



wwPDB EM Validation Summary Report ⓘ

Nov 5, 2022 – 10:46 PM EDT

PDB ID : 5WFS
EMDB ID : EMD-8829
Title : 70S ribosome-EF-Tu H84A complex with GTP and near-cognate tRNA (Complex C4)
Authors : Fislage, M.; Frank, J.
Deposited on : 2017-07-12
Resolution : 3.00 Å(reported)

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

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

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.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

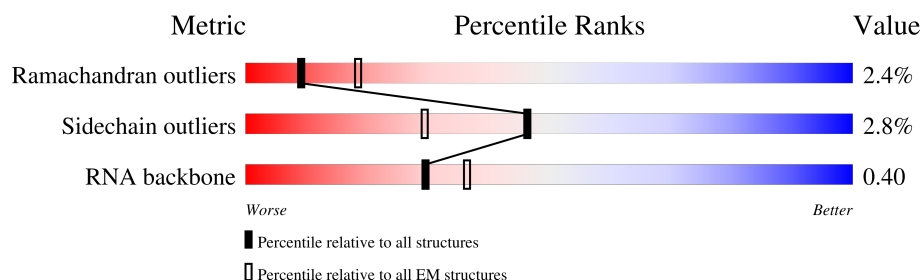
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.00 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	2903	
2	B	120	
3	C	271	
4	D	208	
5	E	200	
6	F	177	
7	G	174	
8	H	149	


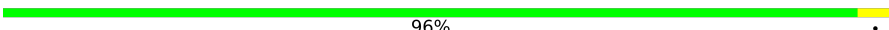
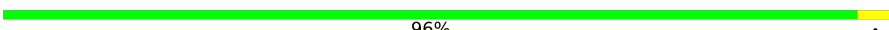
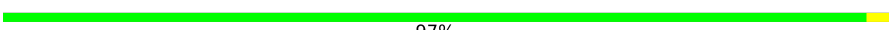
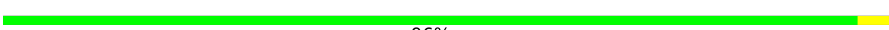





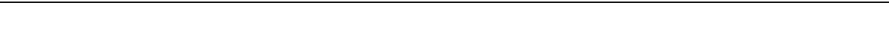

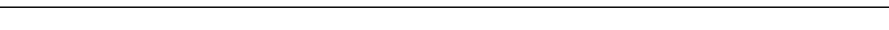
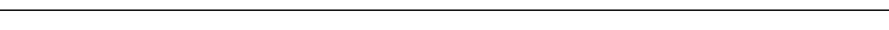
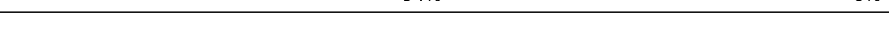
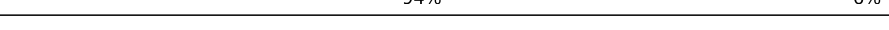
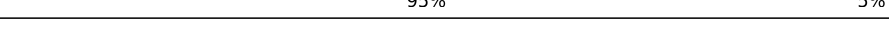
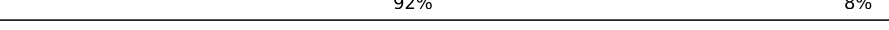

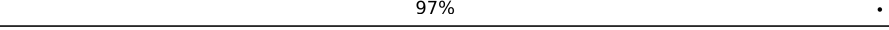
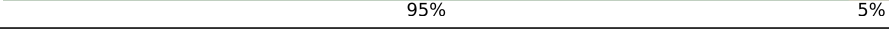




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Mol	Chain	Length	Quality of chain
9	I	141	<div> <div>24%</div> <div>92%</div> <div>7%</div> </div>
10	J	141	<div> <div>98%</div> </div>
11	K	122	<div> <div>94%</div> <div>6%</div> </div>
12	L	143	<div> <div>90%</div> <div>9%</div> </div>
13	M	136	<div> <div>97%</div> </div>
14	N	119	<div> <div>96%</div> </div>
15	O	116	<div> <div>99%</div> </div>
16	P	114	<div> <div>98%</div> </div>
17	Q	115	<div> <div>97%</div> </div>
18	R	102	<div> <div>95%</div> <div>5%</div> </div>
19	S	109	<div> <div>98%</div> </div>
20	T	92	<div> <div>95%</div> <div>5%</div> </div>
21	U	102	<div> <div>94%</div> <div>6%</div> </div>
22	V	92	<div> <div>98%</div> </div>
23	W	75	<div> <div>97%</div> </div>
24	X	77	<div> <div>99%</div> </div>
25	Y	60	<div> <div>97%</div> </div>
26	Z	56	<div> <div>100%</div> </div>
27	0	55	<div> <div>96%</div> </div>
28	1	51	<div> <div>100%</div> </div>
29	2	45	<div> <div>96%</div> </div>
30	3	64	<div> <div>97%</div> </div>
31	4	38	<div> <div>100%</div> </div>
32	5	131	<div> <div>89%</div> <div>92%</div> <div>8%</div> </div>
33	6	66	<div> <div>95%</div> <div>5%</div> </div>

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Mol	Chain	Length	Quality of chain
34	a	1540	
35	b	218	
36	c	206	
37	d	205	
38	e	157	
39	f	100	
40	g	151	
41	h	129	
42	i	127	
43	j	98	
44	k	116	
45	l	121	
46	m	115	
47	n	101	
48	o	88	
49	p	82	
50	q	80	
51	r	65	
52	s	79	
53	t	85	
54	u	65	
55	v	77	
55	w	77	
56	x	12	
57	y	76	

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Mol	Chain	Length	Quality of chain
58	z	393	<div><div></div><div>96%</div><div></div></div>

2 Entry composition

There are 64 unique types of molecules in this entry. The entry contains 155100 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 RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	2900	Total	C	N	O	P	0	0
			62277	27788	11459	20130	2900		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	747	5MC	U	conflict	GB 216643
A	1723	G	A	conflict	GB 216643
A	1847	G	A	conflict	GB 216643

- Molecule 2 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	120	Total	C	N	O	P	0	0
			2572	1145	471	836	120		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	120	A	U	conflict	GB 1199817771

- Molecule 3 is a protein called 50S ribosomal protein L2.

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

- Molecule 4 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	208	Total	C	N	O	S	0	0
			1557	974	287	293	3		

- Molecule 5 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	200	Total	C	N	O	S	0	0
			1544	969	282	289	4		

- Molecule 6 is a protein called 50S ribosomal protein L5.

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

- Molecule 7 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	174	Total	C	N	O	S	0	0
			1304	820	239	243	2		

- Molecule 8 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	149	Total	C	N	O	S	0	0
			1111	699	197	214	1		

- Molecule 9 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	141	Total	C	N	O	S	0	0
			1032	651	179	196	6		

- Molecule 10 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	141	Total	C	N	O	S	0	0
			1120	708	211	197	4		

- Molecule 11 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	122	Total	C	N	O	S	0	0
			938	587	180	165	6		

- Molecule 12 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	143	Total	C	N	O	S	0	0
			1043	649	206	186	2		

- Molecule 13 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	136	Total	C	N	O	S	0	0
			1074	686	205	177	6		

- Molecule 14 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	119	Total	C	N	O	S	0	0
			951	588	195	163	5		

- Molecule 15 is a protein called 50S ribosomal protein L18.

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

- Molecule 16 is a protein called 50S ribosomal protein L19.

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

- Molecule 17 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	115	Total	C	N	O		0	0
			933	595	190	148			

- Molecule 18 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	102	Total	C	N	O	S	0	0
			810	513	152	143	2		

- Molecule 19 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	109	Total	C	N	O	S	0	0
			845	526	162	154	3		

- Molecule 20 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	92	Total	C	N	O	S	0	0
			730	461	138	130	1		

- Molecule 21 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	U	102	Total	C	N	O		0	0
			779	492	146	141			

- Molecule 22 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	V	92	Total	C	N	O	S	0	0
			739	471	135	131	2		

- Molecule 23 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	W	75	Total	C	N	O	S	0	0
			572	355	116	100	1		

- Molecule 24 is a protein called 50S ribosomal protein L28.

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

- Molecule 25 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Y	60	Total	C	N	O	S	0	0
			494	305	96	91	2		

- Molecule 26 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Z	56	Total	C	N	O	S	0	0
			434	273	85	74	2		

- Molecule 27 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	0	55	Total	C	N	O	S	0	0
			434	263	92	78	1		

- Molecule 28 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	1	51	Total	C	N	O	S	0	0
			417	269	76	72			

- Molecule 29 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	2	45	Total	C	N	O	S	0	0
			367	222	88	55	2		

- Molecule 30 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	3	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 31 is a protein called 50S ribosomal protein L36 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	4	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 32 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	5	131	Total	C	N	O	S	0	0
			988	625	175	183	5		

- Molecule 33 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	6	66	Total	C	N	O	S	0	0
			522	323	99	94	6		

- Molecule 34 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	a	1540	Total	C	N	O	P	0	0
			33050	14748	6057	10705	1540		

- Molecule 35 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	b	218	Total	C	N	O	S	0	0
			1704	1081	305	311	7		

- Molecule 36 is a protein called 30S ribosomal protein S3.

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

- Molecule 37 is a protein called 30S ribosomal protein S4.

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

- Molecule 38 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	e	157	Total	C	N	O	S	1	0
			1164	724	221	213	6		

- Molecule 39 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	f	100	Total	C	N	O	S	0	0
			817	515	148	148	6		

- Molecule 40 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	g	151	Total	C	N	O	S	0	0
			1181	735	227	215	4		

- Molecule 41 is a protein called 30S ribosomal protein S8.

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

- Molecule 42 is a protein called 30S ribosomal protein S9.

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

- Molecule 43 is a protein called 30S ribosomal protein S10.

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

- Molecule 44 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	k	116	Total	C	N	O	S	0	0
			869	535	173	158	3		

- Molecule 45 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	l	121	Total	C	N	O	S	0	0
			940	581	193	162	4		

- Molecule 46 is a protein called 30S ribosomal protein S13.

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

- Molecule 47 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	n	101	Total	C	N	O	S	0	0
			810	502	165	140	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
n	35	ALA	-	insertion	UNP B7MCS2

- Molecule 48 is a protein called 30S ribosomal protein S15.

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

- Molecule 49 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	p	82	Total	C	N	O	S	0	0
			649	406	128	114	1		

- Molecule 50 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	q	80	Total	C	N	O	S	0	0
			648	411	121	113	3		

- Molecule 51 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	r	65	Total	C	N	O	S	0	0
			535	339	100	95	1		

- Molecule 52 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	s	79	Total	C	N	O	S	0	0
			637	408	120	107	2		

- Molecule 53 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	t	85	Total	C	N	O	S	0	0
			665	411	137	114	3		

- Molecule 54 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	u	65	Total	C	N	O	S	0	0
			544	335	117	91	1		

- Molecule 55 is a RNA chain called tRNA-fMet.

Mol	Chain	Residues	Atoms						AltConf	Trace
55	v	77	Total 1644	C 733	N 297	O 536	P 77	S 1	0	0
55	w	77	Total 1644	C 733	N 297	O 536	P 77	S 1	0	0

- Molecule 56 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	x	12	Total	C	N	O	P	0	0
			252	113	43	84	12		

- Molecule 57 is a RNA chain called Phe-tRNA-Phe.

Mol	Chain	Residues	Atoms						AltConf	Trace
57	y	76	Total	C	N	O	P	S	0	0
			1632	731	290	533	76	2		

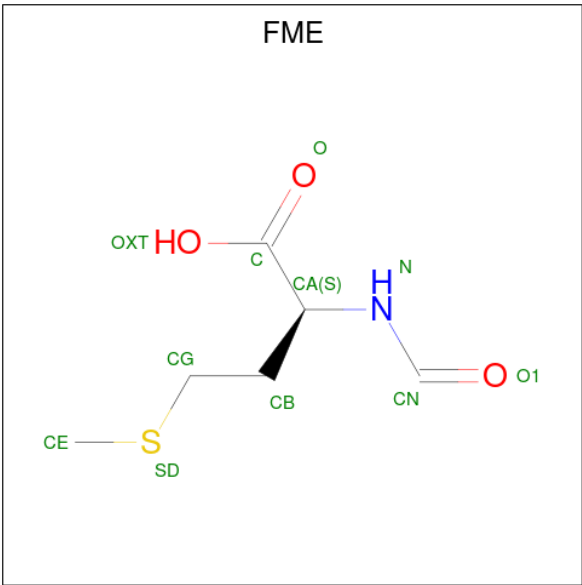
- Molecule 58 is a protein called Elongation factor Tu 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	z	393	Total	C	N	O	S	0	0
			3031	1915	522	581	13		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
z	84	ALA	HIS	engineered mutation	UNP A7ZUJ2

- Molecule 59 is N-FORMYLMETHIONINE (three-letter code: FME) (formula: C₆H₁₁NO₃S).



Mol	Chain	Residues	Atoms					AltConf
59	A	1	Total	C	N	O	S	0
			10	6	1	2	1	

- Molecule 60 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
60	A	1011	Total	Mg	0
			1011	1011	
60	B	37	Total	Mg	0
			37	37	
60	C	1	Total	Mg	0
			1	1	
60	D	2	Total	Mg	0
			2	2	
60	E	1	Total	Mg	0
			1	1	
60	M	2	Total	Mg	0
			2	2	
60	N	1	Total	Mg	0
			1	1	
60	Q	1	Total	Mg	0
			1	1	
60	T	1	Total	Mg	0
			1	1	
60	W	1	Total	Mg	0
			1	1	
60	0	3	Total	Mg	0
			3	3	

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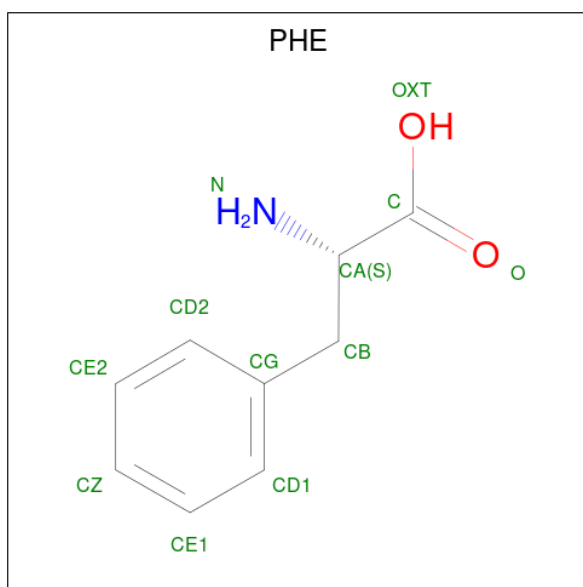
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Mol	Chain	Residues	Atoms		AltConf
60	2	1	Total 1	Mg 1	0
60	a	392	Total 392	Mg 392	0
60	d	1	Total 1	Mg 1	0
60	e	1	Total 1	Mg 1	0
60	i	1	Total 1	Mg 1	0
60	u	1	Total 1	Mg 1	0
60	v	6	Total 6	Mg 6	0
60	w	2	Total 2	Mg 2	0
60	x	1	Total 1	Mg 1	0
60	y	2	Total 2	Mg 2	0
60	z	2	Total 2	Mg 2	0

- Molecule 61 is POTASSIUM ION (three-letter code: K) (formula: K).

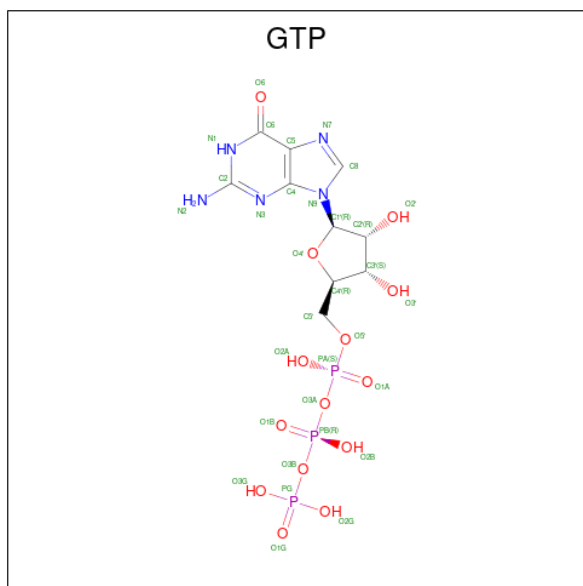
Mol	Chain	Residues	Atoms		AltConf
61	A	6	Total 6	K 6	0
61	a	1	Total 1	K 1	0

- Molecule 62 is PHENYLALANINE (three-letter code: PHE) (formula: C₉H₁₁NO₂).



Mol	Chain	Residues	Atoms				AltConf
62	z	1	Total	C	N	O	0
			11	9	1	1	

- Molecule 63 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



Mol	Chain	Residues	Atoms					AltConf
63	z	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 64 is water.

Mol	Chain	Residues	Atoms	AltConf
64	A	828	Total O 828 828	0
64	B	29	Total O 29 29	0
64	C	5	Total O 5 5	0
64	D	6	Total O 6 6	0
64	E	5	Total O 5 5	0
64	J	4	Total O 4 4	0
64	L	5	Total O 5 5	0
64	N	1	Total O 1 1	0
64	O	1	Total O 1 1	0
64	Q	3	Total O 3 3	0
64	R	1	Total O 1 1	0
64	S	3	Total O 3 3	0
64	W	2	Total O 2 2	0
64	X	3	Total O 3 3	0
64	Y	1	Total O 1 1	0
64	0	2	Total O 2 2	0
64	1	1	Total O 1 1	0
64	2	2	Total O 2 2	0
64	3	1	Total O 1 1	0
64	a	253	Total O 253 253	0
64	c	1	Total O 1 1	0
64	i	1	Total O 1 1	0

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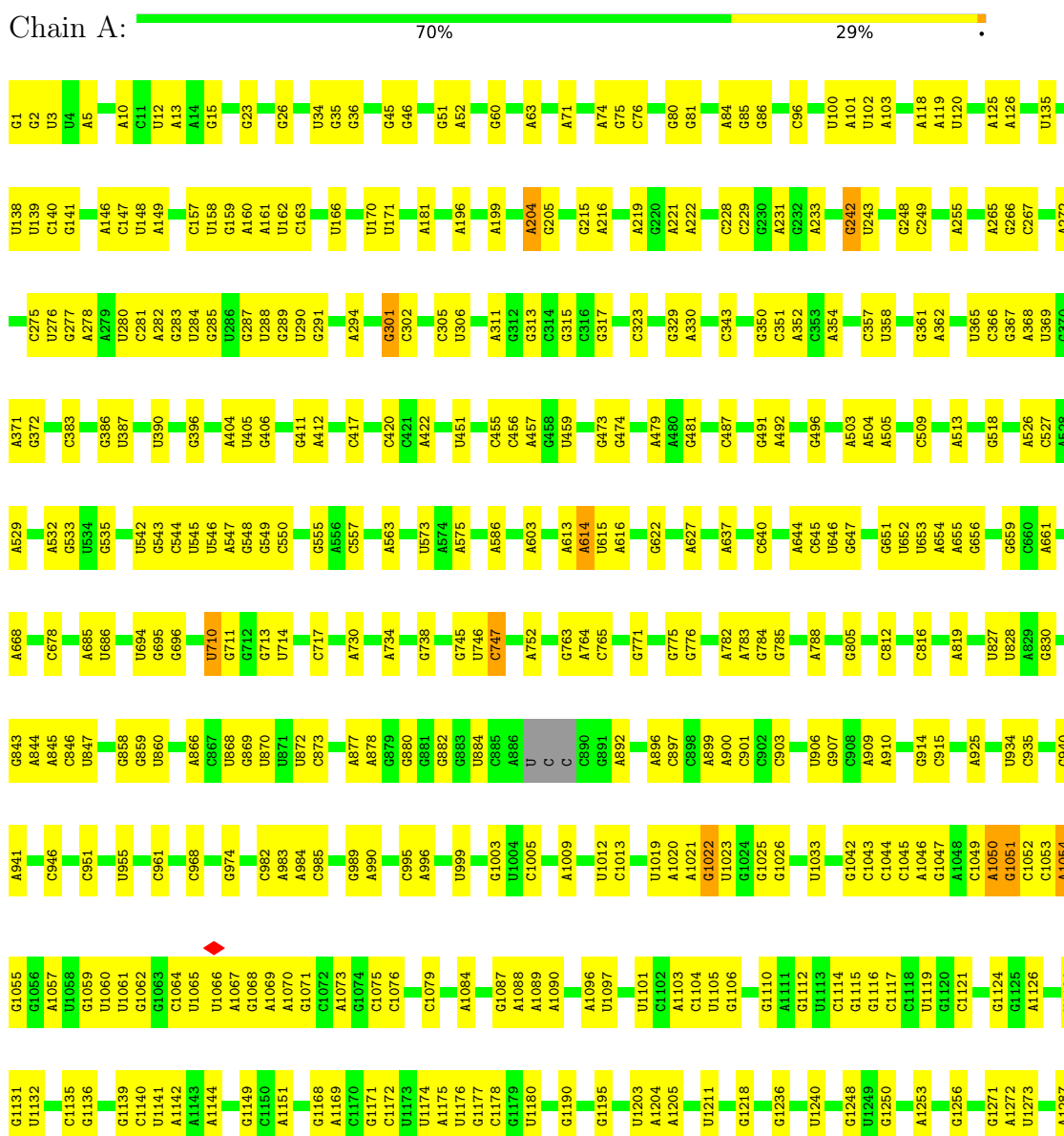
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Mol	Chain	Residues	Atoms		AltConf
64	j	1	Total 1	O 1	0
64	l	2	Total 2	O 2	0
64	m	1	Total 1	O 1	0
64	o	1	Total 1	O 1	0
64	q	1	Total 1	O 1	0
64	s	3	Total 3	O 3	0
64	u	1	Total 1	O 1	0
64	v	3	Total 3	O 3	0
64	w	1	Total 1	O 1	0
64	x	1	Total 1	O 1	0
64	y	2	Total 2	O 2	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: 23S rRNA



A2835	C2723	A2435	G2320	A2191	G2069	U1939	A1679	G1540	C1437	G1288
U2836	A2577	G2436	U2321	U2192	C2072	U1940	G1835	C1541	C1289	
A2837	A2725	G2193	A2322	G2193		C1941	U1693	G1542	C1451	
A2726	U2580	U2441	G2325	U2194	A2077	C1942	G1839	G1543	G1452	G1300
G2729	U2585	G2445	C2326	A2198		U1955	G1842	G1546	A1453	A1301
U2849	U2586	G2446	A2327	A2199	A2080	U1965	G1703		G1456	C1306
C2853	G2732	G2447	G2331	G2204	U2092	C1962	G1847	G1585	U1457	
G2857	U2739	U2448	G2332	G2204	G2093	U1963	G1715	U1588	U1458	A1321
C2858	A2740	U2604	A2333	A2211	A2094	C1965	U1716	U1559	G1459	
G2859	U2605	U2457	U2336	C2214	A2095	A1966	G1857	U1480	U1460	G1343
U2860	U2609	G2458	G2337	C2214	C2096	C1967	A1858	A1566	C1461	U1344
U2861	C2610	A2459	G2337	U2220	A2097	U1970	G1723	G1475	G1345	G1346
G2748	U2613	A2469	G2345	U2220	U2098	U1971	G1724	U1476	U1476	C1350
A2753	U2613	G2346	A2346	G2223	G2100	G1972	G1863	A1572	G1478	C1351
A2758	G2623	G2472	C2347	G2224	U2106	U1976	G1867	U1578	G1479	U1352
U2768	U2473	U2473	C2350	C2226	G2107	U1982	C1870	A1579	C1480	A1353
A2872	G2624	U2474	G2351	C2226	A2108	U1982	A1871	U1729	U1481	
A2873	C2760	A2475	A2352	G2238	U2109	U1982	A1872	G1483	G1482	
C2874	U2629	A2476	A2352	G2239	G2110	U1991	G1873	C1582	G1484	A1365
					U2111	G1992	C1874	A1583	U1485	
A2879	C2636	G2481	G2357	G2246	U2112	U1993	G1875	U1584	A1490	G1368
C2880	G2645	U2491	G2361	G2246	U2113	C1997	A1876	C1585	G1491	A1378
U2881	G2646	U2492	G2361	G2251	U2118	C1997	G1878	U1589	G1492	U1379
A2882	C2646	U2492	G2373	G2251	A2119	G2004	C1881	A1590	C1493	
A2883	U2647	U2493	G2373	C2263	G2120	G2004	A1739	A1591	A1494	C1386
U2884	G2648	G2494	A2377	C2263	G2121	C2021	G1738			A1387
G2885	C2649	C2494	A2377	A2267	U2121	U2022	G1750	C1607	C1498	
A2886			A2378	A2268	G2127	C2023	G1750	A1608		A1392
	A2654	G2502	G2383	A2278	U2131	G2027	C1764	A1609	A1503	
U2891	G2782	G2685	U2384	A2278	U2132	U2028	A1773	A1610	A1504	A1395
G2892	U2783	U2504	C2385	C2283	U2132	G2029	G1776	C1611	A1585	
A2893	U2784	U2505		C2283	G2133	A2030	G1776	C1612	U1506	U1397
G2894	G2688	G2506	G2391	U2506	A2134	A2030			C1507	C1398
	G2689	U2506	A2392	G2286	G2134	A2030			C1508	C1399
U2897	A2670	U2517	A2392	A2287	G2141	A2033			A1509	
A2791	G2671	G2518	G2396	A2287	G2157	A2033			G1510	A1403
C2793				U2292	G2162	A2033				
G2796	G2685	G2518	G2396	U2292	C2145	A2033			A1515	G1407
U2797	U2689	G2523	U2401	G2293	C2146	C2036				G1408
U2798	U2690	G2294	U2402	G2294	A2147	C2043			G1519	G1409
G2799	C2403	C2295	G2403	C2295	G2157	G2049				G1410
C2691	U2296	U2404	U2404	U2296	G2162	A2051			U1522	G1416
G2692	G2692	A2297	G2405	A2297	A2163	A2051			U1523	C1417
G2801	A2406	A2297	A2406	A2297	C2164	G2056			G1524	G1418
A2802	G2407	U2302	U2407	U2302	G2170	G2056			G1529	A1420
G2803	U2408	U2305	U2408	U2305	A2171	G2056				
U2806	G2707	G2306	G2409	U2306	G2171	G2056				
G2807	G2708	G2552	G2410	G2306	A2171	G2056				
G2808	U2712	G2553	G2410	G2307	A2171	G2056				
A2809	U2713	U2554	G2414	G2308	A2171	A2059				
	G2714	A2566	U2423	A2309	U2172	A2060				
U2818	G2718	G2567	C2424	C2311	A2173	G2061				
A2820		U2572	U2429	A2309	G2186	C2063				
A2821		C2573	G2429	A2309	U2189	G2067				
		G2574	A2430	G2315	U2190	U2068				
		C2574		G2319	U2190	U2068				
							</			

• Molecule 2: 5S rRNA

Chain B:  62% 38%

U1	C4	U5	G6	C11	C12	G13	U14	A15	U22	G23	G24	G33	A34	C35	C36	U40	G41	C42	C43	G44	A45	U46	G51	A52	A53	G56	A57	A58	A59	G60	G61	G64	U65	A66	G67	C70	G81	U87	C88	U89	C90	C91	U95	G96	G100
----	----	----	----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------



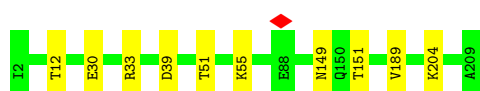
- Molecule 3: 50S ribosomal protein L2

Chain C: 96%



- Molecule 4: 50S ribosomal protein L3

Chain D: 95%



- Molecule 5: 50S ribosomal protein L4

Chain E: 94%



- Molecule 6: 50S ribosomal protein L5

Chain F: 98%



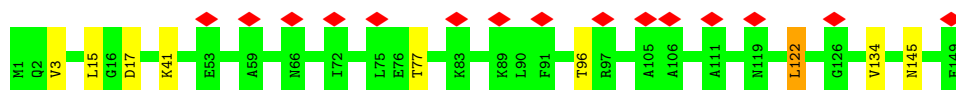
- Molecule 7: 50S ribosomal protein L6

Chain G: 99%



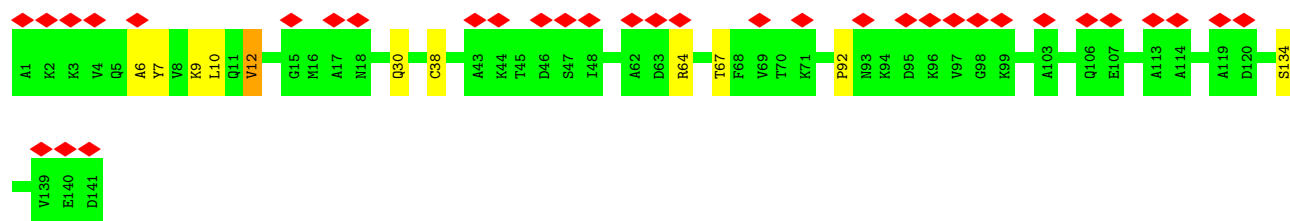
- Molecule 8: 50S ribosomal protein L9

Chain H: 10% 94% 5%



- Molecule 9: 50S ribosomal protein L11

Chain I: 24% 92% 7%



- Molecule 10: 50S ribosomal protein L13

Chain J: 98%



- Molecule 11: 50S ribosomal protein L14

Chain K: 94%



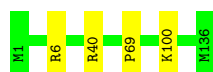
- Molecule 12: 50S ribosomal protein L15

Chain L: 90%



- Molecule 13: 50S ribosomal protein L16

Chain M: 97%



- Molecule 14: 50S ribosomal protein L17

Chain N: 96%



- Molecule 15: 50S ribosomal protein L18

Chain O: 99%



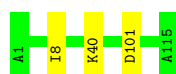
- Molecule 16: 50S ribosomal protein L19

Chain P:  98% .



- Molecule 17: 50S ribosomal protein L20

Chain Q:  97% .



- Molecule 18: 50S ribosomal protein L21

Chain R:  95% 5%



- Molecule 19: 50S ribosomal protein L22

Chain S:  98% .



- Molecule 20: 50S ribosomal protein L23

Chain T:  95% 5%



- Molecule 21: 50S ribosomal protein L24

Chain U:  94% 6%



- Molecule 22: 50S ribosomal protein L25

Chain V:  98% .



- Molecule 23: 50S ribosomal protein L27

Chain W:  97% .



- Molecule 24: 50S ribosomal protein L28

Chain X:  99% .



- Molecule 25: 50S ribosomal protein L29

Chain Y:  97% .



- Molecule 26: 50S ribosomal protein L30

Chain Z:  100%

There are no outlier residues recorded for this chain.

- Molecule 27: 50S ribosomal protein L32

Chain 0:  96% .



- Molecule 28: 50S ribosomal protein L33

Chain 1:  100%

There are no outlier residues recorded for this chain.

- Molecule 29: 50S ribosomal protein L34

Chain 2:  96% .



- Molecule 30: 50S ribosomal protein L35

Chain 3:  97% .




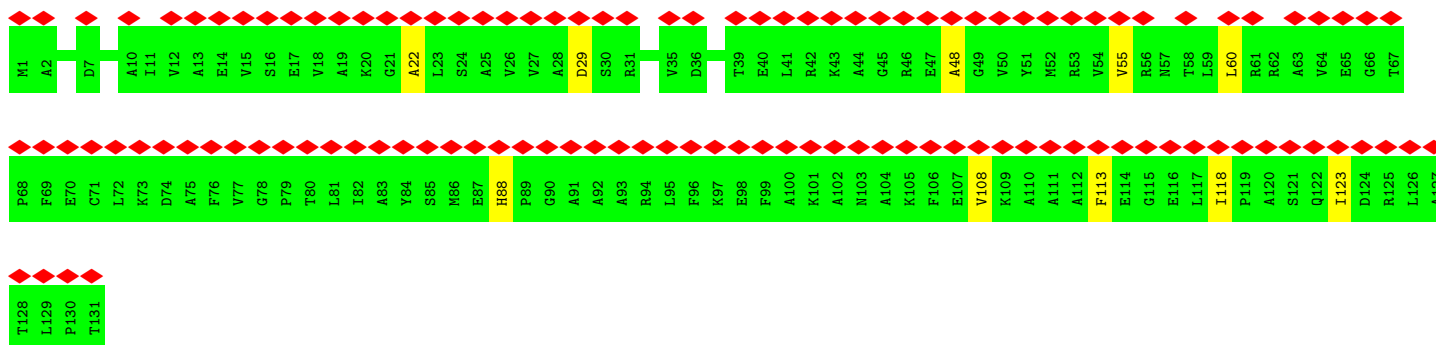
- Molecule 31: 50S ribosomal protein L36 1

Chain 4:  100%

There are no outlier residues recorded for this chain.

- Molecule 32: 50S ribosomal protein L10

Chain 5:  89%
92% 8%



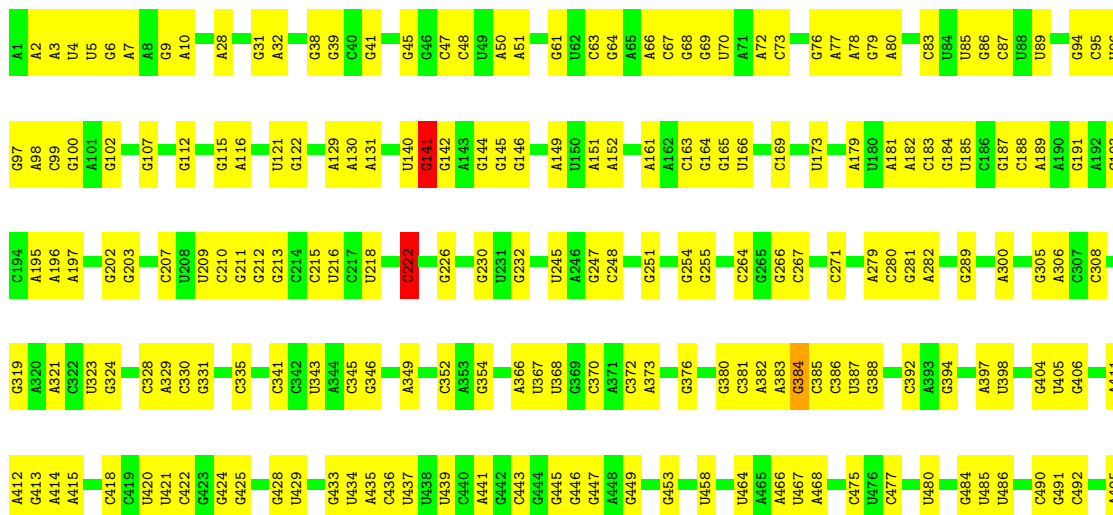
- Molecule 33: 50S ribosomal protein L31

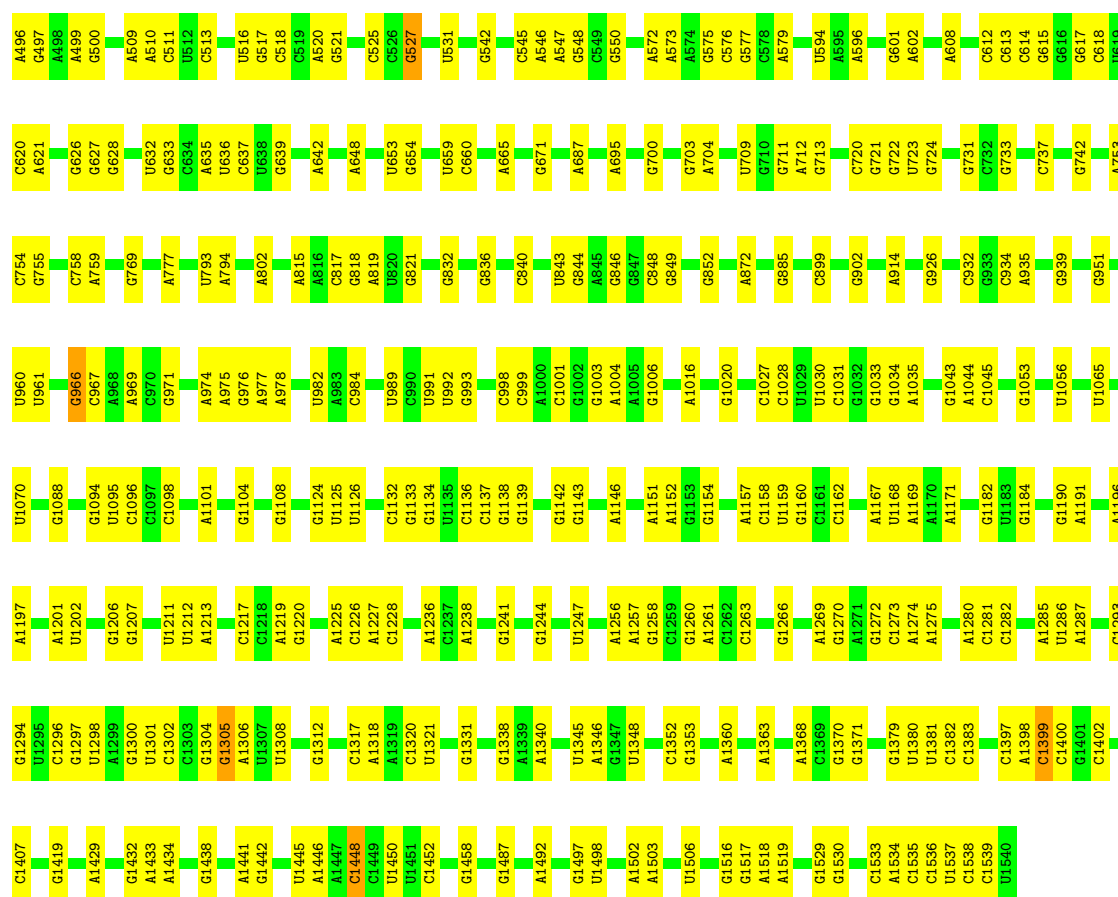
Chain 6:  95% 5%



- Molecule 34: 16S rRNA

Chain a:  67% 32%





- Molecule 35: 30S ribosomal protein S2

Chain b: 96%



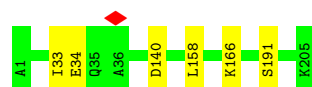
- Molecule 36: 30S ribosomal protein S3

Chain c: 96%

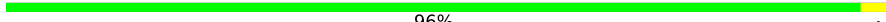


- Molecule 37: 30S ribosomal protein S4

Chain d: 97%



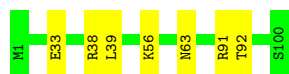
- Molecule 38: 30S ribosomal protein S5

Chain e:  96% .



- Molecule 39: 30S ribosomal protein S6

Chain f:  93% 7%



- Molecule 40: 30S ribosomal protein S7

Chain g:  92% 8%



- Molecule 41: 30S ribosomal protein S8

Chain h:  98% .



- Molecule 42: 30S ribosomal protein S9

Chain i:  94% 5% .



- Molecule 43: 30S ribosomal protein S10

Chain j:  94% 6%



- Molecule 44: 30S ribosomal protein S11

Chain k:  93% 7%



- Molecule 45: 30S ribosomal protein S12

Chain l:  93% 7%



- Molecule 46: 30S ribosomal protein S13

Chain m:  97%



- Molecule 47: 30S ribosomal protein S14

Chain n:  94% 6%



- Molecule 48: 30S ribosomal protein S15

Chain o:  94% 6%



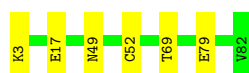
- Molecule 49: 30S ribosomal protein S16

Chain p:  95% 5%




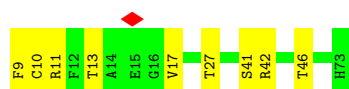
- Molecule 50: 30S ribosomal protein S17

Chain q:  92% 8%



- Molecule 51: 30S ribosomal protein S18

Chain r:  86% 14%



- Molecule 52: 30S ribosomal protein S19

Chain s:  97% .




- Molecule 53: 30S ribosomal protein S20

Chain t:  95% 5%



- Molecule 54: 30S ribosomal protein S21

Chain u:  82% 18%



- Molecule 55: tRNA-fMet

Chain v:  66% 31% .



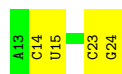
- Molecule 55: tRNA-fMet

Chain w:  8% 53% 42% 5%



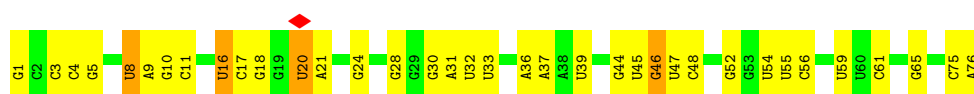
- Molecule 56: mRNA

Chain x:  67% 33%

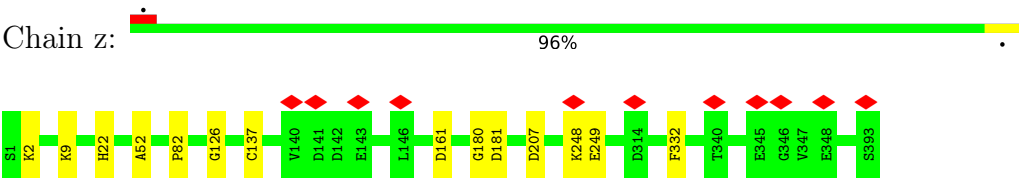


- Molecule 57: Phe-tRNA-Phe

Chain y:  53% 42% 5%



- Molecule 58: Elongation factor Tu 2



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	58475	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	67	Depositor
Minimum defocus (nm)	300	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	51020	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.288	Depositor
Minimum map value	-0.143	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.010	Depositor
Recommended contour level	0.00532	Depositor
Map size (Å)	390.04, 390.04, 390.04	wwPDB
Map dimensions	398, 398, 398	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.98, 0.98, 0.98	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GTP, H2U, OMG, OMU, PSU, 2MA, 5MU, UR3, OMC, 5MC, 4OC, MIA, MG, MA6, 4SU, FME, 7MG, K, 2MG, 3TD, 1MG, 6MZ

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	0.25	1/69174 (0.0%)	0.70	16/107907 (0.0%)
2	B	0.30	1/2876 (0.0%)	0.71	0/4483
3	C	0.35	0/2121	0.70	0/2852
4	D	0.35	0/1578	0.60	0/2124
5	E	0.35	0/1563	0.64	0/2103
6	F	0.38	0/1434	0.61	0/1926
7	G	0.35	0/1324	0.56	0/1794
8	H	0.39	0/1122	0.57	0/1515
9	I	0.43	0/1046	0.60	0/1410
10	J	0.34	0/1143	0.61	0/1540
11	K	0.35	0/947	0.68	0/1268
12	L	0.36	0/1052	0.71	0/1401
13	M	0.37	0/1093	0.63	0/1460
14	N	0.38	0/964	0.71	0/1289
15	O	0.36	0/902	0.63	0/1209
16	P	0.36	0/929	0.64	0/1242
17	Q	0.36	0/946	0.67	0/1260
18	R	0.35	0/823	0.60	0/1100
19	S	0.33	0/852	0.67	0/1142
20	T	0.35	0/736	0.61	0/984
21	U	0.34	0/787	0.57	0/1051
22	V	0.35	0/752	0.55	0/1008
23	W	0.35	0/579	0.64	0/767
24	X	0.36	0/635	0.65	0/848
25	Y	0.38	0/495	0.59	0/658
26	Z	0.36	0/438	0.60	0/586
27	0	0.33	0/440	0.67	0/588
28	1	0.35	0/424	0.56	0/565
29	2	0.38	0/370	0.78	0/487
30	3	0.33	0/513	0.62	0/676
31	4	0.33	0/303	0.65	0/397

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	5	0.43	0/1001	0.58	0/1350
33	6	0.40	0/531	0.54	0/709
34	a	0.26	7/36725 (0.0%)	0.71	10/57285 (0.0%)
35	b	0.37	0/1735	0.54	0/2338
36	c	0.36	0/1651	0.59	0/2225
37	d	0.40	0/1665	0.61	0/2227
38	e	0.35	0/1180	0.61	0/1587
39	f	0.36	0/835	0.59	0/1128
40	g	0.36	0/1195	0.60	0/1602
41	h	0.34	0/989	0.61	0/1326
42	i	0.38	0/1034	0.69	0/1375
43	j	0.36	0/796	0.65	0/1077
44	k	0.36	0/885	0.60	0/1195
45	l	0.37	0/954	0.67	0/1282
46	m	0.36	0/900	0.64	0/1204
47	n	0.37	0/822	0.66	0/1095
48	o	0.35	0/722	0.61	0/964
49	p	0.38	0/659	0.58	0/884
50	q	0.37	0/657	0.65	0/881
51	r	0.40	0/544	0.61	0/731
52	s	0.37	0/652	0.62	0/877
53	t	0.36	0/671	0.61	0/888
54	u	0.45	0/550	0.75	0/728
55	v	0.33	1/1747 (0.1%)	0.68	0/2721
55	w	0.34	1/1747 (0.1%)	0.96	4/2721 (0.1%)
56	x	0.23	0/280	0.73	0/433
57	y	0.33	1/1607 (0.1%)	0.68	0/2501
58	z	0.37	0/3086	0.56	0/4175
All	All	0.30	12/164181 (0.0%)	0.69	30/245149 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
34	a	0	2
All	All	0	3

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	v	0	C	OP3-P	-10.16	1.49	1.61
2	B	1	U	OP3-P	-10.16	1.49	1.61
1	A	1	G	OP3-P	-10.15	1.49	1.61
55	w	1	C	OP3-P	-10.12	1.49	1.61
57	y	1	G	OP3-P	-10.07	1.49	1.61

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	w	117	U	P-O3'-C3'	28.03	153.34	119.70
55	w	117	U	O3'-P-O5'	18.55	139.25	104.00
55	w	117	U	OP1-P-O3'	-9.49	84.33	105.20
34	a	222	C	N1-C2-O2	8.24	123.84	118.90
1	A	1484	U	N1-C1'-C2'	8.16	124.61	114.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1054	A	Sidechain
34	a	141	G	Sidechain
34	a	222	C	Sidechain

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	269/271 (99%)	239 (89%)	27 (10%)	3 (1%)	14	50
4	D	206/208 (99%)	190 (92%)	15 (7%)	1 (0%)	29	68

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	E	198/200 (99%)	178 (90%)	18 (9%)	2 (1%)	15	53
6	F	175/177 (99%)	157 (90%)	16 (9%)	2 (1%)	14	50
7	G	172/174 (99%)	158 (92%)	14 (8%)	0	100	100
8	H	147/149 (99%)	128 (87%)	15 (10%)	4 (3%)	5	26
9	I	139/141 (99%)	109 (78%)	23 (16%)	7 (5%)	2	12
10	J	139/141 (99%)	130 (94%)	8 (6%)	1 (1%)	22	60
11	K	120/122 (98%)	106 (88%)	10 (8%)	4 (3%)	4	21
12	L	141/143 (99%)	117 (83%)	18 (13%)	6 (4%)	2	15
13	M	134/136 (98%)	128 (96%)	5 (4%)	1 (1%)	22	60
14	N	117/119 (98%)	101 (86%)	14 (12%)	2 (2%)	9	39
15	O	114/116 (98%)	105 (92%)	8 (7%)	1 (1%)	17	55
16	P	112/114 (98%)	99 (88%)	12 (11%)	1 (1%)	17	55
17	Q	113/115 (98%)	111 (98%)	2 (2%)	0	100	100
18	R	100/102 (98%)	85 (85%)	12 (12%)	3 (3%)	4	24
19	S	107/109 (98%)	100 (94%)	6 (6%)	1 (1%)	17	55
20	T	90/92 (98%)	81 (90%)	7 (8%)	2 (2%)	6	31
21	U	100/102 (98%)	87 (87%)	9 (9%)	4 (4%)	3	17
22	V	90/92 (98%)	86 (96%)	3 (3%)	1 (1%)	14	50
23	W	73/75 (97%)	68 (93%)	5 (7%)	0	100	100
24	X	75/77 (97%)	69 (92%)	6 (8%)	0	100	100
25	Y	58/60 (97%)	54 (93%)	3 (5%)	1 (2%)	9	39
26	Z	54/56 (96%)	51 (94%)	3 (6%)	0	100	100
27	0	53/55 (96%)	44 (83%)	8 (15%)	1 (2%)	8	36
28	1	49/51 (96%)	43 (88%)	6 (12%)	0	100	100
29	2	43/45 (96%)	40 (93%)	2 (5%)	1 (2%)	6	30
30	3	62/64 (97%)	59 (95%)	3 (5%)	0	100	100
31	4	36/38 (95%)	31 (86%)	5 (14%)	0	100	100
32	5	129/131 (98%)	99 (77%)	21 (16%)	9 (7%)	1	6
33	6	64/66 (97%)	58 (91%)	4 (6%)	2 (3%)	4	23
35	b	216/218 (99%)	186 (86%)	25 (12%)	5 (2%)	6	30
36	c	204/206 (99%)	183 (90%)	15 (7%)	6 (3%)	4	24

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
37	d	203/205 (99%)	183 (90%)	17 (8%)	3 (2%)	10	42
38	e	156/157 (99%)	133 (85%)	21 (14%)	2 (1%)	12	45
39	f	98/100 (98%)	85 (87%)	9 (9%)	4 (4%)	3	16
40	g	149/151 (99%)	131 (88%)	11 (7%)	7 (5%)	2	14
41	h	127/129 (98%)	116 (91%)	11 (9%)	0	100	100
42	i	125/127 (98%)	97 (78%)	24 (19%)	4 (3%)	4	22
43	j	96/98 (98%)	73 (76%)	18 (19%)	5 (5%)	2	12
44	k	114/116 (98%)	97 (85%)	11 (10%)	6 (5%)	2	11
45	l	119/121 (98%)	93 (78%)	19 (16%)	7 (6%)	1	9
46	m	113/115 (98%)	102 (90%)	9 (8%)	2 (2%)	8	37
47	n	99/101 (98%)	84 (85%)	10 (10%)	5 (5%)	2	12
48	o	86/88 (98%)	79 (92%)	4 (5%)	3 (4%)	3	20
49	p	80/82 (98%)	70 (88%)	8 (10%)	2 (2%)	5	28
50	q	78/80 (98%)	67 (86%)	7 (9%)	4 (5%)	2	12
51	r	63/65 (97%)	54 (86%)	6 (10%)	3 (5%)	2	13
52	s	77/79 (98%)	67 (87%)	10 (13%)	0	100	100
53	t	83/85 (98%)	77 (93%)	4 (5%)	2 (2%)	6	29
54	u	63/65 (97%)	41 (65%)	12 (19%)	10 (16%)	0	1
58	z	391/393 (100%)	357 (91%)	22 (6%)	12 (3%)	4	23
All	All	6219/6322 (98%)	5486 (88%)	581 (9%)	152 (2%)	9	29

5 of 152 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	70	LYS
5	E	83	VAL
6	F	11	VAL
11	K	89	ASN
16	P	65	ASN

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	
3	C	216/216 (100%)	207 (96%)	9 (4%)	30	66
4	D	163/163 (100%)	154 (94%)	9 (6%)	21	57
5	E	164/164 (100%)	154 (94%)	10 (6%)	18	53
6	F	148/148 (100%)	145 (98%)	3 (2%)	55	83
7	G	135/135 (100%)	133 (98%)	2 (2%)	65	87
8	H	114/114 (100%)	108 (95%)	6 (5%)	22	58
9	I	109/109 (100%)	104 (95%)	5 (5%)	27	64
10	J	115/115 (100%)	113 (98%)	2 (2%)	60	85
11	K	103/103 (100%)	100 (97%)	3 (3%)	42	76
12	L	102/102 (100%)	93 (91%)	9 (9%)	10	36
13	M	109/109 (100%)	106 (97%)	3 (3%)	43	77
14	N	99/99 (100%)	95 (96%)	4 (4%)	31	68
15	O	86/86 (100%)	86 (100%)	0	100	100
16	P	99/99 (100%)	98 (99%)	1 (1%)	76	91
17	Q	88/88 (100%)	85 (97%)	3 (3%)	37	72
18	R	84/84 (100%)	82 (98%)	2 (2%)	49	79
19	S	92/92 (100%)	91 (99%)	1 (1%)	73	90
20	T	79/79 (100%)	76 (96%)	3 (4%)	33	69
21	U	83/83 (100%)	81 (98%)	2 (2%)	49	79
22	V	77/77 (100%)	76 (99%)	1 (1%)	69	89
23	W	57/57 (100%)	55 (96%)	2 (4%)	36	71
24	X	67/67 (100%)	66 (98%)	1 (2%)	65	87
25	Y	55/55 (100%)	54 (98%)	1 (2%)	59	85
26	Z	47/47 (100%)	47 (100%)	0	100	100
27	0	46/46 (100%)	45 (98%)	1 (2%)	52	81
28	1	46/46 (100%)	46 (100%)	0	100	100
29	2	37/37 (100%)	36 (97%)	1 (3%)	44	77
30	3	51/51 (100%)	49 (96%)	2 (4%)	32	69
31	4	34/34 (100%)	34 (100%)	0	100	100
32	5	100/100 (100%)	99 (99%)	1 (1%)	76	91

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
33	6	59/59 (100%)	58 (98%)	1 (2%)	60	85
35	b	180/180 (100%)	177 (98%)	3 (2%)	60	85
36	c	170/170 (100%)	168 (99%)	2 (1%)	71	90
37	d	172/172 (100%)	169 (98%)	3 (2%)	60	85
38	e	120/119 (101%)	115 (96%)	5 (4%)	30	66
39	f	87/87 (100%)	84 (97%)	3 (3%)	37	72
40	g	124/124 (100%)	119 (96%)	5 (4%)	31	68
41	h	104/104 (100%)	102 (98%)	2 (2%)	57	84
42	i	105/105 (100%)	101 (96%)	4 (4%)	33	69
43	j	86/86 (100%)	85 (99%)	1 (1%)	71	90
44	k	89/89 (100%)	87 (98%)	2 (2%)	52	81
45	l	102/102 (100%)	99 (97%)	3 (3%)	42	76
46	m	93/93 (100%)	91 (98%)	2 (2%)	52	81
47	n	83/83 (100%)	82 (99%)	1 (1%)	71	90
48	o	76/76 (100%)	74 (97%)	2 (3%)	46	78
49	p	65/65 (100%)	63 (97%)	2 (3%)	40	75
50	q	74/74 (100%)	72 (97%)	2 (3%)	44	77
51	r	56/56 (100%)	50 (89%)	6 (11%)	6	26
52	s	70/70 (100%)	68 (97%)	2 (3%)	42	76
53	t	65/65 (100%)	63 (97%)	2 (3%)	40	75
54	u	55/55 (100%)	53 (96%)	2 (4%)	35	70
58	z	325/325 (100%)	323 (99%)	2 (1%)	86	95
All	All	5165/5164 (100%)	5021 (97%)	144 (3%)	46	77

5 of 144 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
43	j	45	ARG
58	z	181	ASP
45	l	77	SER
51	r	9	PHE
11	K	61	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
32	5	4	ASN
53	t	69	ASN
35	b	18	GLN
58	z	135	ASN
44	k	39	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2893/2903 (99%)	815 (28%)	91 (3%)
2	B	119/120 (99%)	44 (36%)	7 (5%)
34	a	1536/1540 (99%)	492 (32%)	0
55	v	76/77 (98%)	23 (30%)	0
55	w	76/77 (98%)	33 (43%)	0
56	x	11/12 (91%)	4 (36%)	0
57	y	74/76 (97%)	30 (40%)	0
All	All	4785/4805 (99%)	1441 (30%)	98 (2%)

5 of 1441 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	2	G
1	A	3	U
1	A	5	A
1	A	10	A
1	A	12	U

5 of 98 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	1538	G
1	A	2192	U
1	A	1607	C
1	A	1884	G
1	A	2401	U

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

52 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	$\# Z > 2$
57	PSU	y	39	57	18,21,22	1.41	2 (11%)	22,30,33	1.86	4 (18%)
1	PSU	A	2605	1,60	18,21,22	1.39	2 (11%)	22,30,33	2.04	4 (18%)
55	4SU	v	7	55	18,21,22	1.66	4 (22%)	26,30,33	2.34	5 (19%)
1	PSU	A	955	1	18,21,22	1.38	2 (11%)	22,30,33	1.95	4 (18%)
34	2MG	a	1516	34	18,26,27	0.96	1 (5%)	16,38,41	1.16	2 (12%)
34	MA6	a	1519	34	19,26,27	1.22	2 (10%)	18,38,41	1.68	4 (22%)
1	7MG	A	2069	1,60	22,26,27	1.53	4 (18%)	29,39,42	2.45	10 (34%)
1	5MC	A	1962	1	18,22,23	0.90	1 (5%)	26,32,35	1.19	3 (11%)
1	2MA	A	2503	1,60	17,25,26	1.02	1 (5%)	17,37,40	1.15	2 (11%)
1	PSU	A	2604	1	18,21,22	1.40	3 (16%)	22,30,33	1.85	4 (18%)
34	7MG	a	527	34	22,26,27	1.48	4 (18%)	29,39,42	2.39	8 (27%)
57	H2U	y	16	57	18,21,22	0.81	1 (5%)	21,30,33	1.49	4 (19%)
55	H2U	w	20	55	18,21,22	0.81	0	21,30,33	1.69	3 (14%)
34	2MG	a	966	34	18,26,27	0.93	0	16,38,41	1.32	3 (18%)
1	6MZ	A	1618	1	18,25,26	1.03	1 (5%)	16,36,39	2.29	5 (31%)
57	5MU	y	54	57	19,22,23	1.40	4 (21%)	28,32,35	2.09	8 (28%)
57	PSU	y	32	57	18,21,22	1.33	2 (11%)	22,30,33	1.91	5 (22%)
1	PSU	A	2504	1	18,21,22	1.37	2 (11%)	22,30,33	1.79	4 (18%)
1	PSU	A	746	1,60	18,21,22	1.38	3 (16%)	22,30,33	1.92	4 (18%)
1	OMC	A	2498	1,60	19,22,23	0.90	1 (5%)	26,31,34	1.18	2 (7%)
1	6MZ	A	2030	1	18,25,26	1.01	1 (5%)	16,36,39	2.28	5 (31%)
55	4SU	w	8	55	18,21,22	1.71	5 (27%)	26,30,33	2.14	5 (19%)
1	2MG	A	1835	1	18,26,27	1.01	1 (5%)	16,38,41	1.14	1 (6%)
55	5MU	v	54	55	19,22,23	1.48	5 (26%)	28,32,35	1.88	8 (28%)
34	4OC	a	1402	60,34	20,23,24	0.81	0	26,32,35	1.31	5 (19%)
34	5MC	a	967	34	18,22,23	1.06	1 (5%)	26,32,35	1.23	4 (15%)
1	OMU	A	2552	1,60	19,22,23	1.36	3 (15%)	26,31,34	2.14	8 (30%)
55	5MU	w	54	55	19,22,23	1.48	4 (21%)	28,32,35	2.04	10 (35%)
34	PSU	a	516	34	18,21,22	1.40	2 (11%)	22,30,33	1.96	5 (22%)
34	2MG	a	1207	60,34	18,26,27	0.98	0	16,38,41	1.11	2 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
57	PSU	y	55	57	18,21,22	1.36	2 (11%)	22,30,33	1.90	5 (22%)
34	5MC	a	1407	34	18,22,23	1.00	1 (5%)	26,32,35	1.29	4 (15%)
1	PSU	A	1911	1	18,21,22	1.35	2 (11%)	22,30,33	1.93	4 (18%)
1	OMG	A	2251	55,1,60	18,26,27	1.04	2 (11%)	19,38,41	1.22	3 (15%)
1	PSU	A	2457	1	18,21,22	1.52	3 (16%)	22,30,33	1.85	5 (22%)
1	H2U	A	2449	1	18,21,22	1.02	2 (11%)	21,30,33	1.51	4 (19%)
34	UR3	a	1498	34	19,22,23	1.08	2 (10%)	26,32,35	1.72	3 (11%)
1	PSU	A	1917	1	18,21,22	1.38	2 (11%)	22,30,33	1.94	4 (18%)
55	H2U	v	20	55	18,21,22	0.90	1 (5%)	21,30,33	1.59	5 (23%)
57	7MG	y	46	57	22,26,27	1.44	4 (18%)	29,39,42	2.36	7 (24%)
1	PSU	A	2580	1	18,21,22	1.47	3 (16%)	22,30,33	1.93	5 (22%)
1	5MC	A	747	1	18,22,23	0.97	2 (11%)	26,32,35	1.60	6 (23%)
1	3TD	A	1915	1,60	18,22,23	7.19	13 (72%)	22,32,35	1.96	3 (13%)
1	5MU	A	1939	1	19,22,23	1.38	5 (26%)	28,32,35	2.00	8 (28%)
34	MA6	a	1518	34	19,26,27	1.34	3 (15%)	18,38,41	1.77	4 (22%)
1	1MG	A	745	1	18,26,27	0.89	0	19,39,42	1.48	3 (15%)
57	H2U	y	20	57	18,21,22	0.84	1 (5%)	21,30,33	1.58	4 (19%)
57	MIA	y	37	57	24,31,32	2.37	6 (25%)	26,44,47	2.65	10 (38%)
1	2MG	A	2445	1	18,26,27	1.11	1 (5%)	16,38,41	1.20	2 (12%)
55	PSU	w	55	55	18,21,22	1.30	2 (11%)	22,30,33	1.93	5 (22%)
55	PSU	v	55	55,60	18,21,22	1.34	3 (16%)	22,30,33	1.85	5 (22%)
57	4SU	y	8	57	18,21,22	1.71	5 (27%)	26,30,33	2.28	7 (26%)

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
57	PSU	y	39	57	-	2/7/25/26	0/2/2/2
1	PSU	A	2605	1,60	-	0/7/25/26	0/2/2/2
55	4SU	v	7	55	-	2/7/25/26	0/2/2/2
1	PSU	A	955	1	-	0/7/25/26	0/2/2/2
34	2MG	a	1516	34	-	0/5/27/28	0/3/3/3
34	MA6	a	1519	34	-	3/7/29/30	0/3/3/3
1	7MG	A	2069	1,60	-	2/7/37/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	5MC	A	1962	1	-	2/7/25/26	0/2/2/2
1	2MA	A	2503	1,60	-	0/3/25/26	0/3/3/3
1	PSU	A	2604	1	-	2/7/25/26	0/2/2/2
34	7MG	a	527	34	-	2/7/37/38	0/3/3/3
57	H2U	y	16	57	-	2/7/38/39	0/2/2/2
55	H2U	w	20	55	-	2/7/38/39	0/2/2/2
34	2MG	a	966	34	-	3/5/27/28	0/3/3/3
1	6MZ	A	1618	1	-	3/5/27/28	0/3/3/3
57	5MU	y	54	57	-	0/7/25/26	0/2/2/2
57	PSU	y	32	57	-	2/7/25/26	0/2/2/2
1	PSU	A	2504	1	-	2/7/25/26	0/2/2/2
1	PSU	A	746	1,60	-	3/7/25/26	0/2/2/2
1	OMC	A	2498	1,60	-	0/9/27/28	0/2/2/2
1	6MZ	A	2030	1	-	3/5/27/28	0/3/3/3
55	4SU	w	8	55	-	6/7/25/26	0/2/2/2
1	2MG	A	1835	1	-	0/5/27/28	0/3/3/3
55	5MU	v	54	55	-	0/7/25/26	0/2/2/2
34	4OC	a	1402	60,34	-	2/9/29/30	0/2/2/2
34	5MC	a	967	34	-	0/7/25/26	0/2/2/2
1	OMU	A	2552	1,60	-	2/9/27/28	0/2/2/2
55	5MU	w	54	55	-	0/7/25/26	0/2/2/2
34	PSU	a	516	34	-	0/7/25/26	0/2/2/2
34	2MG	a	1207	60,34	-	0/5/27/28	0/3/3/3
57	PSU	y	55	57	-	0/7/25/26	0/2/2/2
34	5MC	a	1407	34	-	0/7/25/26	0/2/2/2
1	PSU	A	1911	1	-	0/7/25/26	0/2/2/2
1	OMG	A	2251	55,1,60	-	0/5/27/28	0/3/3/3
1	PSU	A	2457	1	-	2/7/25/26	0/2/2/2
1	H2U	A	2449	1	-	0/7/38/39	0/2/2/2
34	UR3	a	1498	34	-	2/7/25/26	0/2/2/2
1	PSU	A	1917	1	-	2/7/25/26	0/2/2/2
55	H2U	v	20	55	-	5/7/38/39	0/2/2/2
57	7MG	y	46	57	-	4/7/37/38	0/3/3/3
1	PSU	A	2580	1	-	0/7/25/26	0/2/2/2
1	5MC	A	747	1	-	0/7/25/26	0/2/2/2
1	3TD	A	1915	1,60	-	2/7/25/26	0/2/2/2
1	5MU	A	1939	1	-	2/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	MA6	a	1518	34	-	2/7/29/30	0/3/3/3
1	1MG	A	745	1	-	0/3/25/26	0/3/3/3
57	H2U	y	20	57	-	2/7/38/39	0/2/2/2
57	MIA	y	37	57	-	5/11/33/34	0/3/3/3
1	2MG	A	2445	1	-	2/5/27/28	0/3/3/3
55	PSU	w	55	55	-	1/7/25/26	0/2/2/2
55	PSU	v	55	55,60	-	2/7/25/26	0/2/2/2
57	4SU	y	8	57	-	2/7/25/26	0/2/2/2

The worst 5 of 127 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1915	3TD	O4'-C1'	16.38	1.66	1.43
1	A	1915	3TD	C6-C5	15.22	1.53	1.35
1	A	1915	3TD	C2'-C1'	-15.08	1.34	1.53
1	A	1915	3TD	C2-N1	7.61	1.47	1.37
57	y	37	MIA	C13-C14	7.49	1.53	1.32

The worst 5 of 247 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	y	46	7MG	N9-C4-N3	7.89	137.26	125.47
34	a	527	7MG	N9-C4-N3	7.73	137.04	125.47
57	y	37	MIA	C12-C13-C14	-7.64	112.26	127.14
1	A	2069	7MG	N9-C4-N3	7.18	136.21	125.47
55	v	7	4SU	C4-N3-C2	-6.84	120.70	127.34

There are no chirality outliers.

5 of 80 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	746	PSU	C2'-C1'-C5-C4
1	A	746	PSU	O4'-C1'-C5-C6
1	A	2030	6MZ	C4'-C5'-O5'-P
1	A	2030	6MZ	C3'-C4'-C5'-O5'
1	A	2069	7MG	O4'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 1481 ligands modelled in this entry, 1478 are monoatomic - leaving 3 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
62	PHE	z	401	-	10,11,12	0.38	0	10,13,15	0.29	0
63	GTP	z	402	60	26,34,34	0.95	1 (3%)	32,54,54	1.47	5 (15%)
59	FME	A	3001	-	8,9,10	0.53	0	7,9,11	1.07	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
62	PHE	z	401	-	-	1/5/6/8	0/1/1/1
63	GTP	z	402	60	-	7/18/38/38	0/3/3/3
59	FME	A	3001	-	-	0/7/9/11	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
63	z	402	GTP	C6-N1	-2.71	1.33	1.37

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
63	z	402	GTP	PA-O3A-PB	-3.58	120.55	132.83
63	z	402	GTP	PB-O3B-PG	-3.46	120.95	132.83
63	z	402	GTP	C3'-C2'-C1'	3.14	105.71	100.98
63	z	402	GTP	C5-C6-N1	2.46	118.30	113.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
63	z	402	GTP	C8-N7-C5	2.19	107.16	102.99

There are no chirality outliers.

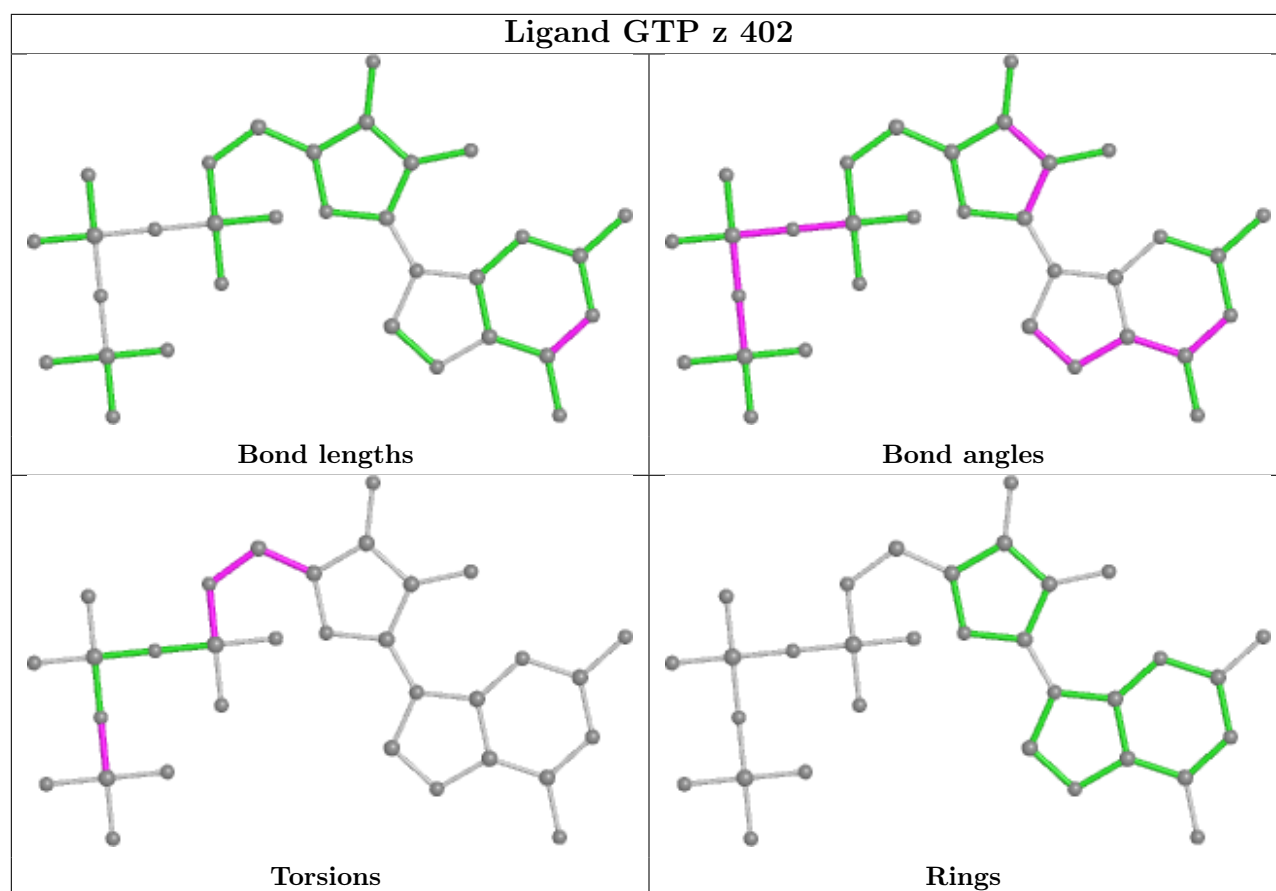
5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
62	z	401	PHE	O-C-CA-CB
63	z	402	GTP	C5'-O5'-PA-O1A
63	z	402	GTP	C5'-O5'-PA-O2A
63	z	402	GTP	C3'-C4'-C5'-O5'
63	z	402	GTP	O4'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

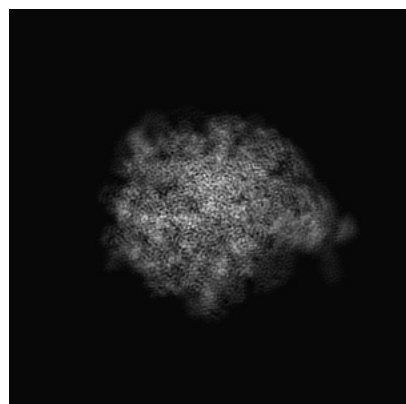
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8829. These allow visual inspection of the internal detail of the map and identification of artifacts.

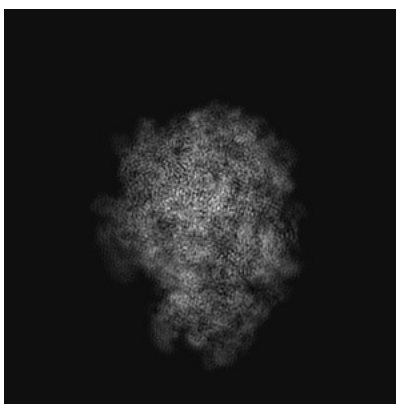
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

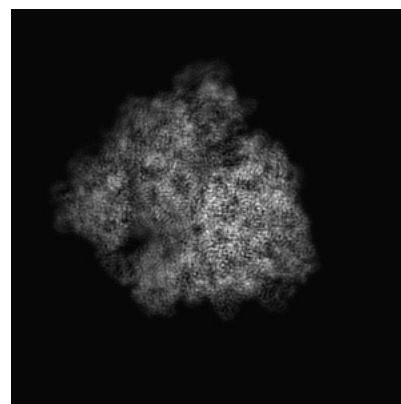
6.1.1 Primary map



X

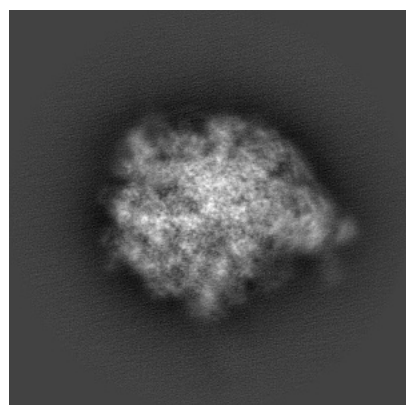


Y

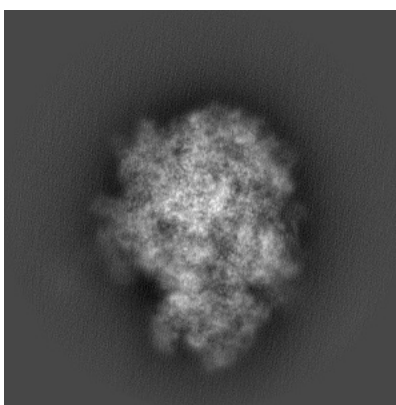


Z

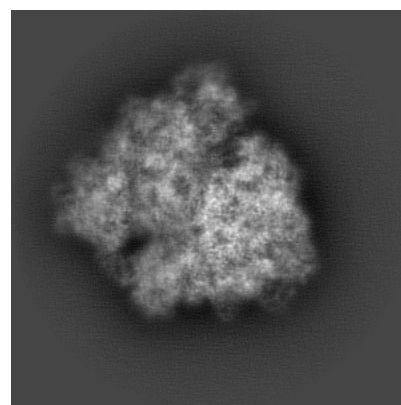
6.1.2 Raw map



X



Y

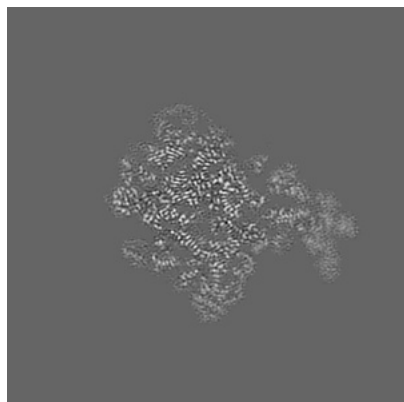


Z

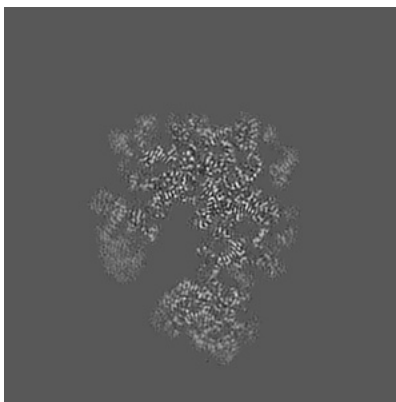
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

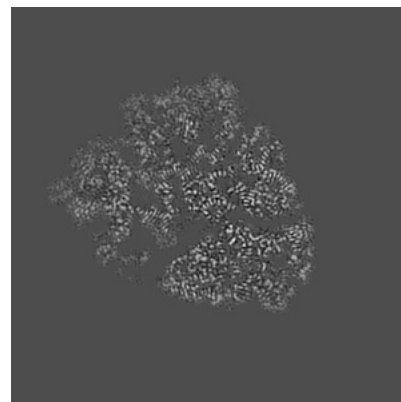
6.2.1 Primary map



X Index: 199

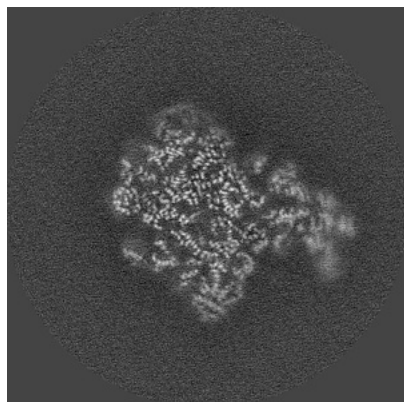


Y Index: 199

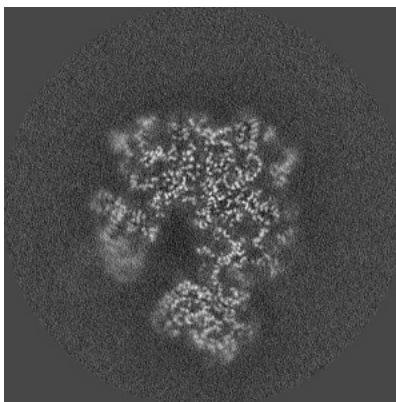


Z Index: 199

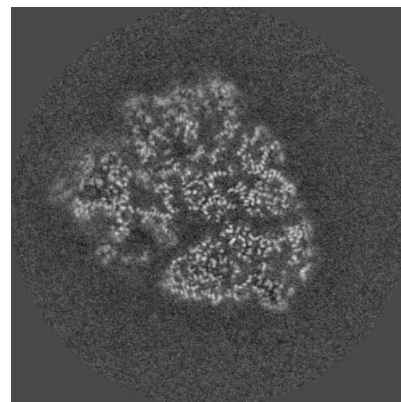
6.2.2 Raw map



X Index: 199



Y Index: 199

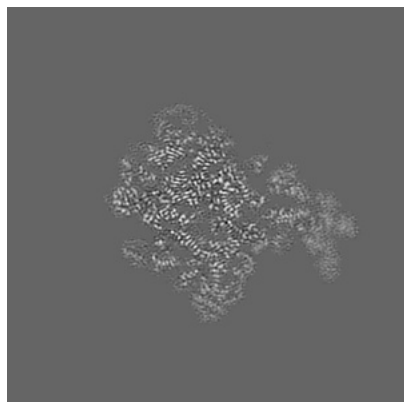


Z Index: 199

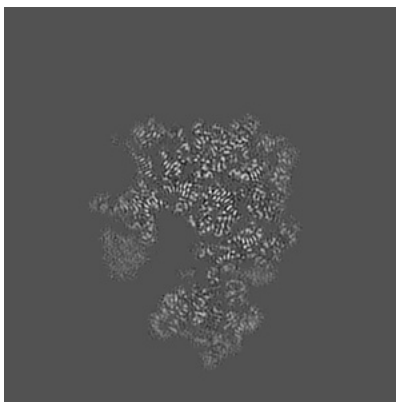
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

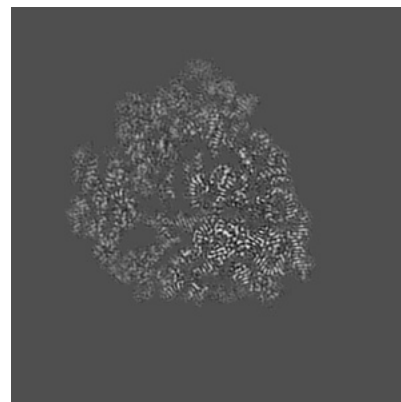
6.3.1 Primary map



X Index: 199

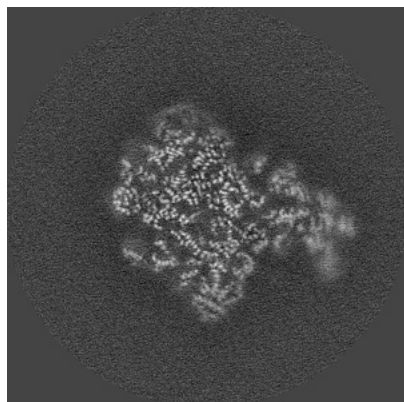


Y Index: 207

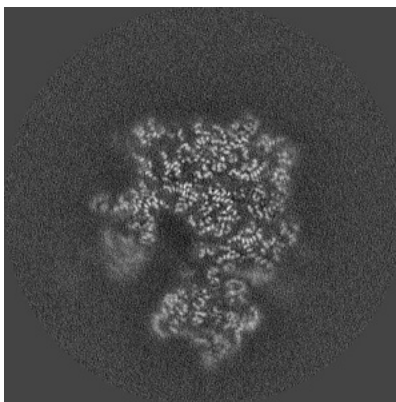


Z Index: 190

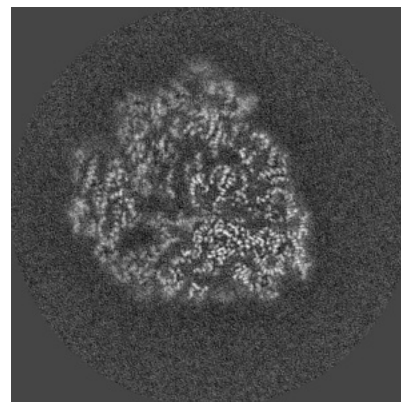
6.3.2 Raw map



X Index: 199



Y Index: 207

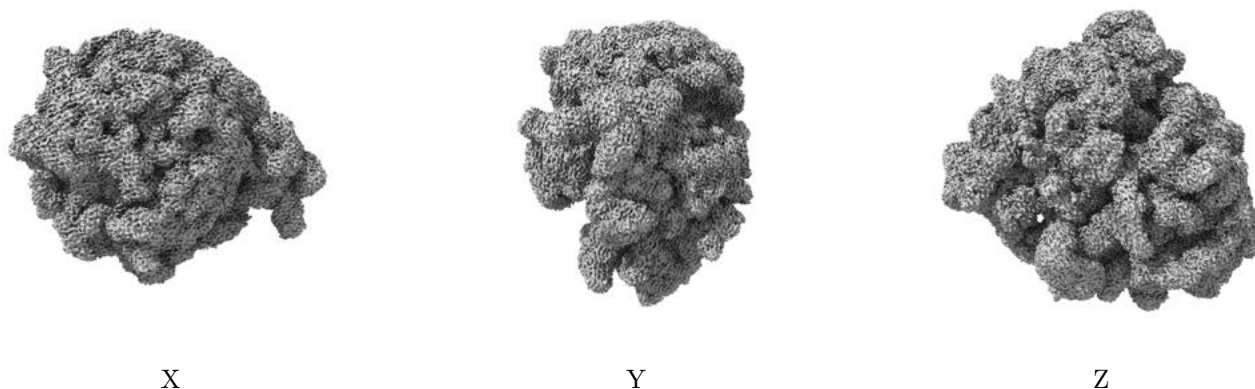


Z Index: 190

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

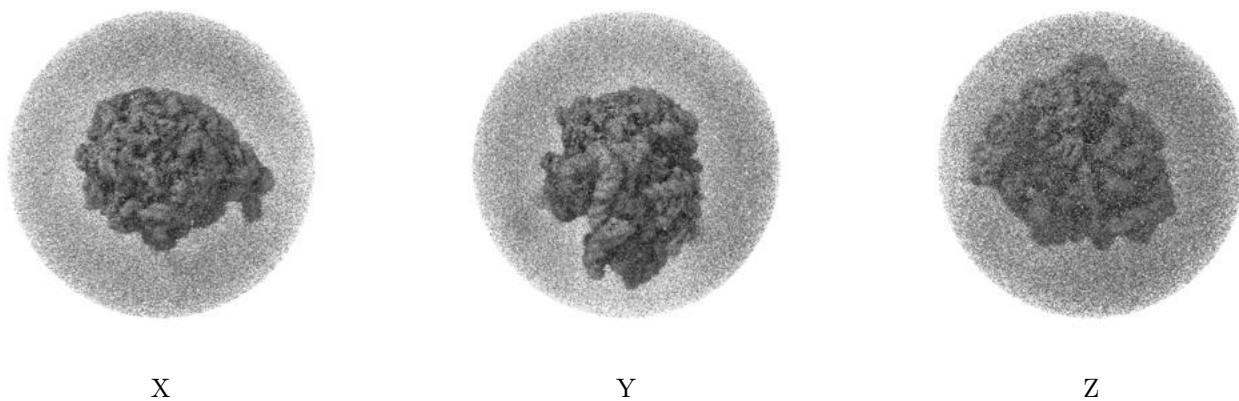
6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.00532. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map



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

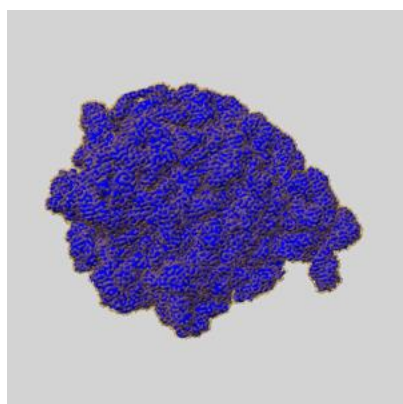
6.5 Mask visualisation [i](#)

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

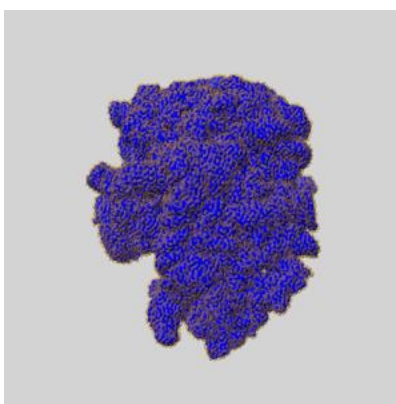
A mask typically either:

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

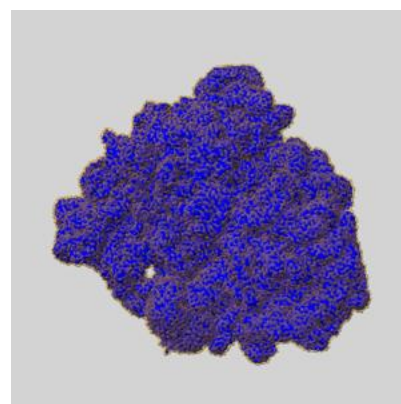
6.5.1 emd_8829_msk_1.map [i](#)



X



Y

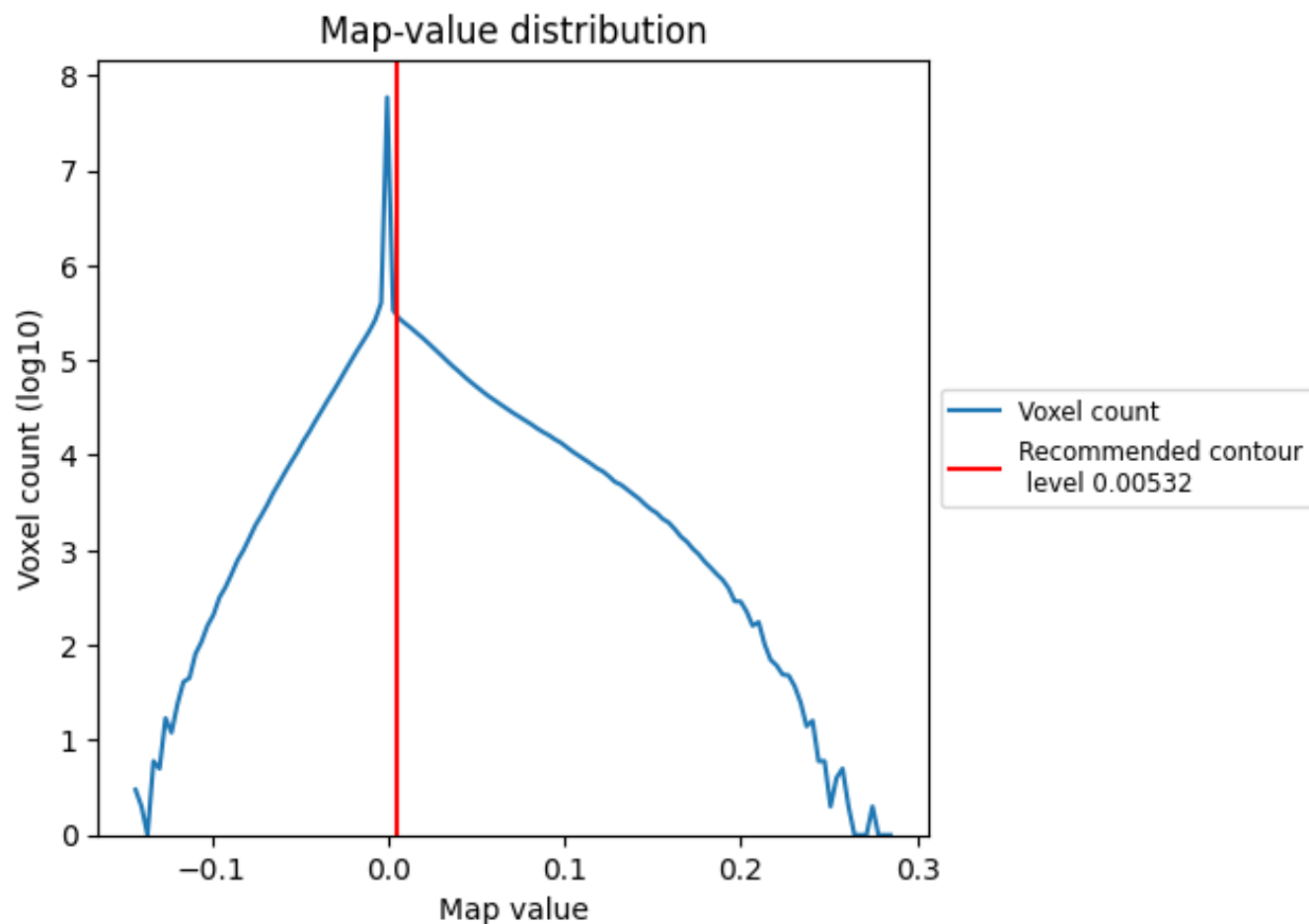


Z

7 Map analysis [i](#)

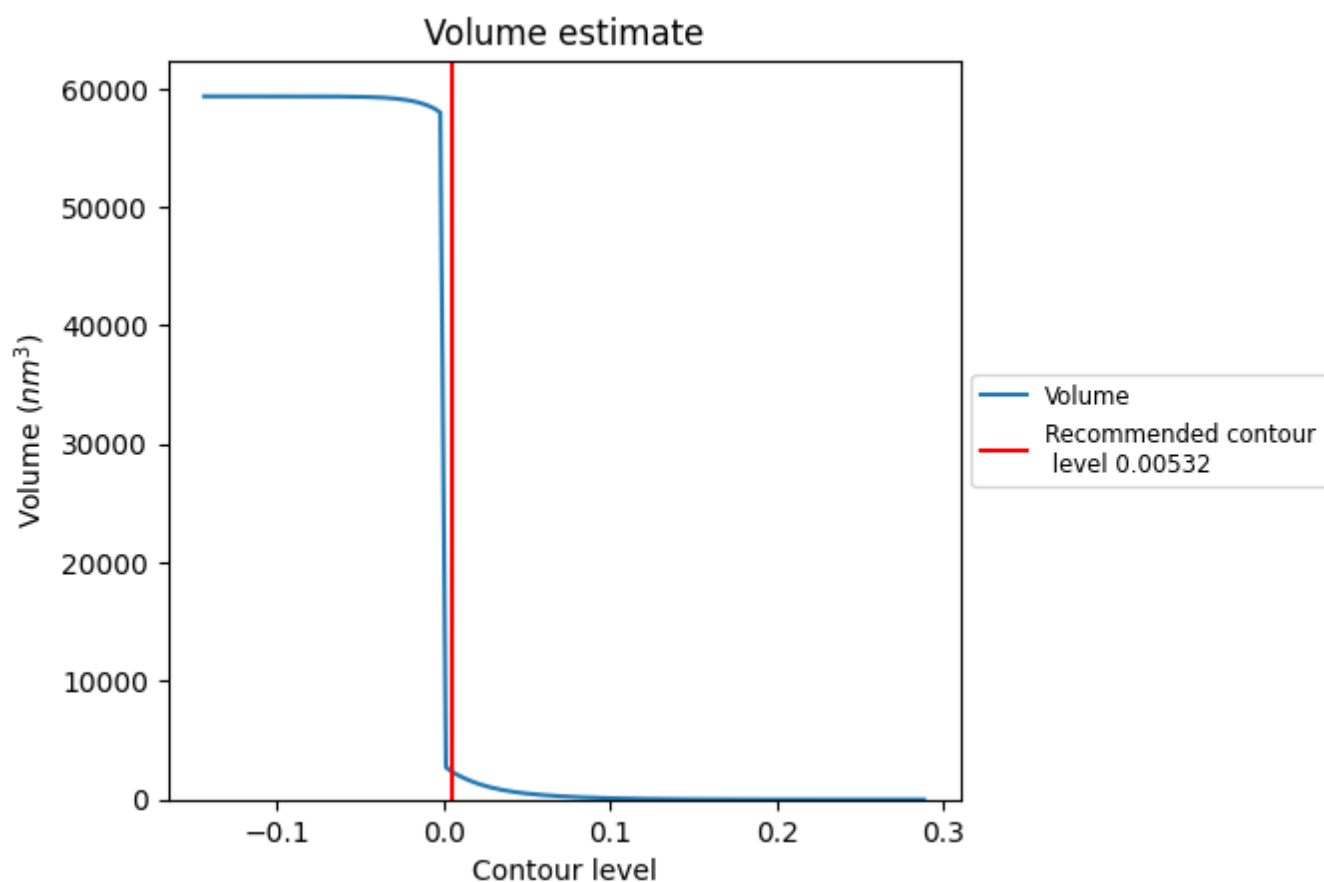
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

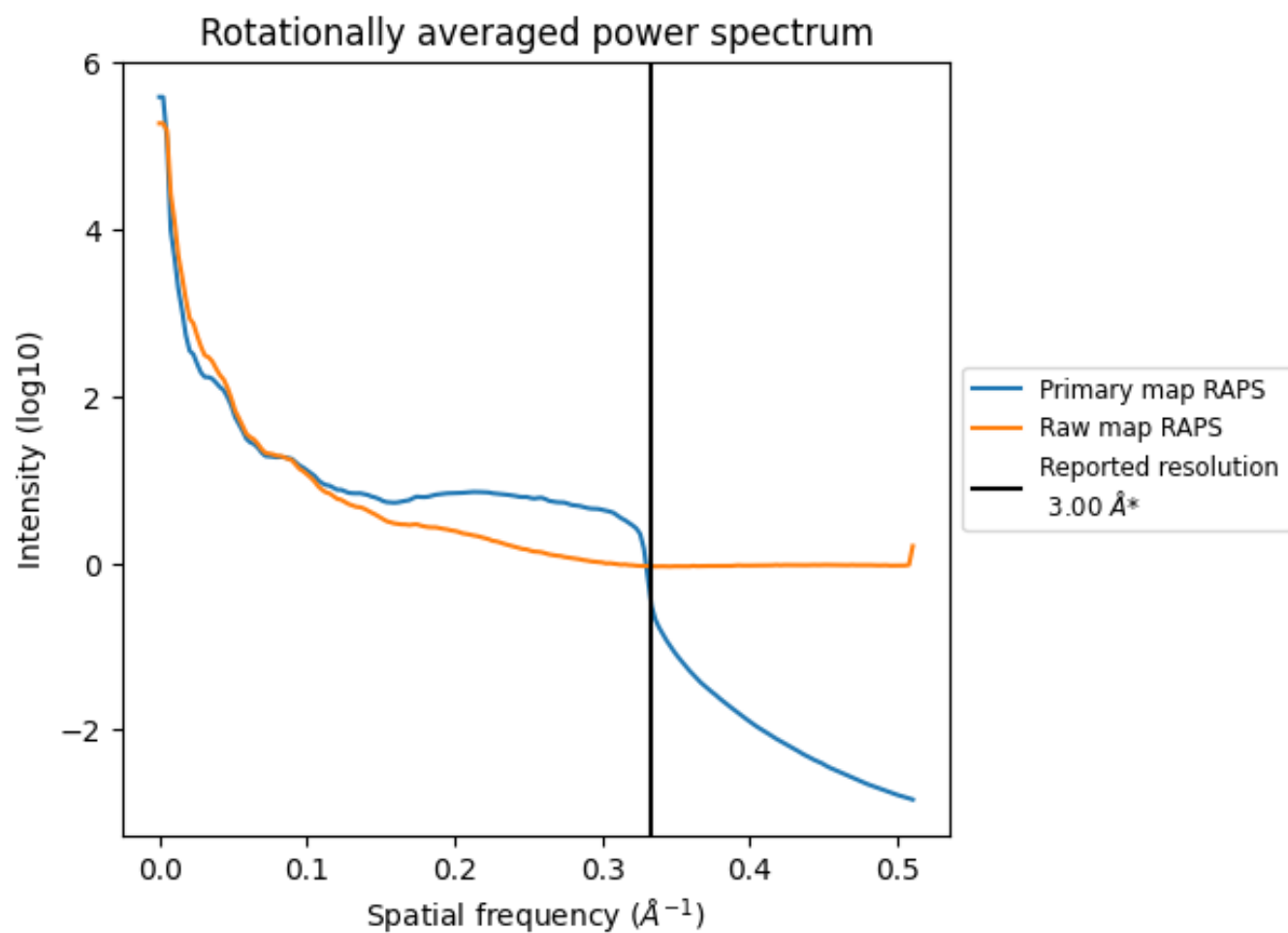
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2339 nm³; this corresponds to an approximate mass of 2113 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](#)

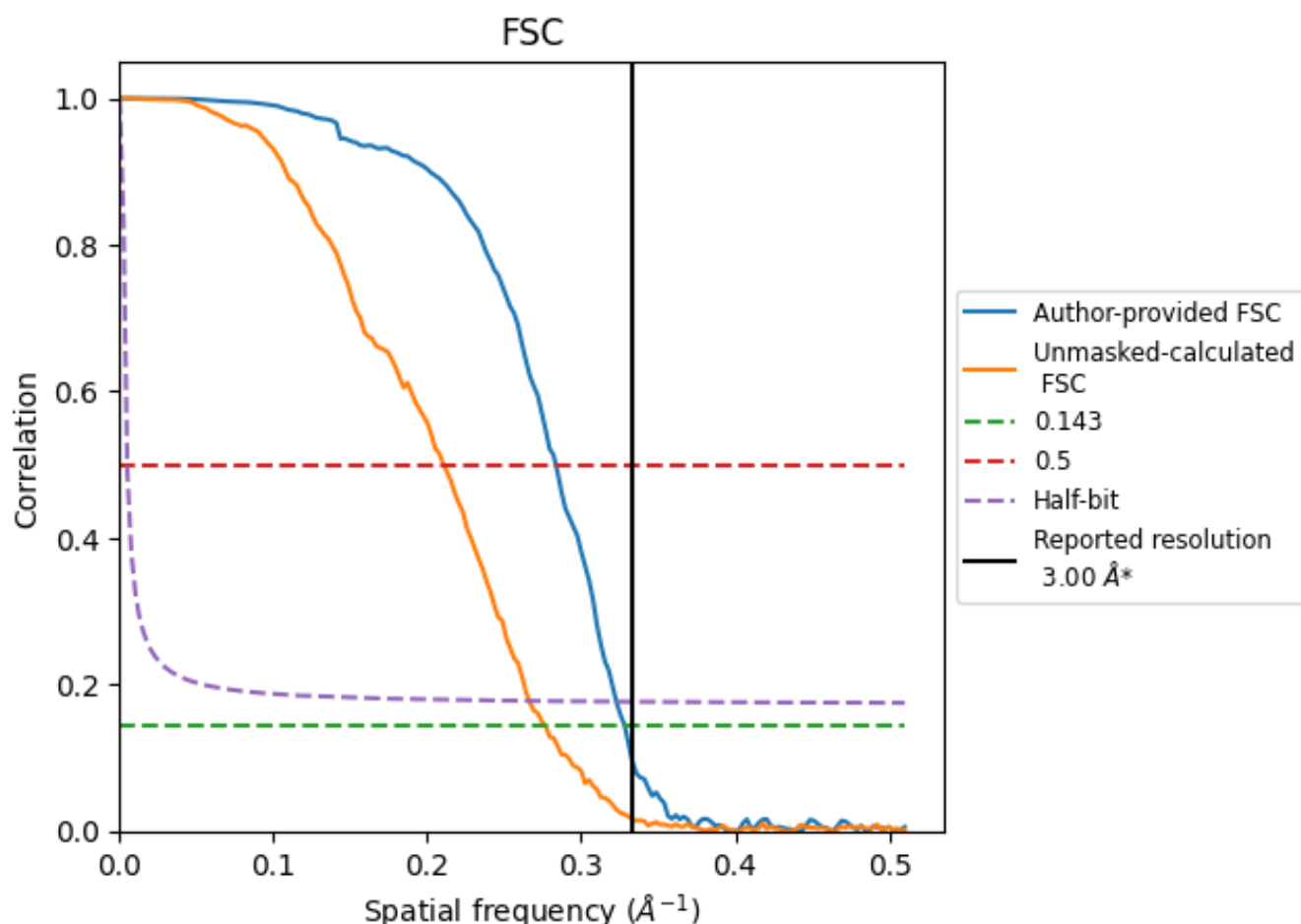


*Reported resolution corresponds to spatial frequency of 0.333 \AA^{-1}

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 0.333 Å⁻¹

8.2 Resolution estimates [i](#)

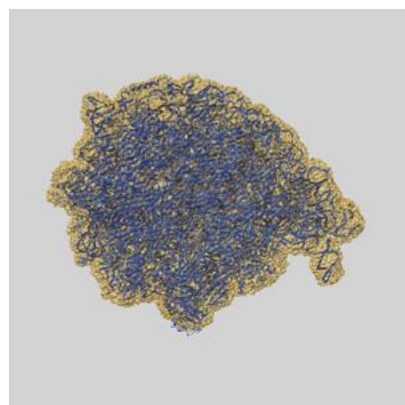
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	3.05	3.53	3.10
Unmasked-calculated*	3.61	4.75	3.76

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.61 differs from the reported value 3.0 by more than 10 %

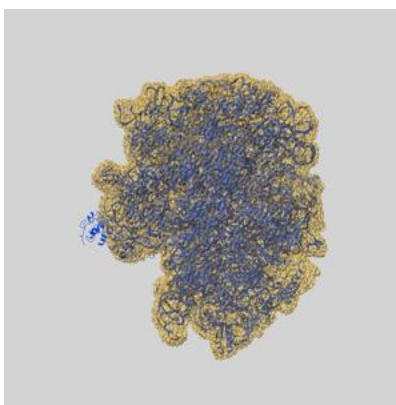
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-8829 and PDB model 5WFS. Per-residue inclusion information can be found in section [3](#) on page [20](#).

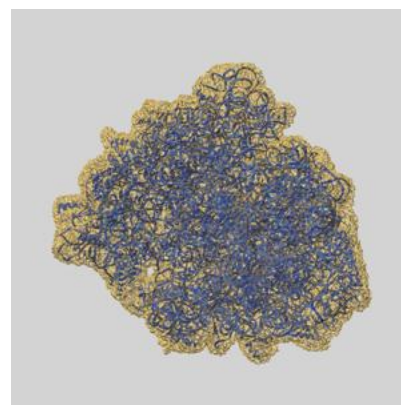
9.1 Map-model overlay [i](#)



X



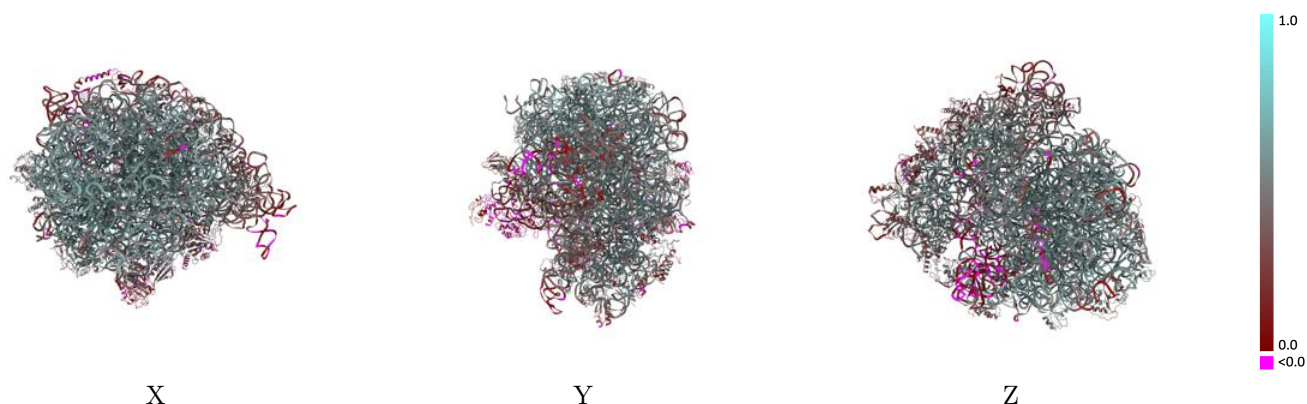
Y



Z

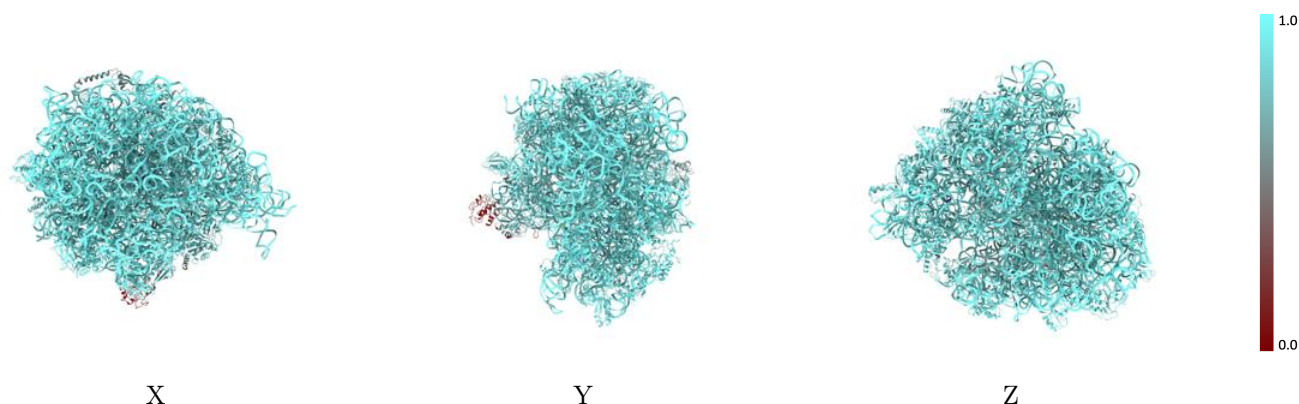
The images above show the 3D surface view of the map at the recommended contour level 0.00532 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



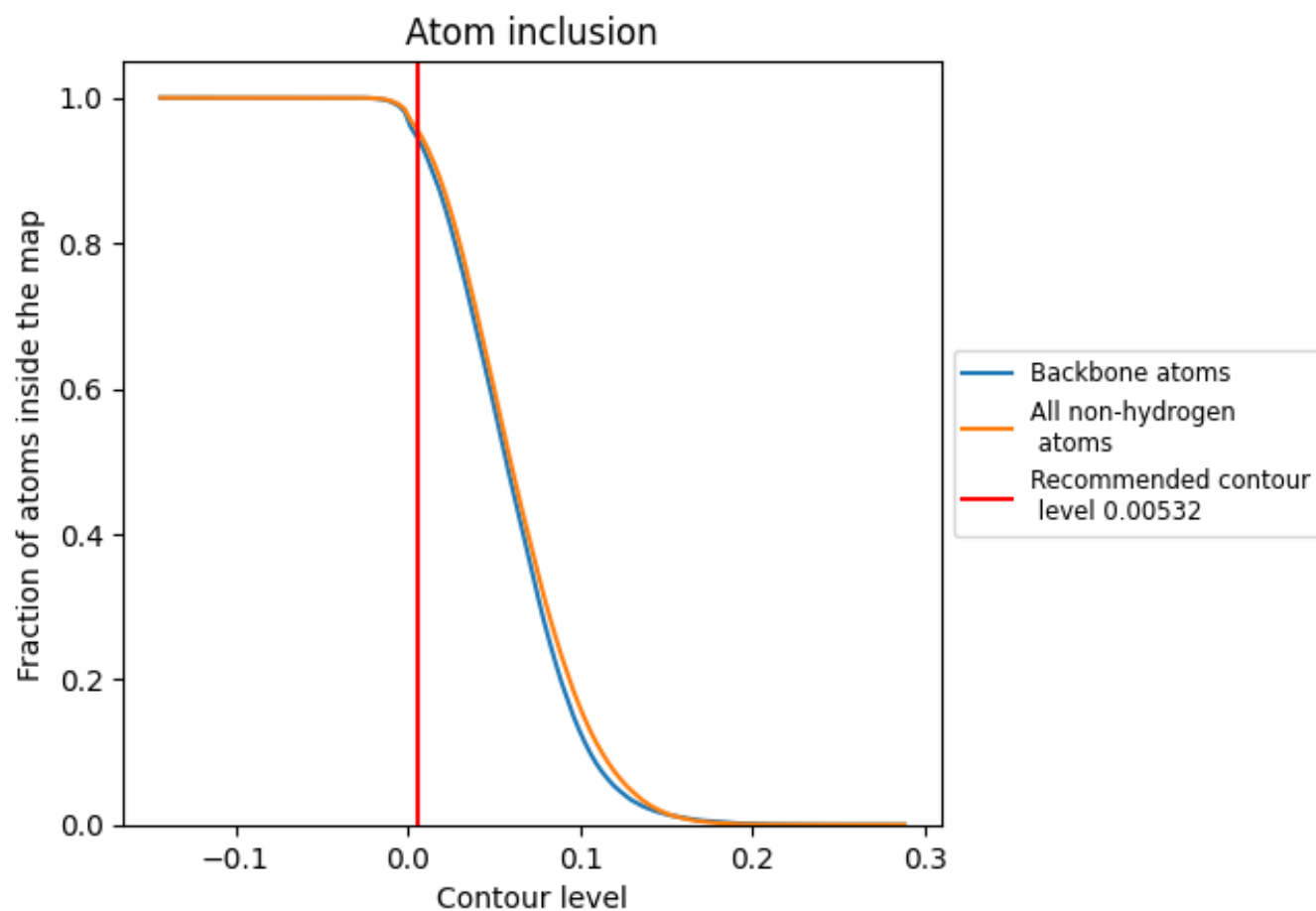
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.00532).







































































9.4 Atom inclusion ⓘ



At the recommended contour level, 95% of all backbone atoms, 96% 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 (0.00532) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9570	 0.4750
0	 0.9620	 0.5080
1	 0.9242	 0.4640
2	 0.9884	 0.5860
3	 0.9837	 0.5760
4	 0.9521	 0.4940
5	 0.1116	 -0.0200
6	 0.8885	 0.3120
A	 0.9874	 0.5350
B	 0.9935	 0.5140
C	 0.9742	 0.5550
D	 0.9661	 0.5260
E	 0.9689	 0.5080
F	 0.9359	 0.4310
G	 0.9366	 0.3790
H	 0.7354	 0.2180
I	 0.6194	 0.0210
J	 0.9652	 0.5270
K	 0.9518	 0.5180
L	 0.9645	 0.5170
M	 0.9693	 0.5180
N	 0.9858	 0.5530
O	 0.9676	 0.4480
P	 0.9572	 0.5080
Q	 0.9564	 0.5500
R	 0.9393	 0.4830
S	 0.9516	 0.5230
T	 0.9343	 0.4560
U	 0.9452	 0.4450
V	 0.9489	 0.4600
W	 0.9641	 0.5480
X	 0.9551	 0.5170
Y	 0.9378	 0.4430
Z	 0.9645	 0.5020
a	 0.9870	 0.4800



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Chain	Atom inclusion	Q-score
b	 0.8955	 0.3360
c	 0.9423	 0.4360
d	 0.8994	 0.2860
e	 0.9533	 0.4820
f	 0.9234	 0.4070
g	 0.9161	 0.3700
h	 0.9490	 0.4840
i	 0.9224	 0.3850
j	 0.8962	 0.3370
k	 0.9456	 0.4300
l	 0.9084	 0.4010
m	 0.9441	 0.4280
n	 0.9499	 0.4390
o	 0.9406	 0.4440
p	 0.8931	 0.2610
q	 0.9146	 0.3710
r	 0.8969	 0.4030
s	 0.9517	 0.4260
t	 0.9200	 0.3290
u	 0.8205	 0.2580
v	 0.9721	 0.4880
w	 0.7454	 0.0740
x	 0.9842	 0.4960
y	 0.9162	 0.2870
z	 0.8294	 0.2520