



wwPDB EM Validation Summary Report ⓘ

Feb 4, 2025 – 10:58 AM EST

PDB ID : 5WDT
EMDB ID : EMD-8813
Title : 70S ribosome-EF-Tu H84A complex with GppNHp
Authors : Fislage, M.; Brown, Z.; Frank, J.
Deposited on : 2017-07-06
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

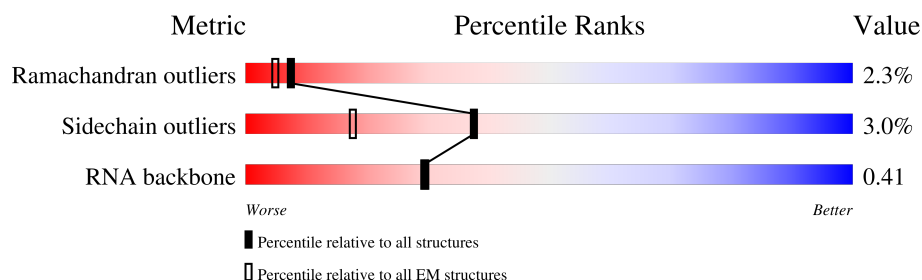
1 Overall quality at a glance

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	


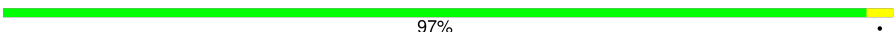
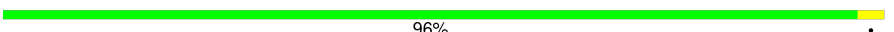









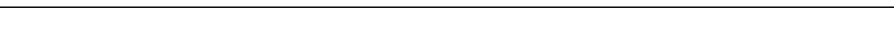

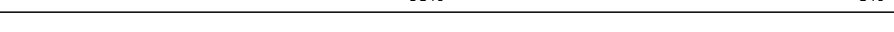
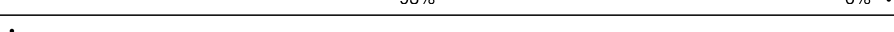
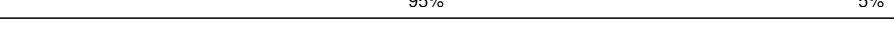
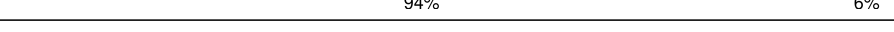

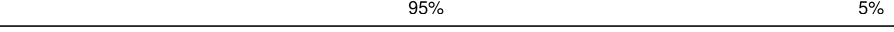
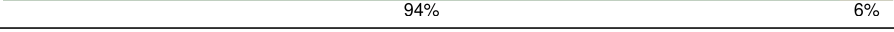




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Mol	Chain	Length	Quality of chain
9	I	141	<div> <div>26%</div> <div>95%</div> <div>5%</div> </div>
10	J	141	<div> <div>97%</div> <div>.</div> </div>
11	K	122	<div> <div>93%</div> <div>7%</div> </div>
12	L	143	<div> <div>90%</div> <div>10%</div> </div>
13	M	136	<div> <div>99%</div> <div>.</div> </div>
14	N	119	<div> <div>97%</div> <div>..</div> </div>
15	O	116	<div> <div>99%</div> <div>.</div> </div>
16	P	114	<div> <div>100%</div> </div>
17	Q	115	<div> <div>97%</div> <div>.</div> </div>
18	R	102	<div> <div>95%</div> <div>5%</div> </div>
19	S	109	<div> <div>95%</div> <div>5%</div> </div>
20	T	92	<div> <div>96%</div> <div>.</div> </div>
21	U	102	<div> <div>95%</div> <div>5%</div> </div>
22	V	92	<div> <div>98%</div> <div>..</div> </div>
23	W	75	<div> <div>97%</div> <div>.</div> </div>
24	X	77	<div> <div>97%</div> <div>.</div> </div>
25	Y	60	<div> <div>98%</div> <div>.</div> </div>
26	Z	56	<div> <div>98%</div> <div>.</div> </div>
27	0	55	<div> <div>98%</div> <div>.</div> </div>
28	1	51	<div> <div>98%</div> <div>.</div> </div>
29	2	45	<div> <div>93%</div> <div>..</div> </div>
30	3	64	<div> <div>95%</div> <div>5%</div> </div>
31	4	38	<div> <div>97%</div> <div>.</div> </div>
32	5	131	<div> <div>77%</div> <div>92%</div> <div>8%</div> </div>
33	6	66	<div> <div>97%</div> <div>.</div> </div>

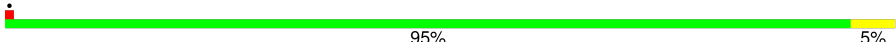
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Mol	Chain	Length	Quality of chain
34	a	1540	 71%29%
35	b	218	 97%.
36	c	206	 96%.
37	d	205	 98%.
38	e	157	 92%8%
39	f	100	 93%6%.
40	g	151	 93%7%
41	h	129	 97%.
42	i	127	 94%6%.
43	j	98	 93%7%
44	k	116	 93%7%
45	l	121	 92%7%.
46	m	115	 97%.
47	n	101	 95%5%.
48	o	88	 93%6%.
49	p	82	 95%5%.
50	q	80	 94%6%
51	r	65	 89%11%.
52	s	79	 95%5%.
53	t	85	 94%6%
54	u	65	 82%17%.
55	v	77	 74%23%.
55	w	77	 51%43%6%.
56	x	12	 92%8%
57	y	76	 54%42%.

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Mol	Chain	Length	Quality of chain
58	z	393	 A horizontal bar chart showing the quality of the chain. The bar is green and extends to 95% of the total length. The remaining 5% is highlighted in yellow. The text '95%' is centered below the green portion, and '5%' is at the end of the yellow portion.

2 Entry composition

There are 64 unique types of molecules in this entry. The entry contains 155275 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 731469900
A	1723	G	A	conflict	GB 731469900
A	1847	G	A	conflict	GB 731469900

- 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 1174070234

- 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.

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 P0AG59

- 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	42	85	12		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
57	y	76	Total	C	N	O	P	S	0	0
			1631	731	290	532	76	2		

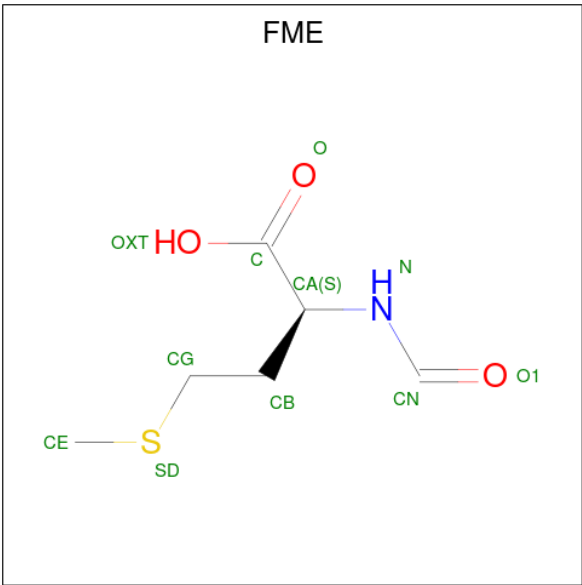
- Molecule 58 is a protein called Elongation factor Tu 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	z	393	Total	C	N	O	S	0	0
			3031	1915	521	582	13		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
z	84	ALA	HIS	engineered mutation	UNP P0CE48

- 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	1325	Total	Mg	0
			1325	1325	
60	B	36	Total	Mg	0
			36	36	
60	C	3	Total	Mg	0
			3	3	
60	D	3	Total	Mg	0
			3	3	
60	E	3	Total	Mg	0
			3	3	
60	L	2	Total	Mg	0
			2	2	
60	M	1	Total	Mg	0
			1	1	
60	N	1	Total	Mg	0
			1	1	
60	Q	2	Total	Mg	0
			2	2	
60	R	1	Total	Mg	0
			1	1	
60	S	1	Total	Mg	0
			1	1	

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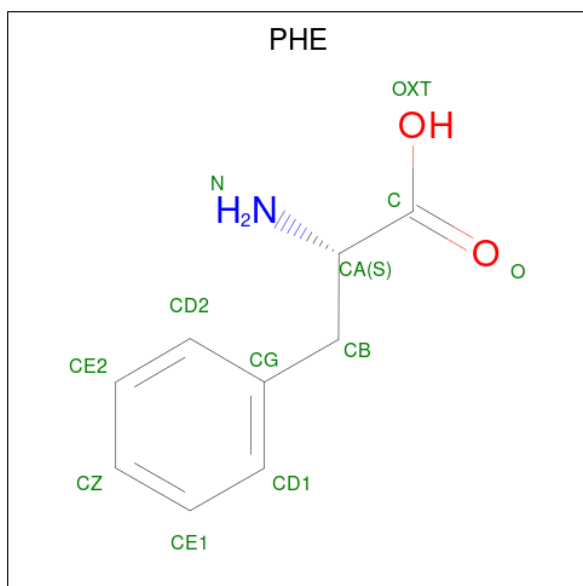
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Mol	Chain	Residues	Atoms		AltConf
60	T	1	Total 1	Mg 1	0
60	X	1	Total 1	Mg 1	0
60	Y	1	Total 1	Mg 1	0
60	Z	2	Total 2	Mg 2	0
60	0	2	Total 2	Mg 2	0
60	3	3	Total 3	Mg 3	0
60	4	1	Total 1	Mg 1	0
60	a	481	Total 481	Mg 481	0
60	d	1	Total 1	Mg 1	0
60	h	1	Total 1	Mg 1	0
60	i	3	Total 3	Mg 3	0
60	s	1	Total 1	Mg 1	0
60	t	1	Total 1	Mg 1	0
60	u	1	Total 1	Mg 1	0
60	v	12	Total 12	Mg 12	0
60	w	1	Total 1	Mg 1	0
60	x	1	Total 1	Mg 1	0
60	y	8	Total 8	Mg 8	0
60	z	4	Total 4	Mg 4	0

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

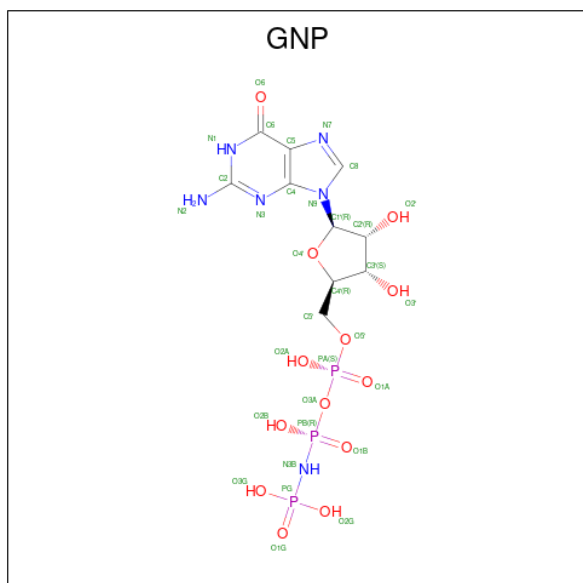
Mol	Chain	Residues	Atoms			AltConf
61	A	5	Total	K		0
			5	5		

- Molecule 62 is PHENYLALANINE (three-letter code: PHE) (formula: $C_9H_{11}NO_2$).



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

- Molecule 63 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (three-letter code: GNP) (formula: $C_{10}H_{17}N_6O_{13}P_3$).



Mol	Chain	Residues	Atoms					AltConf
63	z	1	Total	C	N	O	P	0
			32	10	6	13	3	

- Molecule 64 is water.

Mol	Chain	Residues	Atoms		AltConf
64	A	653	Total	O	0
			653	653	
64	B	22	Total	O	0
			22	22	
64	C	7	Total	O	0
			7	7	
64	D	6	Total	O	0
			6	6	
64	E	6	Total	O	0
			6	6	
64	G	1	Total	O	0
			1	1	
64	J	1	Total	O	0
			1	1	
64	L	6	Total	O	0
			6	6	
64	M	1	Total	O	0
			1	1	
64	N	3	Total	O	0
			3	3	
64	P	1	Total	O	0
			1	1	
64	Q	4	Total	O	0
			4	4	
64	S	2	Total	O	0
			2	2	
64	U	3	Total	O	0
			3	3	
64	W	1	Total	O	0
			1	1	
64	X	3	Total	O	0
			3	3	
64	Y	1	Total	O	0
			1	1	
64	Z	2	Total	O	0
			2	2	
64	0	1	Total	O	0
			1	1	

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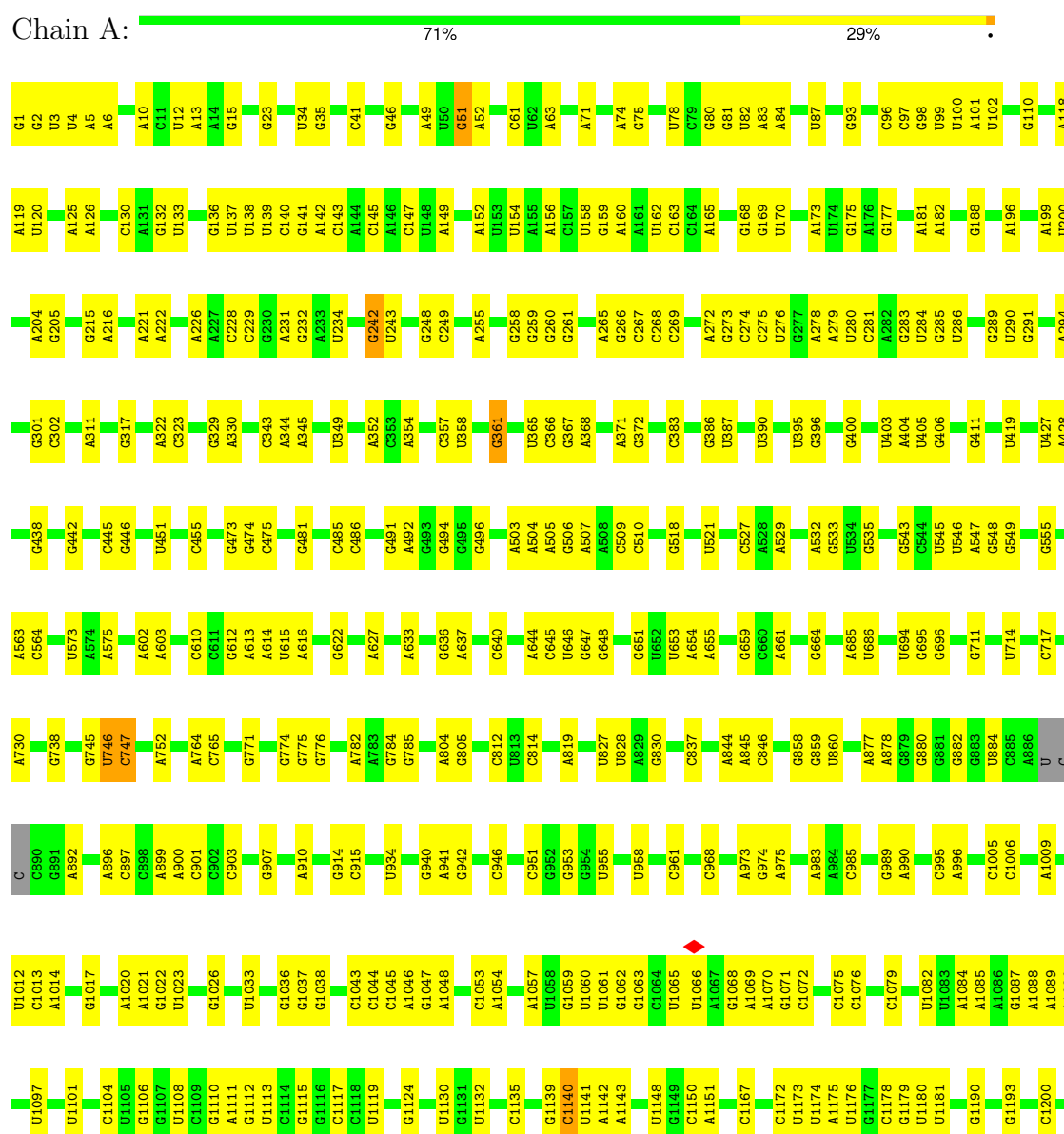
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Mol	Chain	Residues	Atoms		AltConf
64	2	4	Total 4	O 4	0
64	3	1	Total 1	O 1	0
64	4	1	Total 1	O 1	0
64	a	163	Total 163	O 163	0
64	d	1	Total 1	O 1	0
64	h	2	Total 2	O 2	0
64	k	1	Total 1	O 1	0
64	m	3	Total 3	O 3	0
64	o	1	Total 1	O 1	0
64	s	2	Total 2	O 2	0
64	t	1	Total 1	O 1	0
64	u	1	Total 1	O 1	0
64	v	9	Total 9	O 9	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
64	z	2	Total 2	O 2	0

3 Residue-property plots

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



A2826	U2720	G2535	G2399	G2230	A2108	C1967	G1857	U1716	G1567	G1478	A1204
G2844	U2724	A2542	G2400	G2238	U2109	A1970	A1858		G1568	G1479	A1365
A2856	U2725	A2547	U2402	G2239	G2110	U1971	G1862	G1721	A1569		G1210
U2861	A2726	U2547	U2404	G2251	U2113	G1972		G1724		G1482	G1212
G2867	U2727	U2552	G2405	G2252	U2118	U1976	A1866	C1725	A1572	G1483	G1218
A2868	U2728	G2553	A2406	A2278	A2119	U1991	G1867	G1726	A1579	U1484	
A2872	A2733	U2554	U2407	G2283	A2119	G1992	C1868	U1727	A1590	U1485	G1225
A2877	A2734	U2555	U2408	C2283	G2120	U1993	C1870	U1729	G1581	U1486	G1226
G2882	G2735	C2556	U2423	G2286	G2121	U1997	C1872	U1730	G1582	U1487	G1227
A2873		A2566	C2424	A2287	G2127	C1997	G1873	G1731	A1584	A1490	G1236
C2874	G2742	G2567	A2425	A2288				C1732	C1585	G1491	
	U2743				U2131	A2020	A1876	G1735	G1588	G1492	U1391
C2880	U2744	A2572	G2428	U2286	U2132	C2021		U1736	A1494	A1493	A1392
A2883	C2745	C2573	A2429	A2297	G2133	U2022	C1879	G1737	A1495	A1496	C1399
U2884	U2746	U2578	A2430		A2134	C2023		G1738	U1496	U1497	U1402
G2885	G2747	U2580	U2435	U2305	G2141	G2027	G1884	A1739	A1593	A1403	G1248
A2886	A2748	G2581		U2309			A1885	G1740	C1605	A1504	A1253
	C2752	U2585	U2441	A2309	C2145	A2030	A1890	C1741		C1507	G1256
C2895	A2753	U2586		A2311	C2146			A1746	A1508	A1508	G1257
U2897	U2754	G2445	G2445	G2318	A2147	A2033	C1895		A1509	U1411	U1258
U2898		G2446	G2446	G2319	G2157	U2039	U1898	G1750	A1610	U1412	
A2899	A2758	G2603	U2447	G2319		C2043	G1906	U1758	A1616	A1413	A1262
C2901	U2760	U2604	A2448	G2325	G2162	C2043	G1907		C1617	A1414	A1269
C2902	C2762	U2605	U2449	C2326	A2163		G1907	C1764	A1618	U1415	G1270
U2903	A2764	U2609	C2452	C2326	C2164	C2055	C1908			C1417	G1271
	A2765		U2457	C2332		G2056	G1909	U1773	A1634	G1524	A1272
		U2613	U2457	A2333	A2170		G1910			A1419	U1273
	U2768	G2624	C2465	U2334	A2171	A2059	U1911	G1776	U1647	G1527	C1289
A2776		U2629	C2465	U2336	U2172	A2060	A1912		U1648	A1528	C1290
G2777	A2776		A2469	A2336	A2173	G2061	C1913	A1780	G1649	G1529	C1291
A2778	G2777	U2629		C2339	U2180	A2062	C1914			G1530	C1428
		A2634	C2475	A2340			3TD1915		A1654	C1531	
	G2791		A2476	A2340	G2186	G2069	A1916	A1791		G1532	U1294
		C2651		U2344	U2192	C2072	U1917	C1800	G1659	A1532	G1432
U2794	U2794	C2652	C2480	G2345	G2193	A2077	A1918	A1801		C1533	G1300
G2799		U2653	G2484	C2340	U2194		G1674			U1534	A1301
A2800	U2800	A2654		U2350	U2195	A2080	C1675	A1808	G1674	A1535	G1436
G2801	G2801	U2655	G2494	G2357	U2195	G2097	C1691	A1809	G1675	C1536	G1441
	A2802				A2198	U2092	U1692	G1811	C1691	G1537	
U2803	U2803	G2673	C2498	G2361		G2093	U1693		U1692	U1538	
U2804	U2804	G2674	C2499	U2372	G2204	C2096	A1936	G1816	U1692	G1546	C1320
C2805	C2805		G2502	U2372	A2205	C2096	A1937	G1817	C1694	A1549	A1321
C2806	C2806	U2689	G2503	U2378	C2206	A2097	U1938	U1818	G1695		G1332
U2807	U2807	U2690	A2502	A2378	G2206	U2097	U1939		A1700	U1554	
G2808	C2691	C2691	U2504	G2379	A2211	U2098	U1940	A1829	A1705	G1555	U1344
A2809			G2505	G2379	A2212	G2100	C1941		C1706	C1557	C1345
			U2506	G2383	U2213	G2100	C1942	C1833	C1706	C1558	C1349
	G2812	U2707	U2506	U2383	U2213	A2101		U1834		C1558	
				U2384		A2101	U1945	G1835	U1709	U1559	
U2818	C2712	C2712	C2517	U2385	G2221	G2102	C1962			U1468	U1352
G2819	U2713	U2713	A2518	C2385	G2221	C2103	C1962	U1841	U1712	U1563	G1355
G2714	G2714	G2714		G2391	A2225	C2104	C1965	A1713	A1713	G1475	
A2820	C2715	C2715	G2529	A2392	C2226	U2106	A1966	G1847	C1715	C1565	U1476
						C2106	C1966		C1715	C1566	A1359

• Molecule 2: 5S rRNA

Chain B:  70% 30%

U1	G2	C3	C4	U5	G9	C12	G13	U14	C17	G20	G21	U22	U25	G26	C27	U32	G33	A34	C35	C36	C37	C38	G41	C42	G43	G44	G56	C63	G64	A66	G67	G84	U89	C90	G102	G105	A108	A109	C110	C118	A119	A120
----	----	----	----	----	----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	------	------	------	------	------	------	------

- Molecule 3: 50S ribosomal protein L2

Chain C:  96%



- Molecule 4: 50S ribosomal protein L3

Chain D:  94%



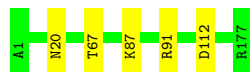
- Molecule 5: 50S ribosomal protein L4

Chain E:  97%



- Molecule 6: 50S ribosomal protein L5

Chain F:  97%



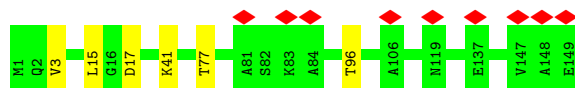
- Molecule 7: 50S ribosomal protein L6

Chain G:  98%

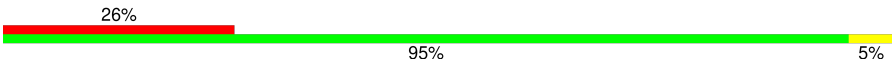


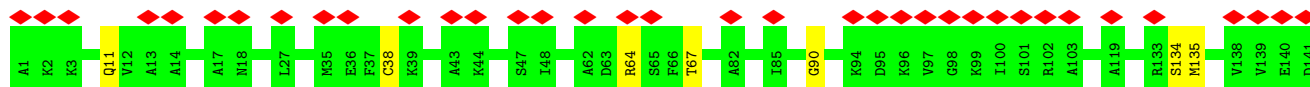
- Molecule 8: 50S ribosomal protein L9

Chain H:  96%



- Molecule 9: 50S ribosomal protein L11

Chain I:  95%



- Molecule 10: 50S ribosomal protein L13

Chain J:  97% .




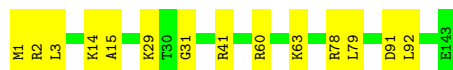
- Molecule 11: 50S ribosomal protein L14

Chain K:  93% 7%



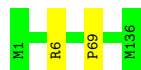
- Molecule 12: 50S ribosomal protein L15

Chain L:  90% 10%



- Molecule 13: 50S ribosomal protein L16

Chain M:  99% .



- Molecule 14: 50S ribosomal protein L17

Chain N:  97% ..



- Molecule 15: 50S ribosomal protein L18

Chain O:  99% .



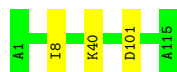
- Molecule 16: 50S ribosomal protein L19

Chain P:  100%

There are no outlier residues recorded for this chain.

- 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:  95% 5%



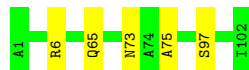
- Molecule 20: 50S ribosomal protein L23

Chain T:  96% .



- Molecule 21: 50S ribosomal protein L24

Chain U:  95% 5%



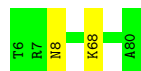
- Molecule 22: 50S ribosomal protein L25

Chain V:  98% ..




- Molecule 23: 50S ribosomal protein L27

Chain W:  97% .



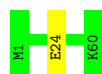
- Molecule 24: 50S ribosomal protein L28

Chain X:  97% .



- Molecule 25: 50S ribosomal protein L29

Chain Y:  98% .



- Molecule 26: 50S ribosomal protein L30

Chain Z:  98% .



- Molecule 27: 50S ribosomal protein L32

Chain 0:  98% .



- Molecule 28: 50S ribosomal protein L33

Chain 1:  98% .



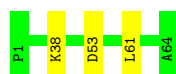
- Molecule 29: 50S ribosomal protein L34

Chain 2:  93% . .



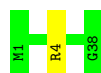
- Molecule 30: 50S ribosomal protein L35

Chain 3:  95% 5%




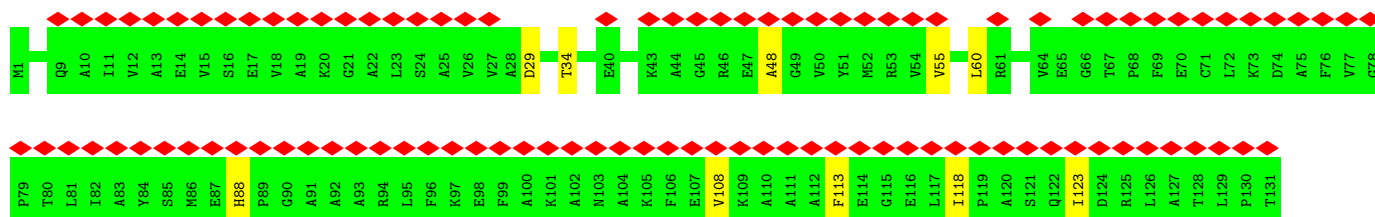
- Molecule 31: 50S ribosomal protein L36

Chain 4:  97% .



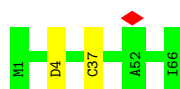
- Molecule 32: 50S ribosomal protein L10

Chain 5:  77% 92% 8%



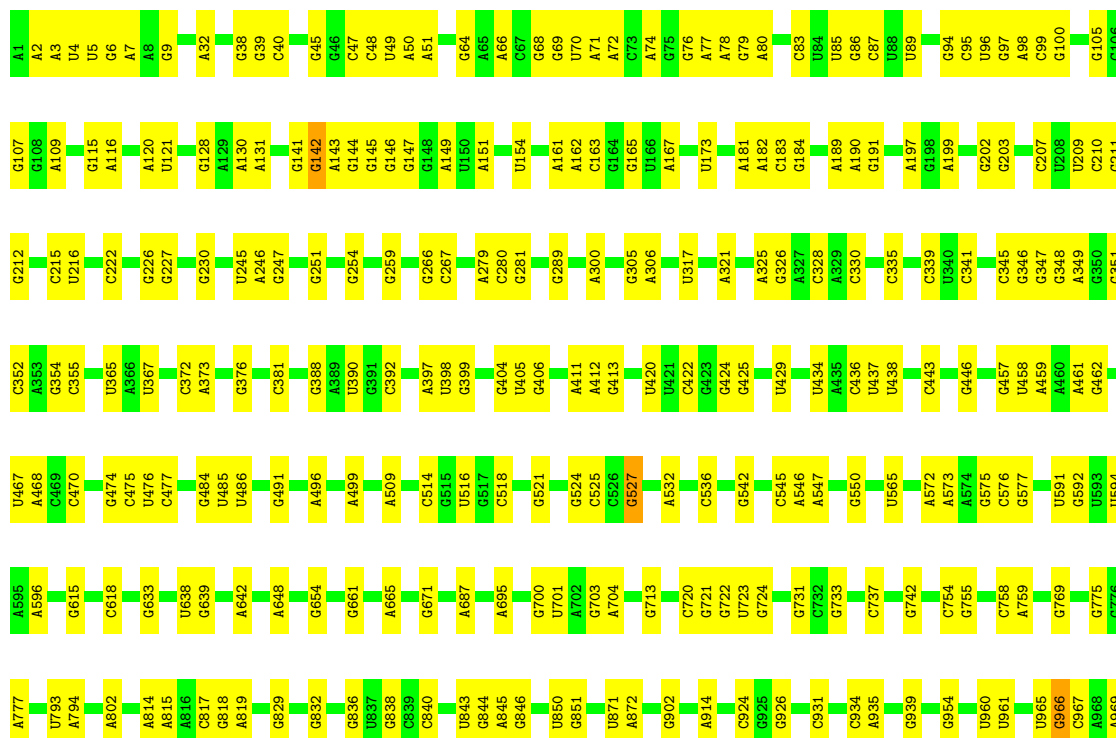
- Molecule 33: 50S ribosomal protein L31

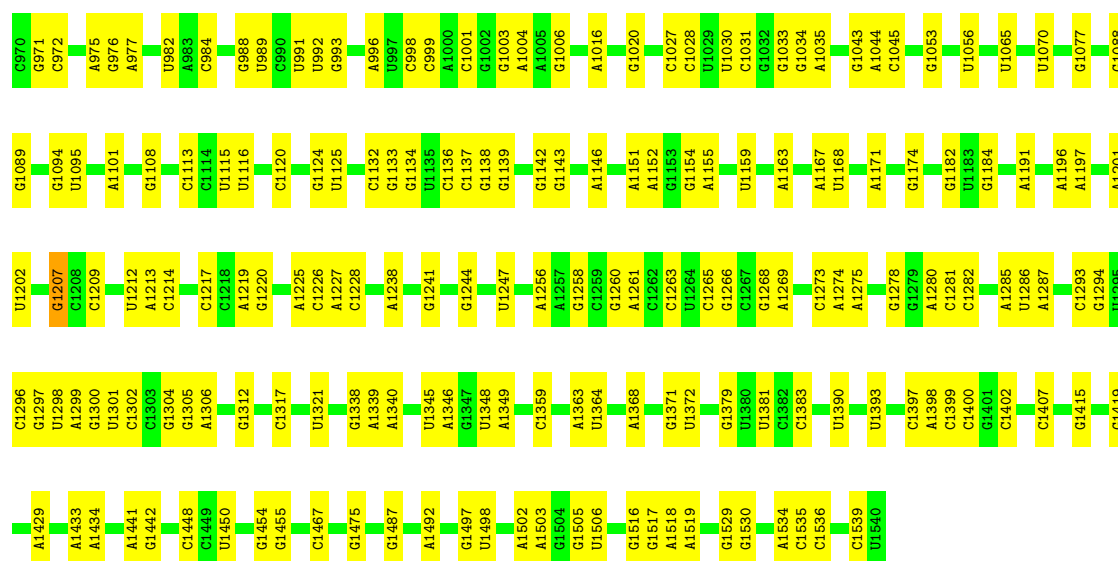
Chain 6:  97% .



- Molecule 34: 16S rRNA

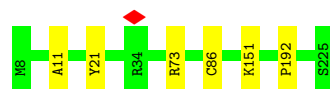
Chain a:  71% 29%





• Molecule 35: 30S ribosomal protein S2

Chain b: 97%



• Molecule 36: 30S ribosomal protein S3

Chain c: 96%



• Molecule 37: 30S ribosomal protein S4

Chain d: 98%



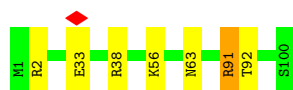
• Molecule 38: 30S ribosomal protein S5

Chain e: 92%



• Molecule 39: 30S ribosomal protein S6

Chain f: 93%



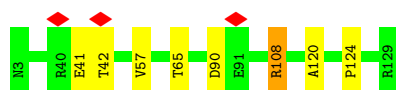
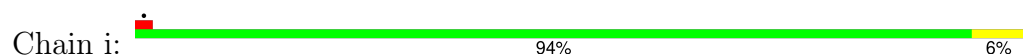
- Molecule 40: 30S ribosomal protein S7



- Molecule 41: 30S ribosomal protein S8



- Molecule 42: 30S ribosomal protein S9



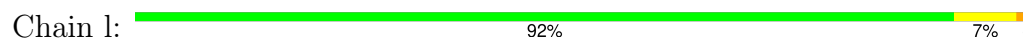
- Molecule 43: 30S ribosomal protein S10



- Molecule 44: 30S ribosomal protein S11



- Molecule 45: 30S ribosomal protein S12



- Molecule 46: 30S ribosomal protein S13





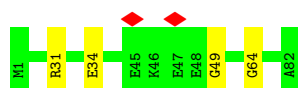
- Molecule 47: 30S ribosomal protein S14



- Molecule 48: 30S ribosomal protein S15



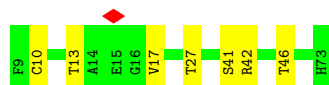
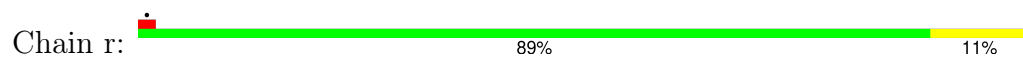
- Molecule 49: 30S ribosomal protein S16



- Molecule 50: 30S ribosomal protein S17



- Molecule 51: 30S ribosomal protein S18

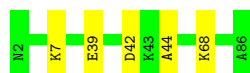


- Molecule 52: 30S ribosomal protein S19



- Molecule 53: 30S ribosomal protein S20

Chain t:  94% 6%



- Molecule 54: 30S ribosomal protein S21

Chain u:  82% 17%



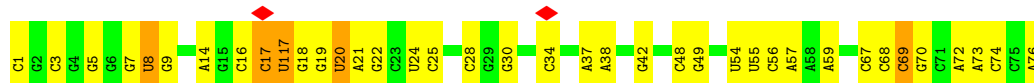
- Molecule 55: tRNA-fMet

Chain v:  74% 23%



- Molecule 55: tRNA-fMet

Chain w:  51% 43% 6%



- Molecule 56: mRNA

Chain x:  92% 8%



- Molecule 57: tRNA-Phe

Chain y:  54% 42%



- Molecule 58: Elongation factor Tu 2

Chain z:  95% 5%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	55276	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)	500	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	51020	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.247	Depositor
Minimum map value	-0.131	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.00558	Depositor
Map size (\AA)	390.04, 390.04, 390.04	wwPDB
Map dimensions	398, 398, 398	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	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: MIA, MG, 5MC, 6MZ, 4OC, OMC, 3TD, 4SU, UR3, H2U, OMU, 5MU, 2MG, PSU, MA6, K, 2MA, FME, 7MG, 1MG, OMG, GNP

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	0.24	1/69174 (0.0%)	0.70	11/107907 (0.0%)
2	B	0.31	1/2876 (0.0%)	0.69	0/4483
3	C	0.34	0/2121	0.66	0/2852
4	D	0.35	0/1578	0.59	0/2124
5	E	0.35	0/1563	0.61	0/2103
6	F	0.37	0/1434	0.59	0/1926
7	G	0.35	0/1324	0.54	0/1794
8	H	0.37	0/1122	0.51	0/1515
9	I	0.41	0/1046	0.60	0/1410
10	J	0.34	0/1143	0.60	0/1540
11	K	0.35	0/947	0.66	0/1268
12	L	0.36	0/1052	0.68	0/1401
13	M	0.36	0/1093	0.61	0/1460
14	N	0.39	0/964	0.68	0/1289
15	O	0.38	0/902	0.63	0/1209
16	P	0.35	0/929	0.63	0/1242
17	Q	0.37	0/946	0.67	0/1260
18	R	0.34	0/823	0.58	0/1100
19	S	0.34	0/852	0.67	0/1142
20	T	0.35	0/736	0.60	0/984
21	U	0.35	0/787	0.57	0/1051
22	V	0.36	0/752	0.57	1/1008 (0.1%)
23	W	0.35	0/579	0.64	0/767
24	X	0.36	0/635	0.65	0/848
25	Y	0.37	0/495	0.61	0/658
26	Z	0.37	0/438	0.59	0/586
27	0	0.35	0/440	0.69	0/588
28	1	0.35	0/424	0.54	0/565
29	2	0.39	0/370	0.77	0/487
30	3	0.35	0/513	0.62	0/676
31	4	0.32	0/303	0.66	0/397

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	5	0.42	0/1001	0.61	0/1350
33	6	0.39	0/531	0.54	0/709
34	a	0.24	0/36725	0.70	3/57285 (0.0%)
35	b	0.37	0/1735	0.53	0/2338
36	c	0.36	0/1651	0.58	0/2225
37	d	0.37	0/1665	0.59	0/2227
38	e	0.36	0/1180	0.61	0/1587
39	f	0.36	0/835	0.65	2/1128 (0.2%)
40	g	0.36	0/1195	0.61	0/1602
41	h	0.34	0/989	0.59	0/1326
42	i	0.39	0/1034	0.68	0/1375
43	j	0.36	0/796	0.65	0/1077
44	k	0.36	0/885	0.60	0/1195
45	l	0.36	0/954	0.69	0/1282
46	m	0.37	0/900	0.64	0/1204
47	n	0.38	0/822	0.65	0/1095
48	o	0.38	0/722	0.74	1/964 (0.1%)
49	p	0.36	0/659	0.61	0/884
50	q	0.37	0/657	0.63	0/881
51	r	0.40	0/544	0.64	0/731
52	s	0.36	0/652	0.61	0/877
53	t	0.37	0/671	0.63	0/888
54	u	0.44	0/550	0.78	0/728
55	v	0.34	1/1747 (0.1%)	0.69	0/2721
55	w	0.46	3/1747 (0.2%)	0.90	5/2721 (0.2%)
56	x	0.21	0/280	0.64	0/433
57	y	0.32	1/1607 (0.1%)	0.67	0/2501
58	z	0.35	0/3086	0.58	0/4175
All	All	0.29	7/164181 (0.0%)	0.68	23/245149 (0.0%)

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	y	1	G	OP3-P	-10.19	1.49	1.61
55	v	0	C	OP3-P	-10.18	1.49	1.61
2	B	1	U	OP3-P	-10.16	1.49	1.61
55	w	1	C	OP3-P	-10.14	1.49	1.61
55	w	117	U	O3'-P	-9.83	1.49	1.61

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	w	17	C	O3'-P-O5'	23.18	148.04	104.00
55	w	17	C	P-O3'-C3'	-13.48	103.52	119.70
55	w	17	C	OP1-P-O3'	-10.56	81.96	105.20
48	o	88	ARG	NE-CZ-NH2	9.56	125.08	120.30
1	A	2712	C	C2'-C3'-O3'	8.01	127.11	109.50

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	269/271 (99%)	242 (90%)	25 (9%)	2 (1%)	19	54
4	D	206/208 (99%)	191 (93%)	14 (7%)	1 (0%)	25	61
5	E	198/200 (99%)	179 (90%)	17 (9%)	2 (1%)	13	46
6	F	175/177 (99%)	155 (89%)	19 (11%)	1 (1%)	22	57
7	G	172/174 (99%)	159 (92%)	13 (8%)	0	100	100
8	H	147/149 (99%)	125 (85%)	19 (13%)	3 (2%)	6	29
9	I	139/141 (99%)	112 (81%)	24 (17%)	3 (2%)	5	27
10	J	139/141 (99%)	131 (94%)	7 (5%)	1 (1%)	19	54
11	K	120/122 (98%)	107 (89%)	9 (8%)	4 (3%)	3	18
12	L	141/143 (99%)	117 (83%)	20 (14%)	4 (3%)	4	21
13	M	134/136 (98%)	126 (94%)	6 (4%)	2 (2%)	8	36
14	N	117/119 (98%)	104 (89%)	11 (9%)	2 (2%)	7	33

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	O	114/116 (98%)	105 (92%)	8 (7%)	1 (1%)	14	49
16	P	112/114 (98%)	97 (87%)	15 (13%)	0	100	100
17	Q	113/115 (98%)	112 (99%)	1 (1%)	0	100	100
18	R	100/102 (98%)	86 (86%)	11 (11%)	3 (3%)	3	20
19	S	107/109 (98%)	98 (92%)	7 (6%)	2 (2%)	6	31
20	T	90/92 (98%)	78 (87%)	10 (11%)	2 (2%)	5	27
21	U	100/102 (98%)	86 (86%)	11 (11%)	3 (3%)	3	20
22	V	90/92 (98%)	84 (93%)	5 (6%)	1 (1%)	12	44
23	W	73/75 (97%)	66 (90%)	7 (10%)	0	100	100
24	X	75/77 (97%)	71 (95%)	4 (5%)	0	100	100
25	Y	58/60 (97%)	53 (91%)	4 (7%)	1 (2%)	7	33
26	Z	54/56 (96%)	51 (94%)	3 (6%)	0	100	100
27	0	53/55 (96%)	48 (91%)	4 (8%)	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%)	55 (89%)	7 (11%)	0	100	100
31	4	36/38 (95%)	30 (83%)	6 (17%)	0	100	100
32	5	129/131 (98%)	99 (77%)	22 (17%)	8 (6%)	1	7
33	6	64/66 (97%)	57 (89%)	6 (9%)	1 (2%)	8	34
35	b	216/218 (99%)	187 (87%)	24 (11%)	5 (2%)	5	26
36	c	204/206 (99%)	184 (90%)	15 (7%)	5 (2%)	4	24
37	d	203/205 (99%)	182 (90%)	19 (9%)	2 (1%)	13	46
38	e	156/157 (99%)	131 (84%)	19 (12%)	6 (4%)	2	15
39	f	98/100 (98%)	85 (87%)	9 (9%)	4 (4%)	2	13
40	g	149/151 (99%)	130 (87%)	12 (8%)	7 (5%)	2	11
41	h	127/129 (98%)	116 (91%)	11 (9%)	0	100	100
42	i	125/127 (98%)	93 (74%)	27 (22%)	5 (4%)	2	14
43	j	96/98 (98%)	73 (76%)	17 (18%)	6 (6%)	1	6
44	k	114/116 (98%)	99 (87%)	10 (9%)	5 (4%)	2	12
45	l	119/121 (98%)	98 (82%)	13 (11%)	8 (7%)	1	5
46	m	113/115 (98%)	103 (91%)	8 (7%)	2 (2%)	7	32

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
47	n	99/101 (98%)	82 (83%)	12 (12%)	5 (5%)	1	10
48	o	86/88 (98%)	78 (91%)	5 (6%)	3 (4%)	3	16
49	p	80/82 (98%)	69 (86%)	9 (11%)	2 (2%)	4	24
50	q	78/80 (98%)	70 (90%)	6 (8%)	2 (3%)	4	23
51	r	63/65 (97%)	53 (84%)	7 (11%)	3 (5%)	2	11
52	s	77/79 (98%)	67 (87%)	10 (13%)	0	100	100
53	t	83/85 (98%)	78 (94%)	3 (4%)	2 (2%)	5	25
54	u	63/65 (97%)	40 (64%)	14 (22%)	9 (14%)	0	1
58	z	391/393 (100%)	352 (90%)	29 (7%)	10 (3%)	4	23
All	All	6219/6322 (98%)	5477 (88%)	602 (10%)	140 (2%)	7	26

5 of 140 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	E	83	VAL
11	K	89	ASN
32	5	55	VAL
32	5	123	ILE
36	c	96	VAL

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%)	208 (96%)	8 (4%)	29	63
4	D	163/163 (100%)	152 (93%)	11 (7%)	13	43
5	E	164/164 (100%)	160 (98%)	4 (2%)	44	74
6	F	148/148 (100%)	144 (97%)	4 (3%)	40	71
7	G	135/135 (100%)	132 (98%)	3 (2%)	47	76
8	H	114/114 (100%)	111 (97%)	3 (3%)	41	72
9	I	109/109 (100%)	105 (96%)	4 (4%)	29	63

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	J	115/115 (100%)	112 (97%)	3 (3%)	41	72
11	K	103/103 (100%)	98 (95%)	5 (5%)	21	54
12	L	102/102 (100%)	92 (90%)	10 (10%)	6	26
13	M	109/109 (100%)	109 (100%)	0	100	100
14	N	99/99 (100%)	97 (98%)	2 (2%)	50	78
15	O	86/86 (100%)	86 (100%)	0	100	100
16	P	99/99 (100%)	99 (100%)	0	100	100
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%)	89 (97%)	3 (3%)	33	67
20	T	79/79 (100%)	77 (98%)	2 (2%)	42	73
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%)	65 (97%)	2 (3%)	36	69
25	Y	55/55 (100%)	55 (100%)	0	100	100
26	Z	47/47 (100%)	46 (98%)	1 (2%)	48	77
27	0	46/46 (100%)	46 (100%)	0	100	100
28	1	46/46 (100%)	45 (98%)	1 (2%)	47	76
29	2	37/37 (100%)	34 (92%)	3 (8%)	9	34
30	3	51/51 (100%)	48 (94%)	3 (6%)	16	47
31	4	34/34 (100%)	33 (97%)	1 (3%)	37	70
32	5	100/100 (100%)	98 (98%)	2 (2%)	50	78
33	6	59/59 (100%)	58 (98%)	1 (2%)	56	81
35	b	180/180 (100%)	179 (99%)	1 (1%)	84	93
36	c	170/170 (100%)	166 (98%)	4 (2%)	44	74
37	d	172/172 (100%)	169 (98%)	3 (2%)	56	81
38	e	120/119 (101%)	114 (95%)	6 (5%)	20	53
39	f	87/87 (100%)	85 (98%)	2 (2%)	45	75
40	g	124/124 (100%)	121 (98%)	3 (2%)	44	74
41	h	104/104 (100%)	100 (96%)	4 (4%)	28	62

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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%)	86 (97%)	3 (3%)	32	66
45	l	102/102 (100%)	98 (96%)	4 (4%)	27	61
46	m	93/93 (100%)	91 (98%)	2 (2%)	47	76
47	n	83/83 (100%)	83 (100%)	0	100	100
48	o	76/76 (100%)	73 (96%)	3 (4%)	27	61
49	p	65/65 (100%)	63 (97%)	2 (3%)	35	68
50	q	74/74 (100%)	71 (96%)	3 (4%)	26	60
51	r	56/56 (100%)	52 (93%)	4 (7%)	12	40
52	s	70/70 (100%)	66 (94%)	4 (6%)	17	49
53	t	65/65 (100%)	62 (95%)	3 (5%)	23	56
54	u	55/55 (100%)	51 (93%)	4 (7%)	11	39
58	z	325/325 (100%)	317 (98%)	8 (2%)	42	73
All	All	5165/5164 (100%)	5011 (97%)	154 (3%)	37	69

5 of 154 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
44	k	126	ARG
54	u	32	ARG
45	l	88	ASP
50	q	63	CYS
58	z	136	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
18	R	11	GLN
20	T	70	HIS
53	t	69	ASN
45	l	72	ASN
15	O	100	HIS

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2892/2903 (99%)	793 (27%)	79 (2%)
2	B	119/120 (99%)	33 (27%)	4 (3%)
34	a	1536/1540 (99%)	435 (28%)	0
55	v	76/77 (98%)	17 (22%)	0
55	w	76/77 (98%)	35 (46%)	0
56	x	11/12 (91%)	1 (9%)	0
57	y	74/76 (97%)	28 (37%)	0
All	All	4784/4805 (99%)	1342 (28%)	83 (1%)

5 of 1342 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	2	G
1	A	3	U
1	A	4	U
1	A	5	A
1	A	6	A

5 of 83 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	1857	G
1	A	2566	A
1	A	1918	A
1	A	2333	A
1	A	2803	G

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

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	55	57	18,21,22	1.39	2 (11%)	21,30,33	2.10	5 (23%)
57	PSU	y	32	57,60	18,21,22	1.37	2 (11%)	21,30,33	2.05	5 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
34	UR3	a	1498	34	19,22,23	1.14	1 (5%)	26,32,35	2.01	5 (19%)
1	H2U	A	2449	1	18,21,22	0.95	2 (11%)	19,30,33	1.74	4 (21%)
34	4OC	a	1402	34	20,23,24	0.85	2 (10%)	25,32,35	1.32	4 (16%)
34	MA6	a	1518	34,60	19,26,27	1.52	4 (21%)	18,38,41	2.56	5 (27%)
1	5MC	A	1962	1	19,22,23	2.00	2 (10%)	26,32,35	1.54	4 (15%)
34	5MC	a	967	34	19,22,23	2.04	2 (10%)	26,32,35	1.55	5 (19%)
1	2MG	A	2445	1,60	18,26,27	0.95	1 (5%)	16,38,41	1.53	3 (18%)
34	MA6	a	1519	34	19,26,27	1.45	4 (21%)	18,38,41	2.46	6 (33%)
1	PSU	A	955	1	18,21,22	1.41	2 (11%)	21,30,33	2.06	4 (19%)
1	6MZ	A	1618	1	17,25,26	1.08	2 (11%)	15,36,39	2.38	5 (33%)
55	4SU	w	8	55	18,21,22	1.82	5 (27%)	25,30,33	2.22	5 (20%)
1	OMC	A	2498	1,60	19,22,23	0.84	0	25,31,34	1.21	2 (8%)
55	5MU	v	54	55	19,22,23	1.47	4 (21%)	27,32,35	1.94	8 (29%)
1	PSU	A	1917	1	18,21,22	1.45	2 (11%)	21,30,33	2.07	5 (23%)
55	H2U	w	20	55	18,21,22	0.82	1 (5%)	19,30,33	1.57	2 (10%)
1	2MG	A	1835	1	18,26,27	1.03	2 (11%)	16,38,41	1.26	2 (12%)
57	H2U	y	16	57	18,21,22	0.81	1 (5%)	19,30,33	1.38	4 (21%)
1	OMG	A	2251	1,55,60	19,26,27	1.03	2 (10%)	21,38,41	1.09	2 (9%)
1	PSU	A	2457	1,60	18,21,22	1.44	2 (11%)	21,30,33	2.04	5 (23%)
1	PSU	A	2504	1	18,21,22	1.43	2 (11%)	21,30,33	2.05	4 (19%)
55	H2U	v	20	55	18,21,22	0.82	1 (5%)	19,30,33	1.68	3 (15%)
57	H2U	y	20	57	18,21,22	0.87	1 (5%)	19,30,33	1.48	4 (21%)
57	PSU	y	39	57	18,21,22	1.41	2 (11%)	21,30,33	1.99	4 (19%)
57	MIA	y	37	57	23,30,32	2.31	5 (21%)	22,42,47	2.58	7 (31%)
34	5MC	a	1407	34	19,22,23	2.02	2 (10%)	26,32,35	1.62	5 (19%)
1	PSU	A	2605	1	18,21,22	1.40	2 (11%)	21,30,33	2.05	4 (19%)
55	PSU	v	55	55	18,21,22	1.38	2 (11%)	21,30,33	2.03	5 (23%)
1	2MA	A	2503	1,60	17,25,26	1.12	2 (11%)	16,37,40	1.32	3 (18%)
34	2MG	a	966	34	18,26,27	1.04	1 (5%)	16,38,41	2.12	5 (31%)
1	5MU	A	1939	1	19,22,23	1.48	4 (21%)	27,32,35	2.05	8 (29%)
1	PSU	A	2580	1	18,21,22	1.53	2 (11%)	21,30,33	2.13	5 (23%)
1	6MZ	A	2030	1,60	17,25,26	1.07	2 (11%)	15,36,39	2.38	5 (33%)
55	5MU	w	54	55	19,22,23	1.50	4 (21%)	27,32,35	2.07	10 (37%)
1	7MG	A	2069	1,60	23,26,27	1.43	2 (8%)	27,39,42	2.53	11 (40%)
1	5MC	A	747	1	19,22,23	1.91	2 (10%)	26,32,35	1.54	5 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
55	4SU	v	7	55	18,21,22	1.81	4 (22%)	25,30,33	2.36	6 (24%)
57	4SU	y	8	57	18,21,22	1.85	5 (27%)	25,30,33	2.38	7 (28%)
34	2MG	a	1207	34	18,26,27	0.93	1 (5%)	16,38,41	2.68	5 (31%)
1	PSU	A	2604	1	18,21,22	1.44	2 (11%)	21,30,33	1.94	4 (19%)
57	5MU	y	54	57	19,22,23	1.43	4 (21%)	27,32,35	2.08	7 (25%)
1	PSU	A	746	1,60	18,21,22	1.42	2 (11%)	21,30,33	1.99	4 (19%)
1	OMU	A	2552	1,60	19,22,23	1.31	3 (15%)	25,31,34	2.04	9 (36%)
34	7MG	a	527	34,60	23,26,27	1.41	2 (8%)	27,39,42	2.52	7 (25%)
34	PSU	a	516	34	18,21,22	1.38	2 (11%)	21,30,33	2.16	5 (23%)
34	2MG	a	1516	34	18,26,27	0.96	1 (5%)	16,38,41	1.57	4 (25%)
57	7MG	y	46	57	23,26,27	1.41	3 (13%)	27,39,42	2.46	7 (25%)
55	PSU	w	55	55	18,21,22	1.32	2 (11%)	21,30,33	2.07	5 (23%)
1	3TD	A	1915	1	19,22,23	7.08	14 (73%)	23,32,35	2.02	5 (21%)
1	PSU	A	1911	1	18,21,22	1.44	2 (11%)	21,30,33	2.16	4 (19%)
1	1MG	A	745	1	19,26,27	1.33	3 (15%)	18,39,42	1.84	5 (27%)

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	55	57	-	0/7/25/26	0/2/2/2
57	PSU	y	32	57,60	-	2/7/25/26	0/2/2/2
34	UR3	a	1498	34	-	2/7/25/26	0/2/2/2
1	H2U	A	2449	1	-	0/7/38/39	0/2/2/2
34	4OC	a	1402	34	-	2/9/29/30	0/2/2/2
34	MA6	a	1518	34,60	-	3/7/29/30	0/3/3/3
1	5MC	A	1962	1	-	2/7/25/26	0/2/2/2
34	5MC	a	967	34	-	0/7/25/26	0/2/2/2
1	2MG	A	2445	1,60	-	2/5/27/28	0/3/3/3
34	MA6	a	1519	34	-	2/7/29/30	0/3/3/3
1	PSU	A	955	1	-	0/7/25/26	0/2/2/2
1	6MZ	A	1618	1	-	0/5/27/28	0/3/3/3
55	4SU	w	8	55	-	6/7/25/26	0/2/2/2
1	OMC	A	2498	1,60	-	0/9/27/28	0/2/2/2
55	5MU	v	54	55	-	2/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	A	1917	1	-	2/7/25/26	0/2/2/2
55	H2U	w	20	55	-	1/7/38/39	0/2/2/2
1	2MG	A	1835	1	-	0/5/27/28	0/3/3/3
57	H2U	y	16	57	-	2/7/38/39	0/2/2/2
1	OMG	A	2251	1,55,60	-	0/5/27/28	0/3/3/3
1	PSU	A	2457	1,60	-	2/7/25/26	0/2/2/2
1	PSU	A	2504	1	-	2/7/25/26	0/2/2/2
55	H2U	v	20	55	-	0/7/38/39	0/2/2/2
57	H2U	y	20	57	-	2/7/38/39	0/2/2/2
57	PSU	y	39	57	-	0/7/25/26	0/2/2/2
57	MIA	y	37	57	-	4/10/32/34	0/3/3/3
34	5MC	a	1407	34	-	0/7/25/26	0/2/2/2
1	PSU	A	2605	1	-	0/7/25/26	0/2/2/2
55	PSU	v	55	55	-	2/7/25/26	0/2/2/2
1	2MA	A	2503	1,60	-	3/3/25/26	0/3/3/3
34	2MG	a	966	34	-	3/5/27/28	0/3/3/3
1	5MU	A	1939	1	-	1/7/25/26	0/2/2/2
1	PSU	A	2580	1	-	0/7/25/26	0/2/2/2
1	6MZ	A	2030	1,60	-	3/5/27/28	0/3/3/3
55	5MU	w	54	55	-	0/7/25/26	0/2/2/2
1	7MG	A	2069	1,60	-	2/7/37/38	0/3/3/3
1	5MC	A	747	1	-	0/7/25/26	0/2/2/2
55	4SU	v	7	55	-	2/7/25/26	0/2/2/2
57	4SU	y	8	57	-	1/7/25/26	0/2/2/2
34	2MG	a	1207	34	-	1/5/27/28	0/3/3/3
1	PSU	A	2604	1	-	0/7/25/26	0/2/2/2
57	5MU	y	54	57	-	0/7/25/26	0/2/2/2
1	PSU	A	746	1,60	-	1/7/25/26	0/2/2/2
1	OMU	A	2552	1,60	-	2/9/27/28	0/2/2/2
34	7MG	a	527	34,60	-	2/7/37/38	0/3/3/3
34	PSU	a	516	34	-	2/7/25/26	0/2/2/2
34	2MG	a	1516	34	-	0/5/27/28	0/3/3/3
57	7MG	y	46	57	-	4/7/37/38	0/3/3/3
55	PSU	w	55	55	-	1/7/25/26	0/2/2/2
1	3TD	A	1915	1	-	4/7/25/26	0/2/2/2
1	PSU	A	1911	1	-	0/7/25/26	0/2/2/2
1	1MG	A	745	1	-	0/3/25/26	0/3/3/3

The worst 5 of 131 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1915	3TD	O4'-C1'	16.51	1.66	1.43
1	A	1915	3TD	C6-C5	15.64	1.52	1.35
1	A	1915	3TD	C2'-C1'	-14.44	1.34	1.53
1	A	1915	3TD	C2-N1	8.58	1.47	1.37
34	a	967	5MC	C5-C4	7.69	1.49	1.44

The worst 5 of 262 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	a	527	7MG	N9-C4-N3	8.12	137.35	125.46
57	y	46	7MG	N9-C4-N3	8.09	137.32	125.46
34	a	1207	2MG	N1-C2-N2	7.72	124.44	116.56
57	y	37	MIA	C12-C13-C14	-7.51	113.53	127.01
1	A	2069	7MG	N9-C4-N3	7.39	136.29	125.46

There are no chirality outliers.

5 of 72 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1915	3TD	O4'-C1'-C5-C4
1	A	1915	3TD	O4'-C1'-C5-C6
1	A	1915	3TD	C3'-C4'-C5'-O5'
1	A	1915	3TD	O4'-C4'-C5'-O5'
1	A	1917	PSU	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 1912 ligands modelled in this entry, 1909 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	$\# Z > 2$
59	FME	A	3001	-	8,9,10	0.63	0	8,9,11	1.92	2 (25%)
63	GNP	z	402	60	29,34,34	2.58	6 (20%)	33,54,54	1.93	9 (27%)
62	PHE	z	401	-	10,11,12	0.45	0	8,13,15	0.17	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
59	FME	A	3001	-	-	2/7/9/11	-
63	GNP	z	402	60	-	2/14/38/38	0/3/3/3
62	PHE	z	401	-	-	1/5/6/8	0/1/1/1

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
63	z	402	GNP	PG-O1G	10.09	1.61	1.46
63	z	402	GNP	C5-C6	4.46	1.49	1.41
63	z	402	GNP	PG-N3B	4.42	1.74	1.63
63	z	402	GNP	PB-N3B	4.23	1.74	1.63
63	z	402	GNP	PG-O2G	-3.25	1.48	1.56

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
63	z	402	GNP	C2-N3-C4	5.32	121.22	115.48
63	z	402	GNP	C2-N1-C6	4.14	121.71	115.96
59	A	3001	FME	C-CA-N	4.03	117.28	109.50
63	z	402	GNP	N3-C2-N1	-3.56	122.68	127.21
63	z	402	GNP	C5-C6-N1	-3.33	118.96	123.42

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
59	A	3001	FME	O1-CN-N-CA
62	z	401	PHE	O-C-CA-CB

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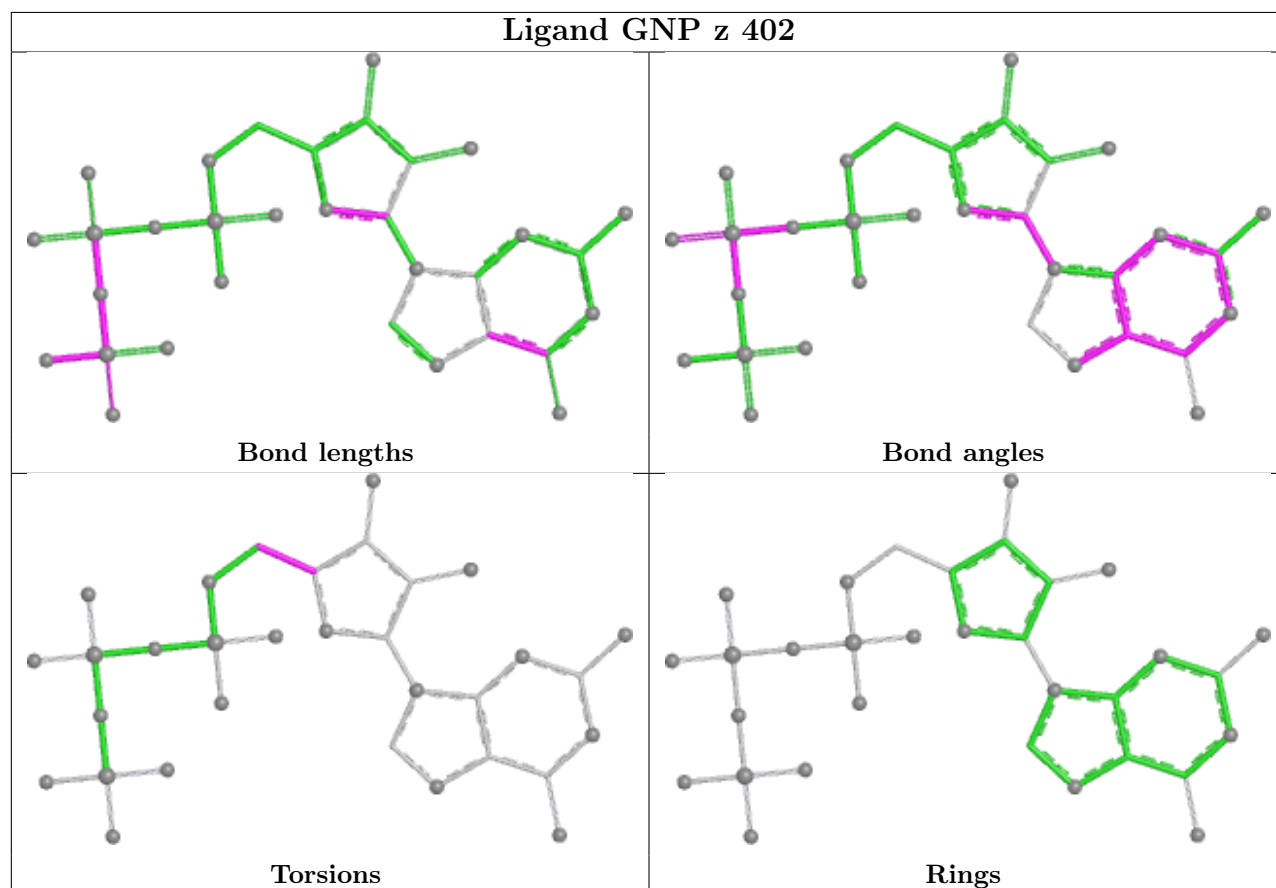
Continued from previous page...

Mol	Chain	Res	Type	Atoms
63	z	402	GNP	O4'-C4'-C5'-O5'
63	z	402	GNP	C3'-C4'-C5'-O5'
59	A	3001	FME	CA-CB-CG-SD

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	2030:6MZ	O3'	2031:A	P	2.28
1	A	1618:6MZ	O3'	1619:G	P	1.81

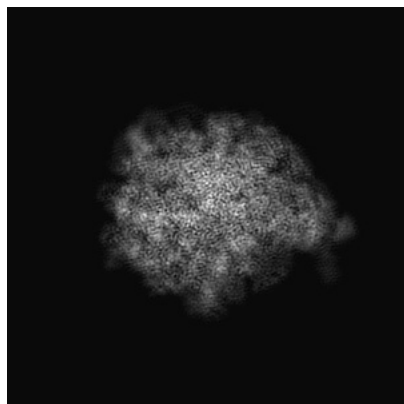
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8813. These allow visual inspection of the internal detail of the map and identification of artifacts.

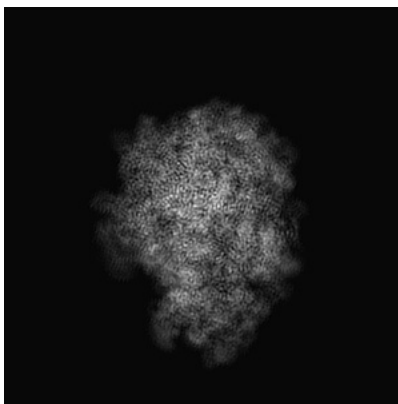
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

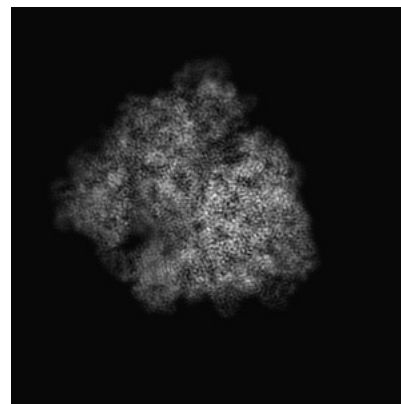
6.1.1 Primary map



X

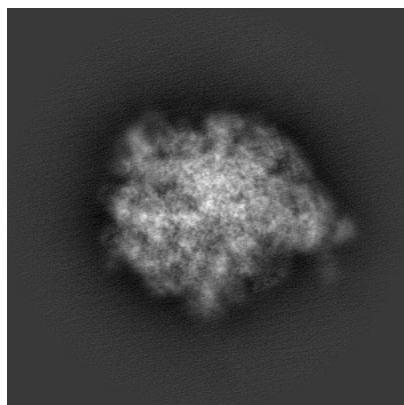


Y

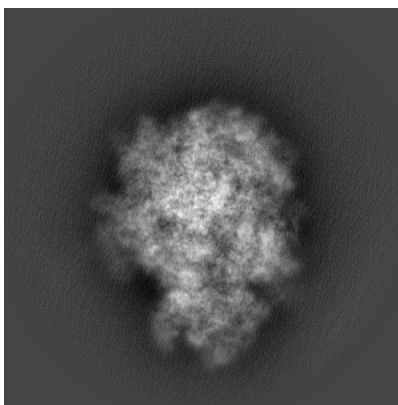


Z

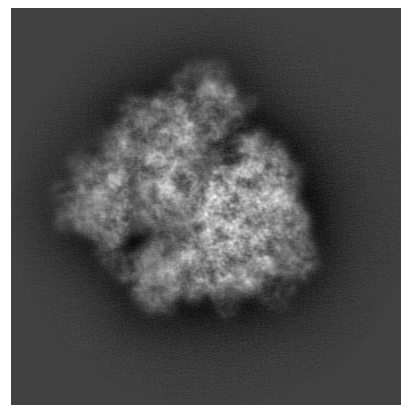
6.1.2 Raw map



X



Y

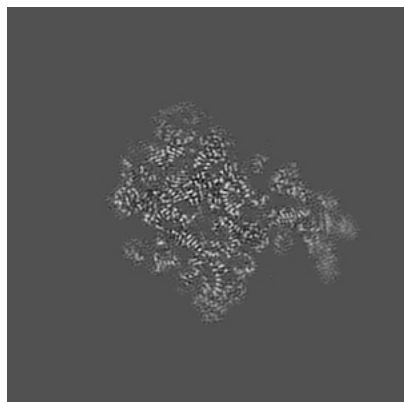


Z

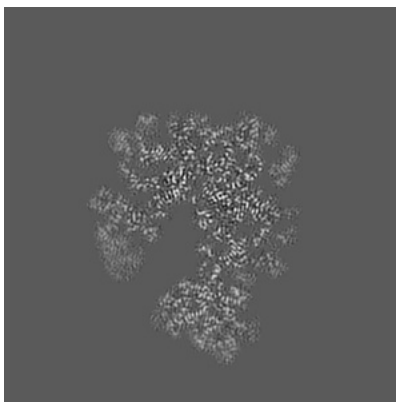
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

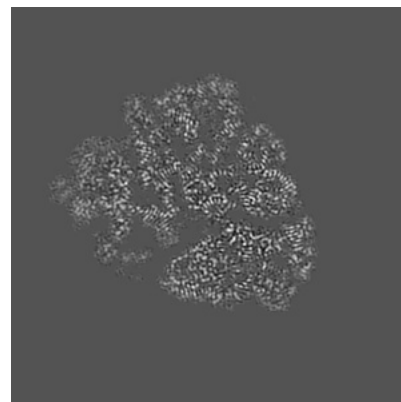
6.2.1 Primary map



X Index: 199

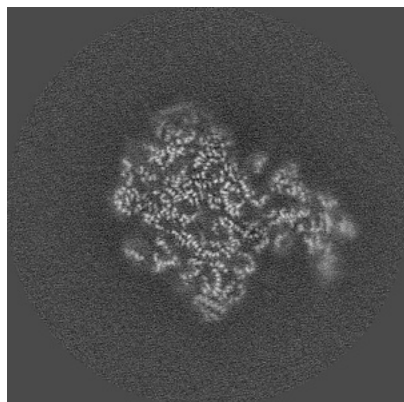


Y Index: 199

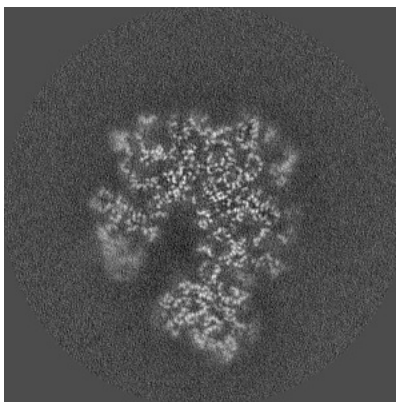


Z Index: 199

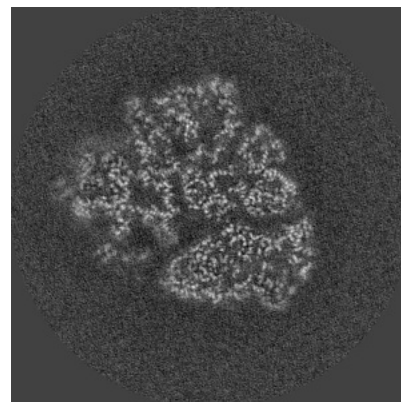
6.2.2 Raw map



X Index: 199



Y Index: 199

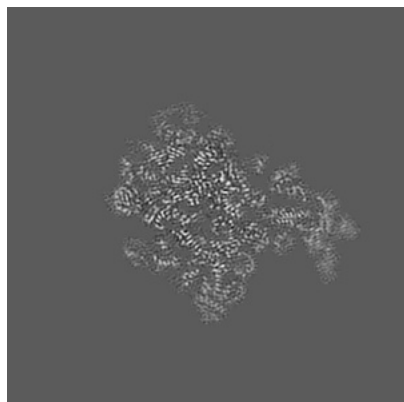


Z Index: 199

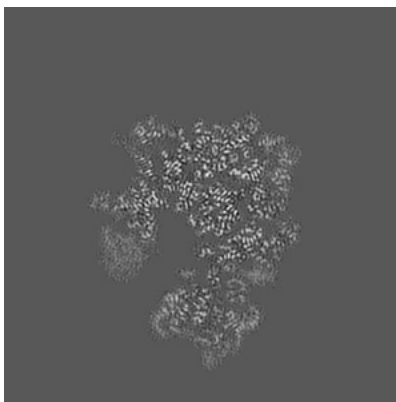
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

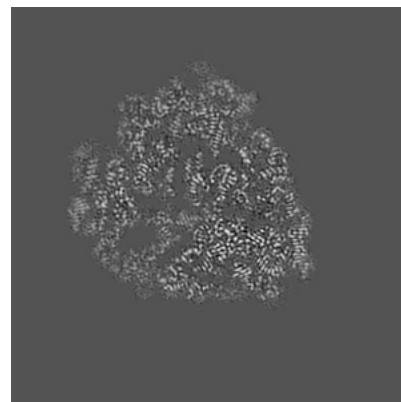
6.3.1 Primary map



X Index: 200

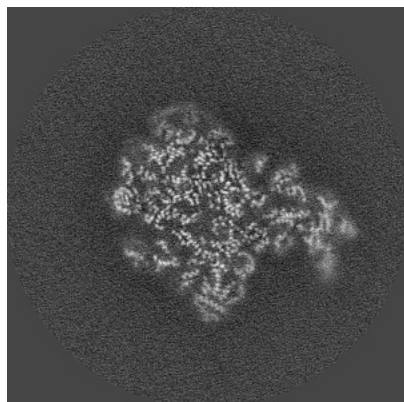


Y Index: 208

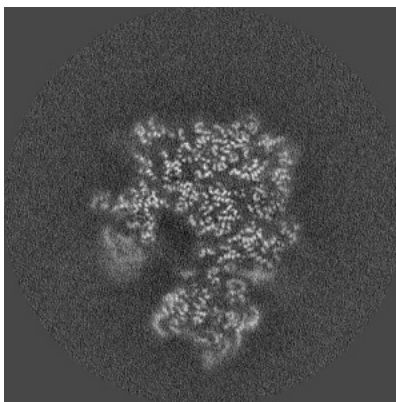


Z Index: 191

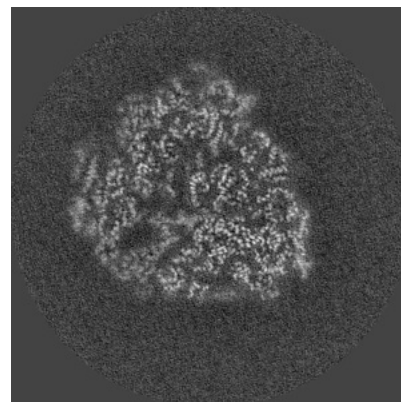
6.3.2 Raw map



X Index: 200



Y Index: 208

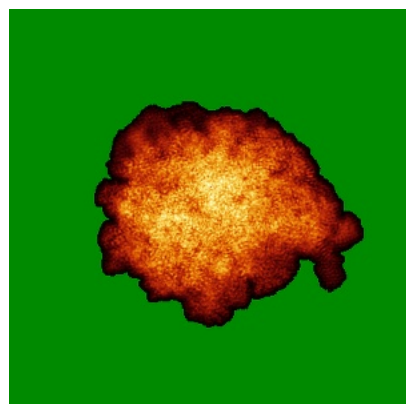


Z Index: 190

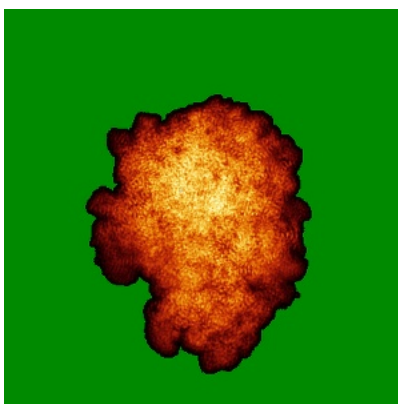
The images above show the largest variance slices of the map in three orthogonal directions.

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

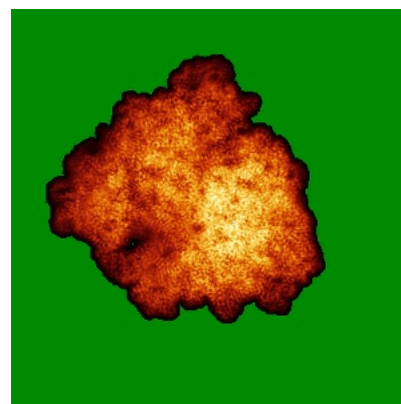
6.4.1 Primary map



X

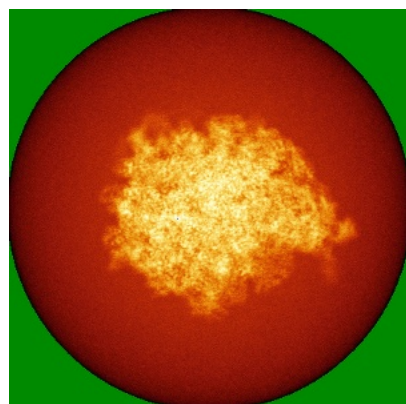


Y

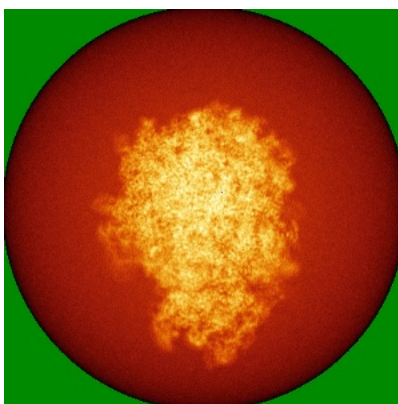


Z

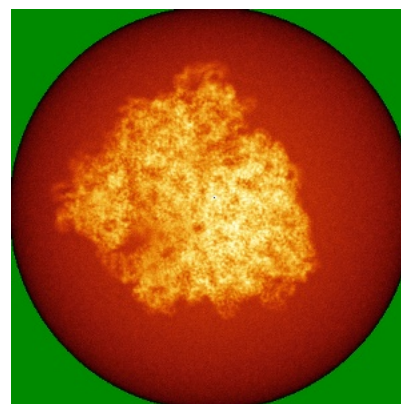
6.4.2 Raw map



X



Y



Z

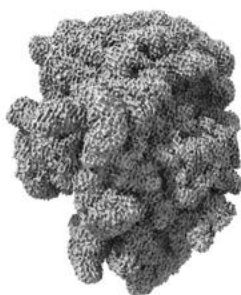
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

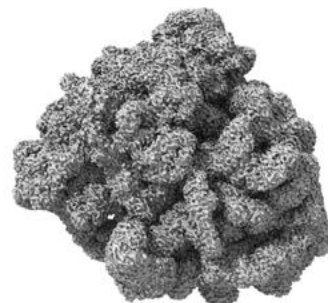
6.5.1 Primary map



X



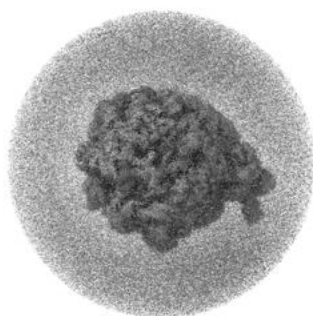
Y



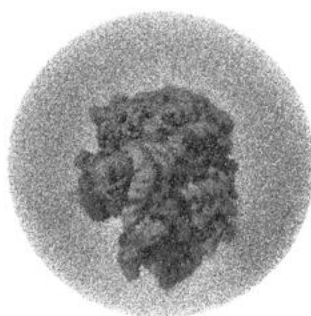
Z

The images above show the 3D surface view of the map at the recommended contour level 0.00558. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

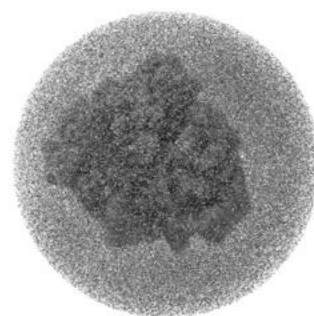
6.5.2 Raw map



X



Y



Z

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

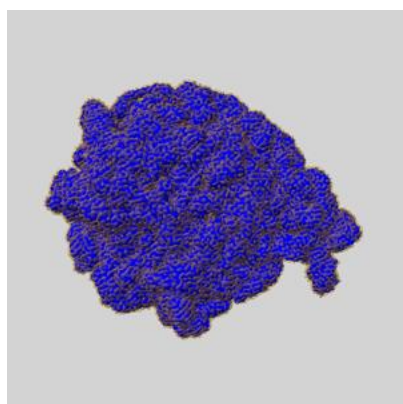
6.6 Mask visualisation [i](#)

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

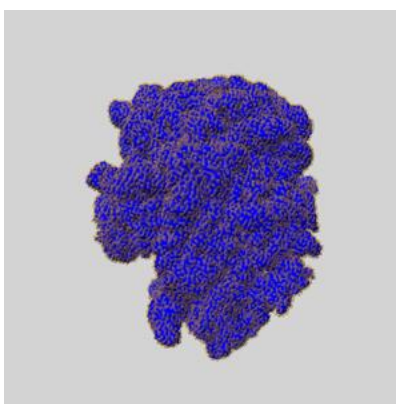
A mask typically either:

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

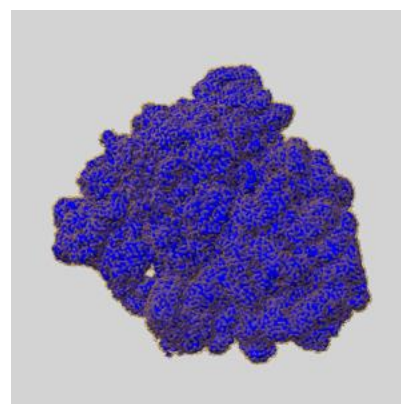
6.6.1 emd_8813_msk_1.map [i](#)



X



Y

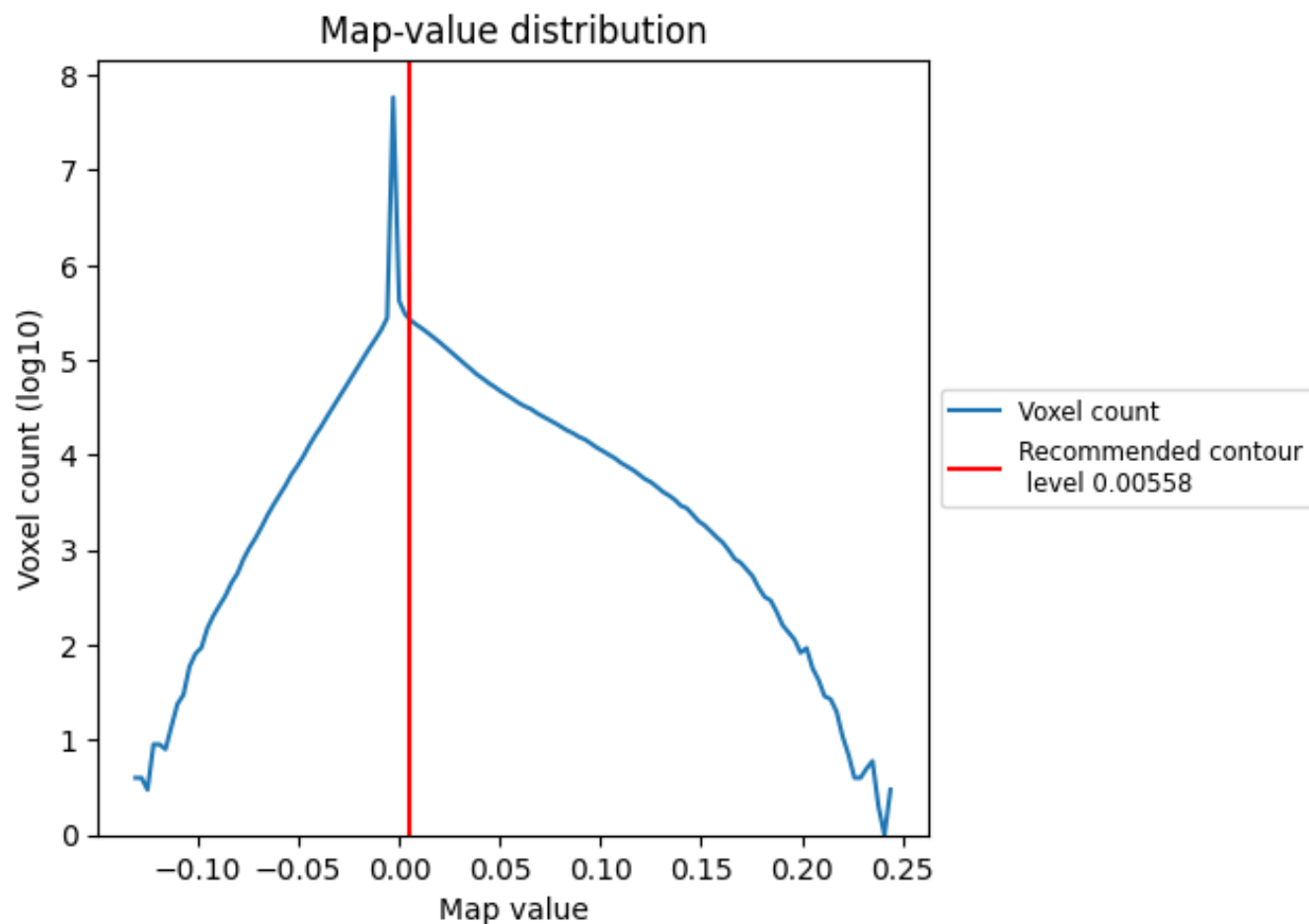


Z

7 Map analysis [i](#)

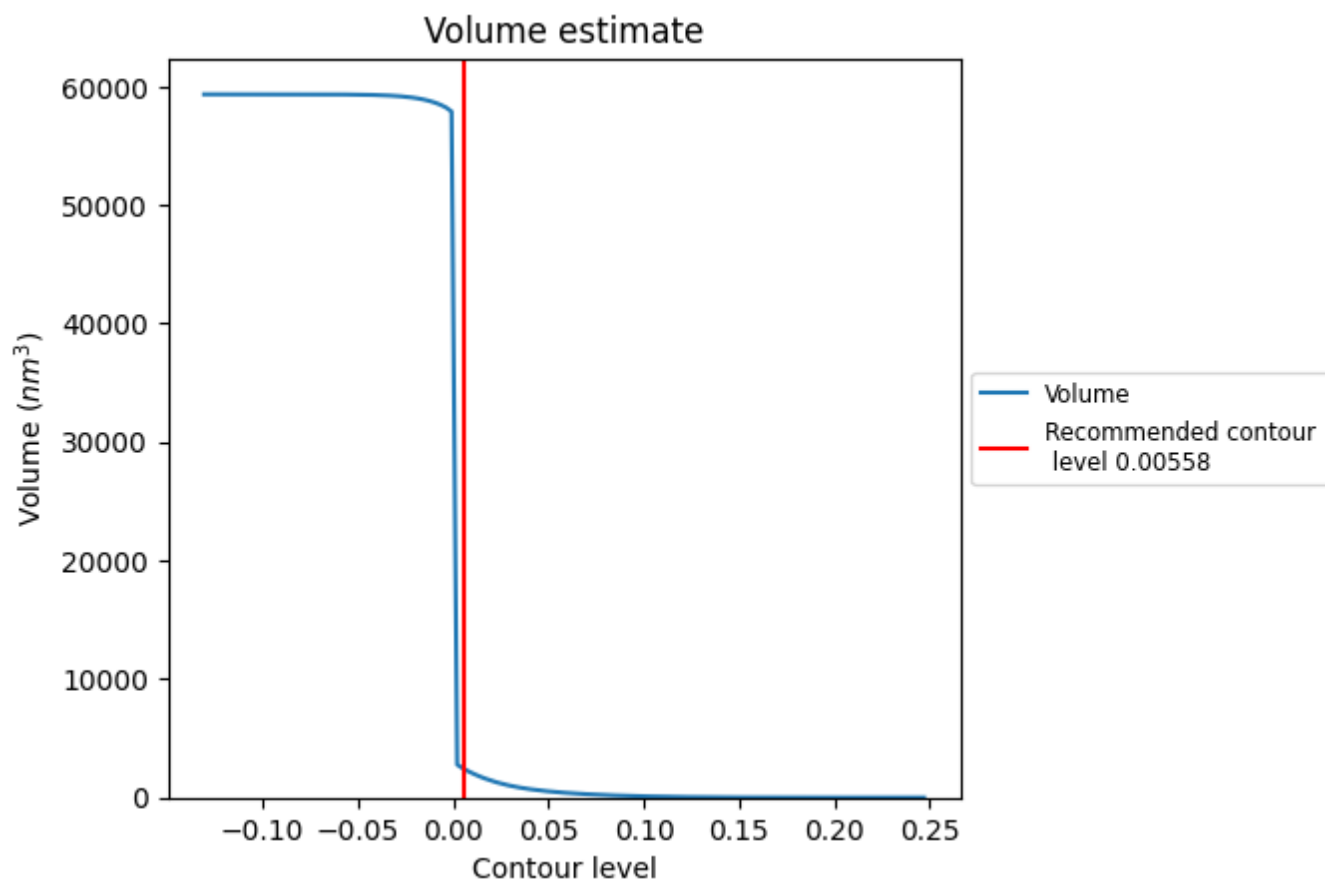
This section contains the results of statistical analysis of the map.

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.

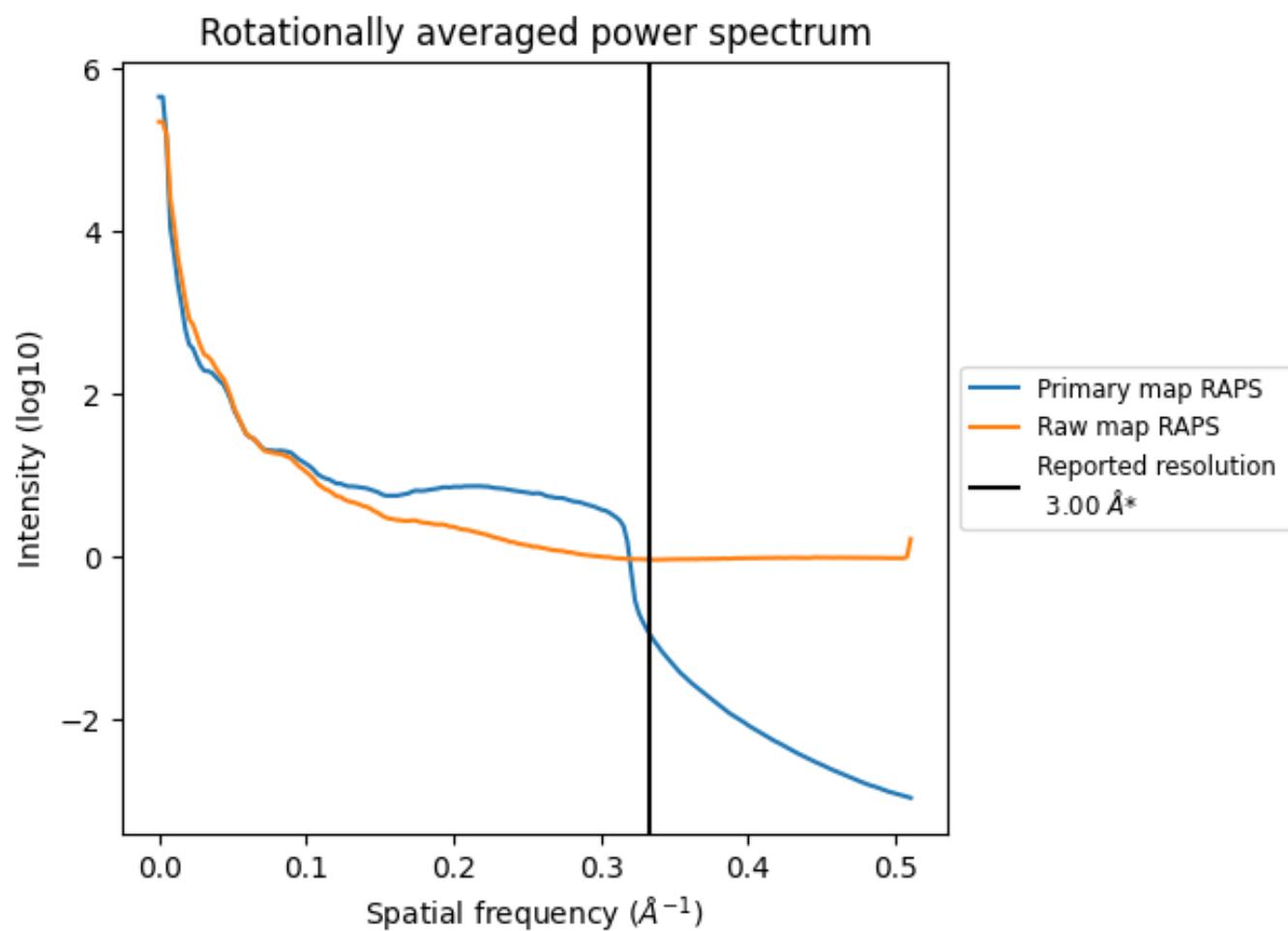
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2421 nm³; this corresponds to an approximate mass of 2187 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 ⓘ

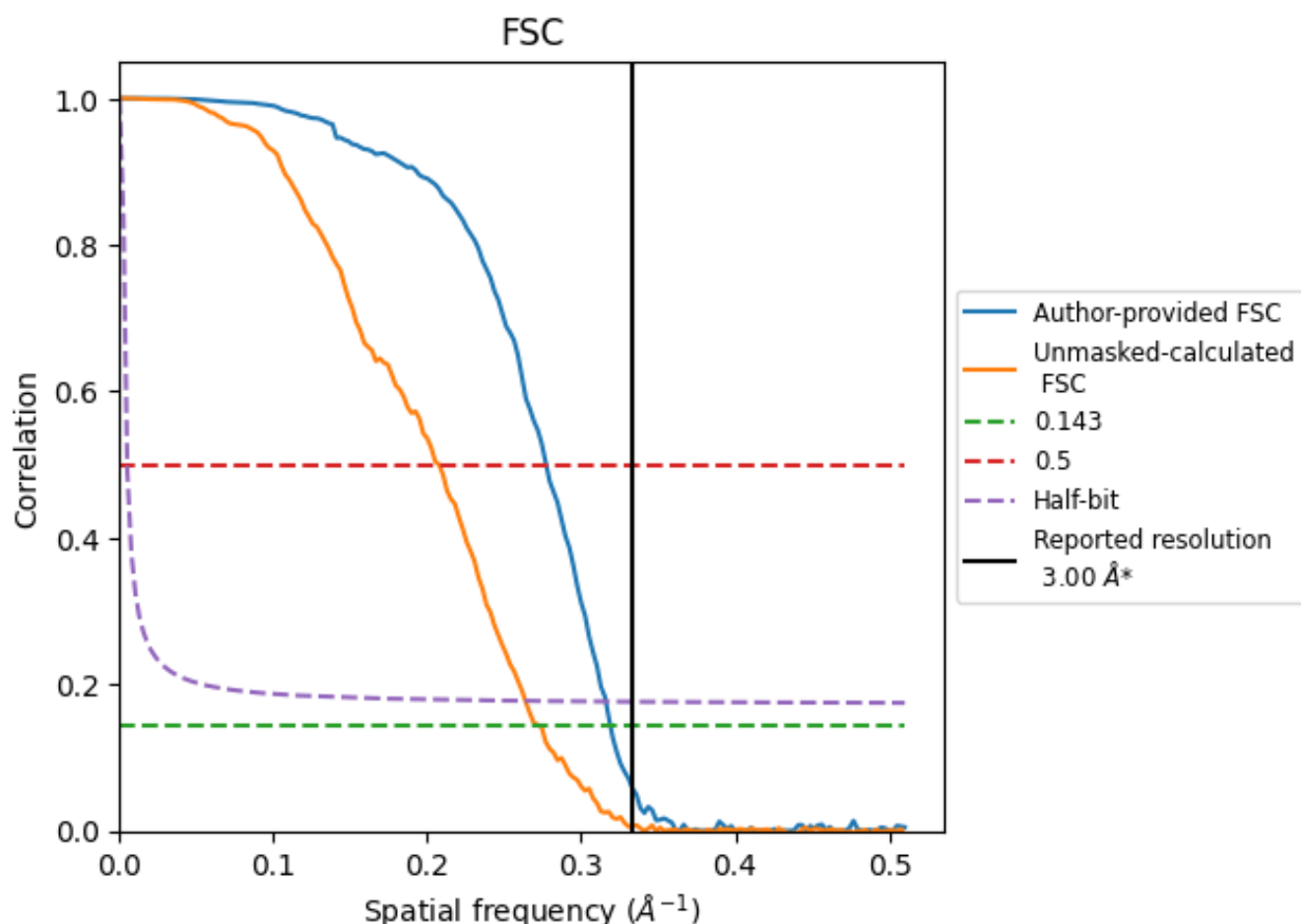


*Reported resolution corresponds to spatial frequency of 0.333 \AA^{-1}

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](#)

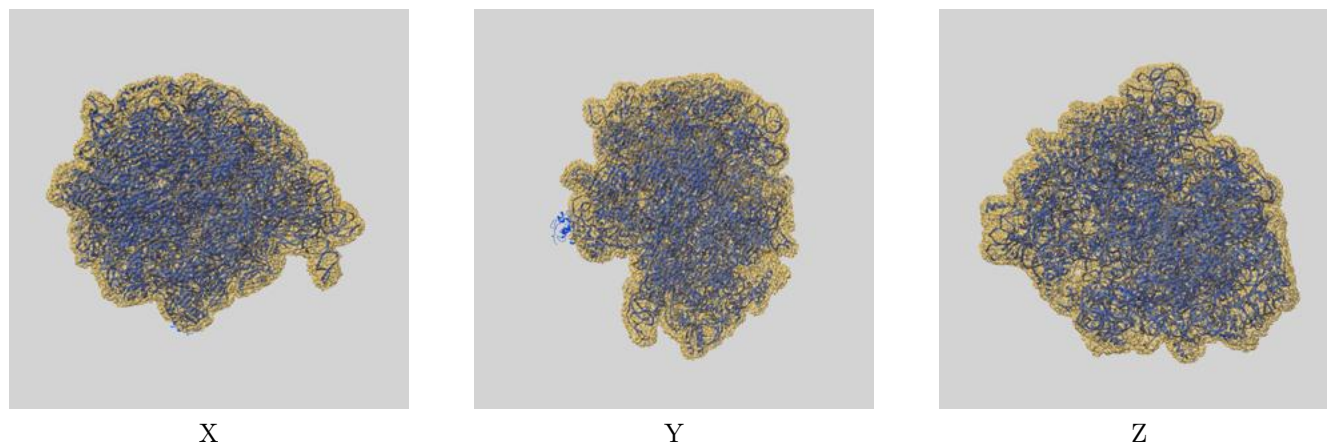
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	3.13	3.61	3.16
Unmasked-calculated*	3.66	4.82	3.79

*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 3.66 differs from the reported value 3.0 by more than 10 %

9 Map-model fit [i](#)

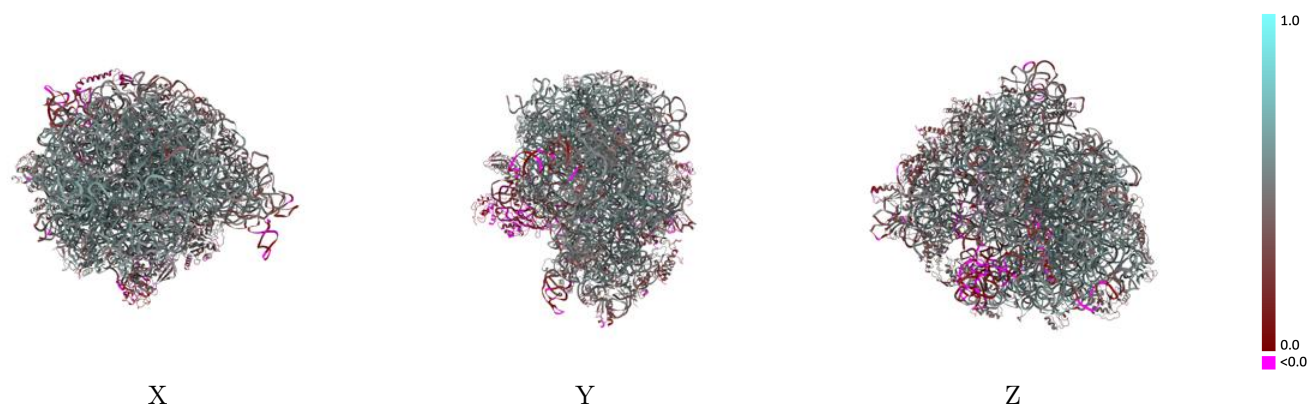
This section contains information regarding the fit between EMDB map EMD-8813 and PDB model 5WDT. Per-residue inclusion information can be found in section [3](#) on page [20](#).

9.1 Map-model overlay [i](#)



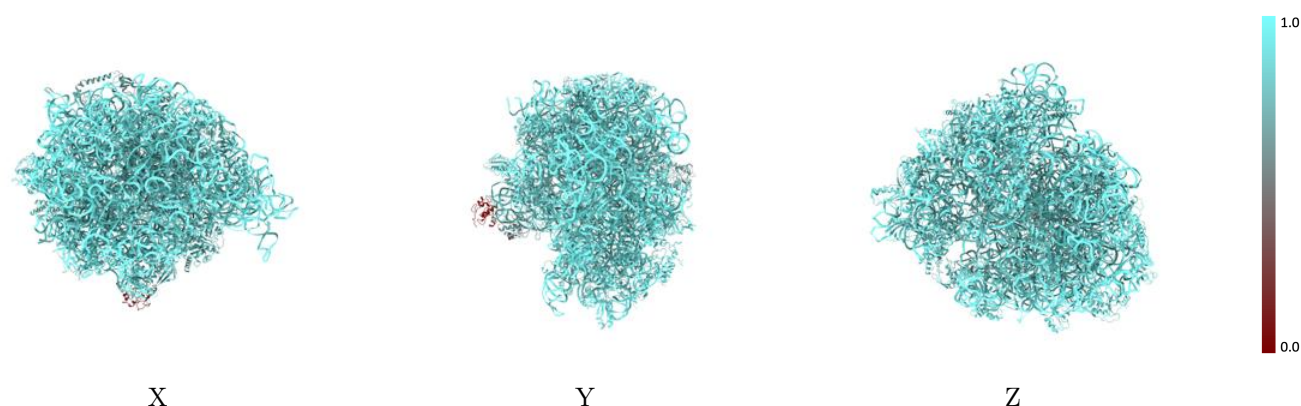
The images above show the 3D surface view of the map at the recommended contour level 0.00558 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



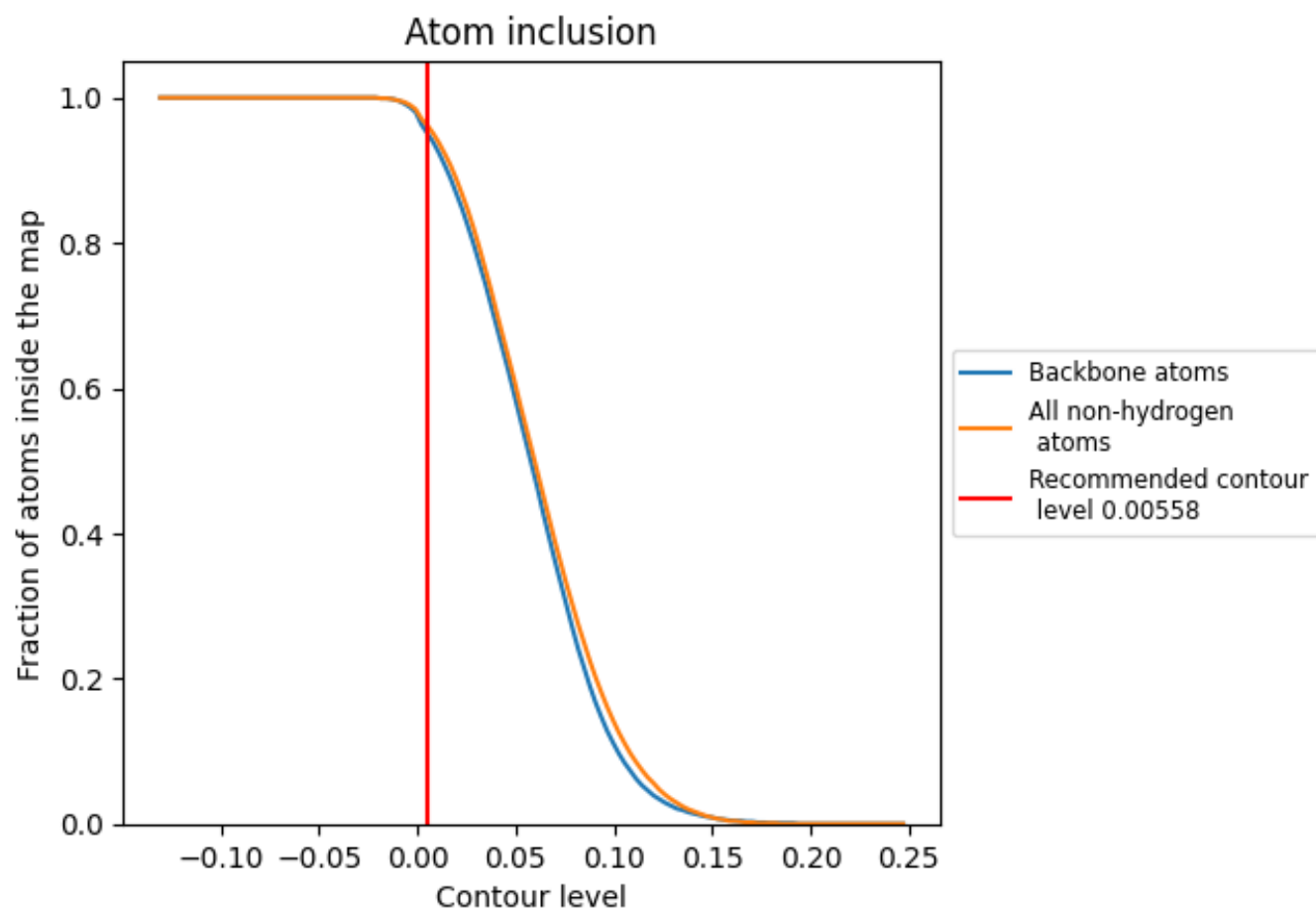
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.00558).







































































9.4 Atom inclusion [i](#)



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 (0.00558) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9600	 0.4690
0	 0.9430	 0.4710
1	 0.9540	 0.4730
2	 0.9680	 0.5660
3	 0.9680	 0.5520
4	 0.9760	 0.5170
5	 0.1950	 0.0080
6	 0.8810	 0.2830
A	 0.9860	 0.5100
B	 0.9950	 0.5060
C	 0.9660	 0.5260
D	 0.9680	 0.5190
E	 0.9510	 0.4730
F	 0.9270	 0.3960
G	 0.9410	 0.3910
H	 0.7410	 0.1690
I	 0.6250	 0.0170
J	 0.9720	 0.5140
K	 0.9380	 0.4980
L	 0.9460	 0.4800
M	 0.9550	 0.4980
N	 0.9690	 0.5250
O	 0.9570	 0.4340
P	 0.9400	 0.4850
Q	 0.9720	 0.5400
R	 0.9390	 0.4660
S	 0.9430	 0.5010
T	 0.9300	 0.4440
U	 0.9480	 0.4300
V	 0.9380	 0.4460
W	 0.9680	 0.5310
X	 0.9520	 0.5040
Y	 0.9300	 0.4080
Z	 0.9510	 0.4930
a	 0.9900	 0.4890



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Chain	Atom inclusion	Q-score
b	 0.9040	 0.3380
c	 0.9450	 0.4310
d	 0.9350	 0.4110
e	 0.9440	 0.4610
f	 0.9150	 0.3890
g	 0.9150	 0.3550
h	 0.9510	 0.4730
i	 0.9220	 0.3720
j	 0.9260	 0.3410
k	 0.9470	 0.4480
l	 0.9450	 0.4870
m	 0.9400	 0.4100
n	 0.9550	 0.4370
o	 0.9540	 0.4570
p	 0.9310	 0.4280
q	 0.9290	 0.4380
r	 0.9180	 0.4040
s	 0.9530	 0.4390
t	 0.9430	 0.4210
u	 0.8110	 0.2700
v	 0.9680	 0.4680
w	 0.8190	 0.1030
x	 0.9840	 0.4830
y	 0.9490	 0.3620
z	 0.8850	 0.3280