wwPDB EM Validation Summary Report

Apr 17, 2024 – 07:23 am BST

PDB ID	:	6Q9A
EMDB ID	:	EMD-4478
Title	:	Structure of tmRNA SmpB bound past E site of E. coli 70S ribosome
Authors	:	Rae, C.D.
Deposited on	:	2018-12-17
Resolution	:	3.70 Å(reported)
Based on initial model	:	5MDZ

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:

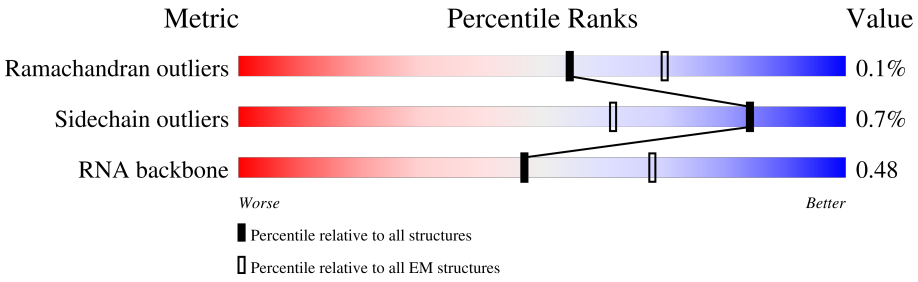
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	1	2903	69% 28%
2	2	1534	74% 24%
3	3	120	71% 26%
4	6	23	26% 100%
5	7	76	62% 32% 7%
6	B	271	100%
7	C	207	99%
8	D	201	100%

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Mol	Chain	Length	Quality of chain
9	E	177	99%
10	F	175	99%
11	G	148	8% 99%
12	H	130	22% 98%
13	I	135	31% 100%
14	J	142	100%
15	K	123	98%
16	L	143	99%
17	M	135	99%
18	N	119	100%
19	O	115	100%
20	P	113	100%
21	Q	117	99%
22	R	102	100%
23	S	109	100%
24	T	94	100%
25	U	101	99%
26	V	93	100%
27	W	75	99%
28	X	77	100%
29	Y	62	98%
30	Z	56	100%
31	a	66	100%
32	b	55	100%
33	c	51	100%

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Mol	Chain	Length	Quality of chain
34	d	45	100%
35	e	64	97%
36	f	38	97%
37	g	225	99%
38	h	208	100%
39	i	205	100%
40	j	156	98%
41	k	104	99%
42	l	152	99%
43	m	129	99%
44	n	127	98%
45	o	99	98%
46	p	116	98%
47	q	122	98%
48	r	116	98%
49	s	100	100%
50	t	87	100%
51	u	82	98%
52	v	80	100%
53	w	66	97%
54	x	83	100%
55	y	85	100%
56	z	70	97%
57	5	118	90% 98%
58	4	363	56% 21% 41% 38%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	6MZ	1	1618	X	-	-	-
1	PSU	1	1911	X	-	-	-
1	3TD	1	1915	X	-	-	-
1	PSU	1	1917	X	-	-	-
1	5MU	1	1939	X	-	-	-
1	6MZ	1	2030	X	-	-	-
1	G7M	1	2069	X	-	-	-
1	OMG	1	2251	X	-	-	-
1	PSU	1	2457	X	-	-	-
1	OMC	1	2498	X	-	-	-
1	2MA	1	2503	X	-	-	-
1	PSU	1	2504	X	-	-	-
1	OMU	1	2552	X	-	-	-
1	PSU	1	2580	X	-	-	-
1	PSU	1	2605	X	-	-	-
1	1MG	1	745	X	-	-	-
1	PSU	1	746	X	-	-	-
1	5MU	1	747	X	-	-	-
1	PSU	1	955	X	-	-	-
2	4OC	2	1402	X	-	-	-
2	PSU	2	516	X	-	-	-
2	7MG	2	527	X	-	-	-

2 Entry composition (i)

There are 61 unique types of molecules in this entry. The entry contains 155169 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 ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	1	2903	62336	27816	11470	20147	2903	0	0

- Molecule 2 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	2	1534	32929	14693	6041	10661	1534	0	0

- Molecule 3 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	3	120	2569	1144	468	837	120	0	0

- Molecule 4 is a protein called Nascent peptide.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	6	23	115	69	23	23	0	0

- Molecule 5 is a RNA chain called P-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
5	7	76	1621	722	289	534	76	0	0

- Molecule 6 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	B	271	2083	1288	423	365	7	0	0

- Molecule 7 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	C	207	Total	C	N	O	S	0	0
			1551	971	286	291	3		

- Molecule 8 is a protein called 50S ribosomal protein L4.

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

- Molecule 9 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	E	177	Total	C	N	O	S	0	0
			1411	899	249	257	6		

- Molecule 10 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	F	175	Total	C	N	O	S	0	0
			1313	826	241	244	2		

- Molecule 11 is a protein called 50S ribosomal protein L9.

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

- Molecule 12 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	H	130	Total	C	N	O	S	0	0
			980	620	174	182	4		

- Molecule 13 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	I	135	Total	C	N	O	S	0	0
			984	622	171	185	6		

- Molecule 14 is a protein called 50S ribosomal protein L13.

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

- Molecule 15 is a protein called 50S ribosomal protein L14.

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

- Molecule 16 is a protein called 50S ribosomal protein L15.

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

- Molecule 17 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	M	135	Total	C	N	O	S	0	0
			1065	681	204	175	5		

- Molecule 18 is a protein called 50S ribosomal protein L17.

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

- Molecule 19 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	O	115	Total	C	N	O	0	0
			884	548	177	159		

- Molecule 20 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	P	113	Total	C	N	O	S	0	0
			908	570	177	160	1		

- Molecule 21 is a protein called 50S ribosomal protein L20.

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

- Molecule 22 is a protein called 50S ribosomal protein L21.

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

- Molecule 23 is a protein called 50S ribosomal protein L22.

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

- Molecule 24 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	T	94	Total 746	C 470	N 140	O 134	S 2	0	0

- Molecule 25 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	U	101	Total 774	C 489	N 145	O 140	0	0

- Molecule 26 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	V	93	Total 747	C 476	N 136	O 132	S 3	0	0

- Molecule 27 is a protein called 50S ribosomal protein L27.

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

- Molecule 28 is a protein called 50S ribosomal protein L28.

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

- Molecule 29 is a protein called 50S ribosomal protein L29.

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

- Molecule 30 is a protein called 50S ribosomal protein L30.

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

- Molecule 31 is a protein called 50S ribosomal protein L31.

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

- Molecule 32 is a protein called 50S ribosomal protein L32.

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

- Molecule 33 is a protein called 50S ribosomal protein L33.

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

- Molecule 34 is a protein called 50S ribosomal protein L34.

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

- Molecule 35 is a protein called 50S ribosomal protein L35.

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

- Molecule 36 is a protein called 50S ribosomal protein L36.

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

- Molecule 37 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	g	225	Total	C	N	O	S	0	0
			1760	1113	316	323	8		

- Molecule 38 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	h	208	Total	C	N	O	S	0	0
			1636	1036	307	290	3		

- Molecule 39 is a protein called 30S ribosomal protein S4.

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

- Molecule 40 is a protein called 30S ribosomal protein S5.

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

- Molecule 41 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	k	104	Total	C	N	O	S	0	0
			848	536	153	152	7		

- Molecule 42 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	l	152	Total	C	N	O	S	0	0
			1191	741	230	216	4		

- Molecule 43 is a protein called 30S ribosomal protein S8.

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

- Molecule 44 is a protein called 30S ribosomal protein S9.

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

- Molecule 45 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	o	99	Total	C	N	O	S	0	0
			790	495	151	143	1		

- Molecule 46 is a protein called 30S ribosomal protein S11.

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

- Molecule 47 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	q	122	Total	C	N	O	S	0	0
			951	588	195	163	5		

- Molecule 48 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	r	116	Total	C	N	O	S	0	0
			900	558	181	158	3		

- Molecule 49 is a protein called 30S ribosomal protein S14.

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

- Molecule 50 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	t	87	Total	C	N	O	S	0	0
			708	436	143	128	1		

- Molecule 51 is a protein called 30S ribosomal protein S16.

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

- Molecule 52 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	v	80	Total	C	N	O	S	0	0
			649	411	121	114	3		

- Molecule 53 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	w	66	Total	C	N	O	S	0	0
			544	344	102	97	1		

- Molecule 54 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	x	83	Total	C	N	O	S	0	0
			663	424	126	111	2		

- Molecule 55 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	y	85	Total	C	N	O	S	0	0
			664	411	137	113	3		

- Molecule 56 is a protein called 30S ribosomal protein S21.

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

- Molecule 57 is a protein called SsrA-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	5	118	Total	C	N	O	S	0	0
			940	601	168	168	3		

- Molecule 58 is a RNA chain called tmRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	4	363	Total	C	N	O	P	0	0
			7758	3465	1410	2520	363		

- Molecule 59 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
59	1	292	Total	Mg	0
			292	292	
59	2	127	Total	Mg	0
			127	127	
59	3	8	Total	Mg	0
			8	8	
59	7	4	Total	Mg	0
			4	4	
59	O	1	Total	Mg	0
			1	1	
59	Q	1	Total	Mg	0
			1	1	
59	b	1	Total	Mg	0
			1	1	
59	f	1	Total	Mg	0
			1	1	
59	i	1	Total	Mg	0
			1	1	
59	s	1	Total	Mg	0
			1	1	

- Molecule 60 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
60	a	1	Total Zn 1 1	0
60	f	1	Total Zn 1 1	0

- Molecule 61 is water.

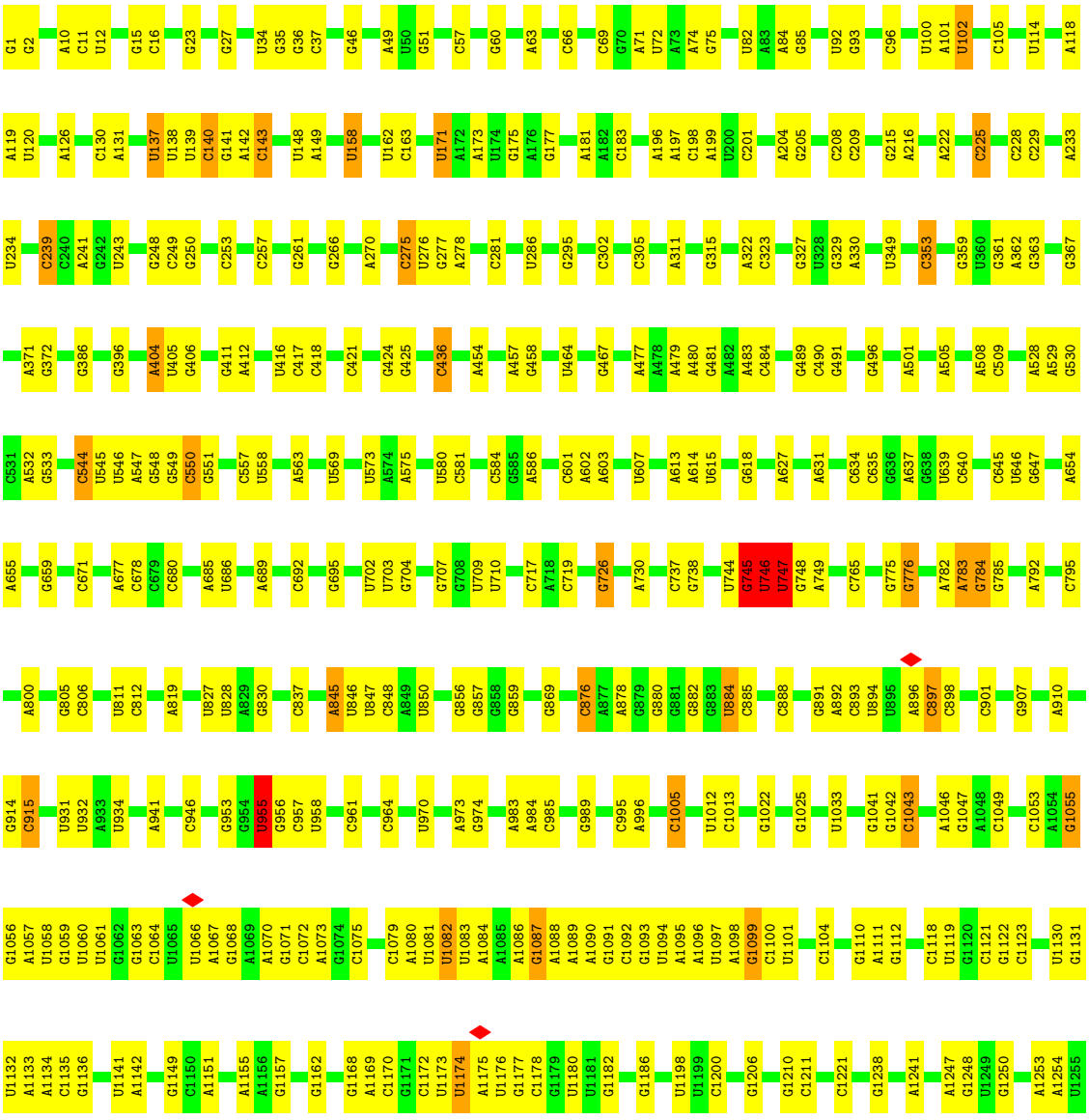
Mol	Chain	Residues	Atoms	AltConf
61	B	2	Total O 2 2	0

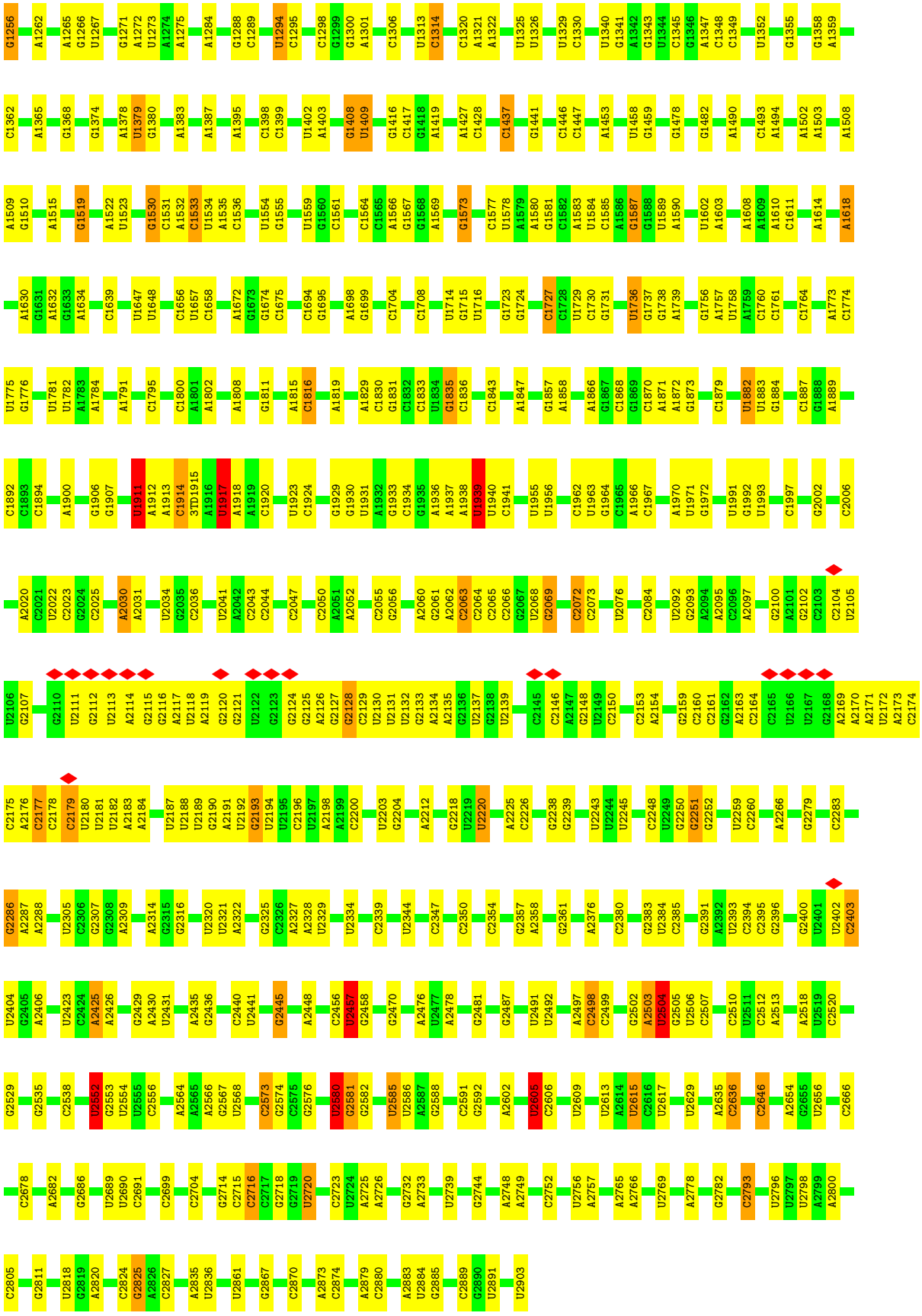
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: 23S ribosomal RNA

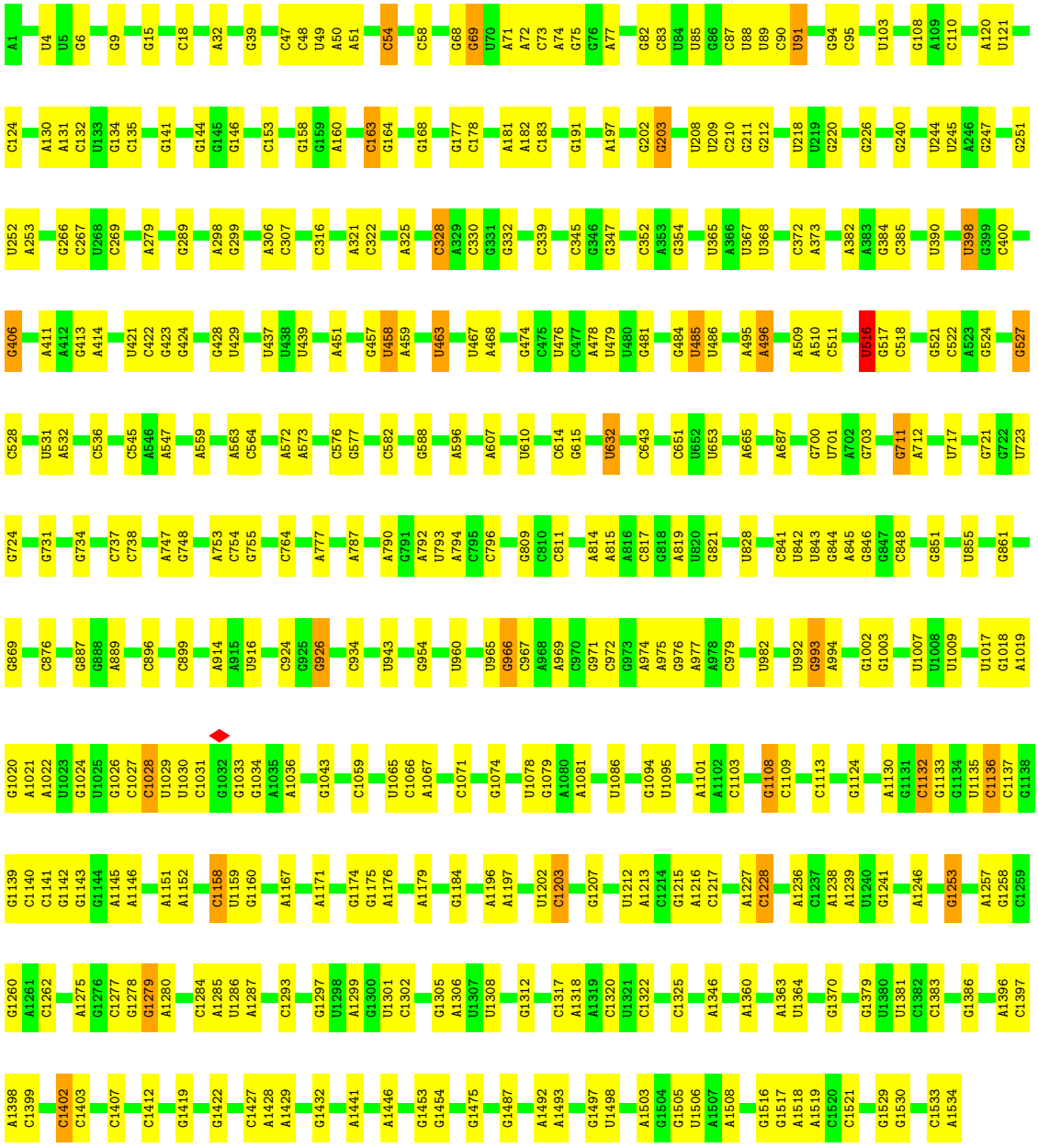
Chain 1:





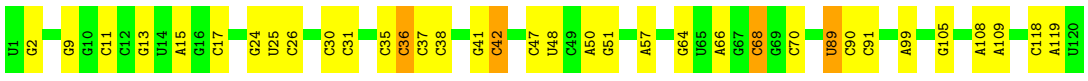
• Molecule 2: 16S ribosomal RNA

Chain 2:



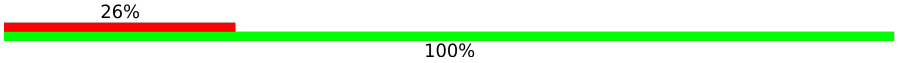
• Molecule 3: 5S ribosomal RNA

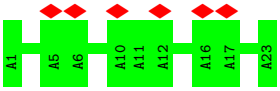
Chain 3:



• Molecule 4: Nascent peptide

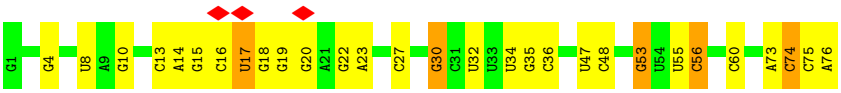
Chain 6:





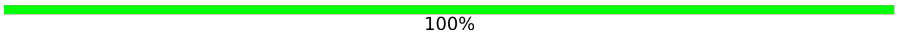
• Molecule 5: P-site tRNA

Chain 7:



• Molecule 6: 50S ribosomal protein L2

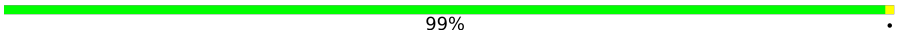
Chain B:



There are no outlier residues recorded for this chain.

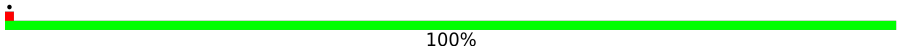
• Molecule 7: 50S ribosomal protein L3

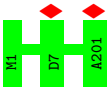
Chain C:



• Molecule 8: 50S ribosomal protein L4

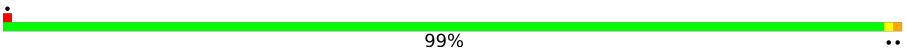
Chain D:

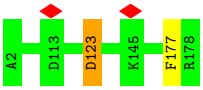




• Molecule 9: 50S ribosomal protein L5

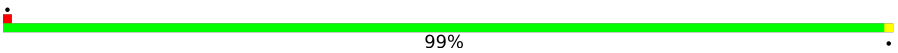
Chain E:

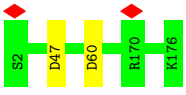




• Molecule 10: 50S ribosomal protein L6

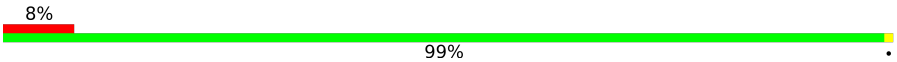
Chain F:

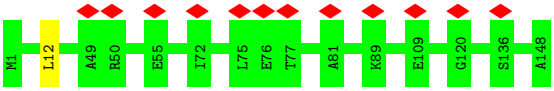




• Molecule 11: 50S ribosomal protein L9

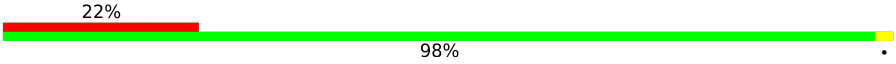
Chain G:

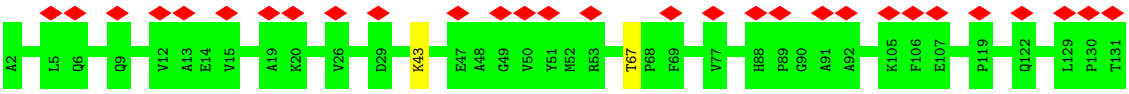




• Molecule 12: 50S ribosomal protein L10

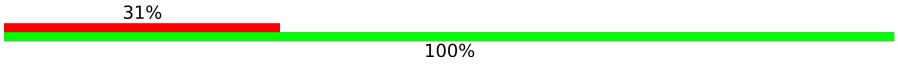
Chain H:

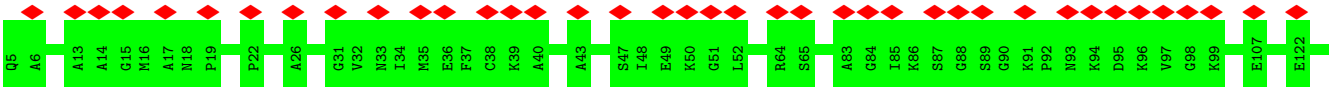




• Molecule 13: 50S ribosomal protein L11

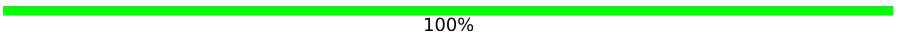
Chain I:





• Molecule 14: 50S ribosomal protein L13

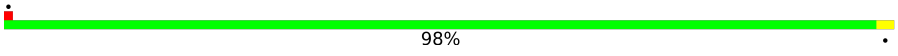
Chain J:

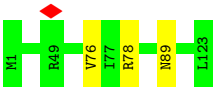


There are no outlier residues recorded for this chain.

• Molecule 15: 50S ribosomal protein L14

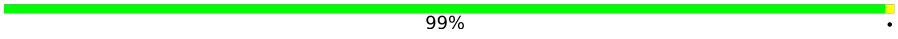
Chain K:

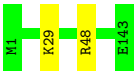




• Molecule 16: 50S ribosomal protein L15

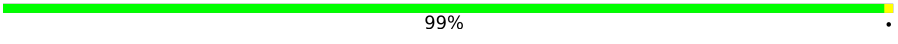
Chain L:





• Molecule 17: 50S ribosomal protein L16

Chain M:

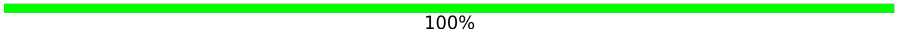


• Molecule 18: 50S ribosomal protein L17

Chain N: 

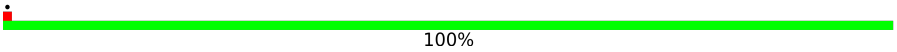
There are no outlier residues recorded for this chain.

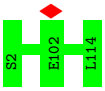
• Molecule 19: 50S ribosomal protein L18

Chain O: 

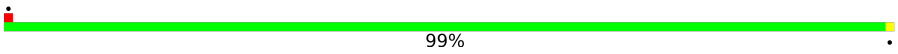
There are no outlier residues recorded for this chain.

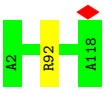
• Molecule 20: 50S ribosomal protein L19

Chain P: 

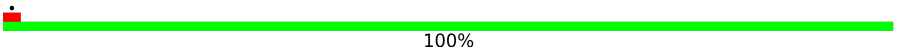


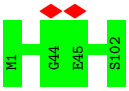
• Molecule 21: 50S ribosomal protein L20

Chain Q: 

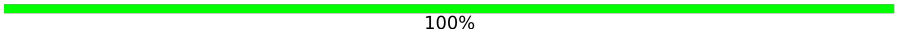


• Molecule 22: 50S ribosomal protein L21

Chain R: 

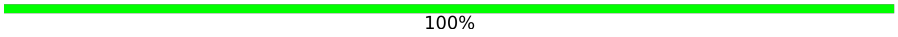


• Molecule 23: 50S ribosomal protein L22

Chain S: 

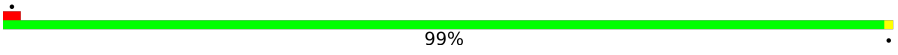
There are no outlier residues recorded for this chain.

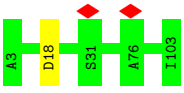
• Molecule 24: 50S ribosomal protein L23

Chain T: 

There are no outlier residues recorded for this chain.

• Molecule 25: 50S ribosomal protein L24

Chain U: 



• Molecule 26: 50S ribosomal protein L25

Chain V: 100%

There are no outlier residues recorded for this chain.

• Molecule 27: 50S ribosomal protein L27

Chain W: 99%

• Molecule 28: 50S ribosomal protein L28

Chain X: 100%

There are no outlier residues recorded for this chain.

• Molecule 29: 50S ribosomal protein L29

Chain Y: 98%

• Molecule 30: 50S ribosomal protein L30

Chain Z: 100%

There are no outlier residues recorded for this chain.

• Molecule 31: 50S ribosomal protein L31

Chain a: 100%

There are no outlier residues recorded for this chain.

• Molecule 32: 50S ribosomal protein L32

Chain b: 100%

There are no outlier residues recorded for this chain.

• Molecule 33: 50S ribosomal protein L33

Chain c: 100%

There are no outlier residues recorded for this chain.

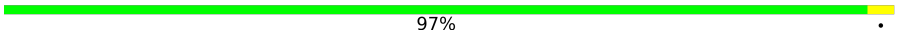
• Molecule 34: 50S ribosomal protein L34

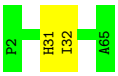
Chain d: 100%

There are no outlier residues recorded for this chain.

• Molecule 35: 50S ribosomal protein L35

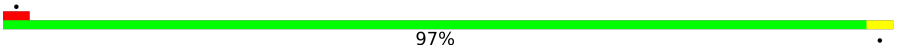
Chain e:

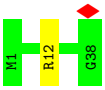




• Molecule 36: 50S ribosomal protein L36

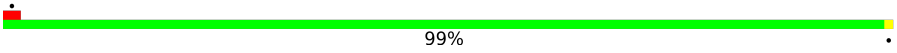
Chain f:

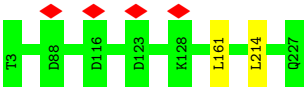




• Molecule 37: 30S ribosomal protein S2

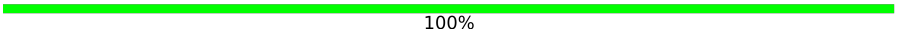
Chain g:





• Molecule 38: 30S ribosomal protein S3

Chain h:



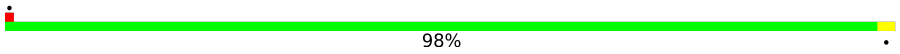
• Molecule 39: 30S ribosomal protein S4

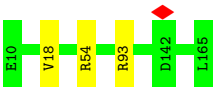
Chain i:

There are no outlier residues recorded for this chain.

• Molecule 40: 30S ribosomal protein S5

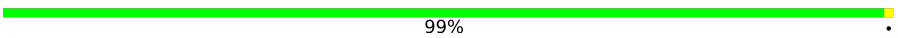
Chain j:





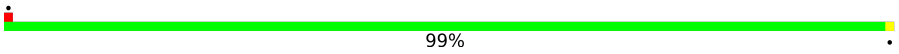
• Molecule 41: 30S ribosomal protein S6

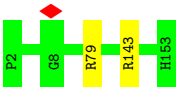
Chain k:



• Molecule 42: 30S ribosomal protein S7

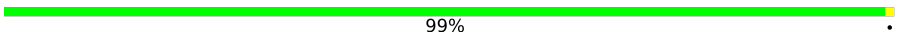
Chain l:





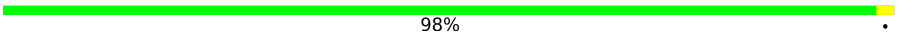
• Molecule 43: 30S ribosomal protein S8

Chain m:



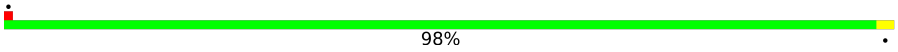
• Molecule 44: 30S ribosomal protein S9

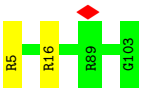
Chain n:



• Molecule 45: 30S ribosomal protein S10

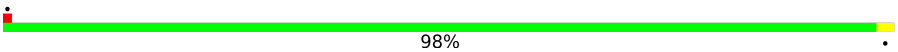
Chain o:

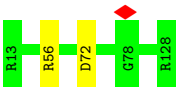




• Molecule 46: 30S ribosomal protein S11

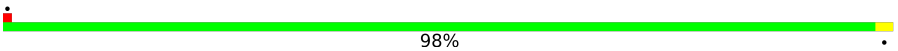
Chain p:

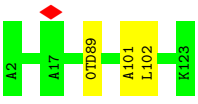




• Molecule 47: 30S ribosomal protein S12

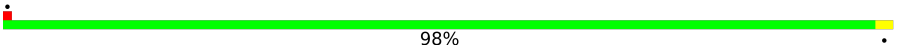
Chain q:

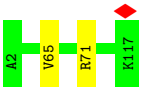




• Molecule 48: 30S ribosomal protein S13

Chain r:





• Molecule 49: 30S ribosomal protein S14

Chain s: 100%

There are no outlier residues recorded for this chain.

• Molecule 50: 30S ribosomal protein S15

Chain t: 100%

There are no outlier residues recorded for this chain.

• Molecule 51: 30S ribosomal protein S16

Chain u: 98%

• Molecule 52: 30S ribosomal protein S17

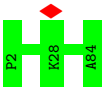
Chain v: 100%

• Molecule 53: 30S ribosomal protein S18

Chain w: 97%

• Molecule 54: 30S ribosomal protein S19

Chain x: 100%



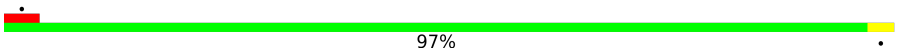
• Molecule 55: 30S ribosomal protein S20

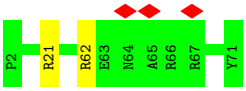
Chain y: 100%

There are no outlier residues recorded for this chain.

• Molecule 56: 30S ribosomal protein S21

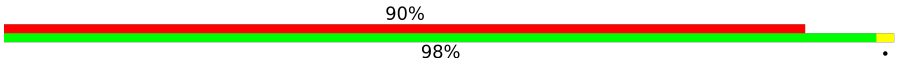
Chain z:

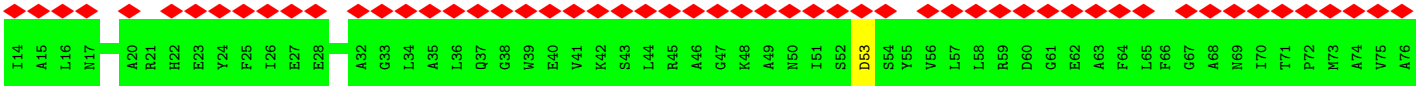


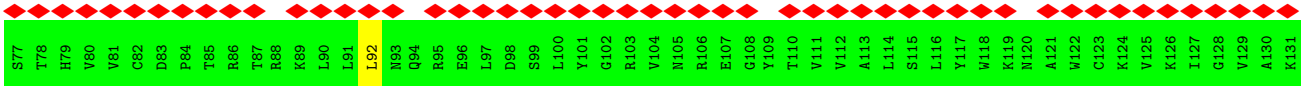


• Molecule 57: SsrA-binding protein

Chain 5:

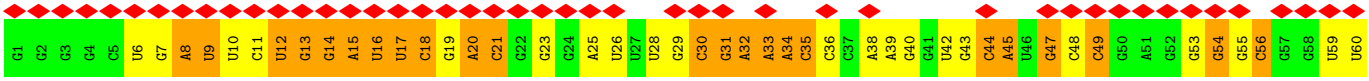


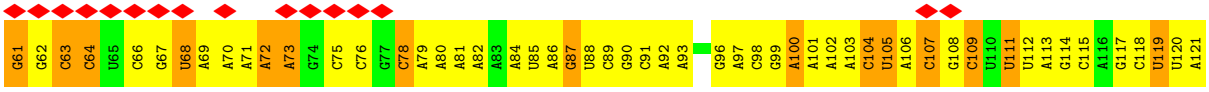


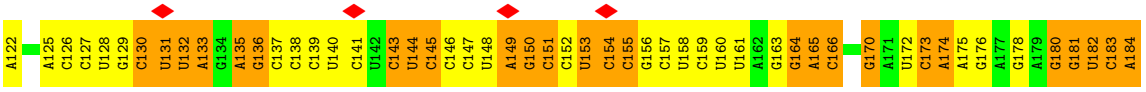


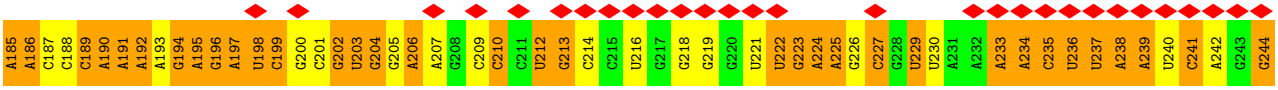
• Molecule 58: tmRNA

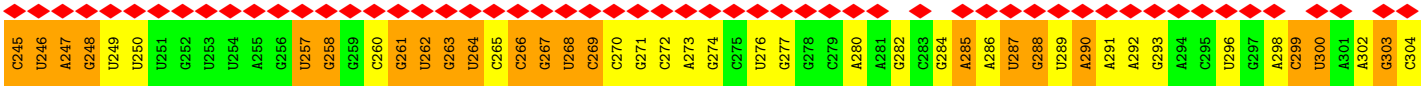
Chain 4:

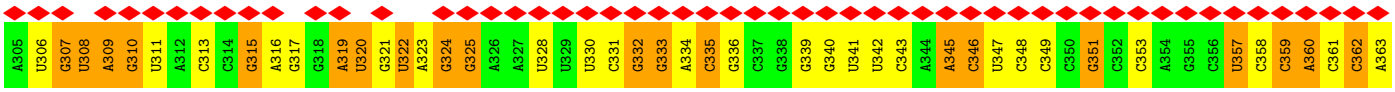












4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	47115	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 ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.517	Depositor
Minimum map value	-0.327	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.018	Depositor
Recommended contour level	0.05	Depositor
Map size (Å)	437.0, 437.0, 437.0	wwPDB
Map dimensions	380, 380, 380	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.15, 1.15, 1.15	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: 2MA, OMC, OMG, 5MC, 6MZ, 2MG, MG, 3TD, G7M, MA6, ZN, UR3, 1MG, 5MU, 0TD, 7MG, 4OC, PSU, OMU

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	1	0.97	2/69285 (0.0%)	1.22	518/108083 (0.5%)
2	2	0.87	1/36587 (0.0%)	1.17	173/57062 (0.3%)
3	3	0.78	0/2872	1.20	30/4478 (0.7%)
4	6	0.29	0/114	0.60	0/158
5	7	0.71	0/1810	1.29	21/2820 (0.7%)
6	B	0.50	0/2122	0.62	0/2852
7	C	0.48	0/1572	0.60	0/2117
8	D	0.43	0/1571	0.58	0/2113
9	E	0.40	0/1435	0.62	1/1926 (0.1%)
10	F	0.39	0/1333	0.59	0/1805
11	G	0.34	0/1112	0.59	0/1503
12	H	0.35	0/993	0.68	0/1340
13	I	0.32	0/998	0.62	0/1348
14	J	0.48	0/1152	0.56	0/1551
15	K	0.50	0/955	0.63	0/1279
16	L	0.43	0/1052	0.56	0/1401
17	M	0.46	0/1084	0.55	0/1450
18	N	0.43	0/964	0.57	0/1289
19	O	0.41	0/894	0.58	0/1198
20	P	0.49	0/920	0.60	0/1231
21	Q	0.57	0/960	0.58	0/1278
22	R	0.47	0/823	0.59	0/1100
23	S	0.45	0/852	0.58	0/1142
24	T	0.42	0/752	0.55	0/1005
25	U	0.37	0/782	0.57	0/1044
26	V	0.41	0/760	0.52	0/1018
27	W	0.47	0/579	0.53	0/767
28	X	0.43	0/635	0.54	0/848
29	Y	0.32	0/502	0.53	0/667
30	Z	0.42	0/438	0.63	0/586
31	a	0.31	0/531	0.56	0/709

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
32	b	0.41	0/440	0.54	0/588
33	c	0.42	0/424	0.58	0/565
34	d	0.46	0/370	0.55	0/487
35	e	0.47	0/513	0.62	0/676
36	f	0.46	0/303	0.58	0/397
37	g	0.35	0/1791	0.59	1/2413 (0.0%)
38	h	0.41	0/1663	0.58	1/2241 (0.0%)
39	i	0.40	0/1665	0.56	0/2227
40	j	0.46	0/1165	0.69	1/1568 (0.1%)
41	k	0.40	0/867	0.56	0/1171
42	l	0.36	0/1206	0.56	0/1617
43	m	0.41	0/989	0.57	0/1326
44	n	0.38	0/1034	0.57	0/1375
45	o	0.37	0/800	0.63	0/1082
46	p	0.41	0/885	0.61	1/1195 (0.1%)
47	q	0.46	0/954	0.65	1/1279 (0.1%)
48	r	0.35	0/909	0.59	0/1215
49	s	0.40	0/817	0.52	0/1088
50	t	0.41	0/716	0.56	0/956
51	u	0.41	0/659	0.60	0/884
52	v	0.39	0/658	0.58	0/881
53	w	0.43	0/553	0.57	0/743
54	x	0.38	0/680	0.54	0/915
55	y	0.36	0/670	0.53	0/888
56	z	0.36	0/597	0.56	0/792
57	5	0.32	0/958	0.73	1/1294 (0.1%)
58	4	0.75	4/8681 (0.0%)	2.10	533/13532 (3.9%)
All	All	0.81	7/167406 (0.0%)	1.15	1282/250563 (0.5%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	1	34	0
2	2	5	0
12	H	0	1
35	e	0	1
42	l	0	1
47	q	0	1
48	r	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
53	w	0	1
58	4	3	0
All	All	42	6

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	586	A	N9-C4	-5.86	1.34	1.37
58	4	237	U	N1-C2	5.69	1.43	1.38
1	1	1614	A	N9-C4	-5.69	1.34	1.37
58	4	32	A	N9-C4	5.27	1.41	1.37
58	4	225	A	N9-C4	5.16	1.41	1.37

The worst 5 of 1282 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
58	4	335	C	O5'-P-OP2	-18.29	88.75	110.70
58	4	173	C	N1-C2-O2	14.29	127.47	118.90
58	4	182	U	O4'-C1'-N1	14.16	119.53	108.20
58	4	146	C	C6-N1-C2	-13.90	114.74	120.30
58	4	154	C	N1-C2-O2	13.88	127.23	118.90

5 of 42 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	1	745	1MG	C4',C3'
1	1	746	PSU	C4',C3'
1	1	747	5MU	C2',C4'
1	1	955	PSU	C4',C3'
1	1	1618	6MZ	C2',C3'

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
12	H	67	THR	Peptide
35	e	31	HIS	Peptide
42	l	79	ARG	Peptide
47	q	101	ALA	Peptide
48	r	65	VAL	Peptide

5.2 Too-close contacts

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

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	6	21/23 (91%)	16 (76%)	5 (24%)	0	100	100
6	B	269/271 (99%)	240 (89%)	29 (11%)	0	100	100
7	C	205/207 (99%)	182 (89%)	23 (11%)	0	100	100
8	D	199/201 (99%)	186 (94%)	13 (6%)	0	100	100
9	E	175/177 (99%)	156 (89%)	17 (10%)	2 (1%)	14	50
10	F	173/175 (99%)	153 (88%)	20 (12%)	0	100	100
11	G	146/148 (99%)	131 (90%)	15 (10%)	0	100	100
12	H	128/130 (98%)	104 (81%)	24 (19%)	0	100	100
13	I	133/135 (98%)	113 (85%)	20 (15%)	0	100	100
14	J	140/142 (99%)	126 (90%)	14 (10%)	0	100	100
15	K	121/123 (98%)	108 (89%)	13 (11%)	0	100	100
16	L	141/143 (99%)	128 (91%)	13 (9%)	0	100	100
17	M	133/135 (98%)	125 (94%)	8 (6%)	0	100	100
18	N	117/119 (98%)	106 (91%)	11 (9%)	0	100	100
19	O	113/115 (98%)	107 (95%)	6 (5%)	0	100	100
20	P	111/113 (98%)	98 (88%)	13 (12%)	0	100	100
21	Q	115/117 (98%)	109 (95%)	6 (5%)	0	100	100
22	R	100/102 (98%)	95 (95%)	5 (5%)	0	100	100
23	S	107/109 (98%)	102 (95%)	5 (5%)	0	100	100
24	T	92/94 (98%)	85 (92%)	7 (8%)	0	100	100
25	U	99/101 (98%)	81 (82%)	18 (18%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	V	91/93 (98%)	87 (96%)	4 (4%)	0	100	100
27	W	73/75 (97%)	68 (93%)	5 (7%)	0	100	100
28	X	75/77 (97%)	72 (96%)	3 (4%)	0	100	100
29	Y	60/62 (97%)	60 (100%)	0	0	100	100
30	Z	54/56 (96%)	47 (87%)	7 (13%)	0	100	100
31	a	64/66 (97%)	58 (91%)	6 (9%)	0	100	100
32	b	53/55 (96%)	50 (94%)	3 (6%)	0	100	100
33	c	49/51 (96%)	45 (92%)	4 (8%)	0	100	100
34	d	43/45 (96%)	38 (88%)	5 (12%)	0	100	100
35	e	62/64 (97%)	54 (87%)	7 (11%)	1 (2%)	9	43
36	f	36/38 (95%)	33 (92%)	3 (8%)	0	100	100
37	g	223/225 (99%)	201 (90%)	22 (10%)	0	100	100
38	h	206/208 (99%)	190 (92%)	16 (8%)	0	100	100
39	i	203/205 (99%)	190 (94%)	13 (6%)	0	100	100
40	j	154/156 (99%)	140 (91%)	14 (9%)	0	100	100
41	k	102/104 (98%)	95 (93%)	7 (7%)	0	100	100
42	l	150/152 (99%)	137 (91%)	13 (9%)	0	100	100
43	m	127/129 (98%)	119 (94%)	8 (6%)	0	100	100
44	n	125/127 (98%)	115 (92%)	10 (8%)	0	100	100
45	o	97/99 (98%)	87 (90%)	10 (10%)	0	100	100
46	p	114/116 (98%)	101 (89%)	13 (11%)	0	100	100
47	q	119/122 (98%)	111 (93%)	8 (7%)	0	100	100
48	r	114/116 (98%)	106 (93%)	8 (7%)	0	100	100
49	s	98/100 (98%)	93 (95%)	5 (5%)	0	100	100
50	t	85/87 (98%)	82 (96%)	3 (4%)	0	100	100
51	u	80/82 (98%)	75 (94%)	5 (6%)	0	100	100
52	v	78/80 (98%)	68 (87%)	10 (13%)	0	100	100
53	w	64/66 (97%)	60 (94%)	4 (6%)	0	100	100
54	x	81/83 (98%)	72 (89%)	9 (11%)	0	100	100
55	y	83/85 (98%)	82 (99%)	1 (1%)	0	100	100
56	z	68/70 (97%)	64 (94%)	4 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
57	5	116/118 (98%)	89 (77%)	27 (23%)	0	100 100
All	All	5985/6092 (98%)	5440 (91%)	542 (9%)	3 (0%)	54 83

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	E	123	ASP
35	e	32	ILE
9	E	177	PHE

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	Percentiles
6	B	216/216 (100%)	216 (100%)	0	100 100
7	C	163/163 (100%)	161 (99%)	2 (1%)	71 84
8	D	165/165 (100%)	165 (100%)	0	100 100
9	E	148/148 (100%)	148 (100%)	0	100 100
10	F	136/136 (100%)	134 (98%)	2 (2%)	65 81
11	G	113/113 (100%)	112 (99%)	1 (1%)	78 88
12	H	99/99 (100%)	98 (99%)	1 (1%)	76 86
13	I	104/104 (100%)	104 (100%)	0	100 100
14	J	116/116 (100%)	116 (100%)	0	100 100
15	K	104/104 (100%)	101 (97%)	3 (3%)	42 66
16	L	102/102 (100%)	100 (98%)	2 (2%)	55 74
17	M	108/108 (100%)	107 (99%)	1 (1%)	78 88
18	N	99/99 (100%)	99 (100%)	0	100 100
19	O	85/85 (100%)	85 (100%)	0	100 100
20	P	98/98 (100%)	98 (100%)	0	100 100
21	Q	89/89 (100%)	88 (99%)	1 (1%)	73 85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
22	R	84/84 (100%)	84 (100%)	0	100	100
23	S	92/92 (100%)	92 (100%)	0	100	100
24	T	81/81 (100%)	81 (100%)	0	100	100
25	U	83/83 (100%)	82 (99%)	1 (1%)	71	84
26	V	78/78 (100%)	78 (100%)	0	100	100
27	W	57/57 (100%)	56 (98%)	1 (2%)	59	77
28	X	67/67 (100%)	67 (100%)	0	100	100
29	Y	54/54 (100%)	53 (98%)	1 (2%)	57	76
30	Z	47/47 (100%)	47 (100%)	0	100	100
31	a	59/59 (100%)	59 (100%)	0	100	100
32	b	46/46 (100%)	46 (100%)	0	100	100
33	c	46/46 (100%)	46 (100%)	0	100	100
34	d	37/37 (100%)	37 (100%)	0	100	100
35	e	51/51 (100%)	51 (100%)	0	100	100
36	f	34/34 (100%)	33 (97%)	1 (3%)	42	66
37	g	187/187 (100%)	186 (100%)	1 (0%)	88	94
38	h	171/171 (100%)	171 (100%)	0	100	100
39	i	172/172 (100%)	172 (100%)	0	100	100
40	j	119/119 (100%)	117 (98%)	2 (2%)	60	79
41	k	91/91 (100%)	90 (99%)	1 (1%)	73	85
42	l	125/125 (100%)	124 (99%)	1 (1%)	81	89
43	m	104/104 (100%)	103 (99%)	1 (1%)	76	86
44	n	105/105 (100%)	103 (98%)	2 (2%)	57	76
45	o	86/86 (100%)	84 (98%)	2 (2%)	50	71
46	p	89/89 (100%)	88 (99%)	1 (1%)	73	85
47	q	102/102 (100%)	102 (100%)	0	100	100
48	r	94/94 (100%)	93 (99%)	1 (1%)	73	85
49	s	83/83 (100%)	83 (100%)	0	100	100
50	t	75/75 (100%)	75 (100%)	0	100	100
51	u	65/65 (100%)	63 (97%)	2 (3%)	40	65
52	v	74/74 (100%)	74 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
53	w	57/57 (100%)	56 (98%)	1 (2%)	59 77
54	x	72/72 (100%)	72 (100%)	0	100 100
55	y	65/65 (100%)	65 (100%)	0	100 100
56	z	60/60 (100%)	58 (97%)	2 (3%)	38 64
57	5	97/97 (100%)	96 (99%)	1 (1%)	76 86
All	All	4954/4954 (100%)	4919 (99%)	35 (1%)	84 91

5 of 35 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
48	r	71	ARG
51	u	1	MET
56	z	21	ARG
21	Q	92	ARG
17	M	7	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 51 such sidechains are listed below:

Mol	Chain	Res	Type
33	c	19	HIS
40	j	132	ASN
57	5	69	ASN
35	e	26	HIS
39	i	59	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	2897/2903 (99%)	701 (24%)	18 (0%)
2	2	1525/1534 (99%)	320 (20%)	2 (0%)
3	3	119/120 (99%)	23 (19%)	0
5	7	75/76 (98%)	25 (33%)	1 (1%)
58	4	362/363 (99%)	220 (60%)	32 (8%)
All	All	4978/4996 (99%)	1289 (25%)	53 (1%)

5 of 1289 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	2	G
1	1	10	A
1	1	15	G
1	1	23	G
1	1	27	G

5 of 53 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
58	4	33	A
58	4	183	C
58	4	333	G
58	4	68	U
58	4	153	U

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	6MZ	1	2030	1	18,25,26	1.94	1 (5%)	16,36,39	2.56	4 (25%)
2	MA6	2	1519	2	18,26,27	1.09	3 (16%)	19,38,41	1.49	2 (10%)
1	2MG	1	1835	1	18,26,27	2.86	6 (33%)	16,38,41	1.56	4 (25%)
1	OMU	1	2552	1	19,22,23	2.71	7 (36%)	26,31,34	2.12	9 (34%)
2	2MG	2	966	2	18,26,27	2.87	5 (27%)	16,38,41	1.47	4 (25%)
1	PSU	1	1917	1	18,21,22	2.05	6 (33%)	22,30,33	2.12	5 (22%)
1	2MA	1	2503	59,1	17,25,26	1.56	3 (17%)	17,37,40	1.35	2 (11%)
2	PSU	2	516	59,2	18,21,22	2.25	6 (33%)	22,30,33	2.24	5 (22%)
2	5MC	2	1407	2	18,22,23	2.08	3 (16%)	26,32,35	1.33	4 (15%)
2	MA6	2	1518	2	18,26,27	1.01	1 (5%)	19,38,41	1.53	2 (10%)
1	5MU	1	747	1	19,22,23	2.50	8 (42%)	28,32,35	3.59	11 (39%)
47	0TD	q	89	47	7,9,10	1.48	0	6,11,13	2.20	2 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	OMC	1	2498	59,1	19,22,23	1.90	6 (31%)	26,31,34	2.20	7 (26%)
1	PSU	1	1911	1	18,21,22	2.01	5 (27%)	22,30,33	2.35	4 (18%)
2	5MC	2	967	2	18,22,23	2.15	3 (16%)	26,32,35	1.46	2 (7%)
1	G7M	1	2069	1	20,26,27	2.81	4 (20%)	17,39,42	1.17	2 (11%)
1	PSU	1	955	1	18,21,22	2.27	6 (33%)	22,30,33	2.45	5 (22%)
1	PSU	1	746	59,1	18,21,22	2.15	6 (33%)	22,30,33	1.90	5 (22%)
1	OMG	1	2251	5,1	18,26,27	3.02	7 (38%)	19,38,41	1.47	3 (15%)
1	PSU	1	2605	1	18,21,22	2.09	6 (33%)	22,30,33	2.22	5 (22%)
2	4OC	2	1402	2	20,23,24	2.45	5 (25%)	26,32,35	2.28	6 (23%)
1	5MU	1	1939	1	19,22,23	2.63	7 (36%)	28,32,35	3.51	10 (35%)
1	5MC	1	1962	1	18,22,23	2.04	3 (16%)	26,32,35	1.52	4 (15%)
1	2MG	1	2445	1	18,26,27	3.04	6 (33%)	16,38,41	1.27	3 (18%)
1	PSU	1	2580	1	18,21,22	2.13	5 (27%)	22,30,33	2.24	6 (27%)
2	2MG	2	1207	2	18,26,27	2.87	5 (27%)	16,38,41	1.40	4 (25%)
2	UR3	2	1498	2	19,22,23	2.94	7 (36%)	26,32,35	1.41	2 (7%)
1	3TD	1	1915	1	18,22,23	2.75	7 (38%)	22,32,35	1.80	4 (18%)
2	7MG	2	527	2	22,26,27	6.22	6 (27%)	29,39,42	2.47	8 (27%)
1	PSU	1	2457	1	18,21,22	2.03	5 (27%)	22,30,33	2.25	5 (22%)
1	PSU	1	2504	1	18,21,22	2.17	5 (27%)	22,30,33	2.26	5 (22%)
1	6MZ	1	1618	1	18,25,26	1.94	1 (5%)	16,36,39	2.12	4 (25%)
2	2MG	2	1516	2	18,26,27	2.85	6 (33%)	16,38,41	1.46	3 (18%)
1	1MG	1	745	1	18,26,27	3.04	6 (33%)	19,39,42	2.12	8 (42%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	6MZ	1	2030	1	2/2/5/6	2/5/27/28	0/3/3/3
2	MA6	2	1519	2	-	6/7/29/30	0/3/3/3
1	2MG	1	1835	1	-	2/5/27/28	0/3/3/3
1	OMU	1	2552	1	2/2/5/5	3/9/27/28	0/2/2/2
2	2MG	2	966	2	-	3/5/27/28	0/3/3/3
1	PSU	1	1917	1	2/2/5/5	3/7/25/26	0/2/2/2
1	2MA	1	2503	59,1	2/2/5/5	2/3/25/26	0/3/3/3

Continued on next page...

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PSU	2	516	59,2	2/2/5/5	3/7/25/26	0/2/2/2
2	5MC	2	1407	2	-	0/7/25/26	0/2/2/2
2	MA6	2	1518	2	-	5/7/29/30	0/3/3/3
1	5MU	1	747	1	2/2/5/5	3/7/25/26	0/2/2/2
47	0TD	q	89	47	-	1/7/12/14	-
1	OMC	1	2498	59,1	1/1/5/5	6/9/27/28	0/2/2/2
1	PSU	1	1911	1	2/2/5/5	3/7/25/26	0/2/2/2
2	5MC	2	967	2	-	0/7/25/26	0/2/2/2
1	G7M	1	2069	1	1/1/5/5	2/3/25/26	0/3/3/3
1	PSU	1	955	1	2/2/5/5	4/7/25/26	0/2/2/2
1	PSU	1	746	59,1	2/2/5/5	4/7/25/26	0/2/2/2
1	PSU	1	2605	1	2/2/5/5	3/7/25/26	0/2/2/2
1	OMG	1	2251	5,1	1/1/5/5	3/5/27/28	0/3/3/3
2	4OC	2	1402	2	2/2/5/6	6/9/29/30	0/2/2/2
1	5MU	1	1939	1	2/2/5/5	1/7/25/26	0/2/2/2
1	5MC	1	1962	1	-	4/7/25/26	0/2/2/2
1	2MG	1	2445	1	-	2/5/27/28	0/3/3/3
1	PSU	1	2580	1	2/2/5/5	3/7/25/26	0/2/2/2
2	2MG	2	1207	2	-	2/5/27/28	0/3/3/3
2	UR3	2	1498	2	-	0/7/25/26	0/2/2/2
1	3TD	1	1915	1	1/1/5/5	5/7/25/26	0/2/2/2
2	7MG	2	527	2	1/1/7/7	3/7/37/38	0/3/3/3
1	PSU	1	2457	1	2/2/5/5	1/7/25/26	0/2/2/2
1	PSU	1	2504	1	2/2/5/5	3/7/25/26	0/2/2/2
1	6MZ	1	1618	1	2/2/5/6	5/5/27/28	0/3/3/3
2	2MG	2	1516	2	-	0/5/27/28	0/3/3/3
1	1MG	1	745	1	2/2/5/5	2/3/25/26	0/3/3/3

The worst 5 of 166 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	527	7MG	C8-N9	-26.70	1.31	1.46
1	1	2069	G7M	O6-C6	9.98	1.43	1.23
1	1	2251	OMG	O6-C6	9.21	1.42	1.23
2	2	1516	2MG	O6-C6	8.89	1.41	1.23
2	2	1207	2MG	O6-C6	8.79	1.41	1.23

The worst 5 of 159 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	1939	5MU	N3-C2-N1	8.55	126.24	114.89
1	1	747	5MU	N3-C2-N1	8.44	126.09	114.89
1	1	747	5MU	C4-N3-C2	-8.06	116.92	127.35
1	1	1939	5MU	C5M-C5-C4	8.01	127.59	118.77
1	1	747	5MU	C5M-C5-C4	7.64	127.18	118.77

5 of 39 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	1	745	1MG	C4'
1	1	745	1MG	C3'
1	1	746	PSU	C4'
1	1	746	PSU	C3'
1	1	747	5MU	C2'

5 of 95 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
47	q	89	0TD	CG-CB-SB-CSB
1	1	745	1MG	C3'-C4'-C5'-O5'
1	1	746	PSU	C2'-C1'-C5-C4
1	1	746	PSU	C2'-C1'-C5-C6
1	1	747	5MU	C3'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 439 ligands modelled in this entry, 439 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	2	3
1	1	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	2	1276:G	O3'	1277:C	P	3.78
1	1	2314:A	O3'	2315:G	P	3.57
1	2	1383:C	O3'	1384:C	P	3.26
1	2	147:G	O3'	148:G	P	3.21

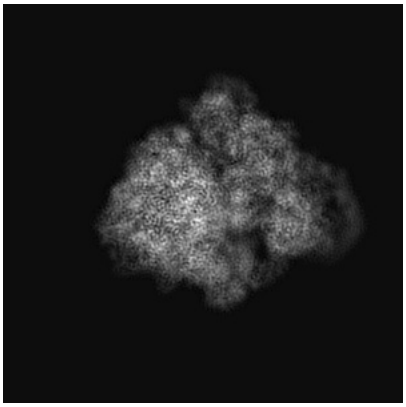
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-4478. These allow visual inspection of the internal detail of the map and identification of artifacts.

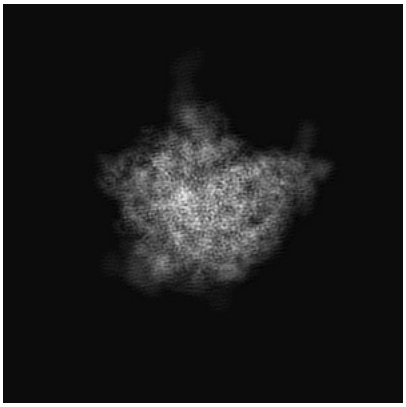
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

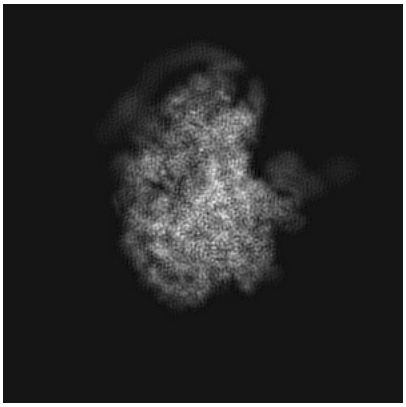
6.1.1 Primary map



X



Y

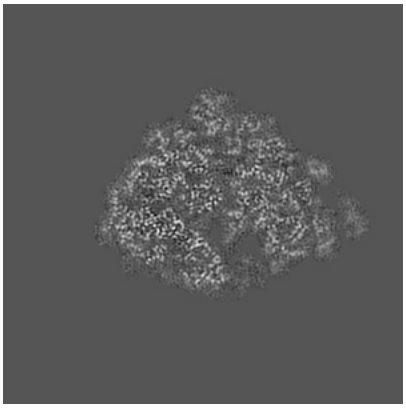


Z

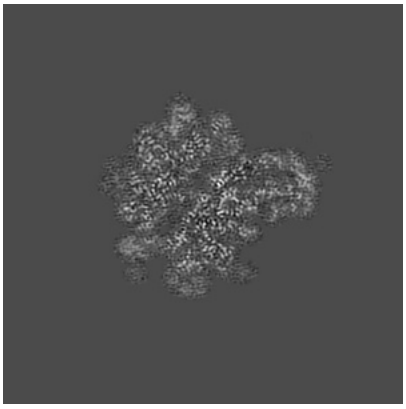
The images above show the map projected in three orthogonal directions.

6.2 Central slices

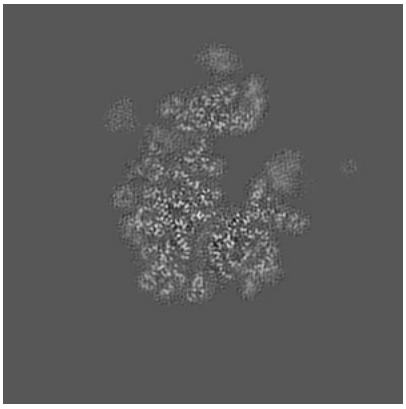
6.2.1 Primary map



X Index: 190



Y Index: 190

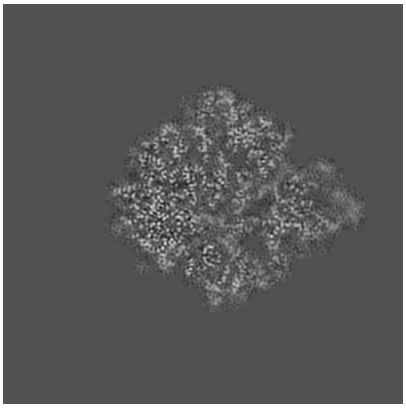


Z Index: 190

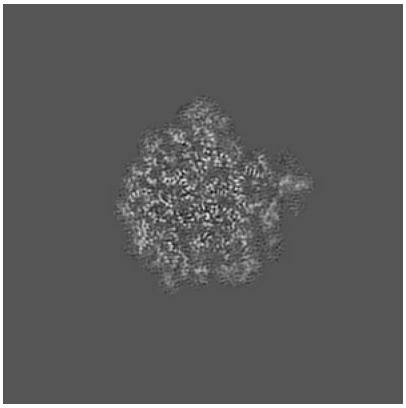
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

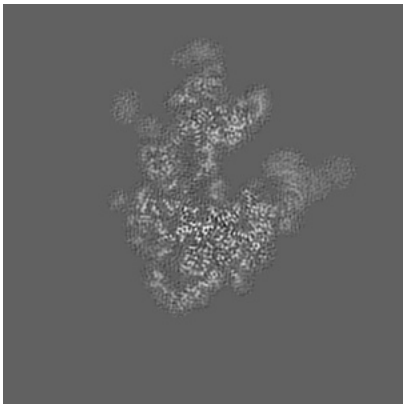
6.3.1 Primary map



X Index: 200



Y Index: 177

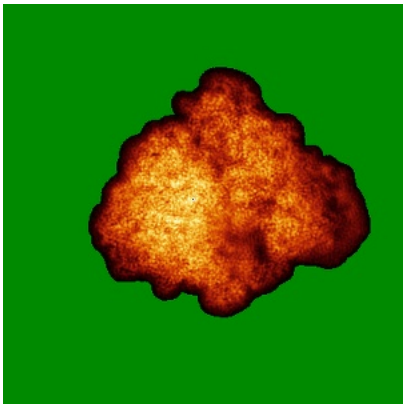


Z Index: 173

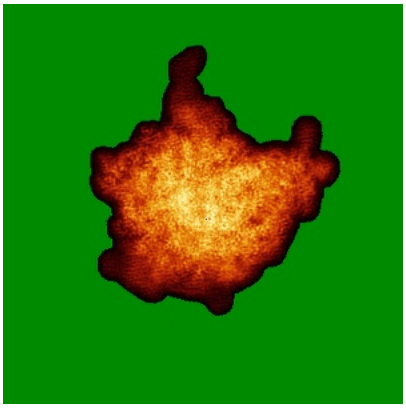
The images above show the largest variance slices of the map in three orthogonal directions.

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

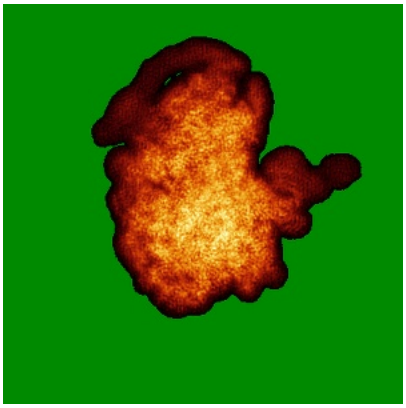
6.4.1 Primary map



X



Y

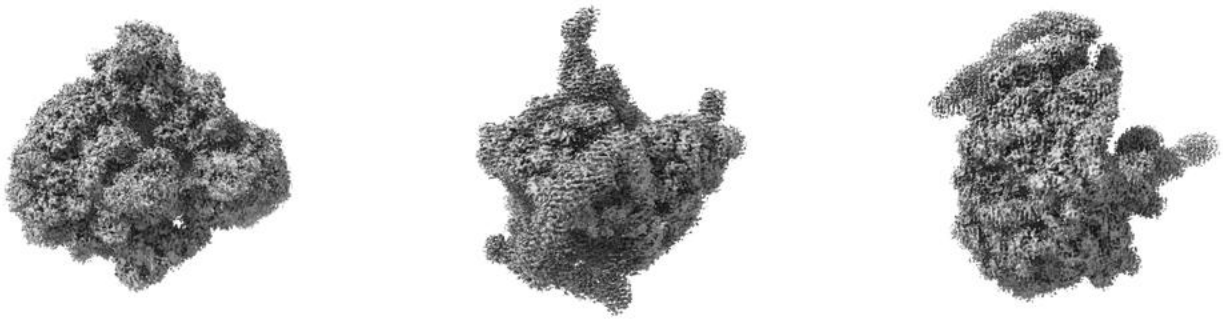


Z

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 0.05. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

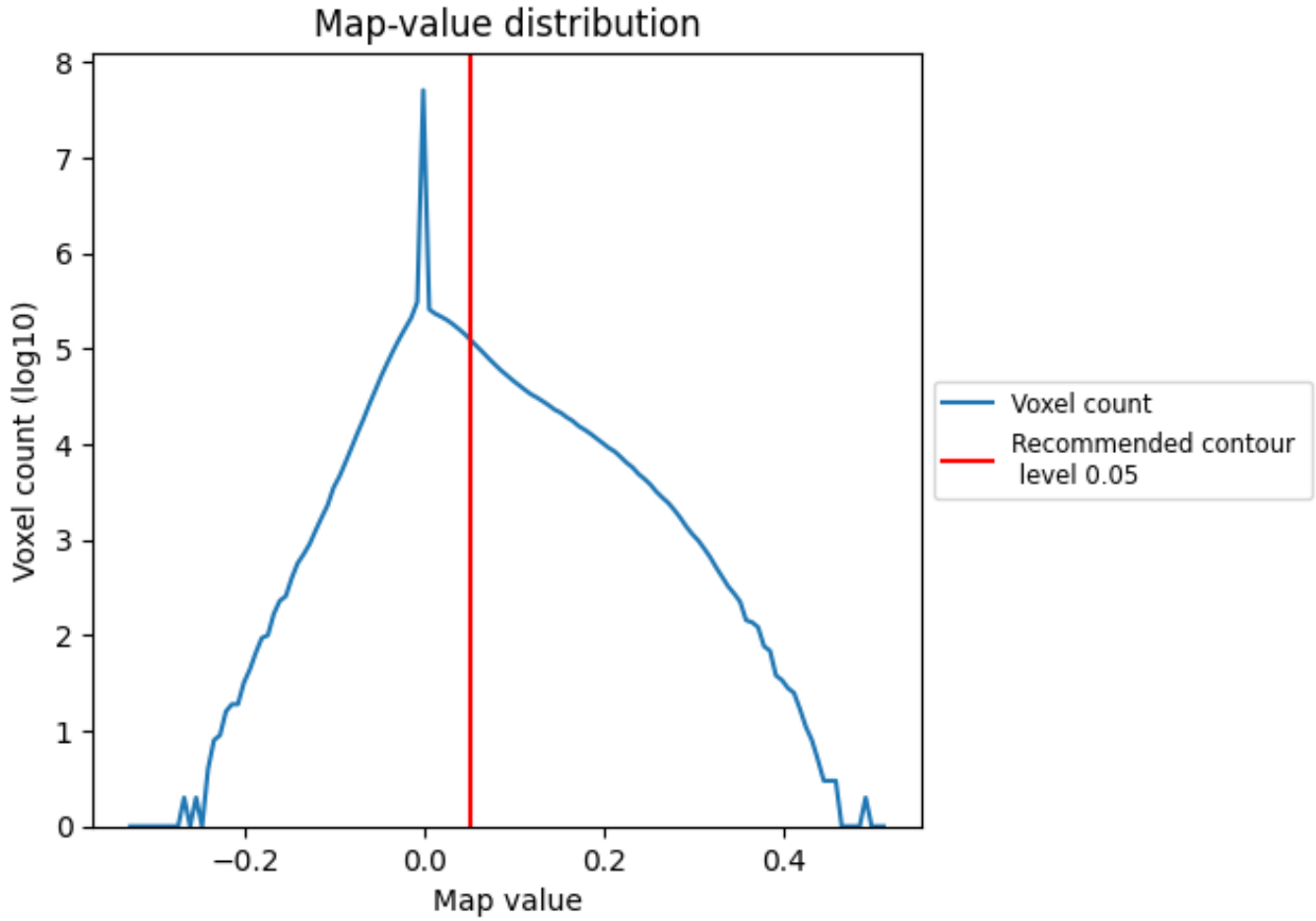
6.6 Mask visualisation (i)

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

7 Map analysis

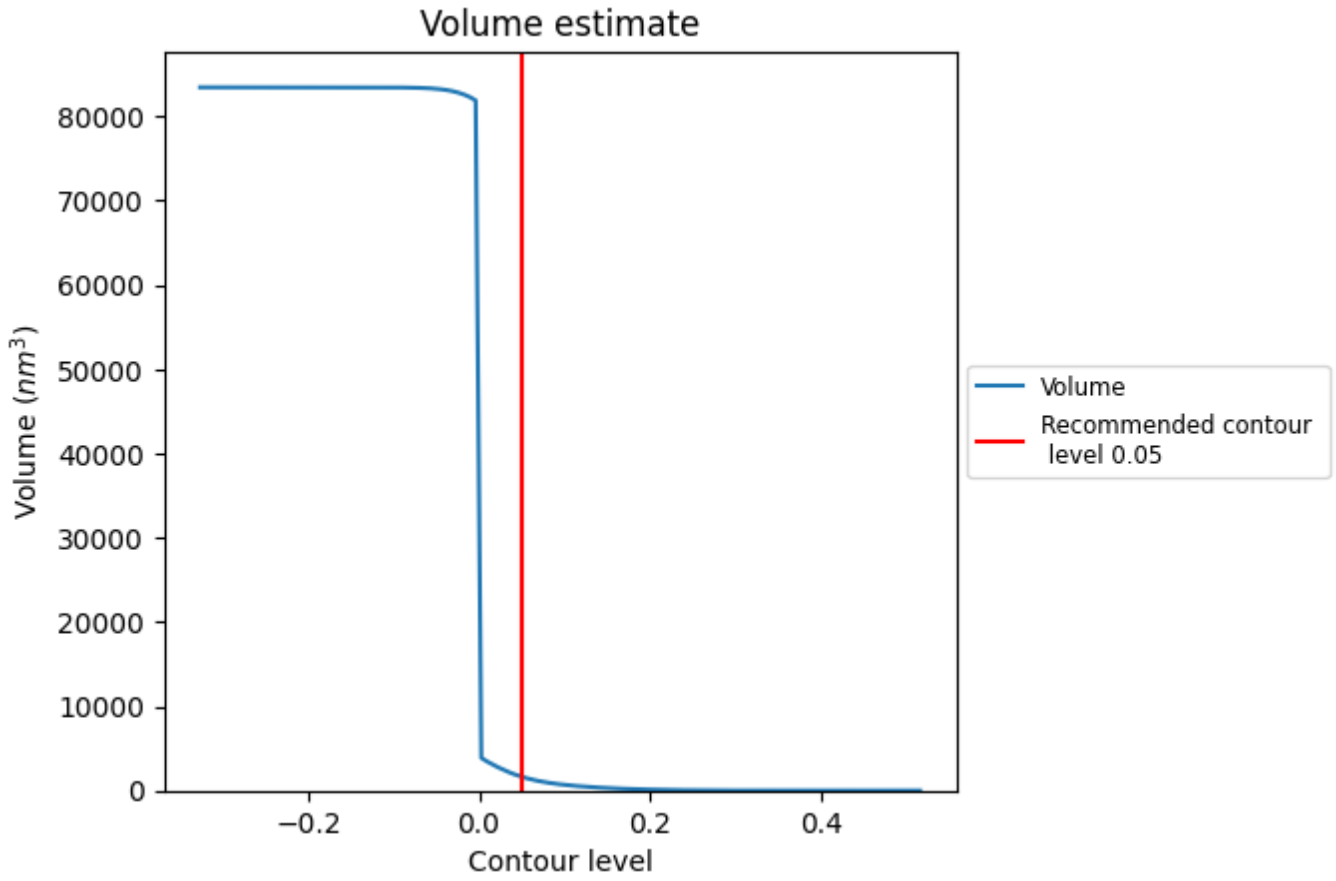
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

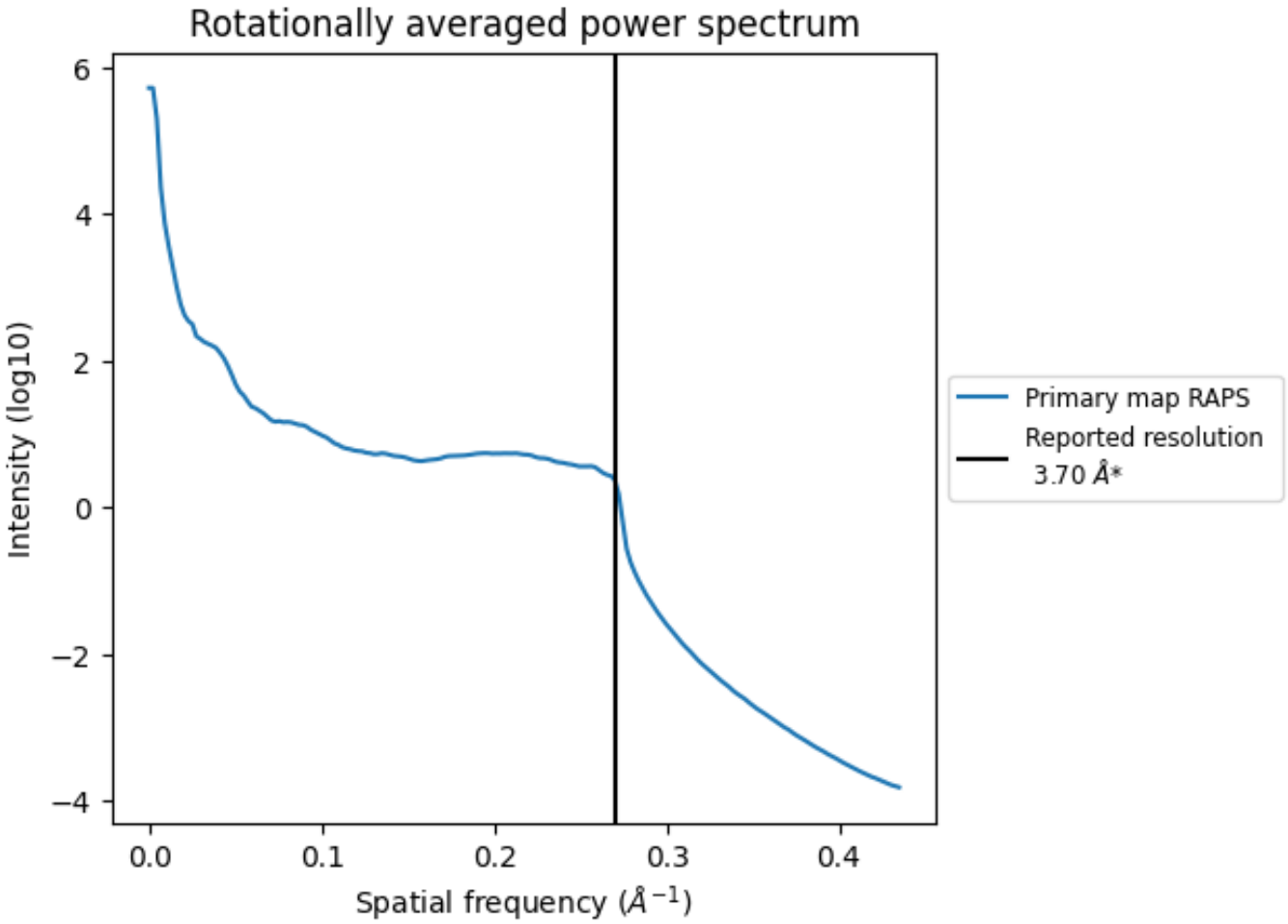
7.2 Volume estimate (i)



The volume at the recommended contour level is 1641 nm^3; this corresponds to an approximate mass of 1482 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 Å^{-1}

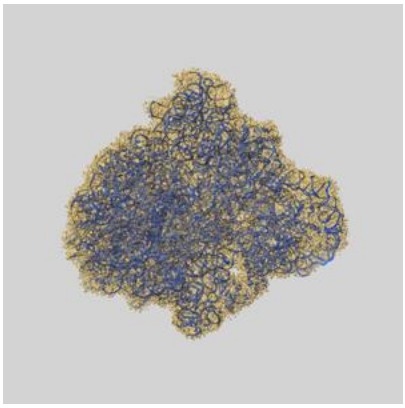
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

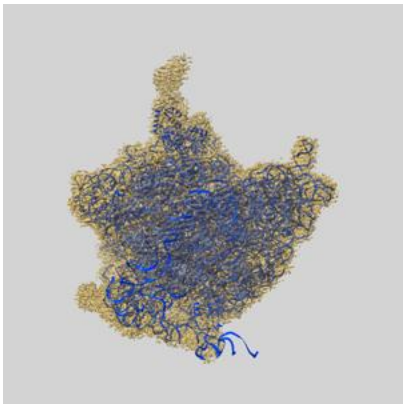
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-4478 and PDB model 6Q9A. Per-residue inclusion information can be found in section 3 on page 16.

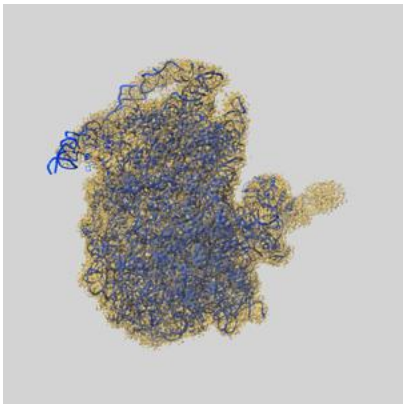
9.1 Map-model overlay



X



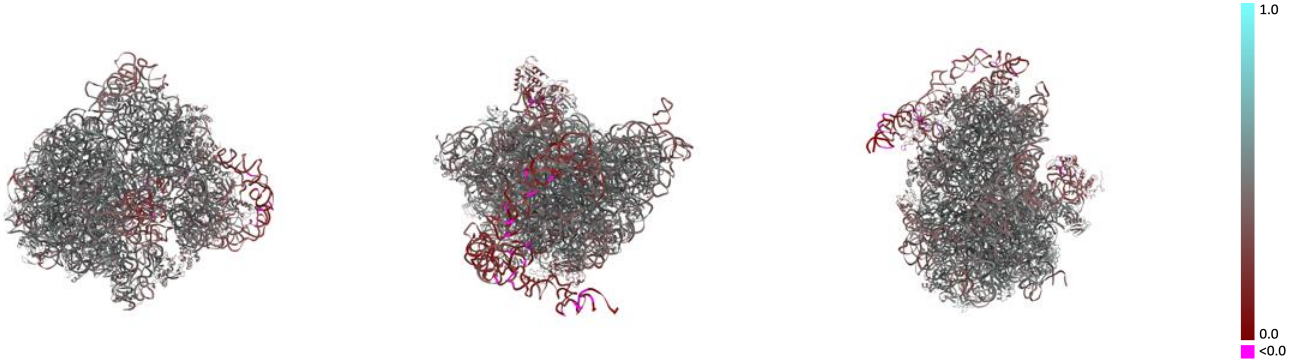
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.05 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.

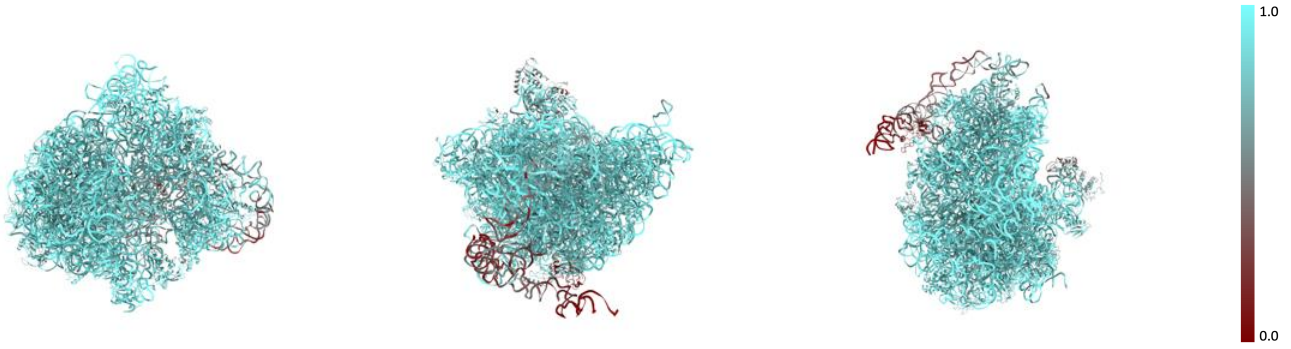
9.2 Q-score mapped to coordinate model (i)



X Y Z

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.

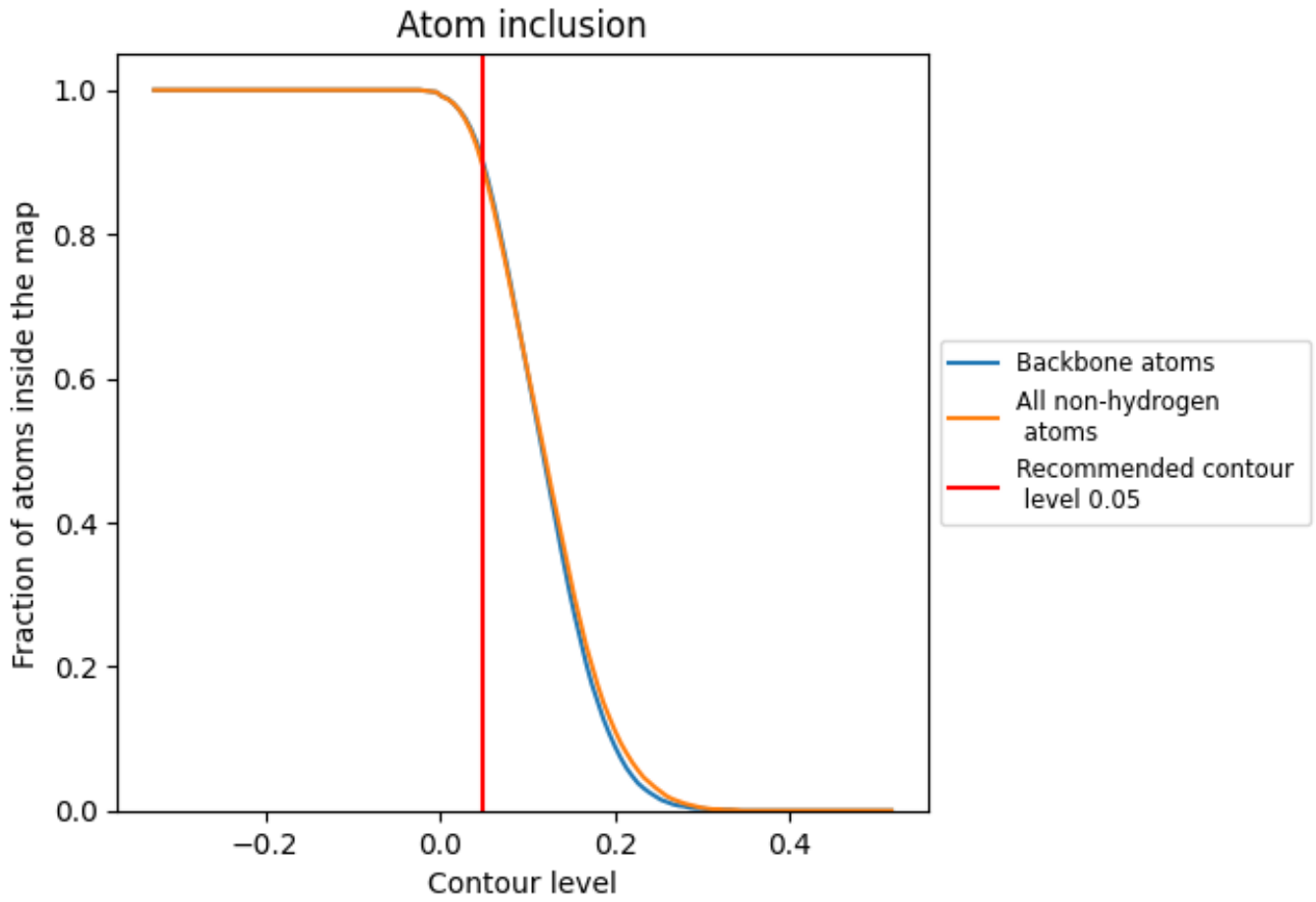
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.05).

9.4 Atom inclusion (i)



At the recommended contour level, 90% of all backbone atoms, 89% 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 (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8910	0.4400
1	0.9460	0.4520
2	0.9620	0.4470
3	0.9600	0.4340
4	0.4070	0.1720
5	0.1950	0.2830
6	0.6170	0.4430
7	0.8820	0.4010
B	0.9020	0.5200
C	0.9000	0.5110
D	0.8700	0.4760
E	0.8710	0.4570
F	0.8910	0.4530
G	0.7570	0.3830
H	0.6220	0.2760
I	0.5530	0.2680
J	0.8990	0.5000
K	0.8660	0.5100
L	0.9010	0.5030
M	0.9000	0.5180
N	0.9130	0.5110
O	0.9090	0.4680
P	0.8830	0.5110
Q	0.8930	0.4990
R	0.8910	0.4990
S	0.8810	0.5060
T	0.8790	0.4840
U	0.8940	0.4730
V	0.8950	0.4810
W	0.9150	0.5310
X	0.8920	0.4980
Y	0.8830	0.4600
Z	0.8960	0.4850
a	0.8560	0.4120
b	0.9190	0.5060

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Chain	Atom inclusion	Q-score
c	0.8560	0.4800
d	0.9190	0.5290
e	0.9140	0.5240
f	0.9050	0.5190
g	0.8360	0.4240
h	0.8430	0.4720
i	0.8660	0.4610
j	0.8740	0.4820
k	0.8890	0.4690
l	0.8500	0.4450
m	0.8740	0.4870
n	0.8990	0.4590
o	0.8310	0.4440
p	0.8570	0.4700
q	0.8850	0.5110
r	0.8850	0.4620
s	0.9020	0.4770
t	0.8950	0.4720
u	0.8850	0.4750
v	0.8630	0.4900
w	0.8850	0.4710
x	0.9160	0.4720
y	0.9140	0.4600
z	0.7660	0.4220