wwPDB EM Validation Summary Report (i)

Apr 16, 2024 – 03:46 am BST

PDB ID	:	7OT5
EMDB ID	:	EMD-13055
Title	:	CspA-70 cotranslational folding intermediate 1
Authors	:	Agirrezabala, X.; Samatova, E.; Macher, M.; Liutkute, M.; Gil-Carton, D.; Novacek, J.; Valle, M.; Rodnina, M.V.
Deposited on	:	2021-06-09
Resolution	:	2.90 Å(reported)
Based on initial model	:	6ORE

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:

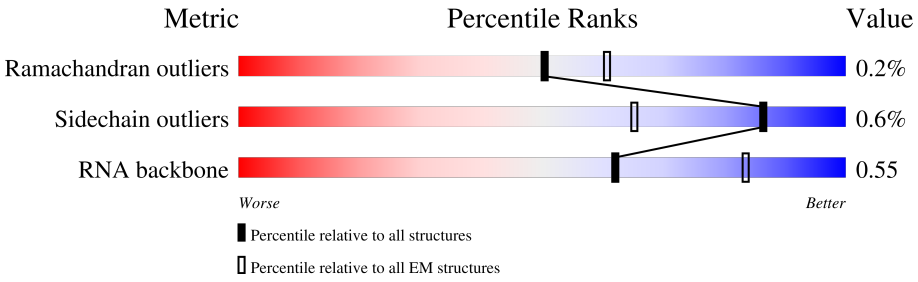
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.90 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	81% 18%
2	2	1534	82% 17%
3	3	120	87% 12%
4	C	271	100%
5	D	209	98%
6	E	201	100%
7	F	177	99%
8	G	175	99%

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Mol	Chain	Length	Quality of chain
9	H	149	47% 98%
10	I	142	100%
11	J	123	99%
12	K	144	99%
13	L	136	99%
14	M	119	100%
15	N	116	100%
16	O	114	100%
17	P	117	100%
18	Q	103	98%
19	R	110	99%
20	S	94	100%
21	T	103	100%
22	U	94	100%
23	V	81	5% 99%
24	W	77	100%
25	X	62	100%
26	Y	58	98%
27	Z	66	6% 100%
28	a	56	100%
29	b	52	100%
30	c	46	100%
31	d	64	97%
32	e	38	100%
33	f	225	99%

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Mol	Chain	Length	Quality of chain
34	g	208	100%
35	h	205	100%
36	i	156	99%
37	j	104	100%
38	k	151	100%
39	l	129	100%
40	m	127	99%
41	n	99	99%
42	o	117	99%
43	p	123	99%
44	q	116	100%
45	r	100	100%
46	s	88	99%
47	t	82	100%
48	u	80	100%
49	v	66	100%
50	w	83	99%
51	x	86	98%
52	y	70	9% 99%
53	4	6	83% 17%
54	z	85	55% 34% 11%
55	B	66	5% 92% 8%

2 Entry composition (i)

There are 57 unique types of molecules in this entry. The entry contains 145365 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 23S rRNA.

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

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

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 rRNA.

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 50S ribosomal protein L2.

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

- Molecule 5 is a protein called 50S ribosomal protein L3.

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

- Molecule 6 is a protein called 50S ribosomal protein L4.

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

- Molecule 7 is a protein called 50S ribosomal protein L5.

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

- Molecule 8 is a protein called 50S ribosomal protein L6.

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

- Molecule 9 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	H	149	Total	C	N	O	S	0	0
			1111	699	197	214	1		

- Molecule 10 is a protein called 50S ribosomal protein L13.

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

- Molecule 11 is a protein called 50S ribosomal protein L14.

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

- Molecule 12 is a protein called 50S ribosomal protein L15.

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

- Molecule 13 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	L	136	Total	C	N	O	S	0	0
			1074	686	205	177	6		

- Molecule 14 is a protein called 50S ribosomal protein L17.

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

- Molecule 15 is a protein called 50S ribosomal protein L18.

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

- Molecule 16 is a protein called 50S ribosomal protein L19.

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

- Molecule 17 is a protein called 50S ribosomal protein L20.

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

- Molecule 18 is a protein called 50S ribosomal protein L21.

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

- Molecule 19 is a protein called 50S ribosomal protein L22.

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

- Molecule 20 is a protein called 50S ribosomal protein L23.

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

- Molecule 21 is a protein called Ribosomal protein L24.

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

- Molecule 22 is a protein called 50S ribosomal protein L25.

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

- Molecule 23 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	V	81	Total 610	C 376	N 123	O 110	S 1	0	0

- Molecule 24 is a protein called 50S ribosomal protein L28.

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

- Molecule 25 is a protein called 50S ribosomal protein L29.

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

- Molecule 26 is a protein called 50S ribosomal protein L30.

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

- Molecule 27 is a protein called 50S ribosomal protein L31.

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

- Molecule 28 is a protein called 50S ribosomal protein L32.

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

- Molecule 29 is a protein called 50S ribosomal protein L33.

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

- Molecule 30 is a protein called 50S ribosomal protein L34.

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

- Molecule 31 is a protein called 50S ribosomal protein L35.

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

- Molecule 32 is a protein called 50S ribosomal protein L36.

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

- Molecule 33 is a protein called 30S ribosomal protein S2.

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

- Molecule 34 is a protein called 30S ribosomal protein S3.

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

- Molecule 35 is a protein called 30S ribosomal protein S4.

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

- Molecule 36 is a protein called 30S ribosomal protein S5.

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

- Molecule 37 is a protein called 30S ribosomal protein S6.

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

- Molecule 38 is a protein called 30S ribosomal protein S7.

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

- Molecule 39 is a protein called 30S ribosomal protein S8.

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

- Molecule 40 is a protein called 30S ribosomal protein S9.

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

- Molecule 41 is a protein called 30S ribosomal protein S10.

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

- Molecule 42 is a protein called 30S ribosomal protein S11.

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

- Molecule 43 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	p	123	Total	C	N	O	S	0	0
			957	591	196	165	5		

- Molecule 44 is a protein called 30S ribosomal protein S13.

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

- Molecule 45 is a protein called 30S ribosomal protein S14.

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

- Molecule 46 is a protein called 30S ribosomal protein S15.

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

- Molecule 47 is a protein called 30S ribosomal protein S16.

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

- Molecule 48 is a protein called 30S ribosomal protein S17.

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

- Molecule 49 is a protein called 30S ribosomal protein S18.

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

- Molecule 50 is a protein called Ribosomal protein S19.

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

- Molecule 51 is a protein called 30S ribosomal protein S20.

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

- Molecule 52 is a protein called 30S ribosomal protein S21.

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

- Molecule 53 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	4	6	Total	C	N	O	P	0	0
			122	55	17	44	6		

- Molecule 54 is a RNA chain called tRNA-Leu.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	z	85	Total	C	N	O	P	0	0
			1830	822	328	595	85		

- Molecule 55 is a protein called Cold shock protein CspB.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	B	66	Total	C	N	O	S	0	0
			496	316	81	98	1		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	45	LYS	LEU	conflict	UNP A0A7U8W1U7
B	61	ALA	GLY	conflict	UNP A0A7U8W1U7

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

Mol	Chain	Residues	Atoms	AltConf
56	1	261	Total Mg 261 261	0
56	2	113	Total Mg 113 113	0
56	3	8	Total Mg 8 8	0
56	C	1	Total Mg 1 1	0
56	D	2	Total Mg 2 2	0
56	P	1	Total Mg 1 1	0
56	T	1	Total Mg 1 1	0
56	a	2	Total Mg 2 2	0
56	h	1	Total Mg 1 1	0
56	m	1	Total Mg 1 1	0
56	q	1	Total Mg 1 1	0
56	z	2	Total Mg 2 2	0

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

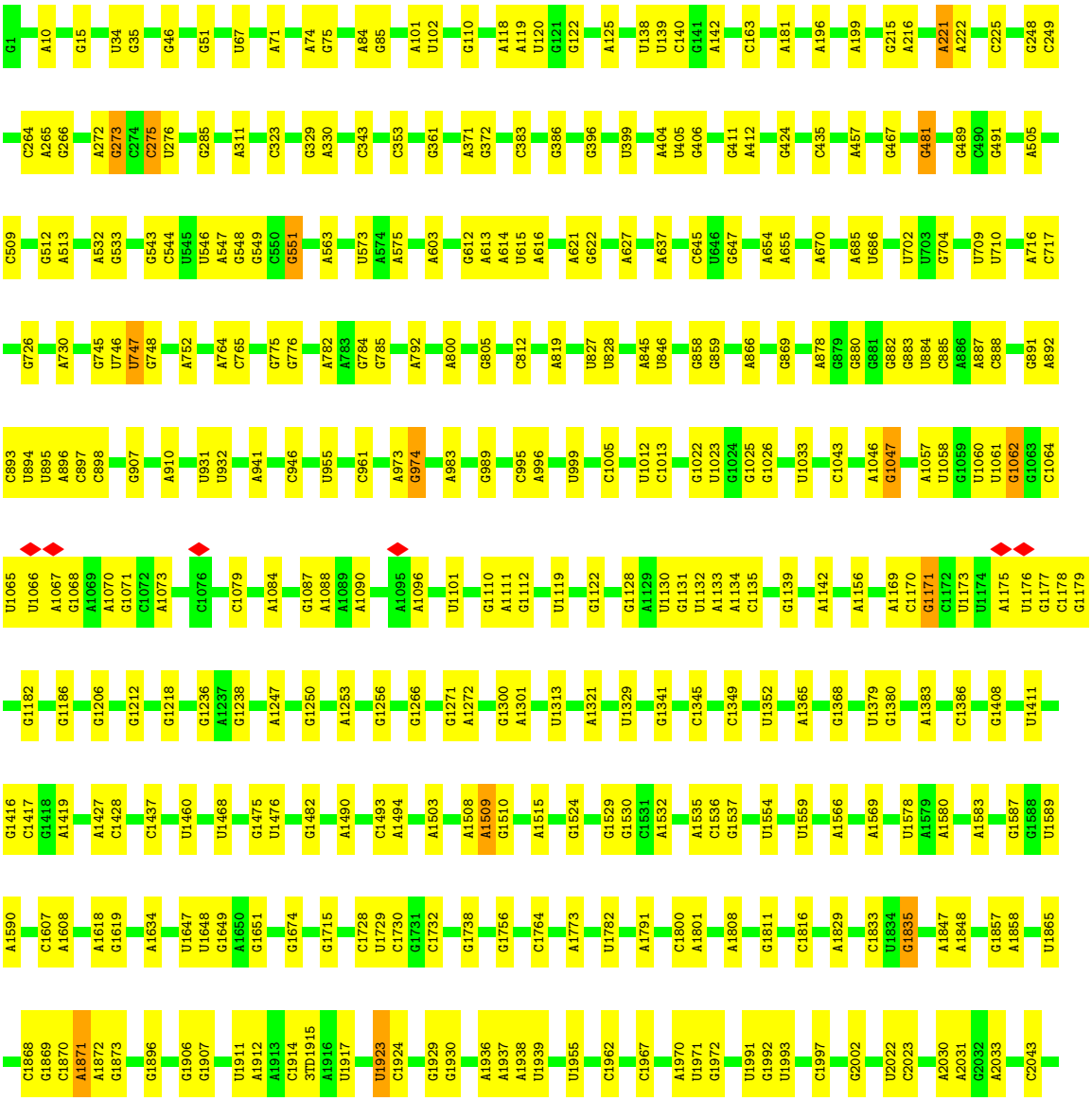
Mol	Chain	Residues	Atoms	AltConf
57	Z	1	Total Zn 1 1	0
57	e	1	Total Zn 1 1	0

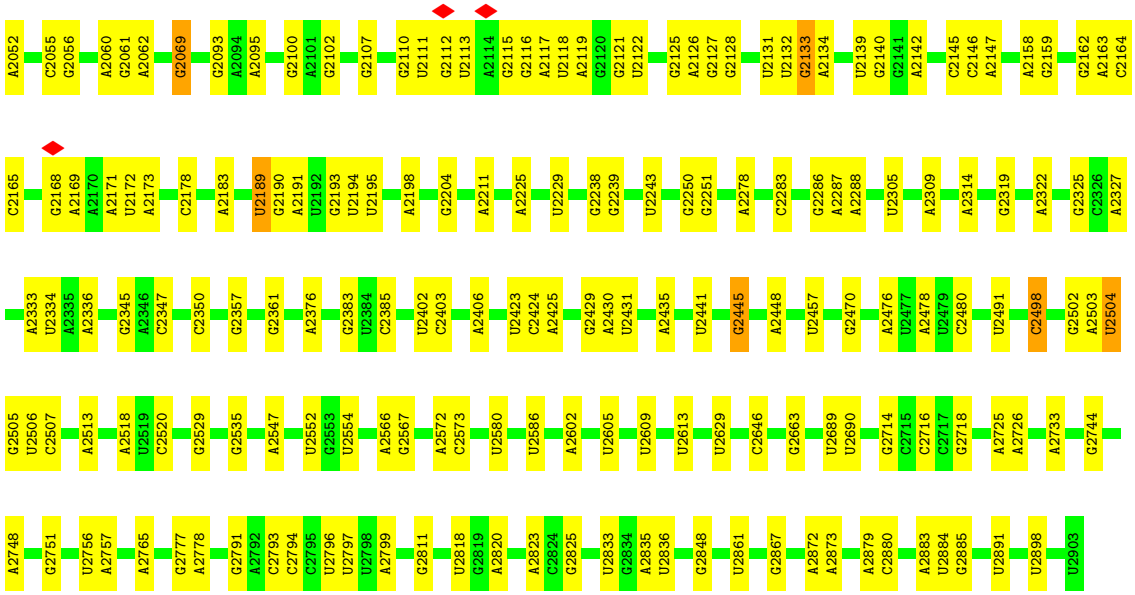
3 Residue-property plots (i)

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 rRNA

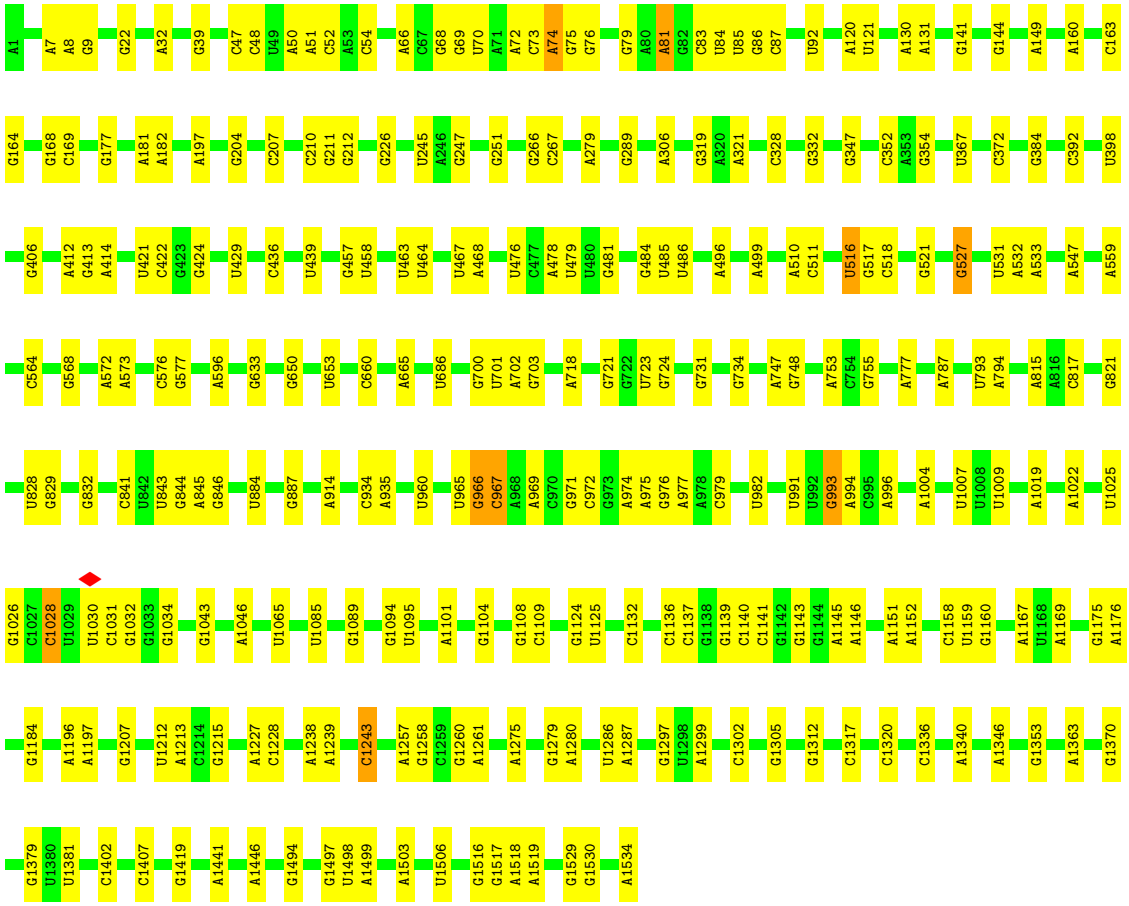
Chain 1:





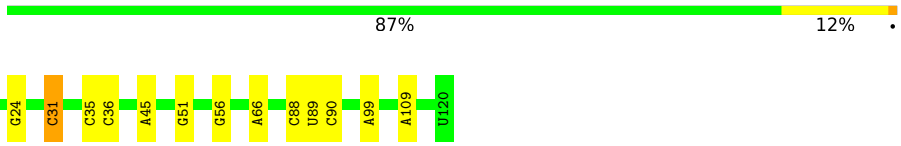
• Molecule 2: 16S rRNA

Chain 2:



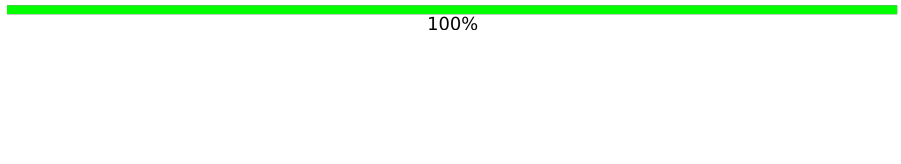
• Molecule 3: 5S rRNA

Chain 3:



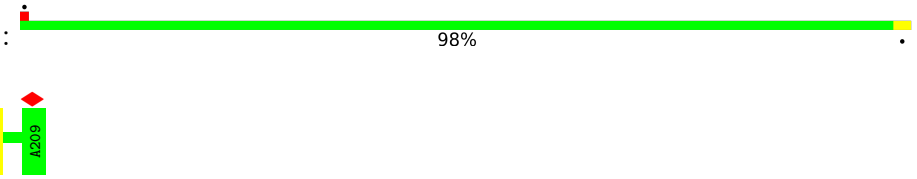
• Molecule 4: 50S ribosomal protein L2

Chain C:



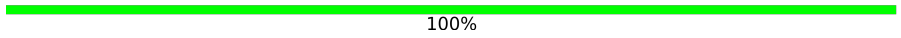
• Molecule 5: 50S ribosomal protein L3

Chain D:



• Molecule 6: 50S ribosomal protein L4

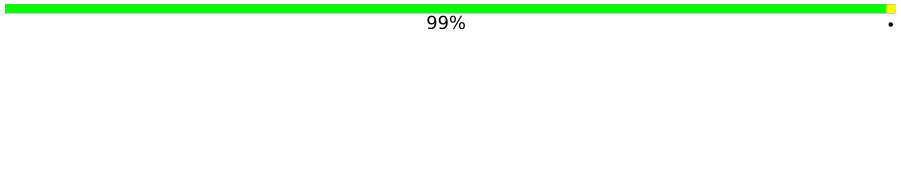
Chain E:



There are no outlier residues recorded for this chain.

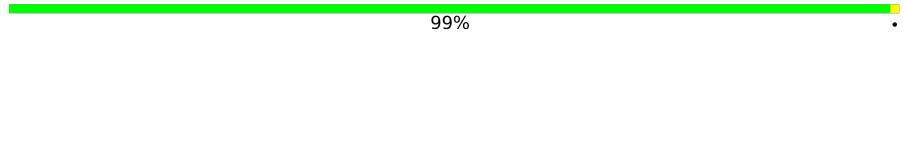
• Molecule 7: 50S ribosomal protein L5

Chain F:



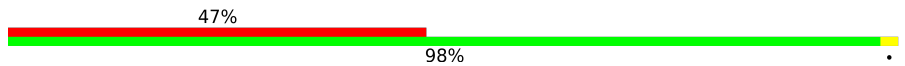
• Molecule 8: 50S ribosomal protein L6

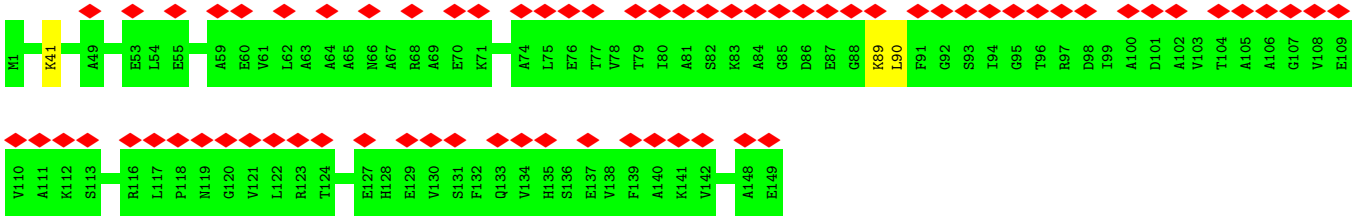
Chain G:



• Molecule 9: 50S ribosomal protein L9

Chain H:



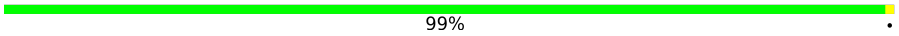


• Molecule 10: 50S ribosomal protein L13

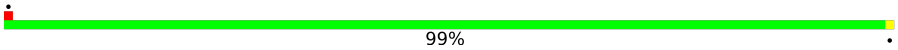
Chain I: 

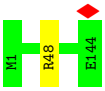
There are no outlier residues recorded for this chain.

• Molecule 11: 50S ribosomal protein L14

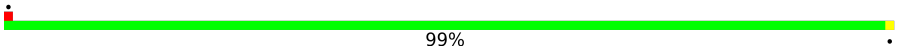
Chain J: 

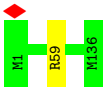
• Molecule 12: 50S ribosomal protein L15

Chain K: 

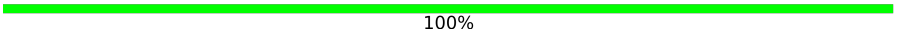


• Molecule 13: 50S ribosomal protein L16

Chain L: 

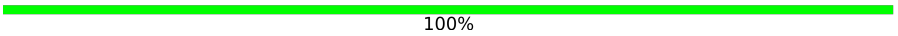


• Molecule 14: 50S ribosomal protein L17

Chain M: 

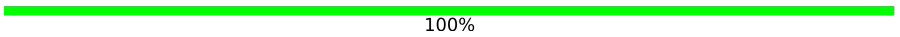
There are no outlier residues recorded for this chain.

• Molecule 15: 50S ribosomal protein L18

Chain N: 

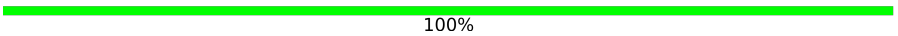
There are no outlier residues recorded for this chain.

• Molecule 16: 50S ribosomal protein L19

Chain O: 

There are no outlier residues recorded for this chain.

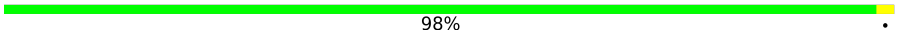
• Molecule 17: 50S ribosomal protein L20

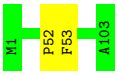
Chain P: 

There are no outlier residues recorded for this chain.

• Molecule 18: 50S ribosomal protein L21

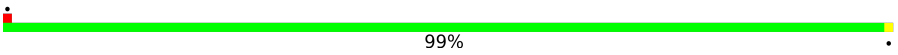
Chain Q:

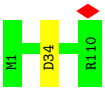




• Molecule 19: 50S ribosomal protein L22

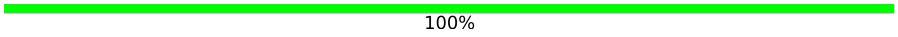
Chain R:





• Molecule 20: 50S ribosomal protein L23

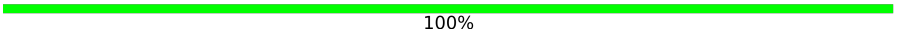
Chain S:



There are no outlier residues recorded for this chain.

• Molecule 21: Ribosomal protein L24

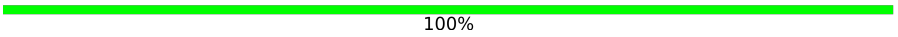
Chain T:



There are no outlier residues recorded for this chain.

• Molecule 22: 50S ribosomal protein L25

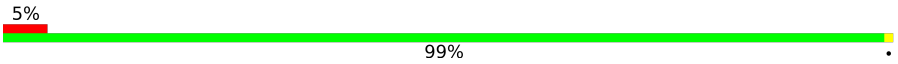
Chain U:

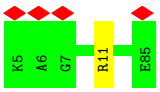


There are no outlier residues recorded for this chain.

• Molecule 23: 50S ribosomal protein L27

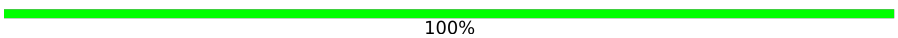
Chain V:





• Molecule 24: 50S ribosomal protein L28

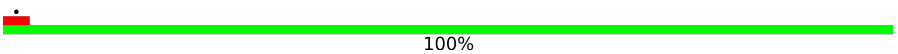
Chain W:



There are no outlier residues recorded for this chain.

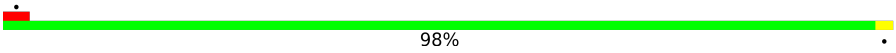
• Molecule 25: 50S ribosomal protein L29

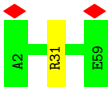
Chain X:



• Molecule 26: 50S ribosomal protein L30

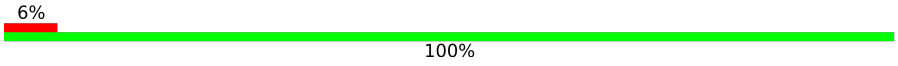
Chain Y:

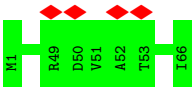




• Molecule 27: 50S ribosomal protein L31

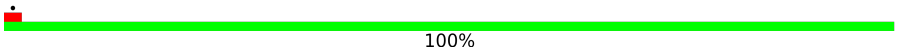
Chain Z:





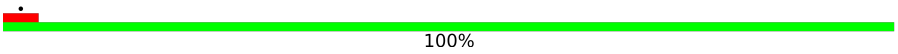
• Molecule 28: 50S ribosomal protein L32

Chain a:



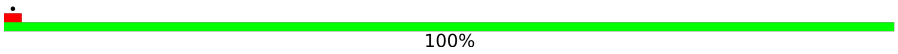
• Molecule 29: 50S ribosomal protein L33

Chain b:



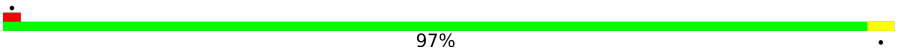
• Molecule 30: 50S ribosomal protein L34

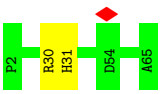
Chain c:



• Molecule 31: 50S ribosomal protein L35

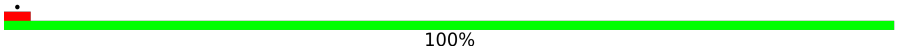
Chain d:





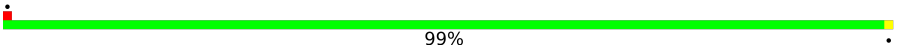
• Molecule 32: 50S ribosomal protein L36

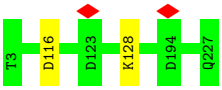
Chain e:



• Molecule 33: 30S ribosomal protein S2

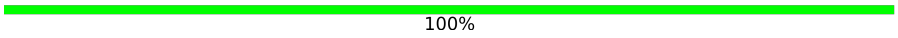
Chain f:





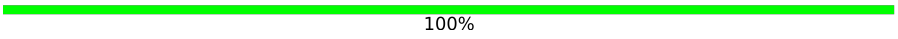
• Molecule 34: 30S ribosomal protein S3

Chain g:



• Molecule 35: 30S ribosomal protein S4

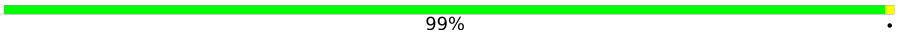
Chain h:



There are no outlier residues recorded for this chain.

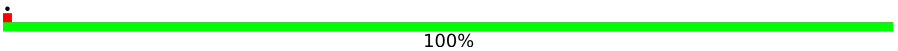
• Molecule 36: 30S ribosomal protein S5

Chain i:



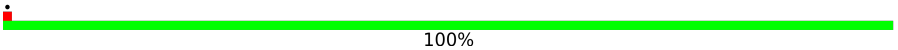
• Molecule 37: 30S ribosomal protein S6

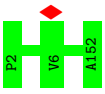
Chain j:



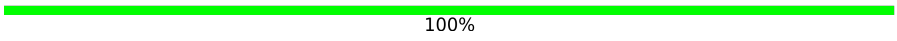
• Molecule 38: 30S ribosomal protein S7

Chain k:



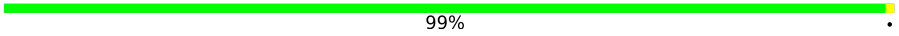


• Molecule 39: 30S ribosomal protein S8

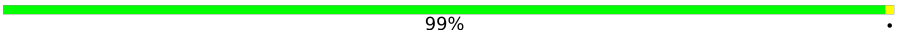
Chain l: 

There are no outlier residues recorded for this chain.

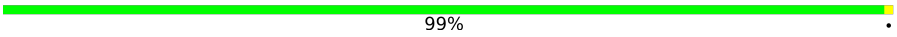
• Molecule 40: 30S ribosomal protein S9

Chain m: 

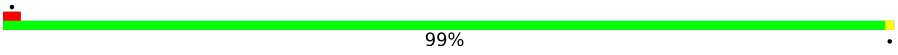
• Molecule 41: 30S ribosomal protein S10

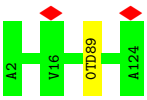
Chain n: 

• Molecule 42: 30S ribosomal protein S11

Chain o: 

• Molecule 43: 30S ribosomal protein S12

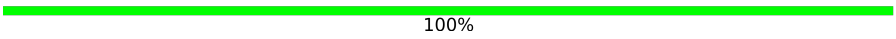
Chain p: 



• Molecule 44: 30S ribosomal protein S13

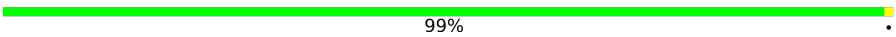
Chain q: 

• Molecule 45: 30S ribosomal protein S14

Chain r: 

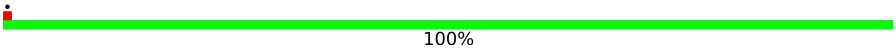
There are no outlier residues recorded for this chain.

• Molecule 46: 30S ribosomal protein S15

Chain s: 

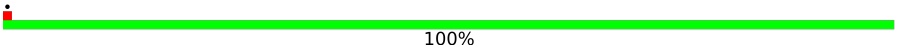
• Molecule 47: 30S ribosomal protein S16

Chain t:



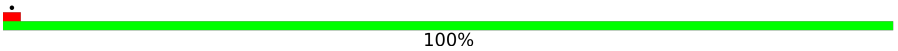
• Molecule 48: 30S ribosomal protein S17

Chain u:



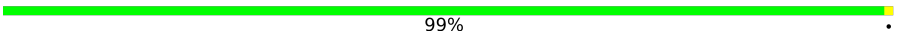
• Molecule 49: 30S ribosomal protein S18

Chain v:



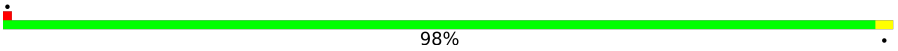
• Molecule 50: Ribosomal protein S19

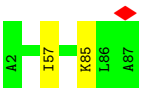
Chain w:



• Molecule 51: 30S ribosomal protein S20

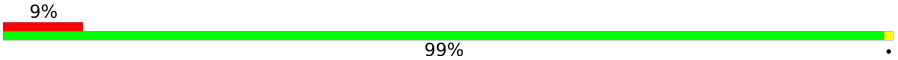
Chain x:

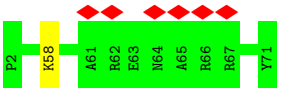




• Molecule 52: 30S ribosomal protein S21

Chain y:



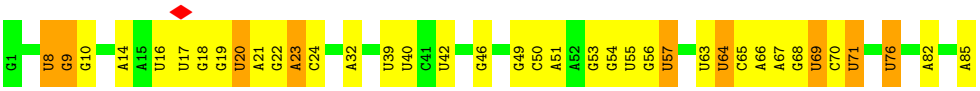


• Molecule 53: mRNA

Chain 4:

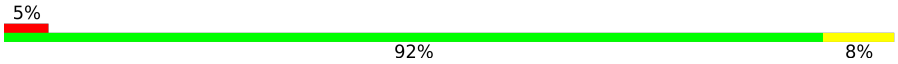
• Molecule 54: tRNA-Leu

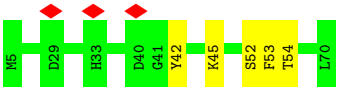
Chain z:



• Molecule 55: Cold shock protein CspB

Chain B:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	26765	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 ($e^-/Å^2$)	2.2	Depositor
Minimum defocus (nm)	-500	Depositor
Maximum defocus (nm)	-2200	Depositor
Magnification	75000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.176	Depositor
Minimum map value	-0.055	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	428.00003, 428.00003, 428.00003	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 2MG, G7M, UR3, ZN, 5MU, 6MZ, 4OC, MA6, 3TD, OMU, 0TD, 5MC, OMG, 1MG, MG, 2MA, PSU, OMC

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	0.92	0/69286	1.00	48/108087 (0.0%)
2	2	0.82	0/36590	0.97	16/57074 (0.0%)
3	3	0.78	0/2872	0.94	2/4478 (0.0%)
4	C	0.63	0/2121	0.60	0/2852
5	D	0.62	0/1586	0.59	0/2134
6	E	0.55	0/1571	0.57	0/2113
7	F	0.47	0/1434	0.58	0/1926
8	G	0.45	0/1333	0.57	0/1805
9	H	0.37	0/1122	0.70	0/1515
10	I	0.62	0/1152	0.56	0/1551
11	J	0.60	0/955	0.59	0/1279
12	K	0.56	0/1062	0.62	0/1413
13	L	0.58	0/1093	0.58	0/1460
14	M	0.59	0/964	0.59	0/1289
15	N	0.51	0/902	0.59	0/1209
16	O	0.60	0/929	0.51	0/1242
17	P	0.68	0/960	0.59	0/1278
18	Q	0.61	0/829	0.64	0/1107
19	R	0.61	0/864	0.62	0/1156
20	S	0.56	0/752	0.55	0/1005
21	T	0.53	0/796	0.57	0/1062
22	U	0.55	0/766	0.59	0/1025
23	V	0.61	0/617	0.58	0/815
24	W	0.57	0/635	0.59	0/848
25	X	0.47	0/502	0.65	0/667
26	Y	0.53	0/452	0.58	0/605
27	Z	0.40	0/531	0.54	0/709
28	a	0.58	0/450	0.63	0/599
29	b	0.50	0/433	0.57	0/576
30	c	0.63	0/380	0.58	0/498
31	d	0.63	0/513	0.60	0/676

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	e	0.59	0/303	0.53	0/397
33	f	0.45	0/1791	0.62	0/2413
34	g	0.50	0/1663	0.58	0/2241
35	h	0.50	0/1665	0.55	0/2227
36	i	0.57	0/1165	0.61	0/1568
37	j	0.49	0/867	0.56	0/1171
38	k	0.47	0/1195	0.59	0/1602
39	l	0.53	0/989	0.57	0/1326
40	m	0.49	0/1034	0.60	0/1375
41	n	0.47	0/800	0.63	0/1082
42	o	0.49	0/893	0.58	0/1205
43	p	0.57	0/960	0.59	0/1286
44	q	0.47	0/909	0.59	0/1215
45	r	0.50	0/817	0.56	0/1088
46	s	0.48	0/722	0.55	0/964
47	t	0.54	0/659	0.60	0/884
48	u	0.48	0/657	0.57	0/881
49	v	0.51	0/553	0.58	0/743
50	w	0.46	0/680	0.53	0/915
51	x	0.48	0/675	0.65	0/895
52	y	0.43	0/597	0.58	0/792
53	4	0.97	0/134	1.30	0/205
54	z	0.83	1/1768 (0.1%)	1.04	4/2759 (0.1%)
55	B	0.42	0/507	0.64	0/682
All	All	0.80	1/156455 (0.0%)	0.90	70/233969 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	z	32	A	N9-C4	-5.83	1.34	1.37

The worst 5 of 70 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	2193	G	C4-N9-C1'	9.56	138.93	126.50
1	1	2193	G	C8-N9-C1'	-8.51	115.94	127.00
1	1	1313	U	C2-N1-C1'	7.81	127.07	117.70
1	1	221	A	O4'-C1'-N9	7.42	114.14	108.20
1	1	1509	A	O4'-C1'-N9	7.37	114.09	108.20

There are no chirality outliers.

There are no planarity outliers.

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	C	269/271 (99%)	257 (96%)	12 (4%)	0	100	100
5	D	207/209 (99%)	201 (97%)	3 (1%)	3 (1%)	11	36
6	E	199/201 (99%)	197 (99%)	2 (1%)	0	100	100
7	F	175/177 (99%)	165 (94%)	9 (5%)	1 (1%)	25	58
8	G	173/175 (99%)	162 (94%)	11 (6%)	0	100	100
9	H	147/149 (99%)	136 (92%)	9 (6%)	2 (1%)	11	36
10	I	140/142 (99%)	137 (98%)	3 (2%)	0	100	100
11	J	121/123 (98%)	119 (98%)	2 (2%)	0	100	100
12	K	142/144 (99%)	139 (98%)	3 (2%)	0	100	100
13	L	134/136 (98%)	130 (97%)	4 (3%)	0	100	100
14	M	117/119 (98%)	114 (97%)	3 (3%)	0	100	100
15	N	114/116 (98%)	111 (97%)	3 (3%)	0	100	100
16	O	112/114 (98%)	111 (99%)	1 (1%)	0	100	100
17	P	115/117 (98%)	114 (99%)	1 (1%)	0	100	100
18	Q	101/103 (98%)	94 (93%)	5 (5%)	2 (2%)	7	27
19	R	108/110 (98%)	107 (99%)	1 (1%)	0	100	100
20	S	92/94 (98%)	90 (98%)	2 (2%)	0	100	100
21	T	101/103 (98%)	93 (92%)	8 (8%)	0	100	100
22	U	92/94 (98%)	89 (97%)	3 (3%)	0	100	100
23	V	79/81 (98%)	72 (91%)	6 (8%)	1 (1%)	12	37
24	W	75/77 (97%)	74 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
25	X	60/62 (97%)	59 (98%)	1 (2%)	0	100	100
26	Y	56/58 (97%)	55 (98%)	1 (2%)	0	100	100
27	Z	64/66 (97%)	60 (94%)	4 (6%)	0	100	100
28	a	54/56 (96%)	52 (96%)	2 (4%)	0	100	100
29	b	50/52 (96%)	49 (98%)	1 (2%)	0	100	100
30	c	44/46 (96%)	44 (100%)	0	0	100	100
31	d	62/64 (97%)	58 (94%)	4 (6%)	0	100	100
32	e	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
33	f	223/225 (99%)	212 (95%)	11 (5%)	0	100	100
34	g	206/208 (99%)	197 (96%)	9 (4%)	0	100	100
35	h	203/205 (99%)	199 (98%)	4 (2%)	0	100	100
36	i	154/156 (99%)	144 (94%)	10 (6%)	0	100	100
37	j	102/104 (98%)	99 (97%)	3 (3%)	0	100	100
38	k	149/151 (99%)	145 (97%)	4 (3%)	0	100	100
39	l	127/129 (98%)	125 (98%)	2 (2%)	0	100	100
40	m	125/127 (98%)	118 (94%)	7 (6%)	0	100	100
41	n	97/99 (98%)	92 (95%)	5 (5%)	0	100	100
42	o	115/117 (98%)	109 (95%)	6 (5%)	0	100	100
43	p	120/123 (98%)	114 (95%)	6 (5%)	0	100	100
44	q	114/116 (98%)	110 (96%)	4 (4%)	0	100	100
45	r	98/100 (98%)	97 (99%)	1 (1%)	0	100	100
46	s	86/88 (98%)	84 (98%)	2 (2%)	0	100	100
47	t	80/82 (98%)	78 (98%)	2 (2%)	0	100	100
48	u	78/80 (98%)	75 (96%)	3 (4%)	0	100	100
49	v	64/66 (97%)	63 (98%)	1 (2%)	0	100	100
50	w	81/83 (98%)	80 (99%)	1 (1%)	0	100	100
51	x	84/86 (98%)	84 (100%)	0	0	100	100
52	y	68/70 (97%)	67 (98%)	1 (2%)	0	100	100
55	B	64/66 (97%)	46 (72%)	17 (27%)	1 (2%)	9	32
All	All	5677/5778 (98%)	5462 (96%)	205 (4%)	10 (0%)	50	78

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	D	152	PRO
5	D	153	GLY
5	D	154	LYS
9	H	90	LEU
18	Q	52	PRO

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
4	C	216/216 (100%)	216 (100%)	0	100 100
5	D	164/164 (100%)	163 (99%)	1 (1%)	86 96
6	E	165/165 (100%)	165 (100%)	0	100 100
7	F	148/148 (100%)	148 (100%)	0	100 100
8	G	136/136 (100%)	135 (99%)	1 (1%)	84 95
9	H	114/114 (100%)	113 (99%)	1 (1%)	78 93
10	I	116/116 (100%)	116 (100%)	0	100 100
11	J	104/104 (100%)	103 (99%)	1 (1%)	76 92
12	K	103/103 (100%)	102 (99%)	1 (1%)	76 92
13	L	109/109 (100%)	108 (99%)	1 (1%)	78 93
14	M	99/99 (100%)	99 (100%)	0	100 100
15	N	86/86 (100%)	86 (100%)	0	100 100
16	O	99/99 (100%)	99 (100%)	0	100 100
17	P	89/89 (100%)	89 (100%)	0	100 100
18	Q	84/84 (100%)	84 (100%)	0	100 100
19	R	93/93 (100%)	92 (99%)	1 (1%)	73 92
20	S	81/81 (100%)	81 (100%)	0	100 100
21	T	84/84 (100%)	84 (100%)	0	100 100
22	U	78/78 (100%)	78 (100%)	0	100 100
23	V	60/60 (100%)	60 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
24	W	67/67 (100%)	67 (100%)	0	100	100
25	X	54/54 (100%)	54 (100%)	0	100	100
26	Y	48/48 (100%)	47 (98%)	1 (2%)	53	81
27	Z	59/59 (100%)	59 (100%)	0	100	100
28	a	47/47 (100%)	47 (100%)	0	100	100
29	b	47/47 (100%)	47 (100%)	0	100	100
30	c	38/38 (100%)	38 (100%)	0	100	100
31	d	51/51 (100%)	49 (96%)	2 (4%)	32	66
32	e	34/34 (100%)	34 (100%)	0	100	100
33	f	187/187 (100%)	185 (99%)	2 (1%)	73	92
34	g	171/171 (100%)	170 (99%)	1 (1%)	86	96
35	h	172/172 (100%)	172 (100%)	0	100	100
36	i	119/119 (100%)	118 (99%)	1 (1%)	81	94
37	j	91/91 (100%)	91 (100%)	0	100	100
38	k	124/124 (100%)	124 (100%)	0	100	100
39	l	104/104 (100%)	104 (100%)	0	100	100
40	m	105/105 (100%)	104 (99%)	1 (1%)	76	92
41	n	86/86 (100%)	85 (99%)	1 (1%)	71	91
42	o	90/90 (100%)	89 (99%)	1 (1%)	73	92
43	p	102/102 (100%)	102 (100%)	0	100	100
44	q	94/94 (100%)	94 (100%)	0	100	100
45	r	83/83 (100%)	83 (100%)	0	100	100
46	s	76/76 (100%)	75 (99%)	1 (1%)	69	90
47	t	65/65 (100%)	65 (100%)	0	100	100
48	u	74/74 (100%)	74 (100%)	0	100	100
49	v	57/57 (100%)	57 (100%)	0	100	100
50	w	72/72 (100%)	71 (99%)	1 (1%)	67	89
51	x	65/65 (100%)	63 (97%)	2 (3%)	40	74
52	y	60/60 (100%)	59 (98%)	1 (2%)	60	86
55	B	52/52 (100%)	48 (92%)	4 (8%)	13	35
All	All	4722/4722 (100%)	4696 (99%)	26 (1%)	86	96

5 of 26 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
40	m	106	ARG
46	s	89	ARG
55	B	52	SER
42	o	56	ARG
50	w	78	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
16	O	56	HIS
31	d	31	HIS
47	t	79	ASN
9	H	43	ASN
9	H	33	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	2898/2903 (99%)	497 (17%)	14 (0%)
2	2	1529/1534 (99%)	253 (16%)	3 (0%)
3	3	119/120 (99%)	16 (13%)	0
53	4	5/6 (83%)	0	1 (20%)
54	z	84/85 (98%)	31 (36%)	0
All	All	4635/4648 (99%)	797 (17%)	18 (0%)

5 of 797 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	10	A
1	1	15	G
1	1	34	U
1	1	35	G
1	1	46	G

5 of 18 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	2	516	PSU
53	4	3	U

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Mol	Chain	Res	Type
2	2	1145	A
1	1	1379	U
1	1	2756	U

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

46 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	2MG	1	2445	1	18,26,27	2.22	7 (38%)	16,38,41	1.35	4 (25%)
54	5MU	z	64	54	19,22,23	1.44	6 (31%)	28,32,35	2.38	10 (35%)
54	5MU	z	57	54	19,22,23	4.71	7 (36%)	28,32,35	3.64	10 (35%)
54	5MU	z	69	54	19,22,23	1.41	6 (31%)	28,32,35	1.92	7 (25%)
1	PSU	1	746	1,56	18,21,22	1.02	1 (5%)	22,30,33	1.77	4 (18%)
1	PSU	1	1911	1	18,21,22	0.98	1 (5%)	22,30,33	1.87	5 (22%)
1	1MG	1	745	1	18,26,27	2.81	5 (27%)	19,39,42	1.32	3 (15%)
54	5MU	z	76	54	19,22,23	1.45	5 (26%)	28,32,35	2.21	7 (25%)
2	G7M	2	527	2	20,26,27	2.31	7 (35%)	17,39,42	1.04	1 (5%)
54	5MU	z	39	54	19,22,23	1.44	6 (31%)	28,32,35	2.20	9 (32%)
2	MA6	2	1519	2	18,26,27	1.18	2 (11%)	19,38,41	3.42	2 (10%)
1	5MU	1	747	1	19,22,23	4.63	7 (36%)	28,32,35	3.73	10 (35%)
1	5MU	1	1939	1,56	19,22,23	4.61	7 (36%)	28,32,35	3.72	9 (32%)
1	OMU	1	2552	1	19,22,23	2.87	8 (42%)	26,31,34	1.64	5 (19%)
54	5MU	z	20	54,56	19,22,23	4.94	7 (36%)	28,32,35	3.63	10 (35%)
2	UR3	2	1498	2,56	19,22,23	2.63	6 (31%)	26,32,35	1.07	2 (7%)
54	5MU	z	55	54	19,22,23	4.79	7 (36%)	28,32,35	3.58	9 (32%)
54	5MU	z	63	54	19,22,23	1.46	6 (31%)	28,32,35	2.18	8 (28%)
1	PSU	1	955	1,56	18,21,22	0.99	2 (11%)	22,30,33	1.93	5 (22%)
1	OMC	1	2498	1,56	19,22,23	2.73	7 (36%)	26,31,34	0.86	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
43	0TD	p	89	43	7,9,10	1.51	1 (14%)	6,11,13	1.91	2 (33%)
1	PSU	1	2457	1	18,21,22	1.02	1 (5%)	22,30,33	1.98	5 (22%)
1	6MZ	1	1618	1	18,25,26	1.78	4 (22%)	16,36,39	3.37	4 (25%)
2	MA6	2	1518	2	18,26,27	1.14	2 (11%)	19,38,41	3.25	2 (10%)
54	5MU	z	8	54	19,22,23	4.71	7 (36%)	28,32,35	3.68	10 (35%)
1	OMG	1	2251	54,1	18,26,27	2.20	7 (38%)	19,38,41	1.42	3 (15%)
1	PSU	1	2605	1	18,21,22	0.98	2 (11%)	22,30,33	1.96	5 (22%)
1	5MC	1	1962	1	18,22,23	3.29	7 (38%)	26,32,35	1.13	3 (11%)
1	6MZ	1	2030	1	18,25,26	1.85	3 (16%)	16,36,39	3.13	3 (18%)
1	PSU	1	2504	1	18,21,22	0.98	2 (11%)	22,30,33	1.82	4 (18%)
54	5MU	z	42	54,2	19,22,23	4.58	7 (36%)	28,32,35	3.73	10 (35%)
1	3TD	1	1915	1	18,22,23	4.07	7 (38%)	22,32,35	1.58	2 (9%)
1	2MA	1	2503	1,56	17,25,26	2.33	5 (29%)	17,37,40	1.35	3 (17%)
54	5MU	z	40	54	19,22,23	1.39	5 (26%)	28,32,35	2.29	12 (42%)
54	5MU	z	71	54	19,22,23	1.44	6 (31%)	28,32,35	2.15	8 (28%)
2	2MG	2	1516	2	18,26,27	2.34	7 (38%)	16,38,41	1.35	4 (25%)
2	5MC	2	967	2	18,22,23	3.44	7 (38%)	26,32,35	1.03	2 (7%)
1	2MG	1	1835	1	18,26,27	2.26	7 (38%)	16,38,41	1.34	3 (18%)
2	2MG	2	1207	2	18,26,27	2.34	7 (38%)	16,38,41	1.35	4 (25%)
1	PSU	1	1917	1	18,21,22	1.06	1 (5%)	22,30,33	1.88	5 (22%)
2	PSU	2	516	2,56	18,21,22	0.98	1 (5%)	22,30,33	1.85	4 (18%)
2	4OC	2	1402	2	20,23,24	2.93	8 (40%)	26,32,35	0.94	0
2	5MC	2	1407	2	18,22,23	3.34	7 (38%)	26,32,35	0.85	1 (3%)
1	PSU	1	2580	1,56	18,21,22	1.01	1 (5%)	22,30,33	1.95	6 (27%)
1	G7M	1	2069	1	20,26,27	2.18	8 (40%)	17,39,42	1.26	2 (11%)
2	2MG	2	966	2	18,26,27	2.39	7 (38%)	16,38,41	1.41	3 (18%)

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	2MG	1	2445	1	-	2/5/27/28	0/3/3/3
54	5MU	z	64	54	-	4/7/25/26	0/2/2/2
54	5MU	z	57	54	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
54	5MU	z	69	54	-	5/7/25/26	0/2/2/2
1	PSU	1	746	1,56	-	1/7/25/26	0/2/2/2
1	PSU	1	1911	1	-	0/7/25/26	0/2/2/2
1	1MG	1	745	1	-	0/3/25/26	0/3/3/3
54	5MU	z	76	54	-	0/7/25/26	0/2/2/2
2	G7M	2	527	2	-	3/3/25/26	0/3/3/3
54	5MU	z	39	54	-	3/7/25/26	0/2/2/2
2	MA6	2	1519	2	-	2/7/29/30	0/3/3/3
1	5MU	1	747	1	-	0/7/25/26	0/2/2/2
1	5MU	1	1939	1,56	-	0/7/25/26	0/2/2/2
1	OMU	1	2552	1	-	0/9/27/28	0/2/2/2
54	5MU	z	20	54,56	-	2/7/25/26	0/2/2/2
2	UR3	2	1498	2,56	-	0/7/25/26	0/2/2/2
54	5MU	z	55	54	-	0/7/25/26	0/2/2/2
54	5MU	z	63	54	-	0/7/25/26	0/2/2/2
1	PSU	1	955	1,56	-	0/7/25/26	0/2/2/2
1	OMC	1	2498	1,56	-	0/9/27/28	0/2/2/2
43	0TD	p	89	43	-	2/7/12/14	-
1	PSU	1	2457	1	-	0/7/25/26	0/2/2/2
1	6MZ	1	1618	1	-	2/5/27/28	0/3/3/3
2	MA6	2	1518	2	-	0/7/29/30	0/3/3/3
54	5MU	z	8	54	-	2/7/25/26	0/2/2/2
1	OMG	1	2251	54,1	-	0/5/27/28	0/3/3/3
1	PSU	1	2605	1	-	0/7/25/26	0/2/2/2
1	5MC	1	1962	1	-	0/7/25/26	0/2/2/2
1	6MZ	1	2030	1	-	2/5/27/28	0/3/3/3
1	PSU	1	2504	1	-	2/7/25/26	0/2/2/2
54	5MU	z	42	54,2	-	0/7/25/26	0/2/2/2
1	3TD	1	1915	1	-	3/7/25/26	0/2/2/2
1	2MA	1	2503	1,56	-	2/3/25/26	0/3/3/3
54	5MU	z	40	54	-	2/7/25/26	0/2/2/2
54	5MU	z	71	54	-	3/7/25/26	0/2/2/2
2	2MG	2	1516	2	-	0/5/27/28	0/3/3/3
2	5MC	2	967	2	-	2/7/25/26	0/2/2/2
1	2MG	1	1835	1	-	2/5/27/28	0/3/3/3
2	2MG	2	1207	2	-	0/5/27/28	0/3/3/3
1	PSU	1	1917	1	-	0/7/25/26	0/2/2/2
2	PSU	2	516	2,56	-	2/7/25/26	0/2/2/2

Continued on next page...

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	4OC	2	1402	2	-	2/9/29/30	0/2/2/2
2	5MC	2	1407	2	-	0/7/25/26	0/2/2/2
1	PSU	1	2580	1,56	-	0/7/25/26	0/2/2/2
1	G7M	1	2069	1	-	1/3/25/26	0/3/3/3
2	2MG	2	966	2	-	0/5/27/28	0/3/3/3

The worst 5 of 237 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	1915	3TD	C6-C5	11.83	1.49	1.35
54	z	20	5MU	C2-N1	11.28	1.56	1.38
54	z	57	5MU	C2-N1	11.11	1.56	1.38
54	z	55	5MU	C2-N1	11.07	1.56	1.38
54	z	20	5MU	C6-N1	10.90	1.56	1.38

The worst 5 of 230 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	1519	MA6	N1-C6-N6	-13.50	102.84	117.06
2	2	1518	MA6	N1-C6-N6	-12.98	103.40	117.06
54	z	8	5MU	C5-C4-N3	12.58	126.05	115.31
54	z	20	5MU	C5-C4-N3	12.49	125.97	115.31
1	1	747	5MU	C5-C4-N3	12.27	125.78	115.31

There are no chirality outliers.

5 of 51 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	1	1618	6MZ	O4'-C4'-C5'-O5'
1	1	1618	6MZ	C3'-C4'-C5'-O5'
1	1	1915	3TD	C2'-C1'-C5-C4
1	1	1915	3TD	O4'-C1'-C5-C4
1	1	1915	3TD	O4'-C1'-C5-C6

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 396 ligands modelled in this entry, 396 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.

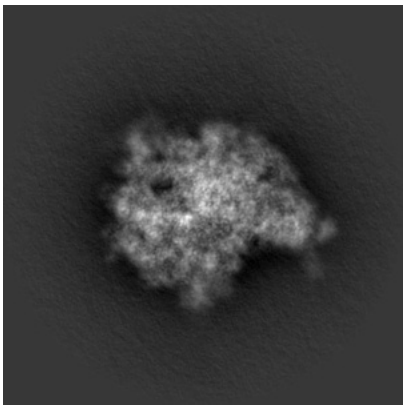
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-13055. These allow visual inspection of the internal detail of the map and identification of artifacts.

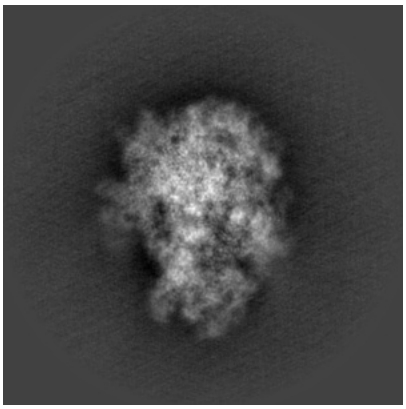
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

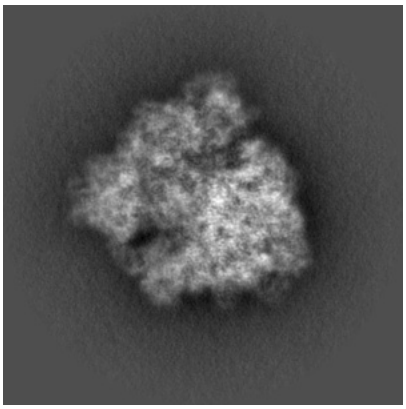
6.1.1 Primary map



X

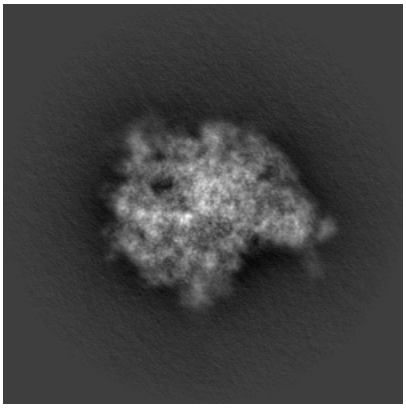


Y

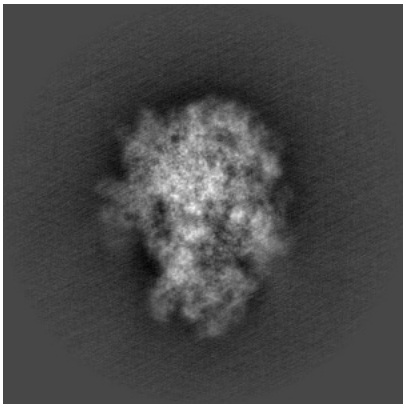


Z

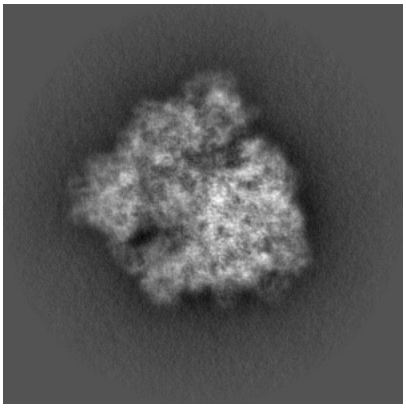
6.1.2 Raw map



X



Y

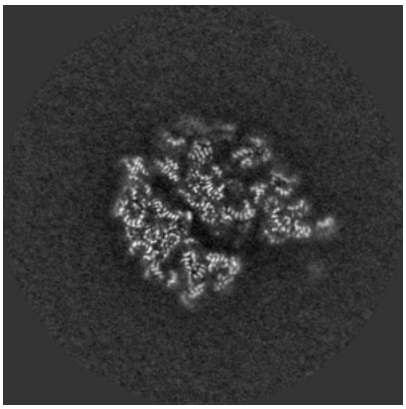


Z

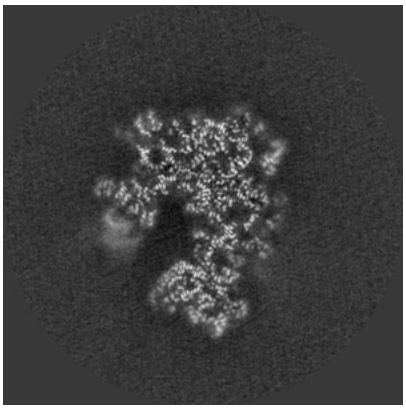
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

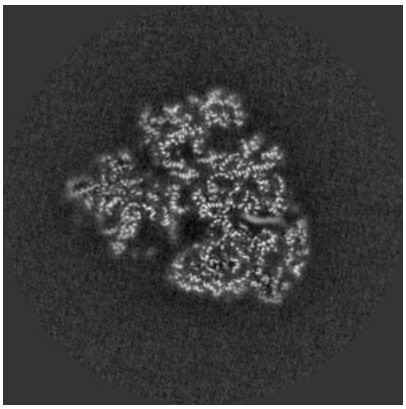
6.2.1 Primary map



X Index: 200

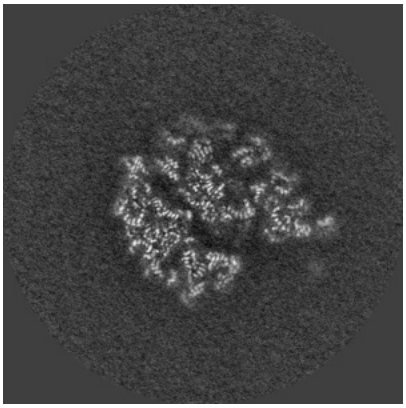


Y Index: 200

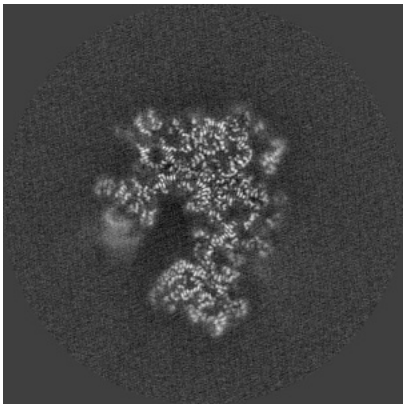


Z Index: 200

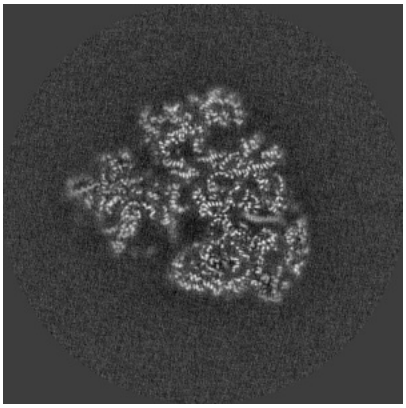
6.2.2 Raw map



X Index: 200



Y Index: 200

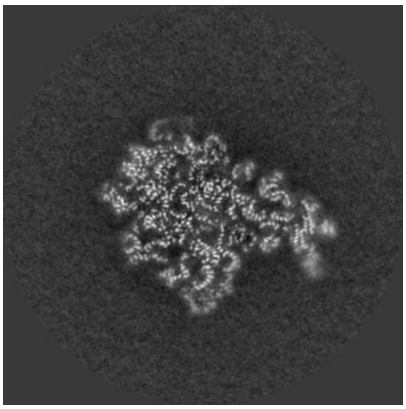


Z Index: 200

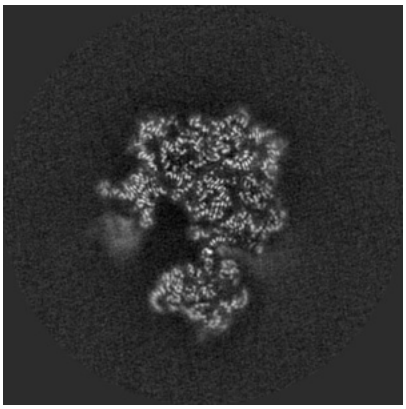
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

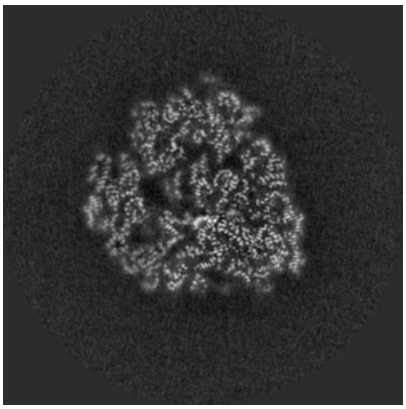
6.3.1 Primary map



X Index: 216

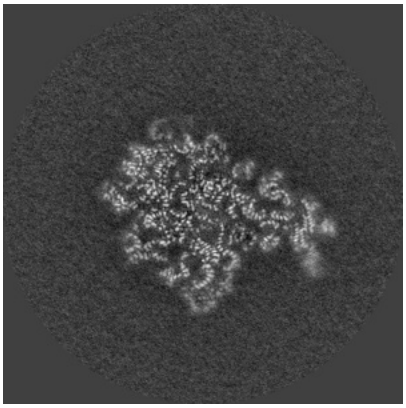


Y Index: 206

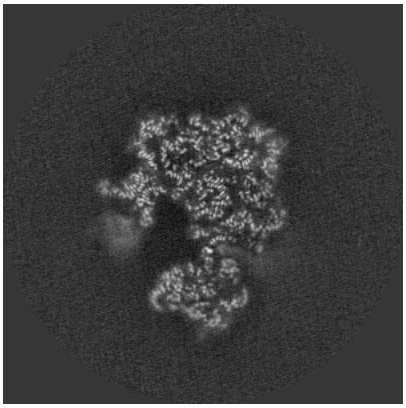


Z Index: 188

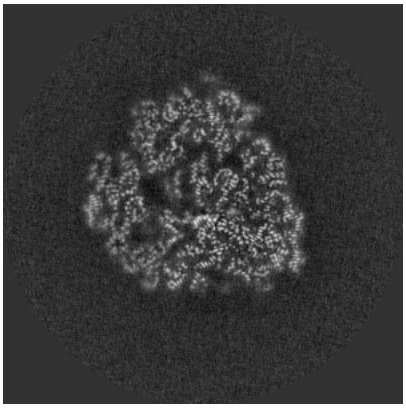
6.3.2 Raw map



X Index: 216



Y Index: 206

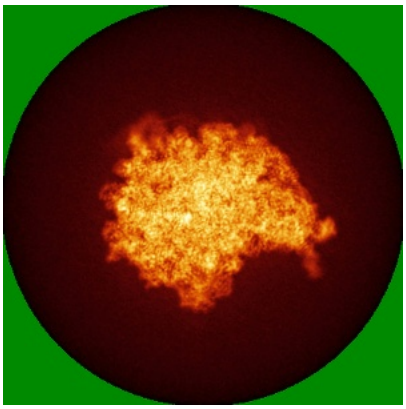


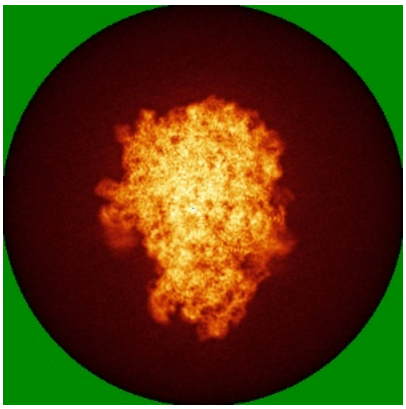
Z Index: 188

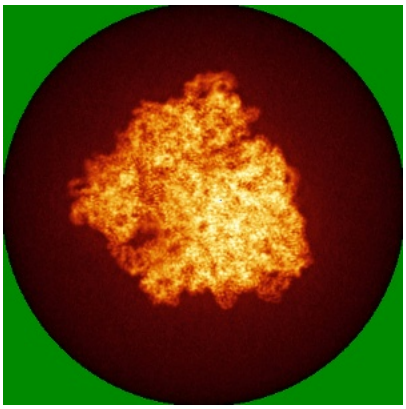
The images above show the largest variance slices of the map in three orthogonal directions.

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

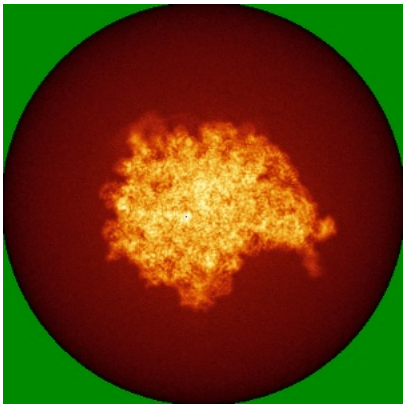
6.4.1 Primary map

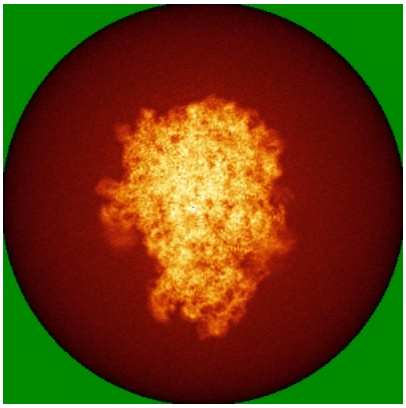

X

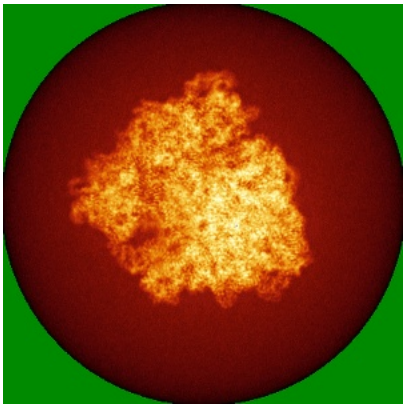

Y


Z

6.4.2 Raw map


X


Y


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.02. 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.

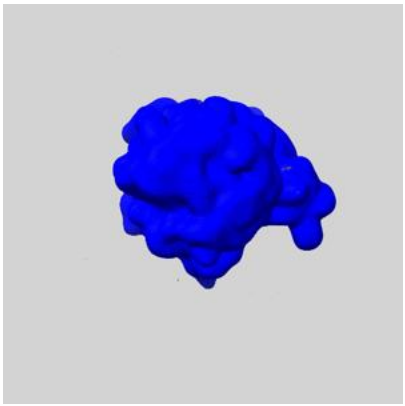
6.6 Mask visualisation (i)

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

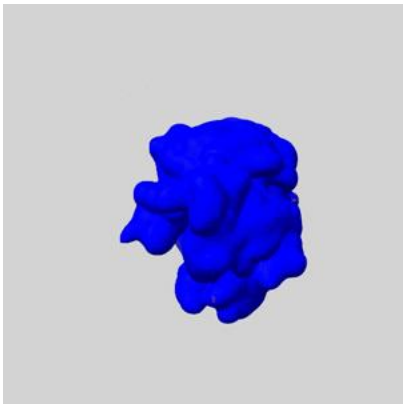
A mask typically either:

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

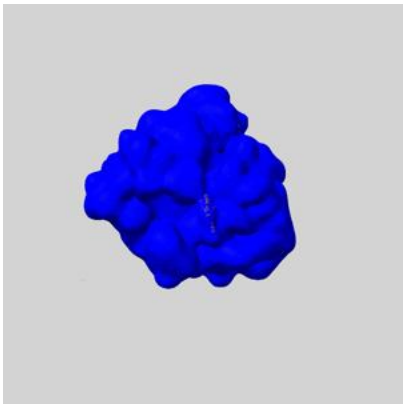
6.6.1 emd_13055_msk_1.map (i)



X



Y

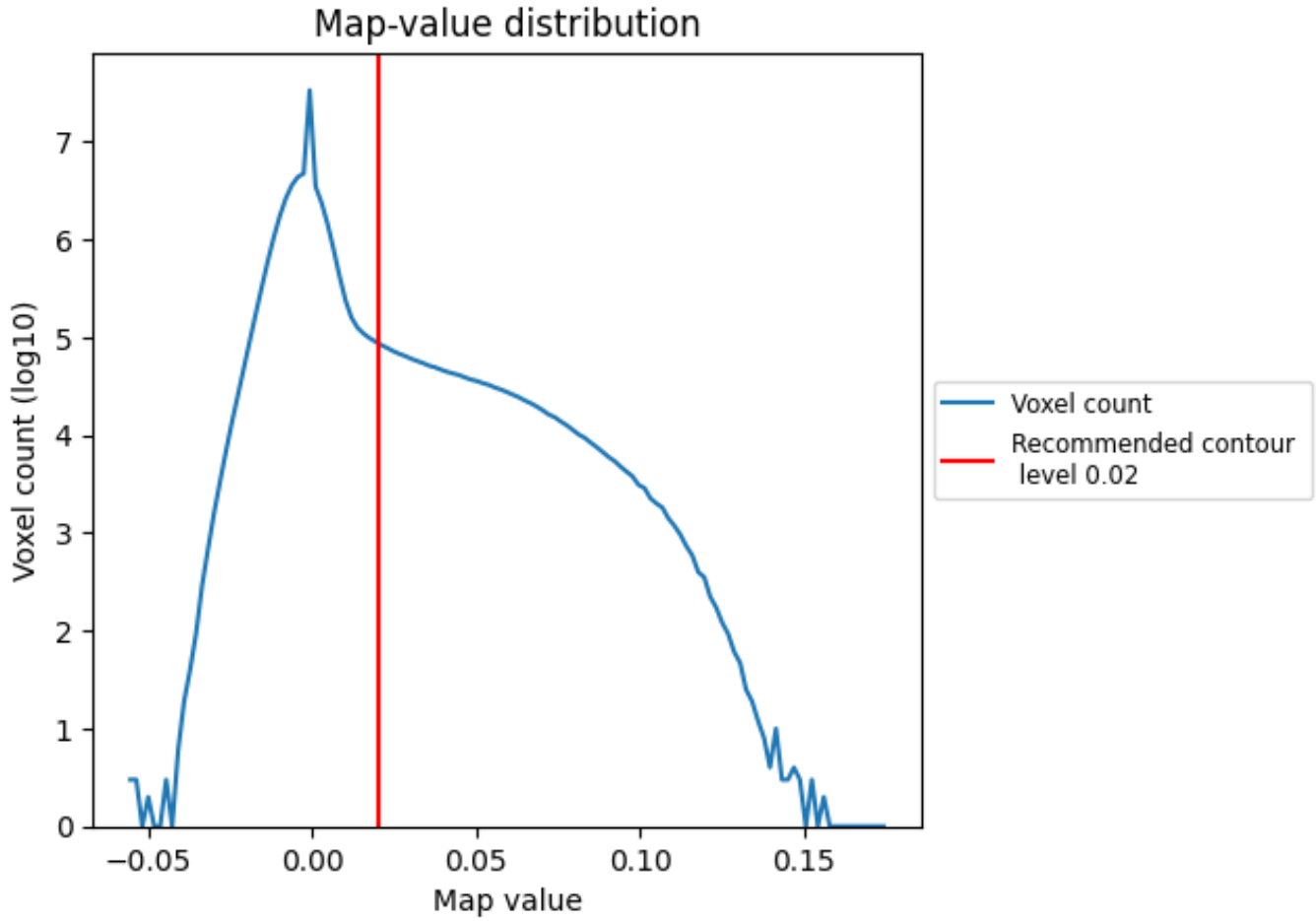


Z

7 Map analysis

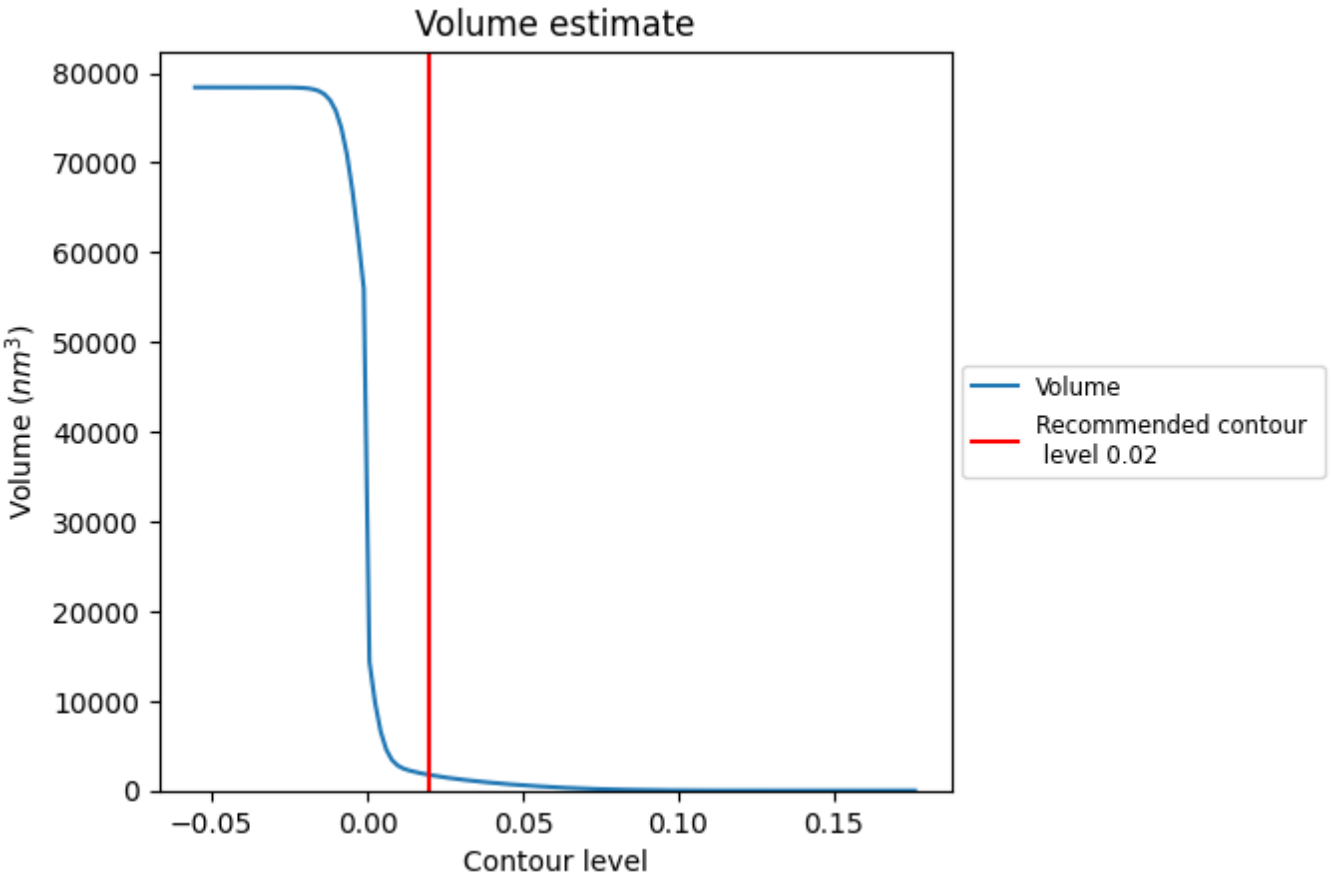
This section contains the results of statistical analysis of the map.

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.

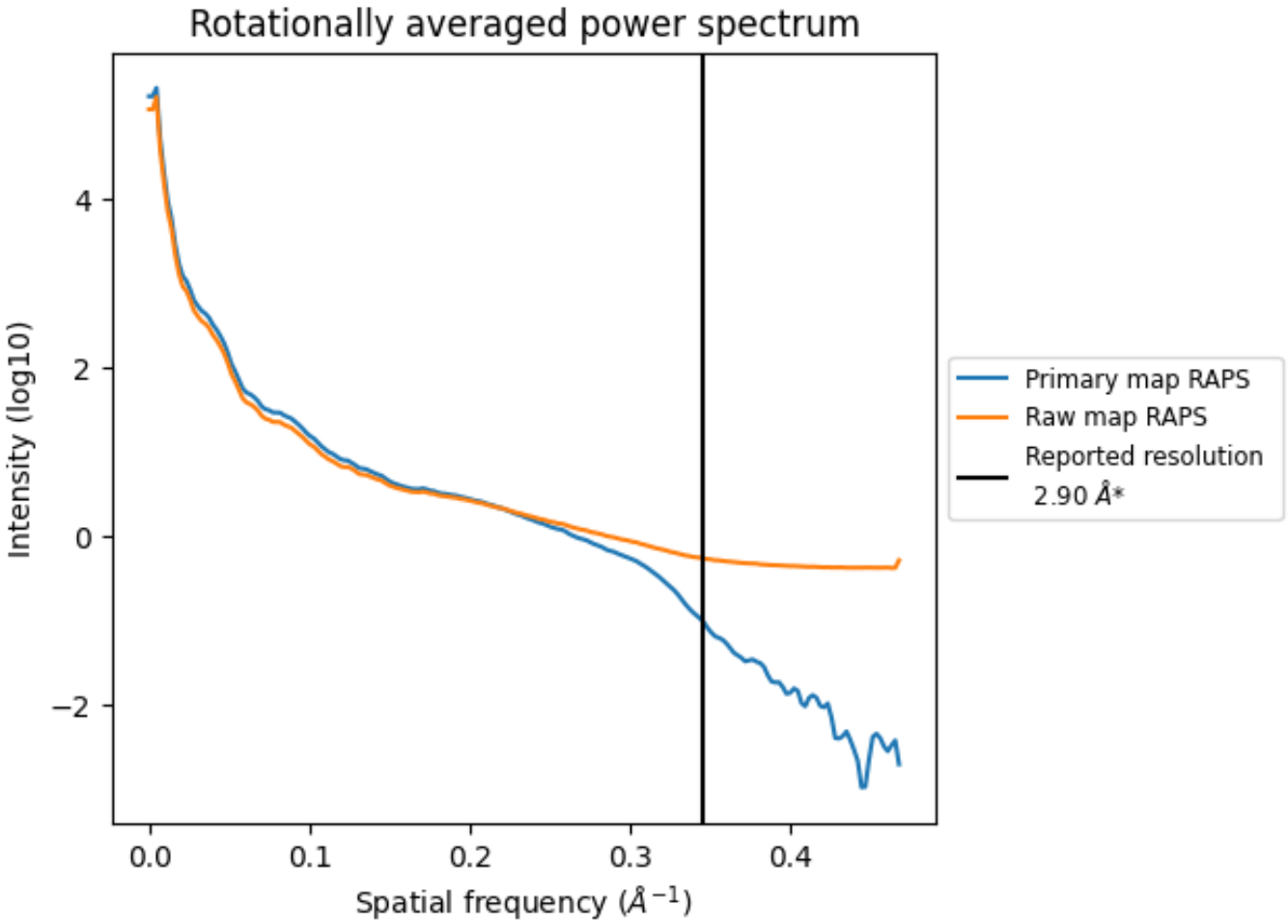
7.2 Volume estimate (i)



The volume at the recommended contour level is 1746 nm^3; this corresponds to an approximate mass of 1577 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)

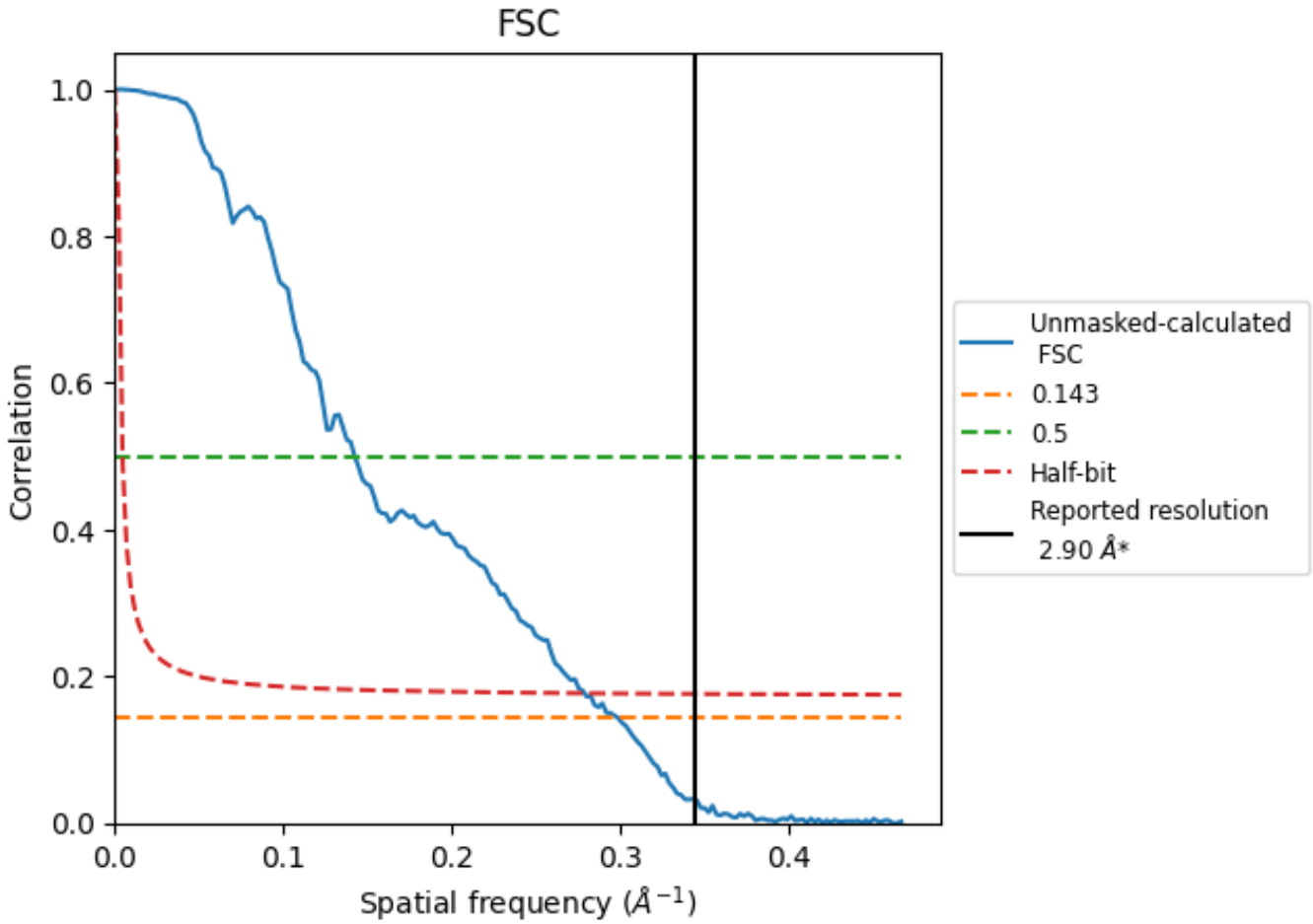


*Reported resolution corresponds to spatial frequency of 0.345 $Å^{-1}$

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 0.345 Å^{-1}

8.2 Resolution estimates (i)

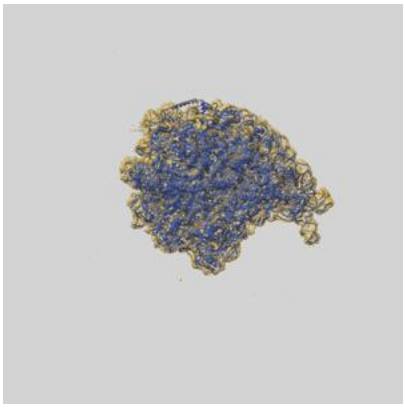
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.34	7.01	3.58

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.34 differs from the reported value 2.9 by more than 10 %

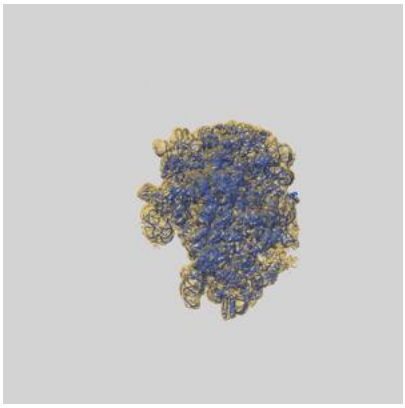
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-13055 and PDB model 7OT5. Per-residue inclusion information can be found in section 3 on page 14.

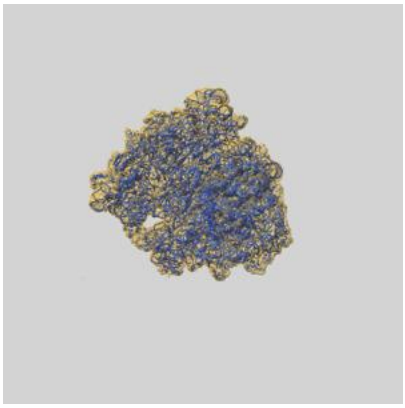
9.1 Map-model overlay



X



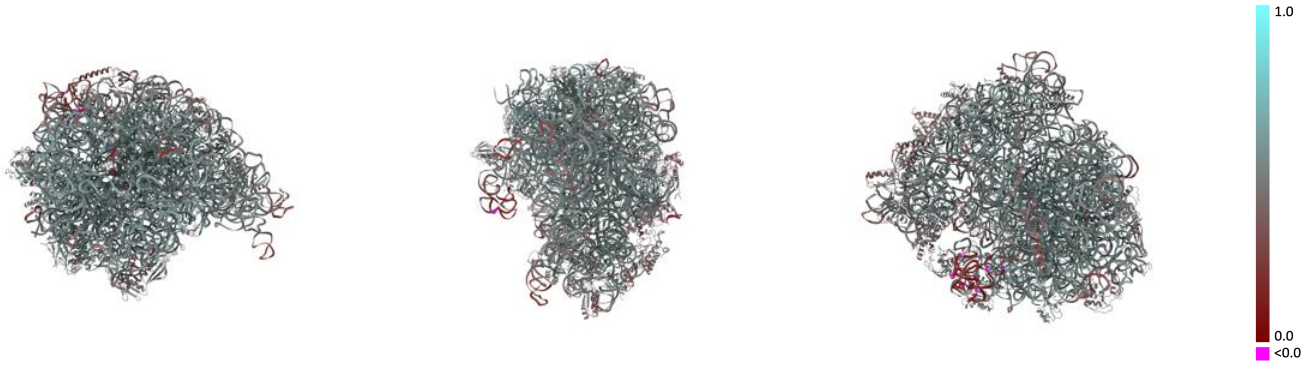
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.02 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.

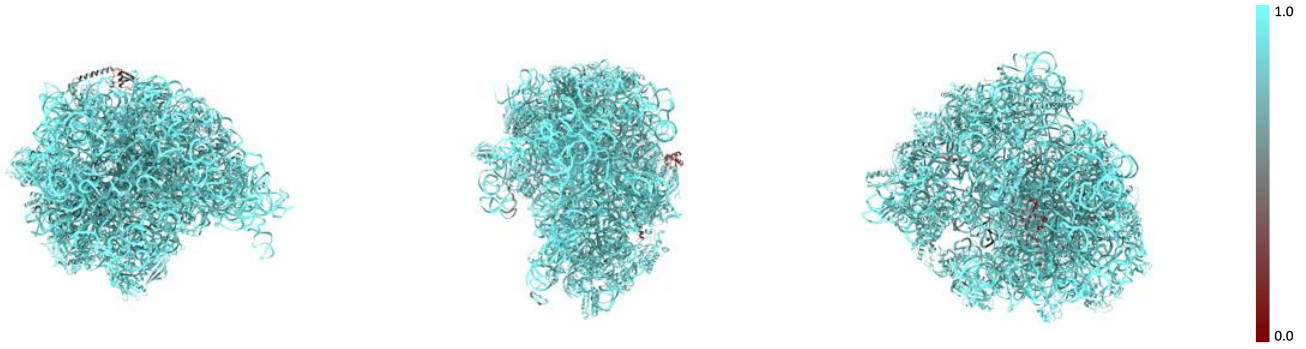
9.2 Q-score mapped to coordinate model



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.

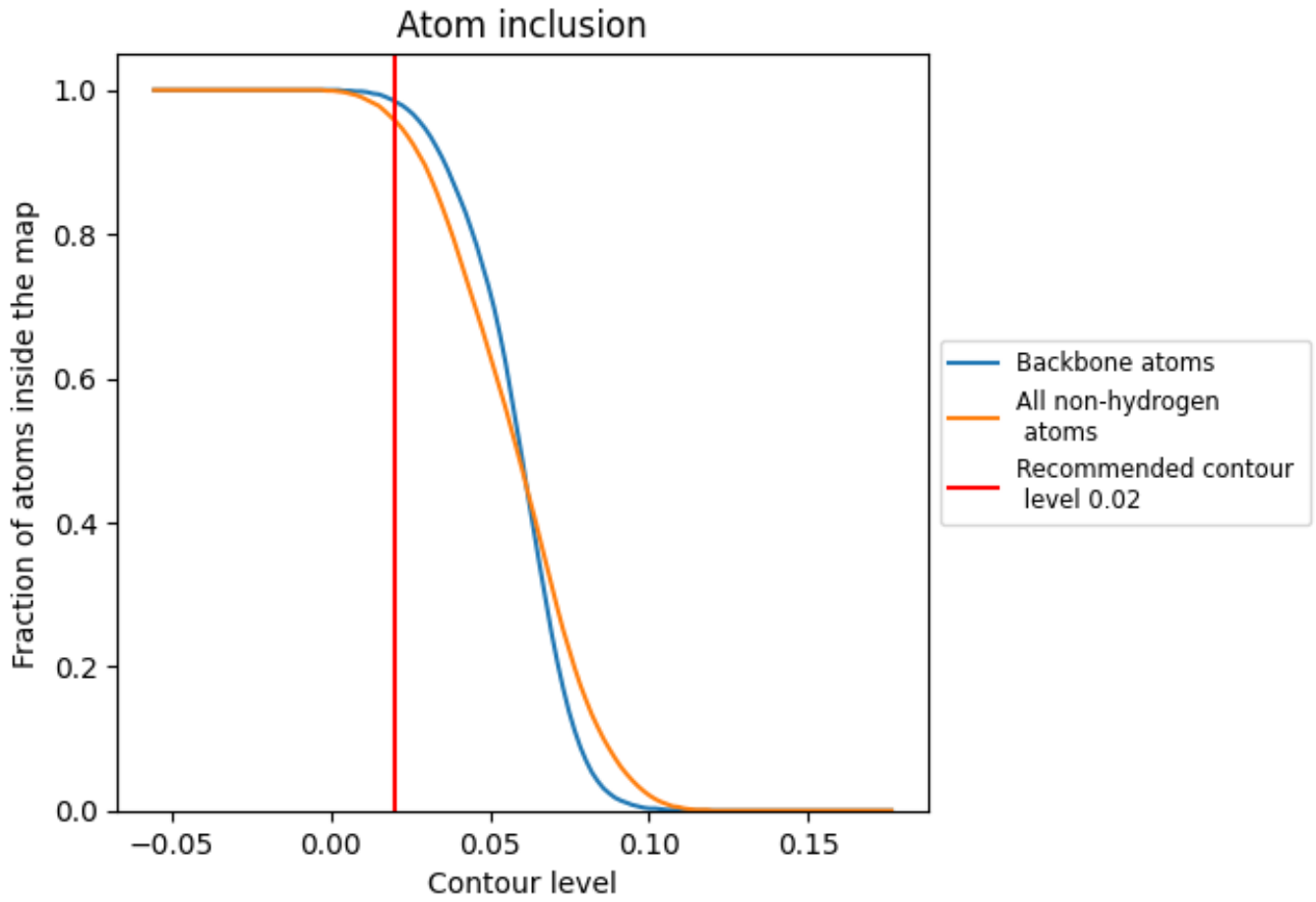
9.3 Atom inclusion mapped to coordinate model



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 (0.02).

9.4 Atom inclusion (i)



At the recommended contour level, 98% of all backbone atoms, 96% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9580	0.5150
1	0.9880	0.5290
2	0.9940	0.5210
3	0.9970	0.5180
4	1.0000	0.5110
B	0.7870	0.2210
C	0.9090	0.5600
D	0.9260	0.5480
E	0.9180	0.5130
F	0.8940	0.4580
G	0.9210	0.4640
H	0.4720	0.3550
I	0.9140	0.5370
J	0.8720	0.5360
K	0.9160	0.5330
L	0.8930	0.5340
M	0.9430	0.5470
N	0.9320	0.4880
O	0.9030	0.5330
P	0.9350	0.5340
Q	0.9270	0.5290
R	0.8890	0.5230
S	0.8750	0.5100
T	0.9160	0.5060
U	0.9130	0.5130
V	0.8840	0.5480
W	0.9080	0.5320
X	0.8790	0.4560
Y	0.9010	0.5240
Z	0.8710	0.4060
a	0.8880	0.5340
b	0.8470	0.5070
c	0.8930	0.5690
d	0.9230	0.5690
e	0.9040	0.5310

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Chain	Atom inclusion	Q-score
f	0.8460	0.4240
g	0.8930	0.4770
h	0.9060	0.4780
i	0.9050	0.5160
j	0.9030	0.4690
k	0.8620	0.4420
l	0.9010	0.5080
m	0.9110	0.4710
n	0.8540	0.4370
o	0.9050	0.4830
p	0.8700	0.5220
q	0.9060	0.4610
r	0.9160	0.4880
s	0.9040	0.4780
t	0.9220	0.4930
u	0.8720	0.4880
v	0.9010	0.4870
w	0.9290	0.4750
x	0.9050	0.4740
y	0.7370	0.4060
z	0.9560	0.4630