9610	 0.8310
z	 0.9600	 0.8260