



wwPDB EM Validation Summary Report ⓘ

Feb 3, 2025 – 09:41 PM EST

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.dev113
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

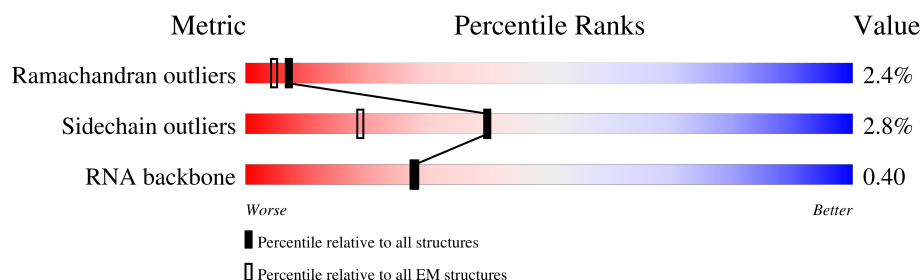
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 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	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	A	2903	
2	B	120	
3	C	271	
4	D	208	
5	E	200	
6	F	177	
7	G	174	
8	H	149	


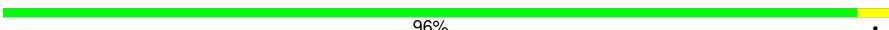
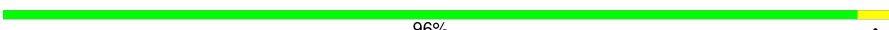
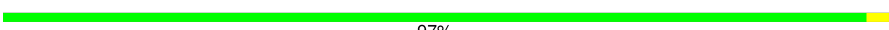






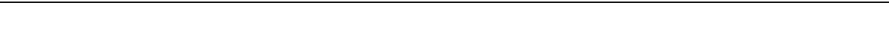

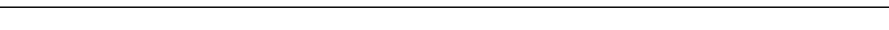
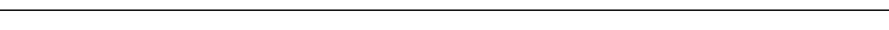
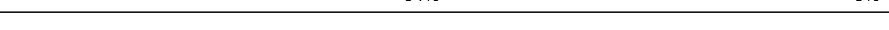
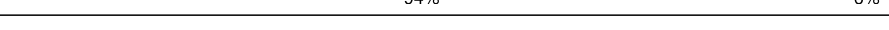
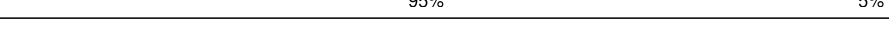
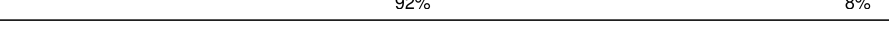

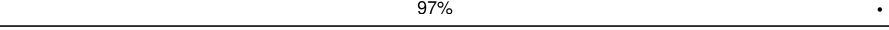
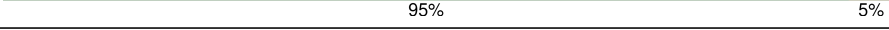




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Mol	Chain	Length	Quality of chain
9	I	141	<div> <div>24%</div> <div>92%</div> <div>7%</div> </div>
10	J	141	<div> <div>98%</div> </div>
11	K	122	<div> <div>94%</div> <div>6%</div> </div>
12	L	143	<div> <div>90%</div> <div>9%</div> </div>
13	M	136	<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		

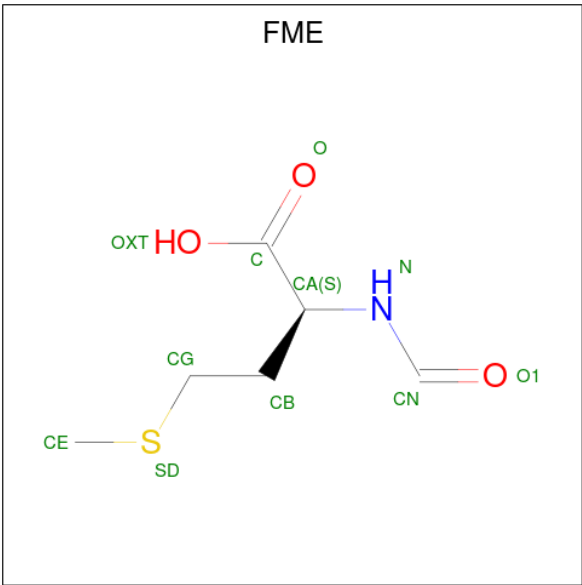
- Molecule 58 is a protein called Elongation factor Tu 2.

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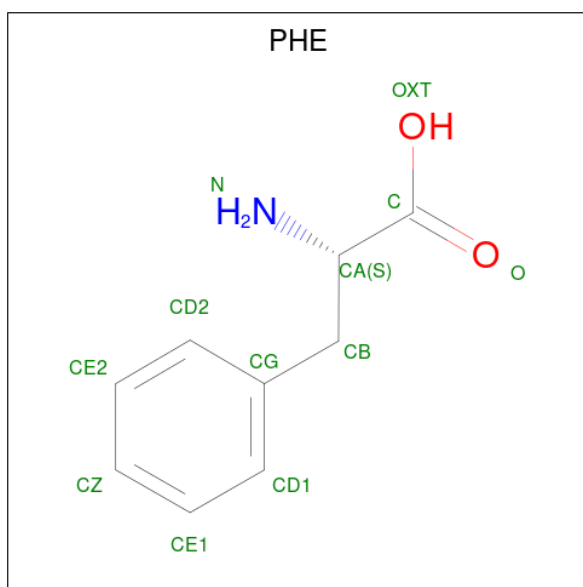
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Mol	Chain	Residues	Atoms		AltConf
60	2	1	Total 1	Mg 1	0
60	a	392	Total 392	Mg 392	0
60	d	1	Total 1	Mg 1	0
60	e	1	Total 1	Mg 1	0
60	i	1	Total 1	Mg 1	0
60	u	1	Total 1	Mg 1	0
60	v	6	Total 6	Mg 6	0
60	w	2	Total 2	Mg 2	0
60	x	1	Total 1	Mg 1	0
60	y	2	Total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

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

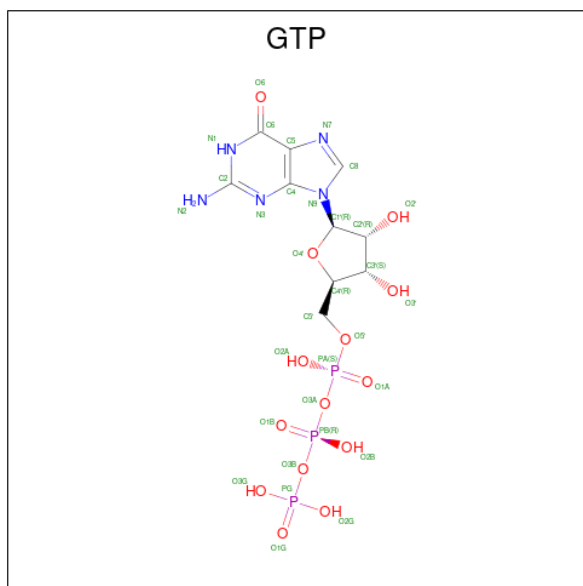
Mol	Chain	Residues	Atoms		AltConf
61	A	6	Total 6	K 6	0
61	a	1	Total 1	K 1	0

- 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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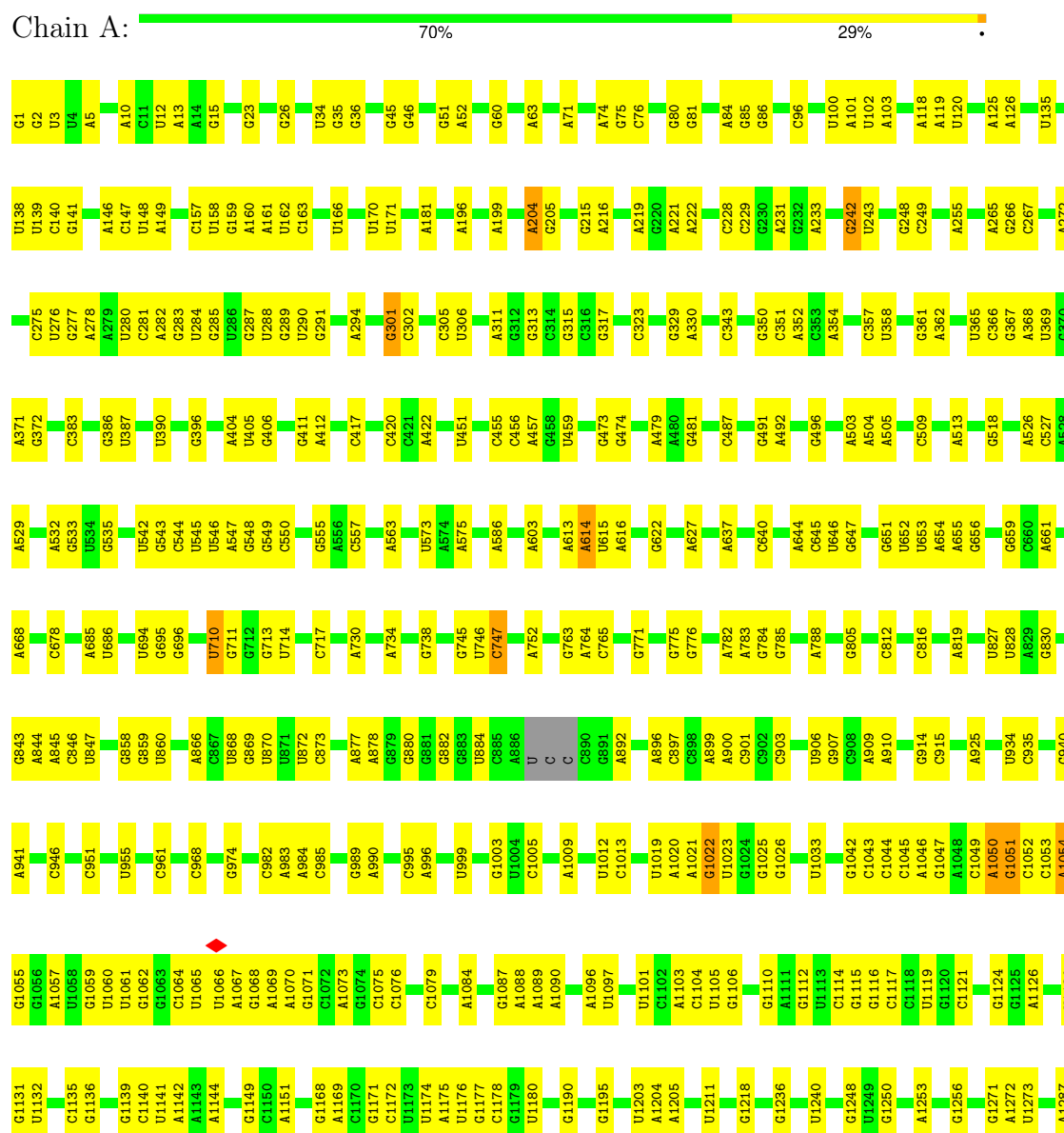
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Mol	Chain	Residues	Atoms		AltConf
64	j	1	Total 1	O 1	0
64	l	2	Total 2	O 2	0
64	m	1	Total 1	O 1	0
64	o	1	Total 1	O 1	0
64	q	1	Total 1	O 1	0
64	s	3	Total 3	O 3	0
64	u	1	Total 1	O 1	0
64	v	3	Total 3	O 3	0
64	w	1	Total 1	O 1	0
64	x	1	Total 1	O 1	0
64	y	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	G2435	U2320	A2191	C2069	U1939	G1835	A1679	G1540	C1437	A2836	U2724	G2436	U2321	A2192	C2070	U1940	G1836	A1679	G1541	C1437	A2837	U2725	G2437	U2322	A2193	C2072	U1941	G1837	A1680	G1542	C1438	A2838	U2726	G2438	U2323	A2194	C2073	U1942	G1838	A1681	G1543	C1439	A2839	U2727	G2439	U2324	A2195	C2074	U1943	G1839	A1682	G1544	C1440	A2840	U2728	G2440	U2325	A2196	C2075	U1944	G1840	A1683	G1545	C1441	A2841	U2729	G2441	U2326	A2197	C2076	U1945	G1841	A1684	G1546	C1442	A2842	U2730	G2442	U2327	A2198	C2077	U1946	G1842	A1685	G1547	C1443	A2843	U2731	G2443	U2328	A2199	C2078	U1947	G1843	A1686	G1548	C1444	A2844	U2732	G2444	U2329	A2200	C2079	U1948	G1844	A1687	G1549	C1445	A2845	U2733	G2445	U2330	A2201	C2080	U1949	G1845	A1688	G1550	C1446	A2846	U2734	G2446	U2331	A2202	C2081	U1950	G1846	A1689	G1551	C1447	A2847	U2735	G2447	U2332	A2203	C2082	U1951	G1847	A1690	G1552	C1448	A2848	U2736	G2448	U2333	A2204	C2083	U1952	G1848	A1691	G1553	C1449	A2849	U2737	G2449	U2334	A2205	C2084	U1953	G1849	A1692	G1554	C1450	A2850	U2738	G2450	U2335	A2206	C2085	U1954	G1850	A1693	G1555	C1451	A2851	U2739	G2451	U2336	A2207	C2086	U1955	G1851	A1694	G1556	C1452	A2852	U2740	G2452	U2337	A2208	C2087	U1956	G1852	A1695	G1557	C1453	A2853	U2741	G2453	U2338	A2209	C2088	U1957	G1853	A1696	G1558	C1454	A2854	U2742	G2454	U2339	A2210	C2089	U1958	G1854	A1697	G1559	C1455	A2855	U2743	G2455	U2340	A2211	C2090	U1959	G1855	A1698	G1560	C1456	A2856	U2744	G2456	U2341	A2212	C2091	U1960	G1856	A1699	G1561	C1457	A2857	U2745	G2457	U2342	A2213	C2092	U1961	G1857	A1700	G1562	C1458	A2858	U2746	G2458	U2343	A2214	C2093	U1962	G1858	A1701	G1563	C1459	A2859	U2747	G2459	U2344	A2215	C2094	U1963	G1859	A1702	G1564	C1460	A2860	U2748	G2460	U2345	A2216	C2095	U1964	G1860	A1703	G1565	C1461	A2861	U2749	G2461	U2346	A2217	C2096	U1965	G1861	A1704	G1566	C1462	A2862	U2750	G2462	U2347	A2218	C2097	U1966	G1862	A1705	G1567	C1463	A2863	U2751	G2463	U2348	A2219	C2098	U1967	G1863	A1706	G1568	C1464	A2864	U2752	G2464	U2349	A2220	C2099	U1968	G1864	A1707	G1569	C1465	A2865	U2753	G2465	U2350	A2221	C2100	U1969	G1865	A1708	G1570	C1466	A2866	U2754	G2466	U2351	A2222	C2101	U1970	G1866	A1709	G1571	C1467	A2867	U2755	G2467	U2352	A2223	C2102	U1971	G1867	A1710	G1572	C1468	A2868	U2756	G2468	U2353	A2224	C2103	U1972	G1868	A1711	G1573	C1469	A2869	U2757	G2469	U2354	A2225	C2104	U1973	G1869	A1712	G1574	C1470	A2870	U2758	G2470	U2355	A2226	C2105	U1974	G1870	A1713	G1575	C1471	A2871	U2759	G2471	U2356	A2227	C2106	U1975	G1871	A1714	G1576	C1472	A2872	U2760	G2472	U2357	A2228	C2107	U1976	G1872	A1715	G1577	C1473	A2873	U2761	G2473	U2358	A2229	C2108	U1977	G1873	A1716	G1578	C1474	A2874	U2762	G2474	U2359	A2230	C2109	U1978	G1874	A1717	G1579	C1475	A2875	U2763	G2475	U2360	A2231	C2110	U1979	G1875	A1718	G1580	C1476	A2876	U2764	G2476	U2361	A2232	C2111	U1980	G1876	A1719	G1581	C1477	A2877	U2765	G2477	U2362	A2233	C2112	U1981	G1877	A1720	G1582	C1478	A2878	U2766	G2478	U2363	A2234	C2113	U1982	G1878	A1721	G1583	C1479	A2879	U2767	G2479	U2364	A2235	C2114	U1983	G1879	A1722	G1584	C1480	A2880	U2768	G2480	U2365	A2236	C2115	U1984	G1880	A1723	G1585	C1481	A2881	U2769	G2481	U2366	A2237	C2116	U1985	G1881	A1724	G1586	C1482	A2882	U2770	G2482	U2367	A2238	C2117	U1986	G1882	A1725	G1587	C1483	A2883	U2771	G2483	U2368	A2239	C2118	U1987	G1883	A1726	G1588	C1484	A2884	U2772	G2484	U2369	A2240	C2119	U1988	G1884	A1727	G1589	C1485	A2885	U2773	G2485	U2370	A2241	C2120	U1989	G1885	A1728	G1590	C1486	A2886	U2774	G2486	U2371	A2242	C2121	U1990	G1886	A1729	G1591	C1487	A2887	U2775	G2487	U2372	A2243	C2122	U1991	G1887	A1730	G1592	C1488	A2888	U2776	G2488	U2373	A2244	C2123	U1992	G1888	A1731	G1593	C1489	A2889	U2777	G2489	U2374	A2245	C2124	U1993	G1889	A1732	G1594	C1490	A2890	U2778	G2490	U2375	A2246	C2125	U1994	G1890	A1733	G1595	C1491	A2891	U2779	G2491	U2376	A2247	C2126	U1995	G1891	A1734	G1596	C1492	A2892	U2780	G2492	U2377	A2248	C2127	U1996	G1892	A1735	G1597	C1493	A2893	U2781	G2493	U2378	A2249	C2128	U1997	G1893	A1736	G1598	C1494	A2894	U2782	G2494	U2379	A2250	C2129	U1998	G1894	A1737	G1599	C1495	A2895	U2783	G2495	U2380	A2251	C2130	U1999	G1895	A1738	G1600	C1496	A2896	U2784	G2496	U2381	A2252	C2131	U2000	G1896	A1739	G1601	C1497	A2897	U2785	G2497	U2382	A2253	C2132	U2001	G1897	A1740	G1602	C1498	A2898	U2786	G2498	U2383	A2254	C2133	U2002	G1898	A1741	G1603	C1499	A2899	U2787	G2499	U2384	A2255	C2134	U2003	G1899	A1742	G1604	C1500	A2900	U2788	G2500	U2385	A2256	C2135	U2004	G1900	A1743	G1605	C1501	A2901	U2789	G2501	U2386	A2257	C2136	U2005	G1901	A1744	G1606	C1502	A2902	U2790	G2502	U2387	A2258	C2137	U2006	G1902	A1745	G1607	C1503	A2903	U2791	G2503	U2388	A2259	C2138	U2007	G1903	A1746	G1608	C1504	A2904	U2792	G2504	U2389	A2260	C2139	U2008	G1904	A1747	G1609	C1505	A2905	U2793	G2505	U2390	A2261	C2140	U2009	G1905	A1748	G1610	C1506	A2906	U2794	G2506	U2391	A2262	C2141	U2010	G1906	A1749	G1611	C1507	A2907	U2795	G2507	U2392	A2263	C2142	U2011	G1907	A1750	G1612	C1508	A2908	U2796	G2508	U2393	A2264	C2143	U2012	G1908	A1751	G1613	C1509	A2909	U2797	G2509	U2394	A2265	C2144	U2013	G1909	A1752	G1614	C1510	A2910	U2798	G2510	U2395	A2266	C2145	U2014	G1910	A1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• 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	A64	U65	A66	G67	C70	G81	U87	C88	U89	C90	C91	U95	G96	G100
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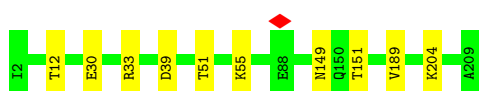
- Molecule 3: 50S ribosomal protein L2

Chain C: 96% .



- Molecule 4: 50S ribosomal protein L3

Chain D: 95% 5% .



- Molecule 5: 50S ribosomal protein L4

Chain E: 94% 6% .



- Molecule 6: 50S ribosomal protein L5

Chain F: 98% ..



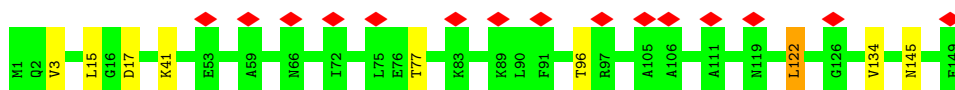
- Molecule 7: 50S ribosomal protein L6

Chain G: 99% .



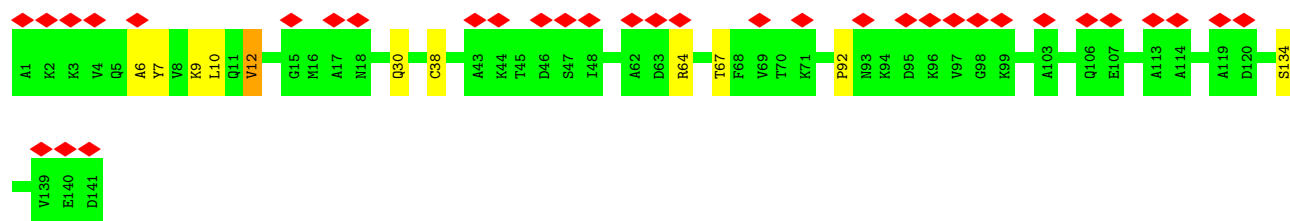
- Molecule 8: 50S ribosomal protein L9

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%



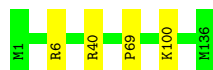
- Molecule 12: 50S ribosomal protein L15

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%



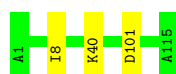
- Molecule 16: 50S ribosomal protein L19

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% .



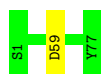
- Molecule 23: 50S ribosomal protein L27

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% .

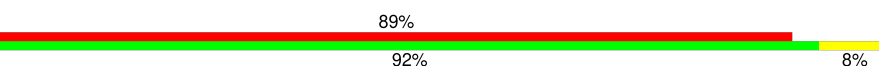


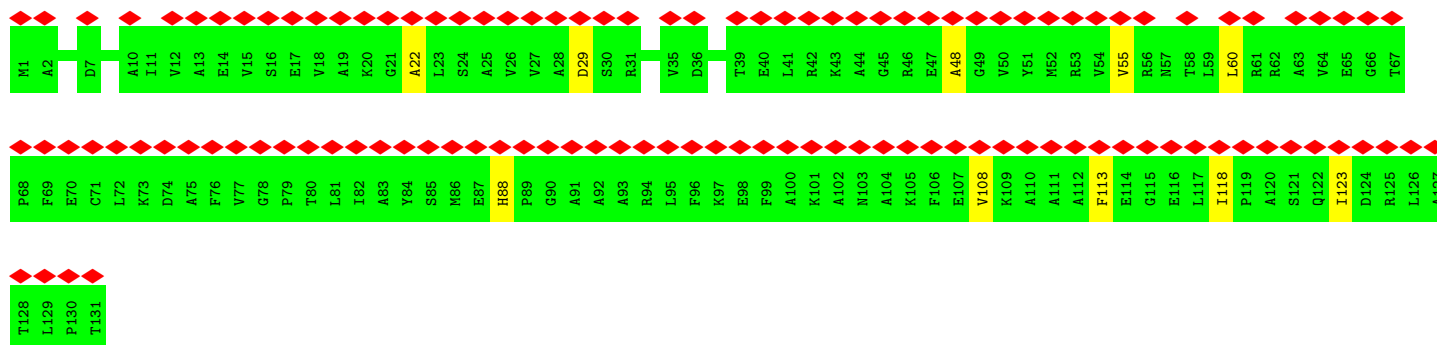
- Molecule 31: 50S ribosomal protein L36 1

Chain 4:  100%

There are no outlier residues recorded for this chain.

- Molecule 32: 50S ribosomal protein L10

Chain 5:  89%
92% 8%



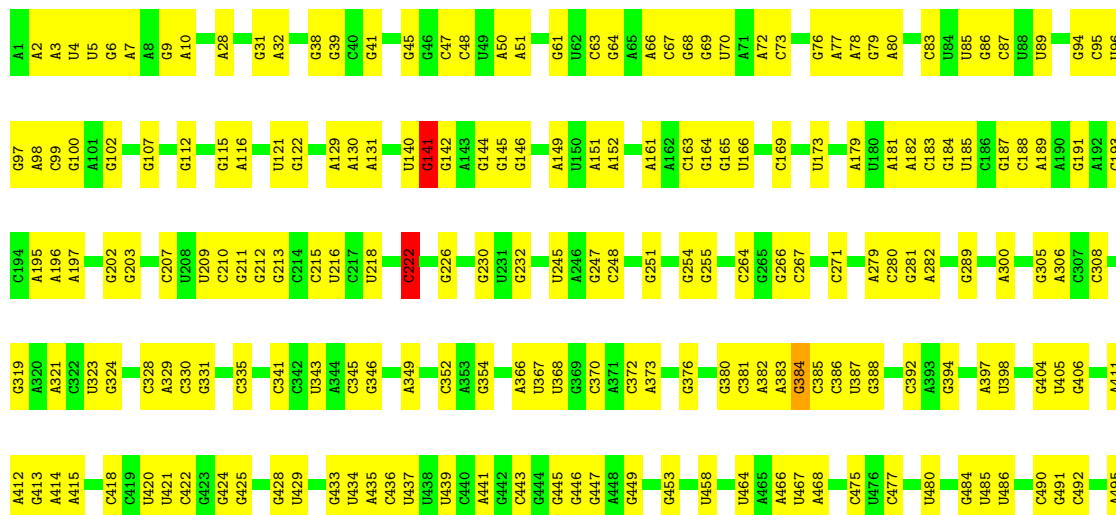
- Molecule 33: 50S ribosomal protein L31

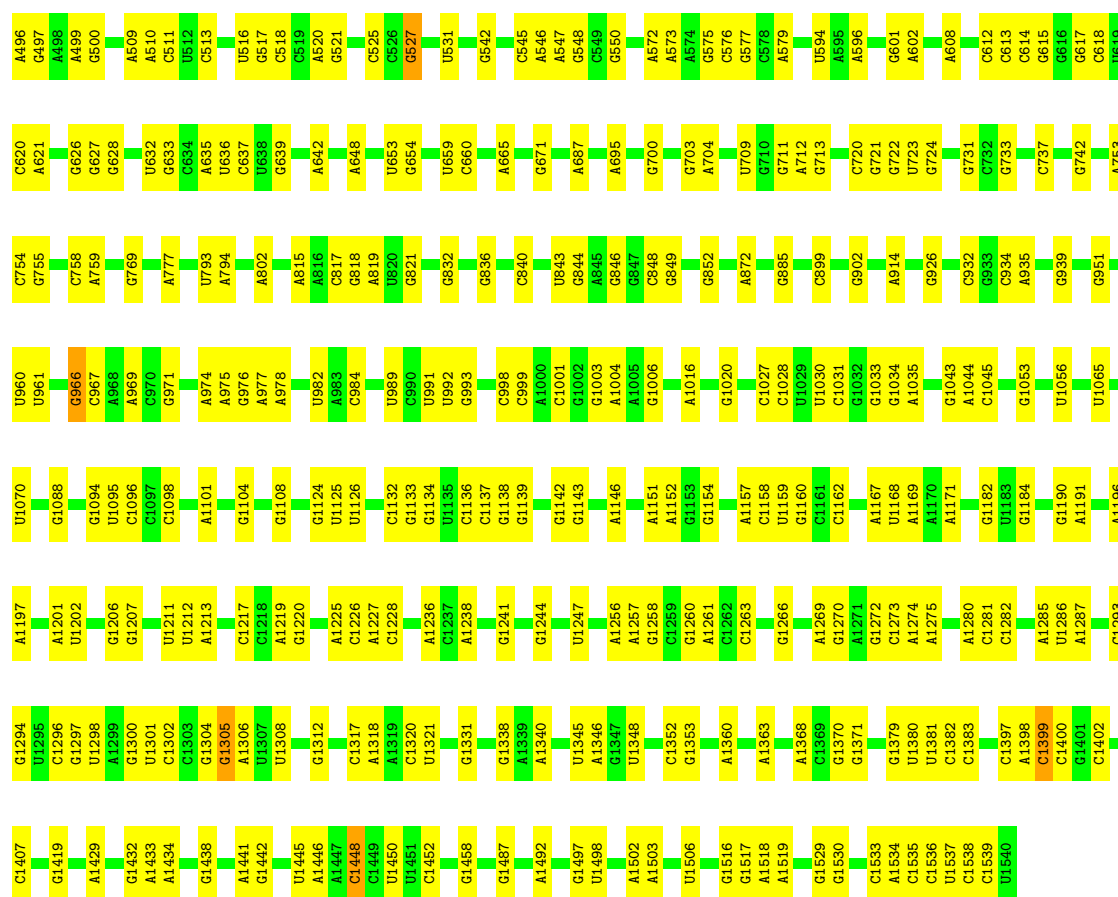
Chain 6:  95% 5%



- Molecule 34: 16S rRNA

Chain a:  67% 32%





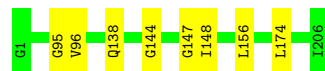
- Molecule 35: 30S ribosomal protein S2

Chain b: 96%



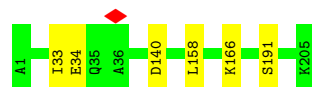
- Molecule 36: 30S ribosomal protein S3

Chain c: 96%



- Molecule 37: 30S ribosomal protein S4

Chain d: 97%



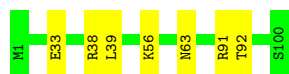
- Molecule 38: 30S ribosomal protein S5

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%

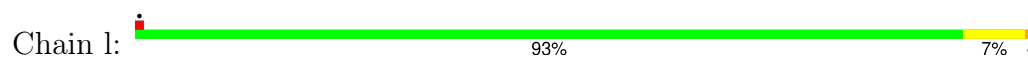


- Molecule 44: 30S ribosomal protein S11

Chain k:  93% 7%



- Molecule 45: 30S ribosomal protein S12



- Molecule 46: 30S ribosomal protein S13



- Molecule 47: 30S ribosomal protein S14



- Molecule 48: 30S ribosomal protein S15



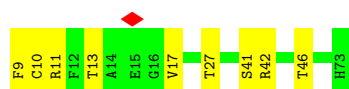
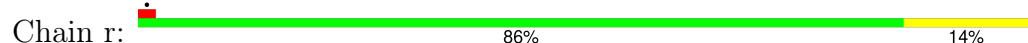
- Molecule 49: 30S ribosomal protein S16



- Molecule 50: 30S ribosomal protein S17



- Molecule 51: 30S ribosomal protein S18



- 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%



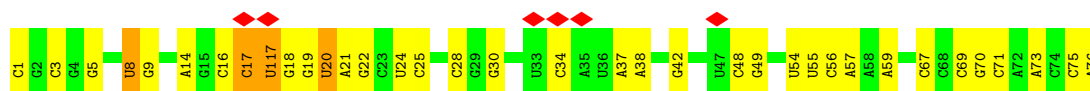
- Molecule 55: tRNA-fMet

Chain v:  66% 31% .



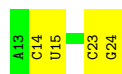
- Molecule 55: tRNA-fMet

Chain w:  8% 53% 42% 5%



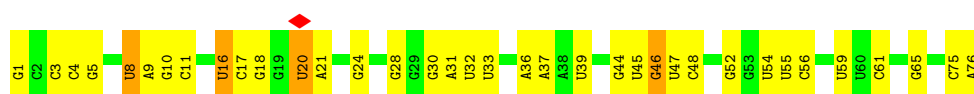
- Molecule 56: mRNA

Chain x:  67% 33%

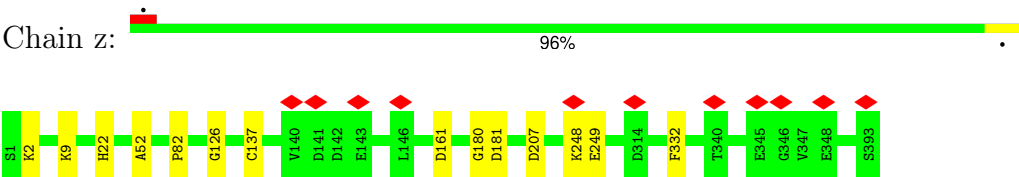


- Molecule 57: Phe-tRNA-Phe

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: H2U, GTP, 3TD, OMG, 1MG, OMU, 4OC, 6MZ, 2MA, 5MC, PSU, OMC, MA6, K, 4SU, 7MG, 2MG, FME, UR3, MIA, MG, 5MU

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%)	12	44
4	D	206/208 (99%)	190 (92%)	15 (7%)	1 (0%)	25	61

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	E	198/200 (99%)	178 (90%)	18 (9%)	2 (1%)	13	46
6	F	175/177 (99%)	157 (90%)	16 (9%)	2 (1%)	12	44
7	G	172/174 (99%)	158 (92%)	14 (8%)	0	100	100
8	H	147/149 (99%)	128 (87%)	15 (10%)	4 (3%)	4	22
9	I	139/141 (99%)	109 (78%)	23 (16%)	7 (5%)	1	10
10	J	139/141 (99%)	130 (94%)	8 (6%)	1 (1%)	19	54
11	K	120/122 (98%)	106 (88%)	10 (8%)	4 (3%)	3	18
12	L	141/143 (99%)	117 (83%)	18 (13%)	6 (4%)	2	13
13	M	134/136 (98%)	128 (96%)	5 (4%)	1 (1%)	19	54
14	N	117/119 (98%)	101 (86%)	14 (12%)	2 (2%)	7	33
15	O	114/116 (98%)	105 (92%)	8 (7%)	1 (1%)	14	49
16	P	112/114 (98%)	99 (88%)	12 (11%)	1 (1%)	14	49
17	Q	113/115 (98%)	111 (98%)	2 (2%)	0	100	100
18	R	100/102 (98%)	85 (85%)	12 (12%)	3 (3%)	3	20
19	S	107/109 (98%)	100 (94%)	6 (6%)	1 (1%)	14	49
20	T	90/92 (98%)	81 (90%)	7 (8%)	2 (2%)	5	27
21	U	100/102 (98%)	87 (87%)	9 (9%)	4 (4%)	2	14
22	V	90/92 (98%)	86 (96%)	3 (3%)	1 (1%)	12	44
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%)	7	33
26	Z	54/56 (96%)	51 (94%)	3 (6%)	0	100	100
27	0	53/55 (96%)	44 (83%)	8 (15%)	1 (2%)	6	31
28	1	49/51 (96%)	43 (88%)	6 (12%)	0	100	100
29	2	43/45 (96%)	40 (93%)	2 (5%)	1 (2%)	5	26
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	4
33	6	64/66 (97%)	58 (91%)	4 (6%)	2 (3%)	3	19
35	b	216/218 (99%)	186 (86%)	25 (12%)	5 (2%)	5	26
36	c	204/206 (99%)	183 (90%)	15 (7%)	6 (3%)	3	20

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
37	d	203/205 (99%)	183 (90%)	17 (8%)	3 (2%)	8	36
38	e	156/157 (99%)	133 (85%)	21 (14%)	2 (1%)	10	39
39	f	98/100 (98%)	85 (87%)	9 (9%)	4 (4%)	2	13
40	g	149/151 (99%)	131 (88%)	11 (7%)	7 (5%)	2	11
41	h	127/129 (98%)	116 (91%)	11 (9%)	0	100	100
42	i	125/127 (98%)	97 (78%)	24 (19%)	4 (3%)	3	19
43	j	96/98 (98%)	73 (76%)	18 (19%)	5 (5%)	1	9
44	k	114/116 (98%)	97 (85%)	11 (10%)	6 (5%)	1	9
45	l	119/121 (98%)	93 (78%)	19 (16%)	7 (6%)	1	7
46	m	113/115 (98%)	102 (90%)	9 (8%)	2 (2%)	7	32
47	n	99/101 (98%)	84 (85%)	10 (10%)	5 (5%)	1	10
48	o	86/88 (98%)	79 (92%)	4 (5%)	3 (4%)	3	16
49	p	80/82 (98%)	70 (88%)	8 (10%)	2 (2%)	4	24
50	q	78/80 (98%)	67 (86%)	7 (9%)	4 (5%)	1	10
51	r	63/65 (97%)	54 (86%)	6 (10%)	3 (5%)	2	11
52	s	77/79 (98%)	67 (87%)	10 (13%)	0	100	100
53	t	83/85 (98%)	77 (93%)	4 (5%)	2 (2%)	5	25
54	u	63/65 (97%)	41 (65%)	12 (19%)	10 (16%)	0	0
58	z	391/393 (100%)	357 (91%)	22 (6%)	12 (3%)	3	19
All	All	6219/6322 (98%)	5486 (88%)	581 (9%)	152 (2%)	7	25

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%)	25	59
4	D	163/163 (100%)	154 (94%)	9 (6%)	18	50
5	E	164/164 (100%)	154 (94%)	10 (6%)	15	46
6	F	148/148 (100%)	145 (98%)	3 (2%)	50	78
7	G	135/135 (100%)	133 (98%)	2 (2%)	60	83
8	H	114/114 (100%)	108 (95%)	6 (5%)	19	51
9	I	109/109 (100%)	104 (95%)	5 (5%)	23	56
10	J	115/115 (100%)	113 (98%)	2 (2%)	56	81
11	K	103/103 (100%)	100 (97%)	3 (3%)	37	70
12	L	102/102 (100%)	93 (91%)	9 (9%)	8	31
13	M	109/109 (100%)	106 (97%)	3 (3%)	38	70
14	N	99/99 (100%)	95 (96%)	4 (4%)	27	61
15	O	86/86 (100%)	86 (100%)	0	100	100
16	P	99/99 (100%)	98 (99%)	1 (1%)	73	88
17	Q	88/88 (100%)	85 (97%)	3 (3%)	32	66
18	R	84/84 (100%)	82 (98%)	2 (2%)	44	74
19	S	92/92 (100%)	91 (99%)	1 (1%)	70	87
20	T	79/79 (100%)	76 (96%)	3 (4%)	28	62
21	U	83/83 (100%)	81 (98%)	2 (2%)	44	74
22	V	77/77 (100%)	76 (99%)	1 (1%)	65	85
23	W	57/57 (100%)	55 (96%)	2 (4%)	31	65
24	X	67/67 (100%)	66 (98%)	1 (2%)	60	83
25	Y	55/55 (100%)	54 (98%)	1 (2%)	54	80
26	Z	47/47 (100%)	47 (100%)	0	100	100
27	0	46/46 (100%)	45 (98%)	1 (2%)	47	76
28	1	46/46 (100%)	46 (100%)	0	100	100
29	2	37/37 (100%)	36 (97%)	1 (3%)	40	71
30	3	51/51 (100%)	49 (96%)	2 (4%)	27	61
31	4	34/34 (100%)	34 (100%)	0	100	100
32	5	100/100 (100%)	99 (99%)	1 (1%)	73	88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
33	6	59/59 (100%)	58 (98%)	1 (2%)	56	81
35	b	180/180 (100%)	177 (98%)	3 (2%)	56	81
36	c	170/170 (100%)	168 (99%)	2 (1%)	67	86
37	d	172/172 (100%)	169 (98%)	3 (2%)	56	81
38	e	120/119 (101%)	115 (96%)	5 (4%)	25	59
39	f	87/87 (100%)	84 (97%)	3 (3%)	32	66
40	g	124/124 (100%)	119 (96%)	5 (4%)	27	61
41	h	104/104 (100%)	102 (98%)	2 (2%)	52	79
42	i	105/105 (100%)	101 (96%)	4 (4%)	28	62
43	j	86/86 (100%)	85 (99%)	1 (1%)	67	86
44	k	89/89 (100%)	87 (98%)	2 (2%)	47	76
45	l	102/102 (100%)	99 (97%)	3 (3%)	37	70
46	m	93/93 (100%)	91 (98%)	2 (2%)	47	76
47	n	83/83 (100%)	82 (99%)	1 (1%)	67	86
48	o	76/76 (100%)	74 (97%)	2 (3%)	41	72
49	p	65/65 (100%)	63 (97%)	2 (3%)	35	68
50	q	74/74 (100%)	72 (97%)	2 (3%)	40	71
51	r	56/56 (100%)	50 (89%)	6 (11%)	5	22
52	s	70/70 (100%)	68 (97%)	2 (3%)	37	70
53	t	65/65 (100%)	63 (97%)	2 (3%)	35	68
54	u	55/55 (100%)	53 (96%)	2 (4%)	30	64
58	z	325/325 (100%)	323 (99%)	2 (1%)	84	93
All	All	5165/5164 (100%)	5021 (97%)	144 (3%)	40	70

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
1	6MZ	A	2030	1	17,25,26	1.06	1 (5%)	15,36,39	2.38	5 (33%)
55	4SU	w	8	55	18,21,22	1.81	5 (27%)	25,30,33	2.22	5 (20%)
1	2MG	A	1835	1	18,26,27	1.01	2 (11%)	16,38,41	1.25	3 (18%)
57	MIA	y	37	57	24,31,32	2.37	6 (25%)	22,44,47	2.61	8 (36%)
1	PSU	A	2605	1,60	18,21,22	1.42	2 (11%)	21,30,33	2.21	4 (19%)
1	2MG	A	2445	1	18,26,27	1.07	2 (11%)	16,38,41	1.48	3 (18%)
1	OMU	A	2552	1,60	19,22,23	1.39	2 (10%)	25,31,34	2.25	8 (32%)
55	H2U	w	20	55	18,21,22	0.82	1 (5%)	19,30,33	1.58	2 (10%)
57	PSU	y	32	57	18,21,22	1.36	2 (11%)	21,30,33	2.05	5 (23%)
57	5MU	y	54	57	19,22,23	1.41	4 (21%)	27,32,35	2.12	8 (29%)
57	PSU	y	55	57	18,21,22	1.40	2 (11%)	21,30,33	2.05	5 (23%)
34	2MG	a	1207	34,60	18,26,27	0.99	0	16,38,41	3.01	4 (25%)
1	PSU	A	2504	1	18,21,22	1.39	2 (11%)	21,30,33	1.94	4 (19%)
55	PSU	w	55	55	18,21,22	1.34	2 (11%)	21,30,33	2.06	5 (23%)
34	MA6	a	1519	34	19,26,27	1.37	4 (21%)	18,38,41	2.38	5 (27%)
34	2MG	a	1516	34	18,26,27	0.98	1 (5%)	16,38,41	1.79	5 (31%)
34	7MG	a	527	34	23,26,27	1.45	4 (17%)	27,39,42	2.48	7 (25%)
34	5MC	a	967	34	19,22,23	1.84	2 (10%)	26,32,35	1.26	3 (11%)
55	5MU	v	54	55	19,22,23	1.49	5 (26%)	27,32,35	1.91	8 (29%)
1	PSU	A	2580	1	18,21,22	1.50	3 (16%)	21,30,33	2.07	5 (23%)
57	H2U	y	20	57	18,21,22	0.85	1 (5%)	19,30,33	1.48	4 (21%)
1	H2U	A	2449	1	18,21,22	1.03	2 (11%)	19,30,33	1.49	3 (15%)
1	5MC	A	747	1	19,22,23	1.84	3 (15%)	26,32,35	1.66	6 (23%)
55	PSU	v	55	60,55	18,21,22	1.38	3 (16%)	21,30,33	1.98	5 (23%)
1	1MG	A	745	1	19,26,27	1.11	1 (5%)	18,39,42	1.85	5 (27%)
57	4SU	y	8	57	18,21,22	1.81	5 (27%)	25,30,33	2.37	7 (28%)
1	PSU	A	1911	1	18,21,22	1.39	2 (11%)	21,30,33	2.08	4 (19%)
1	OMC	A	2498	1,60	19,22,23	0.88	1 (5%)	25,31,34	1.23	2 (8%)
34	MA6	a	1518	34	19,26,27	1.51	5 (26%)	18,38,41	2.64	5 (27%)
34	UR3	a	1498	34	19,22,23	1.09	2 (10%)	26,32,35	1.99	5 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	7MG	A	2069	1,60	23,26,27	1.49	4 (17%)	27,39,42	2.54	10 (37%)
57	PSU	y	39	57	18,21,22	1.45	2 (11%)	21,30,33	2.01	4 (19%)
55	5MU	w	54	55	19,22,23	1.49	4 (21%)	27,32,35	2.08	11 (40%)
34	PSU	a	516	34	18,21,22	1.44	2 (11%)	21,30,33	2.08	5 (23%)
57	7MG	y	46	57	23,26,27	1.43	4 (17%)	27,39,42	2.47	7 (25%)
1	PSU	A	955	1	18,21,22	1.41	3 (16%)	21,30,33	2.10	4 (19%)
57	H2U	y	16	57	18,21,22	0.82	1 (5%)	19,30,33	1.39	4 (21%)
1	5MU	A	1939	1	19,22,23	1.38	5 (26%)	27,32,35	2.04	8 (29%)
1	3TD	A	1915	1,60	19,22,23	7.04	13 (68%)	23,32,35	2.05	4 (17%)
1	PSU	A	1917	1	18,21,22	1.41	2 (11%)	21,30,33	2.09	4 (19%)
1	PSU	A	2457	1	18,21,22	1.55	3 (16%)	21,30,33	2.00	5 (23%)
34	2MG	a	966	34	18,26,27	0.95	1 (5%)	16,38,41	2.22	5 (31%)
34	4OC	a	1402	34,60	20,23,24	0.81	0	25,32,35	1.34	5 (20%)
1	PSU	A	746	1,60	18,21,22	1.41	3 (16%)	21,30,33	2.06	4 (19%)
1	OMG	A	2251	1,60,55	19,26,27	1.02	2 (10%)	21,38,41	1.21	3 (14%)
1	2MA	A	2503	1,60	17,25,26	1.03	1 (5%)	16,37,40	1.53	4 (25%)
34	5MC	a	1407	34	19,22,23	1.68	2 (10%)	26,32,35	1.31	4 (15%)
1	5MC	A	1962	1	19,22,23	1.49	2 (10%)	26,32,35	1.24	3 (11%)
55	H2U	v	20	55	18,21,22	0.91	1 (5%)	19,30,33	1.63	4 (21%)
55	4SU	v	7	55	18,21,22	1.75	4 (22%)	25,30,33	2.42	5 (20%)
1	6MZ	A	1618	1	17,25,26	1.07	1 (5%)	15,36,39	2.38	5 (33%)
1	PSU	A	2604	1	18,21,22	1.42	3 (16%)	21,30,33	1.99	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
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
57	MIA	y	37	57	-	5/11/33/34	0/3/3/3
1	PSU	A	2605	1,60	-	0/7/25/26	0/2/2/2
1	2MG	A	2445	1	-	2/5/27/28	0/3/3/3
1	OMU	A	2552	1,60	-	2/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
55	H2U	w	20	55	-	1/7/38/39	0/2/2/2
57	PSU	y	32	57	-	1/7/25/26	0/2/2/2
57	5MU	y	54	57	-	0/7/25/26	0/2/2/2
57	PSU	y	55	57	-	0/7/25/26	0/2/2/2
34	2MG	a	1207	34,60	-	0/5/27/28	0/3/3/3
1	PSU	A	2504	1	-	2/7/25/26	0/2/2/2
55	PSU	w	55	55	-	1/7/25/26	0/2/2/2
34	MA6	a	1519	34	-	4/7/29/30	0/3/3/3
34	2MG	a	1516	34	-	0/5/27/28	0/3/3/3
34	7MG	a	527	34	-	2/7/37/38	0/3/3/3
34	5MC	a	967	34	-	0/7/25/26	0/2/2/2
55	5MU	v	54	55	-	0/7/25/26	0/2/2/2
1	PSU	A	2580	1	-	0/7/25/26	0/2/2/2
57	H2U	y	20	57	-	2/7/38/39	0/2/2/2
1	H2U	A	2449	1	-	0/7/38/39	0/2/2/2
1	5MC	A	747	1	-	0/7/25/26	0/2/2/2
55	PSU	v	55	60,55	-	2/7/25/26	0/2/2/2
1	1MG	A	745	1	-	0/3/25/26	0/3/3/3
57	4SU	y	8	57	-	1/7/25/26	0/2/2/2
1	PSU	A	1911	1	-	0/7/25/26	0/2/2/2
1	OMC	A	2498	1,60	-	0/9/27/28	0/2/2/2
34	MA6	a	1518	34	-	2/7/29/30	0/3/3/3
34	UR3	a	1498	34	-	2/7/25/26	0/2/2/2
1	7MG	A	2069	1,60	-	2/7/37/38	0/3/3/3
57	PSU	y	39	57	-	2/7/25/26	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
57	7MG	y	46	57	-	4/7/37/38	0/3/3/3
1	PSU	A	955	1	-	0/7/25/26	0/2/2/2
57	H2U	y	16	57	-	2/7/38/39	0/2/2/2
1	5MU	A	1939	1	-	1/7/25/26	0/2/2/2
1	3TD	A	1915	1,60	-	3/7/25/26	0/2/2/2
1	PSU	A	1917	1	-	2/7/25/26	0/2/2/2
1	PSU	A	2457	1	-	1/7/25/26	0/2/2/2
34	2MG	a	966	34	-	3/5/27/28	0/3/3/3
34	4OC	a	1402	34,60	-	2/9/29/30	0/2/2/2
1	PSU	A	746	1,60	-	4/7/25/26	0/2/2/2
1	OMG	A	2251	1,60,55	-	0/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	2MA	A	2503	1,60	-	0/3/25/26	0/3/3/3
34	5MC	a	1407	34	-	0/7/25/26	0/2/2/2
1	5MC	A	1962	1	-	2/7/25/26	0/2/2/2
55	H2U	v	20	55	-	5/7/38/39	0/2/2/2
55	4SU	v	7	55	-	2/7/25/26	0/2/2/2
1	6MZ	A	1618	1	-	3/5/27/28	0/3/3/3
1	PSU	A	2604	1	-	2/7/25/26	0/2/2/2

The worst 5 of 140 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1915	3TD	O4'-C1'	16.11	1.66	1.43
1	A	1915	3TD	C6-C5	16.03	1.53	1.35
1	A	1915	3TD	C2'-C1'	-14.45	1.34	1.53
1	A	1915	3TD	C2-N1	8.02	1.47	1.37
57	y	37	MIA	C13-C14	7.18	1.53	1.32

The worst 5 of 260 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	a	1207	2MG	N1-C2-N2	8.86	125.60	116.56
57	y	37	MIA	C12-C13-C14	-8.22	112.26	127.01
57	y	46	7MG	N9-C4-N3	8.06	137.26	125.46
34	a	527	7MG	N9-C4-N3	7.90	137.04	125.46
1	A	2069	7MG	N9-C4-N3	7.34	136.21	125.46

There are no chirality outliers.

5 of 78 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 oligosaccharides 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	0.39	0	8,13,15	0.19	0
59	FME	A	3001	-	8,9,10	0.52	0	8,9,11	1.03	0
63	GTP	z	402	60	29,34,34	1.02	1 (3%)	35,54,54	1.06	2 (5%)

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

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
63	z	402	GTP	C6-N1	-2.59	1.33	1.37

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
63	z	402	GTP	C8-N7-C5	2.71	107.16	102.55
63	z	402	GTP	C5-C6-N1	2.22	118.30	114.07

There are no chirality outliers.

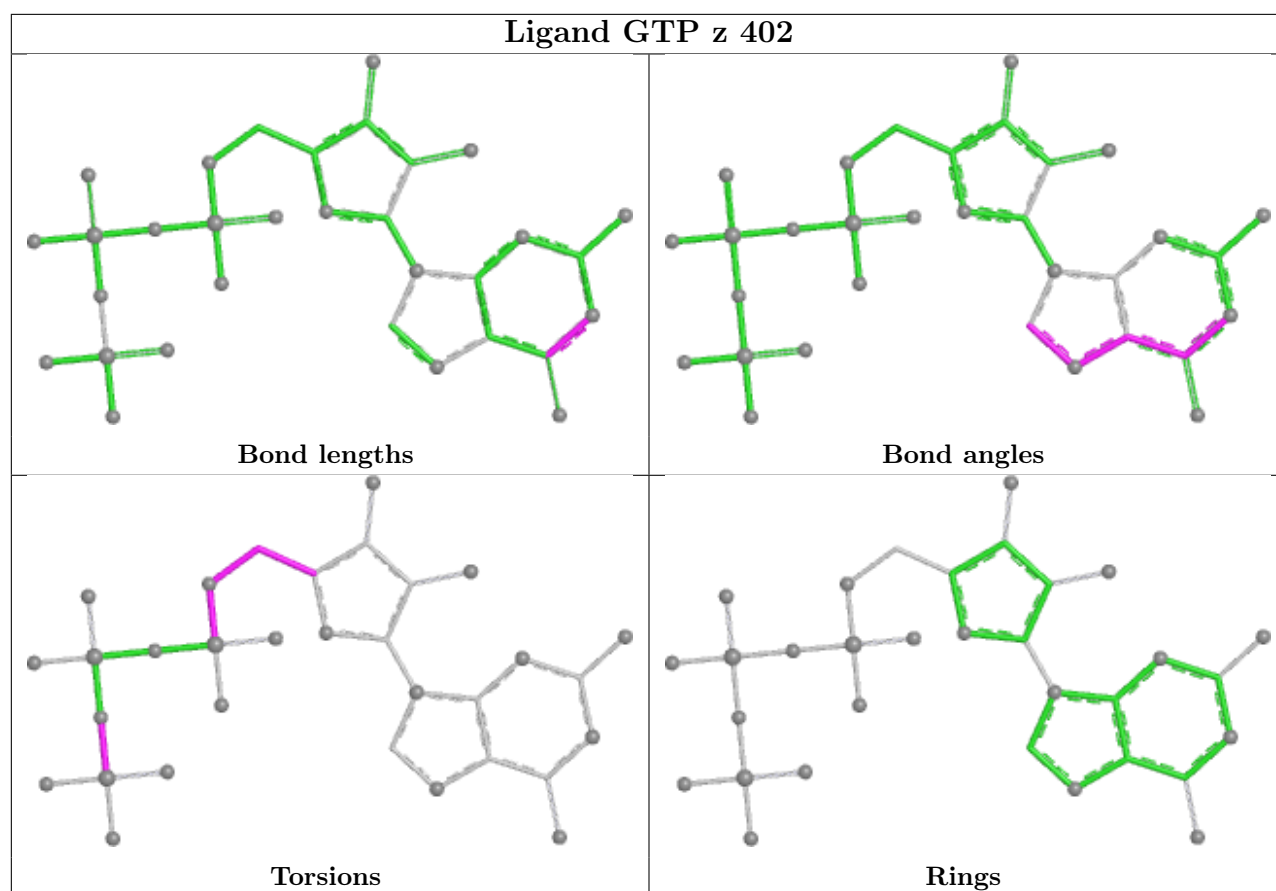
5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
62	z	401	PHE	O-C-CA-CB
63	z	402	GTP	C5'-O5'-PA-O3A
63	z	402	GTP	C5'-O5'-PA-O1A
63	z	402	GTP	C5'-O5'-PA-O2A
63	z	402	GTP	C3'-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.

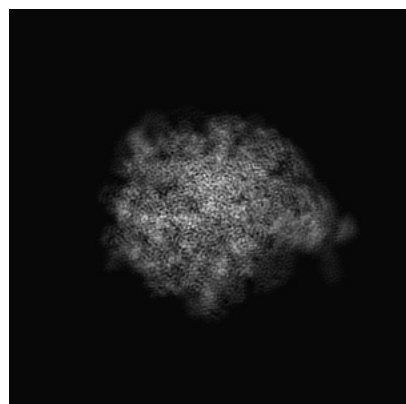
6 Map visualisation [i](#)

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.

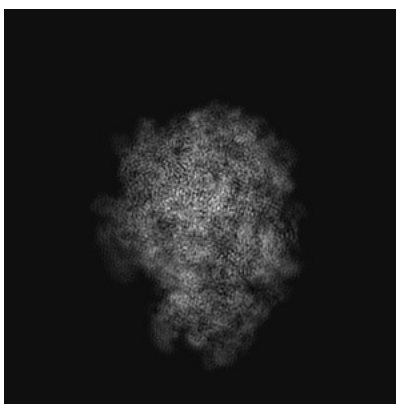
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

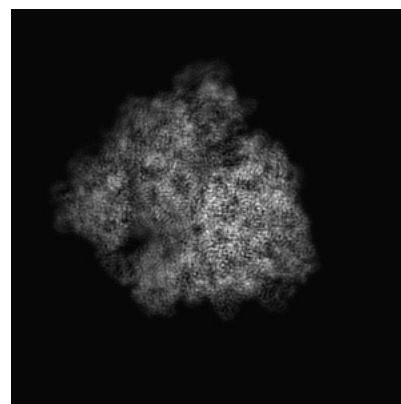
6.1.1 Primary map



X

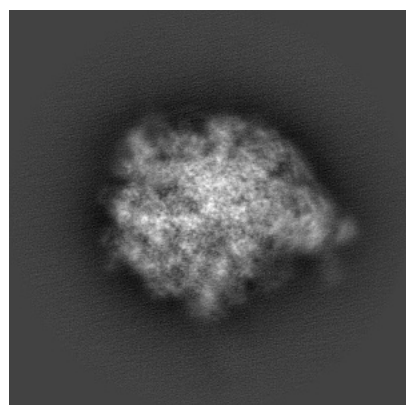


Y

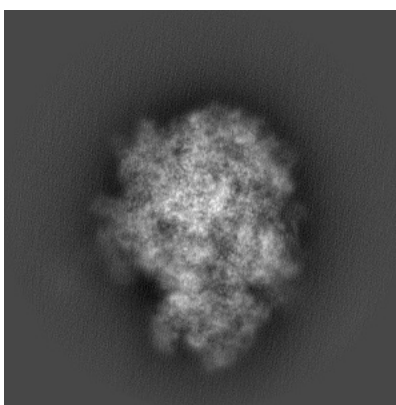


Z

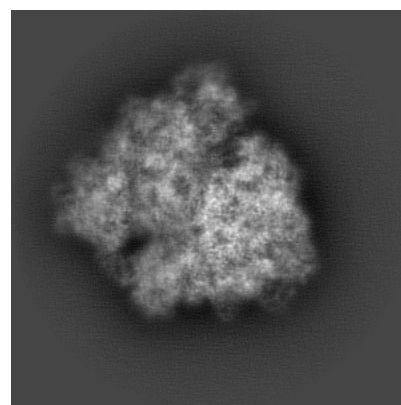
6.1.2 Raw map



X



Y

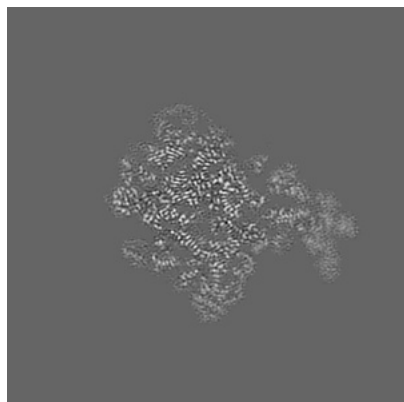


Z

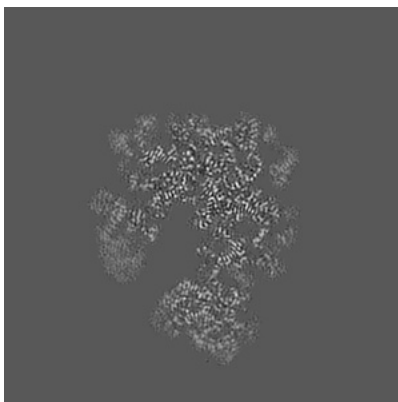
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

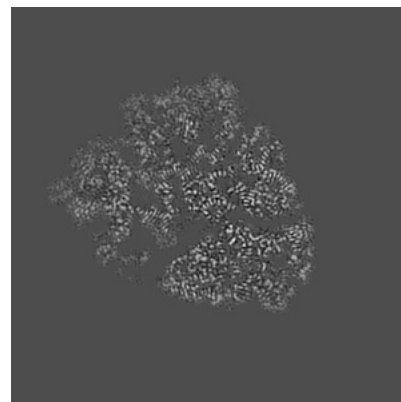
6.2.1 Primary map



X Index: 199

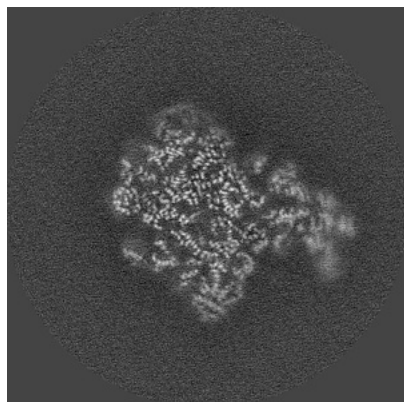


Y Index: 199

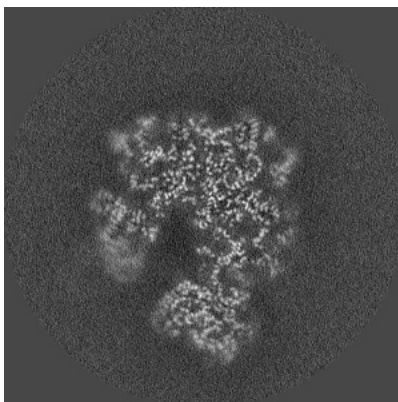


Z Index: 199

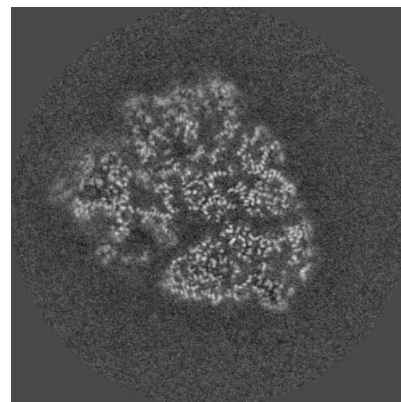
6.2.2 Raw map



X Index: 199



Y Index: 199

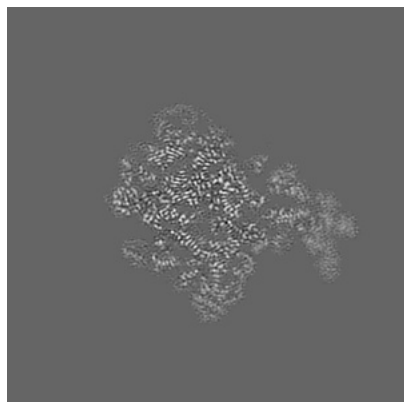


Z Index: 199

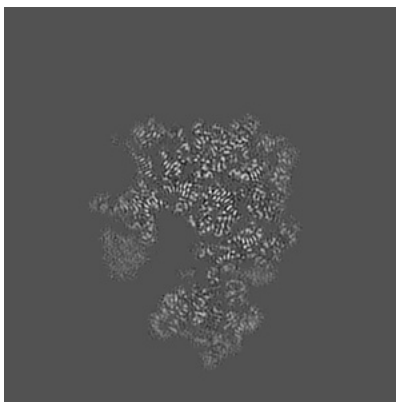
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

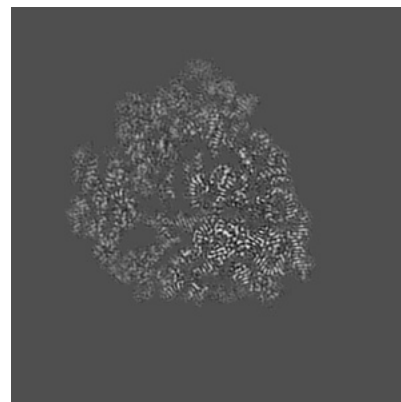
6.3.1 Primary map



X Index: 199

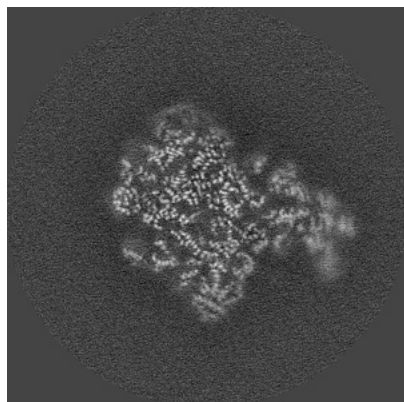


Y Index: 207

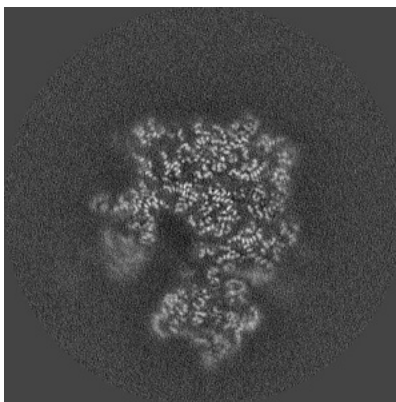


Z Index: 190

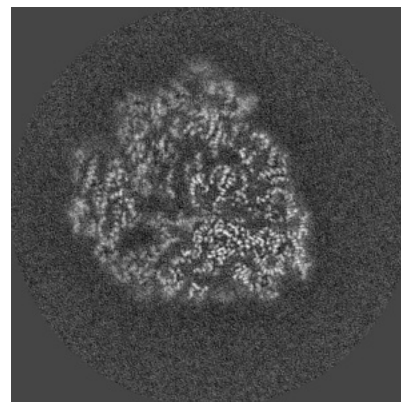
6.3.2 Raw map



X Index: 199



Y Index: 207

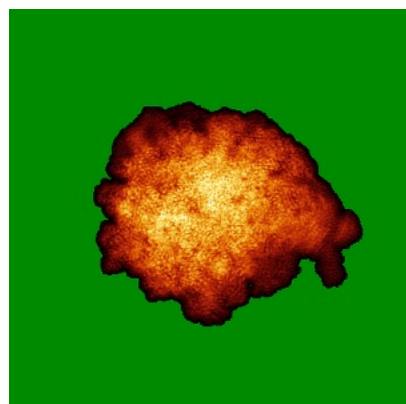


Z Index: 190

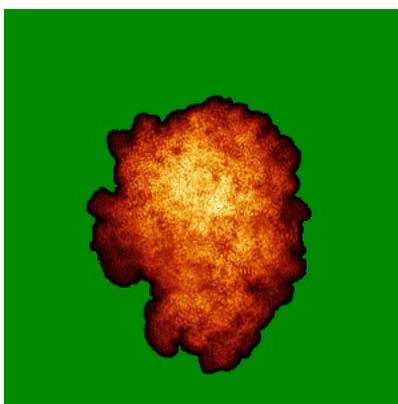
The images above show the largest variance slices of the map in three orthogonal directions.

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

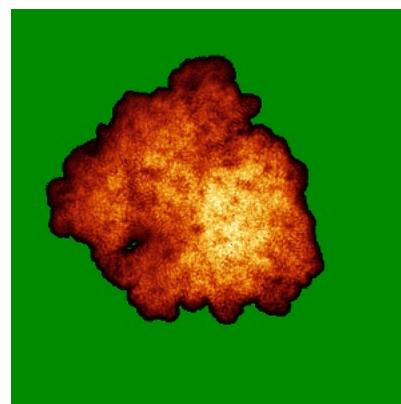
6.4.1 Primary map



X

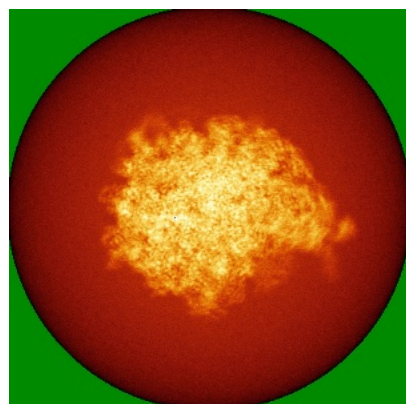


Y

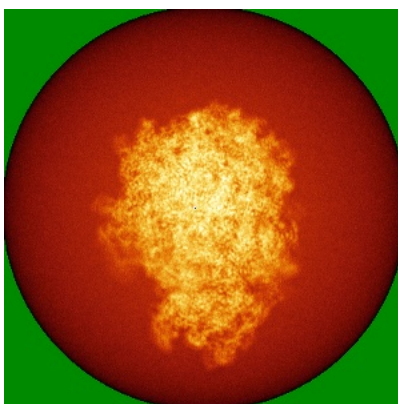


Z

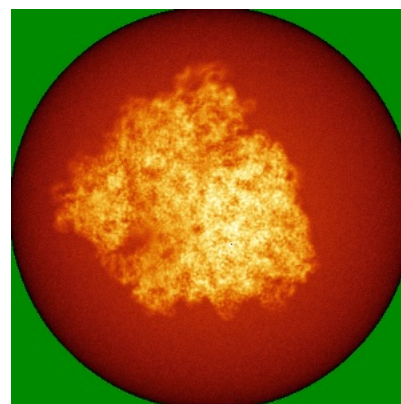
6.4.2 Raw map



X



Y

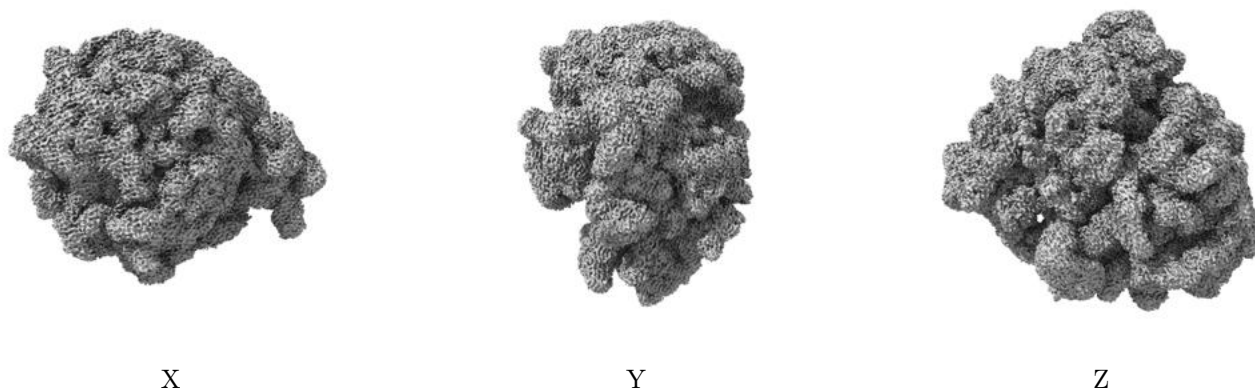


Z

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

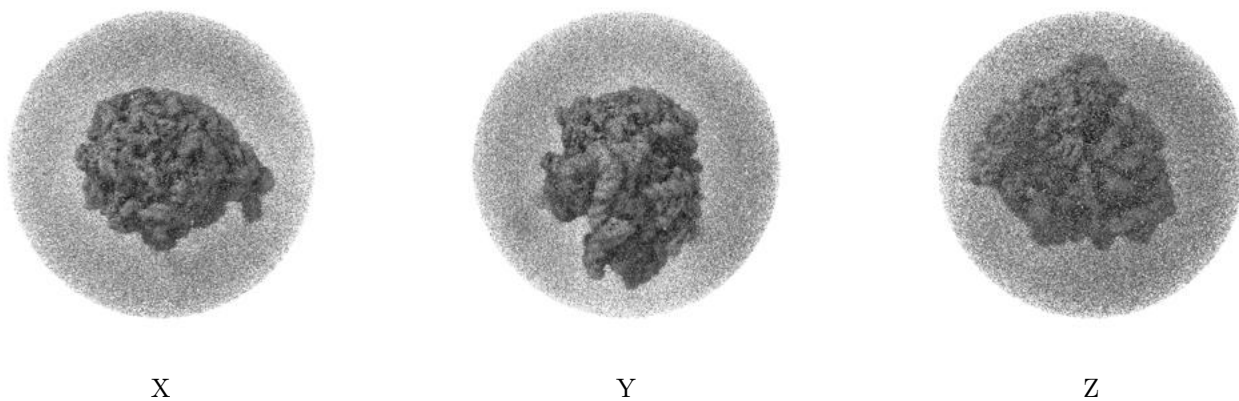
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



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

6.5.2 Raw map



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

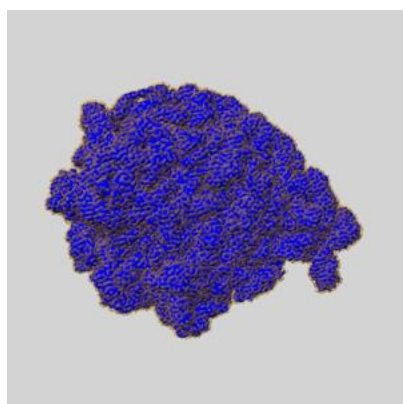
6.6 Mask visualisation [i](#)

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

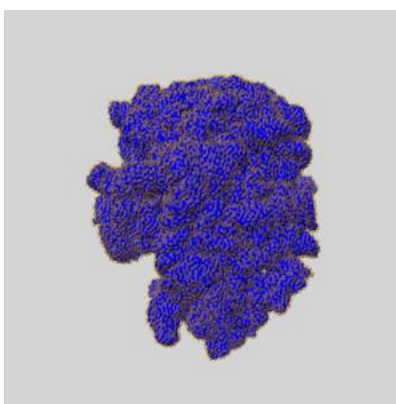
A mask typically either:

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

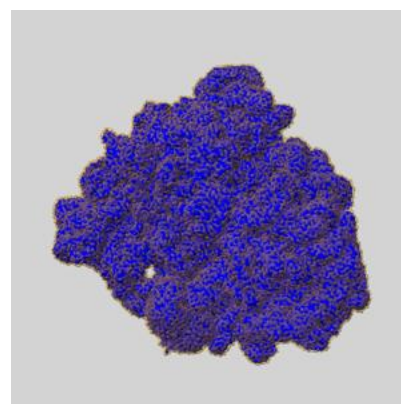
6.6.1 emd_8829_msk_1.map [i](#)



X



Y

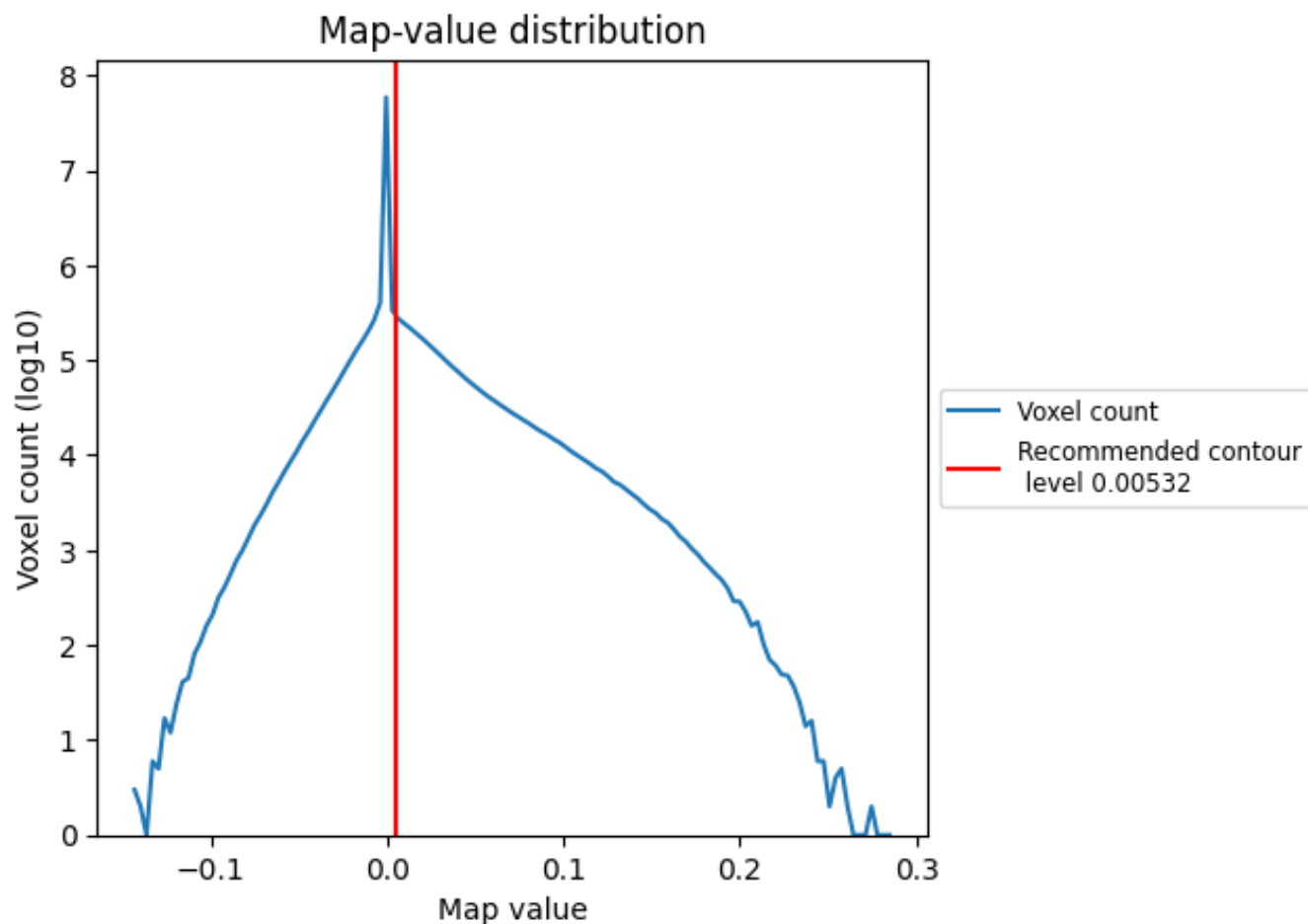


Z

7 Map analysis [i](#)

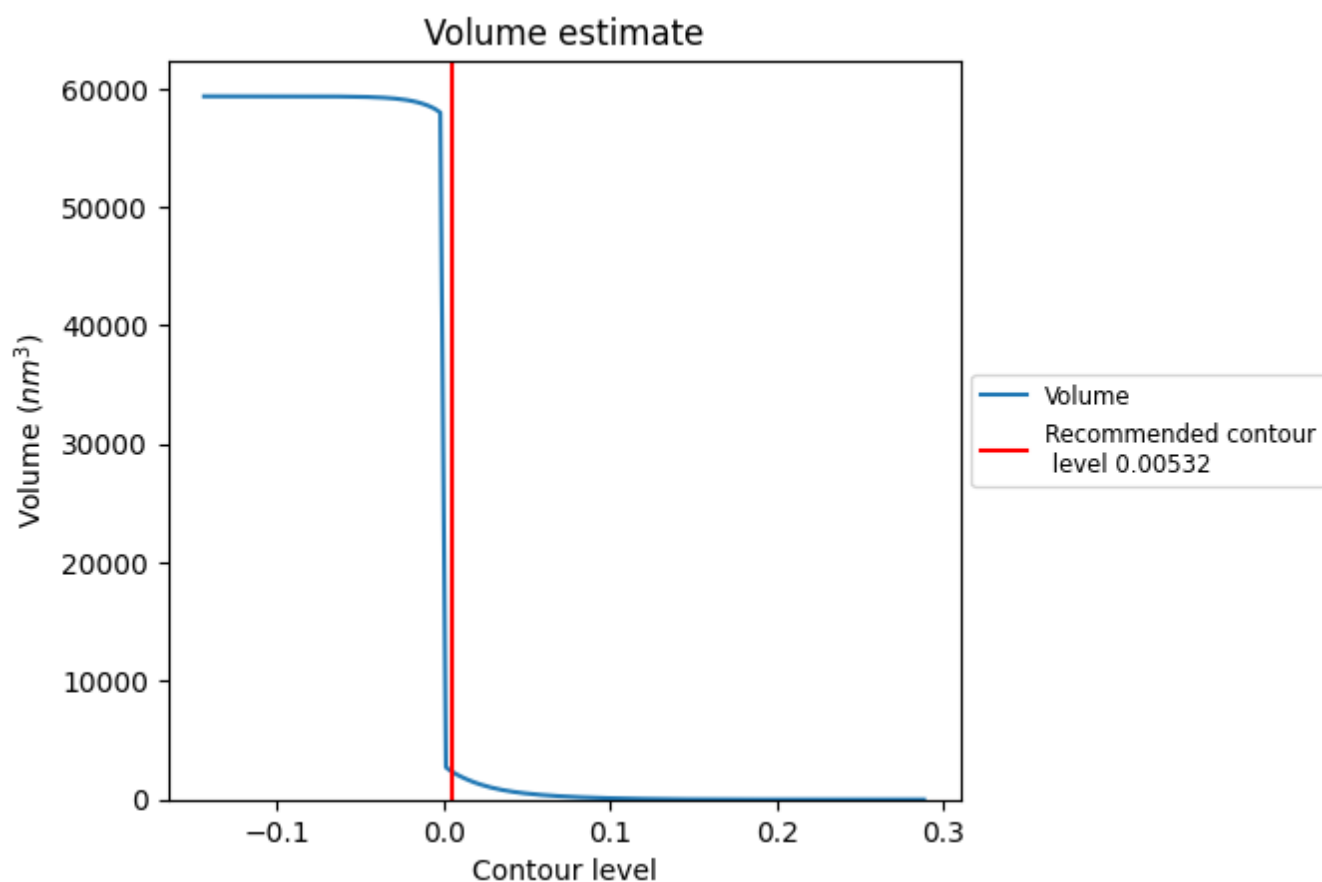
This section contains the results of statistical analysis of the map.

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.

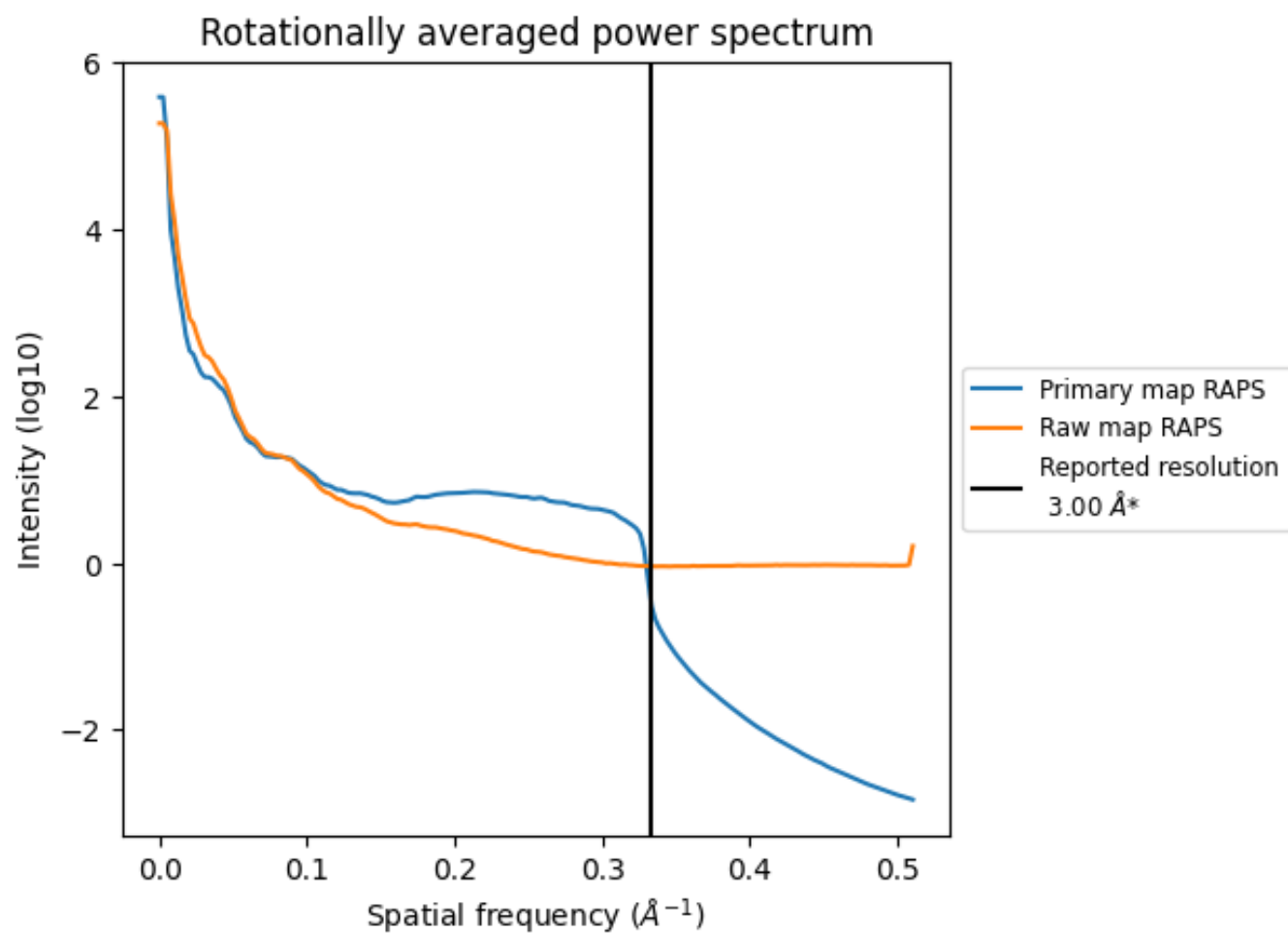
7.2 Volume estimate [i](#)



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 ⓘ

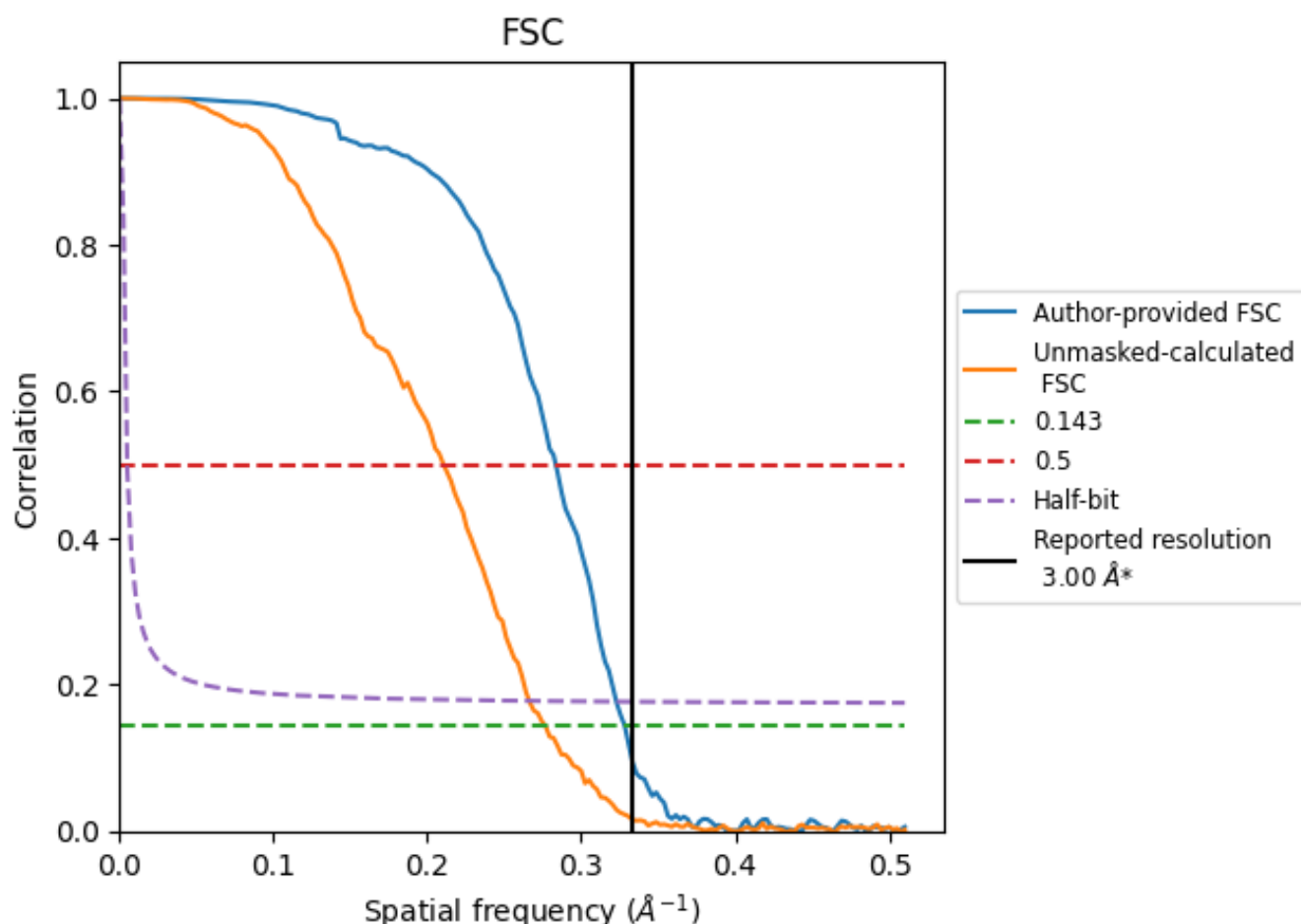


*Reported resolution corresponds to spatial frequency of 0.333 \AA^{-1}

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](#)

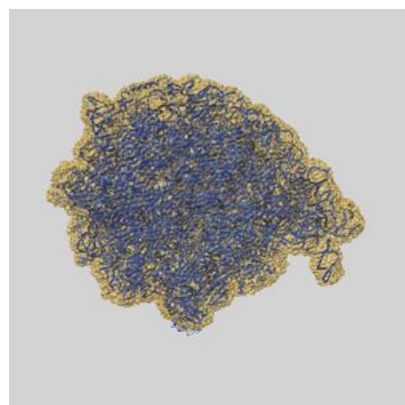
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	3.05	3.53	3.10
Unmasked-calculated*	3.61	4.75	3.76

*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 %

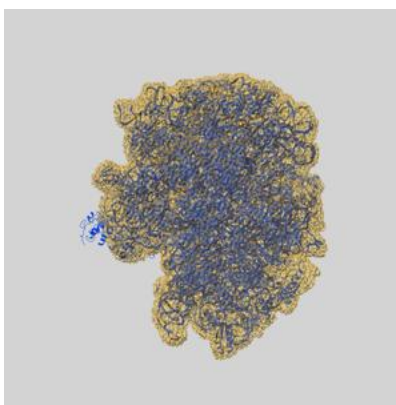
9 Map-model fit [i](#)

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](#).

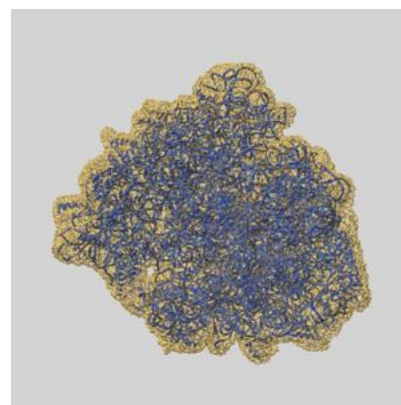
9.1 Map-model overlay [i](#)



X



Y



Z

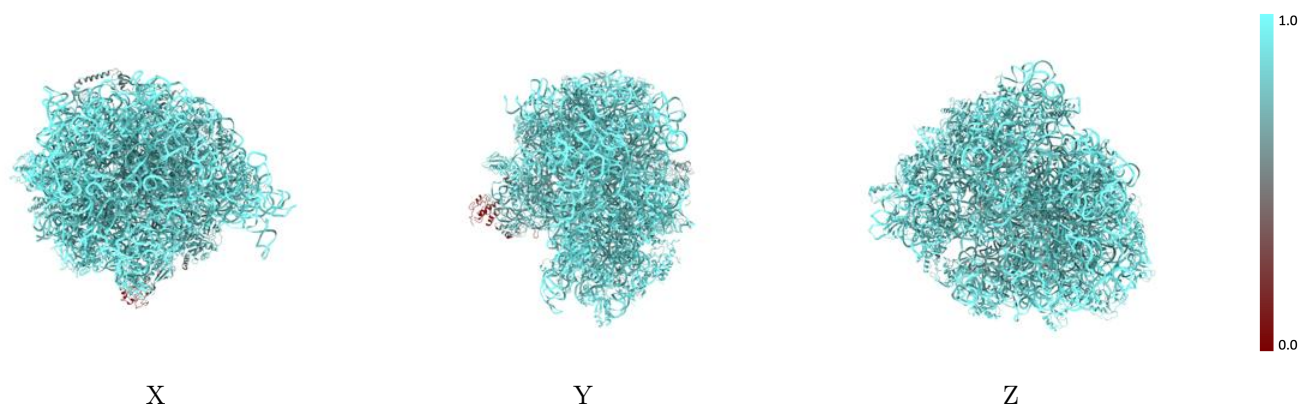
The images above show the 3D surface view of the map at the recommended contour level 0.00532 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



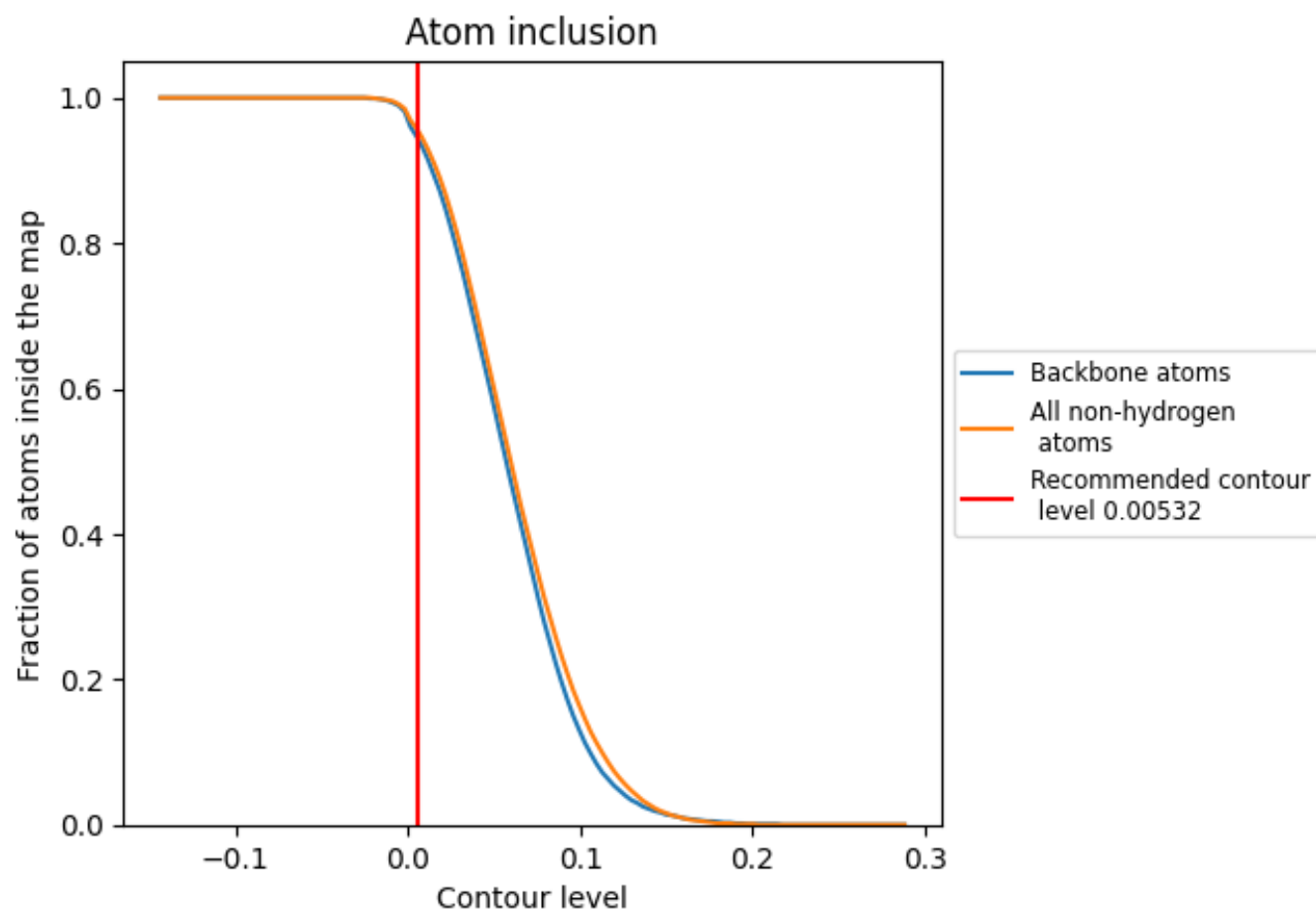
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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	 0.9240	 0.4640
2	 0.9880	 0.5860
3	 0.9840	 0.5760
4	 0.9520	 0.4940
5	 0.1120	 -0.0200
6	 0.8880	 0.3120
A	 0.9870	 0.5350
B	 0.9940	 0.5140
C	 0.9740	 0.5550
D	 0.9660	 0.5260
E	 0.9690	 0.5080
F	 0.9360	 0.4310
G	 0.9370	 0.3790
H	 0.7350	 0.2180
I	 0.6190	 0.0210
J	 0.9650	 0.5270
K	 0.9520	 0.5180
L	 0.9650	 0.5170
M	 0.9690	 0.5180
N	 0.9860	 0.5530
O	 0.9680	 0.4480
P	 0.9570	 0.5080
Q	 0.9560	 0.5500
R	 0.9390	 0.4830
S	 0.9520	 0.5230
T	 0.9340	 0.4560
U	 0.9450	 0.4450
V	 0.9490	 0.4600
W	 0.9640	 0.5480
X	 0.9550	 0.5170
Y	 0.9380	 0.4430
Z	 0.9650	 0.5020
a	 0.9870	 0.4800



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Chain	Atom inclusion	Q-score
b	 0.8950	 0.3360
c	 0.9420	 0.4360
d	 0.8990	 0.2860
e	 0.9530	 0.4820
f	 0.9230	 0.4070
g	 0.9160	 0.3700
h	 0.9490	 0.4840
i	 0.9220	 0.3850
j	 0.8960	 0.3370
k	 0.9460	 0.4300
l	 0.9080	 0.4010
m	 0.9440	 0.4280
n	 0.9500	 0.4390
o	 0.9410	 0.4440
p	 0.8930	 0.2610
q	 0.9150	 0.3710
r	 0.8970	 0.4030
s	 0.9520	 0.4260
t	 0.9200	 0.3290
u	 0.8210	 0.2580
v	 0.9720	 0.4880
w	 0.7450	 0.0740
x	 0.9840	 0.4960
y	 0.9160	 0.2870
z	 0.8290	 0.2520