Full wwPDB EM Validation Report ⓘ

Nov 4, 2023 – 01:59 PM EDT

PDB ID	:	8G6Y
EMDB ID	:	EMD-29788
Title	:	Structure of WT E.coli ribosome 50S subunit with complexed with mRNA, P-site fMet-NH-tRNAfMet and A-site 3-aminopyridine-4-carboxylic acid charged NH-tRNAPhe
Authors	:	Majumdar, C.; Cate, J.H.D.
Deposited on	:	2023-02-16
Resolution	:	2.09 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 ⓘ symbol.

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

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

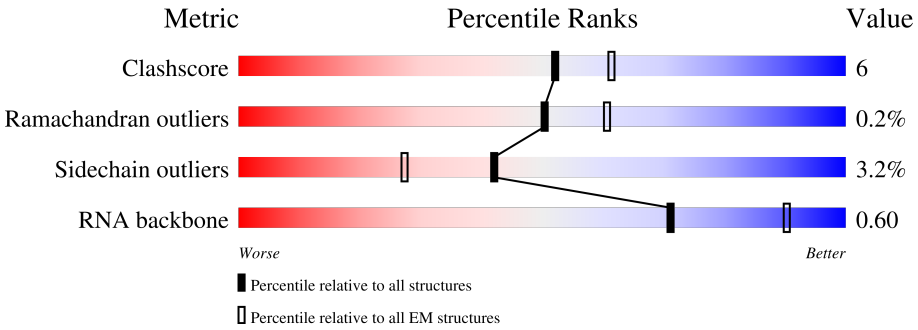
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance

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

The reported resolution of this entry is 2.09 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)
Clashscore	158937	4297
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	0	55	82% 11% 7%
2	1	46	98%
3	2	65	91% 5%
4	3	38	87% 13%
5	4	70	51% 59% 24% 14%
6	X	28	21% 25% 14% 14% 46%
7	Y	76	39% 22% 47% 24%

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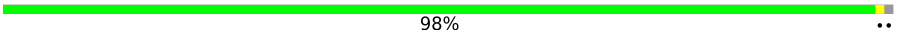
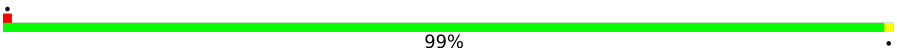
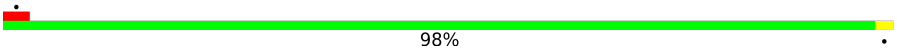
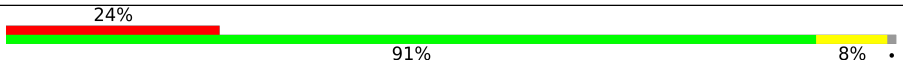
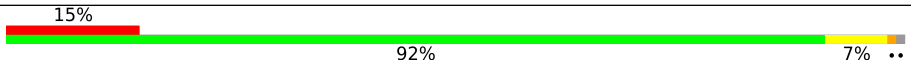
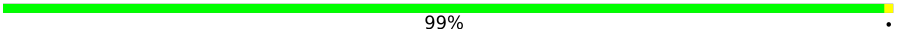
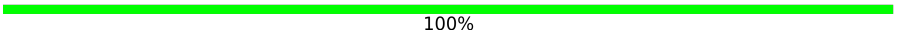
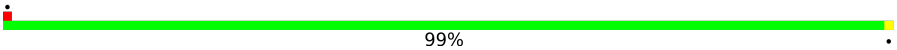
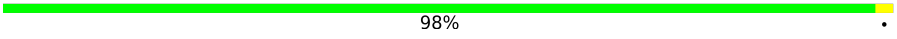
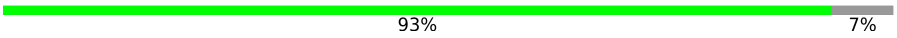
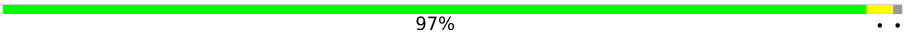
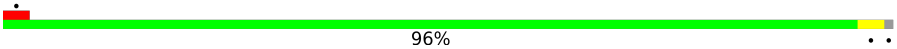
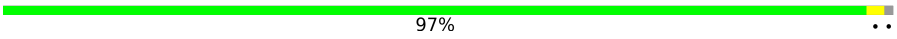
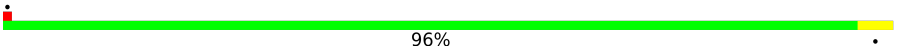
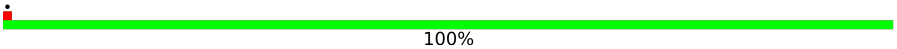
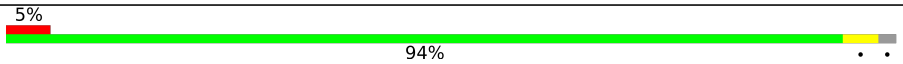
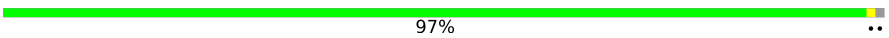
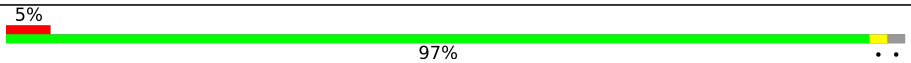
Mol	Chain	Length	Quality of chain
8	Z	76	
9	a	2904	
10	b	120	
11	c	273	
12	d	209	
13	e	201	
14	f	179	
15	g	177	
16	h	149	
17	i	142	
18	j	123	
19	k	144	
20	l	136	
21	m	127	
22	n	117	
23	o	115	
24	p	118	
25	q	103	
26	r	110	
27	s	100	
28	t	104	
29	u	94	
30	v	85	
31	w	78	
32	x	63	

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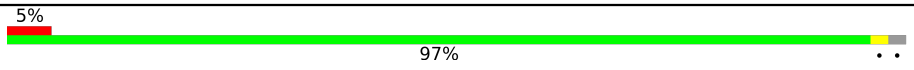
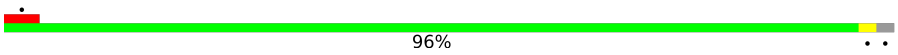
Mol	Chain	Length	Quality of chain
33	y	59	
34	z	57	

2 Entry composition

There are 41 unique types of molecules in this entry. The entry contains 93683 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	0	51	Total	C	N	O	0	0
			417	269	76	72		

- Molecule 2 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 3 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 4 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	3	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 5 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	4	60	Total	C	N	O	S	0	0
			480	299	90	85	6		

- Molecule 6 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	X	15	Total	C	N	O	P	0	0
			317	143	56	103	15		

- Molecule 7 is a RNA chain called A-site tRNA Phe.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	Y	74	Total	C	N	O	P	0	0
			1578	705	285	515	73		

- Molecule 8 is a RNA chain called P-site tRNA fMet.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	Z	75	Total	C	N	O	P	0	0
			1601	713	289	524	75		

- Molecule 9 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	a	2753	Total	C	N	O	P	0	0
			59130	26384	10897	19096	2753		

- Molecule 10 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	b	119	Total	C	N	O	P	0	0
			2549	1135	466	829	119		

- Molecule 11 is a protein called 50S ribosomal protein L2.

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

- Molecule 12 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	d	209	Total	C	N	O	S	0	0
			1566	980	288	294	4		

- Molecule 13 is a protein called 50S ribosomal protein L4.

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

- Molecule 14 is a protein called 50S ribosomal protein L5.

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

- Molecule 15 is a protein called 50S ribosomal protein L6.

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

- Molecule 16 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	h	41	Total	C	N	O	S	0	0
			303	194	54	54	1		

- Molecule 17 is a protein called 50S ribosomal protein L13.

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

- Molecule 18 is a protein called 50S ribosomal protein L14.

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

- Molecule 19 is a protein called 50S ribosomal protein L15.

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

- Molecule 20 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	l	136	Total	C	N	O	S	0	0
			1075	686	205	177	7		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
l	82	MS6	MET	conflict	UNP A1AGK1

- Molecule 21 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	m	118	Total	C	N	O	S	0	0
			945	585	194	161	5		

- Molecule 22 is a protein called 50S ribosomal protein L18.

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

- Molecule 23 is a protein called 50S ribosomal protein L19.

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

- Molecule 24 is a protein called 50S ribosomal protein L20.

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

- Molecule 25 is a protein called Ribosomal protein L21.

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

- Molecule 26 is a protein called 50S ribosomal protein L22.

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

- Molecule 27 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	s	93	Total	C	N	O	S	0	0
			738	466	139	131	2		

- Molecule 28 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	t	102	Total	C	N	O	0	0
			779	492	146	141		

- Molecule 29 is a protein called 50S ribosomal protein L25.

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

- Molecule 30 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	v	76	Total	C	N	O	S	0	0
			576	357	114	104	1		

- Molecule 31 is a protein called 50S ribosomal protein L28.

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

- Molecule 32 is a protein called 50S ribosomal protein L29.

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

- Molecule 33 is a protein called 50S ribosomal protein L30.

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

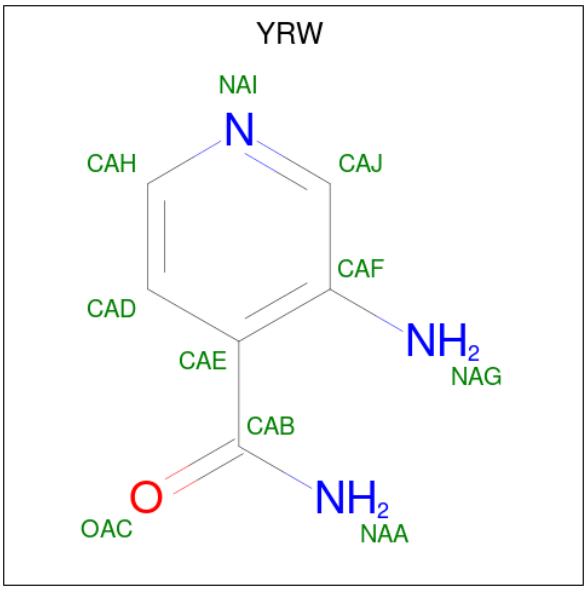
- Molecule 34 is a protein called 50S ribosomal protein L32.

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

- Molecule 35 is ZINC ION (three-letter code: ZN) (formula: Zn).

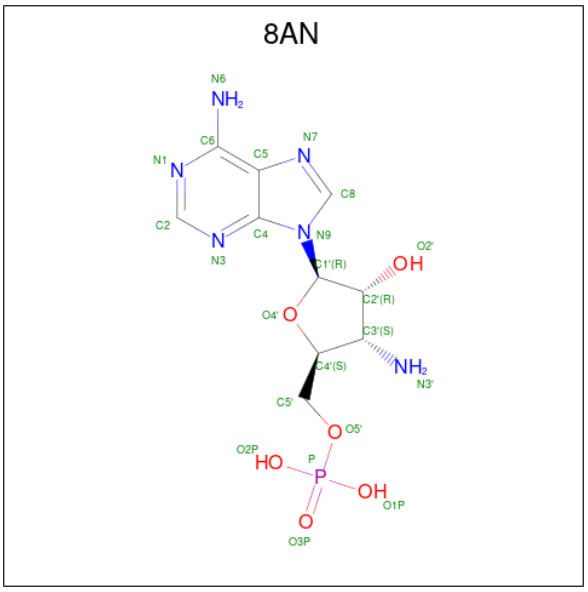
Mol	Chain	Residues	Atoms		AltConf
35	3	1	Total	Zn	0
			1	1	
35	4	1	Total	Zn	0
			1	1	

- Molecule 36 is 3-aminopyridine-4-carboxamide (three-letter code: YRW) (formula: $C_6H_7N_3O$) (labeled as "Ligand of Interest" by depositor).



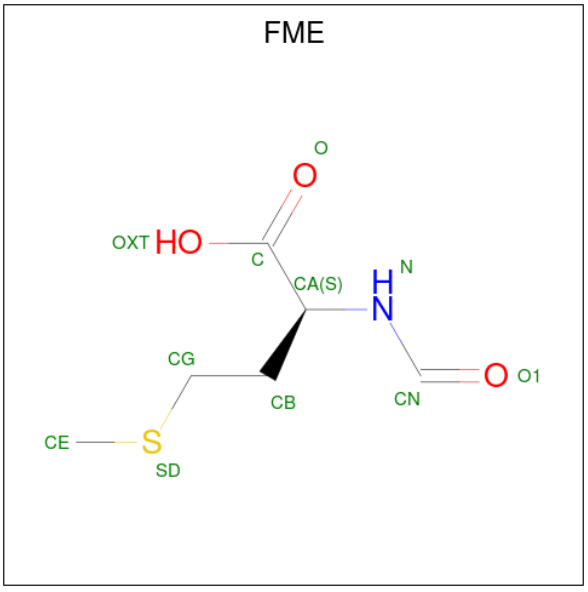
Mol	Chain	Residues	Atoms				AltConf
36	Y	1	Total	C	N	O	0
			10	6	3	1	

- Molecule 37 is 3'-amino-3'-deoxyadenosine 5'-(dihydrogen phosphate) (three-letter code: 8AN) (formula: $C_{10}H_{15}N_6O_6P$).



Mol	Chain	Residues	Atoms					AltConf
37	Z	1	Total	C	N	O	P	0
			22	10	6	5	1	

- Molecule 38 is N-FORMYLMETHIONINE (three-letter code: FME) (formula: $C_6H_{11}NO_3S$).



Mol	Chain	Residues	Atoms					AltConf
38	Z	1	Total	C	N	O	S	0
			10	6	1	2	1	

- Molecule 39 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
39	a	224	Total Mg 224 224	0
39	b	5	Total Mg 5 5	0
39	d	1	Total Mg 1 1	0
39	z	1	Total Mg 1 1	0

- Molecule 40 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	AltConf
40	a	13	Total K 13 13	0
40	c	2	Total K 2 2	0

- Molecule 41 is water.

Mol	Chain	Residues	Atoms	AltConf
41	0	1	Total O 1 1	0
41	1	16	Total O 16 16	0
41	2	22	Total O 22 22	0
41	3	2	Total O 2 2	0
41	Z	1	Total O 1 1	0
41	a	3019	Total O 3019 3019	0
41	b	38	Total O 38 38	0
41	c	84	Total O 84 84	0
41	d	36	Total O 36 36	0
41	e	28	Total O 28 28	0
41	i	9	Total O 9 9	0
41	j	12	Total O 12 12	0

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Mol	Chain	Residues	Atoms	AltConf
41	k	26	Total O 26 26	0
41	l	24	Total O 24 24	0
41	m	21	Total O 21 21	0
41	o	9	Total O 9 9	0
41	p	20	Total O 20 20	0
41	q	12	Total O 12 12	0
41	r	24	Total O 24 24	0
41	s	7	Total O 7 7	0
41	t	1	Total O 1 1	0
41	u	4	Total O 4 4	0
41	v	10	Total O 10 10	0
41	w	9	Total O 9 9	0
41	x	1	Total O 1 1	0
41	z	24	Total O 24 24	0

3 Residue-property plots (i)

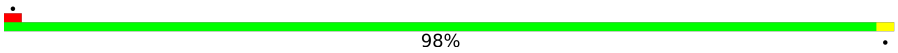
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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.

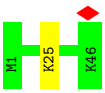
• Molecule 1: 50S ribosomal protein L33

Chain 0:

• Molecule 2: 50S ribosomal protein L34

Chain 1:



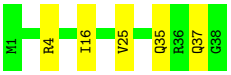


• Molecule 3: 50S ribosomal protein L35

Chain 2:

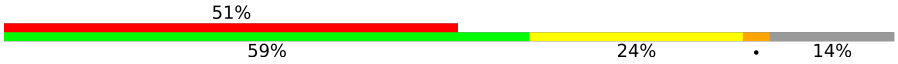
• Molecule 4: 50S ribosomal protein L36

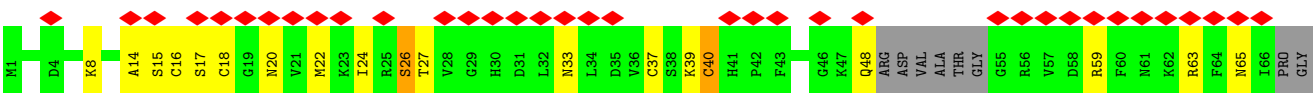
Chain 3:



• Molecule 5: 50S ribosomal protein L31

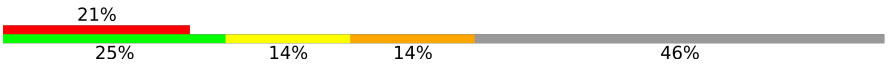
Chain 4:

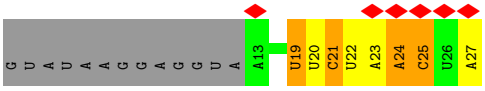




• Molecule 6: mRNA

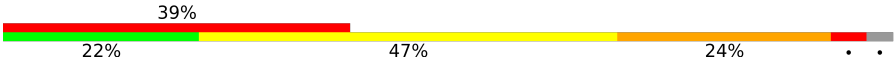
Chain X:

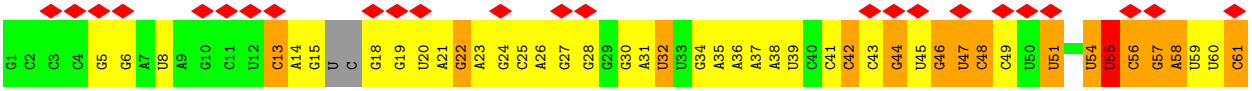


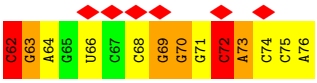


• Molecule 7: A-site tRNA Phe

Chain Y:

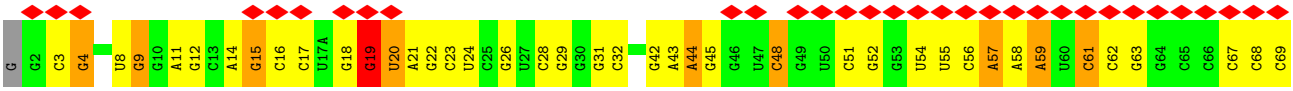


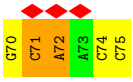




• Molecule 8: P-site tRNA fMet

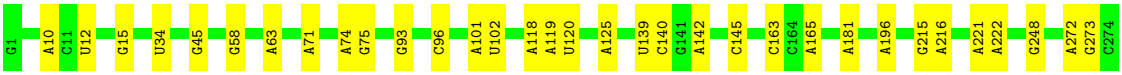
Chain Z:

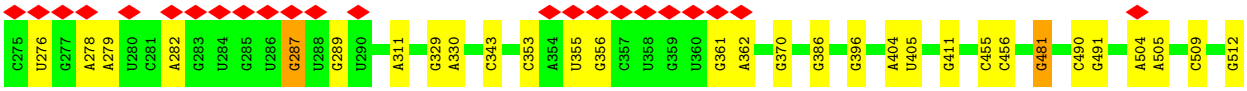


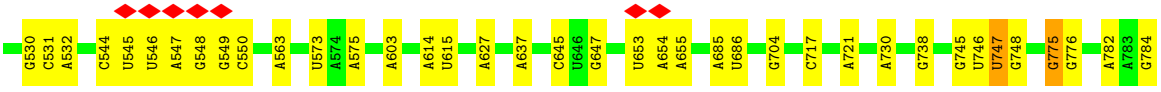


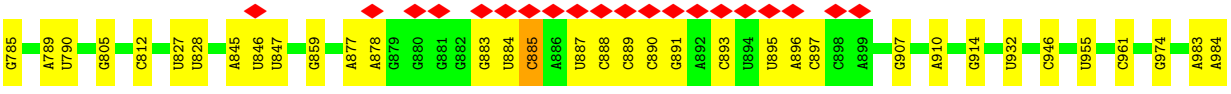
• Molecule 9: 23S rRNA

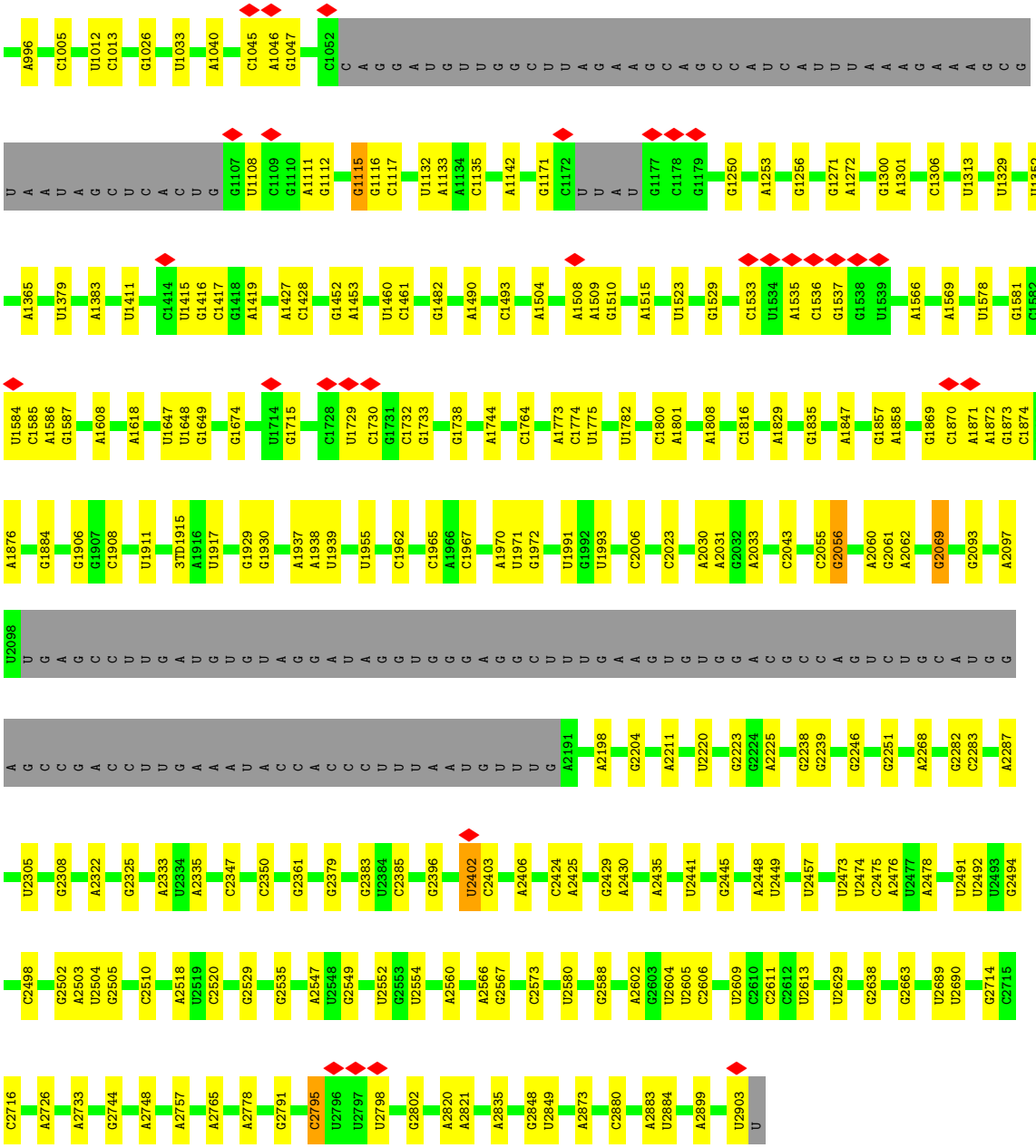
Chain a:









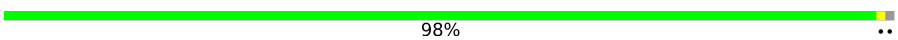


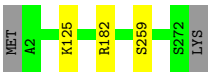
• Molecule 10: 5S rRNA

Chain b:

• Molecule 11: 50S ribosomal protein L2

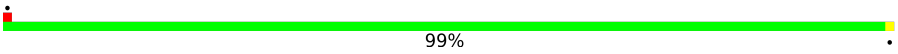
Chain c:

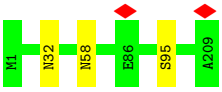




• Molecule 12: 50S ribosomal protein L3

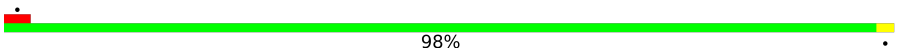
Chain d:

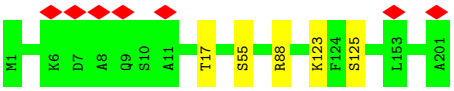




• Molecule 13: 50S ribosomal protein L4

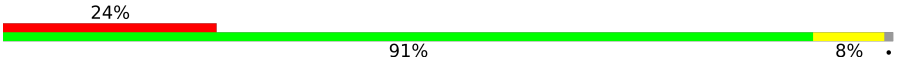
Chain e:

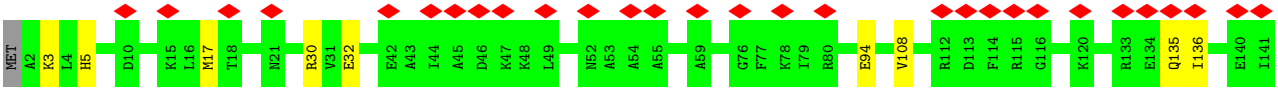


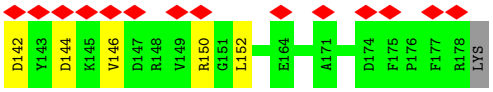


• Molecule 14: 50S ribosomal protein L5

Chain f:

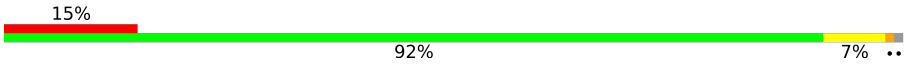


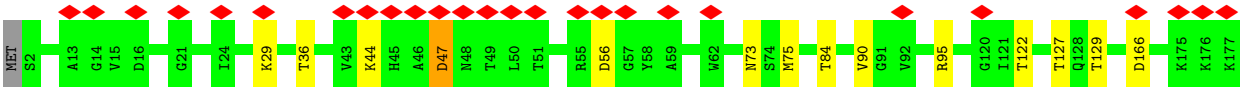




• Molecule 15: 50S ribosomal protein L6

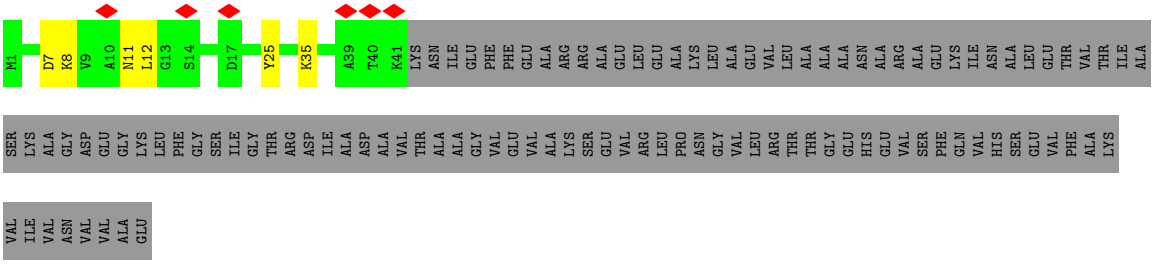
Chain g:





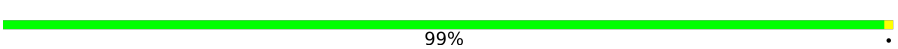
• Molecule 16: 50S ribosomal protein L9

Chain h:



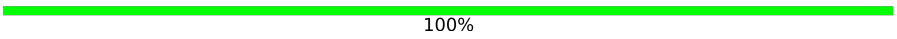
• Molecule 17: 50S ribosomal protein L13

Chain i:



• Molecule 18: 50S ribosomal protein L14

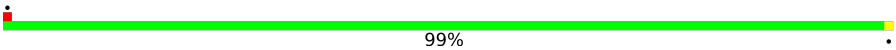
Chain j:



There are no outlier residues recorded for this chain.

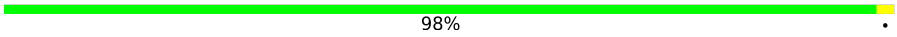
• Molecule 19: 50S ribosomal protein L15

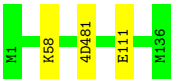
Chain k:



• Molecule 20: 50S ribosomal protein L16

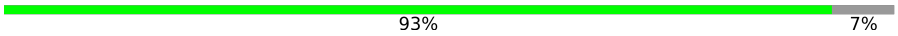
Chain l:

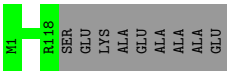




• Molecule 21: 50S ribosomal protein L17

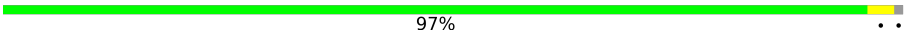
Chain m:





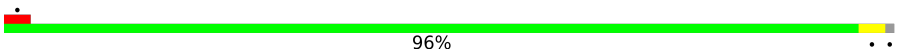
• Molecule 22: 50S ribosomal protein L18

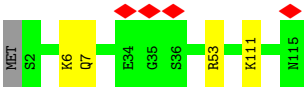
Chain n:



• Molecule 23: 50S ribosomal protein L19

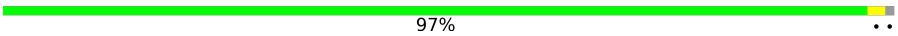
Chain o:





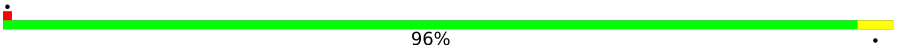
• Molecule 24: 50S ribosomal protein L20

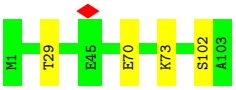
Chain p:



• Molecule 25: Ribosomal protein L21

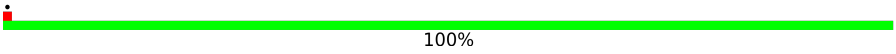
Chain q:





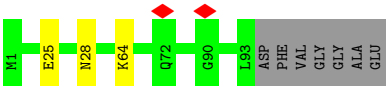
• Molecule 26: 50S ribosomal protein L22

Chain r:



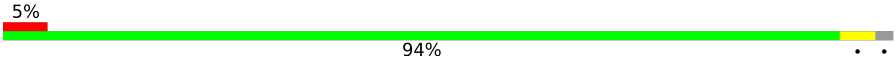
• Molecule 27: 50S ribosomal protein L23

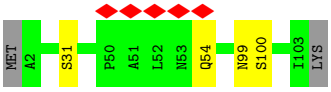
Chain s:



• Molecule 28: 50S ribosomal protein L24

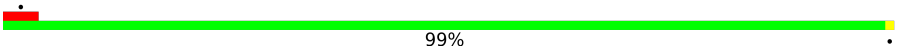
Chain t:

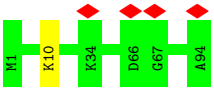




• Molecule 29: 50S ribosomal protein L25

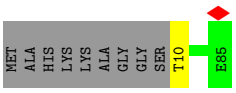
Chain u:





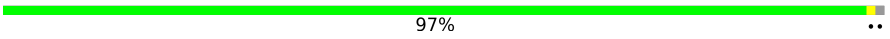
• Molecule 30: 50S ribosomal protein L27

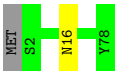
Chain v:



• Molecule 31: 50S ribosomal protein L28

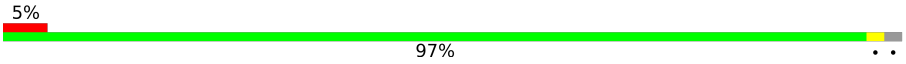
Chain w:

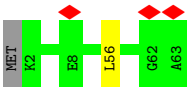




• Molecule 32: 50S ribosomal protein L29

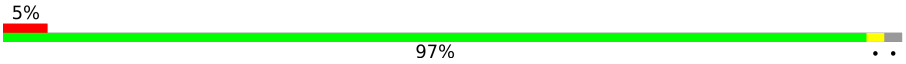
Chain x:

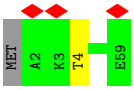




• Molecule 33: 50S ribosomal protein L30

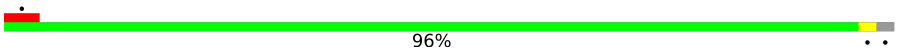
Chain y:

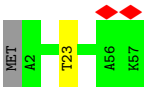




• Molecule 34: 50S ribosomal protein L32

Chain z:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	288552	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	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.377	Depositor
Minimum map value	-0.131	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.0265	Depositor
Map size (Å)	408.704, 408.704, 408.704	wwPDB
Map dimensions	496, 496, 496	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.824, 0.824, 0.824	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 1MG, 4D4, MEQ, OMG, MS6, ZN, MG, K, YRW, H2U, 5MC, 2MG, OMC, FME, 2MA, OMU, 3TD, G7M, 5MU, 8AN, 6MZ, PSU

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	0	0.33	0/424	0.53	0/565
2	1	0.29	0/380	0.51	0/498
3	2	0.32	0/513	0.50	0/676
4	3	0.34	0/303	0.54	0/397
5	4	0.31	0/488	0.52	0/649
6	X	0.55	0/354	0.98	2/548 (0.4%)
7	Y	1.49	18/1763 (1.0%)	1.50	39/2745 (1.4%)
8	Z	0.38	0/1788	0.96	3/2786 (0.1%)
9	a	0.61	7/65651 (0.0%)	0.92	31/102413 (0.0%)
10	b	0.50	0/2850	0.86	0/4444
11	c	0.33	0/2121	0.53	0/2852
12	d	0.32	0/1576	0.52	0/2119
13	e	0.31	0/1571	0.50	0/2113
14	f	0.29	0/1434	0.50	0/1926
15	g	0.32	0/1343	0.55	0/1816
16	h	0.31	0/306	0.64	0/413
17	i	0.33	0/1152	0.49	0/1551
18	j	0.32	0/955	0.54	0/1279
19	k	0.33	0/1062	0.56	0/1413
20	l	0.32	0/1073	0.50	0/1433
21	m	0.33	0/958	0.52	0/1281
22	n	0.31	0/902	0.50	0/1209
23	o	0.34	0/929	0.52	0/1242
24	p	0.33	0/960	0.48	0/1278
25	q	0.33	0/829	0.56	0/1107
26	r	0.31	0/864	0.49	0/1156
27	s	0.30	0/744	0.50	0/994
28	t	0.32	0/787	0.52	0/1051
29	u	0.32	0/766	0.49	0/1025
30	v	0.31	0/583	0.50	0/772
31	w	0.33	0/635	0.53	0/848

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	x	0.28	0/502	0.44	0/667
33	y	0.30	0/453	0.50	0/605
34	z	0.30	0/450	0.52	0/599
All	All	0.57	25/97469 (0.0%)	0.86	75/146470 (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
3	2	0	1
15	g	0	1
31	w	0	1
All	All	0	3

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	Y	8	U	C4-O4	44.59	1.59	1.23
7	Y	73	A	P-O5'	15.81	1.75	1.59
7	Y	73	A	P-OP2	-15.43	1.22	1.49
9	a	2588	G	O3'-P	-13.45	1.45	1.61
9	a	2510	C	O3'-P	11.58	1.75	1.61
7	Y	32	U	N1-C2	11.25	1.48	1.38
9	a	2611	C	O3'-P	11.16	1.74	1.61
7	Y	39	U	N1-C2	10.83	1.48	1.38
7	Y	55	U	N1-C2	10.56	1.48	1.38
7	Y	39	U	C4-C5	-9.99	1.34	1.43
7	Y	32	U	C4-C5	-9.94	1.34	1.43
7	Y	55	U	C4-C5	-9.59	1.34	1.43
9	a	2056	G	O3'-P	9.40	1.72	1.61
9	a	2549	G	O3'-P	9.32	1.72	1.61
9	a	2246	G	O3'-P	7.82	1.70	1.61
9	a	2560	A	O3'-P	7.38	1.70	1.61
7	Y	32	U	C2-N3	-6.08	1.33	1.37
7	Y	54	U	C2-N3	-5.45	1.33	1.37
7	Y	8	U	C2-N3	-5.45	1.33	1.37
7	Y	54	U	N3-C4	-5.32	1.33	1.38
7	Y	8	U	C4-C5	-5.26	1.38	1.43
7	Y	55	U	C2-N3	-5.20	1.34	1.37
7	Y	54	U	C4-C5	5.11	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	Y	39	U	C2-N3	-5.01	1.34	1.37
7	Y	54	U	C5-C6	5.00	1.38	1.34

All (75) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	Y	72	C	O3'-P-O5'	-20.60	64.86	104.00
7	Y	73	A	OP1-P-OP2	17.19	145.38	119.60
7	Y	54	U	N1-C2-N3	12.36	122.31	114.90
7	Y	32	U	N3-C4-C5	12.18	121.91	114.60
7	Y	8	U	C5-C4-O4	-12.15	118.61	125.90
7	Y	55	U	N3-C4-C5	11.88	121.72	114.60
7	Y	39	U	C5-C4-O4	-11.70	118.88	125.90
7	Y	54	U	C2-N3-C4	-11.45	120.13	127.00
7	Y	39	U	N3-C4-C5	11.40	121.44	114.60
7	Y	8	U	C2-N3-C4	-10.94	120.44	127.00
7	Y	8	U	N3-C4-C5	10.89	121.13	114.60
7	Y	32	U	C5-C4-O4	-10.84	119.40	125.90
7	Y	55	U	C5-C4-O4	-10.77	119.44	125.90
7	Y	39	U	C2-N3-C4	-10.16	120.90	127.00
7	Y	32	U	C2-N3-C4	-10.12	120.93	127.00
7	Y	55	U	C2-N3-C4	-10.06	120.96	127.00
9	a	2605	PSU	P-O3'-C3'	-9.87	107.86	119.70
7	Y	54	U	C5-C4-O4	-9.40	120.26	125.90
9	a	2606	C	P-O3'-C3'	-9.21	108.65	119.70
8	Z	72	A	P-O3'-C3'	-9.04	108.85	119.70
7	Y	72	C	OP1-P-O3'	-8.99	85.42	105.20
9	a	512	G	O4'-C1'-N9	8.99	115.39	108.20
7	Y	73	A	P-O5'-C5'	-8.98	106.53	120.90
9	a	2445	2MG	P-O3'-C3'	-8.09	110.00	119.70
9	a	2473	U	N1-C2-O2	7.61	128.13	122.80
7	Y	8	U	N1-C2-N3	7.52	119.41	114.90
7	Y	54	U	N3-C4-C5	7.02	118.81	114.60
7	Y	54	U	C5-C6-N1	-6.87	119.26	122.70
9	a	2473	U	C2-N1-C1'	6.84	125.91	117.70
7	Y	39	U	C6-N1-C2	-6.83	116.90	121.00
7	Y	32	U	C5-C6-N1	-6.74	119.33	122.70
9	a	2473	U	N3-C2-O2	-6.60	117.58	122.20
7	Y	8	U	C5-C6-N1	-6.58	119.41	122.70
9	a	1313	U	C2-N1-C1'	6.56	125.57	117.70
9	a	2848	G	O4'-C1'-N9	6.51	113.41	108.20
7	Y	39	U	N1-C2-N3	6.40	118.74	114.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	a	2638	G	O4'-C1'-N9	6.38	113.31	108.20
8	Z	71	C	P-O3'-C3'	-6.34	112.09	119.70
7	Y	55	U	C5-C6-N1	-6.24	119.58	122.70
9	a	12	U	C2-N1-C1'	5.96	124.86	117.70
7	Y	61	C	C2-N1-C1'	5.95	125.35	118.80
7	Y	55	U	N1-C2-N3	5.94	118.47	114.90
9	a	748	G	O4'-C1'-N9	5.92	112.94	108.20
6	X	21	C	C2-N1-C1'	-5.91	112.30	118.80
9	a	775	G	O4'-C1'-N9	5.90	112.92	108.20
7	Y	73	A	O5'-P-OP1	-5.90	100.39	105.70
7	Y	62	C	N1-C2-O2	5.83	122.40	118.90
7	Y	55	U	C6-N1-C2	-5.78	117.53	121.00
9	a	2282	G	O4'-C1'-N9	5.69	112.75	108.20
9	a	370	G	O4'-C1'-N9	-5.65	103.68	108.20
7	Y	32	U	N1-C2-N3	5.62	118.27	114.90
7	Y	32	U	C6-N1-C2	-5.58	117.65	121.00
9	a	984	A	O4'-C1'-N9	5.58	112.66	108.20
7	Y	62	C	N3-C2-O2	-5.55	118.01	121.90
6	X	21	C	C6-N1-C1'	5.53	127.43	120.80
8	Z	19	G	O4'-C1'-N9	-5.48	103.82	108.20
9	a	885	C	C2-N1-C1'	5.48	124.83	118.80
9	a	1857	G	O4'-C1'-N9	5.47	112.58	108.20
7	Y	54	U	N1-C2-O2	-5.45	118.98	122.80
9	a	2795	C	C2-N1-C1'	5.42	124.76	118.80
9	a	1313	U	N1-C2-O2	5.40	126.58	122.80
9	a	287	G	N3-C4-N9	5.37	129.22	126.00
7	Y	39	U	C5-C6-N1	-5.37	120.01	122.70
9	a	2006	C	C6-N1-C2	-5.36	118.16	120.30
7	Y	13	C	O4'-C1'-N1	5.34	112.47	108.20
9	a	790	U	C5-C6-N1	-5.23	120.08	122.70
9	a	1775	U	C5-C4-O4	-5.21	122.78	125.90
9	a	2402	U	O4'-C1'-N1	5.14	112.31	108.20
9	a	1313	U	C6-N1-C1'	-5.12	114.04	121.20
9	a	481	G	O4'-C1'-N9	5.11	112.28	108.20
9	a	1774	C	N3-C2-O2	-5.05	118.36	121.90
9	a	1411	U	C2-N1-C1'	5.04	123.75	117.70
9	a	1115	G	O4'-C1'-N9	5.02	112.21	108.20
7	Y	54	U	N3-C2-O2	-5.01	118.69	122.20
9	a	704	G	O4'-C1'-N9	5.00	112.20	108.20

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	2	31	HIS	Peptide
15	g	47	ASP	Peptide
31	w	16	ASN	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	417	0	451	3	0
2	1	377	0	418	0	0
3	2	504	0	572	2	0
4	3	302	0	340	5	0
5	4	480	0	478	11	0
6	X	317	0	161	5	0
7	Y	1578	0	800	45	0
8	Z	1601	0	813	27	0
9	a	59130	0	29764	0	0
10	b	2549	0	1290	0	0
11	c	2082	0	2154	0	0
12	d	1566	0	1618	0	0
13	e	1552	0	1619	0	0
14	f	1410	0	1444	0	0
15	g	1323	0	1371	0	0
16	h	303	0	327	0	0
17	i	1129	0	1162	0	0
18	j	946	0	1023	0	0
19	k	1053	0	1129	0	0
20	l	1075	0	1146	0	0
21	m	945	0	989	0	0
22	n	892	0	923	0	0
23	o	917	0	962	0	0
24	p	947	0	1019	0	0
25	q	816	0	839	0	0
26	r	857	0	922	0	0
27	s	738	0	807	0	0
28	t	779	0	831	0	0
29	u	753	0	780	0	0
30	v	576	0	588	0	0
31	w	625	0	652	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	x	501	0	531	0	0
33	y	449	0	488	0	0
34	z	444	0	458	0	0
35	3	1	0	0	0	0
35	4	1	0	0	0	0
36	Y	10	0	0	1	0
37	Z	22	0	11	1	0
38	Z	10	0	10	1	0
39	a	224	0	0	0	0
39	b	5	0	0	0	0
39	d	1	0	0	0	0
39	z	1	0	0	0	0
40	a	13	0	0	0	0
40	c	2	0	0	0	0
41	0	1	0	0	0	0
41	1	16	0	0	0	0
41	2	22	0	0	0	0
41	3	2	0	0	0	0
41	Z	1	0	0	0	0
41	a	3019	0	0	0	0
41	b	38	0	0	0	0
41	c	84	0	0	0	0
41	d	36	0	0	0	0
41	e	28	0	0	0	0
41	i	9	0	0	0	0
41	j	12	0	0	0	0
41	k	26	0	0	0	0
41	l	24	0	0	0	0
41	m	21	0	0	0	0
41	o	9	0	0	0	0
41	p	20	0	0	0	0
41	q	12	0	0	0	0
41	r	24	0	0	0	0
41	s	7	0	0	0	0
41	t	1	0	0	0	0
41	u	4	0	0	0	0
41	v	10	0	0	0	0
41	w	9	0	0	0	0
41	x	1	0	0	0	0
41	z	24	0	0	0	0
All	All	93683	0	58890	100	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including

hydrogen atoms). The all-atom clashscore for this structure is 6.

All (100) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:Y:26:A:N6	7:Y:44:G:H1	1.59	1.00
7:Y:26:A:H61	7:Y:44:G:H1	0.90	0.89
5:4:16:CYS:SG	5:4:37:CYS:HB3	2.15	0.86
5:4:18:CYS:SG	5:4:40:CYS:HB2	2.17	0.84
7:Y:55:U:C5	7:Y:57:G:OP2	2.35	0.80
7:Y:58:A:O2'	7:Y:61:C:N4	2.17	0.77
7:Y:26:A:N1	7:Y:44:G:N2	2.35	0.73
7:Y:51:U:H3	7:Y:63:G:H1	1.34	0.73
7:Y:63:G:H2'	7:Y:64:A:C8	2.29	0.67
7:Y:43:C:H2'	7:Y:44:G:C8	2.30	0.66
6:X:23:A:H4'	6:X:24:A:O4'	1.96	0.66
7:Y:22:G:H2'	7:Y:23:A:H8	1.62	0.64
7:Y:15:G:H22	7:Y:48:C:H42	1.43	0.64
5:4:37:CYS:N	5:4:40:CYS:SG	2.67	0.63
7:Y:18:G:N2	7:Y:58:A:OP1	2.32	0.63
38:Z:102:FME:SD	38:Z:102:FME:N	2.72	0.62
3:2:16:LYS:HE3	3:2:20:GLY:HA2	1.81	0.61
7:Y:23:A:H2'	7:Y:24:G:H8	1.66	0.60
7:Y:23:A:H2'	7:Y:24:G:C8	2.37	0.60
8:Z:44:A:H2'	8:Z:45:G:O4'	2.02	0.60
8:Z:15:G:OP2	8:Z:16:C:N4	2.35	0.59
7:Y:60:U:OP1	7:Y:62:C:N4	2.23	0.59
8:Z:15:G:H22	8:Z:48:C:H42	1.51	0.58
7:Y:55:U:C4	7:Y:57:G:H5'	2.38	0.58
7:Y:21:A:N6	7:Y:46:G:O2'	2.37	0.58
6:X:24:A:H4'	6:X:25:C:OP2	2.03	0.58
7:Y:30:G:H2'	7:Y:31:A:H8	1.70	0.57
8:Z:51:C:H2'	8:Z:52:G:H8	1.70	0.57
8:Z:9:G:H21	8:Z:45:G:H3'	1.69	0.57
7:Y:75:C:H2'	7:Y:76:A:C8	2.40	0.56
7:Y:58:A:O2'	7:Y:60:U:OP2	2.21	0.56
5:4:16:CYS:SG	5:4:17:SER:N	2.79	0.56
6:X:22:U:O4	6:X:23:A:N6	2.36	0.55
8:Z:51:C:H2'	8:Z:52:G:C8	2.42	0.55
8:Z:67:C:H2'	8:Z:68:C:C6	2.42	0.54
4:3:25:VAL:HB	4:3:35:GLN:CG	2.38	0.53
1:0:14:SER:OG	1:0:48:ILE:O	2.22	0.53
8:Z:3:C:H2'	8:Z:4:G:C8	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:Y:101:YRW:NAG	36:Y:101:YRW:OAC	2.38	0.53
8:Z:31:G:H2'	8:Z:32:C:H6	1.74	0.53
8:Z:23:C:H2'	8:Z:24:U:C6	2.45	0.52
5:4:26:SER:OG	5:4:27:THR:N	2.41	0.52
7:Y:15:G:O6	7:Y:48:C:O2	2.28	0.52
8:Z:61:C:H2'	8:Z:62:C:C6	2.46	0.51
7:Y:70:G:H2'	7:Y:71:G:H8	1.74	0.51
8:Z:55:U:H2'	8:Z:57:A:OP2	2.11	0.51
5:4:20:ASN:HD22	5:4:37:CYS:HB2	1.75	0.50
7:Y:63:G:H2'	7:Y:64:A:H8	1.72	0.50
7:Y:26:A:H2'	7:Y:27:G:H8	1.76	0.50
7:Y:70:G:H2'	7:Y:71:G:C8	2.47	0.50
7:Y:43:C:O2'	7:Y:44:G:H5'	2.10	0.49
7:Y:55:U:H3'	7:Y:56:C:H5"	1.93	0.49
8:Z:15:G:H3'	8:Z:16:C:H6	1.77	0.49
7:Y:60:U:H2'	7:Y:61:C:H5	1.78	0.49
8:Z:22:G:H2'	8:Z:23:C:H6	1.77	0.49
7:Y:15:G:H22	7:Y:48:C:N4	2.11	0.48
7:Y:37:A:H2'	7:Y:38:A:O4'	2.14	0.48
4:3:4:ARG:O	4:3:37:GLN:HA	2.15	0.47
5:4:14:ALA:HB2	5:4:24:ILE:HD13	1.97	0.47
7:Y:5:G:H2'	7:Y:6:G:H8	1.79	0.47
7:Y:31:A:C4	7:Y:32:U:C5	3.03	0.47
8:Z:42:G:H2'	8:Z:43:A:O4'	2.15	0.46
8:Z:48:C:C4	8:Z:59:A:C8	3.04	0.46
8:Z:3:C:H2'	8:Z:4:G:H8	1.81	0.46
7:Y:22:G:H2'	7:Y:23:A:C8	2.45	0.46
8:Z:19:G:H4'	8:Z:20:U:OP2	2.15	0.46
7:Y:15:G:N2	7:Y:48:C:H42	2.13	0.46
8:Z:62:C:H2'	8:Z:63:G:H8	1.82	0.45
6:X:20:U:H2'	6:X:21:C:C6	2.51	0.45
7:Y:30:G:C4	7:Y:31:A:C8	3.04	0.45
7:Y:55:U:H5	7:Y:57:G:OP2	1.95	0.45
7:Y:61:C:H3'	7:Y:62:C:O4'	2.16	0.45
7:Y:46:G:H3'	7:Y:47:U:H5"	1.98	0.45
1:0:11:LEU:HB3	1:0:49:TYR:HB3	1.99	0.44
8:Z:9:G:N2	8:Z:45:G:H3'	2.31	0.44
4:3:25:VAL:HB	4:3:35:GLN:HG2	1.99	0.44
8:Z:45:G:H8	8:Z:45:G:OP2	2.00	0.44
3:2:32:ILE:H	3:2:32:ILE:HG13	1.36	0.44
7:Y:54:U:O2	7:Y:58:A:C8	2.71	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:Y:27:G:C4	7:Y:28:G:C8	3.07	0.43
8:Z:67:C:H2'	8:Z:68:C:H6	1.83	0.43
7:Y:25:C:C2	7:Y:26:A:C8	3.07	0.43
4:3:25:VAL:HB	4:3:35:GLN:HG3	2.00	0.43
7:Y:69:G:H8	7:Y:69:G:OP2	2.02	0.42
8:Z:54:U:H2'	8:Z:55:U:O4'	2.19	0.42
4:3:16:ILE:CD1	4:3:25:VAL:HG22	2.49	0.42
5:4:8:LYS:O	5:4:27:THR:HA	2.20	0.42
5:4:15:SER:O	5:4:33:ASN:HA	2.19	0.42
1:0:38:LYS:HB2	1:0:49:TYR:CD1	2.55	0.42
6:X:19:U:O5'	6:X:19:U:H6	2.03	0.41
8:Z:26:G:N3	8:Z:26:G:H2'	2.36	0.41
5:4:8:LYS:HD2	5:4:8:LYS:HA	1.59	0.41
8:Z:11:A:H2'	8:Z:12:G:C8	2.56	0.41
7:Y:72:C:H2'	7:Y:73:A:O4'	2.20	0.41
8:Z:28:C:H2'	8:Z:29:G:H8	1.84	0.41
5:4:37:CYS:SG	5:4:39:LYS:HG2	2.61	0.41
7:Y:41:C:H2'	7:Y:42:C:H6	1.86	0.41
7:Y:24:G:C6	7:Y:25:C:C4	3.09	0.41
7:Y:35:A:H2'	7:Y:36:A:O4'	2.20	0.40
8:Z:75:C:H5"	37:Z:101:8AN:O2P	2.21	0.40

There are no symmetry-related clashes.

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
1	0	49/55 (89%)	49 (100%)	0	0	100 100
2	1	44/46 (96%)	44 (100%)	0	0	100 100
3	2	62/65 (95%)	59 (95%)	2 (3%)	1 (2%)	9 5
4	3	36/38 (95%)	36 (100%)	0	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	4	56/70 (80%)	50 (89%)	6 (11%)	0	100	100
11	c	269/273 (98%)	262 (97%)	7 (3%)	0	100	100
12	d	206/209 (99%)	202 (98%)	4 (2%)	0	100	100
13	e	199/201 (99%)	195 (98%)	4 (2%)	0	100	100
14	f	175/179 (98%)	163 (93%)	12 (7%)	0	100	100
15	g	174/177 (98%)	153 (88%)	20 (12%)	1 (1%)	25	21
16	h	39/149 (26%)	33 (85%)	5 (13%)	1 (3%)	5	2
17	i	140/142 (99%)	139 (99%)	1 (1%)	0	100	100
18	j	121/123 (98%)	119 (98%)	2 (2%)	0	100	100
19	k	142/144 (99%)	137 (96%)	4 (3%)	1 (1%)	22	18
20	l	132/136 (97%)	128 (97%)	4 (3%)	0	100	100
21	m	116/127 (91%)	111 (96%)	5 (4%)	0	100	100
22	n	114/117 (97%)	111 (97%)	2 (2%)	1 (1%)	17	12
23	o	112/115 (97%)	108 (96%)	4 (4%)	0	100	100
24	p	115/118 (98%)	115 (100%)	0	0	100	100
25	q	101/103 (98%)	98 (97%)	3 (3%)	0	100	100
26	r	108/110 (98%)	106 (98%)	2 (2%)	0	100	100
27	s	91/100 (91%)	88 (97%)	3 (3%)	0	100	100
28	t	100/104 (96%)	91 (91%)	8 (8%)	1 (1%)	15	11
29	u	92/94 (98%)	90 (98%)	2 (2%)	0	100	100
30	v	74/85 (87%)	73 (99%)	1 (1%)	0	100	100
31	w	75/78 (96%)	74 (99%)	1 (1%)	0	100	100
32	x	60/63 (95%)	57 (95%)	3 (5%)	0	100	100
33	y	56/59 (95%)	53 (95%)	3 (5%)	0	100	100
34	z	54/57 (95%)	53 (98%)	1 (2%)	0	100	100
All	All	3112/3337 (93%)	2997 (96%)	109 (4%)	6 (0%)	50	49

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	2	32	ILE
15	g	47	ASP
19	k	36	LYS

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Mol	Chain	Res	Type
16	h	35	LYS
22	n	88	LYS
28	t	99	ASN

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
1	0	46/49 (94%)	45 (98%)	1 (2%)	52 57
2	1	38/38 (100%)	37 (97%)	1 (3%)	46 50
3	2	51/52 (98%)	48 (94%)	3 (6%)	19 17
4	3	34/34 (100%)	34 (100%)	0	100 100
5	4	55/62 (89%)	48 (87%)	7 (13%)	4 2
11	c	216/218 (99%)	213 (99%)	3 (1%)	67 73
12	d	163/163 (100%)	160 (98%)	3 (2%)	59 65
13	e	165/165 (100%)	160 (97%)	5 (3%)	41 44
14	f	148/150 (99%)	134 (90%)	14 (10%)	8 5
15	g	137/138 (99%)	124 (90%)	13 (10%)	8 5
16	h	32/114 (28%)	27 (84%)	5 (16%)	2 1
17	i	116/116 (100%)	115 (99%)	1 (1%)	78 84
18	j	104/104 (100%)	104 (100%)	0	100 100
19	k	103/103 (100%)	102 (99%)	1 (1%)	76 82
20	l	107/107 (100%)	105 (98%)	2 (2%)	57 63
21	m	98/103 (95%)	98 (100%)	0	100 100
22	n	86/87 (99%)	84 (98%)	2 (2%)	50 55
23	o	99/100 (99%)	95 (96%)	4 (4%)	31 32
24	p	89/90 (99%)	87 (98%)	2 (2%)	52 57
25	q	84/84 (100%)	80 (95%)	4 (5%)	25 24
26	r	93/93 (100%)	93 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
27	s	80/84 (95%)	77 (96%)	3 (4%)	33 34
28	t	83/85 (98%)	80 (96%)	3 (4%)	35 36
29	u	78/78 (100%)	77 (99%)	1 (1%)	69 75
30	v	57/63 (90%)	56 (98%)	1 (2%)	59 65
31	w	67/68 (98%)	67 (100%)	0	100 100
32	x	54/55 (98%)	53 (98%)	1 (2%)	57 63
33	y	48/49 (98%)	47 (98%)	1 (2%)	53 59
34	z	47/48 (98%)	46 (98%)	1 (2%)	53 59
All	All	2578/2700 (96%)	2496 (97%)	82 (3%)	42 41

All (82) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0	29	THR
2	1	25	LYS
3	2	31	HIS
3	2	32	ILE
3	2	47	LYS
5	4	22	MET
5	4	26	SER
5	4	40	CYS
5	4	48	GLN
5	4	59	ARG
5	4	63	ARG
5	4	65	ASN
11	c	125	LYS
11	c	182	ARG
11	c	259	SER
12	d	32	ASN
12	d	58	ASN
12	d	95	SER
13	e	17	THR
13	e	55	SER
13	e	88	ARG
13	e	123	LYS
13	e	125	SER
14	f	3	LYS
14	f	5	HIS
14	f	17	MET

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Mol	Chain	Res	Type
14	f	30	ARG
14	f	32	GLU
14	f	94	GLU
14	f	108	VAL
14	f	135	GLN
14	f	136	ILE
14	f	142	ASP
14	f	144	ASP
14	f	146	VAL
14	f	150	ARG
14	f	152	LEU
15	g	29	LYS
15	g	36	THR
15	g	44	LYS
15	g	56	ASP
15	g	73	ASN
15	g	75	MET
15	g	84	THR
15	g	90	VAL
15	g	95	ARG
15	g	122	THR
15	g	127	THR
15	g	129	THR
15	g	166	ASP
16	h	7	ASP
16	h	8	LYS
16	h	11	ASN
16	h	12	LEU
16	h	25	TYR
17	i	10	THR
19	k	120	VAL
20	l	58	LYS
20	l	111	GLU
22	n	25	ARG
22	n	63	LYS
23	o	6	LYS
23	o	7	GLN
23	o	53	ARG
23	o	111	LYS
24	p	11	ARG
24	p	51	ARG
25	q	29	THR

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Mol	Chain	Res	Type
25	q	70	GLU
25	q	73	LYS
25	q	102	SER
27	s	25	GLU
27	s	28	ASN
27	s	64	LYS
28	t	31	SER
28	t	54	GLN
28	t	100	SER
29	u	10	LYS
30	v	10	THR
32	x	56	LEU
33	y	4	THR
34	z	23	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
5	4	20	ASN
13	e	115	GLN
23	o	7	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
10	b	118/120 (98%)	19 (16%)	0
6	X	14/28 (50%)	4 (28%)	1 (7%)
7	Y	71/76 (93%)	27 (38%)	1 (1%)
8	Z	74/76 (97%)	22 (29%)	0
9	a	2745/2904 (94%)	331 (12%)	0
All	All	3022/3204 (94%)	403 (13%)	2 (0%)

All (403) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
6	X	19	U
6	X	24	A
6	X	25	C
6	X	27	A
7	Y	13	C

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Mol	Chain	Res	Type
7	Y	14	A
7	Y	19	G
7	Y	20	U
7	Y	22	G
7	Y	34	G
7	Y	42	C
7	Y	44	G
7	Y	45	U
7	Y	46	G
7	Y	47	U
7	Y	48	C
7	Y	49	C
7	Y	51	U
7	Y	55	U
7	Y	56	C
7	Y	57	G
7	Y	58	A
7	Y	59	U
7	Y	62	C
7	Y	63	G
7	Y	66	U
7	Y	68	C
7	Y	69	G
7	Y	70	G
7	Y	72	C
7	Y	74	C
8	Z	4	G
8	Z	8	U
8	Z	9	G
8	Z	14	A
8	Z	15	G
8	Z	17	C
8	Z	18	G
8	Z	19	G
8	Z	20	U
8	Z	21	A
8	Z	44	A
8	Z	48	C
8	Z	56	C
8	Z	57	A
8	Z	58	A
8	Z	59	A

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Mol	Chain	Res	Type
8	Z	61	C
8	Z	69	C
8	Z	70	G
8	Z	71	C
8	Z	72	A
8	Z	74	C
9	a	10	A
9	a	15	G
9	a	34	U
9	a	45	G
9	a	58	G
9	a	63	A
9	a	71	A
9	a	74	A
9	a	75	G
9	a	93	G
9	a	96	C
9	a	101	A
9	a	102	U
9	a	118	A
9	a	119	A
9	a	120	U
9	a	125	A
9	a	139	U
9	a	140	C
9	a	142	A
9	a	145	C
9	a	163	C
9	a	165	A
9	a	181	A
9	a	196	A
9	a	215	G
9	a	216	A
9	a	221	A
9	a	222	A
9	a	248	G
9	a	272	A
9	a	273	G
9	a	276	U
9	a	278	A
9	a	279	A
9	a	282	A

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Mol	Chain	Res	Type
9	a	287	G
9	a	289	G
9	a	311	A
9	a	329	G
9	a	330	A
9	a	343	C
9	a	353	C
9	a	355	U
9	a	356	G
9	a	361	G
9	a	362	A
9	a	386	G
9	a	396	G
9	a	404	A
9	a	405	U
9	a	411	G
9	a	455	C
9	a	456	C
9	a	481	G
9	a	490	C
9	a	491	G
9	a	504	A
9	a	505	A
9	a	509	C
9	a	530	G
9	a	531	C
9	a	532	A
9	a	544	C
9	a	545	U
9	a	546	U
9	a	547	A
9	a	548	G
9	a	549	G
9	a	550	C
9	a	563	A
9	a	573	U
9	a	575	A
9	a	603	A
9	a	614	A
9	a	615	U
9	a	627	A
9	a	637	A

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Mol	Chain	Res	Type
9	a	645	C
9	a	647	G
9	a	653	U
9	a	654	A
9	a	655	A
9	a	685	A
9	a	686	U
9	a	717	C
9	a	721	A
9	a	730	A
9	a	738	G
9	a	747	5MU
9	a	775	G
9	a	776	G
9	a	782	A
9	a	784	G
9	a	785	G
9	a	789	A
9	a	805	G
9	a	812	C
9	a	827	U
9	a	828	U
9	a	845	A
9	a	846	U
9	a	847	U
9	a	859	G
9	a	877	A
9	a	878	A
9	a	883	G
9	a	884	U
9	a	885	C
9	a	887	U
9	a	888	C
9	a	889	C
9	a	890	C
9	a	891	G
9	a	893	C
9	a	895	U
9	a	896	A
9	a	897	C
9	a	907	G
9	a	910	A

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Mol	Chain	Res	Type
9	a	914	G
9	a	932	U
9	a	946	C
9	a	961	C
9	a	974	G
9	a	983	A
9	a	996	A
9	a	1005	C
9	a	1012	U
9	a	1013	C
9	a	1026	G
9	a	1033	U
9	a	1040	A
9	a	1045	C
9	a	1046	A
9	a	1047	G
9	a	1108	U
9	a	1111	A
9	a	1112	G
9	a	1115	G
9	a	1116	G
9	a	1117	C
9	a	1132	U
9	a	1133	A
9	a	1135	C
9	a	1142	A
9	a	1171	G
9	a	1250	G
9	a	1253	A
9	a	1256	G
9	a	1271	G
9	a	1272	A
9	a	1300	G
9	a	1301	A
9	a	1306	C
9	a	1329	U
9	a	1352	U
9	a	1365	A
9	a	1379	U
9	a	1383	A
9	a	1415	U
9	a	1416	G

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Mol	Chain	Res	Type
9	a	1417	C
9	a	1419	A
9	a	1427	A
9	a	1428	C
9	a	1452	G
9	a	1453	A
9	a	1460	U
9	a	1461	C
9	a	1482	G
9	a	1490	A
9	a	1493	C
9	a	1504	A
9	a	1508	A
9	a	1509	A
9	a	1510	G
9	a	1515	A
9	a	1523	U
9	a	1529	G
9	a	1533	C
9	a	1535	A
9	a	1536	C
9	a	1537	G
9	a	1566	A
9	a	1569	A
9	a	1578	U
9	a	1581	G
9	a	1583	A
9	a	1584	U
9	a	1585	C
9	a	1586	A
9	a	1587	G
9	a	1608	A
9	a	1647	U
9	a	1648	U
9	a	1649	G
9	a	1674	G
9	a	1715	G
9	a	1729	U
9	a	1730	C
9	a	1732	C
9	a	1733	G
9	a	1738	G

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Mol	Chain	Res	Type
9	a	1744	A
9	a	1764	C
9	a	1773	A
9	a	1782	U
9	a	1800	C
9	a	1801	A
9	a	1808	A
9	a	1816	C
9	a	1829	A
9	a	1847	A
9	a	1858	A
9	a	1869	G
9	a	1870	C
9	a	1871	A
9	a	1872	A
9	a	1873	G
9	a	1874	C
9	a	1876	A
9	a	1884	G
9	a	1906	G
9	a	1908	C
9	a	1929	G
9	a	1930	G
9	a	1937	A
9	a	1938	A
9	a	1955	U
9	a	1965	C
9	a	1967	C
9	a	1970	A
9	a	1971	U
9	a	1972	G
9	a	1991	U
9	a	1993	U
9	a	2023	C
9	a	2031	A
9	a	2033	A
9	a	2043	C
9	a	2055	C
9	a	2056	G
9	a	2060	A
9	a	2061	G
9	a	2062	A

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Mol	Chain	Res	Type
9	a	2069	G7M
9	a	2093	G
9	a	2097	A
9	a	2198	A
9	a	2204	G
9	a	2211	A
9	a	2220	U
9	a	2223	G
9	a	2225	A
9	a	2238	G
9	a	2239	G
9	a	2268	A
9	a	2283	C
9	a	2287	A
9	a	2305	U
9	a	2308	G
9	a	2322	A
9	a	2325	G
9	a	2333	A
9	a	2335	A
9	a	2347	C
9	a	2350	C
9	a	2361	G
9	a	2379	G
9	a	2383	G
9	a	2385	C
9	a	2396	G
9	a	2402	U
9	a	2403	C
9	a	2406	A
9	a	2424	C
9	a	2425	A
9	a	2429	G
9	a	2430	A
9	a	2435	A
9	a	2441	U
9	a	2448	A
9	a	2474	U
9	a	2475	C
9	a	2476	A
9	a	2478	A
9	a	2491	U

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Mol	Chain	Res	Type
9	a	2492	U
9	a	2494	G
9	a	2502	G
9	a	2505	G
9	a	2518	A
9	a	2520	C
9	a	2529	G
9	a	2535	G
9	a	2547	A
9	a	2554	U
9	a	2566	A
9	a	2567	G
9	a	2573	C
9	a	2602	A
9	a	2609	U
9	a	2613	U
9	a	2629	U
9	a	2663	G
9	a	2689	U
9	a	2690	U
9	a	2714	G
9	a	2716	C
9	a	2726	A
9	a	2733	A
9	a	2744	G
9	a	2748	A
9	a	2757	A
9	a	2765	A
9	a	2778	A
9	a	2791	G
9	a	2795	C
9	a	2798	U
9	a	2802	G
9	a	2820	A
9	a	2821	A
9	a	2835	A
9	a	2849	U
9	a	2873	A
9	a	2880	C
9	a	2883	A
9	a	2884	U
9	a	2899	A

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Mol	Chain	Res	Type
9	a	2903	U
10	b	13	G
10	b	18	G
10	b	25	U
10	b	33	G
10	b	35	C
10	b	36	C
10	b	37	C
10	b	42	C
10	b	45	A
10	b	50	A
10	b	56	G
10	b	57	A
10	b	66	A
10	b	68	C
10	b	89	U
10	b	90	C
10	b	99	A
10	b	109	A
10	b	110	C

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
6	X	24	A
7	Y	13	C

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

26 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	$\#\|Z\| > 2$
9	PSU	a	1911	9	18,21,22	1.33	2 (11%)	22,30,33	1.95	3 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
9	2MG	a	2445	9	18,26,27	1.04	1 (5%)	16,38,41	1.18	3 (18%)
9	PSU	a	2457	9	18,21,22	1.46	4 (22%)	22,30,33	1.88	4 (18%)
9	G7M	a	2069	9	20,26,27	1.11	2 (10%)	17,39,42	0.69	0
9	OMG	a	2251	40,9,8	18,26,27	0.91	1 (5%)	19,38,41	1.13	3 (15%)
9	5MC	a	1962	9	18,22,23	0.89	2 (11%)	26,32,35	1.09	2 (7%)
20	4D4	l	81	20	9,11,12	1.94	2 (22%)	8,13,15	0.97	0
9	H2U	a	2449	9	18,21,22	1.12	2 (11%)	21,30,33	1.65	3 (14%)
9	PSU	a	2604	9	18,21,22	1.45	3 (16%)	22,30,33	1.91	5 (22%)
9	6MZ	a	2030	9	18,25,26	0.79	1 (5%)	16,36,39	2.79	5 (31%)
9	5MU	a	747	9	19,22,23	1.40	5 (26%)	28,32,35	2.13	6 (21%)
9	OMC	a	2498	9,39	19,22,23	0.79	1 (5%)	26,31,34	0.95	1 (3%)
9	OMU	a	2552	9,39	19,22,23	1.22	2 (10%)	26,31,34	1.73	5 (19%)
9	PSU	a	746	9,39	18,21,22	1.32	2 (11%)	22,30,33	1.80	3 (13%)
9	PSU	a	2605	9	18,21,22	1.39	2 (11%)	22,30,33	2.01	4 (18%)
9	PSU	a	955	9	18,21,22	1.37	3 (16%)	22,30,33	1.92	3 (13%)
9	1MG	a	745	9	18,26,27	0.67	0	19,39,42	1.07	2 (10%)
9	PSU	a	2504	40,9	18,21,22	1.39	3 (16%)	22,30,33	1.90	4 (18%)
9	PSU	a	2580	9	18,21,22	1.35	3 (16%)	22,30,33	2.01	4 (18%)
9	6MZ	a	1618	9	18,25,26	0.88	1 (5%)	16,36,39	2.34	3 (18%)
9	PSU	a	1917	9	18,21,22	1.44	2 (11%)	22,30,33	2.00	4 (18%)
9	5MU	a	1939	9	19,22,23	1.38	5 (26%)	28,32,35	2.12	6 (21%)
9	2MA	a	2503	40,9,39	17,25,26	0.95	0	17,37,40	1.01	2 (11%)
12	MEQ	d	150	12	8,9,10	0.45	0	5,10,12	0.25	0
9	3TD	a	1915	9	18,22,23	1.55	4 (22%)	22,32,35	2.02	2 (9%)
9	2MG	a	1835	9	18,26,27	0.93	1 (5%)	16,38,41	1.17	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
9	PSU	a	1911	9	-	0/7/25/26	0/2/2/2
9	2MG	a	2445	9	-	0/5/27/28	0/3/3/3
9	PSU	a	2457	9	-	0/7/25/26	0/2/2/2
9	G7M	a	2069	9	-	1/3/25/26	0/3/3/3
9	OMG	a	2251	40,9,8	-	0/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	5MC	a	1962	9	-	2/7/25/26	0/2/2/2
20	4D4	l	81	20	-	1/11/12/14	-
9	H2U	a	2449	9	-	0/7/38/39	0/2/2/2
9	PSU	a	2604	9	-	0/7/25/26	0/2/2/2
9	6MZ	a	2030	9	-	2/5/27/28	0/3/3/3
9	5MU	a	747	9	-	1/7/25/26	0/2/2/2
9	OMC	a	2498	9,39	-	0/9/27/28	0/2/2/2
9	OMU	a	2552	9,39	-	1/9/27/28	0/2/2/2
9	PSU	a	746	9,39	-	1/7/25/26	0/2/2/2
9	PSU	a	2605	9	-	0/7/25/26	0/2/2/2
9	PSU	a	955	9	-	0/7/25/26	0/2/2/2
9	1MG	a	745	9	-	0/3/25/26	0/3/3/3
9	PSU	a	2504	40,9	-	0/7/25/26	0/2/2/2
9	PSU	a	2580	9	-	0/7/25/26	0/2/2/2
9	6MZ	a	1618	9	-	0/5/27/28	0/3/3/3
9	PSU	a	1917	9	-	0/7/25/26	0/2/2/2
9	5MU	a	1939	9	-	0/7/25/26	0/2/2/2
9	2MA	a	2503	40,9,39	-	2/3/25/26	0/3/3/3
12	MEQ	d	150	12	-	2/8/9/11	-
9	3TD	a	1915	9	-	0/7/25/26	0/2/2/2
9	2MG	a	1835	9	-	0/5/27/28	0/3/3/3

All (54) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	l	81	4D4	CZ-NE	3.94	1.41	1.33
9	a	2504	PSU	C6-C5	3.36	1.39	1.35
9	a	2604	PSU	C4-N3	-3.28	1.32	1.38
9	a	2457	PSU	C6-C5	3.25	1.39	1.35
9	a	955	PSU	C6-C5	3.23	1.39	1.35
9	a	1917	PSU	C4-N3	-3.17	1.33	1.38
9	a	1917	PSU	C6-C5	3.16	1.39	1.35
9	a	2069	G7M	C5-C4	3.11	1.45	1.39
9	a	2605	PSU	C6-C5	3.07	1.38	1.35
9	a	2604	PSU	C6-C5	3.05	1.38	1.35
9	a	2580	PSU	C6-C5	3.04	1.38	1.35
9	a	1915	3TD	C4-N3	-3.01	1.33	1.40
9	a	1911	PSU	C6-C5	2.95	1.38	1.35
9	a	1915	3TD	C6-C5	2.94	1.38	1.35
9	a	2605	PSU	C4-N3	-2.92	1.33	1.38
9	a	955	PSU	C4-N3	-2.90	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	a	2504	PSU	C4-N3	-2.90	1.33	1.38
9	a	2457	PSU	C4-N3	-2.89	1.33	1.38
9	a	1915	3TD	C10-N3	2.87	1.52	1.47
9	a	2552	OMU	C4-N3	-2.87	1.33	1.38
9	a	2449	H2U	C2-N3	-2.86	1.32	1.38
9	a	746	PSU	C4-N3	-2.83	1.33	1.38
9	a	1835	2MG	C6-N1	-2.79	1.33	1.37
9	a	747	5MU	C4-N3	-2.72	1.33	1.38
9	a	1939	5MU	C4-N3	-2.71	1.33	1.38
9	a	2580	PSU	C4-N3	-2.66	1.33	1.38
9	a	2251	OMG	C6-N1	-2.57	1.34	1.37
9	a	2445	2MG	C6-N1	-2.57	1.34	1.37
9	a	747	5MU	C6-C5	2.55	1.38	1.34
9	a	1939	5MU	C6-C5	2.55	1.38	1.34
9	a	2069	G7M	C6-N1	-2.54	1.34	1.37
9	a	1962	5MC	C6-C5	2.52	1.38	1.34
9	a	2449	H2U	C4-N3	-2.50	1.33	1.37
9	a	2552	OMU	C2-N3	-2.48	1.33	1.38
20	l	81	4D4	CZ-NH2	2.48	1.42	1.32
9	a	746	PSU	C6-C5	2.47	1.38	1.35
9	a	1911	PSU	C4-N3	-2.46	1.34	1.38
9	a	1939	5MU	C4-C5	2.43	1.48	1.44
9	a	1915	3TD	C2-N1	-2.38	1.34	1.37
9	a	747	5MU	C4-C5	2.38	1.48	1.44
9	a	1939	5MU	C2-N3	-2.37	1.33	1.38
9	a	747	5MU	C6-N1	-2.33	1.34	1.38
9	a	1962	5MC	C6-N1	-2.33	1.34	1.38
9	a	2604	PSU	C2-N3	-2.32	1.33	1.37
9	a	1939	5MU	C6-N1	-2.32	1.34	1.38
9	a	2580	PSU	O4'-C1'	-2.26	1.40	1.43
9	a	2457	PSU	C2-N3	-2.20	1.33	1.37
9	a	747	5MU	C2-N1	2.19	1.42	1.38
9	a	2457	PSU	C2-N1	-2.12	1.33	1.36
9	a	1618	6MZ	C5-C4	2.09	1.46	1.40
9	a	955	PSU	C2-N3	-2.08	1.33	1.37
9	a	2030	6MZ	C5-C4	2.06	1.46	1.40
9	a	2504	PSU	C2-N3	-2.05	1.34	1.37
9	a	2498	OMC	C6-C5	2.04	1.39	1.35

All (80) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	a	1915	3TD	N1-C2-N3	7.42	121.99	116.14
9	a	2030	6MZ	C2-N1-C6	7.38	122.92	116.59
9	a	1618	6MZ	C2-N1-C6	6.50	122.16	116.59
9	a	1917	PSU	N1-C2-N3	6.40	122.38	115.13
9	a	2605	PSU	N1-C2-N3	6.36	122.34	115.13
9	a	2604	PSU	N1-C2-N3	6.26	122.22	115.13
9	a	2580	PSU	N1-C2-N3	6.14	122.09	115.13
9	a	955	PSU	N1-C2-N3	6.11	122.05	115.13
9	a	2449	H2U	C4-N3-C2	-6.03	120.79	125.79
9	a	2504	PSU	N1-C2-N3	5.99	121.92	115.13
9	a	2457	PSU	N1-C2-N3	5.97	121.89	115.13
9	a	1911	PSU	N1-C2-N3	5.96	121.88	115.13
9	a	746	PSU	N1-C2-N3	5.80	121.70	115.13
9	a	2030	6MZ	C9-N6-C6	-5.79	117.89	122.87
9	a	747	5MU	C4-N3-C2	-5.36	120.41	127.35
9	a	1939	5MU	C4-N3-C2	-5.28	120.52	127.35
9	a	747	5MU	N3-C2-N1	5.26	121.88	114.89
9	a	1939	5MU	N3-C2-N1	4.78	121.24	114.89
9	a	1939	5MU	C5-C4-N3	4.70	119.32	115.31
9	a	2552	OMU	N3-C2-N1	4.49	120.85	114.89
9	a	1618	6MZ	C9-N6-C6	-4.44	119.05	122.87
9	a	2552	OMU	C4-N3-C2	-4.41	120.76	126.58
9	a	2605	PSU	C4-N3-C2	-4.30	120.14	126.34
9	a	1939	5MU	C5-C6-N1	-4.28	118.94	123.34
9	a	747	5MU	C5-C4-N3	4.23	118.92	115.31
9	a	2580	PSU	C4-N3-C2	-4.17	120.33	126.34
9	a	1911	PSU	C4-N3-C2	-4.17	120.34	126.34
9	a	1917	PSU	C4-N3-C2	-4.17	120.34	126.34
9	a	2504	PSU	C4-N3-C2	-4.09	120.44	126.34
9	a	955	PSU	C4-N3-C2	-3.95	120.64	126.34
9	a	1939	5MU	O4-C4-C5	-3.92	120.36	124.90
9	a	746	PSU	C4-N3-C2	-3.90	120.72	126.34
9	a	2457	PSU	C4-N3-C2	-3.90	120.73	126.34
9	a	1915	3TD	C4-N3-C2	-3.89	120.39	124.61
9	a	2604	PSU	C4-N3-C2	-3.84	120.80	126.34
9	a	747	5MU	O4-C4-C5	-3.84	120.45	124.90
9	a	1618	6MZ	N3-C2-N1	-3.83	122.70	128.68
9	a	1911	PSU	O2-C2-N1	-3.69	118.73	122.79
9	a	2030	6MZ	N3-C2-N1	-3.64	122.99	128.68
9	a	1917	PSU	O2-C2-N1	-3.60	118.83	122.79
9	a	747	5MU	C5-C6-N1	-3.58	119.65	123.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	a	1962	5MC	C5-C6-N1	-3.42	119.81	123.34
9	a	2552	OMU	C5-C4-N3	3.41	119.95	114.84
9	a	2030	6MZ	C4-C5-N7	-3.37	105.88	109.40
9	a	1939	5MU	O2-C2-N1	-3.30	118.40	122.79
9	a	2605	PSU	O2-C2-N1	-3.28	119.17	122.79
9	a	2580	PSU	O2-C2-N1	-3.14	119.33	122.79
9	a	2457	PSU	O2-C2-N1	-3.13	119.35	122.79
9	a	747	5MU	O2-C2-N1	-3.08	118.69	122.79
9	a	2552	OMU	O2-C2-N1	-2.92	118.91	122.79
9	a	2504	PSU	O2-C2-N1	-2.90	119.60	122.79
9	a	2030	6MZ	C1'-N9-C4	-2.85	121.62	126.64
9	a	2552	OMU	O4-C4-C5	-2.76	120.30	125.16
9	a	1962	5MC	C5-C4-N3	-2.71	118.75	121.67
9	a	2251	OMG	C5-C6-N1	2.70	118.72	113.95
9	a	955	PSU	O2-C2-N1	-2.66	119.87	122.79
9	a	745	1MG	C8-N7-C5	2.47	107.69	102.99
9	a	746	PSU	O2-C2-N1	-2.44	120.10	122.79
9	a	2503	2MA	C5-C6-N1	2.41	118.18	114.02
9	a	2498	OMC	O2-C2-N3	-2.40	118.43	122.33
9	a	1835	2MG	C8-N7-C5	2.39	107.55	102.99
9	a	2503	2MA	C8-N7-C5	2.35	107.47	102.99
9	a	2605	PSU	C5-C6-N1	-2.35	118.59	122.11
9	a	2580	PSU	O4'-C1'-C2'	2.34	108.45	105.14
9	a	2445	2MG	C8-N7-C5	2.33	107.44	102.99
9	a	2457	PSU	C5-C6-N1	-2.32	118.63	122.11
9	a	2604	PSU	O2-C2-N1	-2.31	120.25	122.79
9	a	2445	2MG	C5-C6-N1	2.29	117.99	113.95
9	a	1835	2MG	C5-C6-N1	2.28	117.97	113.95
9	a	2604	PSU	O2-C2-N3	-2.28	117.53	121.82
9	a	2251	OMG	C8-N7-C5	2.25	107.28	102.99
9	a	745	1MG	C5-C6-N1	2.25	117.28	113.90
9	a	1917	PSU	C5-C6-N1	-2.14	118.90	122.11
9	a	2449	H2U	O2-C2-N1	-2.13	120.44	123.11
9	a	2504	PSU	C5-C6-N1	-2.11	118.95	122.11
9	a	1835	2MG	O6-C6-C5	-2.10	120.27	124.37
9	a	2449	H2U	N3-C2-N1	2.07	118.84	116.65
9	a	2445	2MG	C3'-C2'-C1'	2.06	104.09	100.98
9	a	2251	OMG	O6-C6-C5	-2.06	120.35	124.37
9	a	2604	PSU	C5-C6-N1	-2.04	119.05	122.11

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	d	150	MEQ	NE2-CD-CG-CB
12	d	150	MEQ	OE1-CD-CG-CB
9	a	2030	6MZ	O4'-C4'-C5'-O5'
9	a	747	5MU	C3'-C4'-C5'-O5'
9	a	1962	5MC	C2'-C1'-N1-C6
9	a	2552	OMU	C3'-C2'-O2'-CM2
20	l	81	4D4	NE-CD-CG-CB
9	a	1962	5MC	O4'-C1'-N1-C6
9	a	2069	G7M	O4'-C4'-C5'-O5'
9	a	746	PSU	O4'-C1'-C5-C6
9	a	2030	6MZ	C3'-C4'-C5'-O5'
9	a	2503	2MA	O4'-C4'-C5'-O5'
9	a	2503	2MA	C4'-C5'-O5'-P

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 251 ligands modelled in this entry, 248 are monoatomic - leaving 3 for Mogul analysis.

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	$\#\|Z\| > 2$
37	8AN	Z	101	39,38,8	19,24,25	0.93	1 (5%)	13,35,38	1.00	1 (7%)
36	YRW	Y	101	7	9,10,10	2.91	3 (33%)	10,13,13	1.82	1 (10%)
38	FME	Z	102	37	8,9,10	0.89	0	7,9,11	0.92	0

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
37	8AN	Z	101	39,38,8	-	1/3/25/26	0/3/3/3
36	YRW	Y	101	7	-	0/4/4/4	0/1/1/1
38	FME	Z	102	37	-	4/7/9/11	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	Y	101	YRW	CAE-CAB	-7.60	1.39	1.50
36	Y	101	YRW	CAJ-NAI	2.86	1.40	1.34
37	Z	101	8AN	C3'-N3'	-2.82	1.43	1.47
36	Y	101	YRW	CAH-NAI	2.23	1.40	1.33

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	Y	101	YRW	CAE-CAF-NAG	-4.65	116.53	122.67
37	Z	101	8AN	C5-C6-N6	2.40	124.00	120.35

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
37	Z	101	8AN	C4'-C5'-O5'-P
38	Z	102	FME	N-CA-CB-CG
38	Z	102	FME	CB-CG-SD-CE
38	Z	102	FME	CA-CB-CG-SD
38	Z	102	FME	C-CA-CB-CG

There are no ring outliers.

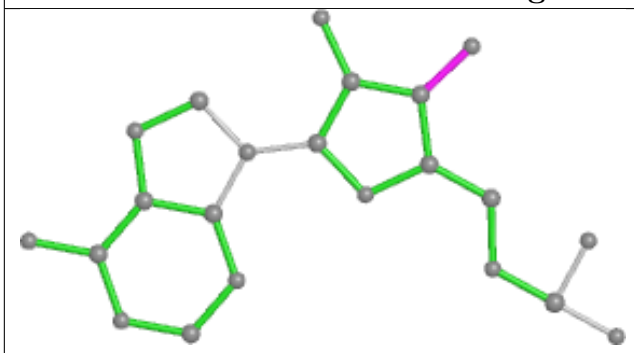
3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
37	Z	101	8AN	1	0
36	Y	101	YRW	1	0
38	Z	102	FME	1	0

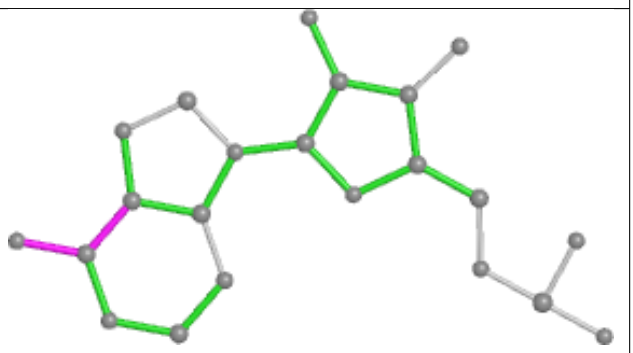
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is

within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

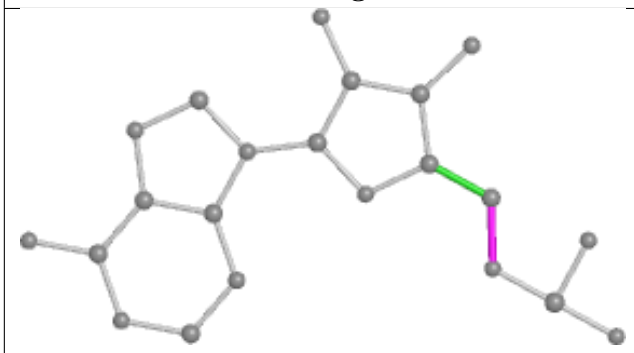
Ligand 8AN Z 101



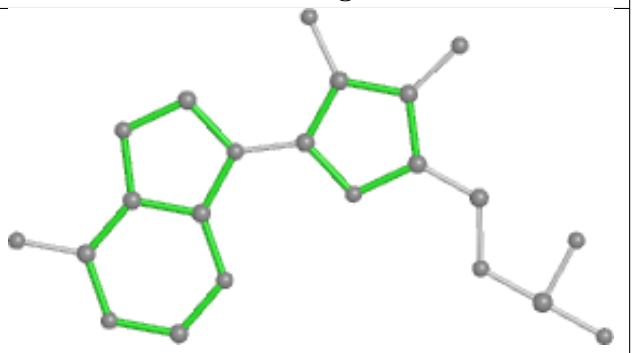
Bond lengths



Bond angles

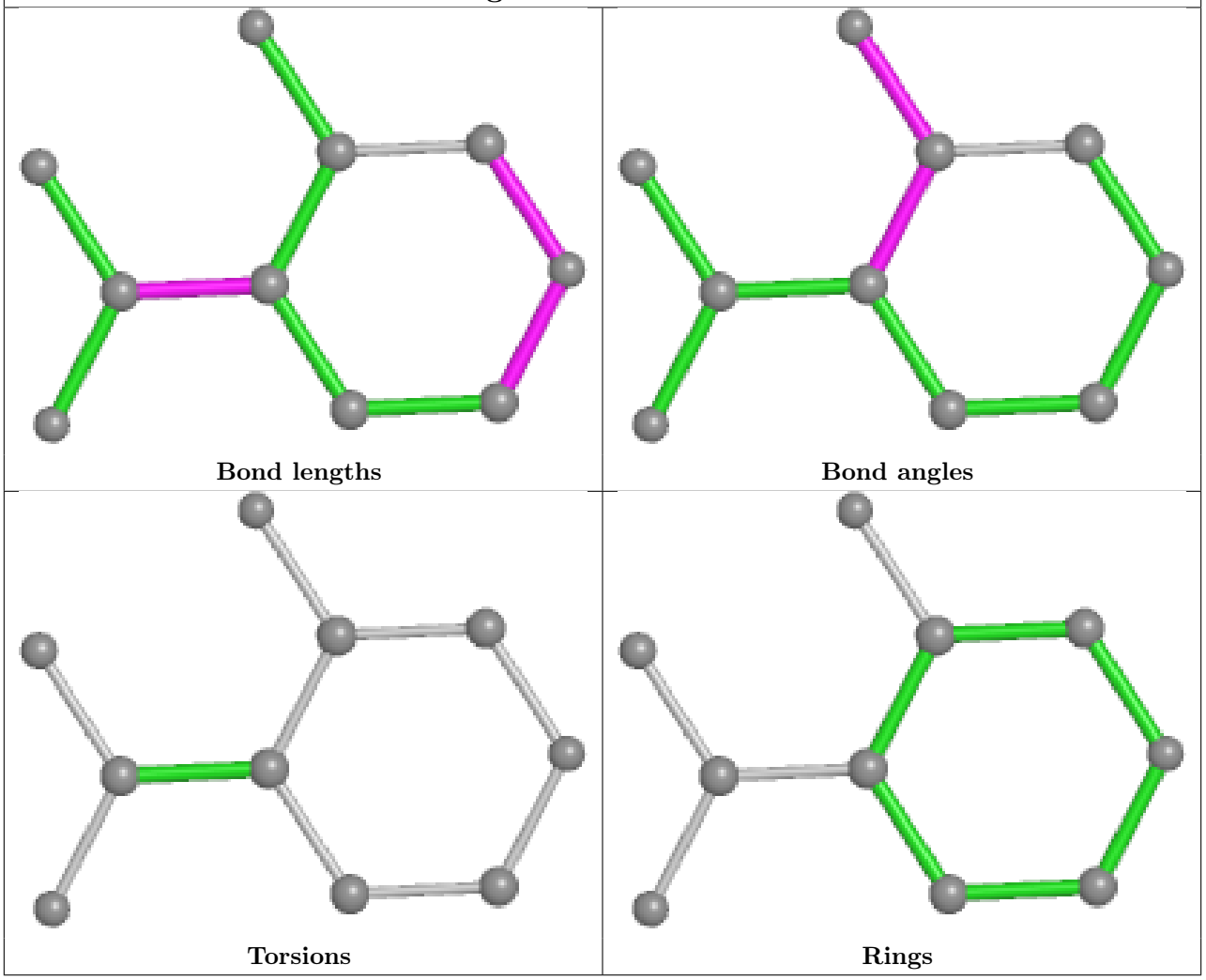


Torsions



Rings

Ligand YRW Y 101



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.

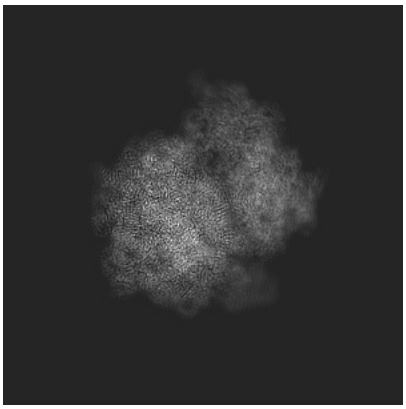
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-29788. These allow visual inspection of the internal detail of the map and identification of artifacts.

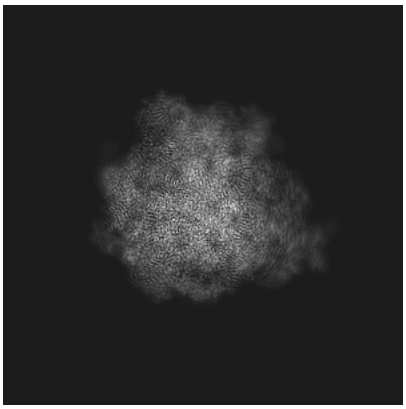
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

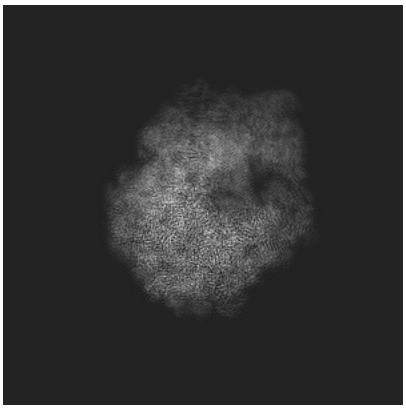
6.1.1 Primary map



X

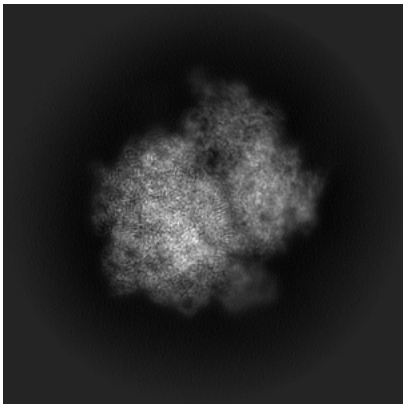


Y

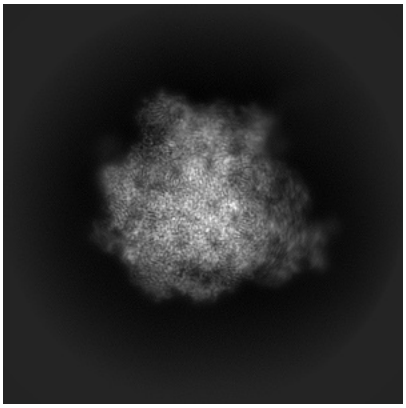


Z

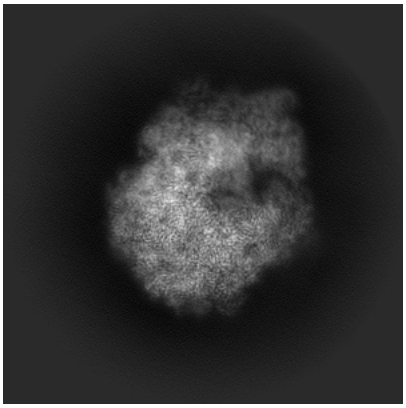
6.1.2 Raw map



X



Y

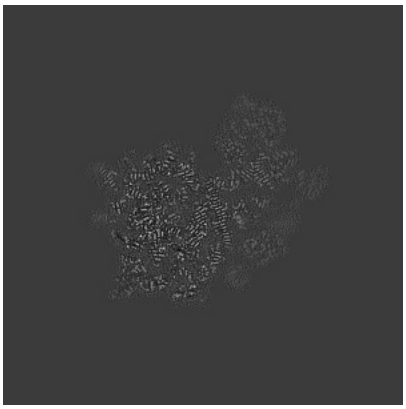


Z

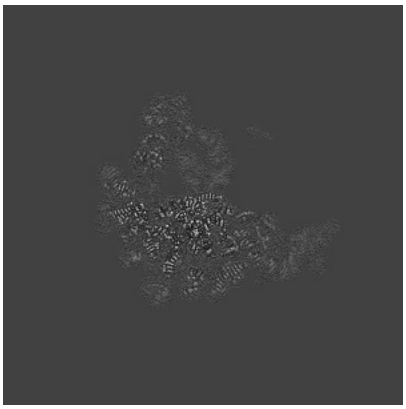
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

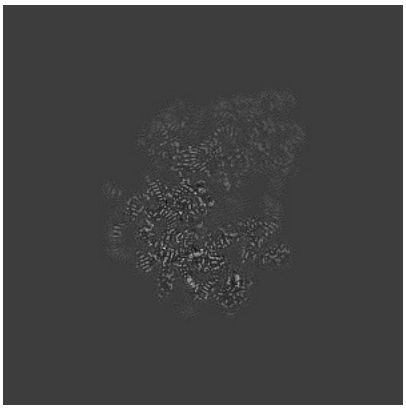
6.2.1 Primary map



X Index: 248

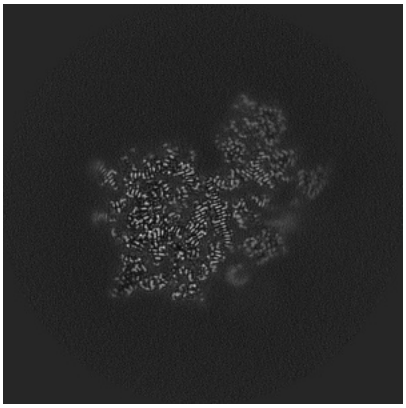


Y Index: 248

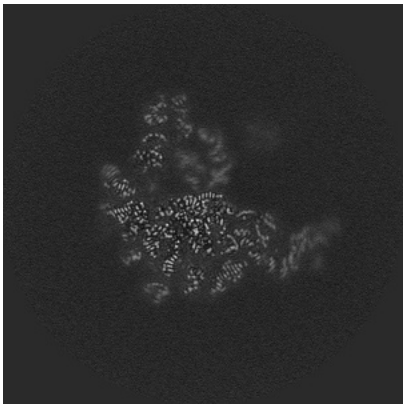


Z Index: 248

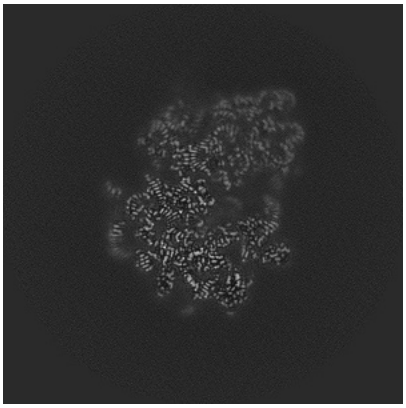
6.2.2 Raw map



X Index: 248



Y Index: 248



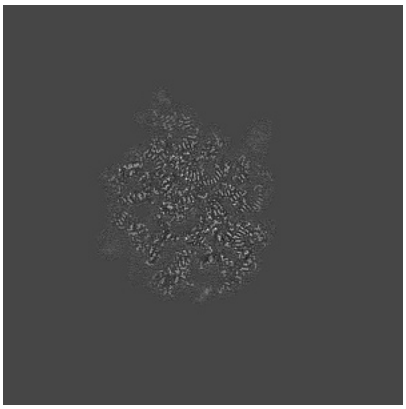
Z Index: 248

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

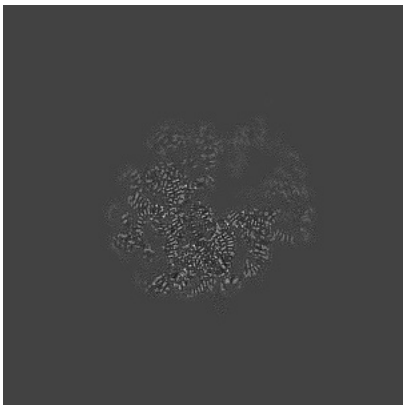
6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 218

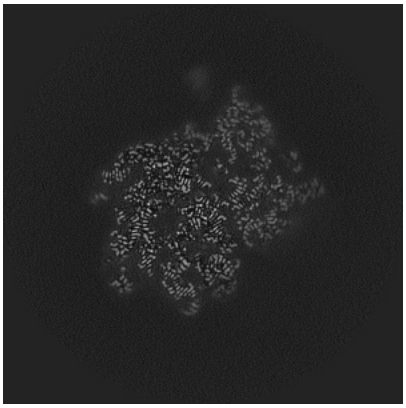


Y Index: 205

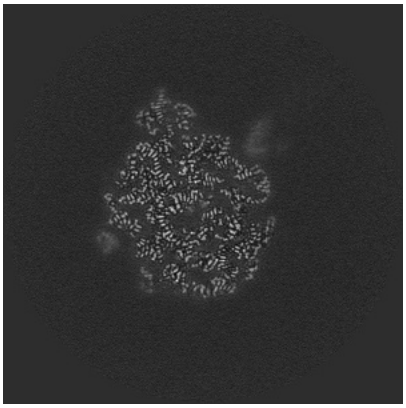


Z Index: 205

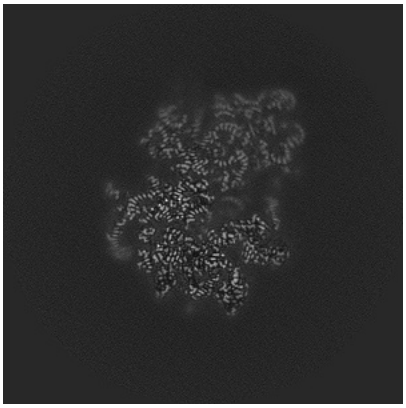
6.3.2 Raw map



X Index: 223



Y Index: 213

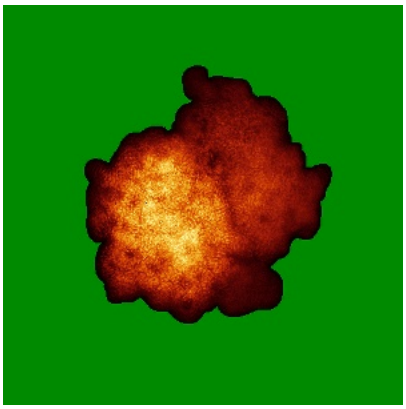


Z Index: 245

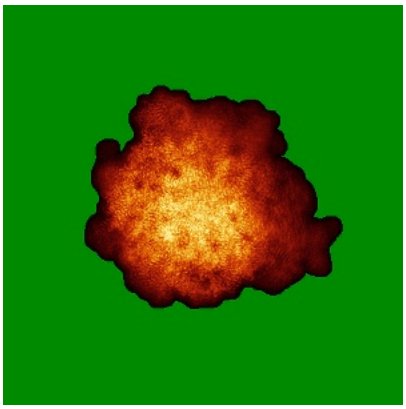
The images above show the largest variance slices of the map in three orthogonal directions.

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

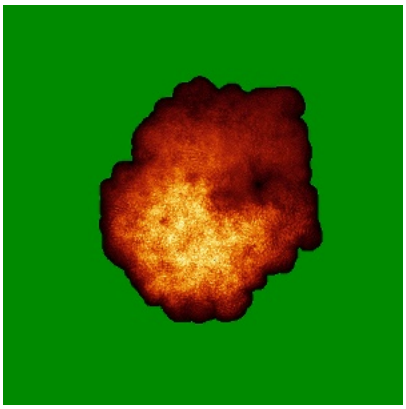
6.4.1 Primary map



X

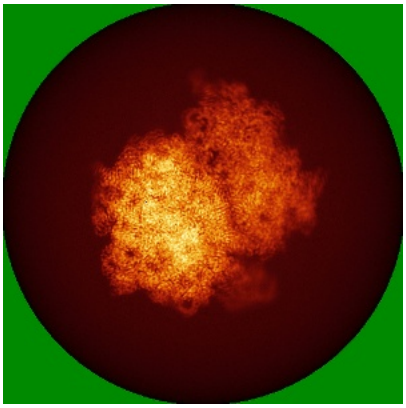


Y

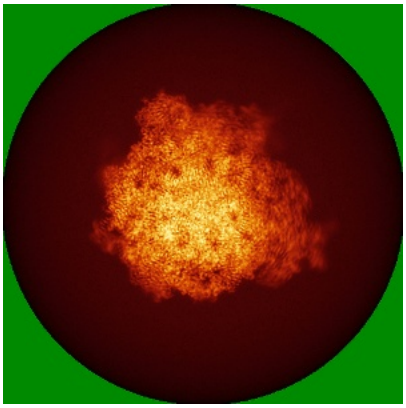


Z

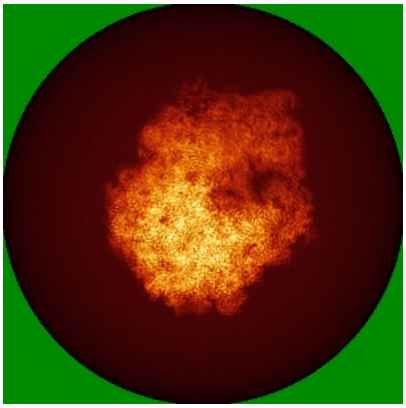
6.4.2 Raw map



X



Y

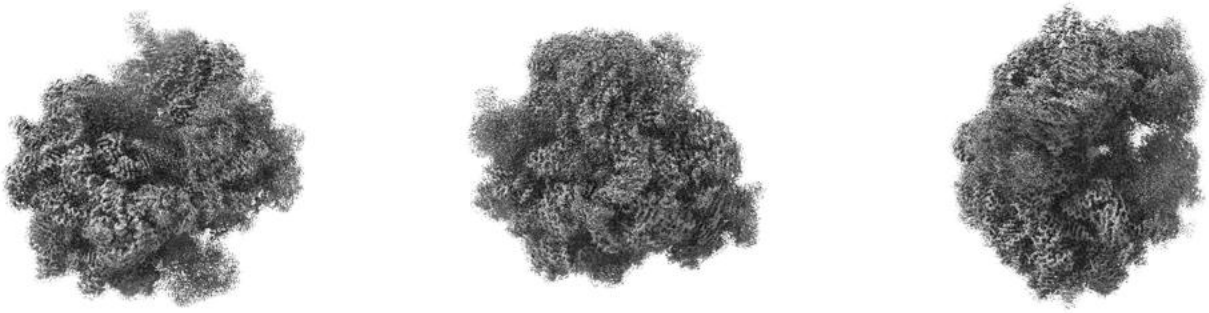


Z

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 0.0265. 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.

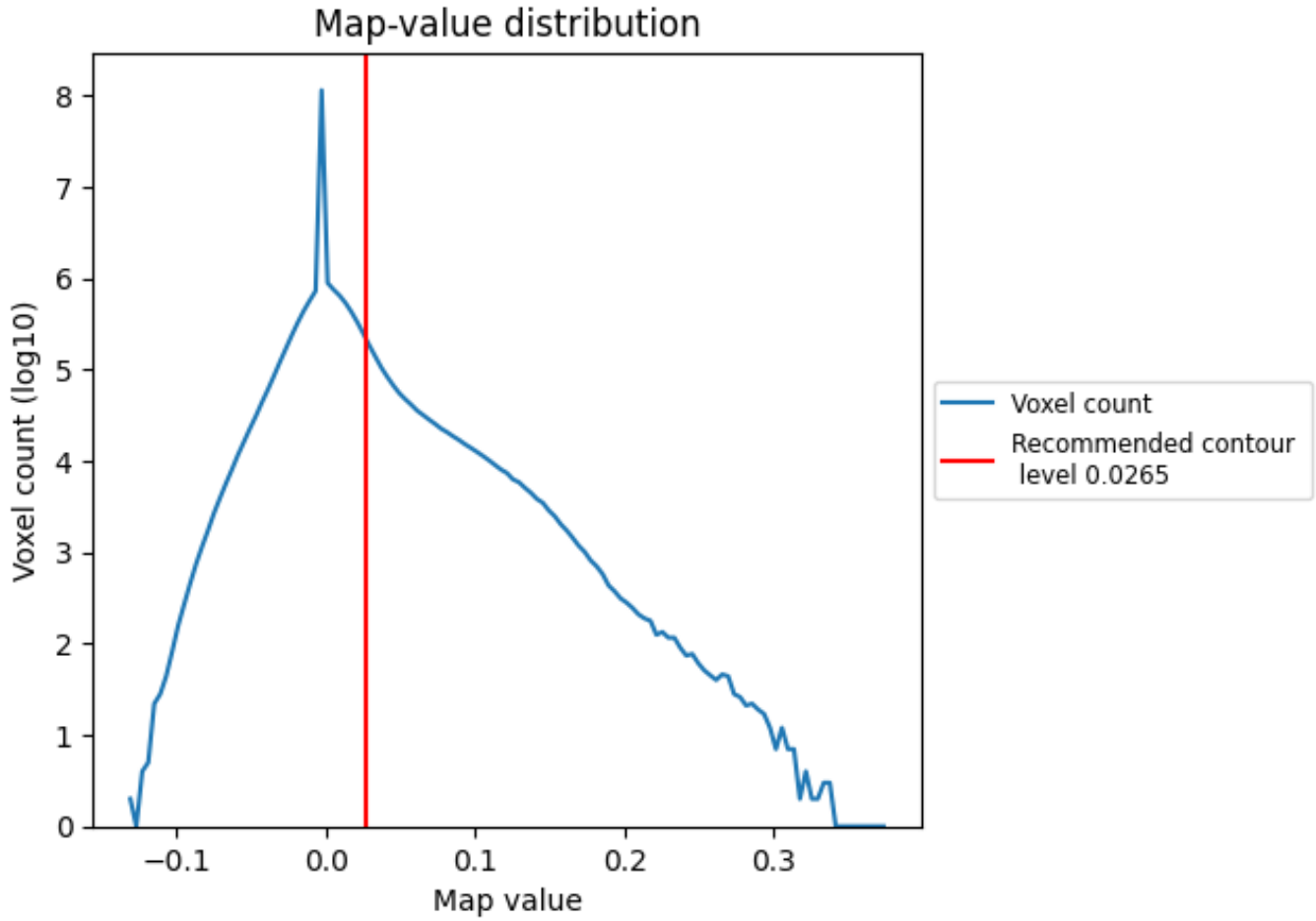
6.6 Mask visualisation (i)

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

7 Map analysis

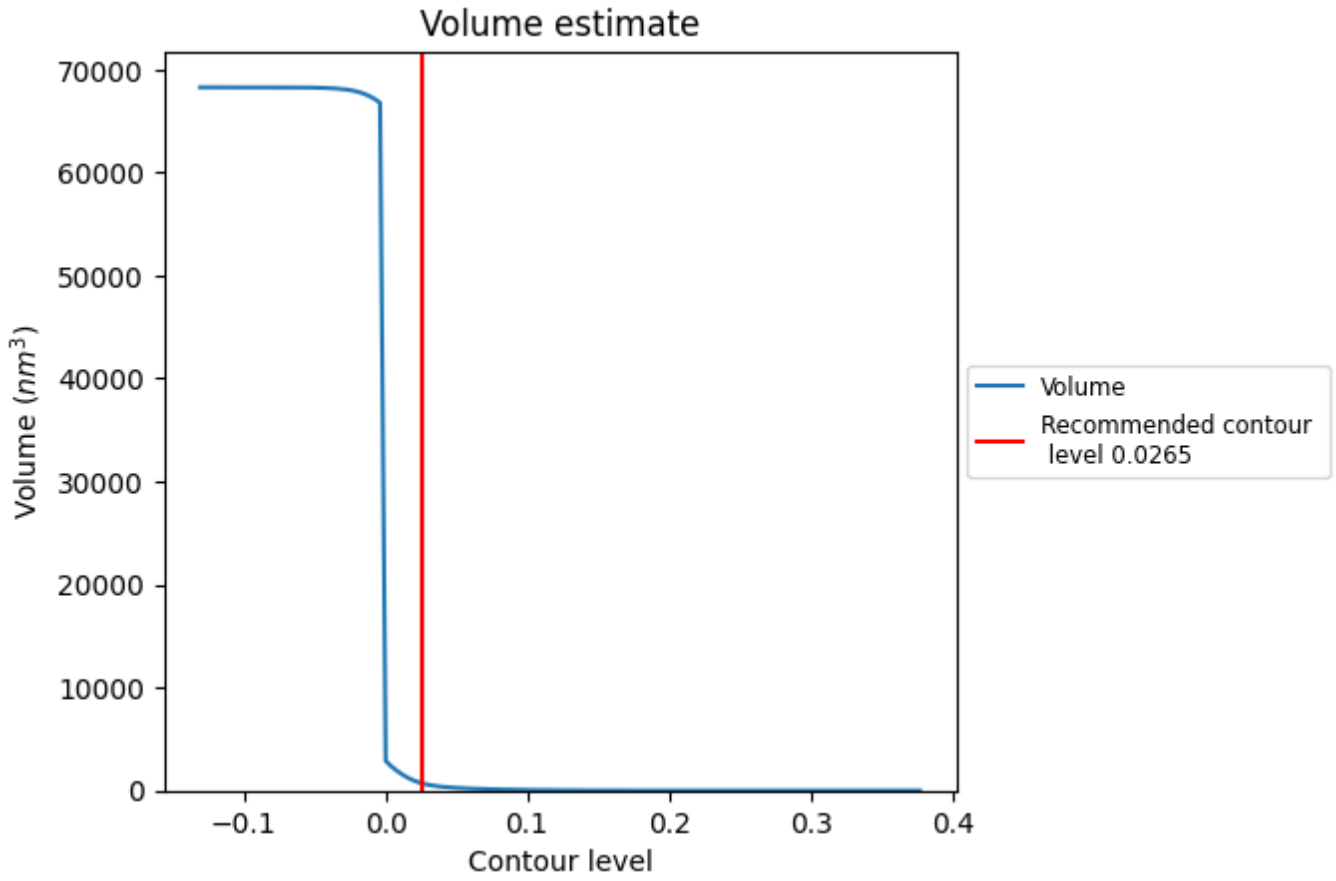
This section contains the results of statistical analysis of the map.

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.

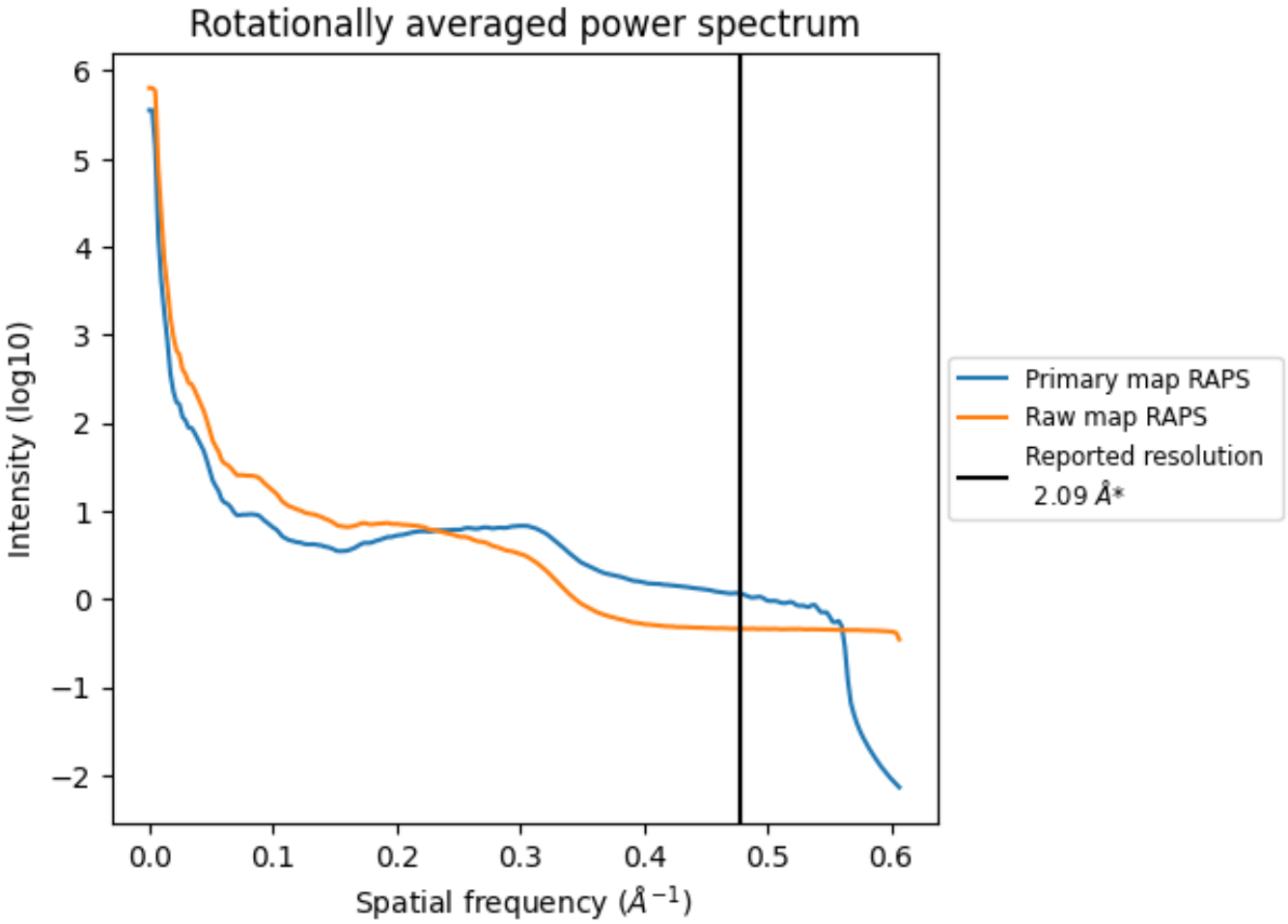
7.2 Volume estimate



The volume at the recommended contour level is 687 nm^3; this corresponds to an approximate mass of 620 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)

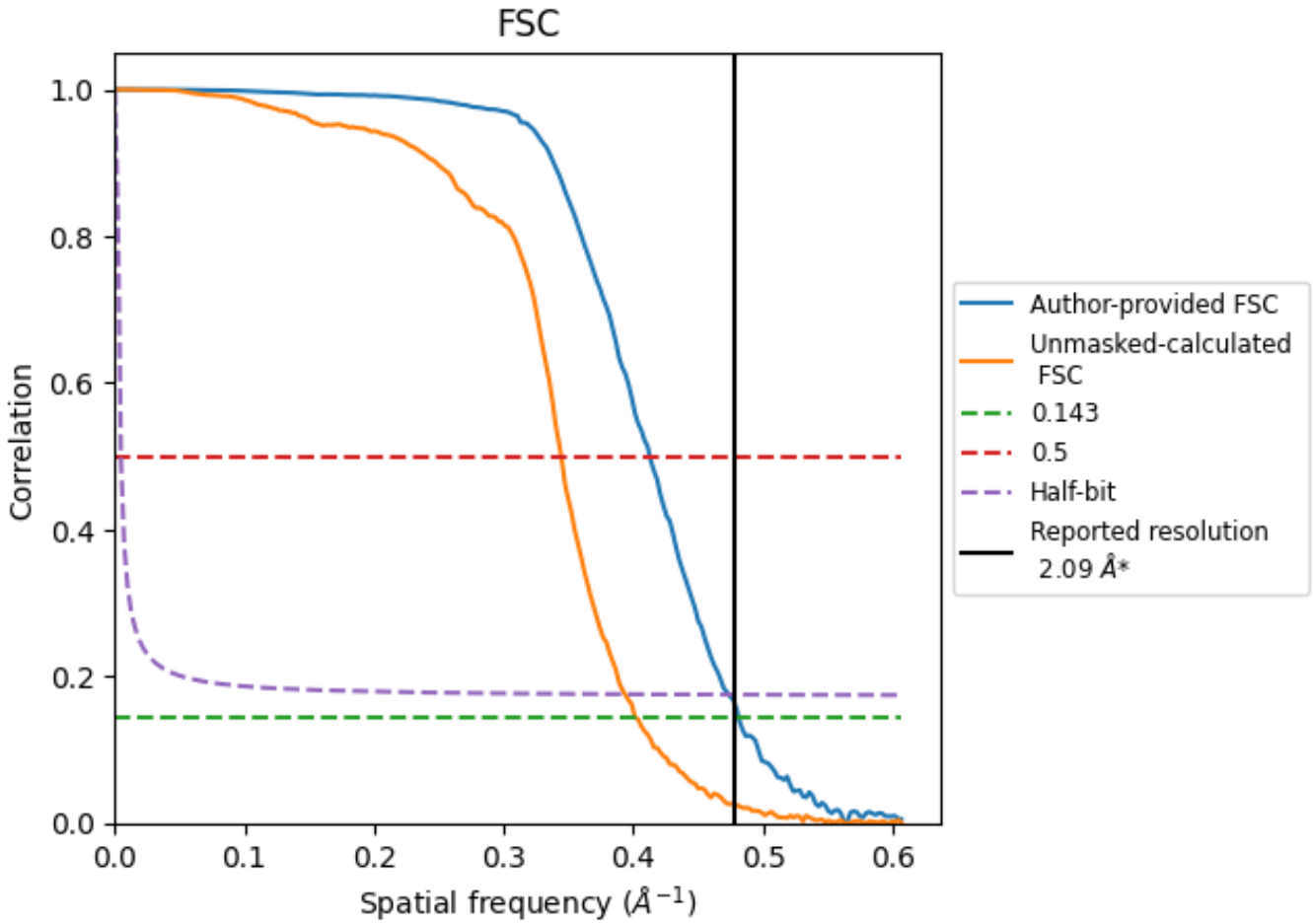


*Reported resolution corresponds to spatial frequency of 0.478 Å^{-1}

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 0.478 $Å^{-1}$

8.2 Resolution estimates (i)

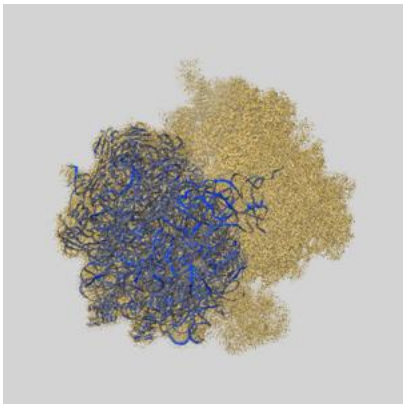
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.09	-	-
Author-provided FSC curve	2.08	2.42	2.11
Unmasked-calculated*	2.49	2.90	2.54

*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 2.49 differs from the reported value 2.09 by more than 10 %

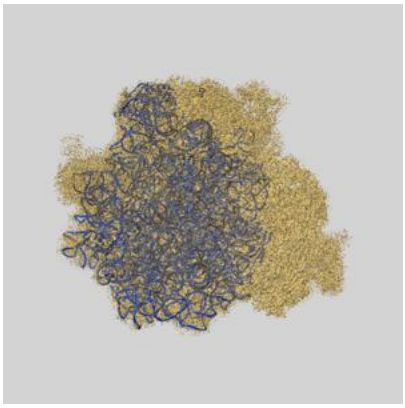
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-29788 and PDB model 8G6Y. Per-residue inclusion information can be found in section 3 on page 14.

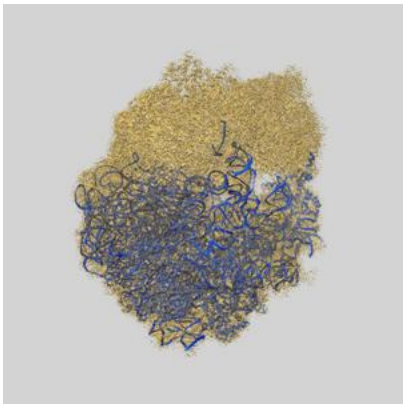
9.1 Map-model overlay



X



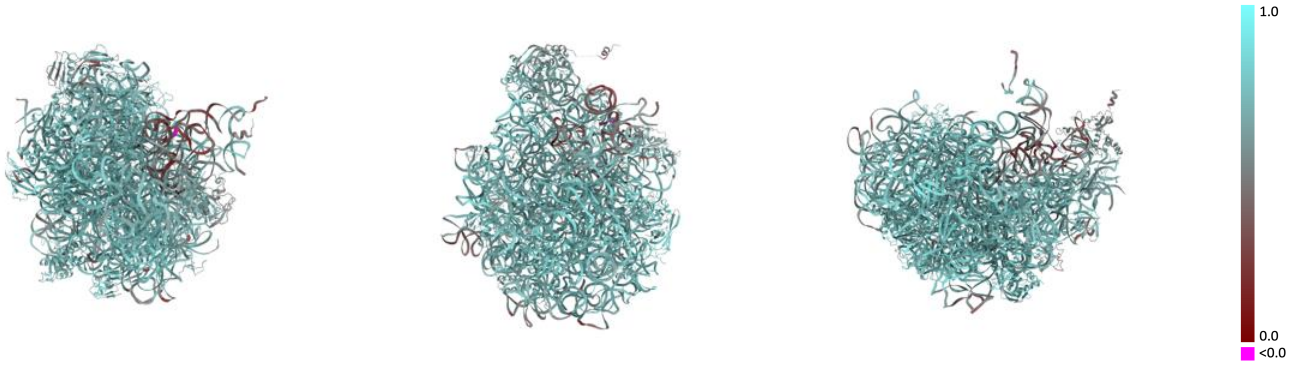
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0265 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

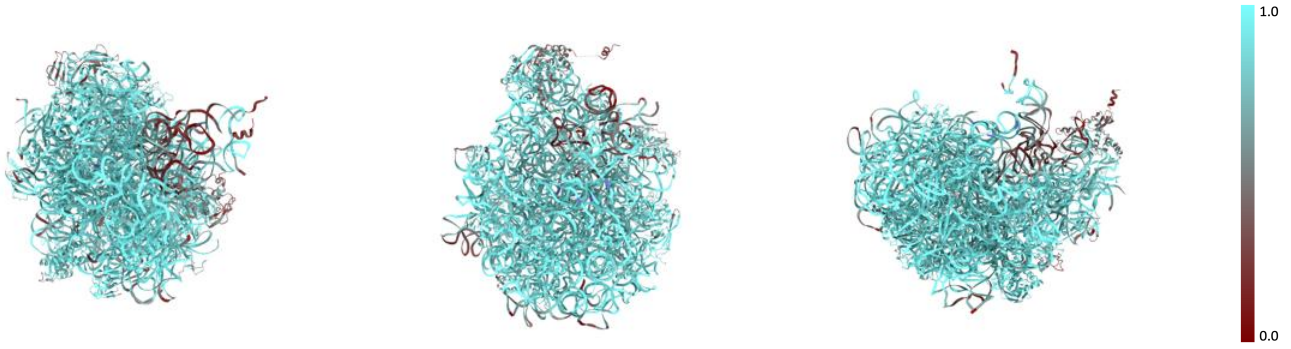
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

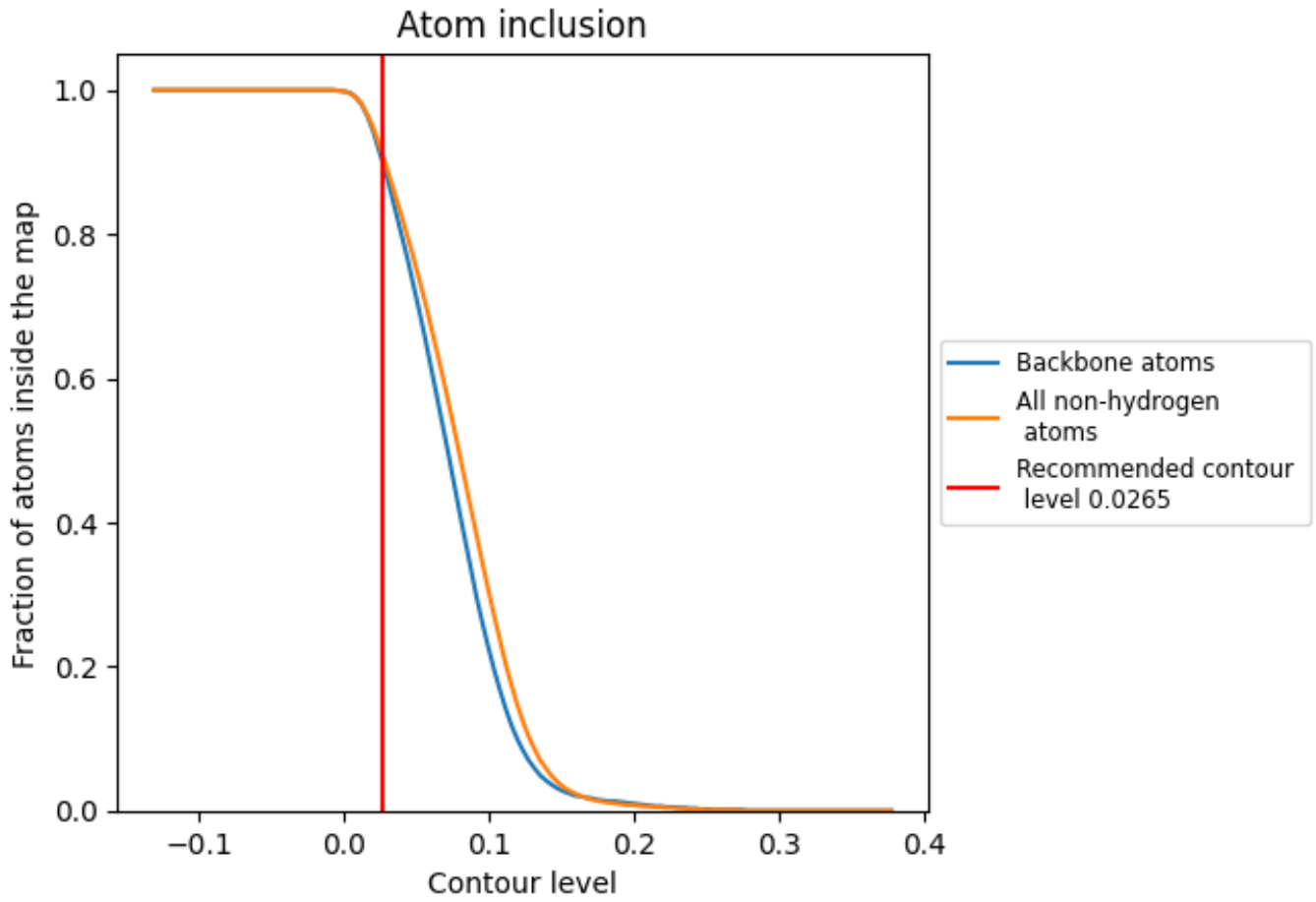
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0265).

9.4 Atom inclusion (i)



At the recommended contour level, 90% of all backbone atoms, 91% 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 (0.0265) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9120	0.7240
0	0.8920	0.7380
1	0.9690	0.8000
2	0.9860	0.7970
3	0.9490	0.7580
4	0.3880	0.5030
X	0.5650	0.5140
Y	0.4730	0.4260
Z	0.5100	0.4750
a	0.9460	0.7360
b	0.9060	0.6800
c	0.9720	0.7820
d	0.9500	0.7820
e	0.9000	0.7420
f	0.5990	0.5890
g	0.6930	0.6070
h	0.7270	0.6540
i	0.9620	0.7840
j	0.9490	0.7730
k	0.9430	0.7620
l	0.9470	0.7680
m	0.9900	0.7930
n	0.8970	0.7120
o	0.9260	0.7630
p	0.9760	0.7950
q	0.9250	0.7510
r	0.9350	0.7730
s	0.8880	0.7270
t	0.8610	0.7000
u	0.8750	0.7190
v	0.9400	0.7790
w	0.9470	0.7560
x	0.8180	0.6840
y	0.9150	0.7540
z	0.9230	0.7660