wwPDB EM Validation Summary Report

Apr 20, 2024 – 01:42 pm BST

PDB ID	:	7ACR
EMDB ID	:	EMD-11718
Title	:	Structure of post-translocated trans-translation complex on E. coli stalled ribosome.
Authors	:	Guyomar, C.; D'Urso, G.; Chat, S.; Giudice, E.; Gillet, R.
Deposited on	:	2020-09-11
Resolution	:	3.44 Å(reported)
Based on initial model	:	4YBB

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 (i)) were used in the production of this report:

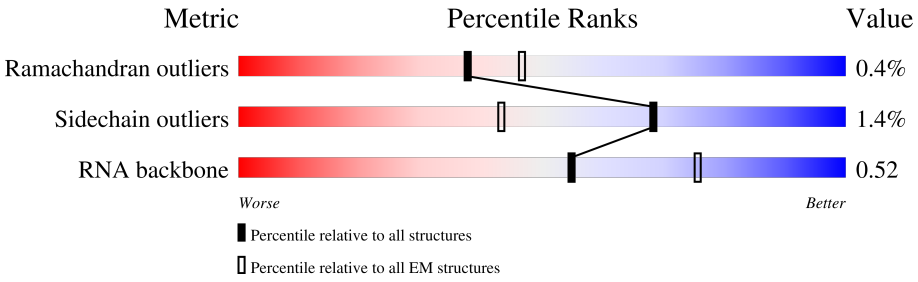
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 3.44 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	78% 22%
2	2	1534	78% 22%
3	3	120	84% 16%
4	4	363	40% 57%
5	5	150	99%
6	A	76	99%
7	B	271	100%
8	C	209	98%

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Mol	Chain	Length	Quality of chain
9	D	201	100%
10	E	177	99%
11	F	175	99%
12	G	149	39% 96%
13	J	142	99%
14	K	123	100%
15	L	144	100%
16	M	136	99%
17	N	119	100%
18	O	116	100%
19	P	114	100%
20	Q	117	100%
21	R	103	98%
22	S	110	100%
23	T	94	100%
24	U	103	100%
25	V	94	100%
26	W	2	100%
27	X	77	100%
28	Y	62	100%
29	Z	58	98%
30	a	65	31% 88% 12%
31	b	56	98%
32	c	52	100%
33	d	46	100%

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Mol	Chain	Length	Quality of chain
34	e	64	98%
35	f	38	100%
36	g	225	97%
37	h	212	99%
38	i	205	100%
39	j	156	100%
40	k	104	100%
41	l	151	22% 100%
42	m	129	100%
43	n	127	54% 42%
44	o	99	99%
45	p	117	100%
46	q	122	99%
47	r	112	10% 99%
48	s	100	96%
49	t	88	100%
50	u	82	100%
51	v	80	100%
52	w	67	99%
53	x	83	22% 98%
54	y	86	100%
55	z	70	99%

2 Entry composition (i)

There are 57 unique types of molecules in this entry. The entry contains 151668 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	62335	27816	11470	20147	2902	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	32927	14693	6041	10660	1533	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 RNA chain called transfer-messenger RNA (tmRNA).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
4	4	363	7755	3466	1410	2518	361	0	0

- Molecule 5 is a protein called SsrA-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	5	150	1209	763	226	216	4	0	0

- Molecule 6 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	A	76	582	360	117	104	1	0	0

- Molecule 7 is a protein called 50S ribosomal protein L2.

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

- Molecule 8 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	C	209	Total	C	N	O	S	0	0
			1565	979	288	294	4		

- Molecule 9 is a protein called 50S ribosomal protein L4.

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

- Molecule 10 is a protein called 50S ribosomal protein L5.

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

- Molecule 11 is a protein called 50S ribosomal protein L6.

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

- Molecule 12 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	G	149	Total	C	N	O	S	0	0
			1110	699	197	213	1		

- Molecule 13 is a protein called 50S ribosomal protein L13.

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

- Molecule 14 is a protein called 50S ribosomal protein L14.

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

- Molecule 15 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	L	144	Total	C	N	O	S	0	0
			1053	654	207	190	2		

- Molecule 16 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	M	136	Total	C	N	O	S	0	0
			1075	686	205	178	6		

- Molecule 17 is a protein called 50S ribosomal protein L17.

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

- Molecule 18 is a protein called 50S ribosomal protein L18.

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

- Molecule 19 is a protein called 50S ribosomal protein L19.

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

- Molecule 20 is a protein called 50S ribosomal protein L20.

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

- Molecule 21 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	R	103	Total	C	N	O	S	0	0
			816	516	153	145	2		

- Molecule 22 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	S	110	Total	C	N	O	S	0	0
			857	532	166	156	3		

- Molecule 23 is a protein called 50S ribosomal protein L23.

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

- Molecule 24 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	U	103	Total	C	N	O	0	0
			788	498	148	142		

- Molecule 25 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	V	94	Total	C	N	O	S	0	0
			753	479	137	134	3		

- Molecule 26 is a protein called Nascent peptide.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	W	2	Total	C	N	O	0	0
			16	12	2	2		

- Molecule 27 is a protein called 50S ribosomal protein L28.

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

- Molecule 28 is a protein called 50S ribosomal protein L29.

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

- Molecule 29 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	Z	58	Total	C	N	O	S	0	0
			448	281	87	78	2		

- Molecule 30 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	a	65	Total	C	N	O	S	0	0
			514	317	98	93	6		

- Molecule 31 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	b	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

- Molecule 32 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
32	c	52	Total	C	N	O	0	0
			426	275	78	73		

- Molecule 33 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	d	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 34 is a protein called 50S ribosomal protein L35.

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

- Molecule 35 is a protein called 50S ribosomal protein L36.

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

- Molecule 36 is a protein called 30S ribosomal protein S2.

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

- Molecule 37 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	h	212	Total	C	N	O	S	0	0
			1658	1049	311	294	4		

- Molecule 38 is a protein called 30S ribosomal protein S4.

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

- Molecule 39 is a protein called 30S ribosomal protein S5.

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

- Molecule 40 is a protein called 30S ribosomal protein S6.

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

- Molecule 41 is a protein called 30S ribosomal protein S7.

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

- Molecule 42 is a protein called 30S ribosomal protein S8.

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

- Molecule 43 is a protein called 30S ribosomal protein S9.

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

- Molecule 44 is a protein called 30S ribosomal protein S10.

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

- Molecule 45 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	p	117	Total	C	N	O	S	0	0
			877	540	174	160	3		

- Molecule 46 is a protein called 30S ribosomal protein S12.

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

- Molecule 47 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	r	112	Total	C	N	O	S	0	0
			867	535	175	154	3		

- Molecule 48 is a protein called 30S ribosomal protein S14.

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

- Molecule 49 is a protein called 30S ribosomal protein S15.

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

- Molecule 50 is a protein called 30S ribosomal protein S16.

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

- Molecule 51 is a protein called 30S ribosomal protein S17.

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

- Molecule 52 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	w	67	Total	C	N	O	S	0	0
			553	350	104	98	1		

- Molecule 53 is a protein called 30S ribosomal protein S19.

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

- Molecule 54 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	y	86	Total	C	N	O	S	0	0
			669	414	138	114	3		

- Molecule 55 is a protein called 30S ribosomal protein S21.

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

- Molecule 56 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
56	1	172	Total Mg 172 172	0
56	2	31	Total Mg 31 31	0
56	3	3	Total Mg 3 3	0
56	C	1	Total Mg 1 1	0
56	O	1	Total Mg 1 1	0
56	Q	1	Total Mg 1 1	0
56	b	1	Total Mg 1 1	0
56	d	1	Total Mg 1 1	0
56	h	1	Total Mg 1 1	0

- Molecule 57 is ZINC ION (three-letter code: ZN) (formula: Zn).

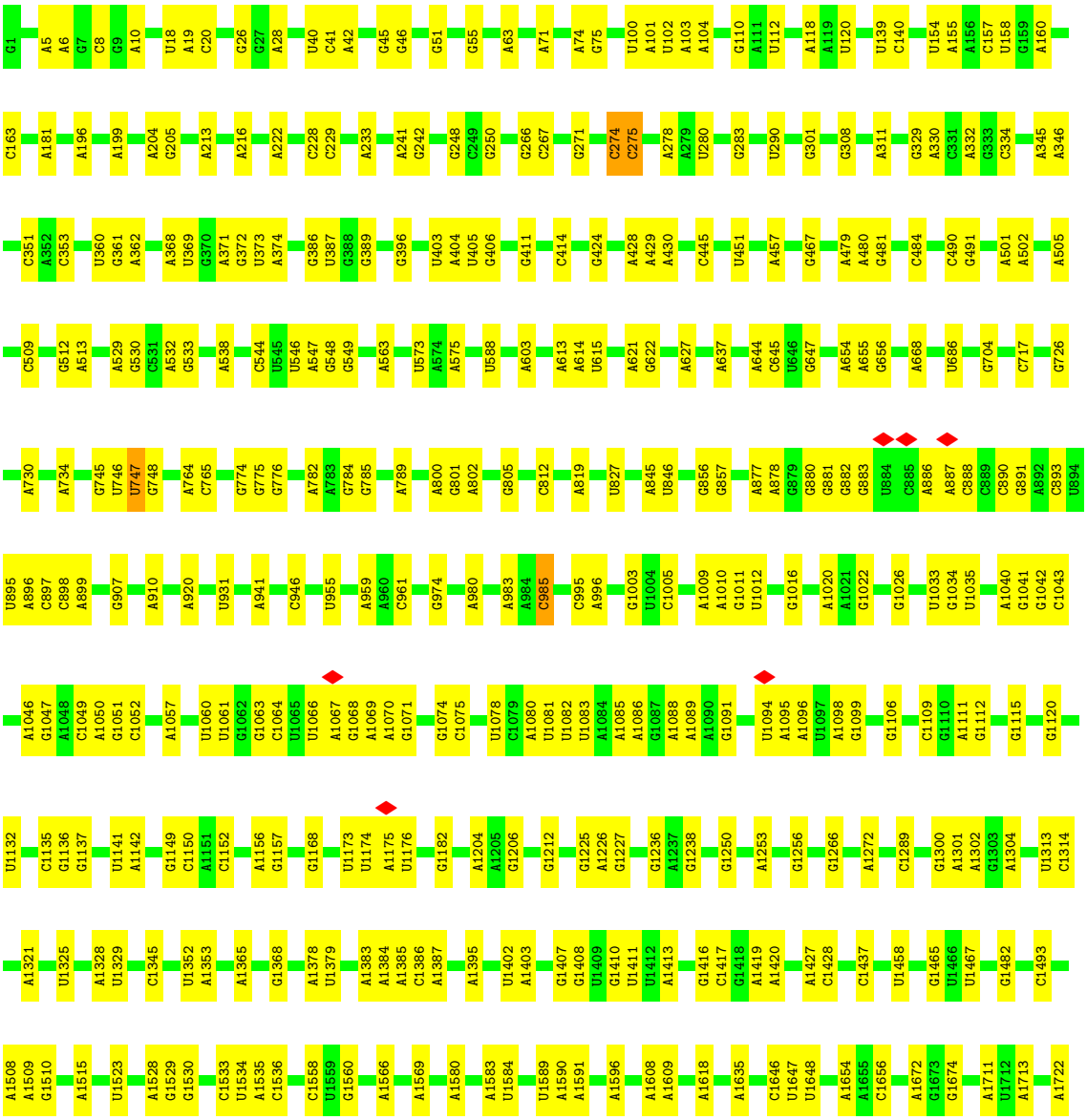
Mol	Chain	Residues	Atoms	AltConf
57	a	1	Total Zn 1 1	0
57	f	1	Total Zn 1 1	0

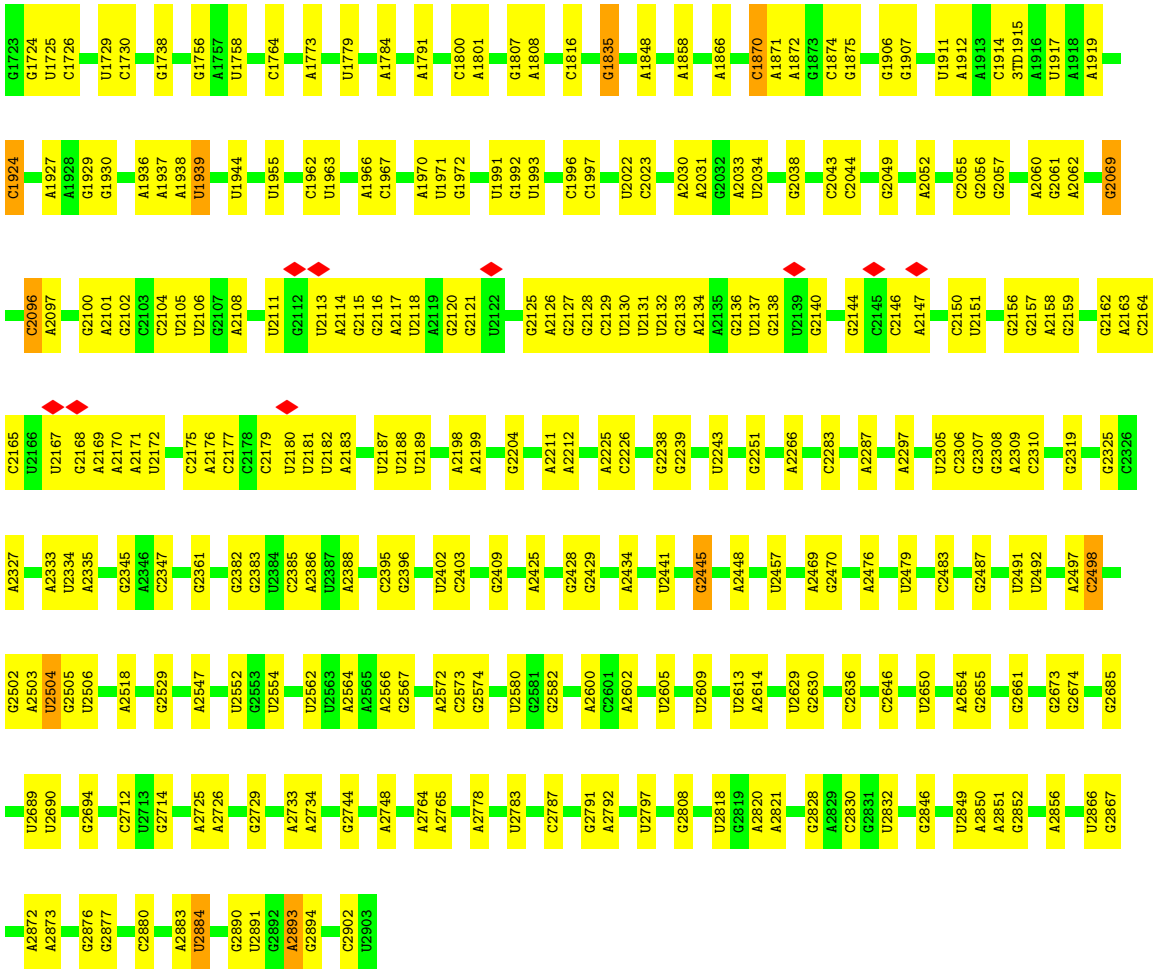
3 Residue-property plots (i)

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

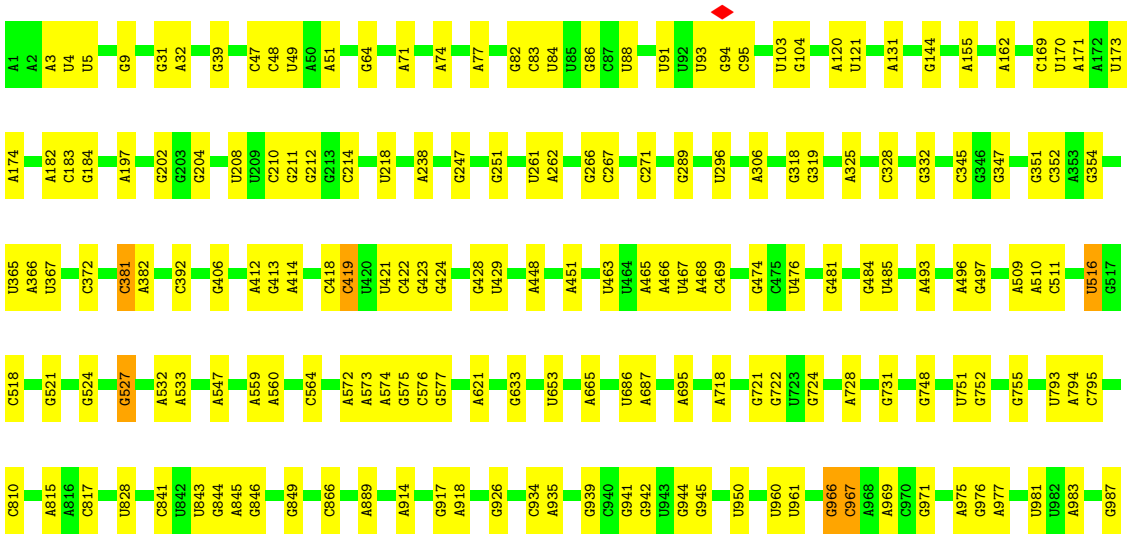
Chain 1:

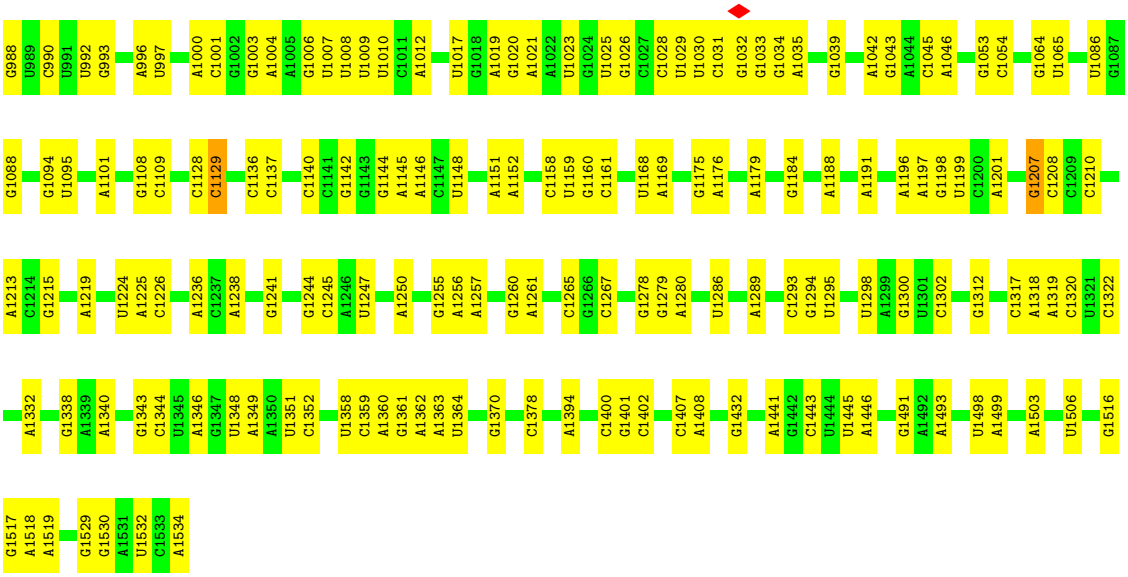




• Molecule 2: 16S ribosomal RNA

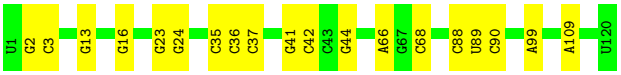
Chain 2:





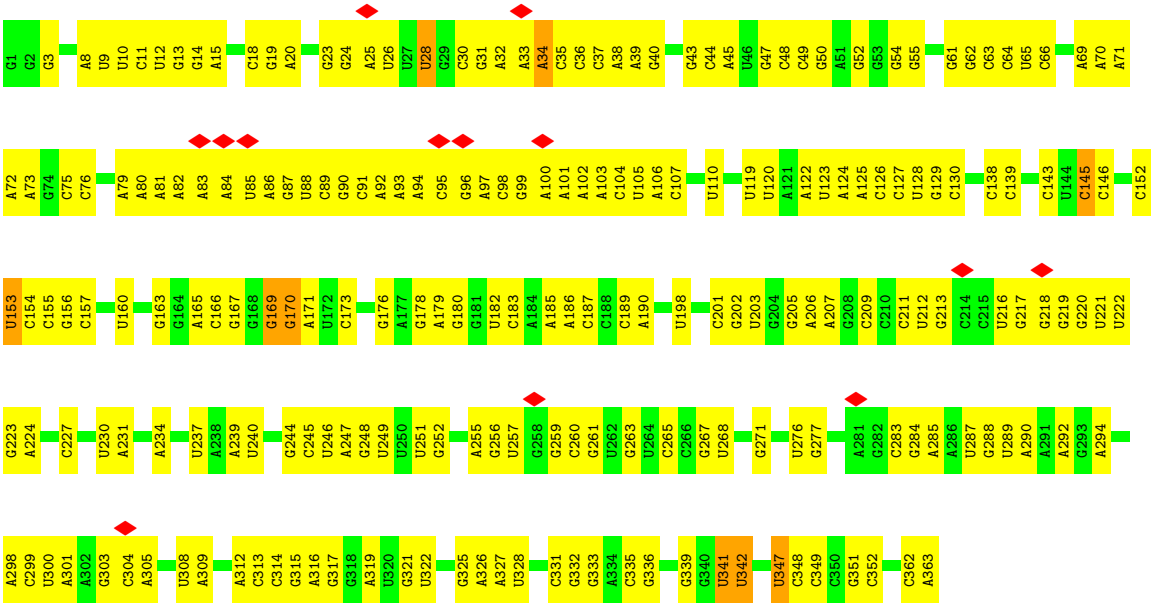
• Molecule 3: 5S ribosomal RNA

Chain 3:



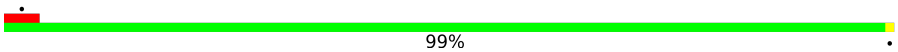
• Molecule 4: transfer-messenger RNA (tmRNA)

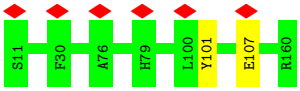
Chain 4:



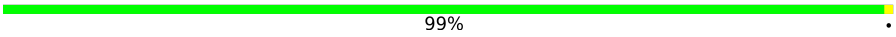
• Molecule 5: SsrA-binding protein

Chain 5:

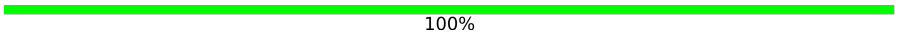




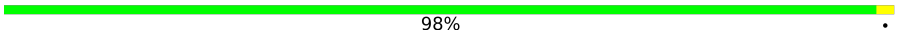
• Molecule 6: 50S ribosomal protein L27

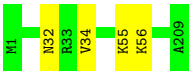
Chain A: 

• Molecule 7: 50S ribosomal protein L2

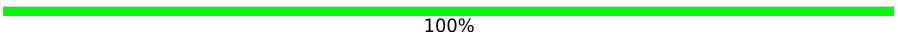
Chain B: 

• Molecule 8: 50S ribosomal protein L3

Chain C: 

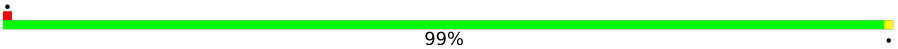


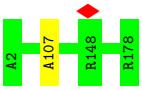
• Molecule 9: 50S ribosomal protein L4

Chain D: 

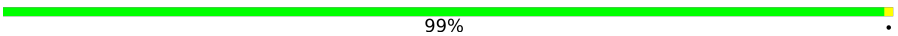
There are no outlier residues recorded for this chain.

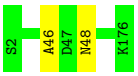
• Molecule 10: 50S ribosomal protein L5

Chain E: 

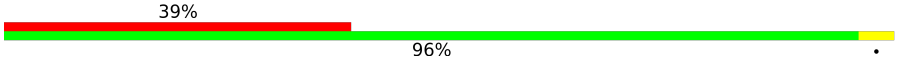


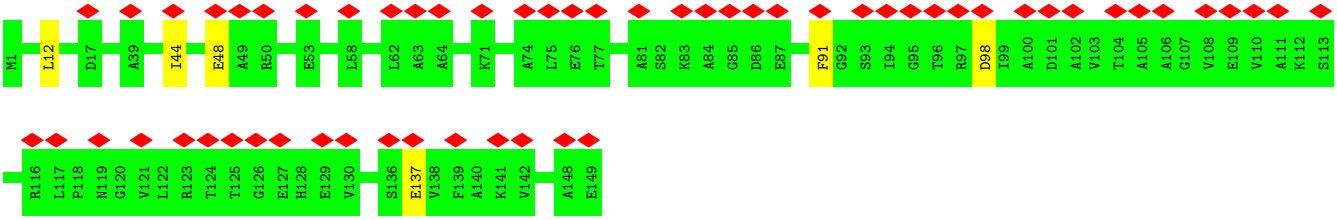
• Molecule 11: 50S ribosomal protein L6

Chain F: 

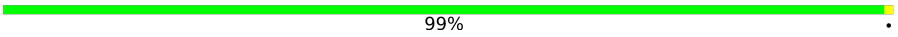


• Molecule 12: 50S ribosomal protein L9

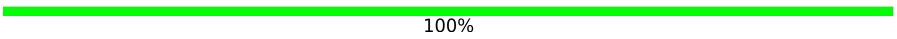
Chain G: 



• Molecule 13: 50S ribosomal protein L13

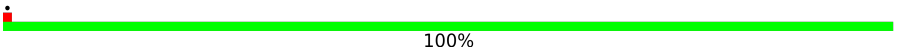
Chain J: 

• Molecule 14: 50S ribosomal protein L14

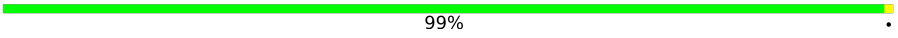
Chain K: 

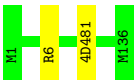
There are no outlier residues recorded for this chain.

• Molecule 15: 50S ribosomal protein L15

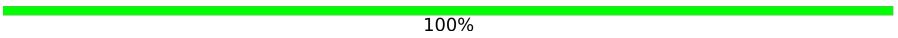
Chain L: 

• Molecule 16: 50S ribosomal protein L16

Chain M: 

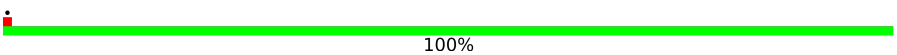


• Molecule 17: 50S ribosomal protein L17

Chain N: 

There are no outlier residues recorded for this chain.

• Molecule 18: 50S ribosomal protein L18

Chain O: 

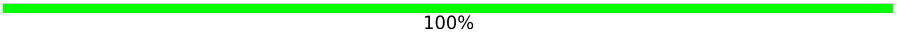
• Molecule 19: 50S ribosomal protein L19

Chain P:

There are no outlier residues recorded for this chain.

• Molecule 20: 50S ribosomal protein L20

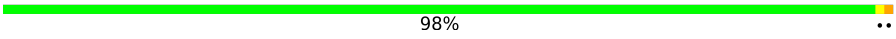
Chain Q:



There are no outlier residues recorded for this chain.

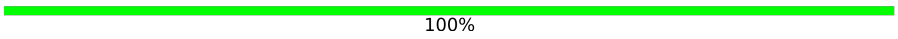
• Molecule 21: 50S ribosomal protein L21

Chain R:



• Molecule 22: 50S ribosomal protein L22

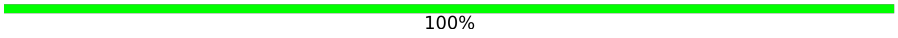
Chain S:



There are no outlier residues recorded for this chain.

• Molecule 23: 50S ribosomal protein L23

Chain T:



There are no outlier residues recorded for this chain.

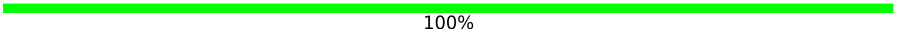
• Molecule 24: 50S ribosomal protein L24

Chain U:

There are no outlier residues recorded for this chain.

• Molecule 25: 50S ribosomal protein L25

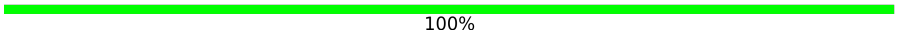
Chain V:



There are no outlier residues recorded for this chain.

• Molecule 26: Nascent peptide

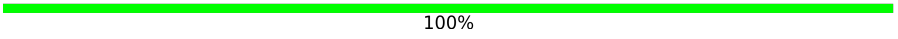
Chain W:



There are no outlier residues recorded for this chain.

• Molecule 27: 50S ribosomal protein L28

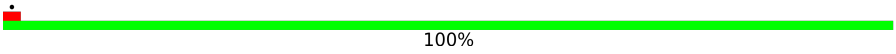
Chain X:

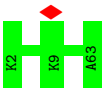


There are no outlier residues recorded for this chain.

• Molecule 28: 50S ribosomal protein L29

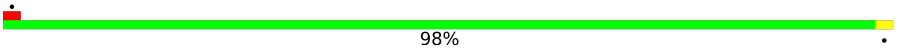
Chain Y:

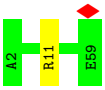




• Molecule 29: 50S ribosomal protein L30

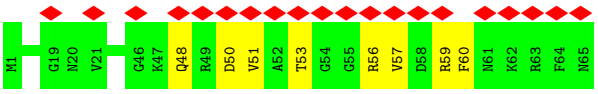
Chain Z:





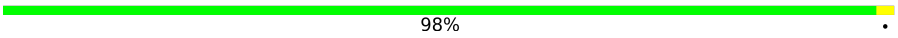
• Molecule 30: 50S ribosomal protein L31

Chain a:



• Molecule 31: 50S ribosomal protein L32

Chain b:



• Molecule 32: 50S ribosomal protein L33

Chain c:

There are no outlier residues recorded for this chain.

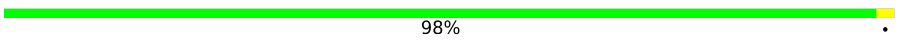
• Molecule 33: 50S ribosomal protein L34

Chain d:

There are no outlier residues recorded for this chain.

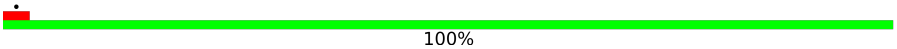
• Molecule 34: 50S ribosomal protein L35

Chain e:



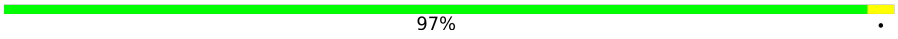
• Molecule 35: 50S ribosomal protein L36

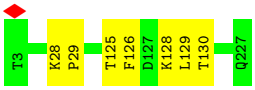
Chain f:



• Molecule 36: 30S ribosomal protein S2

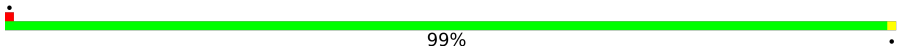
Chain g:





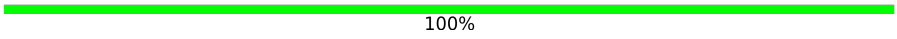
• Molecule 37: 30S ribosomal protein S3

Chain h:



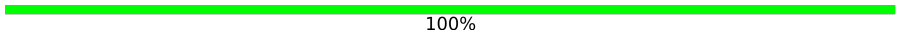
• Molecule 38: 30S ribosomal protein S4

Chain i:



• Molecule 39: 30S ribosomal protein S5

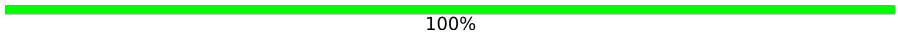
Chain j:



There are no outlier residues recorded for this chain.

• Molecule 40: 30S ribosomal protein S6

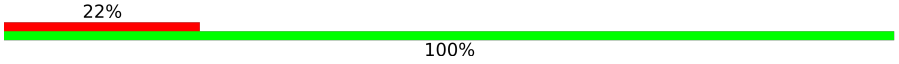
Chain k:

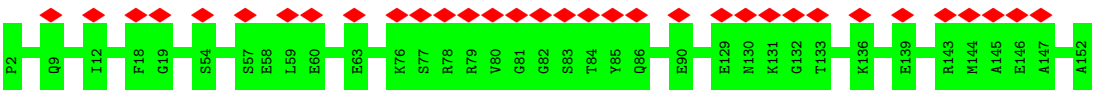


There are no outlier residues recorded for this chain.

• Molecule 41: 30S ribosomal protein S7

Chain l:





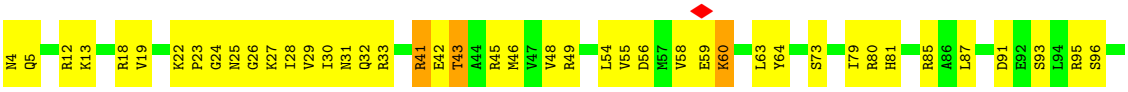
• Molecule 42: 30S ribosomal protein S8

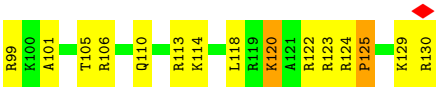
Chain m:

There are no outlier residues recorded for this chain.

• Molecule 43: 30S ribosomal protein S9

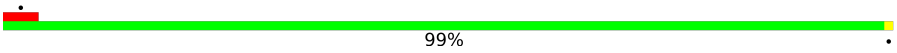
Chain n:

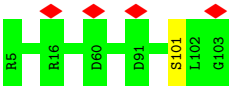




• Molecule 44: 30S ribosomal protein S10

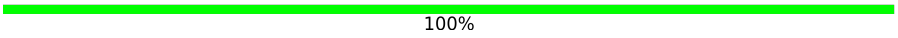
Chain o:





• Molecule 45: 30S ribosomal protein S11

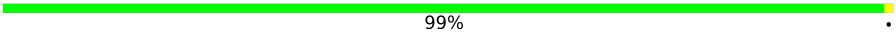
Chain p:



There are no outlier residues recorded for this chain.

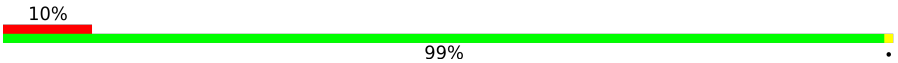
• Molecule 46: 30S ribosomal protein S12

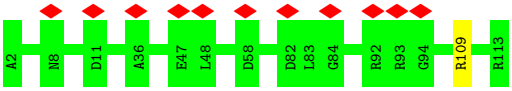
Chain q:



• Molecule 47: 30S ribosomal protein S13

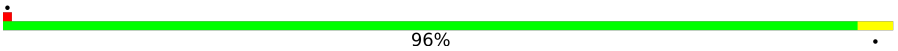
Chain r:

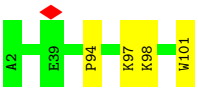




• Molecule 48: 30S ribosomal protein S14

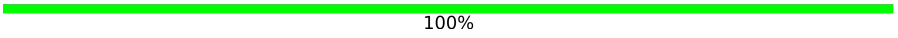
Chain s:





• Molecule 49: 30S ribosomal protein S15

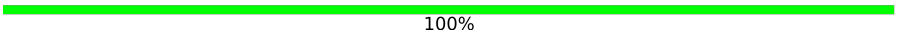
Chain t:



There are no outlier residues recorded for this chain.

• Molecule 50: 30S ribosomal protein S16

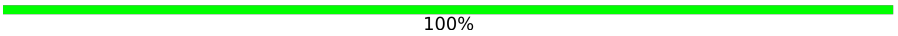
Chain u:



There are no outlier residues recorded for this chain.

• Molecule 51: 30S ribosomal protein S17

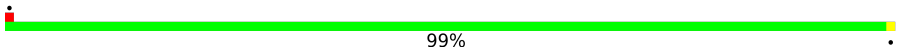
Chain v:

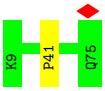


There are no outlier residues recorded for this chain.

• Molecule 52: 30S ribosomal protein S18

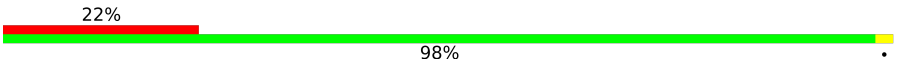
Chain w:

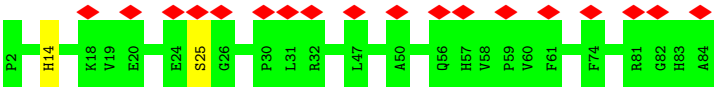




• Molecule 53: 30S ribosomal protein S19

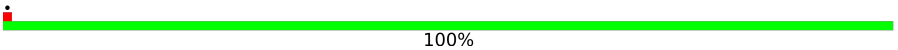
Chain x:





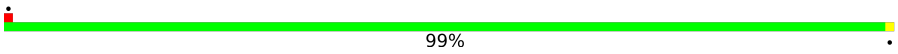
• Molecule 54: 30S ribosomal protein S20

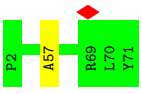
Chain y:



• Molecule 55: 30S ribosomal protein S21

Chain z:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	11059	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	29	Depositor
Minimum defocus (nm)	-700	Depositor
Maximum defocus (nm)	-2000	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 BASE (4k x 4k)	Depositor
Maximum map value	21.822	Depositor
Minimum map value	-9.722	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	2.5	Depositor
Map size (Å)	499.19998, 499.19998, 499.19998	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.04, 1.04, 1.04	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: ZN, G7M, 5MC, OMG, MG, 5MU, 1MG, 0TD, 2MG, UR3, MA6, PSU, 6MZ, 3TD, 2MA, 4D4, OMC, 4OC, 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	0.17	0/69282	0.76	28/108079 (0.0%)
2	2	0.21	0/36585	0.77	18/57064 (0.0%)
3	3	0.15	0/2872	0.73	0/4478
4	4	0.24	0/8608	0.84	10/13418 (0.1%)
5	5	0.25	0/1231	0.57	2/1655 (0.1%)
6	A	0.35	0/589	0.62	1/779 (0.1%)
7	B	0.28	1/2121 (0.0%)	0.48	0/2852
8	C	0.27	0/1586	0.58	1/2134 (0.0%)
9	D	0.24	0/1571	0.44	0/2113
10	E	0.25	0/1434	0.52	1/1926 (0.1%)
11	F	0.27	0/1333	0.56	2/1805 (0.1%)
12	G	0.32	0/1121	0.76	5/1515 (0.3%)
13	J	0.25	0/1152	0.47	0/1551
14	K	0.24	0/955	0.45	0/1279
15	L	0.25	0/1062	0.45	0/1413
16	M	0.26	0/1081	0.54	1/1443 (0.1%)
17	N	0.24	0/964	0.46	0/1289
18	O	0.24	0/902	0.44	0/1209
19	P	0.24	0/929	0.46	0/1242
20	Q	0.23	0/960	0.36	0/1278
21	R	0.27	0/829	0.48	0/1107
22	S	0.24	0/864	0.48	0/1156
23	T	0.23	0/752	0.44	0/1005
24	U	0.26	0/796	0.51	0/1062
25	V	0.25	0/766	0.46	0/1025
26	W	0.27	0/16	0.20	0/20
27	X	0.23	0/635	0.42	0/848
28	Y	0.23	0/502	0.41	0/667
29	Z	0.27	0/452	0.59	1/605 (0.2%)
30	a	0.37	0/523	0.58	0/698
31	b	0.23	0/450	0.55	1/599 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	c	0.23	0/433	0.49	0/576
33	d	0.23	0/380	0.39	0/498
34	e	0.29	0/513	0.63	0/676
35	f	0.23	0/303	0.46	0/397
36	g	0.47	1/1791 (0.1%)	0.61	3/2413 (0.1%)
37	h	0.24	0/1685	0.57	2/2270 (0.1%)
38	i	0.23	0/1665	0.38	0/2227
39	j	0.25	0/1165	0.50	0/1568
40	k	0.23	0/867	0.45	0/1171
41	l	0.24	0/1195	0.43	0/1602
42	m	0.24	0/989	0.43	0/1326
43	n	0.62	0/1034	0.94	2/1375 (0.1%)
44	o	0.23	0/800	0.56	1/1082 (0.1%)
45	p	0.24	0/893	0.45	0/1205
46	q	0.23	0/954	0.45	0/1279
47	r	0.25	0/875	0.51	1/1170 (0.1%)
48	s	0.35	0/817	0.57	0/1088
49	t	0.23	0/722	0.44	0/964
50	u	0.24	0/659	0.47	0/884
51	v	0.23	0/657	0.48	0/881
52	w	0.55	1/562 (0.2%)	0.51	2/754 (0.3%)
53	x	0.27	0/680	0.65	2/915 (0.2%)
54	y	0.23	0/675	0.37	0/895
55	z	0.24	0/597	0.54	1/792 (0.1%)
All	All	0.22	3/163834 (0.0%)	0.71	85/245322 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	g	29	PRO	N-CD	16.27	1.70	1.47
52	w	41	PRO	N-CD	11.76	1.64	1.47
7	B	131	PRO	N-CD	-6.85	1.38	1.47

The worst 5 of 85 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	275	C	C2-N1-C1'	8.70	128.37	118.80
36	g	29	PRO	CA-N-CD	-8.58	99.49	111.50
1	1	275	C	N1-C2-O2	8.57	124.04	118.90
2	2	1129	C	N3-C2-O2	-7.62	116.56	121.90
4	4	146	C	N3-C2-O2	-7.33	116.77	121.90

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	5	148/150 (99%)	131 (88%)	17 (12%)	0	100	100
6	A	74/76 (97%)	72 (97%)	2 (3%)	0	100	100
7	B	269/271 (99%)	261 (97%)	8 (3%)	0	100	100
8	C	207/209 (99%)	196 (95%)	8 (4%)	3 (1%)	11	44
9	D	199/201 (99%)	198 (100%)	1 (0%)	0	100	100
10	E	175/177 (99%)	158 (90%)	17 (10%)	0	100	100
11	F	173/175 (99%)	164 (95%)	9 (5%)	0	100	100
12	G	147/149 (99%)	121 (82%)	25 (17%)	1 (1%)	22	60
13	J	140/142 (99%)	125 (89%)	15 (11%)	0	100	100
14	K	121/123 (98%)	121 (100%)	0	0	100	100
15	L	142/144 (99%)	140 (99%)	2 (1%)	0	100	100
16	M	133/136 (98%)	130 (98%)	3 (2%)	0	100	100
17	N	117/119 (98%)	113 (97%)	4 (3%)	0	100	100
18	O	114/116 (98%)	110 (96%)	4 (4%)	0	100	100
19	P	112/114 (98%)	107 (96%)	5 (4%)	0	100	100
20	Q	115/117 (98%)	112 (97%)	3 (3%)	0	100	100
21	R	101/103 (98%)	96 (95%)	4 (4%)	1 (1%)	15	52
22	S	108/110 (98%)	106 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
23	T	92/94 (98%)	90 (98%)	2 (2%)	0	100	100
24	U	101/103 (98%)	97 (96%)	4 (4%)	0	100	100
25	V	92/94 (98%)	91 (99%)	1 (1%)	0	100	100
27	X	75/77 (97%)	72 (96%)	3 (4%)	0	100	100
28	Y	60/62 (97%)	58 (97%)	2 (3%)	0	100	100
29	Z	56/58 (97%)	53 (95%)	3 (5%)	0	100	100
30	a	63/65 (97%)	49 (78%)	14 (22%)	0	100	100
31	b	54/56 (96%)	53 (98%)	1 (2%)	0	100	100
32	c	50/52 (96%)	50 (100%)	0	0	100	100
33	d	44/46 (96%)	44 (100%)	0	0	100	100
34	e	62/64 (97%)	59 (95%)	2 (3%)	1 (2%)	9	42
35	f	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
36	g	223/225 (99%)	213 (96%)	10 (4%)	0	100	100
37	h	210/212 (99%)	202 (96%)	8 (4%)	0	100	100
38	i	203/205 (99%)	195 (96%)	8 (4%)	0	100	100
39	j	154/156 (99%)	149 (97%)	5 (3%)	0	100	100
40	k	102/104 (98%)	98 (96%)	4 (4%)	0	100	100
41	l	149/151 (99%)	141 (95%)	8 (5%)	0	100	100
42	m	127/129 (98%)	121 (95%)	6 (5%)	0	100	100
43	n	125/127 (98%)	73 (58%)	36 (29%)	16 (13%)	0	4
44	o	97/99 (98%)	87 (90%)	10 (10%)	0	100	100
45	p	115/117 (98%)	110 (96%)	5 (4%)	0	100	100
46	q	119/122 (98%)	112 (94%)	7 (6%)	0	100	100
47	r	110/112 (98%)	102 (93%)	8 (7%)	0	100	100
48	s	98/100 (98%)	95 (97%)	2 (2%)	1 (1%)	15	52
49	t	86/88 (98%)	76 (88%)	10 (12%)	0	100	100
50	u	80/82 (98%)	77 (96%)	3 (4%)	0	100	100
51	v	78/80 (98%)	72 (92%)	6 (8%)	0	100	100
52	w	65/67 (97%)	65 (100%)	0	0	100	100
53	x	81/83 (98%)	77 (95%)	4 (5%)	0	100	100
54	y	84/86 (98%)	81 (96%)	3 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
55	z	68/70 (97%)	65 (96%)	3 (4%)	0	100 100
All	All	5754/5856 (98%)	5423 (94%)	308 (5%)	23 (0%)	38 70

5 of 23 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
43	n	56	ASP
43	n	122	ARG
43	n	5	GLN
43	n	18	ARG
43	n	26	GLY

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
5	5	125/125 (100%)	125 (100%)	0	100 100
6	A	58/58 (100%)	58 (100%)	0	100 100
7	B	216/216 (100%)	216 (100%)	0	100 100
8	C	164/164 (100%)	164 (100%)	0	100 100
9	D	165/165 (100%)	165 (100%)	0	100 100
10	E	148/148 (100%)	148 (100%)	0	100 100
11	F	136/136 (100%)	136 (100%)	0	100 100
12	G	114/114 (100%)	114 (100%)	0	100 100
13	J	116/116 (100%)	114 (98%)	2 (2%)	60 82
14	K	104/104 (100%)	104 (100%)	0	100 100
15	L	103/103 (100%)	103 (100%)	0	100 100
16	M	108/108 (100%)	108 (100%)	0	100 100
17	N	99/99 (100%)	99 (100%)	0	100 100
18	O	86/86 (100%)	86 (100%)	0	100 100
19	P	99/99 (100%)	99 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
20	Q	89/89 (100%)	89 (100%)	0	100 100
21	R	84/84 (100%)	82 (98%)	2 (2%)	49 76
22	S	93/93 (100%)	93 (100%)	0	100 100
23	T	81/81 (100%)	81 (100%)	0	100 100
24	U	84/84 (100%)	84 (100%)	0	100 100
25	V	78/78 (100%)	78 (100%)	0	100 100
26	W	1/1 (100%)	1 (100%)	0	100 100
27	X	67/67 (100%)	67 (100%)	0	100 100
28	Y	54/54 (100%)	54 (100%)	0	100 100
29	Z	48/48 (100%)	48 (100%)	0	100 100
30	a	58/58 (100%)	50 (86%)	8 (14%)	3 18
31	b	47/47 (100%)	47 (100%)	0	100 100
32	c	47/47 (100%)	47 (100%)	0	100 100
33	d	38/38 (100%)	38 (100%)	0	100 100
34	e	51/51 (100%)	51 (100%)	0	100 100
35	f	34/34 (100%)	34 (100%)	0	100 100
36	g	187/187 (100%)	182 (97%)	5 (3%)	44 73
37	h	172/172 (100%)	172 (100%)	0	100 100
38	i	172/172 (100%)	172 (100%)	0	100 100
39	j	119/119 (100%)	119 (100%)	0	100 100
40	k	91/91 (100%)	91 (100%)	0	100 100
41	l	124/124 (100%)	124 (100%)	0	100 100
42	m	104/104 (100%)	104 (100%)	0	100 100
43	n	105/105 (100%)	60 (57%)	45 (43%)	0 0
44	o	86/86 (100%)	86 (100%)	0	100 100
45	p	90/90 (100%)	90 (100%)	0	100 100
46	q	102/102 (100%)	102 (100%)	0	100 100
47	r	90/90 (100%)	90 (100%)	0	100 100
48	s	83/83 (100%)	80 (96%)	3 (4%)	35 66
49	t	76/76 (100%)	76 (100%)	0	100 100
50	u	65/65 (100%)	65 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
51	v	74/74 (100%)	74 (100%)	0	100 100
52	w	58/58 (100%)	58 (100%)	0	100 100
53	x	72/72 (100%)	72 (100%)	0	100 100
54	y	65/65 (100%)	65 (100%)	0	100 100
55	z	60/60 (100%)	60 (100%)	0	100 100
All	All	4790/4790 (100%)	4725 (99%)	65 (1%)	68 85

5 of 65 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
43	n	123	ARG
43	n	125	PRO
43	n	28	ILE
43	n	27	LYS
43	n	129	LYS

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

Mol	Chain	Res	Type
30	a	61	ASN
43	n	126	GLN
37	h	32	ASN
44	o	64	GLN
43	n	4	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	2897/2903 (99%)	614 (21%)	24 (0%)
2	2	1528/1534 (99%)	318 (20%)	14 (0%)
3	3	119/120 (99%)	18 (15%)	1 (0%)
4	4	361/363 (99%)	212 (58%)	13 (3%)
All	All	4905/4920 (99%)	1162 (23%)	52 (1%)

5 of 1162 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	6	A

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Mol	Chain	Res	Type
1	1	8	C
1	1	10	A
1	1	19	A
1	1	20	C

5 of 52 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	2	751	U
2	2	1255	G
4	4	314	C
2	2	845	A
2	2	1042	A

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

38 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	PSU	1	746	56,1	18,21,22	1.09	1 (5%)	22,30,33	1.75	5 (22%)
1	5MC	1	1962	1	18,22,23	3.73	7 (38%)	26,32,35	1.06	2 (7%)
1	6MZ	1	2030	1	18,25,26	1.98	3 (16%)	16,36,39	2.21	5 (31%)
1	PSU	1	955	1	18,21,22	1.09	1 (5%)	22,30,33	1.75	4 (18%)
2	5MC	2	967	2	18,22,23	3.76	7 (38%)	26,32,35	1.01	2 (7%)
2	2MG	2	966	2	18,26,27	2.72	6 (33%)	16,38,41	1.45	3 (18%)
1	PSU	1	2580	1	18,21,22	1.10	2 (11%)	22,30,33	1.88	5 (22%)
1	PSU	1	1917	1	18,21,22	1.08	1 (5%)	22,30,33	1.74	4 (18%)
1	G7M	1	2069	1	20,26,27	2.50	7 (35%)	17,39,42	1.09	1 (5%)
2	MA6	2	1518	2	18,26,27	1.44	2 (11%)	19,38,41	4.24	3 (15%)
1	PSU	1	2605	1	18,21,22	1.11	1 (5%)	22,30,33	1.76	4 (18%)
2	MA6	2	1519	2	18,26,27	1.46	3 (16%)	19,38,41	4.23	3 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
46	0TD	q	89	46	7,9,10	1.47	0	6,11,13	2.26	2 (33%)
16	4D4	M	81	16	9,11,12	2.05	2 (22%)	8,13,15	1.85	3 (37%)
2	G7M	2	527	2	20,26,27	2.50	7 (35%)	17,39,42	1.04	1 (5%)
4	5MU	4	341	4	19,22,23	5.32	5 (26%)	28,32,35	3.52	10 (35%)
1	OMU	1	2552	1	19,22,23	2.98	8 (42%)	26,31,34	1.69	5 (19%)
1	2MG	1	1835	1	18,26,27	2.73	6 (33%)	16,38,41	1.48	3 (18%)
2	4OC	2	1402	2	20,23,24	3.22	8 (40%)	26,32,35	0.88	1 (3%)
4	PSU	4	342	4	18,21,22	1.12	1 (5%)	22,30,33	1.74	3 (13%)
1	3TD	1	1915	1	18,22,23	4.20	6 (33%)	22,32,35	1.60	2 (9%)
1	OMG	1	2251	4,1	18,26,27	2.91	7 (38%)	19,38,41	1.51	4 (21%)
1	2MG	1	2445	1	18,26,27	2.70	6 (33%)	16,38,41	1.44	4 (25%)
1	OMC	1	2498	1	19,22,23	3.39	8 (42%)	26,31,34	0.69	0
1	6MZ	1	1618	1	18,25,26	1.98	3 (16%)	16,36,39	2.08	4 (25%)
1	5MU	1	1939	1	19,22,23	5.27	5 (26%)	28,32,35	3.60	9 (32%)
1	PSU	1	2457	1	18,21,22	1.03	1 (5%)	22,30,33	1.73	4 (18%)
1	PSU	1	1911	1	18,21,22	1.10	1 (5%)	22,30,33	1.77	4 (18%)
4	PSU	4	347	4	18,21,22	1.10	1 (5%)	22,30,33	1.78	5 (22%)
1	1MG	1	745	1	18,26,27	2.61	5 (27%)	19,39,42	1.41	3 (15%)
2	2MG	2	1516	2	18,26,27	2.71	6 (33%)	16,38,41	1.41	3 (18%)
2	2MG	2	1207	2	18,26,27	2.74	6 (33%)	16,38,41	1.40	3 (18%)
1	5MU	1	747	1	19,22,23	5.25	5 (26%)	28,32,35	3.63	9 (32%)
2	5MC	2	1407	2	18,22,23	3.74	7 (38%)	26,32,35	1.00	2 (7%)
1	PSU	1	2504	1	18,21,22	1.14	1 (5%)	22,30,33	1.68	4 (18%)
2	PSU	2	516	2	18,21,22	1.09	1 (5%)	22,30,33	1.75	4 (18%)
1	2MA	1	2503	1	17,25,26	2.54	5 (29%)	17,37,40	1.38	2 (11%)
2	UR3	2	1498	2	19,22,23	3.01	8 (42%)	26,32,35	1.29	1 (3%)

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	PSU	1	746	56,1	-	1/7/25/26	0/2/2/2
1	5MC	1	1962	1	-	4/7/25/26	0/2/2/2
1	6MZ	1	2030	1	-	2/5/27/28	0/3/3/3

Continued on next page...

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	1	955	1	-	0/7/25/26	0/2/2/2
2	5MC	2	967	2	-	1/7/25/26	0/2/2/2
2	2MG	2	966	2	-	2/5/27/28	0/3/3/3
1	PSU	1	2580	1	-	0/7/25/26	0/2/2/2
1	PSU	1	1917	1	-	0/7/25/26	0/2/2/2
1	G7M	1	2069	1	-	2/3/25/26	0/3/3/3
2	MA6	2	1518	2	-	1/7/29/30	0/3/3/3
1	PSU	1	2605	1	-	0/7/25/26	0/2/2/2
2	MA6	2	1519	2	-	2/7/29/30	0/3/3/3
46	0TD	q	89	46	-	1/7/12/14	-
16	4D4	M	81	16	-	4/11/12/14	-
2	G7M	2	527	2	-	2/3/25/26	0/3/3/3
4	5MU	4	341	4	-	5/7/25/26	0/2/2/2
1	OMU	1	2552	1	-	1/9/27/28	0/2/2/2
1	2MG	1	1835	1	-	2/5/27/28	0/3/3/3
2	4OC	2	1402	2	-	0/9/29/30	0/2/2/2
4	PSU	4	342	4	-	3/7/25/26	0/2/2/2
1	3TD	1	1915	1	-	3/7/25/26	0/2/2/2
1	OMG	1	2251	4,1	-	2/5/27/28	0/3/3/3
1	2MG	1	2445	1	-	3/5/27/28	0/3/3/3
1	OMC	1	2498	1	-	2/9/27/28	0/2/2/2
1	6MZ	1	1618	1	-	2/5/27/28	0/3/3/3
1	5MU	1	1939	1	-	2/7/25/26	0/2/2/2
1	PSU	1	2457	1	-	0/7/25/26	0/2/2/2
1	PSU	1	1911	1	-	0/7/25/26	0/2/2/2
4	PSU	4	347	4	-	3/7/25/26	0/2/2/2
1	1MG	1	745	1	-	0/3/25/26	0/3/3/3
2	2MG	2	1516	2	-	0/5/27/28	0/3/3/3
2	2MG	2	1207	2	-	3/5/27/28	0/3/3/3
1	5MU	1	747	1	-	0/7/25/26	0/2/2/2
2	5MC	2	1407	2	-	0/7/25/26	0/2/2/2
1	PSU	1	2504	1	-	4/7/25/26	0/2/2/2
2	PSU	2	516	2	-	6/7/25/26	0/2/2/2
1	2MA	1	2503	1	-	1/3/25/26	0/3/3/3
2	UR3	2	1498	2	-	2/7/25/26	0/2/2/2

The worst 5 of 160 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	4	341	5MU	C6-N1	12.80	1.59	1.38
1	1	1939	5MU	C6-N1	12.70	1.59	1.38
1	1	747	5MU	C6-N1	12.70	1.59	1.38
4	4	341	5MU	C2-N1	12.56	1.58	1.38
1	1	1915	3TD	C6-C5	12.41	1.49	1.35

The worst 5 of 136 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	1518	MA6	N1-C6-N6	-15.62	100.62	117.06
2	2	1519	MA6	N1-C6-N6	-15.62	100.62	117.06
1	1	747	5MU	C5-C4-N3	11.95	125.52	115.31
1	1	1939	5MU	C5-C4-N3	11.93	125.49	115.31
4	4	341	5MU	C5-C4-N3	11.74	125.33	115.31

There are no chirality outliers.

5 of 66 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
16	M	81	4D4	C-CA-CB-OB
16	M	81	4D4	C-CA-CB-CG
16	M	81	4D4	N-CA-CB-OB
16	M	81	4D4	N-CA-CB-CG
1	1	1618	6MZ	N1-C6-N6-C9

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 214 ligands modelled in this entry, 214 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)

There are no chain breaks in this entry.

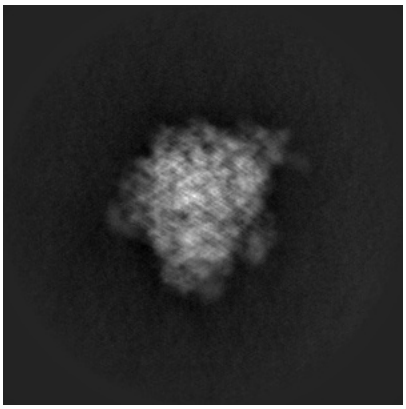
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-11718. These allow visual inspection of the internal detail of the map and identification of artifacts.

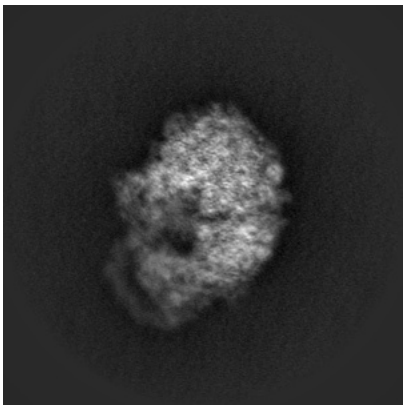
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

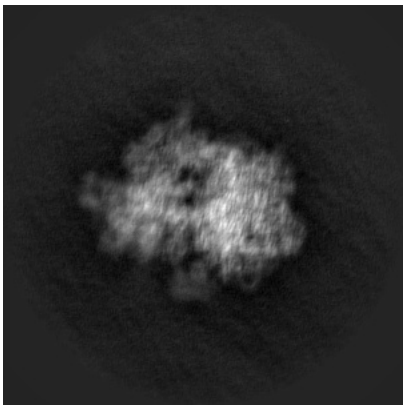
6.1.1 Primary map



X

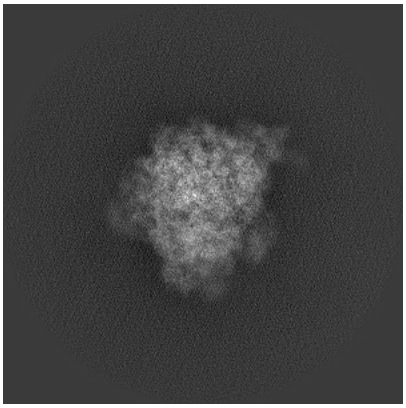


Y

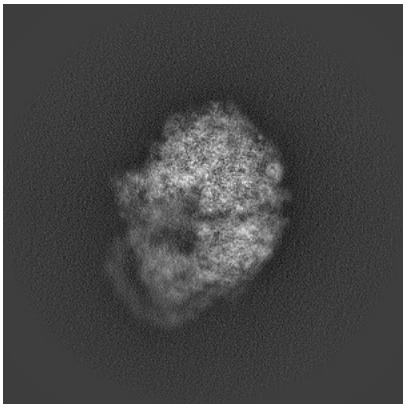


Z

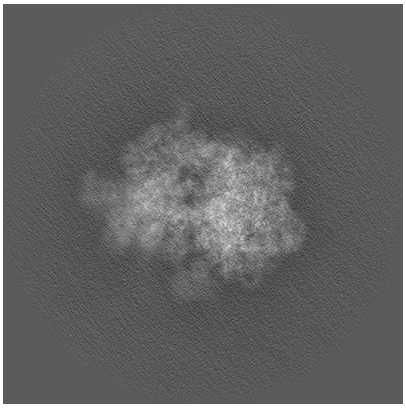
6.1.2 Raw map



X



Y

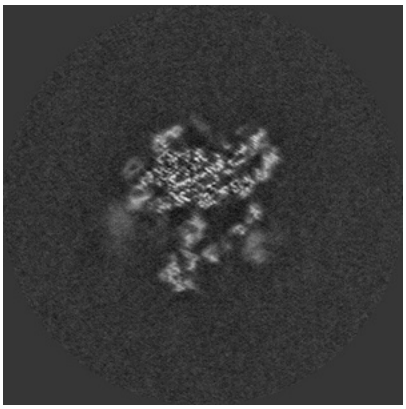


Z

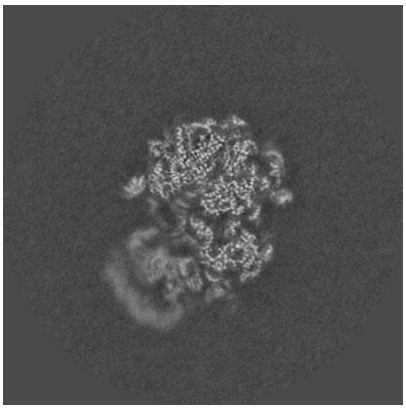
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

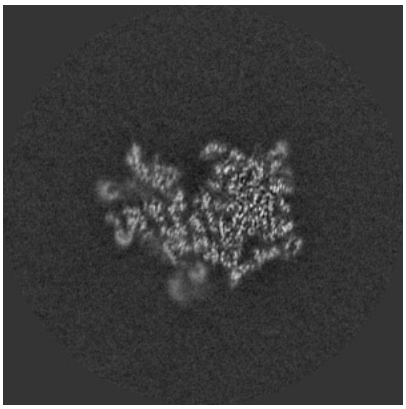
6.2.1 Primary map



X Index: 240

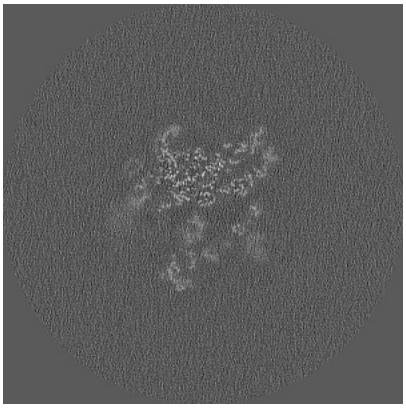


Y Index: 240

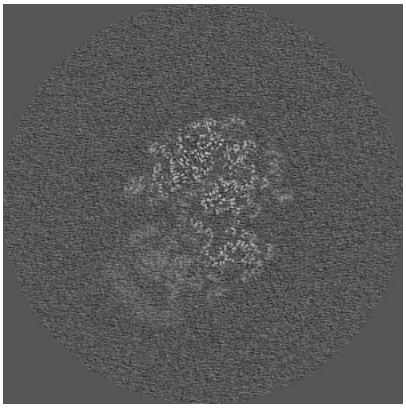


Z Index: 240

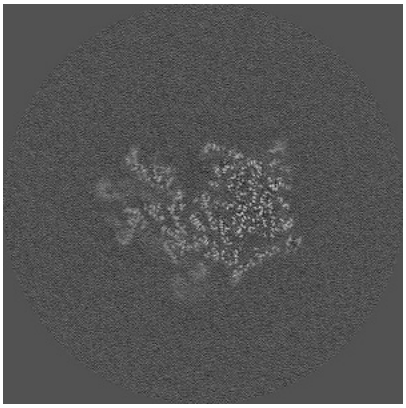
6.2.2 Raw map



X Index: 240



Y Index: 240

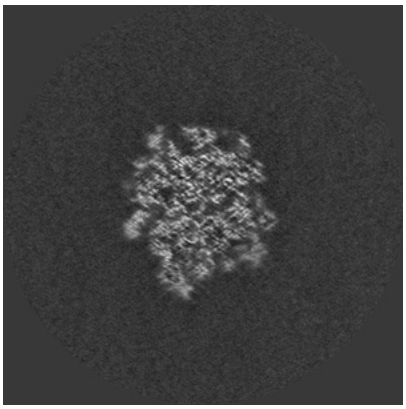


Z Index: 240

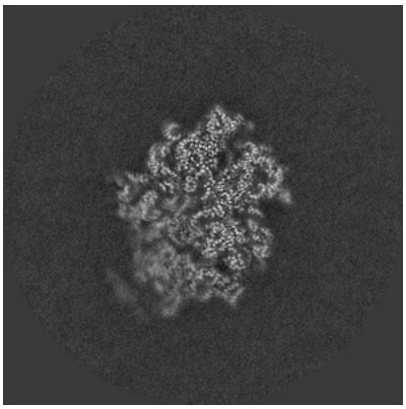
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

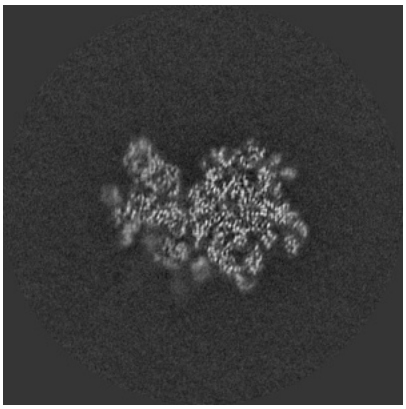
6.3.1 Primary map



X Index: 266

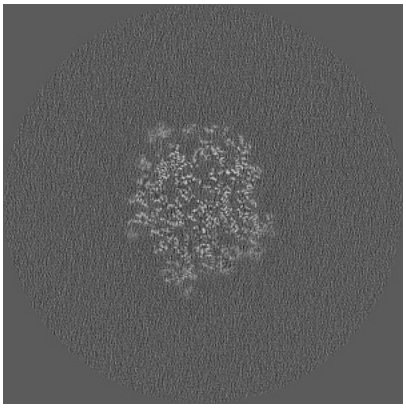


Y Index: 227

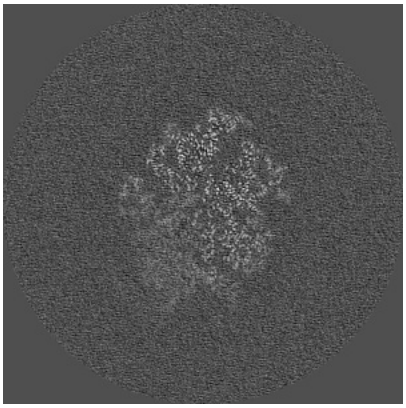


Z Index: 250

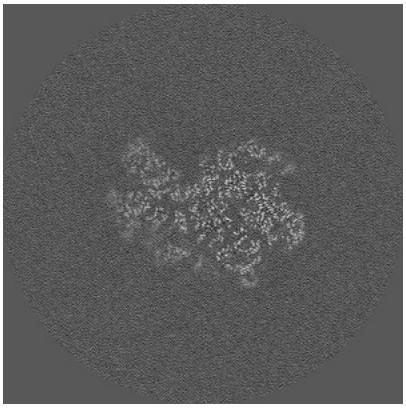
6.3.2 Raw map



X Index: 272



Y Index: 230

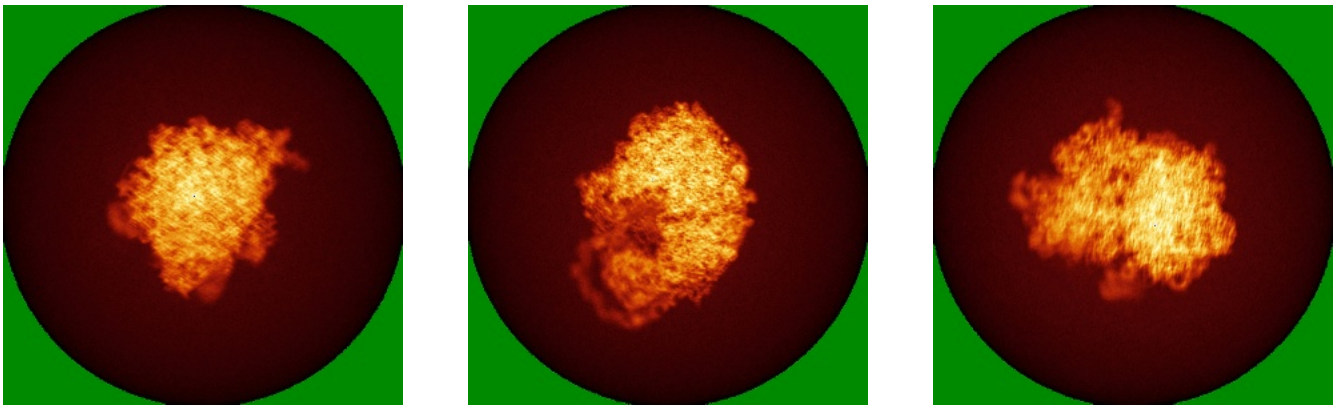


Z Index: 254

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

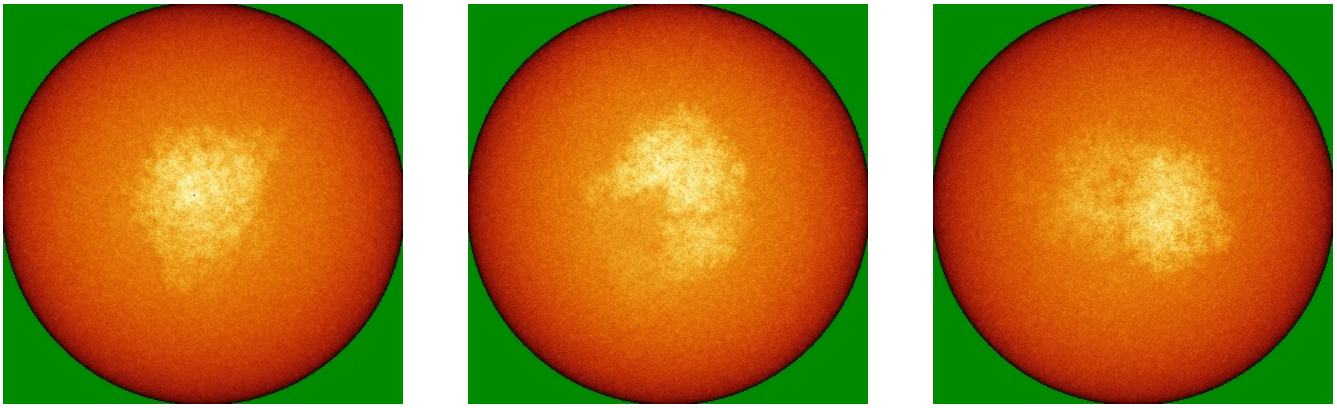
6.4 Orthogonal standard-deviation projections (False-color) (i)

6.4.1 Primary map



X Y Z

6.4.2 Raw map



X Y Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map

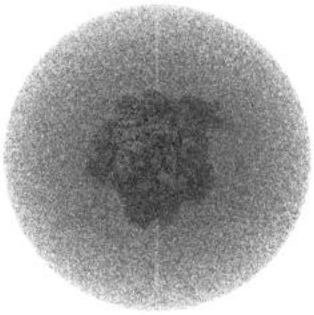
X

Y

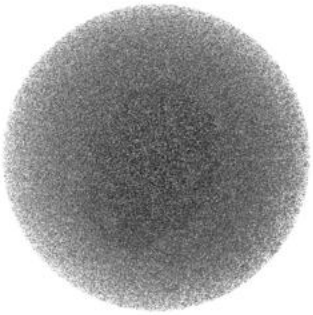
Z

The images above show the 3D surface view of the map at the recommended contour level 2.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

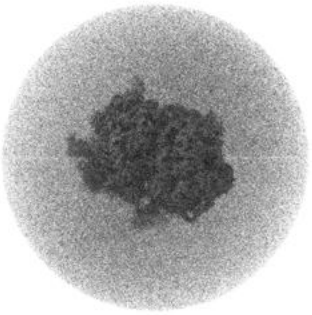
6.5.2 Raw map



X



Y



Z

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

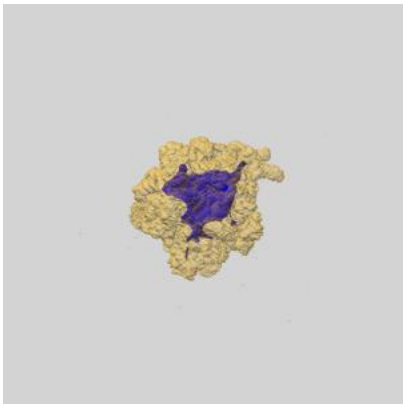
6.6 Mask visualisation (i)

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

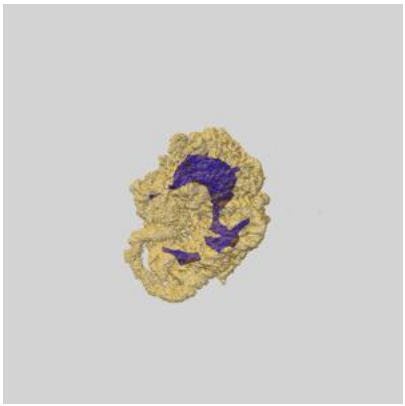
A mask typically either:

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

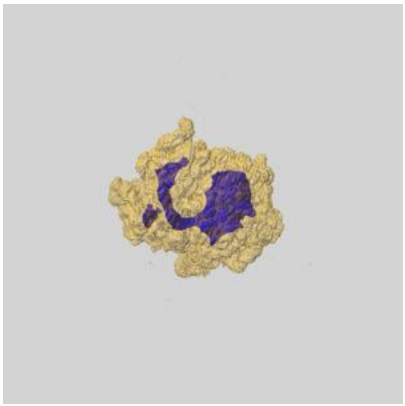
6.6.1 emd_11718_msk_1.map (i)



X



Y

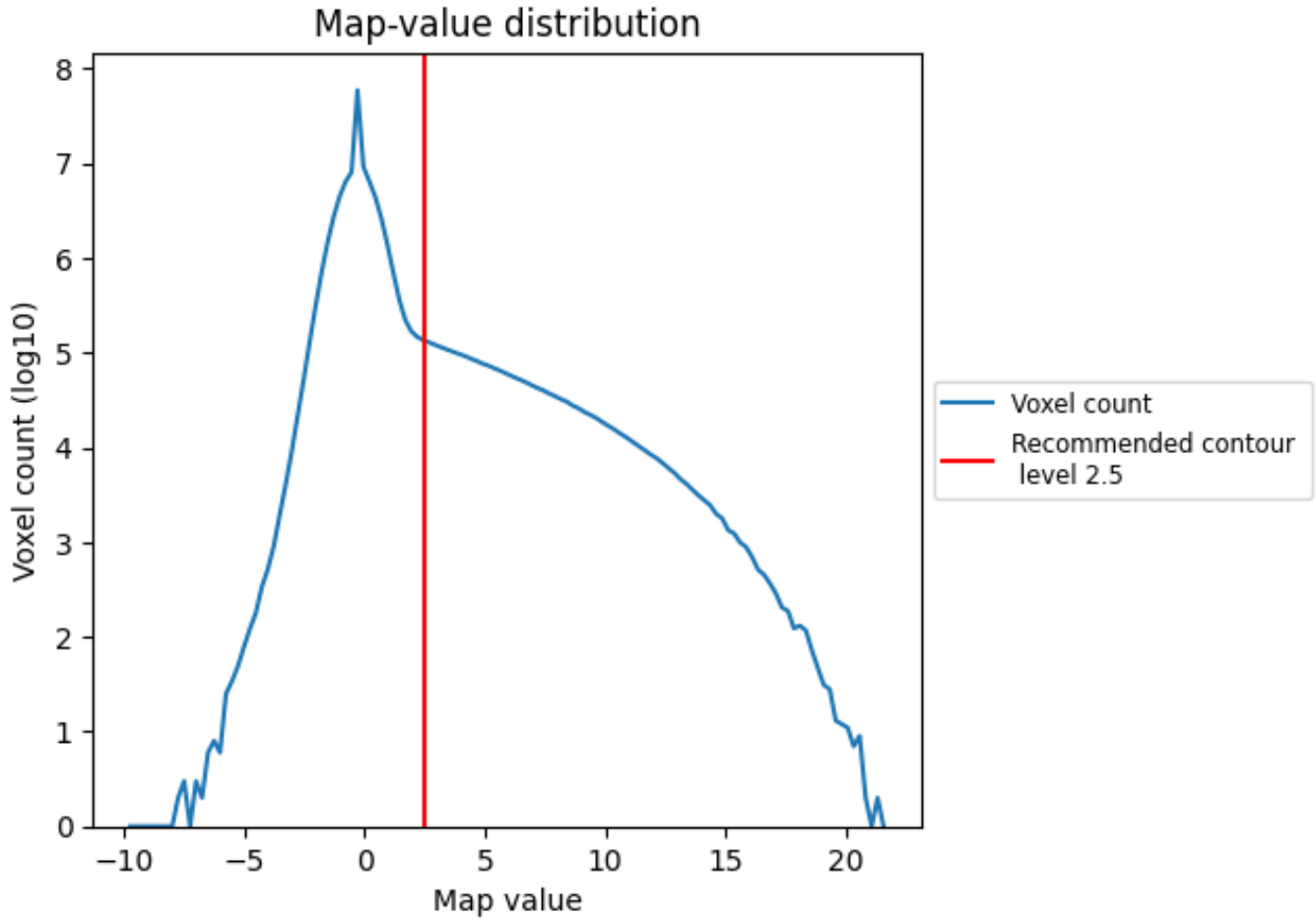


Z

7 Map analysis

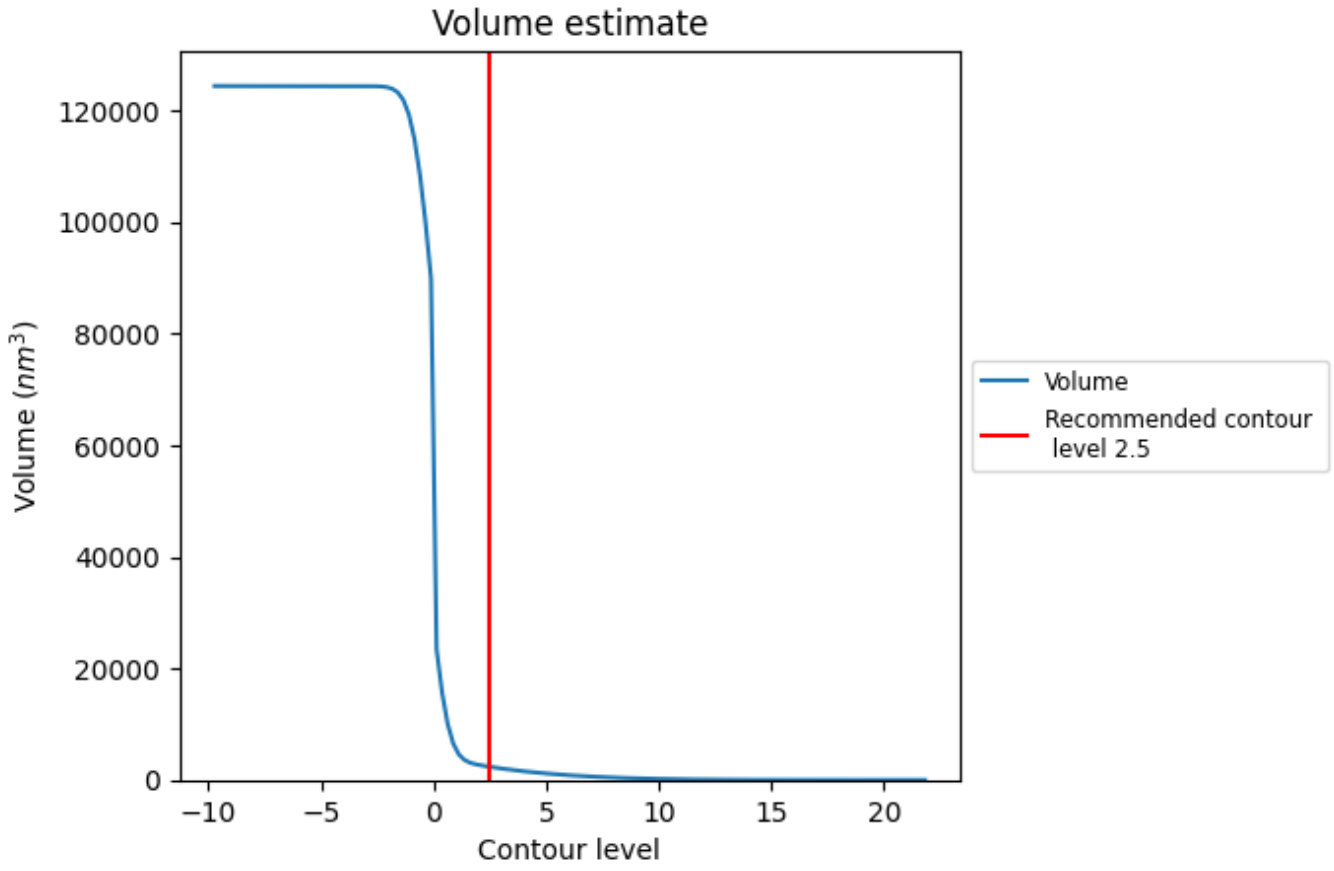
This section contains the results of statistical analysis of the map.

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.

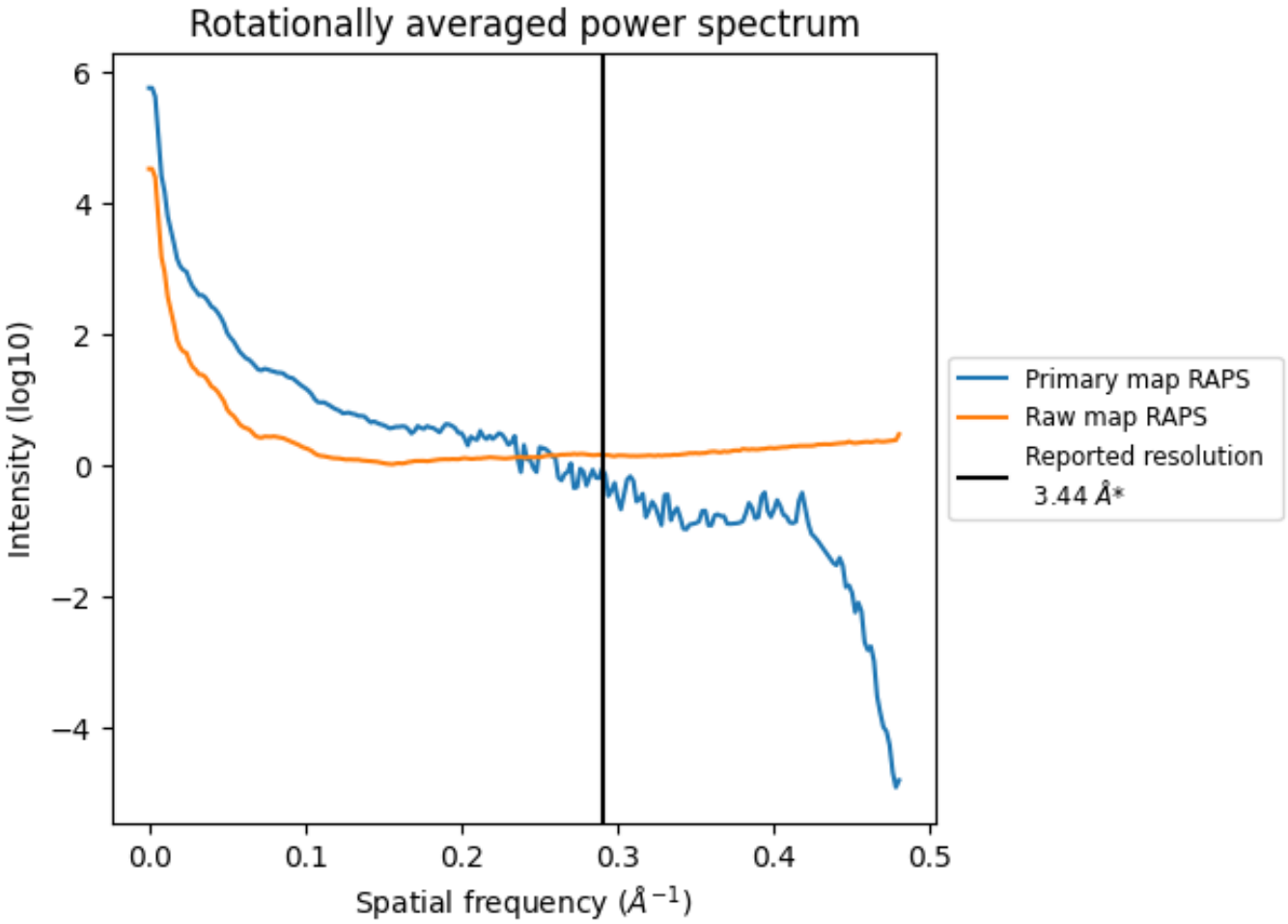
7.2 Volume estimate (i)



The volume at the recommended contour level is 2351 nm^3; this corresponds to an approximate mass of 2123 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)

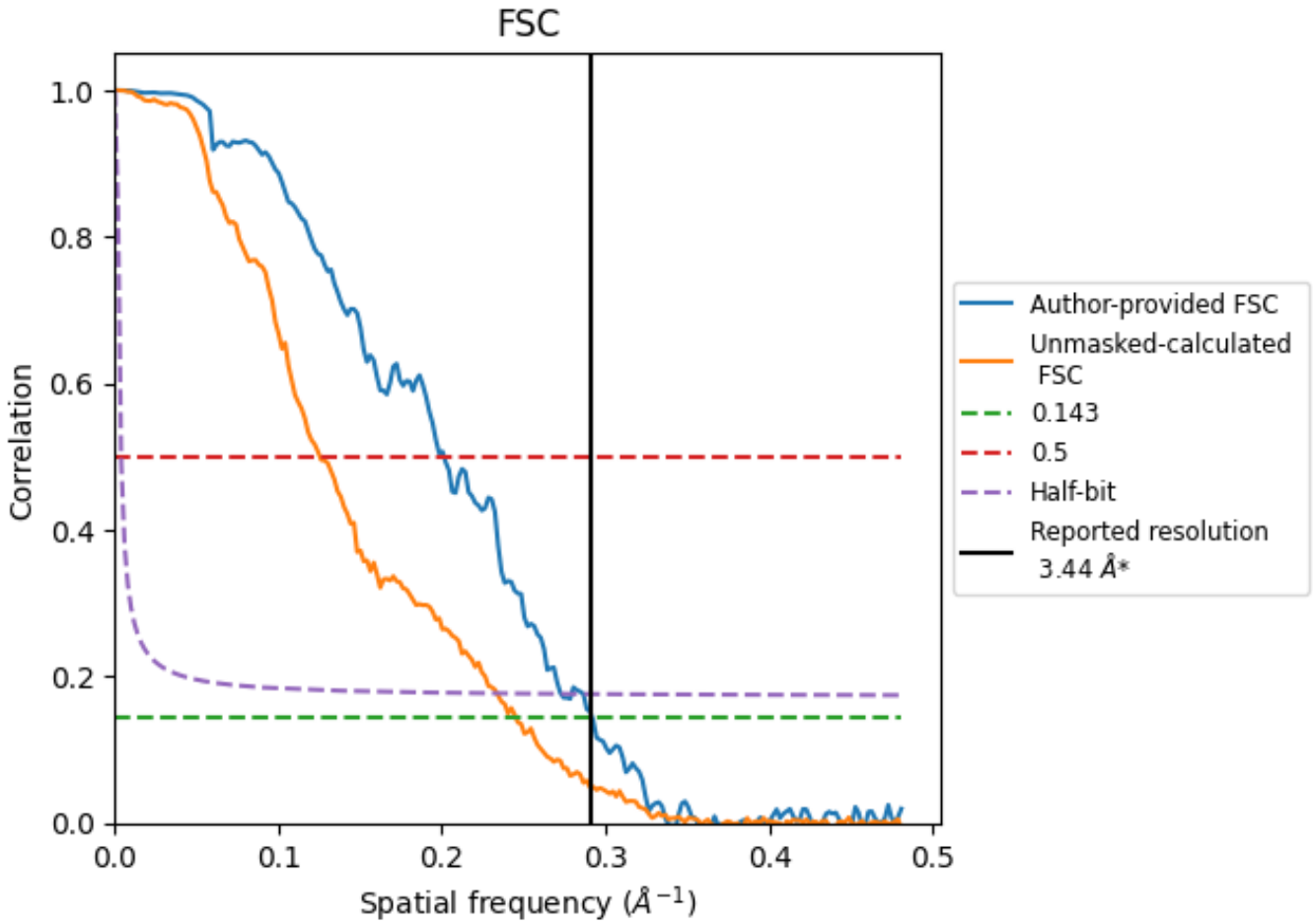


*Reported resolution corresponds to spatial frequency of 0.291 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.291 Å^{-1}

8.2 Resolution estimates (i)

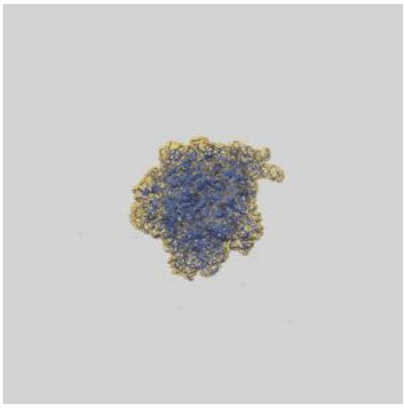
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.44	-	-
Author-provided FSC curve	3.43	4.97	3.67
Unmasked-calculated*	4.08	7.97	4.28

*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 4.08 differs from the reported value 3.44 by more than 10 %

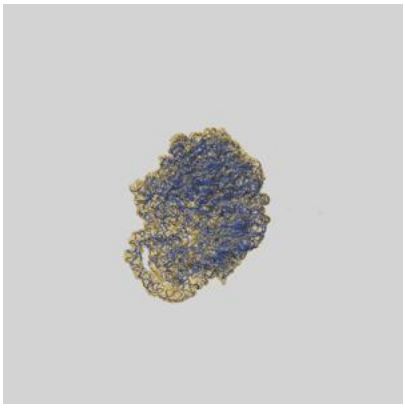
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-11718 and PDB model 7ACR. Per-residue inclusion information can be found in section 3 on page 14.

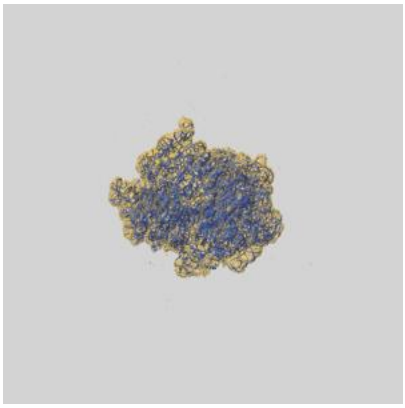
9.1 Map-model overlay



X



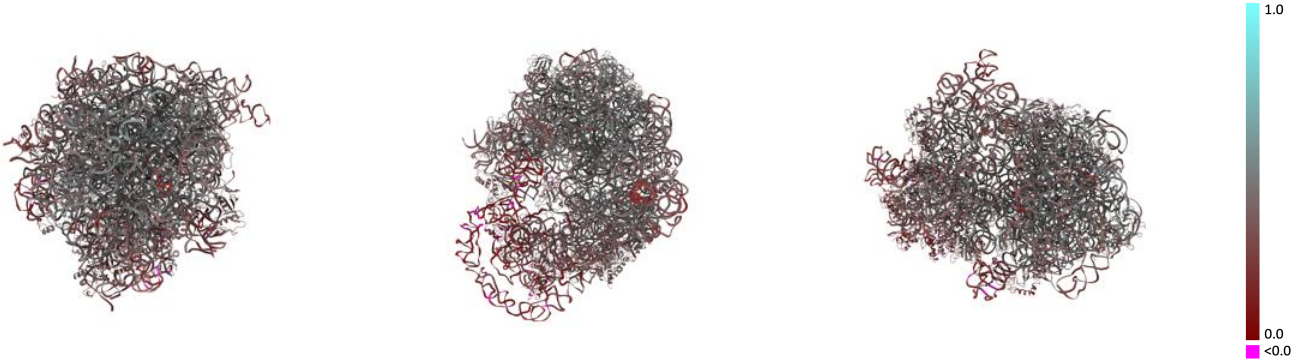
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 2.5 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.

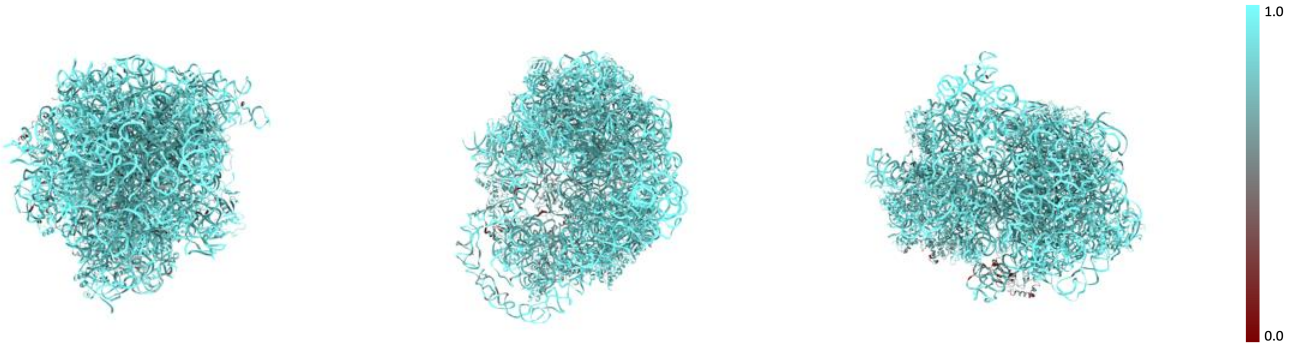
9.2 Q-score mapped to coordinate model (i)



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.

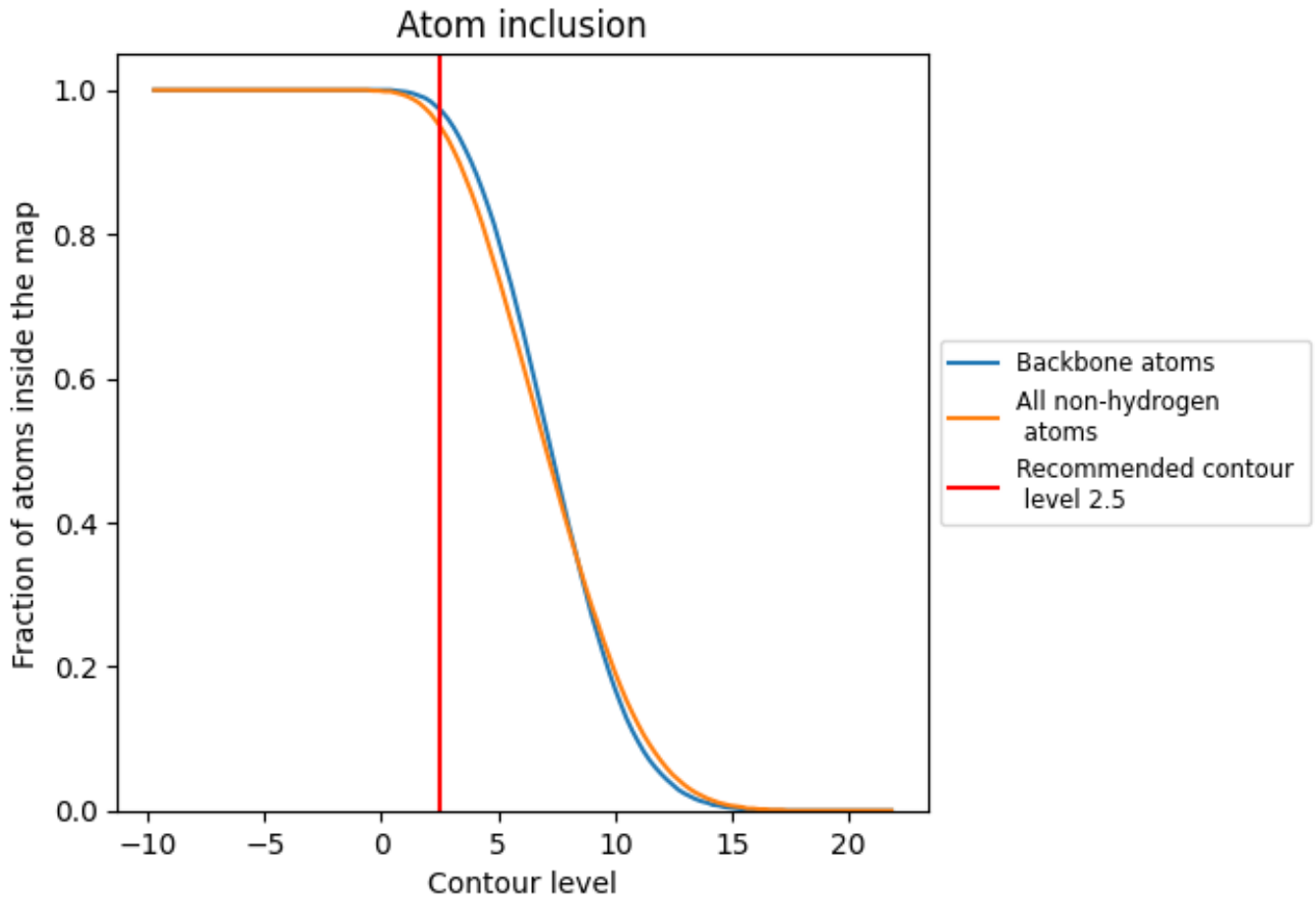
9.3 Atom inclusion mapped to coordinate model (i)



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 (2.5).

9.4 Atom inclusion (i)



At the recommended contour level, 97% of all backbone atoms, 95% 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 (2.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9500	0.3800
1	0.9790	0.4150
2	0.9850	0.3600
3	0.9880	0.3760
4	0.8800	0.1830
5	0.8070	0.3650
A	0.9470	0.4460
B	0.9430	0.4660
C	0.9300	0.4390
D	0.9470	0.4540
E	0.9000	0.2880
F	0.9350	0.3640
G	0.5120	0.2790
J	0.9230	0.4270
K	0.9350	0.4600
L	0.9480	0.4560
M	0.9360	0.4400
N	0.9430	0.4400
O	0.9380	0.3530
P	0.9190	0.4550
Q	0.9420	0.4370
R	0.9330	0.4470
S	0.9410	0.4720
T	0.9300	0.4350
U	0.9370	0.4320
V	0.9290	0.3950
W	0.8120	0.4160
X	0.9200	0.4520
Y	0.9100	0.3590
Z	0.9220	0.4370
a	0.6250	0.2430
b	0.9420	0.4540
c	0.9090	0.4230
d	0.9520	0.4900
e	0.9330	0.4590

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Chain	Atom inclusion	Q-score
f	0.9040	0.4320
g	0.9060	0.3620
h	0.8710	0.2500
i	0.9080	0.3680
j	0.9190	0.4330
k	0.8970	0.3710
l	0.6660	0.1960
m	0.9240	0.4320
n	0.8860	0.2290
o	0.8810	0.2470
p	0.9330	0.4010
q	0.9170	0.4100
r	0.7990	0.2210
s	0.8970	0.2530
t	0.9440	0.3980
u	0.9230	0.4060
v	0.9350	0.3890
w	0.8980	0.3850
x	0.7480	0.1520
y	0.9130	0.3680
z	0.8250	0.3290