

wwPDB EM Validation Summary Report (i)

Feb 25, 2024 – 11:36 PM EST

PDB ID : 6WD4

EMDB ID : EMD-21623

Title: Cryo-EM of elongating ribosome with EF-Tu*GTP elucidates tRNA proof-

reading (Cognate Structure II-B2)

Authors: Loveland, A.B.; Demo, G.; Korostelev, A.A.

Deposited on : 2020-03-31

Resolution : 3.70 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 (i) symbol.

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

The following versions of software and data (see references (1)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev70

Mogul : 1.8.5 (274361), CSD as541be (2020)

MolProbity : 4.02b-467 buster-report : 1.1.7 (2018)

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

MapQ : 1.9.13

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

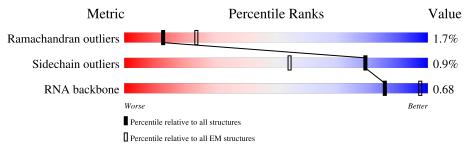
Validation Pipeline (wwPDB-VP) : 2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $ELECTRON\ MICROSCOPY$

The reported resolution of this entry is 3.70 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 $(\# \mathrm{Entries})$	${ m EM~structures} \ (\#{ m Entries})$
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	b	271	97%	
2	c	209	100%	-
3	d	201	99%	
4	e	177	98%	
5	f	176	98%	
6	g	149	7% 98%	
7	h	131	12% 95% 5%	. •
8	i	141	98%	



9 10	j k	142		
	k		99%	•
	11	122	98%	
11	l	143	95% 5%	
12	m	136	99%	
13	n	120	98%	
14		116		
	О		97%	
15	p	114	100% •	
16	q	117	100%	
17	r	103	98%	_
18	s	110	98%	<u>.</u> —
19	t	93	99%	•
20	u	102	95% 5%	
21	v	94	99%	•
22	w	75	100%	•
23	X	77	100%	•
24		63	98%	
	У			
25	Z	58	100%	_
26	В	56	100%	
27	С	50	96%	
28	D	46	100%	_
29	Е	64	97%	•
30	F	38	100%	•
31	G	225	100%	•
32	Н	206	99%	
33	I	205	99%	



Mol	Chain	Length	Quality of chain	
34	J	157	97%	•
35	K	100	91%	9%
36	L	151	100%	
37	M	129	98%	•
38	N	127	95%	5%
39	О	98	95%	5%
40	Р	116	97%	•
41	Q	123	92%	8%
42	R	114	96%	-
43	S	100	98%	
44	Т	88	99%	
45	U		•	•
		82	98%	<u> </u>
46	V	80	96%	•
47	W	65	94%	6%
48	X	79	97%	•
49	Y	85	99%	•
50	Z	65	88% 5%	12%
51	a	223	59% • 40%	
52	3	1539	91%	9%
53	1	2903	88%	12%
54	2	120	92%	8%
55	5	77	92%	8%
55	6	77	92%	8%
56	4	18	83%	17%
57	7	76	82%	18%



Mol	Chain	Length	Quality of chain	
58	8	400	90%	8%



2 Entry composition (i)

There are 61 unique types of molecules in this entry. The entry contains 153083 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

• Molecule 1 is a protein called 50S ribosomal protein L2.

\mathbf{Mol}	Chain	Residues		${f Atoms}$					Trace
1	b	271	Total 2083	C 1288	N 423	O 365	S 7	0	0

• Molecule 2 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	${f Atoms}$					AltConf	Trace
2		209	Total	С	N	О	S	0	0
	C	209	1565	979	288	294	4	0	U

• Molecule 3 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues		At	oms	AltConf	Trace		
3	d	201	Total 1552	C 974	N 283	O 290	S 5	0	0

• Molecule 4 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues		At	oms		AltConf	Trace	
4	e	177	Total 1411	C 899	N 249	O 257	S 6	0	0

• Molecule 5 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues		${f Atoms}$					Trace
5	f	176	Total 1323	C 832	N 243	O 246	S 2	0	0

• Molecule 6 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	CC.	149	Total	С	N	О	S	0	0
0	g	149	1111	699	197	214	1	U	U



• Molecule 7 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues		${f Atoms}$					Trace
7	h	131	Total	С	N	О	S	0	0
'		101	989	625	175	184	5		

• Molecule 8 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues		At	oms			AltConf	Trace
Q	i	141	Total	С	N	О	S	0	0
	1	1,41	1032	651	179	196	6		

• Molecule 9 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues		At	oms			AltConf	Trace
9	j	142	Total 1129	C 714	N 212	O 199	S 4	0	0

• Molecule 10 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues		At	oms	AltConf	Trace		
10	1-	199	Total	С	N	О	S	0	0
10	K	122	939	587	180	166	6	0	U

• Molecule 11 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues		At	oms			AltConf	Trace
11	1	143	Total 1045	C 649	N 206	O 189	S 1	0	0

• Molecule 12 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues		At	oms			AltConf	Trace
12	m	136	Total 1074	C 686	N 205	O 177	S 6	0	0

• Molecule 13 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues		At	oms			AltConf	Trace
13	n	120	Total 961	C 593	N 196	O 167	S 5	0	0

• Molecule 14 is a protein called 50S ribosomal protein L18.



Mo	l Cha	in	Residues		Ato	ms		AltConf	Trace
14	0		116	Total 892	C 552	N 178	O 162	0	0

• Molecule 15 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues		At	oms			AltConf	Trace
15		11/	Total	С	N	О	S	0	0
10	p	114	917	574	179	163	1	U	U

• Molecule 16 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues		Ato	ms	AltConf	Trace	
16	q	117	Total 947	C 604	N 192	O 151	0	0

• Molecule 17 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues		At	oms			AltConf	Trace
17	r	103	Total	С	N	О	S	0	0
11	1	105	816	516	153	145	2	0	U

• Molecule 18 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues		At	oms	AltConf	Trace		
18	s	110	Total 857	C 532	N 166	O 156	S 3	0	0

• Molecule 19 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues		At	oms			AltConf	Trace
10	+	02	Total	С	N	О	S	0	0
19	U	93	739	466	139	132	2	U	U

• Molecule 20 is a protein called 50S ribosomal protein L24.

Mo	l Chain	Residues		Ato	ms	AltConf	Trace	
20	u	102	Total 780	C 492	N 146	O 142	0	0

• Molecule 21 is a protein called 50S ribosomal protein L25.



Mol	Chain	Residues		At	oms	AltConf	Trace		
91	**	0.4	Total	С	N	О	S	0	0
21	V	94	753	479	137	134	3	U	U

• Molecule 22 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues		At	oms	AltConf	Trace		
22	W	75	Total	С	N	0	S	0	0
			575	356	116	102	1		

• Molecule 23 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues		At	oms	AltConf	Trace		
23	х	77	Total 625	C 388	N 129	O 106	S 2	0	0

• Molecule 24 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues		Ato	ms	AltConf	Trace		
24	**	62	Total	С	N	О	S	0	0
24	У	63	509	313	99	95	2	0	U

• Molecule 25 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues		Ato	ms	AltConf	Trace		
25	Z	58	Total 449	C 281	N 87	O 79	S 2	0	0

• Molecule 26 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues		Ato	ms	AltConf	Trace		
26	D	56	Total	С	N	О	S	0	0
20	Б	90	444	269	94	80	1	0	U

• Molecule 27 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues		Aton	ıs	AltConf	Trace	
27	С	50	Total 410	C 263	N 75	O 72	0	0

• Molecule 28 is a protein called 50S ribosomal protein L34.



Mol	Chain	Residues		Ato	ms		AltConf	Trace	
20	D	46	Total	С	N	О	S	0	0
20	ט	40	377	228	90	57	2	0	U

• Molecule 29 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues		Ato	oms	AltConf	Trace		
29	E	64	Total	С	N	О	S	0	0
29	15	04	504	323	105	74	2	U	U

• Molecule 30 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues		Ato	ms	AltConf	Trace		
30	F	38	Total 302	C 185	N 65	O 48	S 4	0	0

• Molecule 31 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues		Ato	AltConf	Trace			
31	G	225	Total 1757	C 1111	N 315	O 323	S 8	0	0

• Molecule 32 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues		Ato	oms		AltConf	Trace	
32	Н	206	Total 1625	C 1028	N 305	O 289	S 3	0	0

• Molecule 33 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues		Ato		AltConf	Trace		
22	T	205	Total	С	N	О	S	0	0
33	1	200	1643	1026	315	298	4		U

• Molecule 34 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues		At	oms	AltConf	Trace		
34	J	157	Total 1157	C 719	N 218	O 214	S 6	0	0

• Molecule 35 is a protein called 30S ribosomal protein S6.



Mol	Chain	Residues		At	oms		AltConf	Trace	
25	I/	100	Total	С	N	О	S	0	0
35	IX.	100	818	515	148	149	6	U	U

• Molecule 36 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues		At	oms	AltConf	Trace		
26	т	151	Total	С	N	О	S	0	0
30	ь	191	1182	735	227	216	4	0	U

• Molecule 37 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues		At	oms		AltConf	Trace	
37	M	129	Total		N	О	S	0	0
	171	120	979	616	173	184	6		

• Molecule 38 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues		At	oms		AltConf	Trace	
20	N	197	Total	С	N	О	S	0	0
30	IN	127	1022	634	206	179	3	0	U

• Molecule 39 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues		At	oms	AltConf	Trace		
39	О	98	Total 787	C 493	N 150	O 143	S 1	0	0

• Molecule 40 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues		At	oms			AltConf	Trace
40	Р	116	Total 870	C 535	N 173	O 159	S 3	0	0

• Molecule 41 is a protein called 30S ribosomal protein S12.

M	ol	Chain	Residues	\mathbf{Atoms}					AltConf	Trace
4	1	Q	123	Total 955	C 590	N 196	O 165	S 4	0	0

• Molecule 42 is a protein called 30S ribosomal protein S13.



Mol	Chain	Residues		At	oms			AltConf	Trace
49	D	11/	Total	С	N	О	S	0	0
42	Λ	114	884	546	178	157	3	U	U

• Molecule 43 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues		At	oms		AltConf	Trace	
43	S	100	Total 805	C 499	N 164	O 139	S 3	0	0

• Molecule 44 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues		At	oms			AltConf	Trace
44	Т	88	Total	С	N	О	S	0	0
	_	00	714	439	144	130	1		

• Molecule 45 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues		At	oms			AltConf	Trace
15	TT	99	Total	С	N	О	S	0	0
45	U	02	649	406	128	114	1	U	U

• Molecule 46 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues		At	oms			AltConf	Trace
16	V	80	Total	С	N	О	S	0	0
40	v	80	649	411	121	114	3	0	U

• Molecule 47 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues		Ato	oms			AltConf	Trace
17	117	65	Total	С	N	О	S	0	0
41	VV	0.0	536	339	100	96	1	U	U

• Molecule 48 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues		At	oms			AltConf	Trace
48	X	79	Total 638	C 408	N 120	O 108	S 2	0	0

• Molecule 49 is a protein called 30S ribosomal protein S20.



Mol	Chain	Residues		At	oms			AltConf	Trace
49	Y	85	Total 665	C 411	N 137	O 114	S 3	0	0

• Molecule 50 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues		Ato	oms			AltConf	Trace
50	7.	65	Total	С	N	О	S	0	0
		00	545	335	117	92	1		

• Molecule 51 is a protein called 50S ribosomal protein L1.

Mol	Chain	Residues		At	oms			AltConf	Trace
51	0	134	Total	С	N	О	S	0	0
91	a	104	1027	645	186	194	2	0	U

• Molecule 52 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues		I	$\mathbf{A}\mathbf{toms}$			AltConf	Trace
52	3	1539	Total 33012	C 14725	N 6052	O 10697	P 1538	0	0

• Molecule 53 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues			Atoms			AltConf	Trace
53	1	2903	Total 62317	C 27801	N 11468	O 20146	P 2902	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	747	С	U	variant	GB 1036415628

• Molecule 54 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues		\mathbf{A}^{1}	toms			AltConf	Trace
54	2	120	Total 2568	C 1145	N 471	O 833	P 119	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2	120	A	-	insertion	GB 1370526515



• Molecule 55 is a RNA chain called tRNAfMet.

Mol	Chain	Residues	${f Atoms}$				AltConf	Trace	
55	5	77	Total	С	N	О	Р	0	0
0.0	3	11	1640	732	297	535	76		
55	6	77	Total	С	N	О	Р	0	0
33	0	11	1640	732	297	535	76	0	0

• Molecule 56 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms				AltConf	Trace	
56	4	18	Total	_	N	0	P	0	0
	_		388	175	76	120	17		

• Molecule 57 is a RNA chain called tRNAPhe.

Mol	Chain	Residues	Atoms				AltConf	Trace	
57	7	76	Total 1619	C 723	N 290	O 531	P 75	0	0

• Molecule 58 is a protein called Elongation factor Tu.

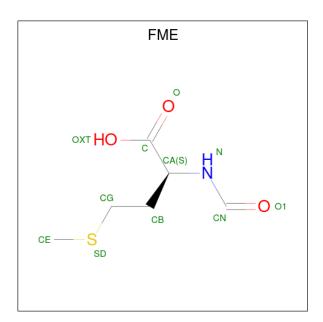
Mol	Chain	Residues	Atoms					AltConf	Trace
58	8	366	Total 2833	C 1796	N 485	O 539	S 13	0	0

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
8	395	SER	-	expression tag	UNP E2QFJ4
8	396	HIS	-	expression tag	UNP E2QFJ4
8	397	HIS	-	expression tag	UNP E2QFJ4
8	398	HIS	-	expression tag	UNP E2QFJ4
8	399	HIS	-	expression tag	UNP E2QFJ4
8	400	HIS	-	expression tag	UNP E2QFJ4
8	401	HIS	-	expression tag	UNP E2QFJ4

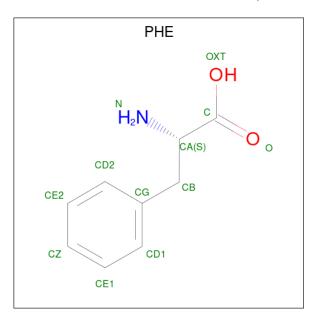
 \bullet Molecule 59 is N-FORMYLMETHIONINE (three-letter code: FME) (formula: $\mathrm{C_6H_{11}NO_3S}).$





Mol	Chain	Residues		Atoms				AltConf
59	5	1	Total	С	N	О	S	0
19	9	1	10	6	1	2	1	0

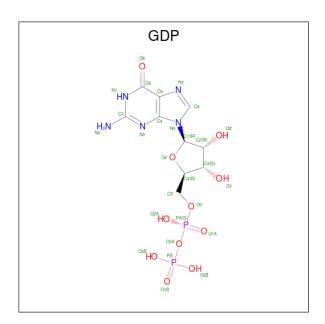
 \bullet Molecule 60 is PHENYLALANINE (three-letter code: PHE) (formula: $\mathrm{C_9H_{11}NO_2}).$



Mol	Chain	Residues	Atoms				AltConf
60	7	1	Total	С	N	О	0
60	1	1	11	9	1	1	U

 \bullet Molecule 61 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2).$





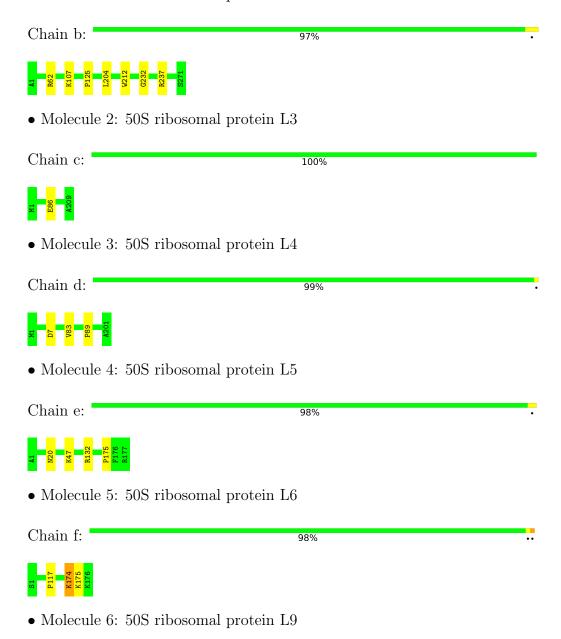
Mol	Chain	Residues		Ato	oms			AltConf
61	0	1	Total	С	N	О	Р	0
01	0	1	28	10	5	11	2	U



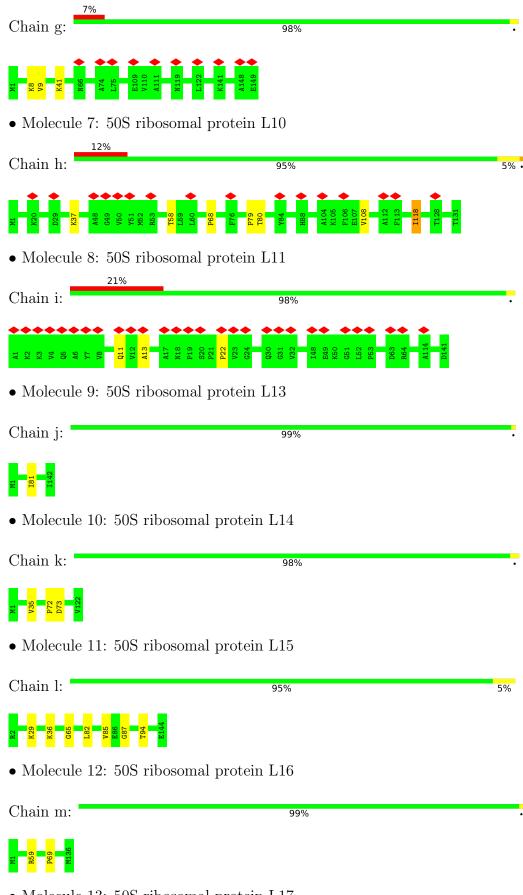
3 Residue-property plots (i)

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: 50S ribosomal protein L2







• Molecule 13: 50S ribosomal protein L17



Chain n: 98% .
MI
• Molecule 14: 50S ribosomal protein L18
Chain o: 97% .
10 10 10 10 10 10 10 10 10 10 10 10 10 1
• Molecule 15: 50S ribosomal protein L19
Chain p: 100%
There are no outlier residues recorded for this chain.
• Molecule 16: 50S ribosomal protein L20
Chain q:
A1177
• Molecule 17: 50S ribosomal protein L21
Chain r: 98%
H
• Molecule 18: 50S ribosomal protein L22
Chain s: 98% .
H H H H H H H H H H H H H H H H H H H
• Molecule 19: 50S ribosomal protein L23
Chain t: 99%
◆◆ ### A Part ### A Part

• Molecule 20: 50S ribosomal protein L24

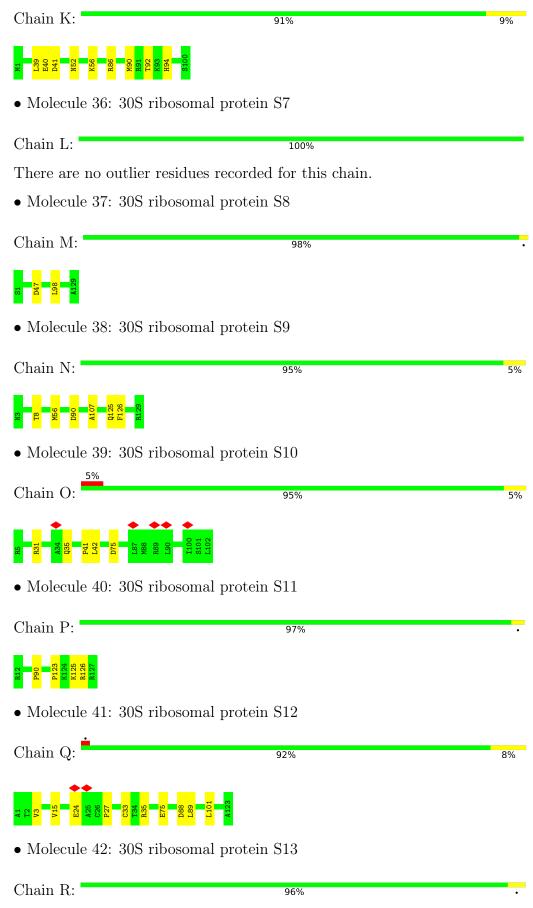


Chain u:	95%	5%
R6 P47 L51	N 102 1102 1102 1102 1102 1102 1102 1102	
• Molecule	21: 50S ribosomal protein L25	
Chain v:	99%	•
M1 D90 A94		
• Molecule	22: 50S ribosomal protein L27	
Chain w:	100%	
There are n	no outlier residues recorded for this chain.	
• Molecule	23: 50S ribosomal protein L28	
Chain x:	100%	
There are a	no outlier residues recorded for this chain.	
• Molecule	24: 50S ribosomal protein L29	
Chain y:	98%	
•		
M1 R7 A63		
M1 R7 A63	25: 50S ribosomal protein L30	
M1 R7 A63	25: 50S ribosomal protein L30	
• Molecule Chain z:		
• Molecule Chain z: There are 1	100%	
• Molecule Chain z: There are 1	no outlier residues recorded for this chain.	
• Molecule Chain z: There are r • Molecule Chain B:	no outlier residues recorded for this chain. 26: 50S ribosomal protein L32	
• Molecule Chain z: There are r • Molecule Chain B: There are r	no outlier residues recorded for this chain. 26: 50S ribosomal protein L32	
• Molecule Chain z: There are r • Molecule Chain B: There are r	100% no outlier residues recorded for this chain. 26: 50S ribosomal protein L32 100% no outlier residues recorded for this chain.	·
 Molecule Chain z: There are r Molecule Chain B: There are r Molecule 	no outlier residues recorded for this chain. 26: 50S ribosomal protein L32 100% no outlier residues recorded for this chain. 27: 50S ribosomal protein L33	

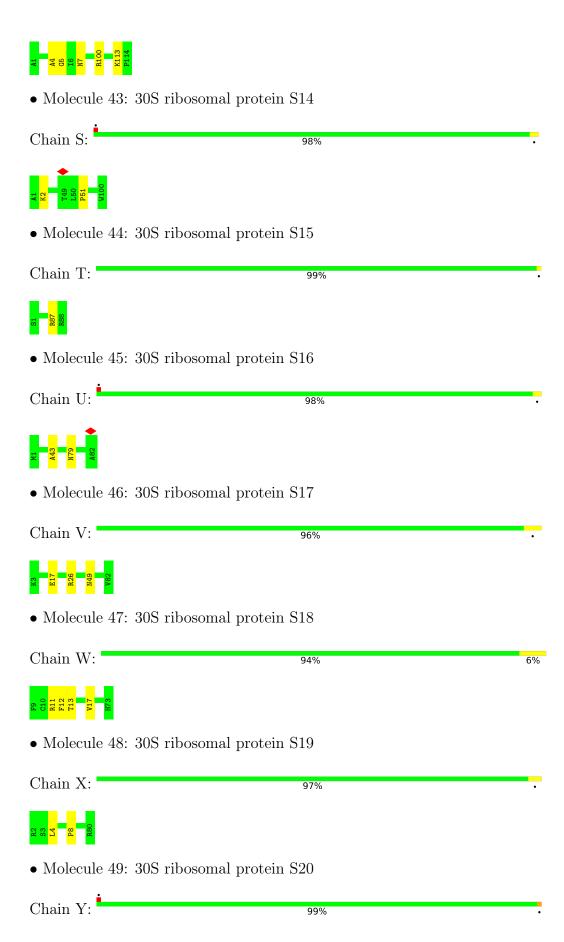


Chain D:
Chain D: 100%
K446
• Molecule 29: 50S ribosomal protein L35
Chain E: 97%
1
• Molecule 30: 50S ribosomal protein L36
Chain F: 100%
There are no outlier residues recorded for this chain.
• Molecule 31: 30S ribosomal protein S2
Chain G: 100%
M122 K127 S228 ◆
• Molecule 32: 30S ribosomal protein S3
Chain H: 99%
L111
• Molecule 33: 30S ribosomal protein S4
Chain I: 99%
M44 K205 K205 K205 K205 K205 K205 K205 K205
• Molecule 34: 30S ribosomal protein S5
Chain J: 97% .
1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
• Molecule 35: 30S ribosomal protein S6













• Molecule 50: 30S ribosomal protein S21

Chain Z: 88% 12%



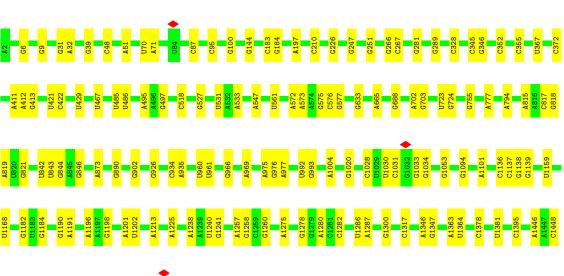
• Molecule 51: 50S ribosomal protein L1

Chain a: 59% • 40%



• Molecule 52: 16S ribosomal RNA

Chain 3: 91% 9%



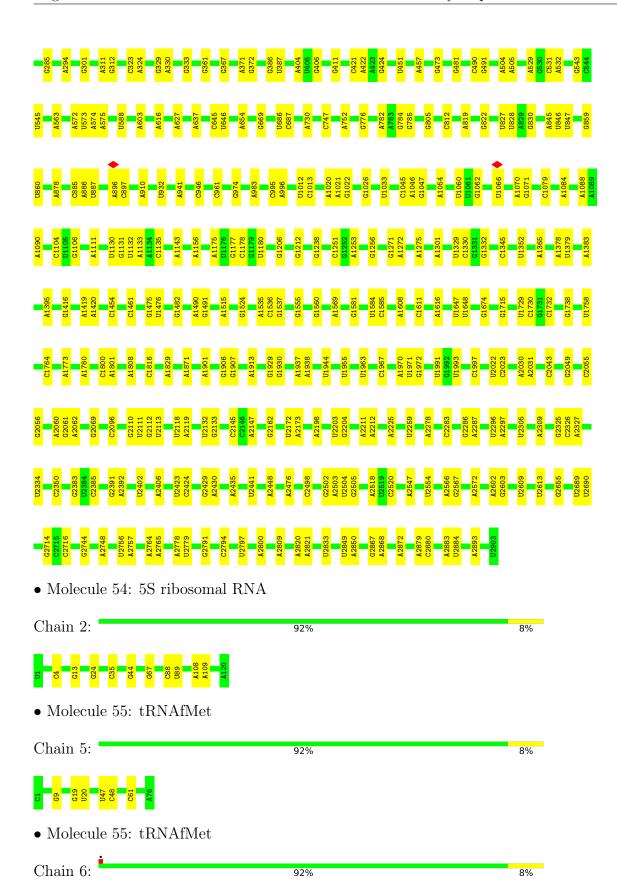


• Molecule 53: 23S ribosomal RNA

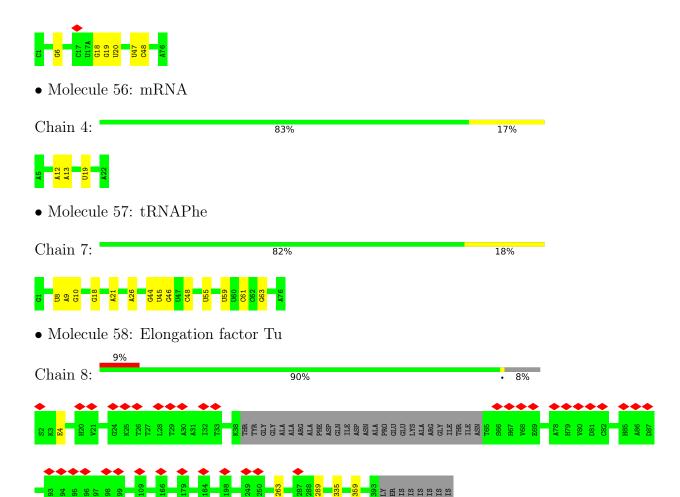
Chain 1: 88% 12%













4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	6805	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE	Depositor
	CORRECTION	
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{Å}^2)$	35	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	18.305	Depositor
Minimum map value	-10.599	Depositor
Average map value	0.113	Depositor
Map value standard deviation	0.860	Depositor
Recommended contour level	1.0	Depositor
Map size (Å)	383.904, 383.904, 383.904	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.333, 1.333, 1.333	Depositor



5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: FME, GDP

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	langles
MIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z >5
1	b	0.25	0/2122	0.59	0/2852
2	С	0.29	0/1586	0.56	0/2134
3	d	0.27	0/1571	0.55	0/2113
4	е	0.30	0/1435	0.55	0/1926
5	f	0.26	0/1343	0.52	0/1816
6	g	0.29	0/1122	0.55	0/1515
7	h	0.31	0/1002	0.64	0/1350
8	i	0.29	0/1046	0.56	0/1410
9	j	0.26	0/1152	0.52	0/1551
10	k	0.26	0/948	0.60	0/1268
11	1	0.27	0/1054	0.59	0/1403
12	m	0.29	0/1093	0.55	0/1460
13	n	0.29	0/974	0.57	0/1301
14	О	0.27	0/902	0.52	0/1209
15	p	0.28	0/929	0.56	0/1242
16	q	0.29	0/960	0.49	0/1278
17	r	0.29	0/829	0.60	0/1107
18	s	0.24	0/864	0.56	0/1156
19	t	0.26	0/745	0.54	0/994
20	u	0.29	0/788	0.58	0/1051
21	V	0.29	0/766	0.57	0/1025
22	W	0.31	0/582	0.53	0/769
23	X	0.29	0/635	0.52	0/848
24	У	0.27	0/510	0.53	0/677
25	Z	0.26	0/453	0.50	0/605
26	В	0.25	0/450	0.54	0/599
27	С	0.32	0/417	0.54	0/554
28	D	0.30	0/380	0.54	0/498
29	Е	0.28	0/513	0.60	0/676
30	F	0.25	0/303	0.59	0/397
31	G	0.29	0/1788	0.54	0/2408
32	Н	0.28	0/1652	0.54	0/2225



N / L 1	Claria.	Bond lengths		Bond	langles
Mol	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5
33	I	0.27	0/1665	0.51	0/2227
34	J	0.28	0/1170	0.62	0/1573
35	K	0.29	0/836	0.60	0/1128
36	L	0.27	0/1196	0.53	0/1602
37	M	0.27	0/989	0.55	0/1326
38	N	0.28	0/1034	0.61	0/1375
39	О	0.27	0/797	0.61	0/1077
40	Р	0.29	0/886	0.60	0/1195
41	Q	0.27	0/969	0.62	0/1300
42	R	0.25	0/893	0.54	0/1193
43	S	0.29	0/817	0.51	0/1088
44	Т	0.26	0/722	0.53	0/964
45	U	0.31	0/659	0.56	0/884
46	V	0.28	0/658	0.64	0/881
47	W	0.30	0/545	0.59	0/731
48	X	0.30	0/653	0.53	0/877
49	Y	0.27	0/671	0.49	0/888
50	Z	0.31	0/551	0.59	0/728
51	a	0.27	0/1034	0.52	0/1387
52	3	0.28	0/36963	0.65	0/57662
53	1	0.26	0/69796	0.65	0/108888
54	2	0.27	0/2872	0.65	0/4479
55	5	0.27	0/1832	0.65	0/2855
55	6	0.28	0/1832	0.66	0/2855
56	4	0.27	0/436	0.62	0/679
57	7	0.28	0/1809	0.65	0/2819
58	8	0.28	0/2885	0.56	0/3902
All	All	0.27	0/166084	0.62	0/247980

There are no bond length outliers.

There are no bond angle outliers.

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.

1 b 269/271 (99%) 236 (88%) 28 (10%) 5 (2%) 8 40 2 c 207/209 (99%) 185 (89%) 21 (10%) 1 (0%) 29 66 3 d 199/201 (99%) 169 (85%) 28 (14%) 2 (1%) 15 51 4 e 175/177 (99%) 154 (88%) 19 (11%) 2 (1%) 14 50 5 f 174/176 (99%) 161 (92%) 10 (6%) 3 (2%) 9 42 6 g 147/149 (99%) 125 (85%) 20 (14%) 2 (1%) 11 45 7 h 129/131 (98%) 95 (74%) 28 (22%) 6 (5%) 2 2 23 8 i 139/141 (99%) 122 (88%) 15 (11%) 2 (1%) 11 45 9 j 140/142 (99%) 127 (91%) 12 (9%) 1 (1%) 22 59 10 k 120/122 (98%) 103 (86%) 14 (12%) 3 (2%) 5 35 11 1 141/143 (99%) 119 (84%) 16 (11%) 6	Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	entiles
3 d 199/201 (99%) 169 (85%) 28 (14%) 2 (1%) 15 51 4 e 175/177 (99%) 154 (88%) 19 (11%) 2 (1%) 14 50 5 f 174/176 (99%) 161 (92%) 10 (6%) 3 (2%) 9 42 6 g 147/149 (99%) 125 (85%) 20 (14%) 2 (1%) 11 45 7 h 129/131 (98%) 95 (74%) 28 (22%) 6 (5%) 2 23 8 i 139/141 (99%) 122 (88%) 15 (11%) 2 (1%) 11 45 9 j 140/142 (99%) 127 (91%) 12 (9%) 1 (1%) 22 59 10 k 120/122 (98%) 103 (86%) 14 (12%) 3 (2%) 5 35 11 1 141/143 (99%) 119 (84%) 16 (11%) 6 (4%) 2 24 12 m 134/136 (98%) 113 (84%) 19 (16%) 2 (2%) 9 42	1	b	269/271 (99%)	236 (88%)	28 (10%)	5 (2%)	8	40
4 e 175/177 (99%) 154 (88%) 19 (11%) 2 (1%) 14 50 5 f 174/176 (99%) 161 (92%) 10 (6%) 3 (2%) 9 42 6 g 147/149 (99%) 125 (85%) 20 (14%) 2 (1%) 11 45 7 h 129/131 (98%) 95 (74%) 28 (22%) 6 (5%) 2 23 8 i 139/141 (99%) 122 (88%) 15 (11%) 2 (1%) 11 45 9 j 140/142 (99%) 127 (91%) 12 (9%) 1 (1%) 22 59 10 k 120/122 (98%) 103 (86%) 14 (12%) 3 (2%) 5 35 11 1 141/143 (99%) 119 (84%) 16 (11%) 6 (4%) 2 24 12 m 134/136 (98%) 113 (84%) 19 (14%) 2 (2%) 10 44 13 n 118/120 (98%) 97 (82%) 19 (16%) 2 (2%) 8 41	2	c	207/209~(99%)	185 (89%)	21 (10%)	1 (0%)	29	66
5 f 174/176 (99%) 161 (92%) 10 (6%) 3 (2%) 9 42 6 g 147/149 (99%) 125 (85%) 20 (14%) 2 (1%) 11 45 7 h 129/131 (98%) 95 (74%) 28 (22%) 6 (5%) 2 23 8 i 139/141 (99%) 122 (88%) 15 (11%) 2 (1%) 11 45 9 j 140/142 (99%) 127 (91%) 12 (9%) 1 (1%) 22 59 10 k 120/122 (98%) 103 (86%) 14 (12%) 3 (2%) 5 35 11 1 141/143 (99%) 119 (84%) 16 (11%) 6 (4%) 2 24 12 m 134/136 (98%) 113 (84%) 19 (14%) 2 (2%) 9 42 14 o 114/116 (98%) 97 (82%) 19 (16%) 2 (2%) 9 42 14 o 114/116 (98%) 99 (87%) 13 (11%) 2 (2%) 9 42	3	d	199/201 (99%)	169 (85%)	28 (14%)	2 (1%)	15	51
6 g 147/149 (99%) 125 (85%) 20 (14%) 2 (1%) 11 45 7 h 129/131 (98%) 95 (74%) 28 (22%) 6 (5%) 2 23 8 i 139/141 (99%) 122 (88%) 15 (11%) 2 (1%) 11 45 9 j 140/142 (99%) 127 (91%) 12 (9%) 1 (1%) 22 59 10 k 120/122 (98%) 103 (86%) 14 (12%) 3 (2%) 5 35 11 1 141/143 (99%) 119 (84%) 16 (11%) 6 (4%) 2 24 12 m 134/136 (98%) 113 (84%) 19 (14%) 2 (2%) 10 44 13 n 118/120 (98%) 97 (82%) 19 (16%) 2 (2%) 9 42 14 o 114/116 (98%) 99 (87%) 13 (11%) 2 (2%) 8 41 15 p 112/114 (98%) 99 (87%) 13 (11%) 2 (2%) 8 41 15 p 112/114 (98%) 99 (87%) 13 (11%) 2 (2%)	4	e	175/177~(99%)	154 (88%)	19 (11%)	2 (1%)	14	50
7 h 129/131 (98%) 95 (74%) 28 (22%) 6 (5%) 2 23 8 i 139/141 (99%) 122 (88%) 15 (11%) 2 (1%) 11 45 9 j 140/142 (99%) 127 (91%) 12 (9%) 1 (1%) 22 59 10 k 120/122 (98%) 103 (86%) 14 (12%) 3 (2%) 5 35 11 1 141/143 (99%) 119 (84%) 16 (11%) 6 (4%) 2 24 12 m 134/136 (98%) 113 (84%) 19 (14%) 2 (2%) 10 44 13 n 118/120 (98%) 97 (82%) 19 (16%) 2 (2%) 9 42 14 o 114/116 (98%) 99 (87%) 13 (11%) 2 (2%) 8 41 15 p 112/114 (98%) 92 (82%) 20 (18%) 0 100 100 16 q 115/117 (98%) 108 (94%) 7 (6%) 0 100 100 17 r 101/103 (98%) 85 (84%) 14 (14%) 2 (2%) 7<	5	f	174/176 (99%)	161 (92%)	10 (6%)	3 (2%)	9	42
8 i 139/141 (99%) 122 (88%) 15 (11%) 2 (1%) 11 45 9 j 140/142 (99%) 127 (91%) 12 (9%) 1 (1%) 22 59 10 k 120/122 (98%) 103 (86%) 14 (12%) 3 (2%) 5 35 11 1 141/143 (99%) 119 (84%) 16 (11%) 6 (4%) 2 24 12 m 134/136 (98%) 113 (84%) 19 (14%) 2 (2%) 10 44 13 n 118/120 (98%) 97 (82%) 19 (16%) 2 (2%) 9 42 14 o 114/116 (98%) 99 (87%) 13 (11%) 2 (2%) 9 42 14 o 114/116 (98%) 99 (87%) 13 (11%) 2 (2%) 8 41 15 p 112/114 (98%) 92 (82%) 20 (18%) 0 100 100 16 q 115/117 (98%) 108 (94%) 7 (6%) 0 100 100 17 r 101/103 (98%) 85 (84%) 14 (14%) 2 (2%) 7	6	g	147/149 (99%)	125 (85%)	20 (14%)	2 (1%)	11	45
9 j 140/142 (99%) 127 (91%) 12 (9%) 1 (1%) 22 59 10 k 120/122 (98%) 103 (86%) 14 (12%) 3 (2%) 5 35 11 1 141/143 (99%) 119 (84%) 16 (11%) 6 (4%) 2 24 12 m 134/136 (98%) 113 (84%) 19 (14%) 2 (2%) 9 42 13 n 118/120 (98%) 97 (82%) 19 (16%) 2 (2%) 9 42 14 o 114/116 (98%) 99 (87%) 13 (11%) 2 (2%) 9 42 14 o 114/116 (98%) 99 (87%) 13 (11%) 2 (2%) 8 41 15 p 112/114 (98%) 92 (82%) 20 (18%) 0 100 100 16 q 115/117 (98%) 108 (94%) 7 (6%) 0 100 100 17 r 101/103 (98%) 85 (84%) 14 (14%) 2 (2%) 7 39 18 s 108/110 (98%) 92 (85%) 15 (14%) 1 (1%) 17<	7	h	129/131 (98%)	95 (74%)	28 (22%)	6 (5%)	2	23
10 k 120/122 (98%) 103 (86%) 14 (12%) 3 (2%) 5 35 11 1 141/143 (99%) 119 (84%) 16 (11%) 6 (4%) 2 2 24 12 m 134/136 (98%) 113 (84%) 19 (14%) 2 (2%) 9 44 13 n 118/120 (98%) 97 (82%) 19 (16%) 2 (2%) 9 42 14 o 114/116 (98%) 99 (87%) 13 (11%) 2 (2%) 8 41 15 p 112/114 (98%) 92 (82%) 20 (18%) 0 100 100 16 q 115/117 (98%) 108 (94%) 7 (6%) 0 100 100 17 r 101/103 (98%) 85 (84%) 14 (14%) 2 (2%) 7 39 18 s 108/110 (98%) 92 (85%) 15 (14%) 1 (1%) 17 54 19 t 91/93 (98%) 83 (91%) 8 (9%) 0 100 100 20 u 100/102 (98%) 85 (85%) 10 (10%) 5 (5%)	8	i	139/141 (99%)	122 (88%)	15 (11%)	2 (1%)	11	45
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	9	j	140/142 (99%)	127 (91%)	12 (9%)	1 (1%)	22	59
12 m 134/136 (98%) 113 (84%) 19 (14%) 2 (2%) 10 44 13 n 118/120 (98%) 97 (82%) 19 (16%) 2 (2%) 9 42 14 o 114/116 (98%) 99 (87%) 13 (11%) 2 (2%) 8 41 15 p 112/114 (98%) 92 (82%) 20 (18%) 0 100 100 16 q 115/117 (98%) 108 (94%) 7 (6%) 0 100 100 17 r 101/103 (98%) 85 (84%) 14 (14%) 2 (2%) 7 39 18 s 108/110 (98%) 92 (85%) 15 (14%) 1 (1%) 17 54 19 t 91/93 (98%) 83 (91%) 8 (9%) 0 100 100 20 u 100/102 (98%) 85 (85%) 10 (10%) 5 (5%) 2 22 21 v 92/94 (98%) 84 (91%) 8 (9%) 0 100 100 22 w 73/75 (97%) 67 (92%) 6 (8%) 0 100 100 </td <td>10</td> <td>k</td> <td>120/122 (98%)</td> <td>103 (86%)</td> <td>14 (12%)</td> <td>3 (2%)</td> <td>5</td> <td>35</td>	10	k	120/122 (98%)	103 (86%)	14 (12%)	3 (2%)	5	35
13 n 118/120 (98%) 97 (82%) 19 (16%) 2 (2%) 9 42 14 o 114/116 (98%) 99 (87%) 13 (11%) 2 (2%) 8 41 15 p 112/114 (98%) 92 (82%) 20 (18%) 0 100 100 16 q 115/117 (98%) 108 (94%) 7 (6%) 0 100 100 17 r 101/103 (98%) 85 (84%) 14 (14%) 2 (2%) 7 39 18 s 108/110 (98%) 92 (85%) 15 (14%) 1 (1%) 17 54 19 t 91/93 (98%) 83 (91%) 8 (9%) 0 100 100 20 u 100/102 (98%) 85 (85%) 10 (10%) 5 (5%) 2 22 21 v 92/94 (98%) 84 (91%) 8 (9%) 0 100 100 22 w 73/75 (97%) 67 (92%) 6 (8%) 0 100 100 23 x 75/77 (97%) 68 (91%) 7 (9%) 0 100 100	11	1	141/143 (99%)	119 (84%)	16 (11%)	6 (4%)	2	24
14 o 114/116 (98%) 99 (87%) 13 (11%) 2 (2%) 8 41 15 p 112/114 (98%) 92 (82%) 20 (18%) 0 100 100 16 q 115/117 (98%) 108 (94%) 7 (6%) 0 100 100 17 r 101/103 (98%) 85 (84%) 14 (14%) 2 (2%) 7 39 18 s 108/110 (98%) 92 (85%) 15 (14%) 1 (1%) 17 54 19 t 91/93 (98%) 83 (91%) 8 (9%) 0 100 100 20 u 100/102 (98%) 85 (85%) 10 (10%) 5 (5%) 2 22 21 v 92/94 (98%) 84 (91%) 8 (9%) 0 100 100 22 w 73/75 (97%) 67 (92%) 6 (8%) 0 100 100 23 x 75/77 (97%) 68 (91%) 7 (9%) 0 100 100 24 y 61/63 (97%) 58 (95%) 3 (5%) 0 100 100	12	m	134/136 (98%)	113 (84%)	19 (14%)	2 (2%)	10	44
15 p 112/114 (98%) 92 (82%) 20 (18%) 0 100 100 16 q 115/117 (98%) 108 (94%) 7 (6%) 0 100 100 17 r 101/103 (98%) 85 (84%) 14 (14%) 2 (2%) 7 39 18 s 108/110 (98%) 92 (85%) 15 (14%) 1 (1%) 17 54 19 t 91/93 (98%) 83 (91%) 8 (9%) 0 100 100 20 u 100/102 (98%) 85 (85%) 10 (10%) 5 (5%) 2 22 21 v 92/94 (98%) 84 (91%) 8 (9%) 0 100 100 22 w 73/75 (97%) 67 (92%) 6 (8%) 0 100 100 23 x 75/77 (97%) 68 (91%) 7 (9%) 0 100 100 24 y 61/63 (97%) 58 (95%) 3 (5%) 0 100 100	13	n	118/120 (98%)	97 (82%)	19 (16%)	2 (2%)	9	42
16 q 115/117 (98%) 108 (94%) 7 (6%) 0 100 100 17 r 101/103 (98%) 85 (84%) 14 (14%) 2 (2%) 7 39 18 s 108/110 (98%) 92 (85%) 15 (14%) 1 (1%) 17 54 19 t 91/93 (98%) 83 (91%) 8 (9%) 0 100 100 20 u 100/102 (98%) 85 (85%) 10 (10%) 5 (5%) 2 22 21 v 92/94 (98%) 84 (91%) 8 (9%) 0 100 100 22 w 73/75 (97%) 67 (92%) 6 (8%) 0 100 100 23 x 75/77 (97%) 68 (91%) 7 (9%) 0 100 100 24 y 61/63 (97%) 58 (95%) 3 (5%) 0 100 100	14	О	114/116 (98%)	99 (87%)	13 (11%)	2 (2%)	8	41
17 r 101/103 (98%) 85 (84%) 14 (14%) 2 (2%) 7 39 18 s 108/110 (98%) 92 (85%) 15 (14%) 1 (1%) 17 54 19 t 91/93 (98%) 83 (91%) 8 (9%) 0 100 100 20 u 100/102 (98%) 85 (85%) 10 (10%) 5 (5%) 2 22 21 v 92/94 (98%) 84 (91%) 8 (9%) 0 100 100 22 w 73/75 (97%) 67 (92%) 6 (8%) 0 100 100 23 x 75/77 (97%) 68 (91%) 7 (9%) 0 100 100 24 y 61/63 (97%) 58 (95%) 3 (5%) 0 100 100	15	p	112/114 (98%)	92 (82%)	20 (18%)	0	100	100
18 s $108/110 (98\%)$ $92 (85\%)$ $15 (14\%)$ $1 (1\%)$ 17 54 19 t $91/93 (98\%)$ $83 (91\%)$ $8 (9\%)$ 0 100 100 20 u $100/102 (98\%)$ $85 (85\%)$ $10 (10\%)$ $5 (5\%)$ 2 22 21 v $92/94 (98\%)$ $84 (91\%)$ $8 (9\%)$ 0 100 100 22 w $73/75 (97\%)$ $67 (92\%)$ $6 (8\%)$ 0 100 100 23 x $75/77 (97\%)$ $68 (91\%)$ $7 (9\%)$ 0 100 100 24 y $61/63 (97\%)$ $58 (95\%)$ $3 (5\%)$ 0 100 100	16	q	115/117 (98%)	108 (94%)	7 (6%)	0	100	100
19 t 91/93 (98%) 83 (91%) 8 (9%) 0 100 100 20 u 100/102 (98%) 85 (85%) 10 (10%) 5 (5%) 2 22 21 v 92/94 (98%) 84 (91%) 8 (9%) 0 100 100 22 w 73/75 (97%) 67 (92%) 6 (8%) 0 100 100 23 x 75/77 (97%) 68 (91%) 7 (9%) 0 100 100 24 y 61/63 (97%) 58 (95%) 3 (5%) 0 100 100	17	r	101/103 (98%)	85 (84%)	14 (14%)	2 (2%)	7	39
20 u 100/102 (98%) 85 (85%) 10 (10%) 5 (5%) 2 22 21 v 92/94 (98%) 84 (91%) 8 (9%) 0 100 100 22 w 73/75 (97%) 67 (92%) 6 (8%) 0 100 100 23 x 75/77 (97%) 68 (91%) 7 (9%) 0 100 100 24 y 61/63 (97%) 58 (95%) 3 (5%) 0 100 100	18	s	108/110 (98%)	92 (85%)	15 (14%)	1 (1%)	17	54
21 v 92/94 (98%) 84 (91%) 8 (9%) 0 100 100 22 w 73/75 (97%) 67 (92%) 6 (8%) 0 100 100 23 x 75/77 (97%) 68 (91%) 7 (9%) 0 100 100 24 y 61/63 (97%) 58 (95%) 3 (5%) 0 100 100	19	t	91/93 (98%)	83 (91%)	8 (9%)	0	100	100
22 w 73/75 (97%) 67 (92%) 6 (8%) 0 100 100 23 x 75/77 (97%) 68 (91%) 7 (9%) 0 100 100 24 y 61/63 (97%) 58 (95%) 3 (5%) 0 100 100	20	u	100/102 (98%)	85 (85%)	10 (10%)	5 (5%)	2	22
23 x 75/77 (97%) 68 (91%) 7 (9%) 0 100 100 24 y 61/63 (97%) 58 (95%) 3 (5%) 0 100 100	21	V	92/94 (98%)	84 (91%)	8 (9%)	0	100	100
24 y 61/63 (97%) 58 (95%) 3 (5%) 0 100 100	22	W	73/75 (97%)	67 (92%)	6 (8%)	0	100	100
	23	X	75/77 (97%)	68 (91%)	7 (9%)	0	100	100
25 z 56/58 (97%) 53 (95%) 3 (5%) 0 100 100	24	У	61/63 (97%)	58 (95%)	3 (5%)	0	100	100
	25	Z	56/58 (97%)	53 (95%)	3 (5%)	0	100	100



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	entiles
26	В	54/56~(96%)	50 (93%)	4 (7%)	0	100	100
27	С	48/50 (96%)	44 (92%)	4 (8%)	0	100	100
28	D	44/46 (96%)	36 (82%)	8 (18%)	0	100	100
29	Е	62/64 (97%)	53 (86%)	7 (11%)	2 (3%)	4	31
30	F	36/38 (95%)	28 (78%)	8 (22%)	0	100	100
31	G	223/225 (99%)	211 (95%)	12 (5%)	0	100	100
32	Н	204/206 (99%)	187 (92%)	16 (8%)	1 (0%)	29	66
33	I	203/205 (99%)	172 (85%)	31 (15%)	0	100	100
34	J	155/157 (99%)	126 (81%)	25 (16%)	4 (3%)	5	34
35	K	98/100 (98%)	79 (81%)	12 (12%)	7 (7%)	1	15
36	L	149/151 (99%)	133 (89%)	16 (11%)	0	100	100
37	M	127/129 (98%)	111 (87%)	15 (12%)	1 (1%)	19	56
38	N	125/127 (98%)	101 (81%)	20 (16%)	4 (3%)	4	31
39	О	96/98 (98%)	82 (85%)	10 (10%)	4 (4%)	3	25
40	Р	114/116 (98%)	89 (78%)	21 (18%)	4 (4%)	3	30
41	Q	121/123 (98%)	95 (78%)	18 (15%)	8 (7%)	1	16
42	R	112/114 (98%)	96 (86%)	13 (12%)	3 (3%)	5	33
43	S	98/100 (98%)	81 (83%)	15 (15%)	2 (2%)	7	39
44	Т	86/88 (98%)	78 (91%)	7 (8%)	1 (1%)	13	48
45	U	80/82 (98%)	68 (85%)	10 (12%)	2 (2%)	5	35
46	V	78/80 (98%)	64 (82%)	12 (15%)	2 (3%)	5	34
47	W	63/65 (97%)	58 (92%)	2 (3%)	3 (5%)	2	22
48	X	77/79 (98%)	65 (84%)	10 (13%)	2 (3%)	5	34
49	Y	83/85 (98%)	77 (93%)	5 (6%)	1 (1%)	13	48
50	Z	63/65 (97%)	45 (71%)	12 (19%)	6 (10%)	0	8
51	a	130/223 (58%)	126 (97%)	4 (3%)	0	100	100
58	8	362/400 (90%)	329 (91%)	31 (9%)	2 (1%)	25	62
All	All	6281/6512 (96%)	5464 (87%)	711 (11%)	106 (2%)	13	42

5 of 106 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	b	204	LEU



Continued from previous page...

Mol	Chain	Res	Type
1	b	232	GLY
2	c	86	GLU
6	g	9	VAL
7	h	108	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Perce	ntiles
1	b	$216/216\ (100\%)$	214 (99%)	2 (1%)	78	88
2	С	164/164~(100%)	164 (100%)	0	100	100
3	d	165/165~(100%)	164 (99%)	1 (1%)	86	93
4	е	148/148 (100%)	146 (99%)	2 (1%)	67	82
5	f	$137/137\ (100\%)$	136 (99%)	1 (1%)	84	91
6	g	114/114~(100%)	113 (99%)	1 (1%)	78	88
7	h	100/100 (100%)	98 (98%)	2 (2%)	55	74
8	i	109/109~(100%)	108 (99%)	1 (1%)	78	88
9	j	$116/116\ (100\%)$	116 (100%)	0	100	100
10	k	103/103~(100%)	103 (100%)	0	100	100
11	1	$102/102\ (100\%)$	101 (99%)	1 (1%)	76	86
12	m	$109/109\ (100\%)$	109 (100%)	0	100	100
13	n	$100/100\ (100\%)$	99 (99%)	1 (1%)	76	86
14	О	86/86~(100%)	84 (98%)	2 (2%)	50	71
15	p	99/99~(100%)	99 (100%)	0	100	100
16	q	89/89 (100%)	89 (100%)	0	100	100
17	r	84/84 (100%)	84 (100%)	0	100	100
18	s	93/93 (100%)	92 (99%)	1 (1%)	73	85
19	t	80/80 (100%)	79 (99%)	1 (1%)	69	83
20	u	83/83 (100%)	83 (100%)	0	100	100



Mol	Chain	Analysed	Rotameric	Outliers	Perce	ntiles
21	v	78/78 (100%)	77 (99%)	1 (1%)	69	83
22	W	57/57~(100%)	57 (100%)	0	100	100
23	X	$67/67\ (100\%)$	67 (100%)	0	100	100
24	У	55/55~(100%)	54 (98%)	1 (2%)	59	77
25	Z	48/48 (100%)	48 (100%)	0	100	100
26	В	47/47 (100%)	47 (100%)	0	100	100
27	С	45/45 (100%)	43 (96%)	2 (4%)	28	58
28	D	38/38 (100%)	38 (100%)	0	100	100
29	E	51/51~(100%)	51 (100%)	0	100	100
30	F	34/34~(100%)	34 (100%)	0	100	100
31	G	186/186 (100%)	185 (100%)	1 (0%)	88	94
32	Н	170/170 (100%)	168 (99%)	2 (1%)	71	84
33	I	172/172 (100%)	170 (99%)	2 (1%)	71	84
34	J	119/119 (100%)	119 (100%)	0	100	100
35	K	87/87 (100%)	85 (98%)	2 (2%)	50	71
36	L	124/124 (100%)	124 (100%)	0	100	100
37	M	104/104 (100%)	103 (99%)	1 (1%)	76	86
38	N	105/105~(100%)	103 (98%)	2 (2%)	57	76
39	О	86/86 (100%)	85 (99%)	1 (1%)	71	84
40	Р	89/89 (100%)	89 (100%)	0	100	100
41	Q	103/103 (100%)	101 (98%)	2 (2%)	57	76
42	R	$92/92\ (100\%)$	90 (98%)	2 (2%)	52	72
43	S	83/83~(100%)	83 (100%)	0	100	100
44	Т	76/76~(100%)	76 (100%)	0	100	100
45	U	65/65~(100%)	65 (100%)	0	100	100
46	V	74/74 (100%)	73 (99%)	1 (1%)	67	82
47	W	$56/56 \; (100\%)$	55 (98%)	1 (2%)	59	77
48	X	70/70~(100%)	70 (100%)	0	100	100
49	Y	$65/65 \; (100\%)$	64 (98%)	1 (2%)	65	81
50	Z	55/55~(100%)	53 (96%)	2 (4%)	35	63
51	a	110/174~(63%)	108 (98%)	2 (2%)	59	77



Mol	Chain	Analysed	Rotameric	Outliers	Perce	entiles
58	8	306/332 (92%)	303 (99%)	3 (1%)	76	86
All	All	5214/5304 (98%)	5169 (99%)	45 (1%)	79	88

5 of 45 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
38	N	56	MET
46	V	26	ARG
38	N	126	PHE
41	Q	89	LEU
49	Y	68	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 89 such sidechains are listed below:

Mol	Chain	Res	Type
33	I	195	ASN
41	Q	4	ASN
34	J	134	ASN
38	N	49	GLN
43	S	3	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
52	3	1538/1539 (99%)	143 (9%)	5 (0%)
53	1	2902/2903 (99%)	330 (11%)	12 (0%)
54	2	119/120 (99%)	9 (7%)	1 (0%)
55	5	76/77~(98%)	6 (7%)	0
55	6	76/77~(98%)	6 (7%)	0
56	4	17/18 (94%)	3 (17%)	0
57	7	75/76 (98%)	14 (18%)	0
All	All	4803/4810 (99%)	511 (10%)	18 (0%)

5 of 511 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
52	3	6	G
52	3	9	G
52	3	31	G



Mol	Chain	Res	Type
52	3	32	A
52	3	39	G

5 of 18 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
53	1	2326	С
54	2	88	С
53	1	2756	U
53	1	859	G
53	1	2296	U

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

3 ligands 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	$\operatorname{Res} \left \operatorname{Link} \right = \operatorname{Bond \ lengths}$				$ \hspace{.05cm} {f B}$	ond ang	cles
WIOI	туре	Chain	nes	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
60	PHE	7	101	57	10,11,12	0.68	0	10,13,15	0.35	0
59	FME	5	101	55	8,9,10	0.50	0	7,9,11	0.87	0
61	GDP	8	501	-	24,30,30	1.65	2 (8%)	30,47,47	1.60	9 (30%)

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.



, ,		. 1.	C 11 1	1 . 1		1 1.0 1
'-' means	no	outhers	of that	: kind	were	identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
60	PHE	7	101	57	-	0/5/6/8	0/1/1/1
59	FME	5	101	55	-	1/7/9/11	-
61	GDP	8	501	-	-	6/12/32/32	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(A)	Ideal(A)
61	8	501	GDP	O4'-C1'	4.49	1.47	1.41
61	8	501	GDP	PB-O1B	3.80	1.62	1.50

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
61	8	501	GDP	C8-N7-C5	3.48	109.63	102.99
61	8	501	GDP	C5-C6-N1	2.70	118.72	113.95
61	8	501	GDP	C2-N1-C6	-2.64	120.23	125.10
61	8	501	GDP	O5'-PA-O1A	-2.62	98.83	109.07
61	8	501	GDP	O4'-C4'-C3'	2.52	110.10	105.11

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
59	5	101	FME	O1-CN-N-CA
61	8	501	GDP	PA-O3A-PB-O2B
61	8	501	GDP	PA-O3A-PB-O3B
61	8	501	GDP	O4'-C4'-C5'-O5'
61	8	501	GDP	C3'-C4'-C5'-O5'

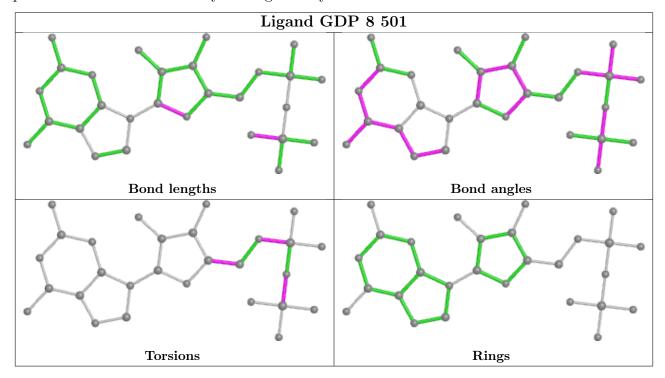
There are no ring outliers.

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 then 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.



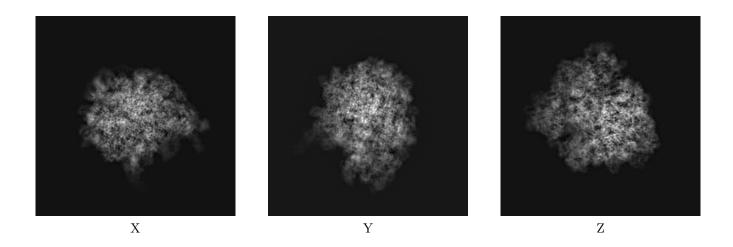
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-21623. These allow visual inspection of the internal detail of the map and identification of artifacts.

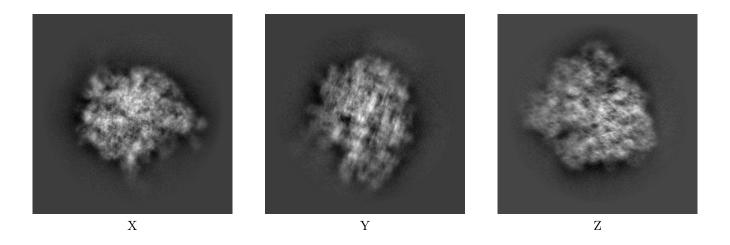
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

6.1.1 Primary map



6.1.2 Raw map

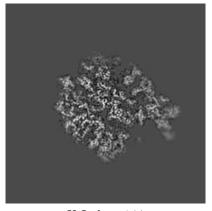


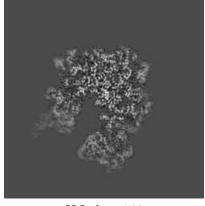
The images above show the map projected in three orthogonal directions.

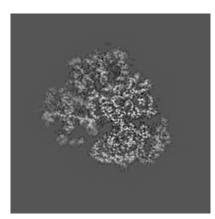


6.2 Central slices (i)

6.2.1 Primary map





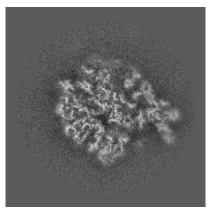


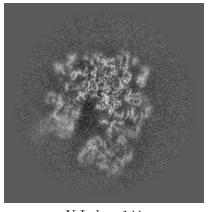
X Index: 144

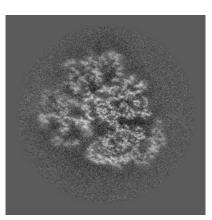
Y Index: 144

Z Index: 144

6.2.2 Raw map







X Index: 144

Y Index: 144

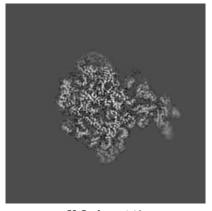
Z Index: 144

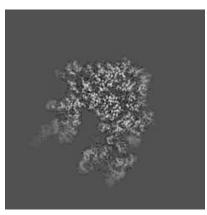
The images above show central slices of the map in three orthogonal directions.

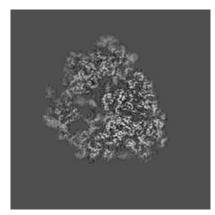


6.3 Largest variance slices (i)

6.3.1 Primary map





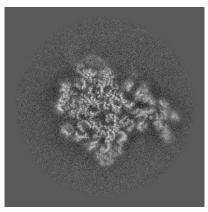


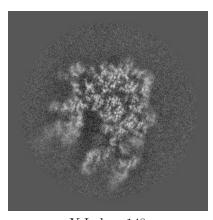
X Index: 149

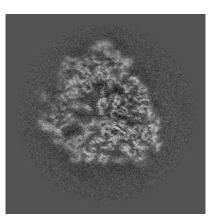
Y Index: 148

Z Index: 135

6.3.2 Raw map







X Index: 149

Y Index: 148

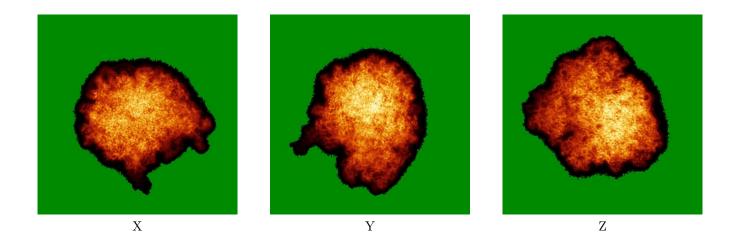
Z Index: 135

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

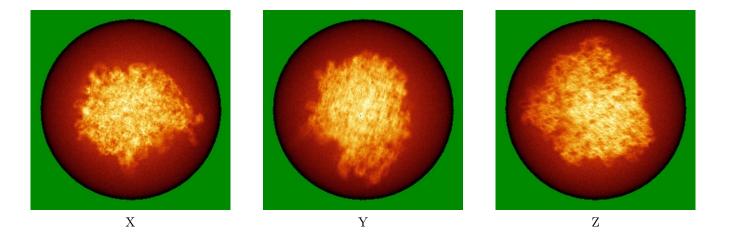


6.4 Orthogonal standard-deviation projections (False-color) (i)

6.4.1 Primary map



6.4.2 Raw map



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.



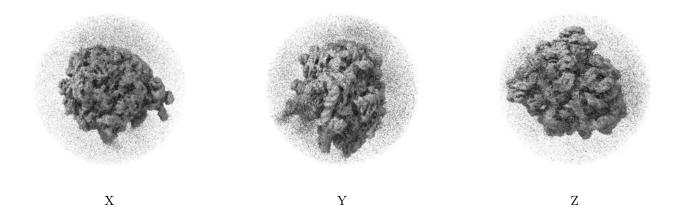
6.5 Orthogonal surface views (i)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 1.0. 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)

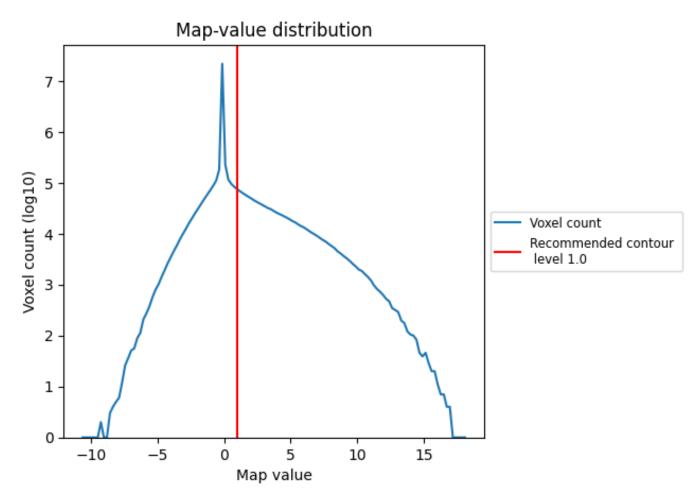
This section was not generated. No masks/segmentation were deposited.



7 Map analysis (i)

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

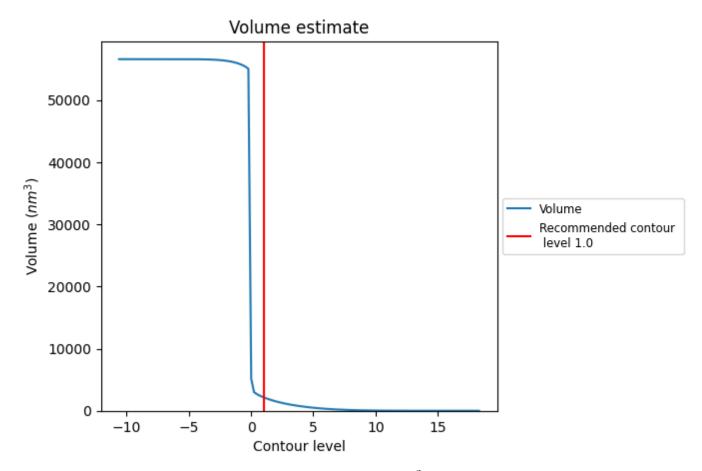
7.1 Map-value distribution (i)



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



7.2 Volume estimate (i)

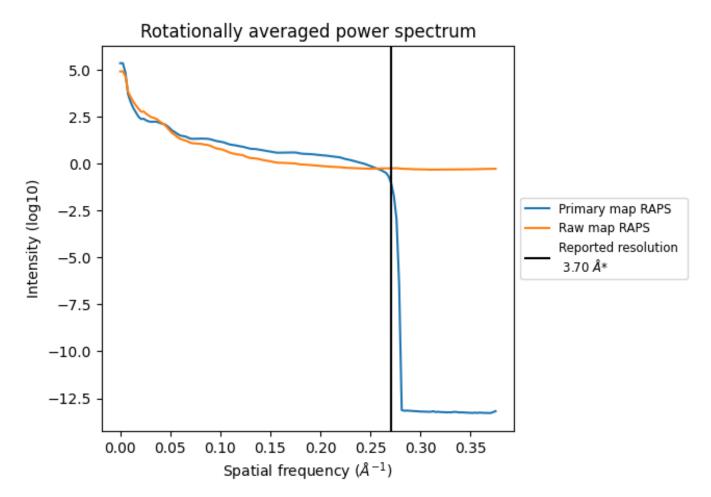


The volume at the recommended contour level is 2174 nm^3 ; this corresponds to an approximate mass of 1964 kDa.

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



7.3 Rotationally averaged power spectrum (i)



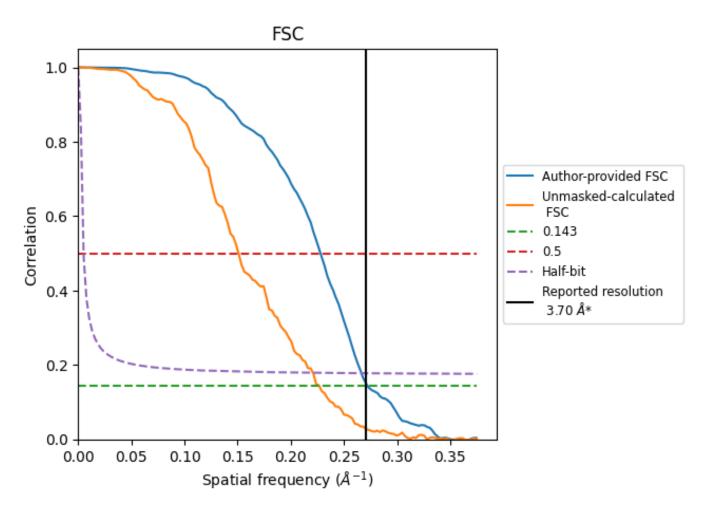
*Reported resolution corresponds to spatial frequency of 0.270 $\rm \mathring{A}^{-1}$



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 0.270 $\rm \mathring{A}^{-1}$



8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
rtesolution estimate (A)	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	3.67	4.39	3.75
Unmasked-calculated*	4.41	6.63	4.53

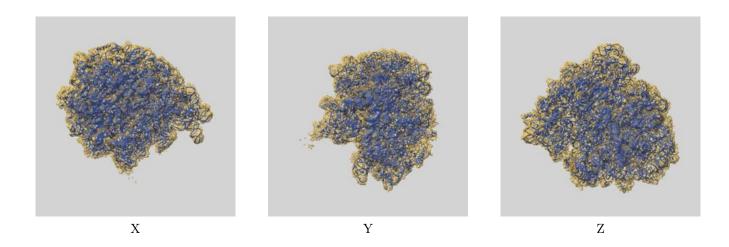
^{*}Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.41 differs from the reported value 3.7 by more than 10 %



9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-21623 and PDB model 6WD4. Per-residue inclusion information can be found in section 3 on page 17.

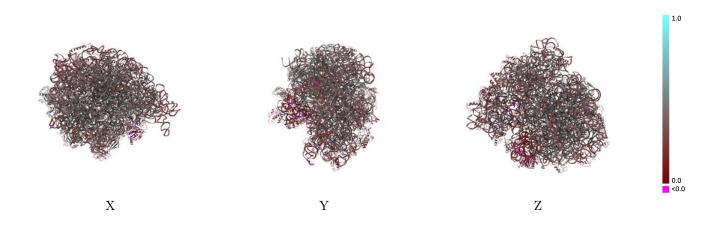
9.1 Map-model overlay (i)



The images above show the 3D surface view of the map at the recommended contour level 1.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

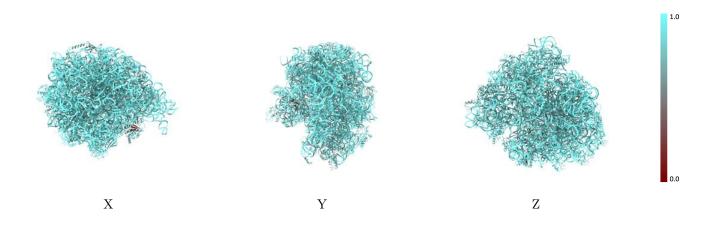


9.2 Q-score mapped to coordinate model (i)



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

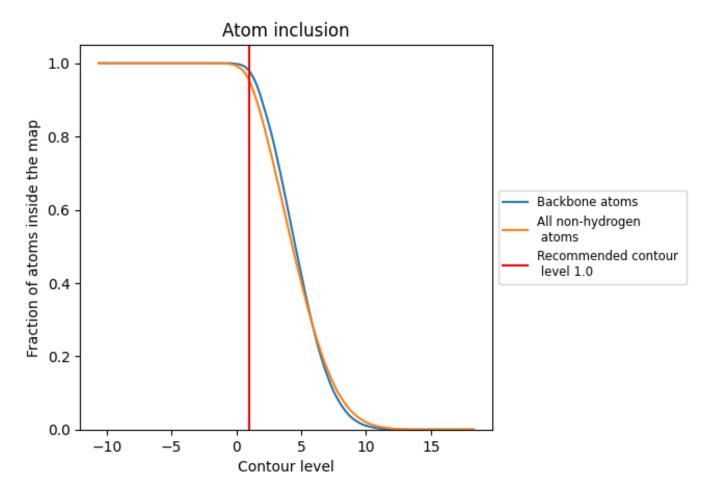
9.3 Atom inclusion mapped to coordinate model (i)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (1.0).



9.4 Atom inclusion (i)



At the recommended contour level, 98% of all backbone atoms, 95% of all non-hydrogen atoms, are inside the map.



9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (1.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9530	0.3610
1	0.9830	0.3810
2	0.9860	0.3380
3	0.9770	0.3510
4	0.8840	0.2510
5	0.9580	0.3000
6	0.8320	0.1500
7	0.9140	0.1910
8	0.8080	0.1840
В	0.9530	0.4320
С	0.8430	0.3760
D	0.9210	0.4480
E	0.9510	0.4640
F	0.8660	0.4320
G	0.8920	0.3130
Н	0.7620	0.3170
I	0.8830	0.3220
J	0.9180	0.3810
K	0.9540	0.3680
L	0.9320	0.3500
M	0.9080	0.3810
N	0.9100	0.3220
О	0.7350	0.2790
P	0.9500	0.3820
Q	0.9050	0.4120
R	0.9350	0.3450
S	0.8220	0.3330
Т	0.9510	0.3770
U	0.9120	0.3880
V	0.9160	0.3960
W	0.9400	0.3680
X	0.9570	0.3300
Y	0.9000	0.3500
Z	0.8650	0.3070
a	0.8340	0.1500



Continued on next page...



 $Continued\ from\ previous\ page...$

Chain	Atom inclusion	Q-score
b	0.9540	0.4520
С	0.9450	0.4470
d	0.9420	0.4060
e	0.9260	0.3360
f	0.9660	0.3690
g	0.7930	0.2920
h	0.7840	0.1630
i	0.7250	0.1970
j	0.9510	0.4400
k	0.9310	0.4460
1	0.9600	0.4240
m	0.9250	0.4470
n	0.9500	0.4360
О	0.9460	0.3720
p	0.9360	0.4320
q	0.9280	0.4250
r	0.9510	0.4130
S	0.9210	0.4300
t	0.9270	0.4040
u	0.9300	0.3860
V	0.9470	0.3920
W	0.9450	0.4570
X	0.9600	0.4310
У	0.9300	0.3350
Z	0.9340	0.4310

