Full wwPDB EM Validation Report (i)

May 27, 2024 – 06:24 AM EDT

PDB ID	:	7ST6
EMDB ID	:	EMD-25420
Title	:	Pre translocation, non-rotated 70S ribosome (Structure I)
Authors	:	Carbone, C.E.; Korostelev, A.A.
Deposited on	:	2021-11-12
Resolution	:	3.00 Å(reported)

This is a Full wwPDB EM Validation 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:

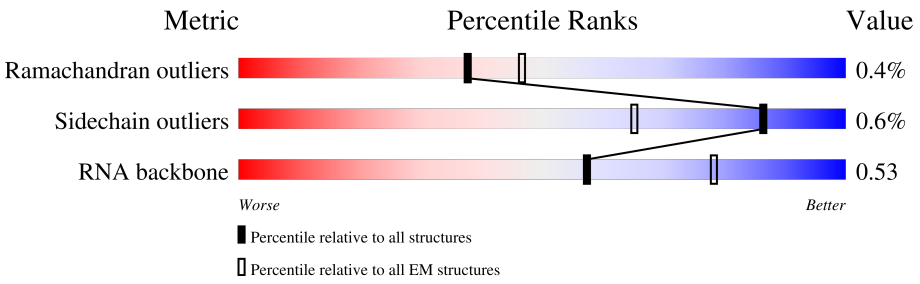
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (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 3.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	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	3	1539	82% 17% •
2	1	2903	85% 14%
3	2	120	82% 15% •
4	5	77	68% 29% •
5	6	77	82% 16% •
5	7	77	56% 62% 34% •
6	b	271	100%
7	c	209	100%

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Mol	Chain	Length	Quality of chain
8	d	201	98%
9	e	177	98%
10	f	176	99%
11	g	149	33% 65%
12	i	142	20% 99%
13	j	142	100%
14	k	122	100%
15	l	143	100%
16	m	136	97%
17	n	120	97%
18	o	116	100%
19	p	114	99%
20	q	117	97%
21	r	103	98%
22	s	110	99%
23	t	93	100%
24	u	102	98%
25	v	94	100%
26	w	75	100%
27	x	77	99%
28	y	63	100%
29	z	58	98%
30	A	66	100%
31	B	56	96%
32	C	50	100%

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Mol	Chain	Length	Quality of chain
33	D	46	100%
34	E	64	97%
35	F	38	97%
36	4	35	40% 9% 49%
37	G	225	96%
38	H	206	99%
39	I	205	99%
40	J	157	98%
41	K	100	98%
42	L	151	100%
43	M	129	100%
44	N	127	97%
45	O	98	98%
46	P	116	97%
47	Q	123	98%
48	R	114	99%
49	S	100	100%
50	T	88	99%
51	U	82	100%
52	V	80	99%
53	W	65	94% 6%
54	X	79	99%
55	Y	85	100%
56	Z	65	91% 9%

2 Entry composition (i)

There are 57 unique types of molecules in this entry. The entry contains 147982 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 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	3	1539	33012	14725	6052	10697	1538	0	0

- Molecule 2 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	1	2903	62317	27801	11468	20146	2902	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	747	C	U	conflict	GB 802133627

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	2	120	2568	1145	471	833	119	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2	120	A	-	insertion	GB 1266961702

- Molecule 4 is a RNA chain called tRNA Pro.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
4	5	77	1647	733	295	542	77	0	0

- Molecule 5 is a RNA chain called tRNA fMet.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
5	7	77	1640	732	297	535	76	0	0
5	6	77	1640	732	297	535	76	0	0

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	f	176	1323	832	243	246	2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	g	52	400	256	73	70	1	0	0

- Molecule 12 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	i	141	1032	651	179	196	6	0	0

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	k	122	939	587	180	166	6	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	l	143	1045	649	206	189	1	0	0

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	n	120	961	593	196	167	5	0	0

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	t	93	739	466	139	132	2	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
24	u	102	780	492	146	142	0	0

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

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

- Molecule 26 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	w	75	575	356	116	102	1	0	0

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	y	63	509	313	99	95	2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	z	58	449	281	87	79	2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	A	66	523	323	99	95	6	0	0

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

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

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
32	C	50	410	263	75	72	0	0

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

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

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

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

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

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

- Molecule 36 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
36	4	18	390	176	80	117	17	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	G	218	1705	1081	305	312	7	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
38	H	206	1625	1028	305	289	3	0	0

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
40	J	157	1157	719	218	214	6	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
41	K	100	818	515	148	149	6	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
42	L	151	1182	735	227	216	4	0	0

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
45	O	98	787	493	150	143	1	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
46	P	116	870	535	173	159	3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
47	Q	123	955	590	196	165	4	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
48	R	114	884	546	178	157	3	0	0

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
53	W	65	536	339	100	96	1	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
54	X	79	638	408	120	108	2	0	0

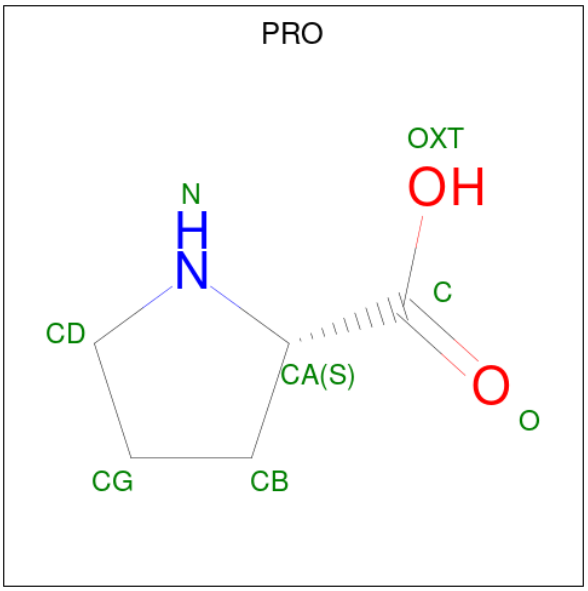
- Molecule 55 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
55	Y	85	665	411	137	114	3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
56	Z	65	545	335	117	92	1	0	0

- Molecule 57 is PROLINE (three-letter code: PRO) (formula: $C_5H_9NO_2$).



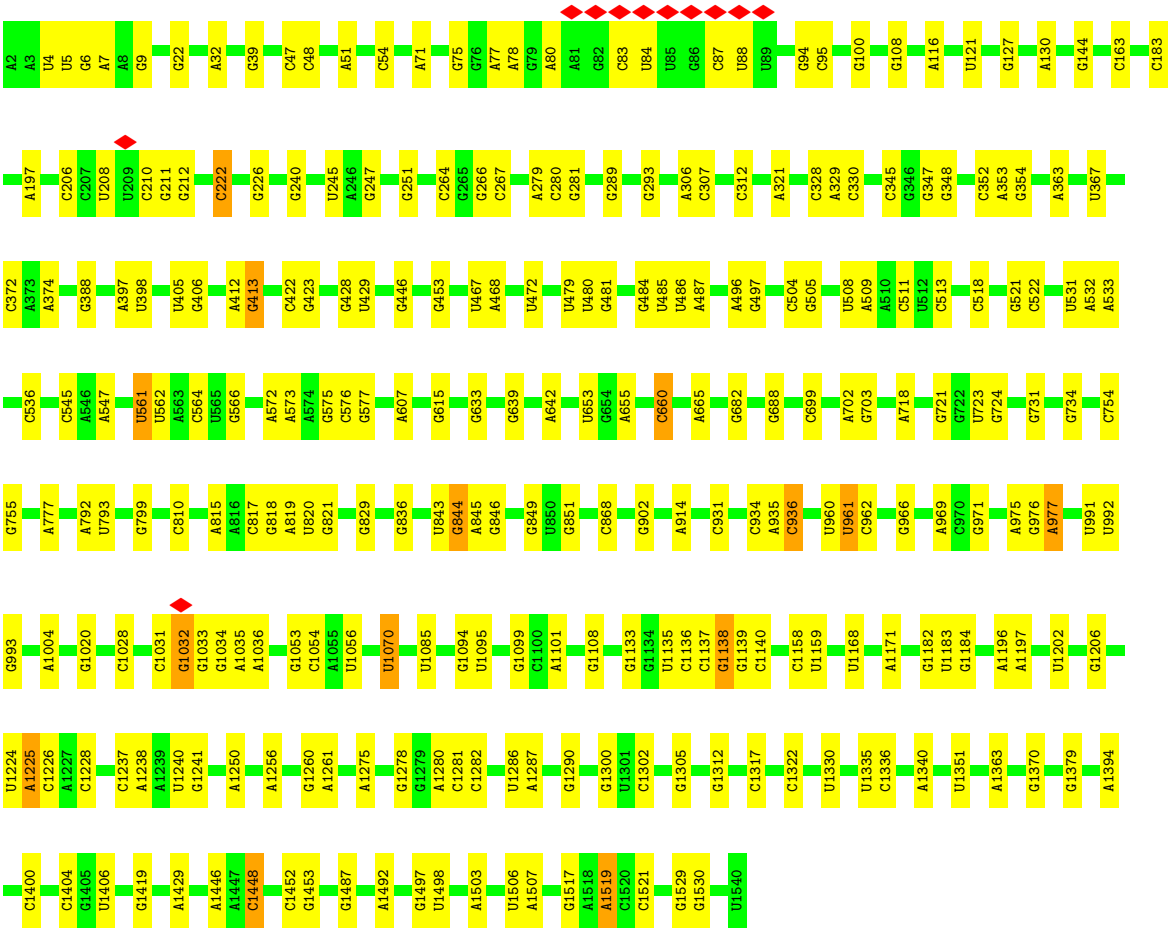
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
57	5	1	7	5	1	1	0

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.

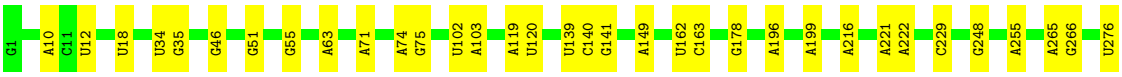
- Molecule 1: 16S rRNA

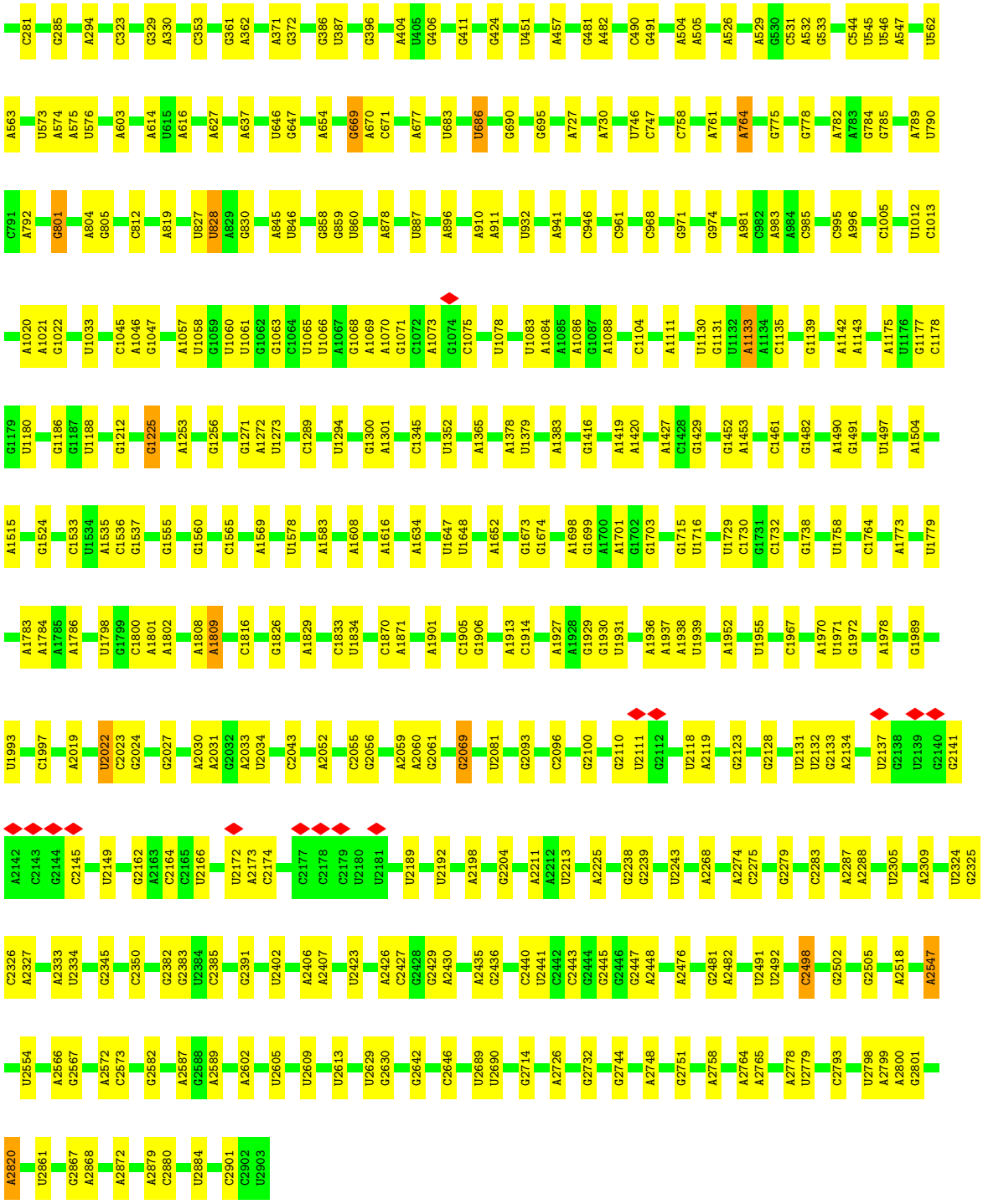
Chain 3:



- Molecule 2: 23S rRNA

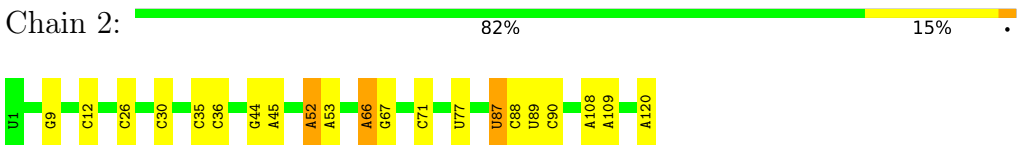
Chain 1:





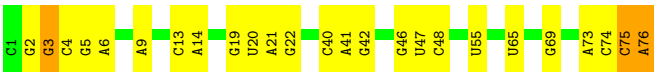
- Molecule 3: 5S rRNA

Chain 2:



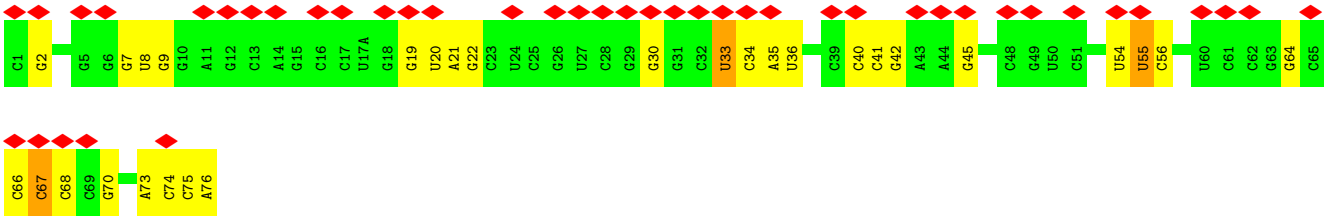
- Molecule 4: tRNA Pro

Chain 5: 68% 29%



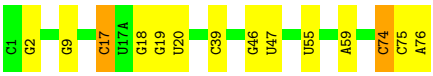
• Molecule 5: tRNA fMet

Chain 7: 56% 62% 34%



• Molecule 5: tRNA fMet

Chain 6: 82% 16%



• Molecule 6: 50S ribosomal protein L2

Chain b: 100%

• Molecule 7: 50S ribosomal protein L3

Chain c: 100%

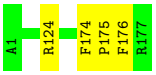
There are no outlier residues recorded for this chain.

• Molecule 8: 50S ribosomal protein L4

Chain d: 98%

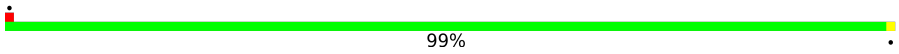
• Molecule 9: 50S ribosomal protein L5

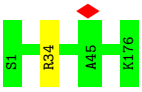
Chain e: 98%



- Molecule 10: 50S ribosomal protein L6

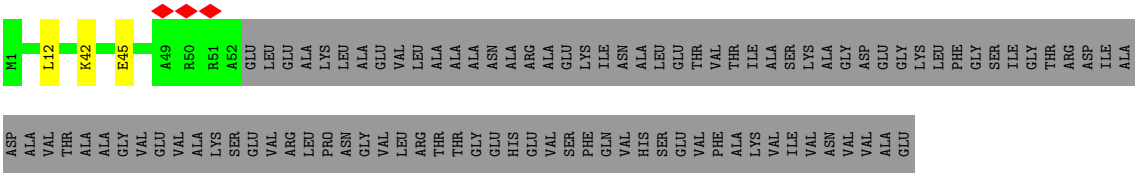
Chain f:





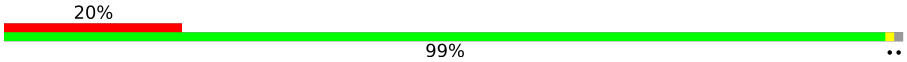
- Molecule 11: 50S ribosomal protein L9

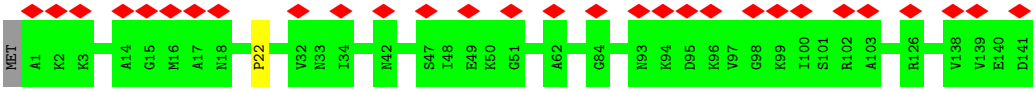
Chain g:



- Molecule 12: 50S ribosomal protein L11

Chain i:





- Molecule 13: 50S ribosomal protein L13

Chain j:

There are no outlier residues recorded for this chain.

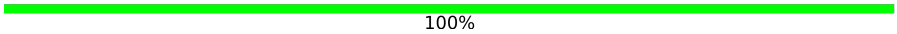
- Molecule 14: 50S ribosomal protein L14

Chain k:

There are no outlier residues recorded for this chain.

- Molecule 15: 50S ribosomal protein L15

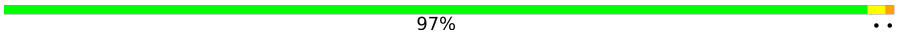
Chain l:

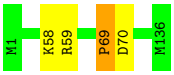


There are no outlier residues recorded for this chain.

- Molecule 16: 50S ribosomal protein L16

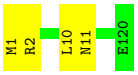
Chain m:





- Molecule 17: 50S ribosomal protein L17

Chain n: 97%



• Molecule 18: 50S ribosomal protein L18

Chain o: 100%

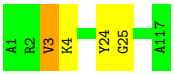
There are no outlier residues recorded for this chain.

• Molecule 19: 50S ribosomal protein L19

Chain p: 99%

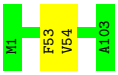
• Molecule 20: 50S ribosomal protein L20

Chain q: 97%



• Molecule 21: 50S ribosomal protein L21

Chain r: 98%



• Molecule 22: 50S ribosomal protein L22

Chain s: 99%

• Molecule 23: 50S ribosomal protein L23

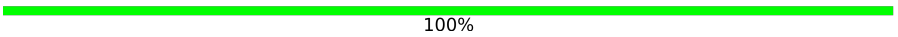
Chain t: 100%

There are no outlier residues recorded for this chain.

• Molecule 24: 50S ribosomal protein L24

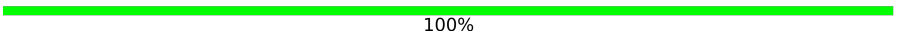
Chain u: 98%

• Molecule 25: 50S ribosomal protein L25

Chain v: 

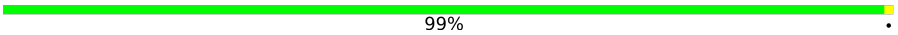
There are no outlier residues recorded for this chain.

• Molecule 26: 50S ribosomal protein L27

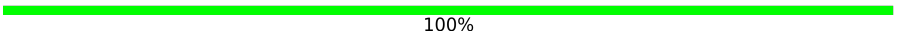
Chain w: 

There are no outlier residues recorded for this chain.

• Molecule 27: 50S ribosomal protein L28

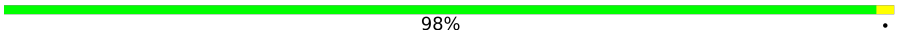
Chain x: 

• Molecule 28: 50S ribosomal protein L29

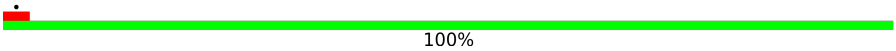
Chain y: 

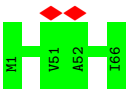
There are no outlier residues recorded for this chain.

• Molecule 29: 50S ribosomal protein L30

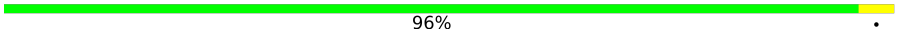
Chain z: 

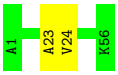
• Molecule 30: 50S ribosomal protein L31

Chain A: 



• Molecule 31: 50S ribosomal protein L32

Chain B: 



• Molecule 32: 50S ribosomal protein L33

Chain C: 100%

There are no outlier residues recorded for this chain.

• Molecule 33: 50S ribosomal protein L34

Chain D: 100%

There are no outlier residues recorded for this chain.

• Molecule 34: 50S ribosomal protein L35

Chain E: 97%

P1 H30 I31 A64

• Molecule 35: 50S ribosomal protein L36

Chain F: 97%

M1 R36 Q37 G38

• Molecule 36: mRNA

Chain 4: 40% 9% 49%

A5 A12 A13 G18 C19 A22 G U U C U A A A A A A A A A A

• Molecule 37: 30S ribosomal protein S2

Chain G: 96%

ALA THR VAL SER MET ARG ASP M8 H14 F29 R94 L128 S225

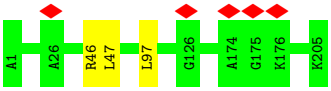
• Molecule 38: 30S ribosomal protein S3

Chain H: 99%

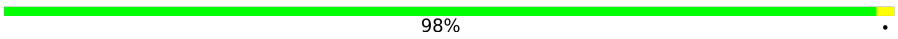
G1 K44 K79 R106 L156 T164 I206

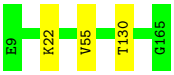
• Molecule 39: 30S ribosomal protein S4

Chain I: 99%

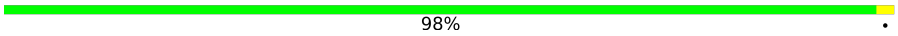


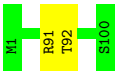
• Molecule 40: 30S ribosomal protein S5

Chain J: 

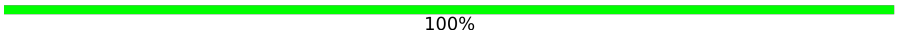


• Molecule 41: 30S ribosomal protein S6

Chain K: 

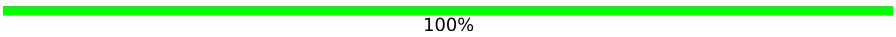


• Molecule 42: 30S ribosomal protein S7

Chain L: 

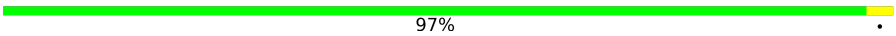
There are no outlier residues recorded for this chain.

• Molecule 43: 30S ribosomal protein S8

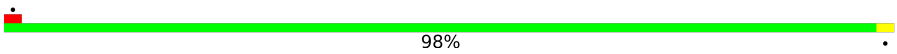
Chain M: 

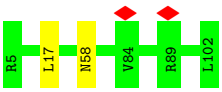
There are no outlier residues recorded for this chain.

• Molecule 44: 30S ribosomal protein S9

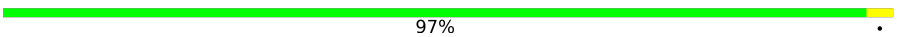
Chain N: 

• Molecule 45: 30S ribosomal protein S10

Chain O: 

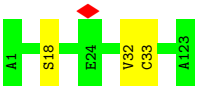


• Molecule 46: 30S ribosomal protein S11

Chain P: 

• Molecule 47: 30S ribosomal protein S12

Chain Q: 98%



• Molecule 48: 30S ribosomal protein S13

Chain R: 99%

• Molecule 49: 30S ribosomal protein S14

Chain S: 100%

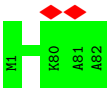
There are no outlier residues recorded for this chain.

• Molecule 50: 30S ribosomal protein S15

Chain T: 99%

• Molecule 51: 30S ribosomal protein S16

Chain U: 100%



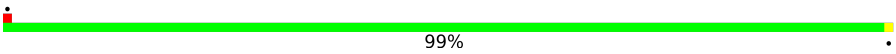
• Molecule 52: 30S ribosomal protein S17

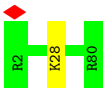
Chain V: 99%

• Molecule 53: 30S ribosomal protein S18

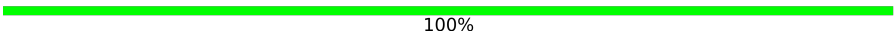
Chain W: 94% 6%

• Molecule 54: 30S ribosomal protein S19

Chain X: 



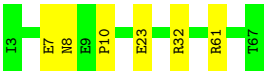
• Molecule 55: 30S ribosomal protein S20

Chain Y: 

There are no outlier residues recorded for this chain.

• Molecule 56: 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	37252	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	40.2	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	14.154	Depositor
Minimum map value	-4.209	Depositor
Average map value	0.009	Depositor
Map value standard deviation	0.866	Depositor
Recommended contour level	1.35	Depositor
Map size (Å)	381.8, 381.8, 381.8	wwPDB
Map dimensions	460, 460, 460	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83, 0.83, 0.83	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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	3	0.82	0/36963	1.01	59/57662 (0.1%)
2	1	0.51	3/69796 (0.0%)	0.73	15/108888 (0.0%)
3	2	0.79	0/2872	1.05	15/4479 (0.3%)
4	5	0.68	0/1840	1.10	11/2868 (0.4%)
5	6	0.74	0/1832	1.38	14/2855 (0.5%)
5	7	0.53	1/1832 (0.1%)	1.15	18/2855 (0.6%)
6	b	0.50	0/2122	0.59	0/2852
7	c	0.46	0/1586	0.59	0/2134
8	d	0.41	0/1571	0.60	1/2113 (0.0%)
9	e	0.41	0/1435	0.58	0/1926
10	f	0.35	0/1343	0.55	0/1816
11	g	0.38	0/405	0.68	0/544
12	i	0.33	0/1046	0.68	0/1410
13	j	0.45	0/1152	0.54	0/1551
14	k	0.46	0/948	0.61	0/1268
15	l	0.45	0/1054	0.58	0/1403
16	m	0.48	0/1093	0.62	1/1460 (0.1%)
17	n	0.41	0/974	0.59	0/1301
18	o	0.36	0/902	0.52	0/1209
19	p	0.46	0/929	0.57	0/1242
20	q	0.49	0/960	0.56	0/1278
21	r	0.45	0/829	0.60	0/1107
22	s	0.41	0/864	0.55	0/1156
23	t	0.38	0/745	0.53	0/994
24	u	0.35	0/788	0.63	0/1051
25	v	0.40	0/766	0.55	0/1025
26	w	0.43	0/582	0.53	0/769
27	x	0.43	0/635	0.57	0/848
28	y	0.32	0/510	0.60	0/677
29	z	0.39	0/453	0.55	0/605
30	A	0.33	0/532	0.52	0/709
31	B	0.43	0/450	0.57	0/599
32	C	0.34	0/417	0.55	0/554
33	D	0.46	0/380	0.59	0/498

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
34	E	0.45	0/513	0.59	0/676
35	F	0.45	0/303	0.64	0/397
36	4	0.78	0/439	0.87	1/684 (0.1%)
37	G	0.34	0/1736	0.58	0/2338
38	H	0.39	0/1652	0.54	0/2225
39	I	0.34	0/1665	0.64	2/2227 (0.1%)
40	J	0.41	0/1170	0.62	0/1573
41	K	0.36	0/836	0.63	0/1128
42	L	0.33	0/1196	0.56	0/1602
43	M	0.41	0/989	0.57	0/1326
44	N	0.35	0/1034	0.63	0/1375
45	O	0.34	0/797	0.65	1/1077 (0.1%)
46	P	0.40	0/886	0.61	0/1195
47	Q	0.40	0/969	0.73	0/1300
48	R	0.35	0/893	0.65	0/1193
49	S	0.35	0/817	0.56	0/1088
50	T	0.37	0/722	0.56	0/964
51	U	0.34	0/659	0.63	0/884
52	V	0.37	0/658	0.59	0/881
53	W	0.39	0/545	0.61	0/731
54	X	0.33	0/653	0.60	0/877
55	Y	0.31	0/671	0.50	0/888
56	Z	0.37	0/551	0.72	0/728
All	All	0.58	4/160960 (0.0%)	0.81	138/241063 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	3	1	0
2	1	0	40
4	5	2	0
5	7	1	0
6	b	0	1
8	d	0	1
9	e	0	1
16	m	0	1
17	n	0	1
20	q	0	2
21	r	0	2

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
24	u	0	1
34	E	0	1
35	F	0	1
37	G	0	1
39	I	0	1
41	K	0	1
44	N	0	1
46	P	0	1
47	Q	0	2
50	T	0	1
52	V	0	1
53	W	0	2
56	Z	0	2
All	All	4	65

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	1	2587	A	O3'-P	10.33	1.73	1.61
2	1	2059	A	O3'-P	-6.63	1.53	1.61
5	7	54	U	C3'-O3'	5.32	1.49	1.42
2	1	2589	A	N9-C4	-5.22	1.34	1.37

All (138) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	6	74	C	OP2-P-O3'	29.71	170.57	105.20
5	6	74	C	P-O3'-C3'	-24.50	90.30	119.70
5	6	74	C	OP1-P-O3'	-18.70	64.06	105.20
5	6	74	C	O3'-P-O5'	-14.65	76.16	104.00
5	7	67	C	N1-C2-O2	11.32	125.69	118.90
5	7	67	C	C2-N1-C1'	11.24	131.16	118.80
2	1	2587	A	P-O3'-C3'	-10.69	106.88	119.70
5	7	55	U	C2'-C3'-O3'	9.43	130.25	109.50
2	1	2587	A	OP2-P-O3'	8.73	124.42	105.20
1	3	1158	C	N1-C2-O2	8.46	123.97	118.90
1	3	1158	C	C2-N1-C1'	8.37	128.00	118.80
1	3	1521	C	N1-C2-O2	8.34	123.90	118.90
5	7	67	C	C6-N1-C1'	-8.22	110.93	120.80
5	7	67	C	N3-C2-O2	-8.18	116.18	121.90
3	2	26	C	N1-C2-O2	8.03	123.72	118.90
1	3	1032	G	C2'-C3'-O3'	8.01	127.11	109.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	3	844	G	N3-C4-C5	-7.94	124.63	128.60
1	3	844	G	C4-N9-C1'	7.86	136.72	126.50
5	7	41	C	N1-C2-O2	7.42	123.35	118.90
1	3	844	G	N3-C4-N9	7.32	130.39	126.00
1	3	522	C	N1-C2-O2	7.32	123.29	118.90
1	3	936	C	N1-C2-O2	7.20	123.22	118.90
8	d	116	ASP	CB-CG-OD2	7.05	124.65	118.30
1	3	1519	A	N7-C8-N9	6.98	117.29	113.80
3	2	87	U	N1-C2-O2	6.98	127.68	122.80
5	6	17	C	C5-C6-N1	6.97	124.49	121.00
1	3	1158	C	N3-C2-O2	-6.93	117.05	121.90
4	5	76	A	C4'-C3'-O3'	6.88	126.76	113.00
1	3	522	C	N3-C2-O2	-6.82	117.12	121.90
3	2	26	C	C2-N1-C1'	6.71	126.19	118.80
3	2	87	U	C2-N1-C1'	6.67	125.71	117.70
5	7	67	C	C6-N1-C2	-6.61	117.66	120.30
4	5	55	U	C2-N1-C1'	6.60	125.62	117.70
5	7	41	C	N3-C2-O2	-6.59	117.29	121.90
5	6	74	C	N1-C2-O2	6.58	122.85	118.90
1	3	931	C	N1-C2-O2	6.56	122.84	118.90
4	5	76	A	C2'-C3'-O3'	6.55	124.18	113.70
3	2	87	U	N3-C2-O2	-6.51	117.64	122.20
1	3	936	C	N3-C2-O2	-6.49	117.36	121.90
1	3	844	G	C8-N9-C1'	-6.46	118.60	127.00
1	3	1351	U	N1-C2-O2	6.44	127.31	122.80
3	2	26	C	N3-C2-O2	-6.43	117.40	121.90
5	6	75	C	O5'-P-OP1	-6.41	99.93	105.70
36	4	18	G	P-O3'-C3'	6.38	127.36	119.70
1	3	754	C	C2-N1-C1'	6.38	125.81	118.80
4	5	75	C	C2'-C3'-O3'	6.36	123.87	113.70
5	7	67	C	C5-C6-N1	6.35	124.18	121.00
39	I	97	LEU	CA-CB-CG	6.35	129.91	115.30
1	3	1158	C	C6-N1-C1'	-6.29	113.26	120.80
4	5	40	C	N1-C2-O2	6.28	122.67	118.90
1	3	962	C	N1-C2-O2	6.26	122.65	118.90
2	1	2324	U	N1-C1'-C2'	6.20	122.06	114.00
1	3	931	C	N3-C2-O2	-6.14	117.60	121.90
2	1	2059	A	O3'-P-O5'	-6.12	92.36	104.00
1	3	1519	A	C8-N9-C4	-6.06	103.38	105.80
5	7	66	C	C6-N1-C2	-6.02	117.89	120.30
5	7	33	U	P-O3'-C3'	5.99	126.88	119.70
1	3	699	C	N1-C2-O2	5.96	122.48	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	3	1521	C	N3-C2-O2	-5.94	117.74	121.90
4	5	3	G	P-O3'-C3'	5.94	126.83	119.70
5	6	55	U	C2-N1-C1'	5.89	124.77	117.70
1	3	307	C	N1-C2-O2	5.87	122.42	118.90
3	2	26	C	C6-N1-C2	-5.85	117.96	120.30
5	6	55	U	N3-C2-O2	-5.82	118.12	122.20
5	6	74	C	N3-C2-O2	-5.82	117.83	121.90
3	2	52	A	P-O3'-C3'	5.78	126.64	119.70
1	3	1228	C	N1-C2-O2	5.78	122.36	118.90
1	3	844	G	C2-N3-C4	5.76	114.78	111.90
2	1	746	U	N1-C1'-C2'	5.75	121.47	114.00
1	3	1330	U	N3-C2-O2	-5.73	118.19	122.20
1	3	413	G	N3-C4-C5	-5.73	125.74	128.60
2	1	686	U	N1-C1'-C2'	5.65	121.35	114.00
1	3	545	C	N1-C2-O2	5.64	122.29	118.90
5	6	55	U	N1-C2-O2	5.63	126.74	122.80
1	3	1070	U	N3-C2-O2	-5.62	118.27	122.20
1	3	1351	U	N3-C2-O2	-5.61	118.27	122.20
3	2	12	C	N1-C2-O2	5.59	122.25	118.90
1	3	561	U	C2-N1-C1'	5.57	124.38	117.70
1	3	792	A	O4'-C1'-N9	5.55	112.64	108.20
4	5	40	C	N3-C2-O2	-5.54	118.02	121.90
3	2	66	A	P-O3'-C3'	5.54	126.34	119.70
3	2	77	U	N3-C2-O2	-5.53	118.33	122.20
1	3	1140	C	N1-C2-O2	5.53	122.22	118.90
5	7	55	U	C4'-C3'-O3'	5.53	124.05	113.00
1	3	977	A	C4-N9-C1'	5.52	136.24	126.30
1	3	961	U	N3-C2-O2	-5.52	118.34	122.20
3	2	71	C	N1-C2-O2	5.50	122.20	118.90
5	6	17	C	C6-N1-C2	-5.50	118.10	120.30
16	m	69	PRO	C-N-CA	5.44	135.29	121.70
1	3	54	C	C6-N1-C2	-5.43	118.13	120.30
1	3	513	C	C6-N1-C2	-5.43	118.13	120.30
1	3	660	C	N1-C2-O2	5.42	122.15	118.90
5	6	39	C	C6-N1-C2	-5.40	118.14	120.30
1	3	561	U	N1-C2-O2	5.36	126.55	122.80
1	3	977	A	N3-C4-N9	5.36	131.69	127.40
1	3	264	C	C6-N1-C2	-5.33	118.17	120.30
2	1	1952	A	N9-C1'-C2'	5.33	120.93	114.00
2	1	727	A	N9-C1'-C2'	5.33	120.92	114.00
5	7	41	C	C2-N1-C1'	5.32	124.66	118.80
4	5	47	U	N1-C2-O2	5.31	126.52	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	1	2059	A	OP2-P-O3'	5.30	116.86	105.20
1	3	1138	G	C4-N9-C1'	5.29	133.37	126.50
1	3	1498	U	N3-C2-O2	-5.27	118.51	122.20
3	2	12	C	C2-N1-C1'	5.27	124.60	118.80
1	3	1228	C	N3-C2-O2	-5.25	118.22	121.90
1	3	1138	G	N3-C4-N9	5.25	129.15	126.00
2	1	2443	C	N1-C2-O2	5.25	122.05	118.90
1	3	504	C	C6-N1-C2	-5.25	118.20	120.30
1	3	222	C	N1-C2-O2	5.25	122.05	118.90
2	1	1133	A	O4'-C1'-N9	5.24	112.39	108.20
45	O	17	LEU	CA-CB-CG	5.23	127.33	115.30
5	7	68	C	N1-C2-O2	5.22	122.03	118.90
1	3	54	C	N1-C2-O2	5.22	122.03	118.90
5	7	55	U	OP2-P-O3'	5.22	116.68	105.20
5	7	68	C	N3-C2-O2	-5.21	118.25	121.90
1	3	810	C	N3-C2-O2	-5.21	118.25	121.90
5	7	40	C	N3-C2-O2	-5.21	118.26	121.90
1	3	961	U	N1-C2-O2	5.18	126.43	122.80
5	7	40	C	N1-C2-O2	5.18	122.01	118.90
1	3	1519	A	C5-N7-C8	-5.17	101.31	103.90
3	2	26	C	C5-C6-N1	5.17	123.58	121.00
1	3	1225	A	C4-N9-C1'	5.17	135.60	126.30
4	5	13	C	N1-C2-O2	5.17	122.00	118.90
2	1	2443	C	N3-C2-O2	-5.16	118.29	121.90
1	3	1406	U	N3-C2-O2	-5.15	118.60	122.20
5	6	74	C	C6-N1-C2	-5.15	118.24	120.30
1	3	222	C	C6-N1-C2	-5.11	118.26	120.30
2	1	669	G	N9-C1'-C2'	5.09	120.62	114.00
1	3	312	C	N1-C2-O2	5.09	121.95	118.90
4	5	47	U	N3-C2-O2	-5.09	118.64	122.20
1	3	754	C	N1-C2-O2	5.08	121.95	118.90
2	1	2820	A	N9-C1'-C2'	5.07	120.59	114.00
39	I	97	LEU	CB-CG-CD2	-5.07	102.38	111.00
1	3	1448	C	N1-C2-O2	5.07	121.94	118.90
3	2	77	U	N1-C2-O2	5.06	126.34	122.80
2	1	790	U	N1-C1'-C2'	5.05	120.56	114.00
4	5	55	U	N3-C2-O2	-5.04	118.67	122.20
1	3	1070	U	N1-C2-O2	5.03	126.32	122.80

All (4) chirality outliers are listed below:

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Mol	Chain	Res	Type	Atom
1	3	1032	G	C3'
4	5	75	C	C3'
4	5	76	A	C3'
5	7	55	U	C3'

All (65) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	1	1133	A	Sidechain
2	1	1188	U	Sidechain
2	1	1225	G	Sidechain
2	1	1652	A	Sidechain
2	1	1673	G	Sidechain
2	1	1701	A	Sidechain
2	1	1779	U	Sidechain
2	1	1798	U	Sidechain
2	1	18	U	Sidechain
2	1	1809	A	Sidechain
2	1	1826	G	Sidechain
2	1	1834	U	Sidechain
2	1	1905	C	Sidechain
2	1	1927	A	Sidechain
2	1	1978	A	Sidechain
2	1	1989	G	Sidechain
2	1	2019	A	Sidechain
2	1	2022	U	Sidechain
2	1	2024	G	Sidechain
2	1	2034	U	Sidechain
2	1	2069	G	Sidechain
2	1	2081	U	Sidechain
2	1	2274	A	Sidechain
2	1	2275	C	Sidechain
2	1	2391	G	Sidechain
2	1	2498	C	Sidechain
2	1	2547	A	Sidechain
2	1	2605	U	Sidechain
2	1	2732	G	Sidechain
2	1	562	U	Sidechain
2	1	576	U	Sidechain
2	1	683	U	Sidechain
2	1	690	G	Sidechain

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Mol	Chain	Res	Type	Group
2	1	761	A	Sidechain
2	1	764	A	Sidechain
2	1	778	G	Sidechain
2	1	801	G	Sidechain
2	1	804	A	Sidechain
2	1	828	U	Sidechain
2	1	971	G	Sidechain
34	E	30	HIS	Peptide
35	F	36	ARG	Peptide
37	G	14	HIS	Peptide
39	I	46	ARG	Peptide
41	K	91	ARG	Peptide
44	N	56	MET	Peptide
46	P	125	LYS	Peptide
47	Q	18	SER	Peptide
47	Q	32	VAL	Peptide
50	T	87	ARG	Peptide
52	V	49	ASN	Peptide
53	W	16	GLY	Peptide
53	W	19	GLU	Peptide
56	Z	23	GLU	Peptide
56	Z	7	GLU	Peptide
6	b	131	MET	Peptide
8	d	82	GLY	Peptide
9	e	174	PHE	Peptide
16	m	58	LYS	Peptide
17	n	10	LEU	Peptide
20	q	24	TYR	Peptide
20	q	3	VAL	Peptide
21	r	53	PHE	Peptide
21	r	54	VAL	Peptide
24	u	99	SER	Peptide

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	
6	b	269/271 (99%)	244 (91%)	25 (9%)	0	100	100
7	c	207/209 (99%)	190 (92%)	17 (8%)	0	100	100
8	d	199/201 (99%)	184 (92%)	15 (8%)	0	100	100
9	e	175/177 (99%)	158 (90%)	15 (9%)	2 (1%)	14	50
10	f	174/176 (99%)	158 (91%)	16 (9%)	0	100	100
11	g	50/149 (34%)	44 (88%)	5 (10%)	1 (2%)	7	34
12	i	139/142 (98%)	116 (84%)	23 (16%)	0	100	100
13	j	140/142 (99%)	128 (91%)	12 (9%)	0	100	100
14	k	120/122 (98%)	106 (88%)	14 (12%)	0	100	100
15	l	141/143 (99%)	129 (92%)	12 (8%)	0	100	100
16	m	134/136 (98%)	126 (94%)	5 (4%)	3 (2%)	6	31
17	n	118/120 (98%)	101 (86%)	16 (14%)	1 (1%)	19	57
18	o	114/116 (98%)	109 (96%)	5 (4%)	0	100	100
19	p	112/114 (98%)	103 (92%)	9 (8%)	0	100	100
20	q	115/117 (98%)	104 (90%)	8 (7%)	3 (3%)	5	27
21	r	101/103 (98%)	87 (86%)	14 (14%)	0	100	100
22	s	108/110 (98%)	100 (93%)	8 (7%)	0	100	100
23	t	91/93 (98%)	82 (90%)	9 (10%)	0	100	100
24	u	100/102 (98%)	83 (83%)	17 (17%)	0	100	100
25	v	92/94 (98%)	87 (95%)	5 (5%)	0	100	100
26	w	73/75 (97%)	67 (92%)	6 (8%)	0	100	100
27	x	75/77 (97%)	72 (96%)	2 (3%)	1 (1%)	12	45
28	y	61/63 (97%)	55 (90%)	6 (10%)	0	100	100
29	z	56/58 (97%)	52 (93%)	4 (7%)	0	100	100
30	A	64/66 (97%)	59 (92%)	5 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
31	B	54/56 (96%)	48 (89%)	4 (7%)	2 (4%)	3	19
32	C	48/50 (96%)	41 (85%)	7 (15%)	0	100	100
33	D	44/46 (96%)	42 (96%)	2 (4%)	0	100	100
34	E	62/64 (97%)	58 (94%)	3 (5%)	1 (2%)	9	40
35	F	36/38 (95%)	32 (89%)	4 (11%)	0	100	100
37	G	216/225 (96%)	189 (88%)	27 (12%)	0	100	100
38	H	204/206 (99%)	194 (95%)	10 (5%)	0	100	100
39	I	203/205 (99%)	172 (85%)	31 (15%)	0	100	100
40	J	155/157 (99%)	138 (89%)	17 (11%)	0	100	100
41	K	98/100 (98%)	83 (85%)	14 (14%)	1 (1%)	15	53
42	L	149/151 (99%)	130 (87%)	19 (13%)	0	100	100
43	M	127/129 (98%)	118 (93%)	9 (7%)	0	100	100
44	N	125/127 (98%)	102 (82%)	23 (18%)	0	100	100
45	O	96/98 (98%)	84 (88%)	11 (12%)	1 (1%)	15	53
46	P	114/116 (98%)	98 (86%)	14 (12%)	2 (2%)	8	37
47	Q	121/123 (98%)	90 (74%)	30 (25%)	1 (1%)	19	57
48	R	112/114 (98%)	99 (88%)	12 (11%)	1 (1%)	17	55
49	S	98/100 (98%)	83 (85%)	15 (15%)	0	100	100
50	T	86/88 (98%)	76 (88%)	10 (12%)	0	100	100
51	U	80/82 (98%)	69 (86%)	11 (14%)	0	100	100
52	V	78/80 (98%)	67 (86%)	11 (14%)	0	100	100
53	W	63/65 (97%)	53 (84%)	9 (14%)	1 (2%)	9	40
54	X	77/79 (98%)	71 (92%)	6 (8%)	0	100	100
55	Y	83/85 (98%)	78 (94%)	5 (6%)	0	100	100
56	Z	63/65 (97%)	43 (68%)	18 (29%)	2 (3%)	4	22
All	All	5620/5825 (96%)	5002 (89%)	595 (11%)	23 (0%)	38	72

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	e	175	PRO
17	n	11	ASN
27	x	25	LYS

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Mol	Chain	Res	Type
9	e	176	PHE
16	m	70	ASP
20	q	4	LYS
53	W	13	THR
16	m	69	PRO
41	K	92	THR
11	g	12	LEU
16	m	59	ARG
31	B	23	ALA
34	E	31	ILE
48	R	5	GLY
56	Z	8	ASN
45	O	58	ASN
46	P	126	ARG
47	Q	33	CYS
20	q	3	VAL
20	q	25	GLY
56	Z	10	PRO
31	B	24	VAL
46	P	88	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	
6	b	216/216 (100%)	216 (100%)	0	100	100
7	c	164/164 (100%)	164 (100%)	0	100	100
8	d	165/165 (100%)	163 (99%)	2 (1%)	71	90
9	e	148/148 (100%)	147 (99%)	1 (1%)	84	94
10	f	137/137 (100%)	136 (99%)	1 (1%)	84	94
11	g	41/114 (36%)	39 (95%)	2 (5%)	25	61
12	i	109/110 (99%)	108 (99%)	1 (1%)	78	92
13	j	116/116 (100%)	116 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	k	103/103 (100%)	103 (100%)	0	100	100
15	l	102/102 (100%)	102 (100%)	0	100	100
16	m	109/109 (100%)	109 (100%)	0	100	100
17	n	100/100 (100%)	98 (98%)	2 (2%)	55	83
18	o	86/86 (100%)	86 (100%)	0	100	100
19	p	99/99 (100%)	98 (99%)	1 (1%)	76	91
20	q	89/89 (100%)	89 (100%)	0	100	100
21	r	84/84 (100%)	84 (100%)	0	100	100
22	s	93/93 (100%)	92 (99%)	1 (1%)	73	90
23	t	80/80 (100%)	80 (100%)	0	100	100
24	u	83/83 (100%)	82 (99%)	1 (1%)	71	90
25	v	78/78 (100%)	78 (100%)	0	100	100
26	w	57/57 (100%)	57 (100%)	0	100	100
27	x	67/67 (100%)	67 (100%)	0	100	100
28	y	55/55 (100%)	55 (100%)	0	100	100
29	z	48/48 (100%)	47 (98%)	1 (2%)	53	82
30	A	59/59 (100%)	59 (100%)	0	100	100
31	B	47/47 (100%)	47 (100%)	0	100	100
32	C	45/45 (100%)	45 (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
37	G	180/186 (97%)	179 (99%)	1 (1%)	86	95
38	H	170/170 (100%)	167 (98%)	3 (2%)	59	85
39	I	172/172 (100%)	171 (99%)	1 (1%)	86	95
40	J	119/119 (100%)	116 (98%)	3 (2%)	47	79
41	K	87/87 (100%)	87 (100%)	0	100	100
42	L	124/124 (100%)	124 (100%)	0	100	100
43	M	104/104 (100%)	104 (100%)	0	100	100
44	N	105/105 (100%)	102 (97%)	3 (3%)	42	76
45	O	86/86 (100%)	86 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
46	P	89/89 (100%)	89 (100%)	0	100	100
47	Q	103/103 (100%)	103 (100%)	0	100	100
48	R	92/92 (100%)	92 (100%)	0	100	100
49	S	83/83 (100%)	83 (100%)	0	100	100
50	T	76/76 (100%)	76 (100%)	0	100	100
51	U	65/65 (100%)	65 (100%)	0	100	100
52	V	74/74 (100%)	74 (100%)	0	100	100
53	W	56/56 (100%)	55 (98%)	1 (2%)	59	85
54	X	70/70 (100%)	69 (99%)	1 (1%)	67	88
55	Y	65/65 (100%)	65 (100%)	0	100	100
56	Z	55/55 (100%)	53 (96%)	2 (4%)	35	70
All	All	4678/4758 (98%)	4650 (99%)	28 (1%)	86	95

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	d	14	VAL
8	d	188	MET
9	e	124	ARG
10	f	34	ARG
11	g	42	LYS
11	g	45	GLU
12	i	22	PRO
17	n	1	MET
17	n	2	ARG
19	p	52	ARG
22	s	11	ARG
24	u	35	VAL
29	z	40	THR
37	G	29	PHE
38	H	106	ARG
38	H	156	LEU
38	H	164	THR
39	I	47	LEU
40	J	22	LYS
40	J	55	VAL
40	J	130	THR
44	N	60	LEU

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Mol	Chain	Res	Type
44	N	65	THR
44	N	122	ARG
53	W	70	THR
54	X	28	LYS
56	Z	32	ARG
56	Z	61	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (63) such sidechains are listed below:

Mol	Chain	Res	Type
6	b	24	HIS
6	b	69	ASN
6	b	89	ASN
6	b	142	ASN
6	b	259	ASN
7	c	49	GLN
7	c	134	HIS
7	c	150	GLN
8	d	62	GLN
8	d	195	GLN
9	e	4	HIS
9	e	62	GLN
9	e	80	GLN
10	f	47	ASN
10	f	87	GLN
12	i	29	GLN
12	i	104	GLN
14	k	3	GLN
14	k	5	GLN
15	l	104	GLN
17	n	11	ASN
19	p	2	ASN
19	p	114	ASN
20	q	55	GLN
20	q	58	GLN
21	r	18	GLN
21	r	82	HIS
22	s	7	HIS
23	t	59	ASN
23	t	92	ASN
27	x	16	ASN
28	y	31	GLN

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Mol	Chain	Res	Type
29	z	8	GLN
30	A	20	ASN
31	B	4	GLN
31	B	5	ASN
33	D	6	GLN
33	D	16	HIS
34	E	30	HIS
35	F	37	GLN
38	H	31	ASN
38	H	122	GLN
38	H	138	GLN
38	H	139	ASN
39	I	135	GLN
39	I	197	HIS
40	J	76	ASN
40	J	121	ASN
42	L	96	ASN
43	M	3	GLN
44	N	30	ASN
45	O	58	ASN
46	P	80	ASN
47	Q	4	ASN
48	R	7	ASN
48	R	99	GLN
49	S	59	GLN
50	T	27	GLN
51	U	79	ASN
52	V	30	HIS
54	X	51	HIS
54	X	68	HIS
55	Y	69	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	3	1538/1539 (99%)	247 (16%)	3 (0%)
2	1	2902/2903 (99%)	377 (12%)	12 (0%)
3	2	119/120 (99%)	16 (13%)	2 (1%)
36	4	17/35 (48%)	3 (17%)	1 (5%)
4	5	76/77 (98%)	20 (26%)	3 (3%)
5	6	76/77 (98%)	11 (14%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
5	7	76/77 (98%)	23 (30%)	2 (2%)
All	All	4804/4828 (99%)	697 (14%)	23 (0%)

All (697) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	3	5	U
1	3	6	G
1	3	7	A
1	3	9	G
1	3	22	G
1	3	32	A
1	3	39	G
1	3	47	C
1	3	48	C
1	3	51	A
1	3	71	A
1	3	75	G
1	3	77	A
1	3	78	A
1	3	80	A
1	3	83	C
1	3	84	U
1	3	87	C
1	3	88	U
1	3	94	G
1	3	95	C
1	3	100	G
1	3	108	G
1	3	116	A
1	3	121	U
1	3	127	G
1	3	130	A
1	3	144	G
1	3	163	C
1	3	183	C
1	3	197	A
1	3	206	C
1	3	208	U
1	3	210	C
1	3	211	G
1	3	212	G

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Mol	Chain	Res	Type
1	3	222	C
1	3	226	G
1	3	240	G
1	3	245	U
1	3	247	G
1	3	251	G
1	3	266	G
1	3	267	C
1	3	279	A
1	3	280	C
1	3	281	G
1	3	289	G
1	3	293	G
1	3	306	A
1	3	321	A
1	3	328	C
1	3	329	A
1	3	330	C
1	3	345	C
1	3	347	G
1	3	348	G
1	3	352	C
1	3	353	A
1	3	354	G
1	3	363	A
1	3	367	U
1	3	372	C
1	3	374	A
1	3	388	G
1	3	397	A
1	3	398	U
1	3	405	U
1	3	406	G
1	3	412	A
1	3	413	G
1	3	422	C
1	3	423	G
1	3	428	G
1	3	429	U
1	3	446	G
1	3	453	G
1	3	467	U

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Mol	Chain	Res	Type
1	3	468	A
1	3	472	U
1	3	479	U
1	3	480	U
1	3	481	G
1	3	484	G
1	3	485	U
1	3	486	U
1	3	487	A
1	3	496	A
1	3	497	G
1	3	505	G
1	3	508	U
1	3	509	A
1	3	511	C
1	3	518	C
1	3	521	G
1	3	531	U
1	3	532	A
1	3	533	A
1	3	536	C
1	3	547	A
1	3	561	U
1	3	562	U
1	3	564	C
1	3	566	G
1	3	572	A
1	3	573	A
1	3	575	G
1	3	576	C
1	3	577	G
1	3	607	A
1	3	615	G
1	3	633	G
1	3	639	G
1	3	642	A
1	3	653	U
1	3	655	A
1	3	660	C
1	3	665	A
1	3	682	G
1	3	688	G

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Mol	Chain	Res	Type
1	3	702	A
1	3	703	G
1	3	718	A
1	3	721	G
1	3	723	U
1	3	724	G
1	3	731	G
1	3	734	G
1	3	755	G
1	3	777	A
1	3	793	U
1	3	799	G
1	3	815	A
1	3	817	C
1	3	818	G
1	3	819	A
1	3	820	U
1	3	821	G
1	3	829	G
1	3	836	G
1	3	843	U
1	3	844	G
1	3	845	A
1	3	846	G
1	3	849	G
1	3	851	G
1	3	868	C
1	3	902	G
1	3	914	A
1	3	934	C
1	3	935	A
1	3	936	C
1	3	960	U
1	3	961	U
1	3	966	G
1	3	969	A
1	3	971	G
1	3	975	A
1	3	976	G
1	3	977	A
1	3	991	U
1	3	992	U

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Mol	Chain	Res	Type
1	3	993	G
1	3	1004	A
1	3	1020	G
1	3	1028	C
1	3	1031	C
1	3	1032	G
1	3	1033	G
1	3	1034	G
1	3	1036	A
1	3	1053	G
1	3	1054	C
1	3	1056	U
1	3	1070	U
1	3	1085	U
1	3	1094	G
1	3	1095	U
1	3	1099	G
1	3	1101	A
1	3	1108	G
1	3	1133	G
1	3	1135	U
1	3	1136	C
1	3	1137	C
1	3	1138	G
1	3	1139	G
1	3	1159	U
1	3	1168	U
1	3	1171	A
1	3	1182	G
1	3	1183	U
1	3	1184	G
1	3	1196	A
1	3	1197	A
1	3	1202	U
1	3	1206	G
1	3	1224	U
1	3	1225	A
1	3	1226	C
1	3	1237	C
1	3	1238	A
1	3	1240	U
1	3	1241	G

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Mol	Chain	Res	Type
1	3	1250	A
1	3	1256	A
1	3	1260	G
1	3	1261	A
1	3	1275	A
1	3	1278	G
1	3	1280	A
1	3	1281	C
1	3	1282	C
1	3	1286	U
1	3	1287	A
1	3	1290	G
1	3	1300	G
1	3	1302	C
1	3	1305	G
1	3	1312	G
1	3	1317	C
1	3	1322	C
1	3	1335	U
1	3	1336	C
1	3	1340	A
1	3	1363	A
1	3	1370	G
1	3	1379	G
1	3	1394	A
1	3	1400	C
1	3	1404	C
1	3	1419	G
1	3	1429	A
1	3	1446	A
1	3	1448	C
1	3	1452	C
1	3	1453	G
1	3	1487	G
1	3	1492	A
1	3	1497	G
1	3	1503	A
1	3	1506	U
1	3	1507	A
1	3	1517	G
1	3	1519	A
1	3	1529	G

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Mol	Chain	Res	Type
1	3	1530	G
2	1	10	A
2	1	12	U
2	1	34	U
2	1	35	G
2	1	46	G
2	1	51	G
2	1	55	G
2	1	63	A
2	1	71	A
2	1	74	A
2	1	75	G
2	1	102	U
2	1	103	A
2	1	119	A
2	1	120	U
2	1	139	U
2	1	140	C
2	1	141	G
2	1	149	A
2	1	162	U
2	1	163	C
2	1	178	G
2	1	196	A
2	1	199	A
2	1	216	A
2	1	221	A
2	1	222	A
2	1	229	C
2	1	248	G
2	1	255	A
2	1	265	A
2	1	266	G
2	1	276	U
2	1	281	C
2	1	285	G
2	1	294	A
2	1	323	C
2	1	329	G
2	1	330	A
2	1	353	C
2	1	361	G

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Mol	Chain	Res	Type
2	1	362	A
2	1	371	A
2	1	372	G
2	1	386	G
2	1	387	U
2	1	396	G
2	1	404	A
2	1	406	G
2	1	411	G
2	1	424	G
2	1	451	U
2	1	457	A
2	1	481	G
2	1	482	A
2	1	491	G
2	1	504	A
2	1	505	A
2	1	526	A
2	1	529	A
2	1	531	C
2	1	532	A
2	1	533	G
2	1	544	C
2	1	545	U
2	1	546	U
2	1	547	A
2	1	563	A
2	1	573	U
2	1	574	A
2	1	575	A
2	1	603	A
2	1	614	A
2	1	616	A
2	1	627	A
2	1	637	A
2	1	646	U
2	1	647	G
2	1	654	A
2	1	669	G
2	1	670	A
2	1	671	C
2	1	677	A

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Mol	Chain	Res	Type
2	1	686	U
2	1	695	G
2	1	730	A
2	1	747	C
2	1	758	C
2	1	764	A
2	1	775	G
2	1	782	A
2	1	784	G
2	1	785	G
2	1	789	A
2	1	792	A
2	1	801	G
2	1	805	G
2	1	812	C
2	1	819	A
2	1	827	U
2	1	828	U
2	1	830	G
2	1	845	A
2	1	846	U
2	1	858	G
2	1	860	U
2	1	878	A
2	1	887	U
2	1	896	A
2	1	910	A
2	1	911	A
2	1	932	U
2	1	941	A
2	1	946	C
2	1	961	C
2	1	968	C
2	1	974	G
2	1	981	A
2	1	983	A
2	1	985	C
2	1	995	C
2	1	996	A
2	1	1005	C
2	1	1012	U
2	1	1013	C

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Mol	Chain	Res	Type
2	1	1021	A
2	1	1022	G
2	1	1033	U
2	1	1045	C
2	1	1046	A
2	1	1047	G
2	1	1057	A
2	1	1058	U
2	1	1060	U
2	1	1061	U
2	1	1063	G
2	1	1065	U
2	1	1066	U
2	1	1068	G
2	1	1069	A
2	1	1070	A
2	1	1071	G
2	1	1073	A
2	1	1075	C
2	1	1078	U
2	1	1083	U
2	1	1084	A
2	1	1086	A
2	1	1088	A
2	1	1104	C
2	1	1111	A
2	1	1131	G
2	1	1135	C
2	1	1139	G
2	1	1142	A
2	1	1143	A
2	1	1175	A
2	1	1177	G
2	1	1178	C
2	1	1180	U
2	1	1186	G
2	1	1212	G
2	1	1225	G
2	1	1253	A
2	1	1256	G
2	1	1271	G
2	1	1272	A

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Mol	Chain	Res	Type
2	1	1273	U
2	1	1289	C
2	1	1294	U
2	1	1300	G
2	1	1301	A
2	1	1345	C
2	1	1352	U
2	1	1365	A
2	1	1378	A
2	1	1379	U
2	1	1383	A
2	1	1416	G
2	1	1419	A
2	1	1420	A
2	1	1427	A
2	1	1429	G
2	1	1452	G
2	1	1453	A
2	1	1461	C
2	1	1482	G
2	1	1490	A
2	1	1491	G
2	1	1497	U
2	1	1504	A
2	1	1515	A
2	1	1524	G
2	1	1533	C
2	1	1535	A
2	1	1536	C
2	1	1537	G
2	1	1555	G
2	1	1560	G
2	1	1565	C
2	1	1569	A
2	1	1578	U
2	1	1583	A
2	1	1608	A
2	1	1616	A
2	1	1634	A
2	1	1647	U
2	1	1648	U
2	1	1674	G

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Mol	Chain	Res	Type
2	1	1698	A
2	1	1699	G
2	1	1703	G
2	1	1715	G
2	1	1716	U
2	1	1729	U
2	1	1730	C
2	1	1732	C
2	1	1738	G
2	1	1758	U
2	1	1764	C
2	1	1773	A
2	1	1783	A
2	1	1784	A
2	1	1786	A
2	1	1800	C
2	1	1801	A
2	1	1802	A
2	1	1808	A
2	1	1809	A
2	1	1816	C
2	1	1829	A
2	1	1833	C
2	1	1870	C
2	1	1871	A
2	1	1901	A
2	1	1906	G
2	1	1913	A
2	1	1914	C
2	1	1929	G
2	1	1931	U
2	1	1936	A
2	1	1937	A
2	1	1938	A
2	1	1939	U
2	1	1955	U
2	1	1967	C
2	1	1970	A
2	1	1971	U
2	1	1972	G
2	1	1993	U
2	1	1997	C

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Mol	Chain	Res	Type
2	1	2022	U
2	1	2023	C
2	1	2027	G
2	1	2030	A
2	1	2031	A
2	1	2033	A
2	1	2043	C
2	1	2052	A
2	1	2055	C
2	1	2056	G
2	1	2060	A
2	1	2061	G
2	1	2069	G
2	1	2093	G
2	1	2096	C
2	1	2100	G
2	1	2110	G
2	1	2111	U
2	1	2118	U
2	1	2119	A
2	1	2123	G
2	1	2128	G
2	1	2131	U
2	1	2132	U
2	1	2133	G
2	1	2134	A
2	1	2137	U
2	1	2141	G
2	1	2145	C
2	1	2149	U
2	1	2162	G
2	1	2164	C
2	1	2166	U
2	1	2172	U
2	1	2173	A
2	1	2174	C
2	1	2189	U
2	1	2192	U
2	1	2198	A
2	1	2204	G
2	1	2211	A
2	1	2213	U

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Mol	Chain	Res	Type
2	1	2225	A
2	1	2238	G
2	1	2239	G
2	1	2243	U
2	1	2268	A
2	1	2279	G
2	1	2283	C
2	1	2287	A
2	1	2288	A
2	1	2305	U
2	1	2309	A
2	1	2325	G
2	1	2326	C
2	1	2327	A
2	1	2333	A
2	1	2334	U
2	1	2345	G
2	1	2350	C
2	1	2382	G
2	1	2383	G
2	1	2385	C
2	1	2402	U
2	1	2406	A
2	1	2407	A
2	1	2423	U
2	1	2426	A
2	1	2427	C
2	1	2429	G
2	1	2430	A
2	1	2435	A
2	1	2436	G
2	1	2440	C
2	1	2441	U
2	1	2445	G
2	1	2447	G
2	1	2448	A
2	1	2476	A
2	1	2482	A
2	1	2491	U
2	1	2492	U
2	1	2498	C
2	1	2502	G

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Mol	Chain	Res	Type
2	1	2505	G
2	1	2518	A
2	1	2547	A
2	1	2554	U
2	1	2566	A
2	1	2567	G
2	1	2572	A
2	1	2573	C
2	1	2582	G
2	1	2602	A
2	1	2609	U
2	1	2613	U
2	1	2629	U
2	1	2630	G
2	1	2642	G
2	1	2646	C
2	1	2689	U
2	1	2690	U
2	1	2714	G
2	1	2726	A
2	1	2744	G
2	1	2748	A
2	1	2751	G
2	1	2758	A
2	1	2764	A
2	1	2765	A
2	1	2778	A
2	1	2779	U
2	1	2793	C
2	1	2798	U
2	1	2799	A
2	1	2800	A
2	1	2801	G
2	1	2820	A
2	1	2861	U
2	1	2867	G
2	1	2868	A
2	1	2872	A
2	1	2879	A
2	1	2880	C
2	1	2884	U
2	1	2901	C

Continued on next page...

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Mol	Chain	Res	Type
3	2	9	G
3	2	30	C
3	2	35	C
3	2	36	C
3	2	44	G
3	2	45	A
3	2	53	A
3	2	66	A
3	2	67	G
3	2	87	U
3	2	88	C
3	2	89	U
3	2	90	C
3	2	108	A
3	2	109	A
3	2	120	A
4	5	2	G
4	5	4	C
4	5	5	G
4	5	6	A
4	5	9	A
4	5	14	A
4	5	19	G
4	5	20	U
4	5	21	A
4	5	22	G
4	5	41	A
4	5	42	G
4	5	46	G
4	5	48	C
4	5	65	U
4	5	69	G
4	5	73	A
4	5	74	C
4	5	75	C
4	5	76	A
5	7	2	G
5	7	7	G
5	7	8	U
5	7	9	G
5	7	19	G
5	7	20	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	7	21	A
5	7	22	G
5	7	30	G
5	7	34	C
5	7	35	A
5	7	36	U
5	7	42	G
5	7	45	G
5	7	55	U
5	7	56	C
5	7	64	G
5	7	67	C
5	7	70	G
5	7	73	A
5	7	74	C
5	7	75	C
5	7	76	A
36	4	12	A
36	4	13	A
36	4	19	C
5	6	2	G
5	6	9	G
5	6	17	C
5	6	18	G
5	6	19	G
5	6	20	U
5	6	46	G
5	6	47	U
5	6	59	A
5	6	74	C
5	6	76	A

All (23) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	3	4	U
1	3	1032	G
1	3	1035	A
2	1	481	G
2	1	490	C
2	1	784	G
2	1	859	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	1	1020	A
2	1	1130	U
2	1	1715	G
2	1	1783	A
2	1	1801	A
2	1	1930	G
2	1	2326	C
2	1	2481	G
3	2	52	A
3	2	66	A
4	5	3	G
4	5	41	A
4	5	75	C
5	7	33	U
5	7	55	U
36	4	18	G

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

1 ligand is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
57	PRO	5	101	4	5,7,8	3.47	3 (60%)	7,8,10	1.49	1 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
57	PRO	5	101	4	-	0/0/9/11	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	5	101	PRO	CD-N	-5.38	1.29	1.49
57	5	101	PRO	O-C	4.77	1.39	1.19
57	5	101	PRO	CB-CA	-2.48	1.32	1.51

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
57	5	101	PRO	O-C-CA	-2.92	117.13	124.78

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.

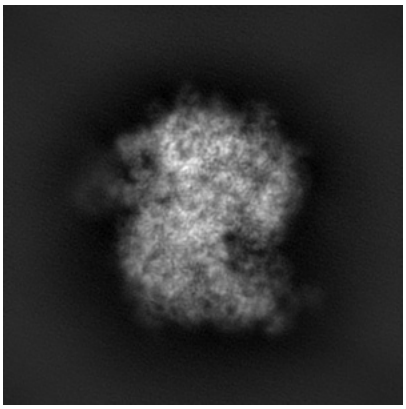
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-25420. These allow visual inspection of the internal detail of the map and identification of artifacts.

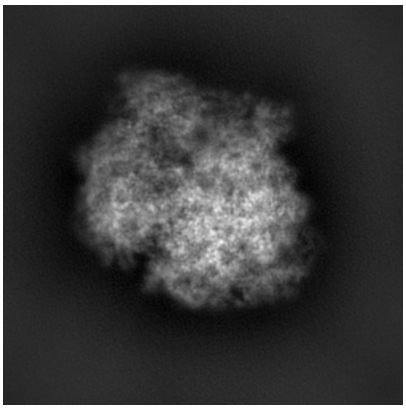
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

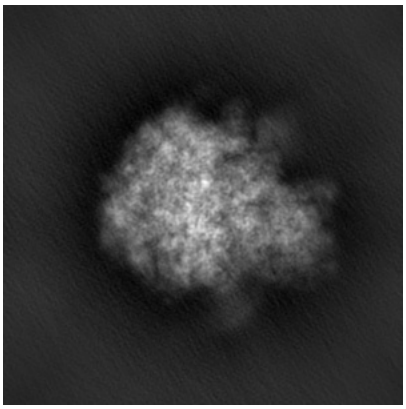
6.1.1 Primary map



X

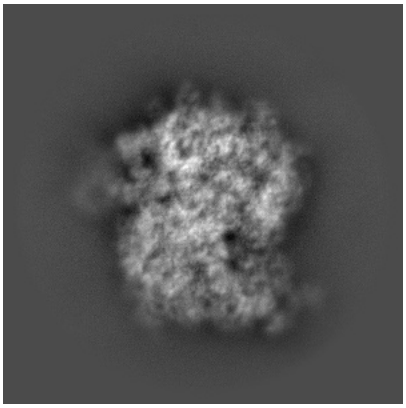


Y

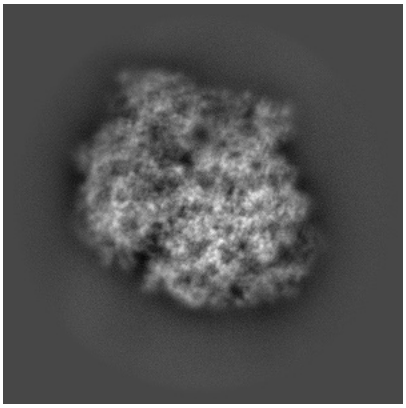


Z

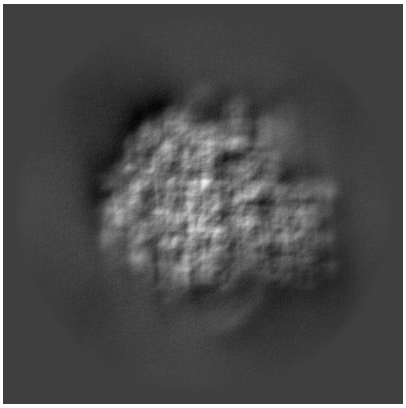
6.1.2 Raw map



X



Y

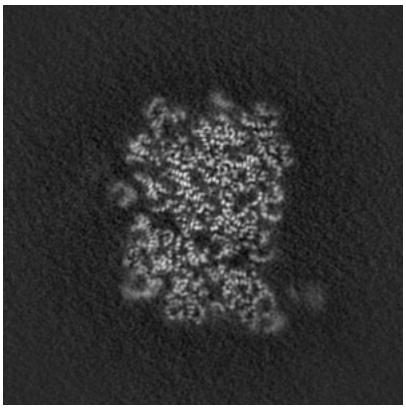


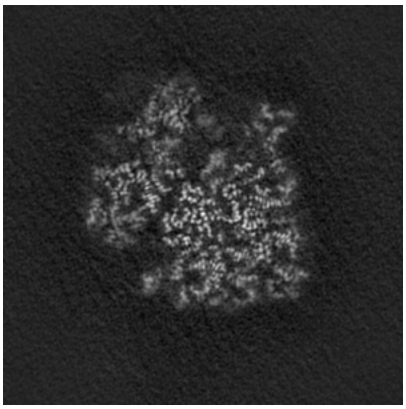
Z

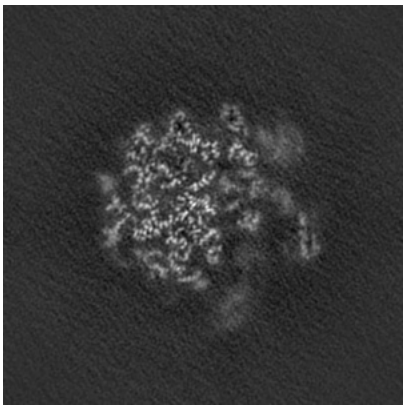
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

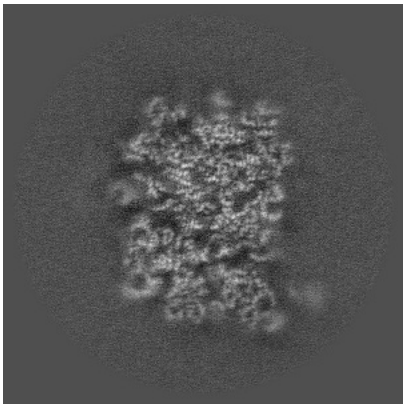
6.2.1 Primary map

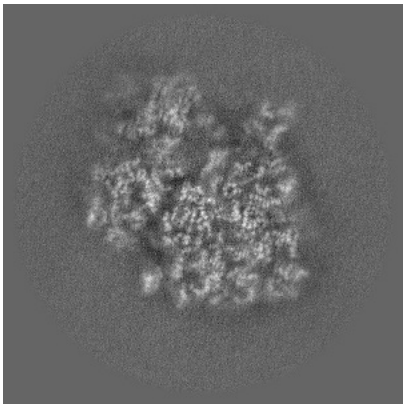

X Index: 230

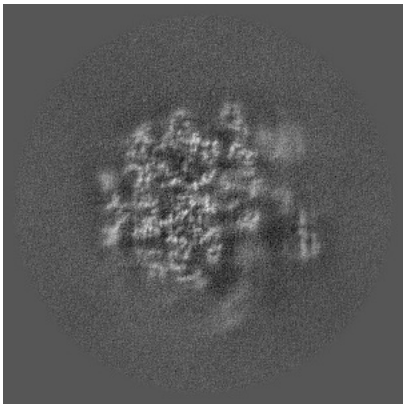

Y Index: 230


Z Index: 230

6.2.2 Raw map


X Index: 230

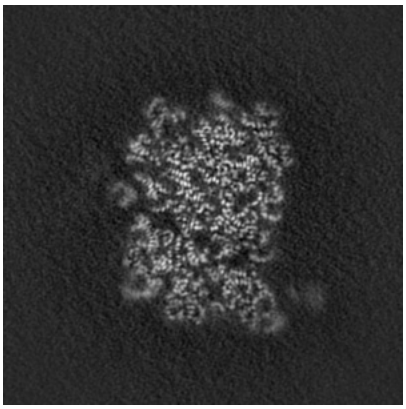

Y Index: 230

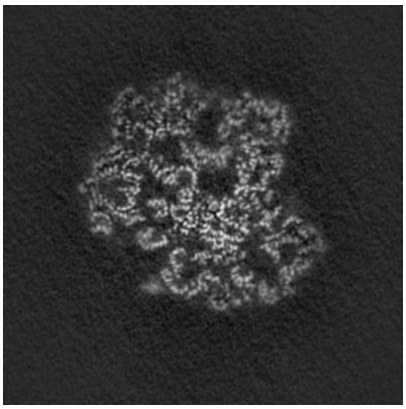

Z Index: 230

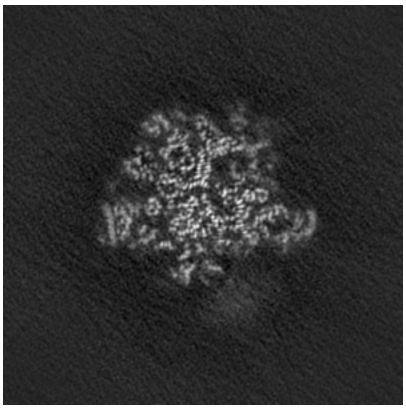
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

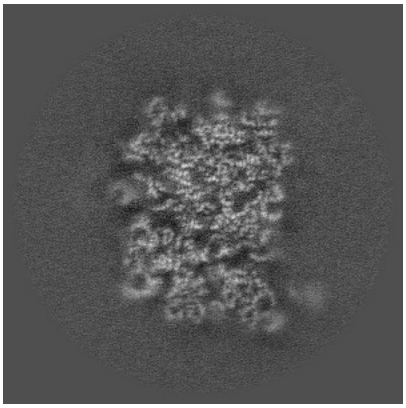
6.3.1 Primary map

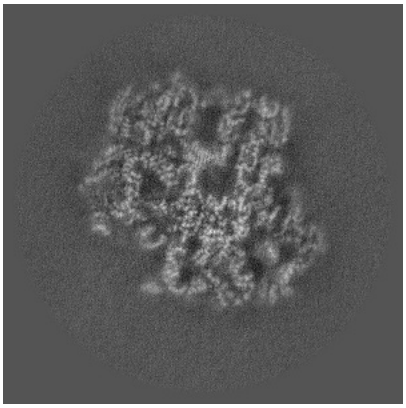

X Index: 230

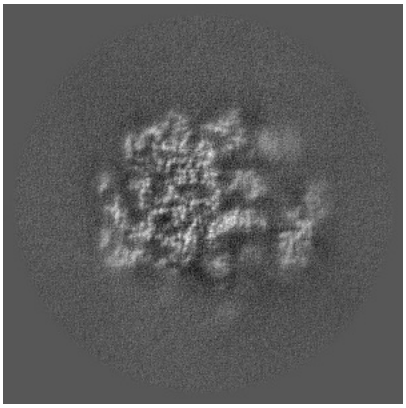

Y Index: 213


Z Index: 279

6.3.2 Raw map


X Index: 230

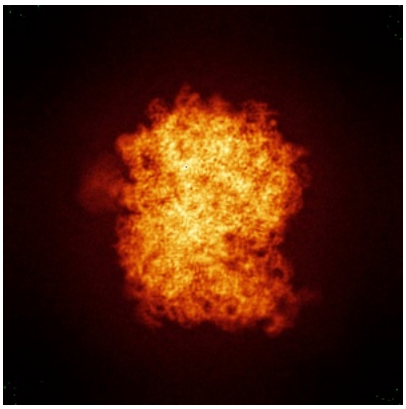

Y Index: 210

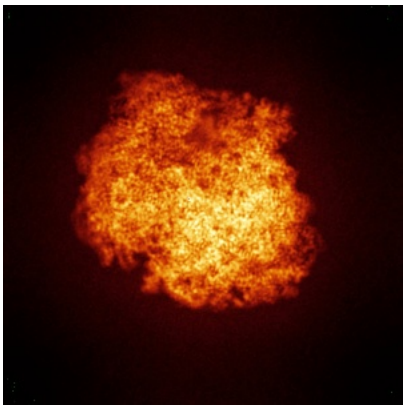

Z Index: 220

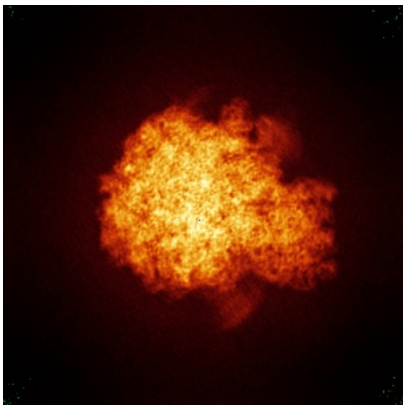
The images above show the largest variance slices of the map in three orthogonal directions.

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

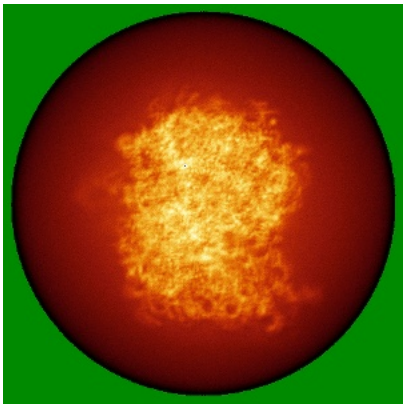
6.4.1 Primary map

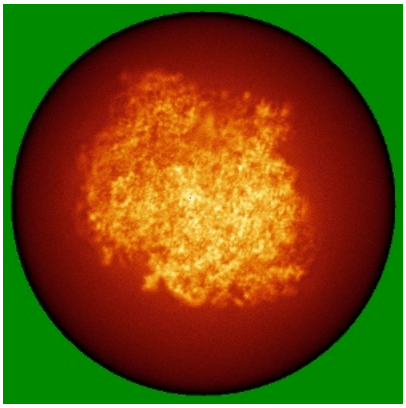

X

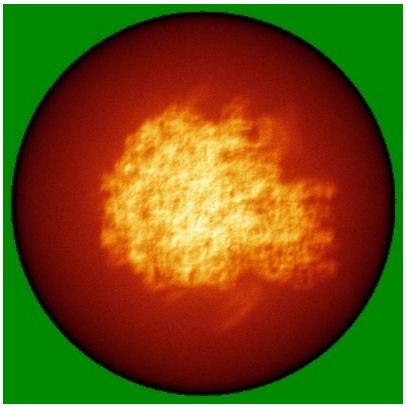

Y


Z

6.4.2 Raw map


X

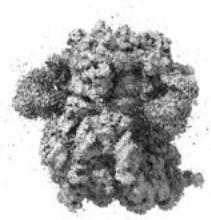

Y


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



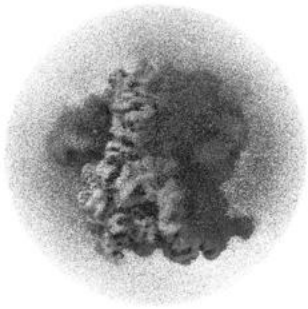
X

Y

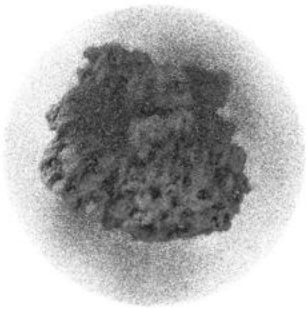
Z

The images above show the 3D surface view of the map at the recommended contour level 1.35. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

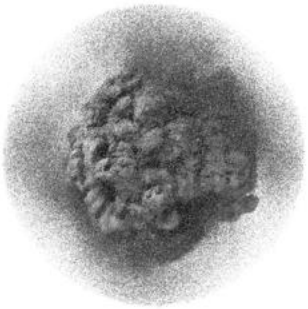
6.5.2 Raw map



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.

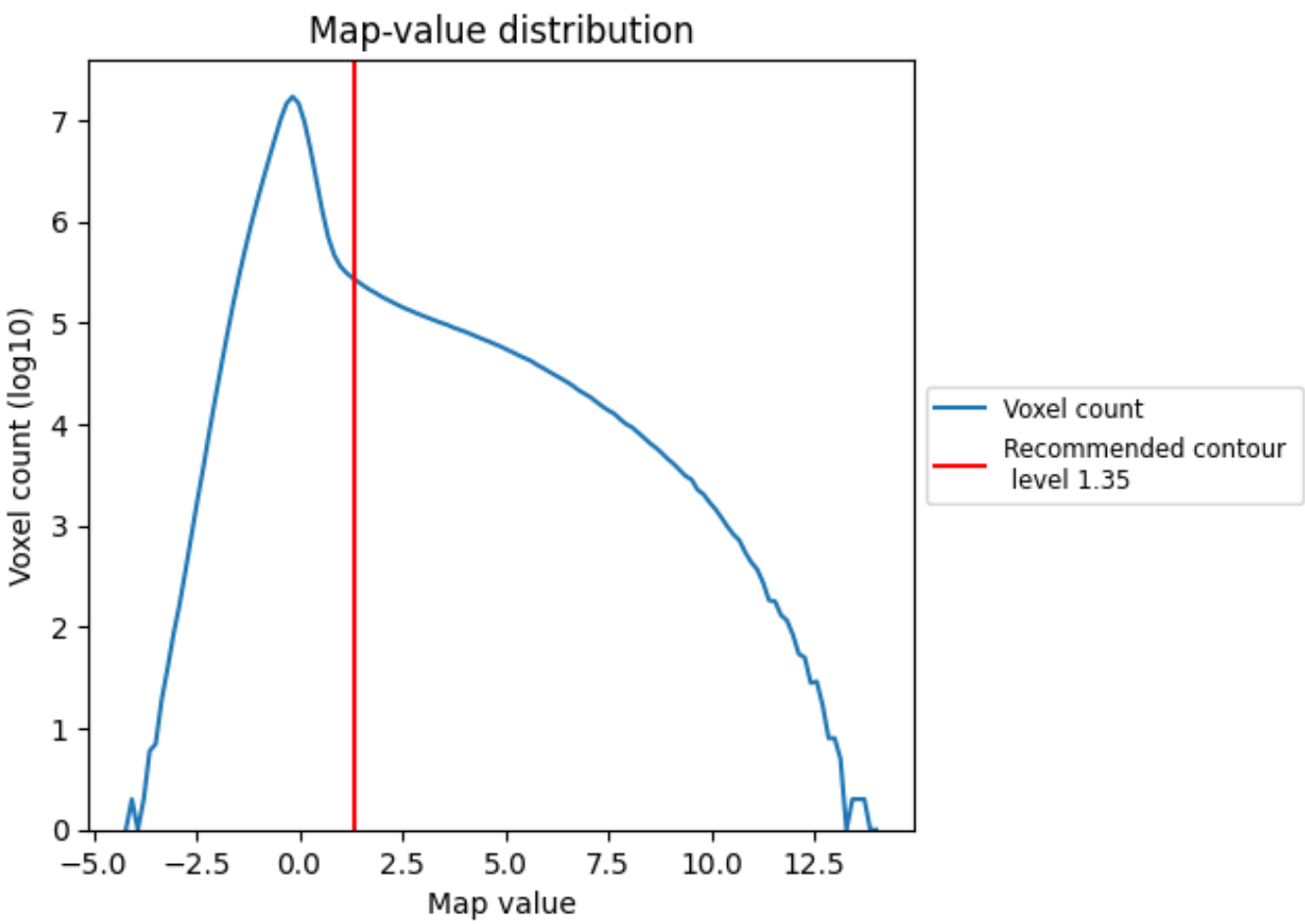
6.6 Mask visualisation (i)

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

7 Map analysis (i)

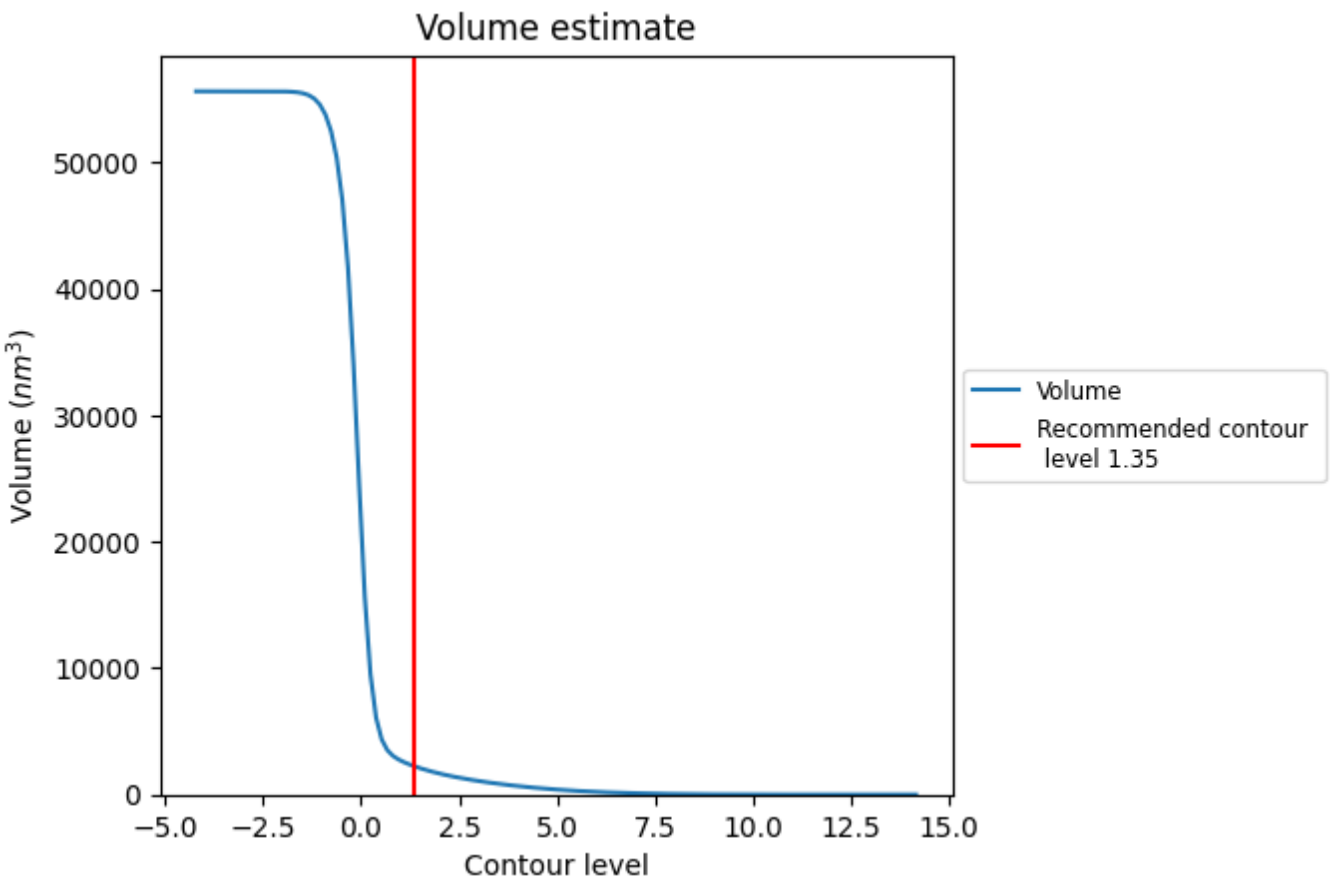
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

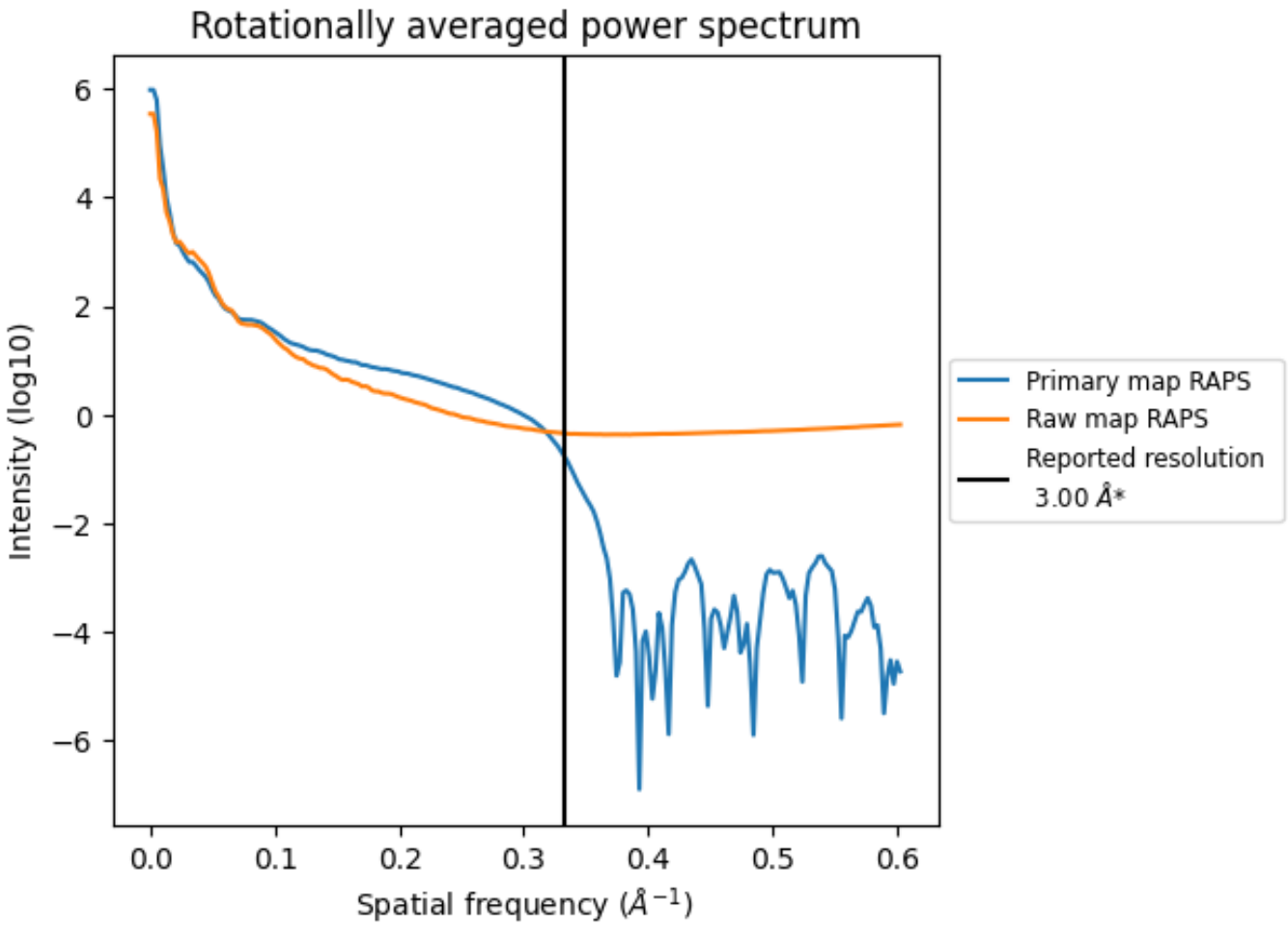
7.2 Volume estimate (i)



The volume at the recommended contour level is 2252 nm^3; this corresponds to an approximate mass of 2034 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)

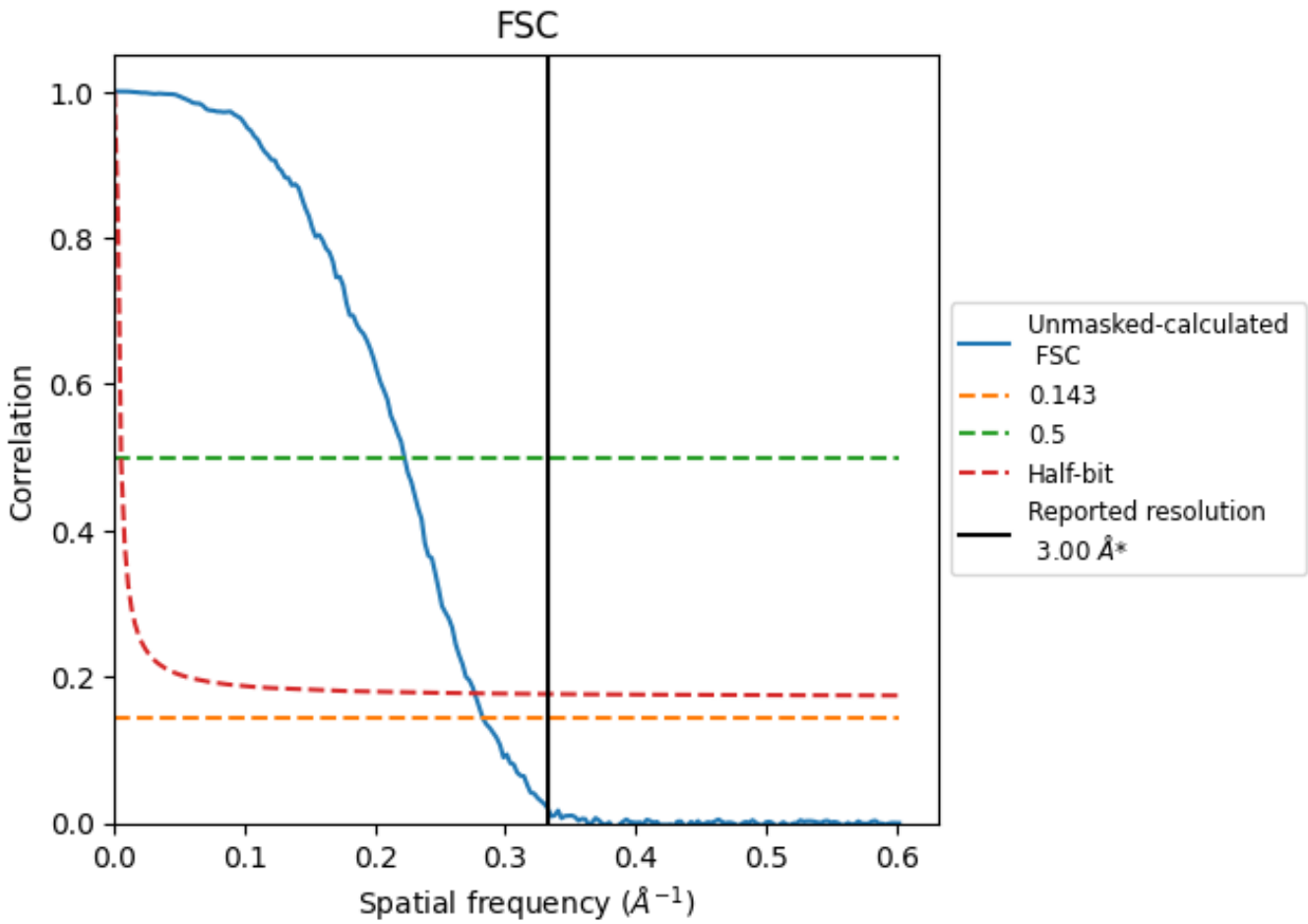


*Reported resolution corresponds to spatial frequency of 0.333 Å^{-1}

8 Fourier-Shell correlation (i)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC (i)



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

8.2 Resolution estimates (i)

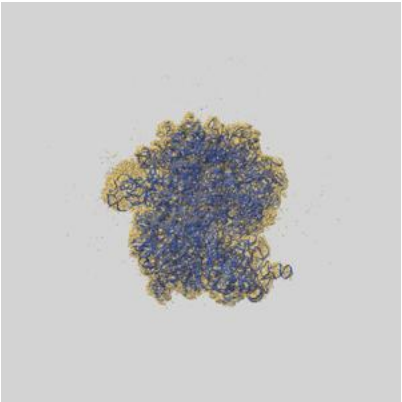
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.54	4.49	3.62

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

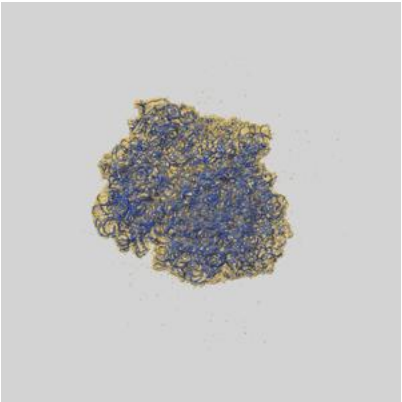
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-25420 and PDB model 7ST6. Per-residue inclusion information can be found in section 3 on page 14.

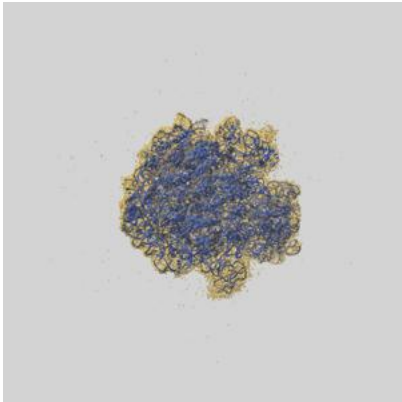
9.1 Map-model overlay (i)



X



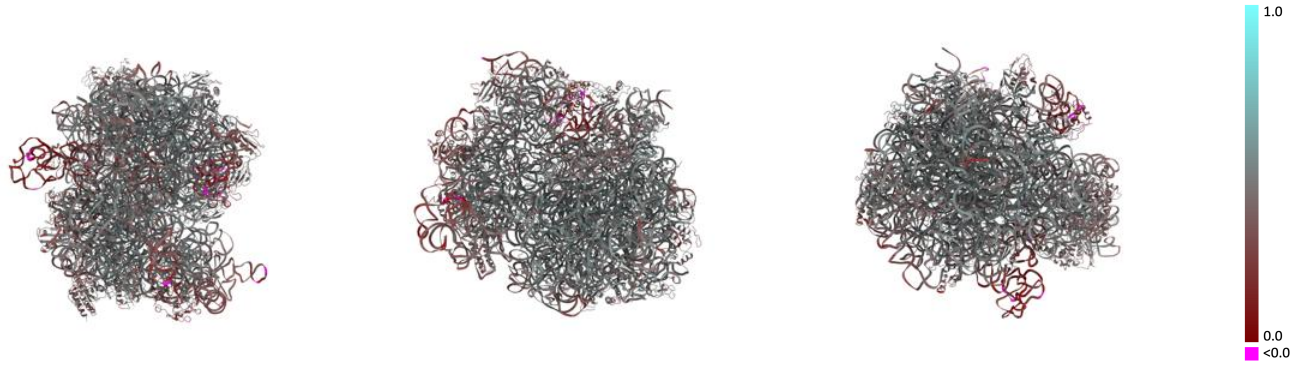
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 1.35 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.

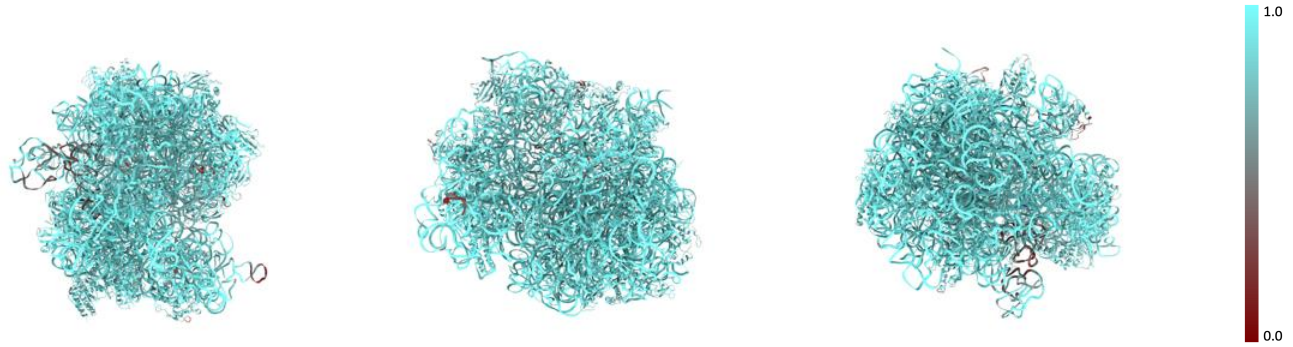
9.2 Q-score mapped to coordinate model (i)



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.

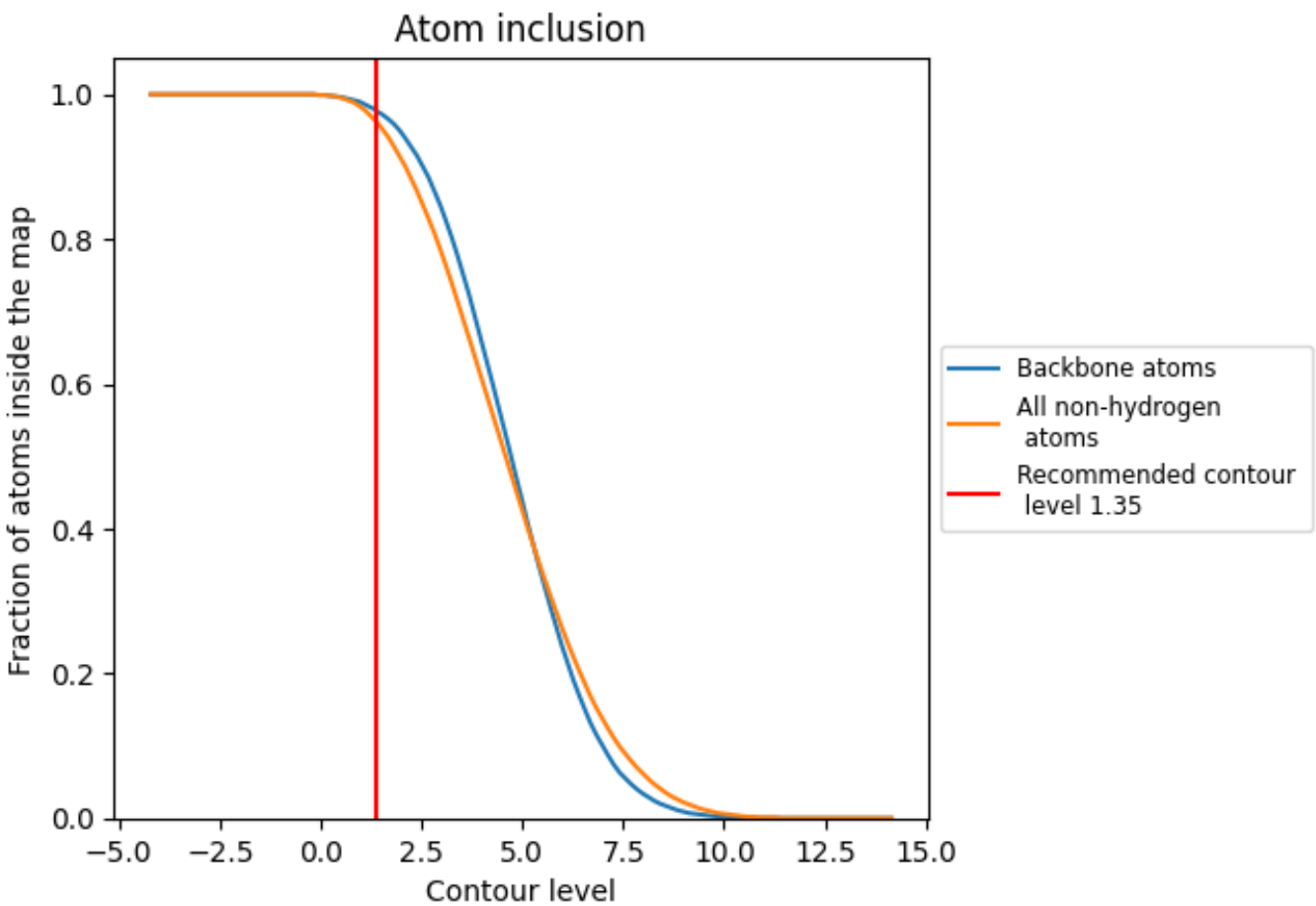
9.3 Atom inclusion mapped to coordinate model (i)



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 (1.35).

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 (i)

The table lists the average atom inclusion at the recommended contour level (1.35) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9640	0.4500
1	0.9870	0.4610
2	0.9950	0.4690
3	0.9860	0.4510
4	0.9510	0.3680
5	0.9900	0.4360
6	0.9970	0.4620
7	0.3890	0.2140
A	0.9040	0.3850
B	0.9790	0.4930
C	0.9500	0.4560
D	0.9780	0.4940
E	0.9780	0.5100
F	0.9490	0.4910
G	0.8810	0.3980
H	0.8840	0.4570
I	0.8650	0.3460
J	0.9490	0.4680
K	0.9550	0.4000
L	0.9130	0.3990
M	0.9500	0.4620
N	0.9110	0.4140
O	0.8160	0.4130
P	0.9630	0.4590
Q	0.9260	0.4210
R	0.9390	0.4240
S	0.9300	0.4350
T	0.9830	0.4460
U	0.9030	0.4020
V	0.9750	0.4120
W	0.9710	0.4410
X	0.9240	0.4300
Y	0.9180	0.3950
Z	0.8710	0.3280
b	0.9790	0.5090

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Chain	Atom inclusion	Q-score
c	0.9750	0.4970
d	0.9340	0.4470
e	0.9510	0.4240
f	0.9180	0.4110
g	0.8320	0.3760
i	0.7020	0.1810
j	0.9710	0.4920
k	0.9650	0.5000
l	0.9690	0.4910
m	0.9760	0.5060
n	0.9720	0.4800
o	0.9640	0.4540
p	0.9540	0.4980
q	0.9650	0.4870
r	0.9330	0.4780
s	0.9680	0.4690
t	0.9590	0.4510
u	0.9350	0.4380
v	0.9430	0.4720
w	0.9930	0.5200
x	0.9750	0.4840
y	0.9030	0.3840
z	0.9540	0.4810