Full wwPDB EM Validation Report (i)

May 19, 2024 – 11:50 am BST

PDB ID	:	6YSU
EMDB ID	:	EMD-10908
Title	:	Structure of the P+0 ArfB-ribosome complex in the post-hydrolysis state
Authors	:	Chan, K.-H.; Petrychenko, V.; Mueller, C.; Maracci, C.; Holtkamp, W.; Wilson, D.N.; Fischer, N.; Rodnina, M.V.
Deposited on	:	2020-04-23
Resolution	:	3.70 Å(reported)
Based on initial models	:	5O2R, 4V95, 4RB7, 5AFI

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:

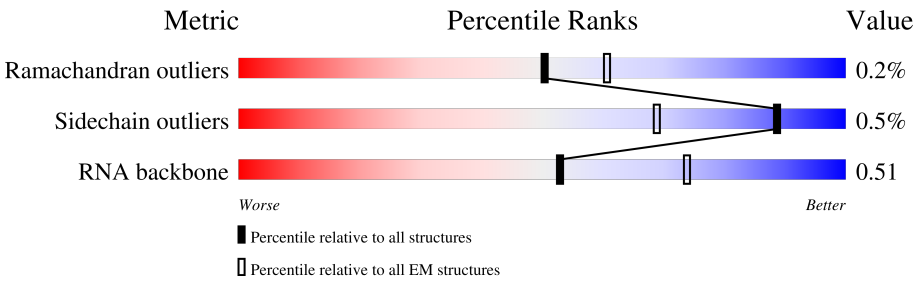
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.70 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	0	57	98%
2	1	55	91% 9%
3	2	46	98%
4	3	65	95%
5	4	38	100%
6	5	165	79% 21%
7	A	2903	74% 25%
8	B	120	79% 18%

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Mol	Chain	Length	Quality of chain
9	C	273	99%
10	D	209	100%
11	E	201	100%
12	F	179	98%
13	G	177	99%
14	H	149	100%
15	I	142	99%
16	J	142	99%
17	K	123	98%
18	L	144	99%
19	M	136	100%
20	N	127	94% 6%
21	O	117	97%
22	P	115	99%
23	Q	118	99%
24	R	103	100%
25	S	110	100%
26	T	100	93% 7%
27	U	104	98%
28	V	94	100%
29	W	85	88% 12%
30	X	78	99%
31	Y	63	97%
32	Z	59	98%
33	a	1542	73% 26%

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Mol	Chain	Length	Quality of chain
34	b	240	90% 9%
35	c	233	88% 12%
36	d	206	98%
37	e	167	93% 6%
38	f	135	74% 26%
39	g	179	83% 16%
40	h	130	99%
41	i	130	97%
42	j	103	92% 5%
43	k	129	90% 10%
44	l	124	99%
45	m	118	95%
46	n	102	99%
47	o	89	98%
48	p	82	99%
49	q	84	93% 5%
50	r	75	75% 25%
51	s	92	89% 11%
52	t	87	97%
53	u	71	90% 8%
54	v	14	100%
55	w	76	46% 46% 8%
56	x	15	33% 7% 60%
57	y	140	99%

2 Entry composition (i)

There are 60 unique types of molecules in this entry. The entry contains 146398 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 L32.

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

- Molecule 2 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	1	50	409	263	75	71	0	0

- Molecule 3 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	2	46	377	228	90	57	2	0	0

- Molecule 4 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	3	64	504	323	105	74	2	0	0

- Molecule 5 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	4	38	302	185	65	48	4	0	0

- Molecule 6 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
6	5	131	647	385	131	131	0	0

- Molecule 7 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
7	A	2903	62336	27815	11468	20150	2903	0	0

- Molecule 8 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
8	B	120	2570	1144	468	838	120	0	0

- Molecule 9 is a protein called 50S ribosomal protein L2.

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

- Molecule 10 is a protein called 50S ribosomal protein L3.

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

- Molecule 11 is a protein called 50S ribosomal protein L4.

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

- Molecule 12 is a protein called 50S ribosomal protein L5.

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

- Molecule 13 is a protein called 50S ribosomal protein L6.

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

- Molecule 14 is a protein called 50S ribosomal protein L9.

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

- Molecule 15 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
15	I	141	693	411	141	141	0	0

- Molecule 16 is a protein called 50S ribosomal protein L13.

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

- Molecule 17 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	K	122	938	587	180	165	6	0	0

- Molecule 18 is a protein called 50S ribosomal protein L15.

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

- Molecule 19 is a protein called 50S ribosomal protein L16.

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

- Molecule 20 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	N	120	960	593	196	166	5	0	0

- Molecule 21 is a protein called 50S ribosomal protein L18.

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

- Molecule 22 is a protein called 50S ribosomal protein L19.

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

- Molecule 23 is a protein called 50S ribosomal protein L20.

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

- Molecule 24 is a protein called 50S ribosomal protein L21.

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

- Molecule 25 is a protein called 50S ribosomal protein L22.

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

- Molecule 26 is a protein called 50S ribosomal protein L23.

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

- Molecule 27 is a protein called 50S ribosomal protein L24.

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

- Molecule 28 is a protein called 50S ribosomal protein L25.

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

- Molecule 29 is a protein called 50S ribosomal protein L27.

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

- Molecule 30 is a protein called 50S ribosomal protein L28.

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

- Molecule 31 is a protein called 50S ribosomal protein L29.

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

- Molecule 32 is a protein called 50S ribosomal protein L30.

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

- Molecule 33 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
33	a	1540	33050	14748	6057	10705	1540	0	0

- Molecule 34 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	b	218	1704	1081	305	311	7	0	0

- Molecule 35 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	c	206	1624	1028	305	288	3	0	0

- Molecule 36 is a protein called 30S ribosomal protein S4.

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

- Molecule 37 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	e	157	1141	709	218	208	6	0	0

- Molecule 38 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
38	f	100	817	515	148	148	6	0	0

- Molecule 39 is a protein called 30S ribosomal protein S7.

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

- Molecule 40 is a protein called 30S ribosomal protein S8.

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

- Molecule 41 is a protein called 30S ribosomal protein S9.

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

- Molecule 42 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
42	j	98	786	493	150	142	1	0	0

- Molecule 43 is a protein called 30S ribosomal protein S11.

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

- Molecule 44 is a protein called 30S ribosomal protein S12.

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

- Molecule 45 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
45	m	114	883	546	178	156	3	0	0

- Molecule 46 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
46	n	101	799	498	165	133	3	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
n	35	ALA	-	insertion	UNP C3SR07

- Molecule 47 is a protein called 30S ribosomal protein S15.

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

- Molecule 48 is a protein called 30S ribosomal protein S16.

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

- Molecule 49 is a protein called 30S ribosomal protein S17.

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

- Molecule 50 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
50	r	56	464	293	88	83	0	0

- Molecule 51 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
51	s	82	658	421	125	110	2	0	0

- Molecule 52 is a protein called 30S ribosomal protein S20.

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

- Molecule 53 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
53	u	65	506	313	105	87	1	0	0

- Molecule 54 is a protein called Api137.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
54	v	14	121	80	25	16	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
v	10	ARG	GLN	engineered mutation	UNP Q8WSY8

- Molecule 55 is a RNA chain called P-site tRNAPhe.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	N	O	P	S		
55	w	76	1631	731	291	531	76	2	0	0

- Molecule 56 is a RNA chain called RNA (5'-R(P*AP*UP*GP*UP*UP*C)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
56	x	6	125	56	19	44	6	0	0

- Molecule 57 is a protein called Alternative stalled-ribosome rescue factor B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
57	y	139	1078	666	215	195	2	0	0

- Molecule 58 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
58	0	2	2	2	0
58	3	1	1	1	0
58	A	244	244	244	0
58	B	5	5	5	0
58	C	2	2	2	0
58	D	2	2	2	0
58	L	1	1	1	0
58	X	1	1	1	0
58	a	93	93	93	0
58	m	1	1	1	0

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Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
58	w	4	4	4	0

- Molecule 59 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
59	4	1	1	1	0

- Molecule 60 is SODIUM ION (three-letter code: NA) (formula: Na).

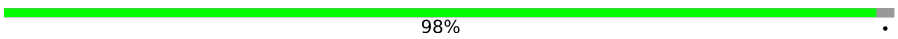
Mol	Chain	Residues	Atoms		AltConf
			Total	Na	
60	A	1	1	1	0

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.

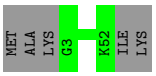
- Molecule 1: 50S ribosomal protein L32

Chain 0:



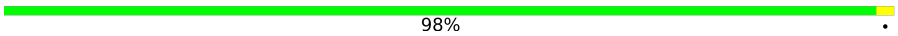
- Molecule 2: 50S ribosomal protein L33

Chain 1:



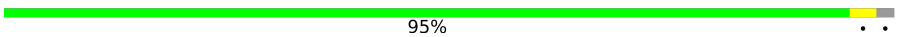
- Molecule 3: 50S ribosomal protein L34

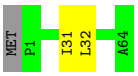
Chain 2:



- Molecule 4: 50S ribosomal protein L35

Chain 3:





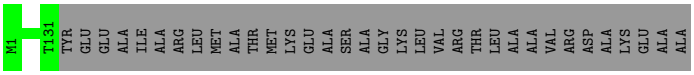
- Molecule 5: 50S ribosomal protein L36

Chain 4:

There are no outlier residues recorded for this chain.

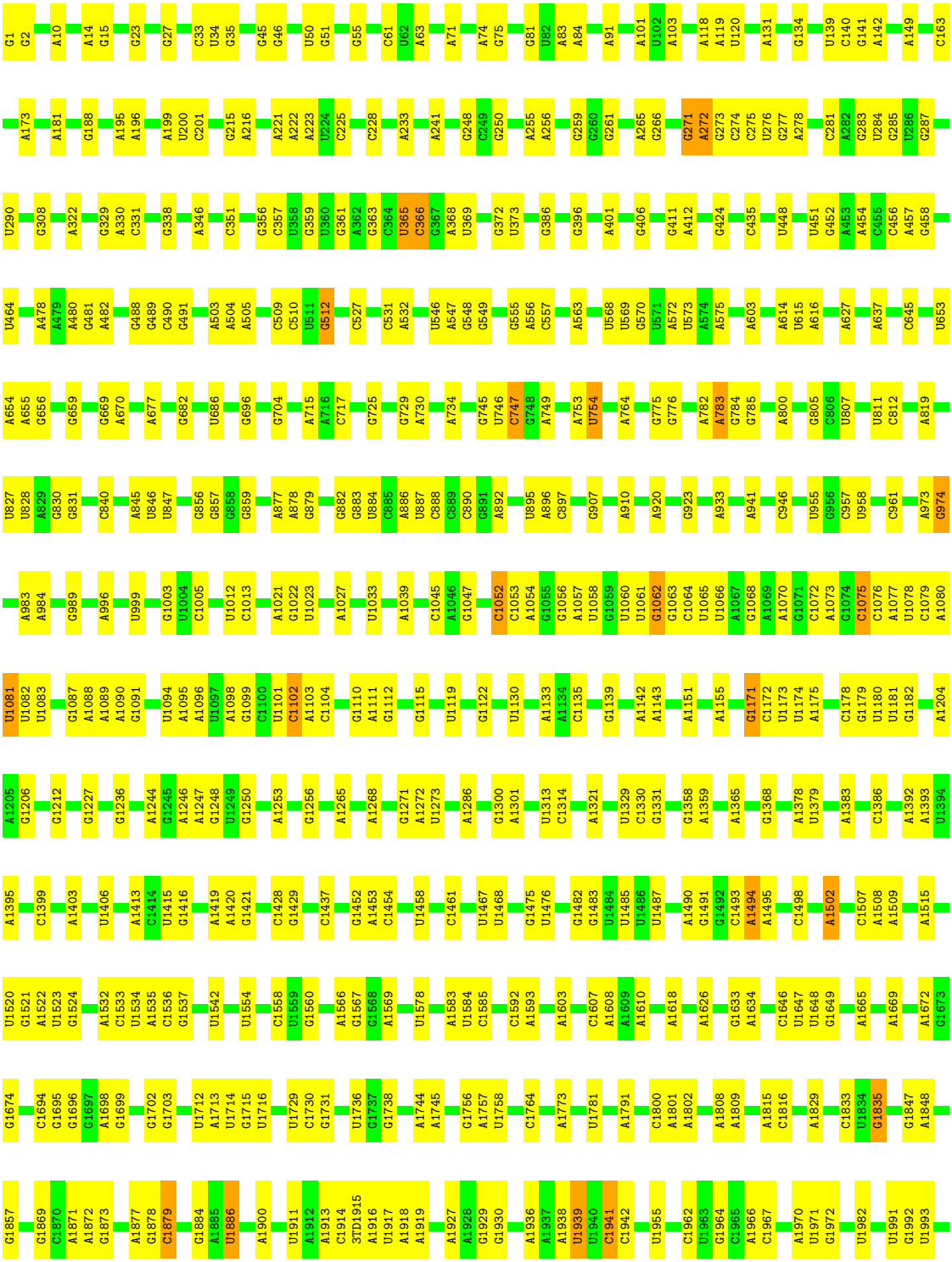
- Molecule 6: 50S ribosomal protein L10

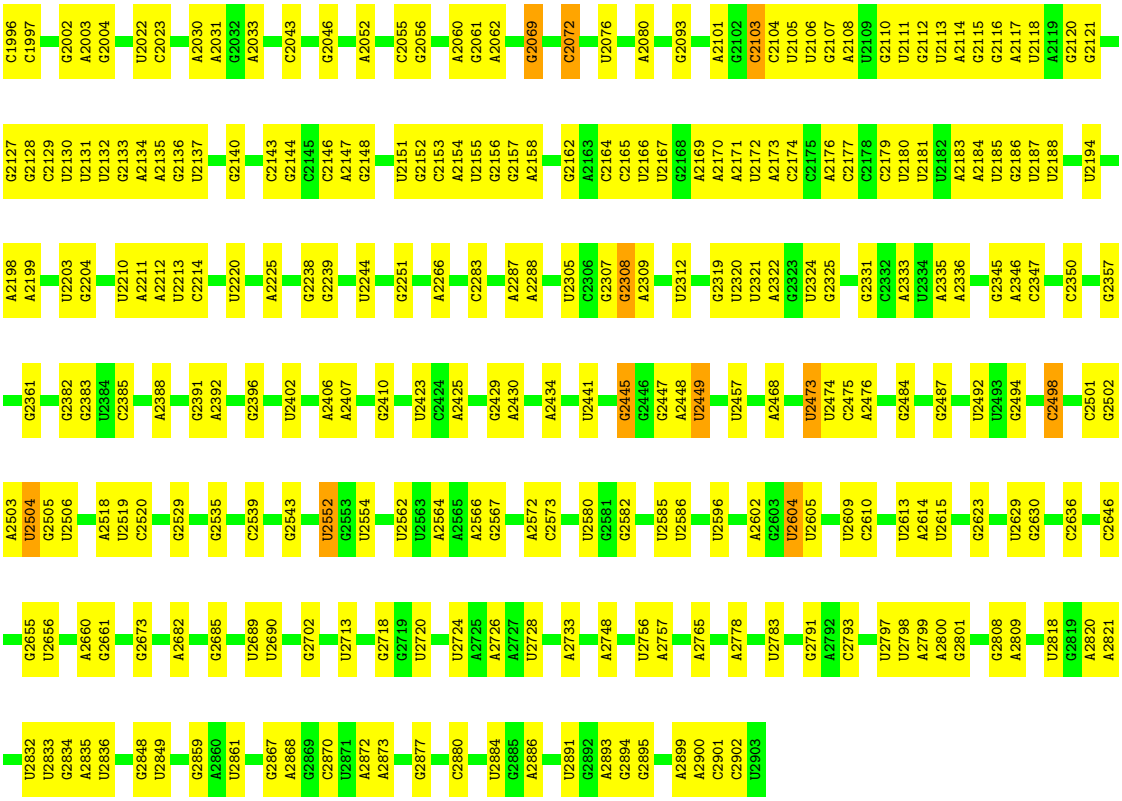
Chain 5:



- Molecule 7: 23S ribosomal RNA

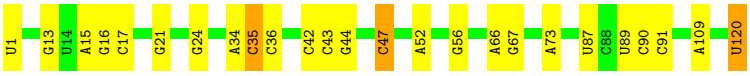
Chain A: 74% 25%





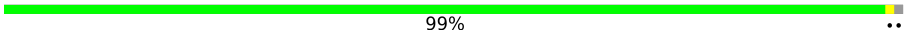
- Molecule 8: 5S ribosomal RNA

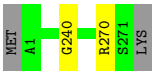
Chain B:



- Molecule 9: 50S ribosomal protein L2

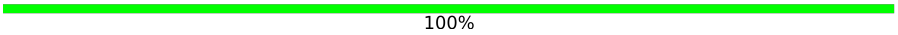
Chain C:





- Molecule 10: 50S ribosomal protein L3

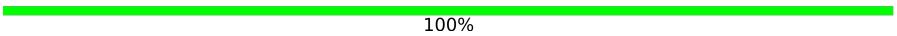
Chain D:



There are no outlier residues recorded for this chain.

- Molecule 11: 50S ribosomal protein L4

Chain E:

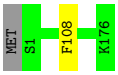


• Molecule 12: 50S ribosomal protein L5

Chain F: 98%

• Molecule 13: 50S ribosomal protein L6

Chain G: 99%



• Molecule 14: 50S ribosomal protein L9

Chain H: 100%

There are no outlier residues recorded for this chain.

• Molecule 15: 50S ribosomal protein L11

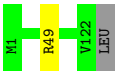
Chain I: 99%

• Molecule 16: 50S ribosomal protein L13

Chain J: 99%

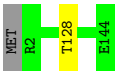
• Molecule 17: 50S ribosomal protein L14

Chain K: 98%



• Molecule 18: 50S ribosomal protein L15

Chain L: 99%



• Molecule 19: 50S ribosomal protein L16

Chain M: 100%

There are no outlier residues recorded for this chain.

• Molecule 20: 50S ribosomal protein L17

Chain N: 94% 6%

M1 E120 LYS ALA GLU ALA ALA ALA GLU

• Molecule 21: 50S ribosomal protein L18

Chain O: 97%

MET D2 Y36 K63 F117

• Molecule 22: 50S ribosomal protein L19

Chain P: 99%

MET S1 N114

• Molecule 23: 50S ribosomal protein L20

Chain Q: 99%

MET A1 A117

• Molecule 24: 50S ribosomal protein L21

Chain R: 100%

There are no outlier residues recorded for this chain.

• Molecule 25: 50S ribosomal protein L22

Chain S: 100%

There are no outlier residues recorded for this chain.

• Molecule 26: 50S ribosomal protein L23

Chain T: 93% 7%

M1 L93 ASP PHE VAL GLY GLY ALA GLU

• Molecule 27: 50S ribosomal protein L24

Chain U: 98%

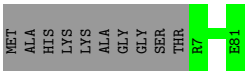
• Molecule 28: 50S ribosomal protein L25

Chain V: 100%

There are no outlier residues recorded for this chain.

• Molecule 29: 50S ribosomal protein L27

Chain W: 88% 12%



• Molecule 30: 50S ribosomal protein L28

Chain X: 99%

• Molecule 31: 50S ribosomal protein L29

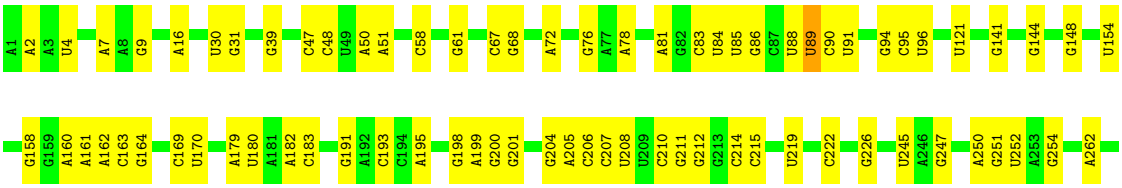
Chain Y: 97%

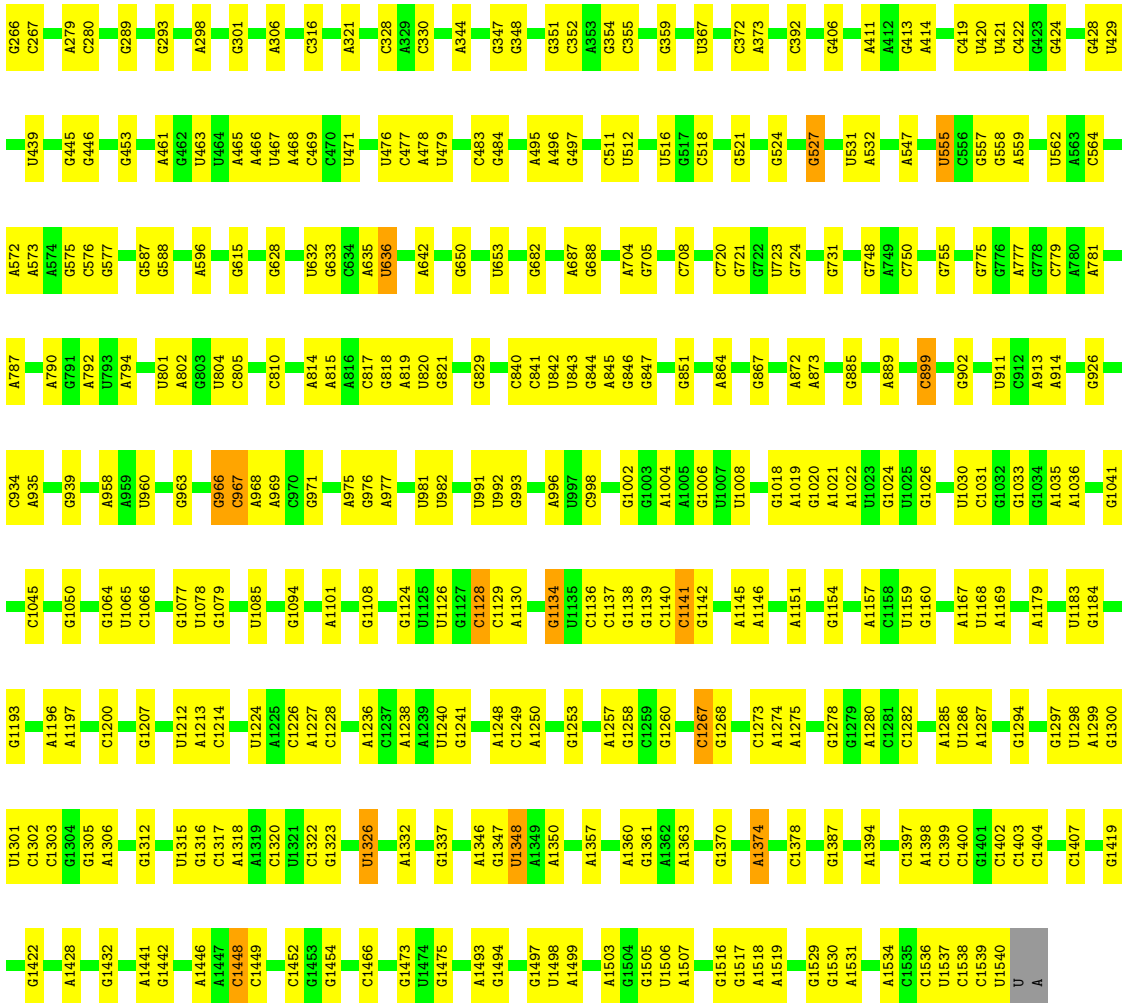
• Molecule 32: 50S ribosomal protein L30

Chain Z: 98%

• Molecule 33: 16S ribosomal RNA

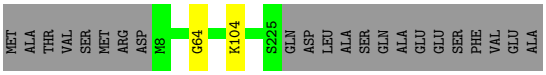
Chain a: 73% 26%





- Molecule 34: 30S ribosomal protein S2

Chain b:

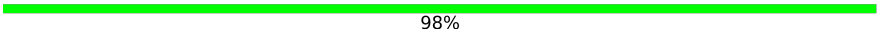


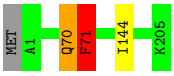
- Molecule 35: 30S ribosomal protein S3

Chain c:

- Molecule 36: 30S ribosomal protein S4

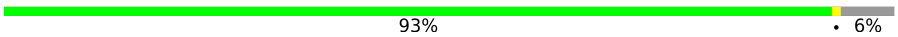
Chain d:

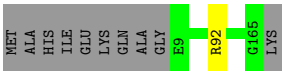




- Molecule 37: 30S ribosomal protein S5

Chain e:





- Molecule 38: 30S ribosomal protein S6

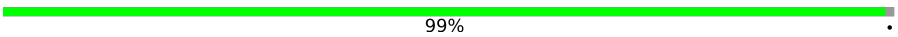
Chain f:

- Molecule 39: 30S ribosomal protein S7

Chain g:

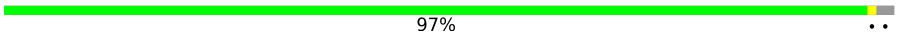
- Molecule 40: 30S ribosomal protein S8

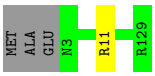
Chain h:



- Molecule 41: 30S ribosomal protein S9

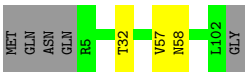
Chain i:





- Molecule 42: 30S ribosomal protein S10

Chain j:



- Molecule 43: 30S ribosomal protein S11

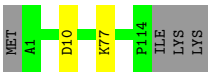
Chain k:

- Molecule 44: 30S ribosomal protein S12

Chain l: 99%

• Molecule 45: 30S ribosomal protein S13

Chain m: 95%



• Molecule 46: 30S ribosomal protein S14

Chain n: 99%

• Molecule 47: 30S ribosomal protein S15

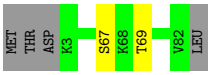
Chain o: 98%

• Molecule 48: 30S ribosomal protein S16

Chain p: 99%

• Molecule 49: 30S ribosomal protein S17

Chain q: 93% 5%

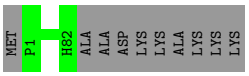


• Molecule 50: 30S ribosomal protein S18

Chain r: 75% 25%

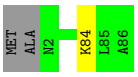
• Molecule 51: 30S ribosomal protein S19

Chain s: 89% 11%



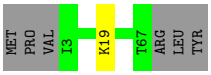
• Molecule 52: 30S ribosomal protein S20

Chain t: 97%



• Molecule 53: 30S ribosomal protein S21

Chain u: 90% 8%



• Molecule 54: Api137

Chain v: 100%

There are no outlier residues recorded for this chain.

• Molecule 55: P-site tRNAPhe

Chain w: 46% 46% 8%

• Molecule 56: RNA (5'-R(P*AP*UP*GP*UP*UP*C)-3')

Chain x: 33% 7% 60%

• Molecule 57: Alternative stalled-ribosome rescue factor B

Chain y: 99%

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	60692	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	25	Depositor
Minimum defocus (nm)	1100	Depositor
Maximum defocus (nm)	2300	Depositor
Magnification	59000	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	14.417	Depositor
Minimum map value	-7.317	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	0.015	Depositor
Map size (Å)	347.328, 347.328, 347.328	wwPDB
Map dimensions	324, 324, 324	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.072, 1.072, 1.072	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: MIA, 4SU, MG, 5MC, 5MU, 6MZ, MA6, 2MG, ZN, 4OC, PSU, UR3, 1MG, OMG, 3TD, OMU, 2MA, G7M, OMC, NA

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	0.41	0/450	0.55	0/599
2	1	0.41	0/416	0.49	0/554
3	2	0.40	0/380	0.54	0/498
4	3	0.41	0/513	0.53	0/676
5	4	0.38	0/303	0.49	0/397
6	5	0.25	0/646	0.50	0/898
7	A	0.83	9/69263 (0.0%)	0.93	90/108050 (0.1%)
8	B	0.67	2/2873 (0.1%)	0.92	4/4478 (0.1%)
9	C	0.45	0/2121	0.53	0/2852
10	D	0.44	0/1586	0.55	0/2134
11	E	0.39	0/1571	0.49	0/2113
12	F	0.32	0/1434	0.48	0/1926
13	G	0.36	0/1343	0.50	0/1816
14	H	0.34	0/1122	0.53	0/1515
15	I	0.25	0/692	0.44	0/960
16	J	0.44	0/1152	0.50	0/1551
17	K	0.41	0/947	0.53	0/1268
18	L	0.41	0/1054	0.57	0/1403
19	M	0.41	0/1093	0.49	0/1460
20	N	0.41	0/973	0.52	0/1301
21	O	0.34	0/902	0.49	0/1209
22	P	0.41	0/929	0.49	0/1242
23	Q	0.50	0/960	0.46	0/1278
24	R	0.40	0/829	0.51	0/1107
25	S	0.39	0/864	0.49	0/1156
26	T	0.37	0/744	0.50	0/994
27	U	0.39	0/787	0.49	0/1051
28	V	0.40	0/766	0.48	0/1025
29	W	0.42	0/582	0.46	0/769
30	X	0.40	0/635	0.48	0/848
31	Y	0.35	0/510	0.59	1/677 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	Z	0.38	0/453	0.53	0/605
33	a	0.67	2/36725 (0.0%)	0.89	26/57285 (0.0%)
34	b	0.31	0/1735	0.48	0/2338
35	c	0.34	0/1651	0.47	0/2225
36	d	0.44	0/1665	0.59	3/2227 (0.1%)
37	e	0.38	0/1154	0.53	0/1554
38	f	0.35	0/835	0.50	0/1128
39	g	0.30	0/1195	0.47	0/1602
40	h	0.37	0/989	0.49	0/1326
41	i	0.33	0/1034	0.51	0/1375
42	j	0.32	0/796	0.55	0/1077
43	k	0.34	0/885	0.48	0/1195
44	l	0.40	0/969	0.52	0/1300
45	m	0.29	0/892	0.48	0/1193
46	n	0.32	0/811	0.46	0/1081
47	o	0.32	0/722	0.46	0/964
48	p	0.35	0/659	0.51	0/884
49	q	0.39	0/657	0.55	0/881
50	r	0.35	0/471	0.45	0/633
51	s	0.31	0/675	0.48	0/908
52	t	0.31	0/671	0.44	0/888
53	u	0.30	0/512	0.49	0/683
54	v	0.31	0/128	0.42	0/175
55	w	1.25	12/1650 (0.7%)	1.11	9/2569 (0.4%)
56	x	0.61	0/138	0.86	0/212
57	y	0.28	0/1090	0.45	0/1461
All	All	0.69	25/157602 (0.0%)	0.83	133/235574 (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
36	d	0	2

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	w	20	U	C2-N3	17.27	1.49	1.37
55	w	16	U	C5-C6	16.84	1.49	1.34
55	w	16	U	C2-N3	16.80	1.49	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	w	20	U	C5-C6	16.74	1.49	1.34
55	w	20	U	N1-C2	16.43	1.53	1.38
55	w	16	U	N1-C2	16.26	1.53	1.38
7	A	2449	U	C5-C6	15.98	1.48	1.34
7	A	2449	U	C2-N3	15.45	1.48	1.37
7	A	2449	U	N1-C2	14.31	1.51	1.38
55	w	20	U	C4-C5	10.90	1.53	1.43
55	w	16	U	C4-C5	10.83	1.53	1.43
7	A	1	G	OP3-P	-10.80	1.48	1.61
8	B	1	U	OP3-P	-10.53	1.48	1.61
7	A	2449	U	C4-C5	10.01	1.52	1.43
55	w	20	U	N3-C4	9.29	1.46	1.38
55	w	20	U	N1-C6	9.18	1.46	1.38
55	w	16	U	N3-C4	8.92	1.46	1.38
55	w	16	U	N1-C6	8.74	1.45	1.38
7	A	2449	U	N3-C4	7.79	1.45	1.38
7	A	2449	U	N1-C6	7.72	1.44	1.38
33	a	89	U	O3'-P	6.29	1.68	1.61
8	B	120	U	C1'-N1	5.20	1.56	1.48
33	a	1374	A	N9-C4	-5.20	1.34	1.37
7	A	783	A	N9-C4	-5.08	1.34	1.37
7	A	452	G	N9-C4	-5.05	1.33	1.38

All (133) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	A	2449	U	C2-N3-C4	-13.54	118.87	127.00
7	A	366	C	C2-N1-C1'	11.70	131.67	118.80
55	w	16	U	C2-N3-C4	-11.70	119.98	127.00
55	w	20	U	C2-N3-C4	-11.60	120.04	127.00
7	A	366	C	N1-C2-O2	10.94	125.46	118.90
7	A	2449	U	C5-C4-O4	-10.34	119.69	125.90
7	A	366	C	C6-N1-C1'	-10.30	108.44	120.80
55	w	20	U	C5-C4-O4	-10.27	119.74	125.90
7	A	2449	U	N3-C4-C5	10.04	120.62	114.60
55	w	16	U	C5-C4-O4	-9.57	120.16	125.90
33	a	1348	U	C2-N1-C1'	9.28	128.83	117.70
55	w	20	U	N3-C4-C5	9.23	120.14	114.60
7	A	2449	U	N1-C2-N3	9.15	120.39	114.90
36	d	71	PHE	N-CA-C	-9.01	86.68	111.00
55	w	16	U	N1-C2-N3	8.79	120.17	114.90
7	A	1102	C	C2-N1-C1'	8.73	128.40	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	A	753	A	N9-C4-C5	-8.43	102.43	105.80
7	A	753	A	C6-C5-N7	-8.22	126.54	132.30
55	w	16	U	N3-C4-C5	8.20	119.52	114.60
33	a	89	U	P-O3'-C3'	8.13	129.46	119.70
7	A	753	A	C4-N9-C1'	8.13	140.93	126.30
7	A	753	A	C8-N9-C1'	-8.12	113.09	127.70
7	A	366	C	C5-C6-N1	8.07	125.03	121.00
55	w	20	U	N1-C2-N3	7.83	119.60	114.90
7	A	2870	C	N3-C2-O2	-7.72	116.50	121.90
33	a	1466	C	N3-C2-O2	-7.63	116.56	121.90
7	A	753	A	N3-C4-N9	7.62	133.49	127.40
7	A	1313	U	C2-N1-C1'	7.60	126.83	117.70
7	A	271	G	N3-C2-N2	7.60	125.22	119.90
7	A	1102	C	N1-C2-O2	7.51	123.41	118.90
7	A	2449	U	C5-C6-N1	-7.33	119.04	122.70
7	A	271	G	C4-C5-N7	7.21	113.69	110.80
7	A	452	G	N3-C4-N9	-7.20	121.68	126.00
33	a	810	C	N3-C2-O2	-7.01	116.99	121.90
36	d	70	GLN	CA-C-N	-7.01	101.78	117.20
8	B	35	C	C2-N1-C1'	6.99	126.48	118.80
8	B	35	C	N1-C2-O2	6.97	123.08	118.90
7	A	1502	A	N9-C4-C5	-6.91	103.04	105.80
7	A	1731	G	N3-C4-N9	-6.85	121.89	126.00
7	A	271	G	N9-C4-C5	-6.83	102.67	105.40
7	A	271	G	C6-C5-N7	-6.82	126.31	130.40
7	A	2506	U	C2-N1-C1'	6.71	125.76	117.70
33	a	1128	C	N1-C2-O2	6.70	122.92	118.90
33	a	1448	C	C2-N1-C1'	6.68	126.15	118.80
7	A	271	G	C8-N9-C1'	-6.60	118.41	127.00
7	A	271	G	O4'-C1'-N9	6.60	113.48	108.20
7	A	1102	C	C6-N1-C1'	-6.54	112.95	120.80
33	a	1348	U	C6-N1-C1'	-6.48	112.12	121.20
7	A	1052	C	C2'-C3'-O3'	6.47	124.06	113.70
7	A	271	G	N3-C4-N9	6.47	129.88	126.00
33	a	1348	U	N1-C2-O2	6.42	127.29	122.80
7	A	1879	C	N1-C2-O2	6.39	122.73	118.90
33	a	636	U	C2-N1-C1'	6.38	125.36	117.70
33	a	998	C	N3-C2-O2	-6.32	117.48	121.90
7	A	1171	G	O4'-C1'-N9	6.26	113.20	108.20
7	A	272	A	C6-C5-N7	-6.23	127.94	132.30
7	A	271	G	C4-N9-C1'	6.21	134.57	126.50
7	A	271	G	N1-C2-N2	-6.19	110.63	116.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	A	2473	U	N1-C2-O2	6.16	127.11	122.80
7	A	754	U	N3-C2-O2	-6.11	117.92	122.20
7	A	2506	U	N1-C2-O2	6.10	127.07	122.80
33	a	1348	U	N3-C2-O2	-6.02	117.98	122.20
7	A	2103	C	N3-C2-O2	-6.01	117.69	121.90
7	A	2783	U	C5-C4-O4	5.99	129.50	125.90
33	a	1128	C	N3-C2-O2	-5.95	117.73	121.90
7	A	2194	U	N3-C2-O2	-5.93	118.05	122.20
7	A	753	A	C4-C5-N7	5.91	113.66	110.70
7	A	2103	C	N1-C2-O2	5.90	122.44	118.90
7	A	1313	U	N1-C2-O2	5.85	126.89	122.80
7	A	1075	C	N1-C2-O2	5.84	122.41	118.90
7	A	1102	C	N3-C2-O2	-5.83	117.82	121.90
33	a	1374	A	C2-N3-C4	-5.81	107.70	110.60
7	A	2072	C	C2-N1-C1'	5.79	125.17	118.80
7	A	754	U	C5-C4-O4	5.69	129.32	125.90
7	A	2539	C	C2-N1-C1'	5.67	125.04	118.80
7	A	2783	U	N3-C2-O2	-5.67	118.23	122.20
55	w	16	U	C5-C6-N1	-5.65	119.88	122.70
7	A	452	G	N3-C4-C5	5.64	131.42	128.60
7	A	366	C	C4-C5-C6	-5.63	114.58	117.40
7	A	753	A	C4-C5-C6	5.60	119.80	117.00
7	A	1886	U	C2-N1-C1'	5.59	124.40	117.70
7	A	452	G	N3-C2-N2	-5.56	116.01	119.90
7	A	974	G	C4-N9-C1'	5.55	133.72	126.50
7	A	2473	U	C2-N1-C1'	5.54	124.34	117.70
7	A	1502	A	C4-C5-N7	5.53	113.46	110.70
7	A	1313	U	C6-N1-C1'	-5.50	113.50	121.20
7	A	366	C	C5-C4-N4	-5.50	116.35	120.20
7	A	1081	U	C2-N1-C1'	5.48	124.27	117.70
7	A	1941	C	C2-N1-C1'	5.47	124.82	118.80
7	A	1731	G	C4-N9-C1'	-5.46	119.40	126.50
7	A	2506	U	N3-C2-O2	-5.46	118.38	122.20
7	A	1314	C	C2-N1-C1'	5.44	124.79	118.80
31	Y	18	LEU	N-CA-CB	5.44	121.27	110.40
7	A	1879	C	N3-C2-O2	-5.43	118.10	121.90
33	a	1134	G	N3-C4-N9	-5.43	122.74	126.00
36	d	70	GLN	C-N-CA	-5.42	108.14	121.70
33	a	1141	C	N3-C2-O2	-5.41	118.11	121.90
7	A	1731	G	C8-N9-C1'	5.37	133.98	127.00
7	A	2308	G	OP1-P-O3'	5.35	116.96	105.20
7	A	2308	G	P-O3'-C3'	5.34	126.11	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	A	2901	C	N1-C2-O2	5.34	122.10	118.90
33	a	1326	U	C2-N1-C1'	5.32	124.08	117.70
7	A	1313	U	N3-C2-O2	-5.30	118.49	122.20
7	A	1075	C	C2-N1-C1'	5.29	124.62	118.80
8	B	35	C	C6-N1-C1'	-5.29	114.45	120.80
33	a	1267	C	P-O3'-C3'	5.29	126.05	119.70
33	a	1374	A	C5-C6-N1	-5.29	115.06	117.70
7	A	365	U	C2-N3-C4	-5.26	123.85	127.00
7	A	1502	A	C6-C5-N7	-5.22	128.64	132.30
7	A	365	U	C5-C4-O4	-5.21	122.77	125.90
7	A	195	A	N1-C6-N6	5.21	121.73	118.60
7	A	974	G	C6-C5-N7	-5.21	127.28	130.40
33	a	471	U	C2-N1-C1'	5.20	123.94	117.70
7	A	1062	G	C8-N9-C1'	-5.19	120.25	127.00
33	a	215	C	C2-N1-C1'	5.18	124.50	118.80
7	A	2449	U	N1-C2-O2	-5.18	119.17	122.80
7	A	2244	U	C5-C4-O4	-5.16	122.80	125.90
7	A	1941	C	N1-C2-O2	5.12	121.97	118.90
33	a	899	C	N1-C2-O2	5.12	121.97	118.90
7	A	1062	G	C4-N9-C1'	5.11	133.14	126.50
7	A	1731	G	N3-C4-C5	5.10	131.15	128.60
7	A	366	C	N1-C2-N3	-5.10	115.63	119.20
7	A	2473	U	N3-C2-O2	-5.09	118.63	122.20
33	a	775	G	C2-N3-C4	-5.09	109.36	111.90
33	a	555	U	N3-C2-O2	-5.08	118.64	122.20
7	A	2901	C	C2-N1-C1'	5.07	124.38	118.80
33	a	899	C	N3-C2-O2	-5.07	118.35	121.90
33	a	1128	C	C2-N1-C1'	5.06	124.37	118.80
8	B	47	C	C2-N1-C1'	5.04	124.34	118.80
7	A	512	G	O4'-C1'-N9	5.03	112.23	108.20
33	a	215	C	N1-C2-O2	5.01	121.91	118.90
7	A	1494	A	O4'-C1'-N9	5.01	112.21	108.20
7	A	2244	U	N3-C4-O4	5.01	122.90	119.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
36	d	70	GLN	Mainchain
36	d	71	PHE	Mainchain

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	
1	0	54/57 (95%)	47 (87%)	7 (13%)	0	100	100
2	1	48/55 (87%)	46 (96%)	2 (4%)	0	100	100
3	2	44/46 (96%)	41 (93%)	3 (7%)	0	100	100
4	3	62/65 (95%)	52 (84%)	8 (13%)	2 (3%)	4	31
5	4	36/38 (95%)	31 (86%)	5 (14%)	0	100	100
6	5	129/165 (78%)	104 (81%)	25 (19%)	0	100	100
9	C	269/273 (98%)	237 (88%)	31 (12%)	1 (0%)	34	69
10	D	207/209 (99%)	182 (88%)	25 (12%)	0	100	100
11	E	199/201 (99%)	181 (91%)	18 (9%)	0	100	100
12	F	175/179 (98%)	152 (87%)	23 (13%)	0	100	100
13	G	174/177 (98%)	159 (91%)	14 (8%)	1 (1%)	25	62
14	H	147/149 (99%)	115 (78%)	32 (22%)	0	100	100
15	I	139/142 (98%)	110 (79%)	29 (21%)	0	100	100
16	J	140/142 (99%)	128 (91%)	12 (9%)	0	100	100
17	K	120/123 (98%)	102 (85%)	18 (15%)	0	100	100
18	L	141/144 (98%)	117 (83%)	23 (16%)	1 (1%)	22	59
19	M	134/136 (98%)	107 (80%)	27 (20%)	0	100	100
20	N	118/127 (93%)	106 (90%)	12 (10%)	0	100	100
21	O	114/117 (97%)	105 (92%)	9 (8%)	0	100	100
22	P	112/115 (97%)	100 (89%)	12 (11%)	0	100	100
23	Q	115/118 (98%)	112 (97%)	3 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
24	R	101/103 (98%)	87 (86%)	14 (14%)	0	100	100
25	S	108/110 (98%)	99 (92%)	9 (8%)	0	100	100
26	T	91/100 (91%)	74 (81%)	17 (19%)	0	100	100
27	U	100/104 (96%)	87 (87%)	13 (13%)	0	100	100
28	V	92/94 (98%)	88 (96%)	4 (4%)	0	100	100
29	W	73/85 (86%)	69 (94%)	4 (6%)	0	100	100
30	X	75/78 (96%)	66 (88%)	9 (12%)	0	100	100
31	Y	61/63 (97%)	54 (88%)	7 (12%)	0	100	100
32	Z	56/59 (95%)	52 (93%)	4 (7%)	0	100	100
34	b	216/240 (90%)	188 (87%)	27 (12%)	1 (0%)	29	66
35	c	204/233 (88%)	188 (92%)	16 (8%)	0	100	100
36	d	203/206 (98%)	170 (84%)	32 (16%)	1 (0%)	29	66
37	e	155/167 (93%)	141 (91%)	14 (9%)	0	100	100
38	f	98/135 (73%)	88 (90%)	10 (10%)	0	100	100
39	g	149/179 (83%)	138 (93%)	11 (7%)	0	100	100
40	h	127/130 (98%)	114 (90%)	13 (10%)	0	100	100
41	i	125/130 (96%)	105 (84%)	20 (16%)	0	100	100
42	j	96/103 (93%)	72 (75%)	22 (23%)	2 (2%)	7	38
43	k	114/129 (88%)	101 (89%)	13 (11%)	0	100	100
44	l	121/124 (98%)	95 (78%)	26 (22%)	0	100	100
45	m	112/118 (95%)	94 (84%)	18 (16%)	0	100	100
46	n	99/102 (97%)	87 (88%)	12 (12%)	0	100	100
47	o	86/89 (97%)	83 (96%)	3 (4%)	0	100	100
48	p	80/82 (98%)	71 (89%)	9 (11%)	0	100	100
49	q	78/84 (93%)	60 (77%)	16 (20%)	2 (3%)	5	34
50	r	54/75 (72%)	48 (89%)	6 (11%)	0	100	100
51	s	80/92 (87%)	73 (91%)	7 (9%)	0	100	100
52	t	83/87 (95%)	79 (95%)	4 (5%)	0	100	100
53	u	63/71 (89%)	53 (84%)	10 (16%)	0	100	100
54	v	12/14 (86%)	8 (67%)	4 (33%)	0	100	100
57	y	137/140 (98%)	132 (96%)	5 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	5926/6304 (94%)	5198 (88%)	717 (12%)	11 (0%)	50 78

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	3	31	ILE
49	q	67	SER
4	3	32	LEU
18	L	128	THR
49	q	69	THR
13	G	108	PHE
42	j	58	ASN
36	d	144	ILE
9	C	240	GLY
34	b	64	GLY
42	j	57	VAL

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	47/48 (98%)	47 (100%)	0	100 100
2	1	45/49 (92%)	45 (100%)	0	100 100
3	2	38/38 (100%)	37 (97%)	1 (3%)	46 69
4	3	51/52 (98%)	51 (100%)	0	100 100
5	4	34/34 (100%)	34 (100%)	0	100 100
9	C	216/218 (99%)	215 (100%)	1 (0%)	88 94
10	D	164/164 (100%)	164 (100%)	0	100 100
11	E	165/165 (100%)	164 (99%)	1 (1%)	86 93
12	F	148/150 (99%)	146 (99%)	2 (1%)	67 82
13	G	137/138 (99%)	137 (100%)	0	100 100
14	H	114/114 (100%)	114 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	J	116/116 (100%)	115 (99%)	1 (1%)	78	88
17	K	103/104 (99%)	102 (99%)	1 (1%)	76	86
18	L	102/103 (99%)	102 (100%)	0	100	100
19	M	109/109 (100%)	109 (100%)	0	100	100
20	N	100/103 (97%)	100 (100%)	0	100	100
21	O	86/87 (99%)	84 (98%)	2 (2%)	50	71
22	P	99/100 (99%)	99 (100%)	0	100	100
23	Q	89/90 (99%)	89 (100%)	0	100	100
24	R	84/84 (100%)	84 (100%)	0	100	100
25	S	93/93 (100%)	93 (100%)	0	100	100
26	T	80/84 (95%)	80 (100%)	0	100	100
27	U	83/85 (98%)	83 (100%)	0	100	100
28	V	78/78 (100%)	78 (100%)	0	100	100
29	W	57/63 (90%)	57 (100%)	0	100	100
30	X	67/68 (98%)	67 (100%)	0	100	100
31	Y	55/55 (100%)	54 (98%)	1 (2%)	59	77
32	Z	48/49 (98%)	48 (100%)	0	100	100
34	b	180/198 (91%)	179 (99%)	1 (1%)	86	93
35	c	170/190 (90%)	169 (99%)	1 (1%)	86	93
36	d	172/173 (99%)	171 (99%)	1 (1%)	86	93
37	e	114/126 (90%)	113 (99%)	1 (1%)	78	88
38	f	87/116 (75%)	87 (100%)	0	100	100
39	g	124/147 (84%)	122 (98%)	2 (2%)	62	80
40	h	104/105 (99%)	104 (100%)	0	100	100
41	i	105/107 (98%)	104 (99%)	1 (1%)	76	86
42	j	86/90 (96%)	85 (99%)	1 (1%)	71	84
43	k	89/99 (90%)	89 (100%)	0	100	100
44	l	103/104 (99%)	103 (100%)	0	100	100
45	m	92/96 (96%)	90 (98%)	2 (2%)	52	72
46	n	79/84 (94%)	79 (100%)	0	100	100
47	o	76/77 (99%)	75 (99%)	1 (1%)	69	83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
48	p	65/65 (100%)	64 (98%)	1 (2%)	65	81
49	q	74/78 (95%)	74 (100%)	0	100	100
50	r	49/65 (75%)	49 (100%)	0	100	100
51	s	72/79 (91%)	72 (100%)	0	100	100
52	t	65/66 (98%)	64 (98%)	1 (2%)	65	81
53	u	46/61 (75%)	45 (98%)	1 (2%)	52	72
54	v	14/14 (100%)	14 (100%)	0	100	100
57	y	112/115 (97%)	112 (100%)	0	100	100
All	All	4686/4896 (96%)	4662 (100%)	24 (0%)	89	94

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	2	25	LYS
9	C	270	ARG
11	E	7	ASP
12	F	132	ARG
12	F	149	ARG
16	J	53	TYR
17	K	49	ARG
21	O	36	TYR
21	O	63	LYS
31	Y	7	ARG
34	b	104	LYS
35	c	106	ARG
36	d	71	PHE
37	e	92	ARG
39	g	4	ARG
39	g	28	ILE
41	i	11	ARG
42	j	32	THR
45	m	10	ASP
45	m	77	LYS
47	o	88	ARG
48	p	25	ARG
52	t	84	LYS
53	u	19	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (65)

such sidechains are listed below:

Mol	Chain	Res	Type
2	1	44	GLN
4	3	25	HIS
4	3	27	ASN
4	3	30	HIS
5	4	13	ASN
9	C	24	HIS
9	C	52	HIS
9	C	196	ASN
10	D	32	ASN
10	D	136	ASN
12	F	4	HIS
12	F	20	ASN
14	H	11	ASN
14	H	28	ASN
14	H	66	ASN
14	H	135	HIS
14	H	145	ASN
16	J	58	ASN
17	K	93	GLN
19	M	13	HIS
19	M	60	GLN
20	N	9	GLN
21	O	38	GLN
22	P	9	GLN
22	P	65	ASN
23	Q	36	GLN
23	Q	70	GLN
23	Q	71	ASN
24	R	18	GLN
24	R	89	HIS
26	T	59	ASN
27	U	98	ASN
28	V	24	ASN
28	V	44	HIS
35	c	101	ASN
35	c	122	GLN
36	d	125	ASN
36	d	135	GLN
36	d	139	ASN
37	e	121	ASN
37	e	134	ASN
38	f	63	ASN

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Mol	Chain	Res	Type
41	i	24	ASN
41	i	30	ASN
41	i	49	GLN
41	i	74	GLN
41	i	125	GLN
42	j	15	HIS
42	j	20	GLN
42	j	58	ASN
42	j	64	GLN
43	k	27	ASN
43	k	80	ASN
44	l	4	ASN
46	n	71	HIS
47	o	27	GLN
47	o	34	GLN
47	o	61	GLN
48	p	26	ASN
48	p	79	ASN
49	q	46	HIS
51	s	56	HIS
52	t	12	GLN
57	y	28	GLN
57	y	29	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
33	a	1536/1542 (99%)	395 (25%)	0
55	w	74/76 (97%)	38 (51%)	0
56	x	5/15 (33%)	1 (20%)	0
7	A	2898/2903 (99%)	710 (24%)	49 (1%)
8	B	119/120 (99%)	23 (19%)	1 (0%)
All	All	4632/4656 (99%)	1167 (25%)	50 (1%)

All (1167) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
7	A	2	G
7	A	10	A
7	A	14	A
7	A	15	G

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Mol	Chain	Res	Type
7	A	23	G
7	A	27	G
7	A	33	C
7	A	34	U
7	A	35	G
7	A	45	G
7	A	46	G
7	A	50	U
7	A	51	G
7	A	55	G
7	A	61	C
7	A	63	A
7	A	71	A
7	A	74	A
7	A	75	G
7	A	81	G
7	A	83	A
7	A	84	A
7	A	91	A
7	A	101	A
7	A	103	A
7	A	118	A
7	A	119	A
7	A	120	U
7	A	131	A
7	A	134	G
7	A	139	U
7	A	140	C
7	A	141	G
7	A	142	A
7	A	149	A
7	A	163	C
7	A	173	A
7	A	181	A
7	A	188	G
7	A	196	A
7	A	199	A
7	A	200	U
7	A	201	C
7	A	215	G
7	A	216	A
7	A	221	A

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Mol	Chain	Res	Type
7	A	222	A
7	A	223	A
7	A	225	C
7	A	228	C
7	A	233	A
7	A	241	A
7	A	248	G
7	A	250	G
7	A	255	A
7	A	256	A
7	A	259	G
7	A	261	G
7	A	265	A
7	A	266	G
7	A	271	G
7	A	272	A
7	A	273	G
7	A	274	C
7	A	275	C
7	A	276	U
7	A	277	G
7	A	278	A
7	A	281	C
7	A	284	U
7	A	285	G
7	A	287	G
7	A	290	U
7	A	308	G
7	A	322	A
7	A	329	G
7	A	330	A
7	A	331	C
7	A	338	G
7	A	346	A
7	A	351	C
7	A	356	G
7	A	357	C
7	A	359	G
7	A	361	G
7	A	363	G
7	A	365	U
7	A	366	C

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Mol	Chain	Res	Type
7	A	368	A
7	A	369	U
7	A	372	G
7	A	373	U
7	A	386	G
7	A	396	G
7	A	401	A
7	A	406	G
7	A	411	G
7	A	412	A
7	A	424	G
7	A	435	C
7	A	448	U
7	A	451	U
7	A	454	A
7	A	456	C
7	A	457	A
7	A	458	G
7	A	464	U
7	A	478	A
7	A	480	A
7	A	481	G
7	A	482	A
7	A	488	G
7	A	489	G
7	A	490	C
7	A	491	G
7	A	503	A
7	A	504	A
7	A	505	A
7	A	509	C
7	A	510	C
7	A	512	G
7	A	527	C
7	A	531	C
7	A	532	A
7	A	546	U
7	A	547	A
7	A	548	G
7	A	549	G
7	A	556	A
7	A	557	C

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Mol	Chain	Res	Type
7	A	563	A
7	A	568	U
7	A	569	U
7	A	570	G
7	A	572	A
7	A	573	U
7	A	575	A
7	A	603	A
7	A	614	A
7	A	615	U
7	A	616	A
7	A	627	A
7	A	637	A
7	A	645	C
7	A	653	U
7	A	654	A
7	A	655	A
7	A	656	G
7	A	659	G
7	A	670	A
7	A	677	A
7	A	682	G
7	A	686	U
7	A	696	G
7	A	704	G
7	A	715	A
7	A	717	C
7	A	725	G
7	A	729	G
7	A	730	A
7	A	734	A
7	A	747	5MC
7	A	749	A
7	A	754	U
7	A	764	A
7	A	775	G
7	A	776	G
7	A	782	A
7	A	783	A
7	A	784	G
7	A	785	G
7	A	800	A

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Mol	Chain	Res	Type
7	A	805	G
7	A	807	U
7	A	811	U
7	A	812	C
7	A	819	A
7	A	827	U
7	A	828	U
7	A	831	G
7	A	845	A
7	A	846	U
7	A	847	U
7	A	856	G
7	A	857	G
7	A	859	G
7	A	877	A
7	A	878	A
7	A	879	G
7	A	882	G
7	A	883	G
7	A	884	U
7	A	886	A
7	A	887	U
7	A	888	C
7	A	890	C
7	A	892	A
7	A	895	U
7	A	896	A
7	A	897	C
7	A	907	G
7	A	910	A
7	A	920	A
7	A	923	G
7	A	933	A
7	A	941	A
7	A	946	C
7	A	957	C
7	A	958	U
7	A	961	C
7	A	973	A
7	A	974	G
7	A	983	A
7	A	984	A

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Mol	Chain	Res	Type
7	A	989	G
7	A	996	A
7	A	999	U
7	A	1003	G
7	A	1005	C
7	A	1012	U
7	A	1013	C
7	A	1022	G
7	A	1023	U
7	A	1027	A
7	A	1033	U
7	A	1039	A
7	A	1045	C
7	A	1047	G
7	A	1052	C
7	A	1053	C
7	A	1054	A
7	A	1056	G
7	A	1057	A
7	A	1058	U
7	A	1060	U
7	A	1061	U
7	A	1062	G
7	A	1063	G
7	A	1064	C
7	A	1065	U
7	A	1066	U
7	A	1068	G
7	A	1070	A
7	A	1072	C
7	A	1073	A
7	A	1075	C
7	A	1076	C
7	A	1077	A
7	A	1078	U
7	A	1079	C
7	A	1080	A
7	A	1081	U
7	A	1082	U
7	A	1083	U
7	A	1087	G
7	A	1088	A

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Mol	Chain	Res	Type
7	A	1089	A
7	A	1090	A
7	A	1091	G
7	A	1094	U
7	A	1096	A
7	A	1098	A
7	A	1099	G
7	A	1101	U
7	A	1102	C
7	A	1103	A
7	A	1104	C
7	A	1110	G
7	A	1111	A
7	A	1112	G
7	A	1115	G
7	A	1119	U
7	A	1122	G
7	A	1130	U
7	A	1133	A
7	A	1135	C
7	A	1139	G
7	A	1142	A
7	A	1143	A
7	A	1151	A
7	A	1155	A
7	A	1171	G
7	A	1172	C
7	A	1173	U
7	A	1174	U
7	A	1175	A
7	A	1178	C
7	A	1179	G
7	A	1180	U
7	A	1181	U
7	A	1204	A
7	A	1206	G
7	A	1212	G
7	A	1227	G
7	A	1236	G
7	A	1244	A
7	A	1246	A
7	A	1247	A

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Mol	Chain	Res	Type
7	A	1248	G
7	A	1250	G
7	A	1253	A
7	A	1256	G
7	A	1265	A
7	A	1268	A
7	A	1271	G
7	A	1272	A
7	A	1273	U
7	A	1286	A
7	A	1300	G
7	A	1301	A
7	A	1321	A
7	A	1329	U
7	A	1330	C
7	A	1359	A
7	A	1365	A
7	A	1368	G
7	A	1378	A
7	A	1379	U
7	A	1383	A
7	A	1386	C
7	A	1392	A
7	A	1393	A
7	A	1395	A
7	A	1403	A
7	A	1406	U
7	A	1413	A
7	A	1415	U
7	A	1416	G
7	A	1419	A
7	A	1420	A
7	A	1421	G
7	A	1428	C
7	A	1429	G
7	A	1437	C
7	A	1452	G
7	A	1453	A
7	A	1454	C
7	A	1458	U
7	A	1461	C
7	A	1467	U

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Mol	Chain	Res	Type
7	A	1468	U
7	A	1475	G
7	A	1476	U
7	A	1482	G
7	A	1483	G
7	A	1485	U
7	A	1487	U
7	A	1490	A
7	A	1491	G
7	A	1493	C
7	A	1494	A
7	A	1495	A
7	A	1498	C
7	A	1502	A
7	A	1507	C
7	A	1508	A
7	A	1509	A
7	A	1515	A
7	A	1520	U
7	A	1521	G
7	A	1522	A
7	A	1523	U
7	A	1524	G
7	A	1532	A
7	A	1533	C
7	A	1534	U
7	A	1535	A
7	A	1536	C
7	A	1537	G
7	A	1542	U
7	A	1554	U
7	A	1558	C
7	A	1560	G
7	A	1566	A
7	A	1567	G
7	A	1569	A
7	A	1578	U
7	A	1583	A
7	A	1584	U
7	A	1585	C
7	A	1592	C
7	A	1593	A

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Mol	Chain	Res	Type
7	A	1603	A
7	A	1607	C
7	A	1608	A
7	A	1610	A
7	A	1626	A
7	A	1633	G
7	A	1634	A
7	A	1646	C
7	A	1647	U
7	A	1648	U
7	A	1649	G
7	A	1665	A
7	A	1669	A
7	A	1672	A
7	A	1674	G
7	A	1694	C
7	A	1695	G
7	A	1696	G
7	A	1698	A
7	A	1699	G
7	A	1702	G
7	A	1703	G
7	A	1712	U
7	A	1713	A
7	A	1714	U
7	A	1715	G
7	A	1716	U
7	A	1729	U
7	A	1730	C
7	A	1736	U
7	A	1738	G
7	A	1744	A
7	A	1745	A
7	A	1756	G
7	A	1757	A
7	A	1758	U
7	A	1764	C
7	A	1773	A
7	A	1781	U
7	A	1791	A
7	A	1800	C
7	A	1801	A

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Mol	Chain	Res	Type
7	A	1802	A
7	A	1808	A
7	A	1809	A
7	A	1815	A
7	A	1816	C
7	A	1829	A
7	A	1833	C
7	A	1835	2MG
7	A	1848	A
7	A	1857	G
7	A	1869	G
7	A	1871	A
7	A	1872	A
7	A	1873	G
7	A	1877	A
7	A	1878	G
7	A	1879	C
7	A	1884	G
7	A	1886	U
7	A	1900	A
7	A	1913	A
7	A	1914	C
7	A	1916	A
7	A	1918	A
7	A	1919	A
7	A	1927	A
7	A	1929	G
7	A	1930	G
7	A	1936	A
7	A	1938	A
7	A	1939	5MU
7	A	1941	C
7	A	1942	C
7	A	1955	U
7	A	1964	G
7	A	1966	A
7	A	1967	C
7	A	1970	A
7	A	1971	U
7	A	1972	G
7	A	1982	U
7	A	1991	U

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Mol	Chain	Res	Type
7	A	1992	G
7	A	1993	U
7	A	1996	C
7	A	1997	C
7	A	2002	G
7	A	2004	G
7	A	2022	U
7	A	2023	C
7	A	2031	A
7	A	2033	A
7	A	2043	C
7	A	2046	G
7	A	2052	A
7	A	2055	C
7	A	2056	G
7	A	2060	A
7	A	2061	G
7	A	2062	A
7	A	2069	G7M
7	A	2072	C
7	A	2076	U
7	A	2080	A
7	A	2093	G
7	A	2101	A
7	A	2103	C
7	A	2104	C
7	A	2105	U
7	A	2106	U
7	A	2107	G
7	A	2108	A
7	A	2110	G
7	A	2111	U
7	A	2112	G
7	A	2113	U
7	A	2114	A
7	A	2115	G
7	A	2116	G
7	A	2118	U
7	A	2120	G
7	A	2121	G
7	A	2127	G
7	A	2128	G

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Mol	Chain	Res	Type
7	A	2129	C
7	A	2130	U
7	A	2131	U
7	A	2132	U
7	A	2133	G
7	A	2134	A
7	A	2135	A
7	A	2136	G
7	A	2137	U
7	A	2140	G
7	A	2143	C
7	A	2144	G
7	A	2146	C
7	A	2147	A
7	A	2148	G
7	A	2151	U
7	A	2152	G
7	A	2153	C
7	A	2154	A
7	A	2155	U
7	A	2156	G
7	A	2157	G
7	A	2158	A
7	A	2162	G
7	A	2164	C
7	A	2165	C
7	A	2166	U
7	A	2167	U
7	A	2169	A
7	A	2170	A
7	A	2171	A
7	A	2172	U
7	A	2173	A
7	A	2174	C
7	A	2176	A
7	A	2177	C
7	A	2179	C
7	A	2180	U
7	A	2181	U
7	A	2183	A
7	A	2184	A
7	A	2185	U

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Mol	Chain	Res	Type
7	A	2186	G
7	A	2187	U
7	A	2188	U
7	A	2198	A
7	A	2199	A
7	A	2203	U
7	A	2204	G
7	A	2210	U
7	A	2211	A
7	A	2212	A
7	A	2213	U
7	A	2214	C
7	A	2220	U
7	A	2225	A
7	A	2238	G
7	A	2239	G
7	A	2266	A
7	A	2283	C
7	A	2287	A
7	A	2288	A
7	A	2305	U
7	A	2307	G
7	A	2308	G
7	A	2309	A
7	A	2312	U
7	A	2319	G
7	A	2320	U
7	A	2321	U
7	A	2322	A
7	A	2325	G
7	A	2331	G
7	A	2333	A
7	A	2335	A
7	A	2336	A
7	A	2345	G
7	A	2346	A
7	A	2347	C
7	A	2350	C
7	A	2357	G
7	A	2361	G
7	A	2382	G
7	A	2383	G

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Mol	Chain	Res	Type
7	A	2385	C
7	A	2388	A
7	A	2392	A
7	A	2396	G
7	A	2402	U
7	A	2406	A
7	A	2407	A
7	A	2410	G
7	A	2423	U
7	A	2425	A
7	A	2429	G
7	A	2430	A
7	A	2434	A
7	A	2441	U
7	A	2445	2MG
7	A	2447	G
7	A	2448	A
7	A	2449	U
7	A	2468	A
7	A	2473	U
7	A	2474	U
7	A	2475	C
7	A	2476	A
7	A	2484	G
7	A	2487	G
7	A	2492	U
7	A	2494	G
7	A	2498	OMC
7	A	2501	C
7	A	2502	G
7	A	2504	PSU
7	A	2505	G
7	A	2518	A
7	A	2519	U
7	A	2520	C
7	A	2529	G
7	A	2535	G
7	A	2543	G
7	A	2552	OMU
7	A	2554	U
7	A	2562	U
7	A	2564	A

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Mol	Chain	Res	Type
7	A	2566	A
7	A	2567	G
7	A	2572	A
7	A	2573	C
7	A	2582	G
7	A	2585	U
7	A	2586	U
7	A	2596	U
7	A	2602	A
7	A	2604	PSU
7	A	2609	U
7	A	2610	C
7	A	2613	U
7	A	2614	A
7	A	2615	U
7	A	2623	G
7	A	2629	U
7	A	2630	G
7	A	2636	C
7	A	2646	C
7	A	2655	G
7	A	2656	U
7	A	2660	A
7	A	2661	G
7	A	2673	G
7	A	2682	A
7	A	2685	G
7	A	2689	U
7	A	2690	U
7	A	2702	G
7	A	2713	U
7	A	2718	G
7	A	2720	U
7	A	2724	U
7	A	2726	A
7	A	2728	U
7	A	2733	A
7	A	2748	A
7	A	2757	A
7	A	2765	A
7	A	2778	A
7	A	2791	G

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Mol	Chain	Res	Type
7	A	2793	C
7	A	2797	U
7	A	2798	U
7	A	2799	A
7	A	2800	A
7	A	2801	G
7	A	2809	A
7	A	2818	U
7	A	2820	A
7	A	2821	A
7	A	2832	U
7	A	2833	U
7	A	2834	G
7	A	2835	A
7	A	2836	U
7	A	2848	G
7	A	2849	U
7	A	2859	G
7	A	2861	U
7	A	2867	G
7	A	2868	A
7	A	2872	A
7	A	2873	A
7	A	2877	G
7	A	2880	C
7	A	2884	U
7	A	2886	A
7	A	2891	U
7	A	2893	A
7	A	2894	G
7	A	2895	G
7	A	2899	A
7	A	2900	A
7	A	2902	C
8	B	13	G
8	B	15	A
8	B	16	G
8	B	17	C
8	B	21	G
8	B	24	G
8	B	35	C
8	B	36	C

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Mol	Chain	Res	Type
8	B	42	C
8	B	43	C
8	B	44	G
8	B	47	C
8	B	52	A
8	B	56	G
8	B	66	A
8	B	67	G
8	B	73	A
8	B	87	U
8	B	89	U
8	B	90	C
8	B	91	C
8	B	109	A
8	B	120	U
33	a	2	A
33	a	4	U
33	a	7	A
33	a	9	G
33	a	16	A
33	a	30	U
33	a	31	G
33	a	39	G
33	a	47	C
33	a	48	C
33	a	50	A
33	a	51	A
33	a	58	C
33	a	61	G
33	a	67	C
33	a	68	G
33	a	72	A
33	a	76	G
33	a	78	A
33	a	81	A
33	a	83	C
33	a	84	U
33	a	85	U
33	a	86	G
33	a	88	U
33	a	89	U
33	a	90	C

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Mol	Chain	Res	Type
33	a	91	U
33	a	94	G
33	a	95	C
33	a	96	U
33	a	121	U
33	a	141	G
33	a	144	G
33	a	148	G
33	a	154	U
33	a	158	G
33	a	160	A
33	a	161	A
33	a	162	A
33	a	163	C
33	a	164	G
33	a	169	C
33	a	170	U
33	a	179	A
33	a	180	U
33	a	182	A
33	a	183	C
33	a	191	G
33	a	193	C
33	a	195	A
33	a	198	G
33	a	199	A
33	a	200	G
33	a	201	G
33	a	204	G
33	a	205	A
33	a	206	C
33	a	207	C
33	a	208	U
33	a	210	C
33	a	211	G
33	a	212	G
33	a	214	C
33	a	219	U
33	a	222	C
33	a	226	G
33	a	245	U
33	a	247	G

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Mol	Chain	Res	Type
33	a	250	A
33	a	251	G
33	a	252	U
33	a	254	G
33	a	262	A
33	a	266	G
33	a	267	C
33	a	279	A
33	a	280	C
33	a	289	G
33	a	293	G
33	a	298	A
33	a	301	G
33	a	306	A
33	a	316	C
33	a	321	A
33	a	328	C
33	a	330	C
33	a	344	A
33	a	347	G
33	a	348	G
33	a	351	G
33	a	352	C
33	a	354	G
33	a	355	C
33	a	359	G
33	a	367	U
33	a	372	C
33	a	373	A
33	a	392	C
33	a	406	G
33	a	411	A
33	a	413	G
33	a	414	A
33	a	419	C
33	a	420	U
33	a	421	U
33	a	422	C
33	a	424	G
33	a	428	G
33	a	429	U
33	a	439	U

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Mol	Chain	Res	Type
33	a	445	G
33	a	446	G
33	a	453	G
33	a	461	A
33	a	463	U
33	a	465	A
33	a	466	A
33	a	467	U
33	a	468	A
33	a	469	C
33	a	476	U
33	a	477	C
33	a	478	A
33	a	479	U
33	a	483	C
33	a	484	G
33	a	495	A
33	a	496	A
33	a	497	G
33	a	511	C
33	a	512	U
33	a	518	C
33	a	521	G
33	a	524	G
33	a	527	G7M
33	a	531	U
33	a	532	A
33	a	547	A
33	a	555	U
33	a	557	G
33	a	558	G
33	a	559	A
33	a	562	U
33	a	564	C
33	a	572	A
33	a	573	A
33	a	575	G
33	a	576	C
33	a	577	G
33	a	587	G
33	a	588	G
33	a	596	A

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Mol	Chain	Res	Type
33	a	615	G
33	a	628	G
33	a	632	U
33	a	633	G
33	a	635	A
33	a	636	U
33	a	642	A
33	a	650	G
33	a	653	U
33	a	682	G
33	a	687	A
33	a	688	G
33	a	704	A
33	a	705	G
33	a	708	C
33	a	720	C
33	a	721	G
33	a	723	U
33	a	724	G
33	a	731	G
33	a	748	G
33	a	750	C
33	a	755	G
33	a	777	A
33	a	779	C
33	a	781	A
33	a	787	A
33	a	790	A
33	a	792	A
33	a	794	A
33	a	801	U
33	a	802	A
33	a	804	U
33	a	805	C
33	a	814	A
33	a	815	A
33	a	817	C
33	a	818	G
33	a	819	A
33	a	820	U
33	a	821	G
33	a	829	G

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Mol	Chain	Res	Type
33	a	840	C
33	a	841	C
33	a	842	U
33	a	843	U
33	a	844	G
33	a	845	A
33	a	846	G
33	a	847	G
33	a	851	G
33	a	864	A
33	a	867	G
33	a	872	A
33	a	873	A
33	a	885	G
33	a	889	A
33	a	899	C
33	a	902	G
33	a	911	U
33	a	913	A
33	a	914	A
33	a	926	G
33	a	934	C
33	a	935	A
33	a	939	G
33	a	958	A
33	a	960	U
33	a	963	G
33	a	966	2MG
33	a	967	5MC
33	a	968	A
33	a	969	A
33	a	971	G
33	a	975	A
33	a	976	G
33	a	977	A
33	a	981	U
33	a	982	U
33	a	991	U
33	a	992	U
33	a	993	G
33	a	996	A
33	a	1002	G

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Mol	Chain	Res	Type
33	a	1004	A
33	a	1006	G
33	a	1008	U
33	a	1018	G
33	a	1019	A
33	a	1020	G
33	a	1021	A
33	a	1022	A
33	a	1024	G
33	a	1026	G
33	a	1030	U
33	a	1031	C
33	a	1033	G
33	a	1035	A
33	a	1036	A
33	a	1041	G
33	a	1045	C
33	a	1050	G
33	a	1064	G
33	a	1065	U
33	a	1066	C
33	a	1077	G
33	a	1078	U
33	a	1079	G
33	a	1085	U
33	a	1094	G
33	a	1101	A
33	a	1108	G
33	a	1124	G
33	a	1126	U
33	a	1128	C
33	a	1129	C
33	a	1130	A
33	a	1134	G
33	a	1136	C
33	a	1137	C
33	a	1138	G
33	a	1139	G
33	a	1140	C
33	a	1141	C
33	a	1142	G
33	a	1145	A

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Mol	Chain	Res	Type
33	a	1146	A
33	a	1151	A
33	a	1154	G
33	a	1157	A
33	a	1159	U
33	a	1160	G
33	a	1167	A
33	a	1168	U
33	a	1169	A
33	a	1179	A
33	a	1183	U
33	a	1184	G
33	a	1193	G
33	a	1196	A
33	a	1197	A
33	a	1200	C
33	a	1212	U
33	a	1213	A
33	a	1214	C
33	a	1224	U
33	a	1226	C
33	a	1227	A
33	a	1228	C
33	a	1236	A
33	a	1238	A
33	a	1240	U
33	a	1241	G
33	a	1248	A
33	a	1249	C
33	a	1250	A
33	a	1253	G
33	a	1257	A
33	a	1258	G
33	a	1260	G
33	a	1267	C
33	a	1268	G
33	a	1273	C
33	a	1274	A
33	a	1275	A
33	a	1278	G
33	a	1280	A
33	a	1282	C

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Mol	Chain	Res	Type
33	a	1285	A
33	a	1286	U
33	a	1287	A
33	a	1294	G
33	a	1297	G
33	a	1298	U
33	a	1299	A
33	a	1300	G
33	a	1301	U
33	a	1302	C
33	a	1303	C
33	a	1305	G
33	a	1306	A
33	a	1312	G
33	a	1315	U
33	a	1316	G
33	a	1317	C
33	a	1318	A
33	a	1320	C
33	a	1322	C
33	a	1323	G
33	a	1326	U
33	a	1332	A
33	a	1337	G
33	a	1346	A
33	a	1347	G
33	a	1348	U
33	a	1350	A
33	a	1357	A
33	a	1360	A
33	a	1361	G
33	a	1363	A
33	a	1370	G
33	a	1374	A
33	a	1378	C
33	a	1387	G
33	a	1394	A
33	a	1397	C
33	a	1398	A
33	a	1399	C
33	a	1400	C
33	a	1403	C

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Mol	Chain	Res	Type
33	a	1404	C
33	a	1419	G
33	a	1422	G
33	a	1428	A
33	a	1432	G
33	a	1441	A
33	a	1442	G
33	a	1446	A
33	a	1448	C
33	a	1449	C
33	a	1452	C
33	a	1454	G
33	a	1473	G
33	a	1475	G
33	a	1493	A
33	a	1494	G
33	a	1497	G
33	a	1499	A
33	a	1503	A
33	a	1505	G
33	a	1506	U
33	a	1507	A
33	a	1517	G
33	a	1529	G
33	a	1530	G
33	a	1531	A
33	a	1534	A
33	a	1536	C
33	a	1537	U
33	a	1538	C
33	a	1539	C
33	a	1540	U
55	w	2	C
55	w	4	C
55	w	5	G
55	w	6	G
55	w	7	A
55	w	8	4SU
55	w	9	A
55	w	10	G
55	w	12	U
55	w	13	C

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Mol	Chain	Res	Type
55	w	14	A
55	w	15	G
55	w	16	U
55	w	17	C
55	w	18	G
55	w	19	G
55	w	20	U
55	w	21	A
55	w	38	A
55	w	46	G7M
55	w	47	U
55	w	48	C
55	w	49	C
55	w	51	C
55	w	54	5MU
55	w	55	PSU
55	w	58	A
55	w	60	U
55	w	62	C
55	w	63	G
55	w	64	A
55	w	67	C
55	w	68	C
55	w	69	G
55	w	70	G
55	w	71	G
55	w	74	C
55	w	76	A
56	x	15	G

All (50) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
7	A	141	G
7	A	274	C
7	A	283	G
7	A	481	G
7	A	482	A
7	A	555	G
7	A	556	A
7	A	669	G
7	A	747	5MC

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Mol	Chain	Res	Type
7	A	784	G
7	A	830	G
7	A	840	C
7	A	1021	A
7	A	1052	C
7	A	1078	U
7	A	1095	A
7	A	1110	G
7	A	1182	G
7	A	1300	G
7	A	1331	G
7	A	1358	G
7	A	1399	C
7	A	1420	A
7	A	1490	A
7	A	1520	U
7	A	1533	C
7	A	1715	G
7	A	1847	G
7	A	1877	A
7	A	1941	C
7	A	2003	A
7	A	2117	A
7	A	2128	G
7	A	2135	A
7	A	2143	C
7	A	2185	U
7	A	2187	U
7	A	2287	A
7	A	2308	G
7	A	2324	U
7	A	2391	G
7	A	2406	A
7	A	2474	U
7	A	2655	G
7	A	2660	A
7	A	2756	U
7	A	2798	U
7	A	2808	G
7	A	2820	A
8	B	34	A

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

41 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	$\#\|Z\| > 2$
7	2MA	A	2503	7,58	17,25,26	2.50	5 (29%)	17,37,40	1.29	2 (11%)
7	PSU	A	2605	7	18,21,22	1.05	2 (11%)	22,30,33	1.87	5 (22%)
7	6MZ	A	2030	7	18,25,26	1.78	5 (27%)	16,36,39	2.45	4 (25%)
7	PSU	A	746	7,58	18,21,22	1.05	2 (11%)	22,30,33	1.70	3 (13%)
7	OMC	A	2498	7,58	19,22,23	2.78	7 (36%)	26,31,34	0.93	2 (7%)
7	5MC	A	747	7	18,22,23	3.40	7 (38%)	26,32,35	1.17	3 (11%)
55	5MU	w	54	55	19,22,23	4.84	7 (36%)	28,32,35	3.64	8 (28%)
7	2MG	A	1835	7	18,26,27	2.36	7 (38%)	16,38,41	1.46	4 (25%)
7	PSU	A	2504	7	18,21,22	1.09	2 (11%)	22,30,33	1.80	4 (18%)
33	4OC	a	1402	33	20,23,24	3.17	8 (40%)	26,32,35	0.89	1 (3%)
55	MIA	w	37	55	24,31,32	2.53	4 (16%)	26,44,47	3.07	8 (30%)
7	6MZ	A	1618	7	18,25,26	1.76	4 (22%)	16,36,39	1.94	4 (25%)
7	OMU	A	2552	7,58	19,22,23	2.85	7 (36%)	26,31,34	1.83	4 (15%)
7	PSU	A	2457	7	18,21,22	0.98	2 (11%)	22,30,33	1.75	4 (18%)
33	5MC	a	967	33	18,22,23	3.52	7 (38%)	26,32,35	1.03	1 (3%)
7	PSU	A	2580	7	18,21,22	1.11	3 (16%)	22,30,33	1.93	6 (27%)
55	G7M	w	46	55	20,26,27	2.13	6 (30%)	17,39,42	1.22	3 (17%)
7	PSU	A	1911	7	18,21,22	1.05	1 (5%)	22,30,33	1.84	5 (22%)
7	2MG	A	2445	7	18,26,27	2.37	7 (38%)	16,38,41	1.47	4 (25%)
33	2MG	a	1207	33	18,26,27	2.49	7 (38%)	16,38,41	1.46	4 (25%)
7	5MU	A	1939	7,58	19,22,23	4.59	7 (36%)	28,32,35	3.81	10 (35%)
55	PSU	w	55	55	18,21,22	1.11	1 (5%)	22,30,33	1.82	5 (22%)
7	PSU	A	1917	7	18,21,22	1.08	1 (5%)	22,30,33	1.90	4 (18%)
7	G7M	A	2069	7	20,26,27	3.87	9 (45%)	17,39,42	1.00	1 (5%)
33	UR3	a	1498	33	19,22,23	2.69	6 (31%)	26,32,35	1.59	4 (15%)
55	PSU	w	32	55	18,21,22	1.47	3 (16%)	22,30,33	1.94	4 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
33	MA6	a	1518	33	18,26,27	1.35	2 (11%)	19,38,41	3.17	2 (10%)
33	G7M	a	527	33	20,26,27	3.99	10 (50%)	17,39,42	1.03	1 (5%)
33	PSU	a	516	33,58	18,21,22	1.03	2 (11%)	22,30,33	1.71	5 (22%)
33	MA6	a	1519	33	18,26,27	1.35	2 (11%)	19,38,41	3.28	2 (10%)
55	PSU	w	39	55	18,21,22	1.03	1 (5%)	22,30,33	1.70	2 (9%)
7	3TD	A	1915	7	18,22,23	4.43	7 (38%)	22,32,35	1.74	4 (18%)
7	PSU	A	2604	7	18,21,22	1.34	2 (11%)	22,30,33	1.94	4 (18%)
55	4SU	w	8	55	18,21,22	3.70	8 (44%)	26,30,33	2.20	4 (15%)
7	5MC	A	1962	7	18,22,23	3.46	7 (38%)	26,32,35	1.12	1 (3%)
33	2MG	a	966	33	18,26,27	2.39	7 (38%)	16,38,41	1.46	4 (25%)
33	2MG	a	1516	33	18,26,27	2.40	7 (38%)	16,38,41	1.41	4 (25%)
7	PSU	A	955	7	18,21,22	1.07	3 (16%)	22,30,33	1.67	4 (18%)
7	1MG	A	745	7	18,26,27	2.57	5 (27%)	19,39,42	1.51	4 (21%)
33	5MC	a	1407	33	18,22,23	3.54	7 (38%)	26,32,35	1.06	2 (7%)
7	OMG	A	2251	55,7,58	18,26,27	2.48	8 (44%)	19,38,41	1.54	4 (21%)

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
7	2MA	A	2503	7,58	-	2/3/25/26	0/3/3/3
7	PSU	A	2605	7	-	0/7/25/26	0/2/2/2
7	6MZ	A	2030	7	-	5/5/27/28	0/3/3/3
7	PSU	A	746	7,58	-	3/7/25/26	0/2/2/2
7	OMC	A	2498	7,58	-	4/9/27/28	0/2/2/2
7	5MC	A	747	7	-	3/7/25/26	0/2/2/2
55	5MU	w	54	55	-	3/7/25/26	0/2/2/2
7	2MG	A	1835	7	-	2/5/27/28	0/3/3/3
7	PSU	A	2504	7	-	2/7/25/26	0/2/2/2
33	4OC	a	1402	33	-	1/9/29/30	0/2/2/2
55	MIA	w	37	55	-	4/11/33/34	0/3/3/3
7	6MZ	A	1618	7	-	3/5/27/28	0/3/3/3
7	OMU	A	2552	7,58	-	5/9/27/28	0/2/2/2
7	PSU	A	2457	7	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	5MC	a	967	33	-	2/7/25/26	0/2/2/2
7	PSU	A	2580	7	-	0/7/25/26	0/2/2/2
55	G7M	w	46	55	-	3/3/25/26	0/3/3/3
7	PSU	A	1911	7	-	0/7/25/26	0/2/2/2
7	2MG	A	2445	7	-	2/5/27/28	0/3/3/3
33	2MG	a	1207	33	-	0/5/27/28	0/3/3/3
7	5MU	A	1939	7,58	-	2/7/25/26	0/2/2/2
55	PSU	w	55	55	-	5/7/25/26	0/2/2/2
7	PSU	A	1917	7	-	0/7/25/26	0/2/2/2
7	G7M	A	2069	7	-	1/3/25/26	0/3/3/3
33	UR3	a	1498	33	-	4/7/25/26	0/2/2/2
55	PSU	w	32	55	-	2/7/25/26	0/2/2/2
33	MA6	a	1518	33	-	2/7/29/30	0/3/3/3
33	G7M	a	527	33	-	3/3/25/26	0/3/3/3
33	PSU	a	516	33,58	-	0/7/25/26	0/2/2/2
33	MA6	a	1519	33	-	2/7/29/30	0/3/3/3
55	PSU	w	39	55	-	3/7/25/26	0/2/2/2
7	3TD	A	1915	7	-	2/7/25/26	0/2/2/2
7	PSU	A	2604	7	-	2/7/25/26	0/2/2/2
55	4SU	w	8	55	-	2/7/25/26	0/2/2/2
7	5MC	A	1962	7	-	4/7/25/26	0/2/2/2
33	2MG	a	966	33	-	0/5/27/28	0/3/3/3
33	2MG	a	1516	33	-	0/5/27/28	0/3/3/3
7	PSU	A	955	7	-	0/7/25/26	0/2/2/2
7	1MG	A	745	7	-	0/3/25/26	0/3/3/3
33	5MC	a	1407	33	-	0/7/25/26	0/2/2/2
7	OMG	A	2251	55,7,58	-	0/5/27/28	0/3/3/3

All (205) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	1915	3TD	C6-C5	14.14	1.51	1.35
55	w	54	5MU	C2-N1	11.21	1.56	1.38
55	w	54	5MU	C6-N1	10.36	1.55	1.38
55	w	54	5MU	C4-C5	10.11	1.61	1.44
33	a	527	G7M	C8-N7	9.86	1.51	1.33
7	A	1939	5MU	C2-N1	9.82	1.54	1.38
7	A	2069	G7M	C8-N7	9.79	1.51	1.33
33	a	527	G7M	C8-N9	9.78	1.51	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	1939	5MU	C6-N1	9.72	1.54	1.38
7	A	2069	G7M	C8-N9	9.60	1.50	1.33
7	A	1939	5MU	C4-C5	9.48	1.60	1.44
33	a	1407	5MC	C6-C5	9.41	1.50	1.34
33	a	967	5MC	C6-C5	9.16	1.49	1.34
7	A	1962	5MC	C6-C5	8.90	1.49	1.34
7	A	747	5MC	C6-C5	8.83	1.49	1.34
7	A	1915	3TD	C2-N1	8.33	1.48	1.37
7	A	1939	5MU	C4-N3	-8.29	1.23	1.38
55	w	8	4SU	C4-N3	8.17	1.46	1.37
55	w	54	5MU	C4-N3	-7.84	1.24	1.38
7	A	2503	2MA	C2-N3	7.70	1.47	1.31
55	w	37	MIA	C13-C14	7.31	1.53	1.32
33	a	1498	UR3	C2-N1	7.16	1.48	1.38
33	a	1402	4OC	C4-N3	7.16	1.45	1.32
55	w	37	MIA	C2-S10	6.91	1.81	1.75
55	w	8	4SU	C2-N3	6.84	1.50	1.38
7	A	2552	OMU	C2-N1	6.70	1.49	1.38
7	A	2552	OMU	C2-N3	6.43	1.49	1.38
33	a	967	5MC	C4-N3	6.35	1.44	1.34
7	A	1962	5MC	C4-N3	6.28	1.44	1.34
7	A	745	1MG	C2-N3	6.24	1.45	1.34
55	w	8	4SU	C2-N1	6.24	1.48	1.38
33	a	1402	4OC	C6-C5	6.18	1.49	1.35
33	a	1407	5MC	C4-N3	6.09	1.44	1.34
7	A	1962	5MC	C2-N3	6.06	1.48	1.36
7	A	2552	OMU	C6-C5	6.01	1.49	1.35
33	a	1402	4OC	C2-N3	5.95	1.48	1.36
33	a	967	5MC	C2-N3	5.93	1.48	1.36
7	A	745	1MG	C2-N2	5.93	1.44	1.34
33	a	1498	UR3	C6-C5	5.88	1.48	1.35
7	A	747	5MC	C2-N3	5.83	1.48	1.36
33	a	1407	5MC	C2-N3	5.76	1.48	1.36
7	A	747	5MC	C4-N3	5.75	1.43	1.34
55	w	54	5MU	C6-C5	5.71	1.44	1.34
55	w	8	4SU	C6-C5	5.66	1.48	1.35
33	a	527	G7M	C2-N3	5.64	1.46	1.33
55	w	37	MIA	C6-N6	5.62	1.44	1.34
7	A	1939	5MU	C6-C5	5.53	1.43	1.34
7	A	2069	G7M	C2-N3	5.45	1.46	1.33
7	A	2498	OMC	C6-C5	5.43	1.47	1.35
7	A	2498	OMC	C2-N3	5.43	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	1915	3TD	C2-N3	5.39	1.50	1.38
33	a	1207	2MG	C2-N2	5.35	1.45	1.33
33	a	1402	4OC	C4-N4	5.27	1.46	1.35
33	a	1516	2MG	C2-N2	5.23	1.45	1.33
7	A	2498	OMC	C4-N4	5.18	1.46	1.33
7	A	2251	OMG	C2-N3	5.16	1.45	1.33
7	A	1618	6MZ	C6-N6	5.14	1.43	1.35
7	A	1835	2MG	C2-N2	5.14	1.44	1.33
7	A	1915	3TD	C6-N1	5.14	1.44	1.36
33	a	966	2MG	C2-N2	5.13	1.44	1.33
55	w	46	G7M	C4-N3	5.04	1.49	1.37
7	A	2445	2MG	C2-N2	4.94	1.44	1.33
55	w	8	4SU	C4-S4	-4.92	1.59	1.68
7	A	2030	6MZ	C6-N6	4.85	1.43	1.35
7	A	2498	OMC	C4-N3	4.84	1.44	1.34
33	a	1207	2MG	C4-N3	4.77	1.48	1.37
7	A	1835	2MG	C4-N3	4.75	1.48	1.37
33	a	1207	2MG	C2-N1	4.75	1.44	1.36
33	a	527	G7M	C2-N2	4.72	1.45	1.34
7	A	745	1MG	C4-N3	4.72	1.48	1.37
33	a	966	2MG	C4-N3	4.70	1.48	1.37
33	a	1407	5MC	C6-N1	4.68	1.46	1.38
7	A	2503	2MA	C4-N3	4.65	1.48	1.37
33	a	1498	UR3	C2-N3	4.65	1.48	1.39
7	A	2251	OMG	C4-N3	4.63	1.48	1.37
33	a	1516	2MG	C4-N3	4.62	1.48	1.37
7	A	2251	OMG	C2-N2	4.57	1.45	1.34
33	a	1516	2MG	C2-N1	4.55	1.44	1.36
33	a	527	G7M	C6-N1	4.52	1.44	1.37
33	a	966	2MG	C2-N1	4.52	1.43	1.36
7	A	2445	2MG	C4-N3	4.50	1.48	1.37
7	A	2069	G7M	C2-N2	4.50	1.44	1.34
7	A	2445	2MG	C2-N1	4.44	1.43	1.36
55	w	8	4SU	C5-C4	4.42	1.48	1.42
33	a	1407	5MC	C4-N4	4.32	1.45	1.34
7	A	1835	2MG	C2-N1	4.29	1.43	1.36
33	a	967	5MC	C4-N4	4.28	1.45	1.34
7	A	747	5MC	C4-N4	4.25	1.45	1.34
7	A	1962	5MC	C4-N4	4.23	1.45	1.34
33	a	967	5MC	C6-N1	4.16	1.45	1.38
7	A	747	5MC	C6-N1	4.14	1.45	1.38
7	A	747	5MC	C2-N1	4.12	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	2069	G7M	C6-N1	4.11	1.44	1.37
7	A	1962	5MC	C6-N1	4.07	1.45	1.38
33	a	967	5MC	C2-N1	4.03	1.48	1.40
55	w	46	G7M	C2-N2	4.01	1.43	1.34
55	w	46	G7M	C2-N3	4.01	1.42	1.33
33	a	527	G7M	C4-N3	3.95	1.46	1.37
7	A	2498	OMC	C2-N1	3.93	1.48	1.40
33	a	1407	5MC	C2-N1	3.90	1.48	1.40
55	w	46	G7M	C6-N1	3.86	1.43	1.37
7	A	1962	5MC	C2-N1	3.85	1.48	1.40
7	A	2069	G7M	C4-N3	3.77	1.46	1.37
33	a	1402	4OC	C5-C4	3.73	1.48	1.40
55	w	55	PSU	C6-C5	3.69	1.39	1.35
33	a	527	G7M	C2-N1	3.66	1.46	1.37
33	a	1402	4OC	C2-N1	3.66	1.47	1.40
33	a	1207	2MG	C6-N1	3.60	1.43	1.37
7	A	2552	OMU	C4-N3	3.56	1.44	1.38
33	a	966	2MG	C6-N1	3.45	1.43	1.37
7	A	2069	G7M	C2-N1	3.32	1.45	1.37
7	A	2251	OMG	C6-N1	3.31	1.42	1.37
33	a	1516	2MG	C6-N1	3.30	1.42	1.37
7	A	2251	OMG	C5-C4	-3.18	1.35	1.43
7	A	2445	2MG	C6-N1	3.17	1.42	1.37
7	A	2604	PSU	C6-C5	3.16	1.39	1.35
55	w	32	PSU	C6-C5	3.16	1.39	1.35
7	A	1835	2MG	C6-N1	3.14	1.42	1.37
55	w	8	4SU	C6-N1	3.14	1.45	1.38
33	a	1518	MA6	C2-N3	3.10	1.37	1.32
33	a	1402	4OC	C6-N1	3.10	1.45	1.38
7	A	1915	3TD	O2-C2	-3.10	1.17	1.23
33	a	1519	MA6	C2-N3	3.10	1.37	1.32
33	a	1519	MA6	C5-C4	-3.08	1.32	1.40
55	w	37	MIA	C5-C4	-3.06	1.32	1.40
33	a	1518	MA6	C5-C4	-3.04	1.32	1.40
7	A	745	1MG	C5-C4	-3.03	1.35	1.43
33	a	1402	4OC	O2-C2	-3.03	1.18	1.23
33	a	1207	2MG	C5-C6	3.01	1.53	1.47
7	A	1911	PSU	C6-C5	3.00	1.38	1.35
7	A	1917	PSU	C6-C5	2.99	1.38	1.35
7	A	2030	6MZ	C5-C4	-2.98	1.33	1.40
55	w	39	PSU	C6-C5	2.96	1.38	1.35
7	A	2445	2MG	C5-C4	-2.91	1.35	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	1835	2MG	C5-C4	-2.91	1.35	1.43
7	A	1939	5MU	O4-C4	-2.90	1.18	1.23
7	A	2504	PSU	C6-C5	2.90	1.38	1.35
33	a	967	5MC	O2-C2	-2.88	1.18	1.23
7	A	1939	5MU	O2-C2	-2.87	1.17	1.23
55	w	32	PSU	C2'-C1'	-2.87	1.50	1.53
7	A	1962	5MC	O2-C2	-2.83	1.18	1.23
33	a	516	PSU	C6-C5	2.83	1.38	1.35
33	a	1516	2MG	C5-C6	2.82	1.53	1.47
33	a	1498	UR3	C6-N1	2.82	1.44	1.38
33	a	966	2MG	C5-C4	-2.80	1.35	1.43
33	a	1207	2MG	C5-C4	-2.79	1.36	1.43
7	A	746	PSU	C6-C5	2.78	1.38	1.35
33	a	1516	2MG	C5-C4	-2.77	1.36	1.43
7	A	2498	OMC	C6-N1	2.77	1.44	1.38
7	A	2498	OMC	O2-C2	-2.76	1.18	1.23
33	a	1407	5MC	O2-C2	-2.75	1.18	1.23
7	A	747	5MC	O2-C2	-2.74	1.18	1.23
7	A	1618	6MZ	C5-C4	-2.70	1.33	1.40
55	w	54	5MU	O4-C4	-2.64	1.18	1.23
7	A	1915	3TD	O4-C4	-2.64	1.17	1.23
7	A	955	PSU	C6-C5	2.63	1.38	1.35
7	A	2605	PSU	C6-C5	2.62	1.38	1.35
7	A	1835	2MG	C5-C6	2.61	1.52	1.47
7	A	2604	PSU	C4-N3	-2.60	1.34	1.38
33	a	527	G7M	C5-C6	2.58	1.52	1.45
33	a	966	2MG	C5-C6	2.58	1.52	1.47
7	A	2069	G7M	O6-C6	-2.58	1.18	1.23
7	A	2445	2MG	C5-C6	2.56	1.52	1.47
55	w	32	PSU	C4-N3	-2.54	1.34	1.38
33	a	1498	UR3	O4-C4	-2.54	1.18	1.23
7	A	2580	PSU	O4'-C1'	-2.53	1.40	1.43
55	w	8	4SU	O2-C2	-2.52	1.18	1.23
7	A	2580	PSU	C6-C5	2.52	1.38	1.35
7	A	2503	2MA	C5-C4	-2.52	1.36	1.43
7	A	1915	3TD	C4-N3	2.48	1.45	1.40
7	A	2251	OMG	C5-C6	2.46	1.52	1.47
7	A	2445	2MG	O6-C6	-2.44	1.18	1.23
7	A	2251	OMG	O6-C6	-2.44	1.18	1.23
7	A	1835	2MG	O6-C6	-2.44	1.18	1.23
7	A	2503	2MA	C2-N1	2.43	1.44	1.36
33	a	1498	UR3	O2-C2	-2.42	1.18	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	2503	2MA	C6-N1	2.42	1.43	1.38
7	A	2251	OMG	C2-N1	2.40	1.43	1.37
33	a	527	G7M	O6-C6	-2.39	1.18	1.23
33	a	1516	2MG	O6-C6	-2.39	1.18	1.23
7	A	2030	6MZ	C6-N1	-2.37	1.30	1.34
7	A	2605	PSU	C4-C5	-2.35	1.37	1.44
7	A	2552	OMU	C6-N1	2.34	1.43	1.38
33	a	966	2MG	O6-C6	-2.33	1.18	1.23
33	a	1207	2MG	O6-C6	-2.32	1.18	1.23
7	A	745	1MG	O6-C6	-2.27	1.18	1.22
7	A	2580	PSU	C4-C5	-2.27	1.37	1.44
55	w	54	5MU	O2-C2	-2.26	1.18	1.23
7	A	2069	G7M	C5-C6	2.21	1.51	1.45
55	w	46	G7M	C2-N1	2.20	1.43	1.37
55	w	46	G7M	C5-C6	2.14	1.51	1.45
7	A	2457	PSU	C4-C5	-2.14	1.38	1.44
7	A	955	PSU	O4'-C1'	-2.14	1.40	1.43
7	A	746	PSU	C4-C5	-2.11	1.38	1.44
7	A	2030	6MZ	C9-N6	-2.11	1.41	1.45
7	A	1618	6MZ	C6-N1	-2.09	1.31	1.34
7	A	2457	PSU	O4'-C1'	-2.08	1.41	1.43
7	A	955	PSU	C4-C5	-2.08	1.38	1.44
7	A	2030	6MZ	C5-N7	-2.07	1.32	1.39
33	a	516	PSU	O4'-C1'	-2.06	1.41	1.43
33	a	527	G7M	C5-C4	2.05	1.43	1.39
7	A	2552	OMU	C5-C4	2.04	1.48	1.43
7	A	2552	OMU	O4-C4	-2.04	1.20	1.24
7	A	2504	PSU	O4'-C1'	-2.03	1.41	1.43
7	A	1618	6MZ	C9-N6	-2.01	1.41	1.45

All (154) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	a	1519	MA6	N1-C6-N6	-13.08	103.29	117.06
33	a	1518	MA6	N1-C6-N6	-12.51	103.89	117.06
7	A	1939	5MU	C5-C4-N3	12.43	125.92	115.31
55	w	54	5MU	C5-C4-N3	12.17	125.70	115.31
7	A	1939	5MU	C5-C6-N1	-11.04	111.99	123.34
55	w	54	5MU	C5-C6-N1	-9.91	113.14	123.34
55	w	37	MIA	C11-S10-C2	8.99	108.98	102.27
55	w	37	MIA	C12-C13-C14	-8.12	111.33	127.14
55	w	8	4SU	C4-N3-C2	-7.65	119.90	127.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
55	w	32	PSU	N1-C2-N3	6.12	122.07	115.13
7	A	2604	PSU	N1-C2-N3	5.98	121.91	115.13
7	A	2552	OMU	C4-N3-C2	-5.74	119.01	126.58
7	A	1915	3TD	N1-C2-N3	5.61	120.56	116.14
55	w	8	4SU	C5-C4-N3	5.60	119.88	114.69
7	A	2030	6MZ	N3-C2-N1	-5.55	120.01	128.68
7	A	1618	6MZ	N3-C2-N1	-5.48	120.11	128.68
7	A	1939	5MU	C4-N3-C2	-5.39	120.38	127.35
33	a	1518	MA6	N3-C2-N1	-5.30	120.40	128.68
7	A	1939	5MU	O4-C4-C5	-5.28	118.78	124.90
33	a	1519	MA6	N3-C2-N1	-5.26	120.45	128.68
7	A	2030	6MZ	C9-N6-C6	-4.99	118.57	122.87
7	A	1917	PSU	N1-C2-N3	4.93	120.72	115.13
55	w	37	MIA	C15-C14-C13	-4.90	108.47	122.65
7	A	1917	PSU	C4-N3-C2	-4.86	119.34	126.34
7	A	2605	PSU	C4-N3-C2	-4.84	119.36	126.34
55	w	39	PSU	C4-N3-C2	-4.74	119.51	126.34
7	A	2504	PSU	N1-C2-N3	4.72	120.48	115.13
7	A	2580	PSU	C4-N3-C2	-4.71	119.55	126.34
7	A	1911	PSU	C4-N3-C2	-4.70	119.56	126.34
7	A	746	PSU	C4-N3-C2	-4.70	119.57	126.34
7	A	2457	PSU	C4-N3-C2	-4.68	119.59	126.34
7	A	2580	PSU	N1-C2-N3	4.64	120.39	115.13
55	w	54	5MU	C5M-C5-C4	4.63	123.87	118.77
7	A	1911	PSU	N1-C2-N3	4.62	120.36	115.13
7	A	1939	5MU	N3-C2-N1	4.60	120.99	114.89
33	a	1498	UR3	C4-N3-C2	-4.59	120.24	124.56
55	w	55	PSU	N1-C2-N3	4.57	120.30	115.13
55	w	54	5MU	C4-N3-C2	-4.56	121.45	127.35
55	w	54	5MU	O4-C4-C5	-4.52	119.66	124.90
7	A	2030	6MZ	C1'-N9-C4	-4.51	118.72	126.64
7	A	2504	PSU	C4-N3-C2	-4.48	119.89	126.34
7	A	2605	PSU	N1-C2-N3	4.47	120.20	115.13
55	w	54	5MU	C5M-C5-C6	-4.44	116.91	122.85
55	w	39	PSU	N1-C2-N3	4.36	120.06	115.13
55	w	55	PSU	C4-N3-C2	-4.34	120.08	126.34
7	A	745	1MG	C5-C6-N1	4.26	120.31	113.90
33	a	516	PSU	C4-N3-C2	-4.21	120.27	126.34
7	A	955	PSU	C4-N3-C2	-4.20	120.29	126.34
7	A	746	PSU	N1-C2-N3	4.16	119.85	115.13
7	A	2552	OMU	N3-C2-N1	4.14	120.39	114.89
7	A	955	PSU	N1-C2-N3	4.08	119.75	115.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	a	516	PSU	N1-C2-N3	4.07	119.74	115.13
55	w	37	MIA	C16-C14-C13	-4.06	110.91	122.65
7	A	2457	PSU	N1-C2-N3	4.05	119.71	115.13
7	A	2604	PSU	C4-N3-C2	-3.99	120.59	126.34
55	w	54	5MU	N3-C2-N1	3.98	120.18	114.89
7	A	2030	6MZ	C2-N1-C6	3.92	119.95	116.59
33	a	1498	UR3	C1'-N1-C2	3.86	123.51	116.99
55	w	37	MIA	S10-C2-N1	3.84	129.31	116.01
7	A	1939	5MU	C5M-C5-C6	-3.84	117.72	122.85
7	A	1962	5MC	C5-C6-N1	-3.80	119.43	123.34
7	A	2552	OMU	C5-C4-N3	3.73	120.42	114.84
55	w	32	PSU	C4-N3-C2	-3.67	121.05	126.34
7	A	2503	2MA	C5-C6-N1	3.67	120.35	114.02
33	a	1207	2MG	C5-C6-N1	3.63	120.37	113.95
7	A	1835	2MG	C5-C6-N1	3.62	120.34	113.95
7	A	1915	3TD	C4-N3-C2	-3.61	120.69	124.61
55	w	37	MIA	N3-C2-N1	-3.61	120.34	126.98
55	w	8	4SU	C5-C4-S4	-3.56	119.88	124.47
55	w	32	PSU	O2-C2-N1	-3.55	118.89	122.79
55	w	8	4SU	N3-C2-N1	3.53	119.57	114.89
7	A	2251	OMG	C5-C6-N1	3.50	120.13	113.95
33	a	1516	2MG	C5-C6-N1	3.43	120.01	113.95
33	a	966	2MG	C5-C6-N1	3.41	119.98	113.95
7	A	2445	2MG	C5-C6-N1	3.40	119.96	113.95
7	A	1939	5MU	C5M-C5-C4	3.39	122.50	118.77
7	A	2604	PSU	O2-C2-N1	-3.34	119.11	122.79
7	A	1939	5MU	O2-C2-N1	-3.30	118.39	122.79
33	a	967	5MC	C5-C6-N1	-3.24	120.01	123.34
33	a	1498	UR3	C6-N1-C2	-3.22	118.91	121.79
55	w	37	MIA	C2-N3-C4	3.15	119.66	115.32
7	A	2445	2MG	CM2-N2-C2	-3.14	116.92	123.86
7	A	747	5MC	C5-C6-N1	-3.11	120.13	123.34
7	A	955	PSU	O2-C2-N1	-3.11	119.37	122.79
7	A	1618	6MZ	C2-N1-C6	3.09	119.24	116.59
7	A	2251	OMG	C2-N1-C6	-3.07	119.45	125.10
7	A	2605	PSU	O2-C2-N1	-3.04	119.44	122.79
33	a	1407	5MC	C5-C6-N1	-3.02	120.23	123.34
7	A	1911	PSU	O2-C2-N1	-3.01	119.47	122.79
33	a	516	PSU	O2-C2-N1	-2.98	119.51	122.79
7	A	2069	G7M	C2-N1-C6	-2.98	119.61	125.10
55	w	55	PSU	O2-C2-N1	-2.95	119.54	122.79
7	A	2552	OMU	O4-C4-C5	-2.87	120.11	125.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
55	w	46	G7M	C2-N1-C6	-2.86	119.82	125.10
55	w	54	5MU	O4-C4-N3	-2.86	114.64	120.12
7	A	1618	6MZ	C9-N6-C6	-2.82	120.44	122.87
55	w	37	MIA	C16-C14-C15	-2.82	108.39	114.60
7	A	2457	PSU	O2-C2-N1	-2.78	119.72	122.79
33	a	527	G7M	C2-N1-C6	-2.78	119.98	125.10
7	A	2251	OMG	O6-C6-C5	-2.75	119.00	124.37
33	a	1498	UR3	O2-C2-N3	-2.71	117.52	121.34
33	a	1207	2MG	C8-N7-C5	2.70	108.13	102.99
33	a	1516	2MG	C8-N7-C5	2.69	108.11	102.99
7	A	2580	PSU	O2-C2-N1	-2.67	119.85	122.79
7	A	1917	PSU	O2-C2-N1	-2.63	119.89	122.79
7	A	2580	PSU	O4'-C1'-C2'	2.60	108.81	105.14
7	A	1917	PSU	C6-N1-C2	-2.59	120.03	122.68
7	A	2580	PSU	C6-N1-C2	-2.55	120.07	122.68
7	A	745	1MG	O6-C6-C5	-2.55	119.68	124.19
7	A	1939	5MU	O4-C4-N3	-2.51	115.30	120.12
7	A	955	PSU	C6-N1-C2	-2.51	120.12	122.68
33	a	966	2MG	C8-N7-C5	2.50	107.76	102.99
7	A	1835	2MG	CM2-N2-C2	-2.50	118.34	123.86
33	a	966	2MG	O6-C6-C5	-2.49	119.50	124.37
33	a	966	2MG	CM2-N2-C2	-2.49	118.36	123.86
7	A	1835	2MG	C8-N7-C5	2.49	107.73	102.99
7	A	745	1MG	C8-N7-C5	2.47	107.69	102.99
7	A	2503	2MA	C8-N7-C5	2.46	107.68	102.99
33	a	1207	2MG	O6-C6-C5	-2.45	119.59	124.37
7	A	2504	PSU	C6-N1-C2	-2.44	120.19	122.68
33	a	516	PSU	C6-N1-C2	-2.43	120.20	122.68
7	A	1618	6MZ	C1'-N9-C4	-2.43	122.37	126.64
7	A	746	PSU	O2-C2-N1	-2.42	120.13	122.79
55	w	55	PSU	C6-N1-C2	-2.41	120.22	122.68
33	a	516	PSU	O4'-C1'-C2'	2.41	108.54	105.14
7	A	2504	PSU	C6-C5-C4	2.40	119.88	118.20
7	A	2251	OMG	C8-N7-C5	2.35	107.46	102.99
55	w	55	PSU	C6-C5-C4	2.35	119.84	118.20
55	w	46	G7M	CN7-N7-C8	-2.34	114.15	125.43
7	A	2445	2MG	O6-C6-C5	-2.34	119.81	124.37
33	a	1516	2MG	CM2-N2-C2	-2.33	118.71	123.86
7	A	1835	2MG	O6-C6-C5	-2.30	119.88	124.37
7	A	1915	3TD	C10-N3-C4	2.28	121.17	117.69
33	a	1402	4OC	C6-C5-C4	2.27	119.74	116.96
7	A	2498	OMC	O2-C2-N3	-2.26	118.65	122.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	A	2445	2MG	C8-N7-C5	2.24	107.26	102.99
7	A	2605	PSU	C6-N1-C2	-2.24	120.39	122.68
33	a	1516	2MG	O6-C6-C5	-2.22	120.03	124.37
55	w	32	PSU	C3'-C2'-C1'	2.13	104.12	101.64
7	A	1911	PSU	C6-N1-C2	-2.13	120.50	122.68
7	A	2580	PSU	C6-C5-C4	2.12	119.68	118.20
33	a	1207	2MG	CM2-N2-C2	-2.11	119.21	123.86
7	A	1939	5MU	C6-C5-C4	2.10	119.78	118.03
7	A	2498	OMC	C1'-N1-C2	2.10	123.10	118.42
7	A	1911	PSU	C6-C5-C4	2.09	119.66	118.20
7	A	2604	PSU	C5-C6-N1	-2.08	118.98	122.11
7	A	747	5MC	CM5-C5-C6	-2.08	120.07	122.85
7	A	745	1MG	CM1-N1-C6	2.07	120.38	117.55
33	a	1407	5MC	O2-C2-N3	-2.07	118.97	122.33
55	w	46	G7M	C3'-C2'-C1'	2.06	104.08	100.98
7	A	1915	3TD	C6-C5-C4	2.05	119.64	118.22
7	A	2457	PSU	O4'-C1'-C2'	2.04	108.02	105.14
7	A	2605	PSU	O4-C4-C5	-2.03	118.74	124.05
7	A	747	5MC	O2-C2-N3	-2.03	119.03	122.33

There are no chirality outliers.

All (78) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	746	PSU	C2'-C1'-C5-C6
7	A	747	5MC	C3'-C4'-C5'-O5'
7	A	1618	6MZ	N1-C6-N6-C9
7	A	1915	3TD	O4'-C1'-C5-C4
7	A	1915	3TD	O4'-C1'-C5-C6
7	A	1962	5MC	C2'-C1'-N1-C6
7	A	2030	6MZ	N1-C6-N6-C9
7	A	2030	6MZ	C3'-C4'-C5'-O5'
7	A	2445	2MG	C3'-C4'-C5'-O5'
7	A	2504	PSU	O4'-C4'-C5'-O5'
7	A	2604	PSU	C3'-C4'-C5'-O5'
33	a	527	G7M	C3'-C4'-C5'-O5'
33	a	967	5MC	O4'-C4'-C5'-O5'
33	a	967	5MC	C3'-C4'-C5'-O5'
33	a	1402	4OC	C1'-C2'-O2'-CM2
33	a	1498	UR3	O4'-C1'-N1-C6
33	a	1498	UR3	O4'-C1'-N1-C2
33	a	1518	MA6	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
33	a	1518	MA6	C3'-C4'-C5'-O5'
55	w	8	4SU	O4'-C4'-C5'-O5'
55	w	32	PSU	O4'-C1'-C5-C4
55	w	32	PSU	O4'-C1'-C5-C6
55	w	37	MIA	C5-C6-N6-C12
55	w	37	MIA	C12-C13-C14-C16
55	w	39	PSU	C2'-C1'-C5-C4
55	w	39	PSU	O4'-C1'-C5-C4
55	w	39	PSU	O4'-C1'-C5-C6
55	w	46	G7M	O4'-C4'-C5'-O5'
55	w	55	PSU	C2'-C1'-C5-C4
55	w	55	PSU	O4'-C1'-C5-C6
7	A	2552	OMU	O4'-C1'-N1-C2
7	A	1962	5MC	C2'-C1'-N1-C2
7	A	1939	5MU	C3'-C4'-C5'-O5'
7	A	1939	5MU	O4'-C4'-C5'-O5'
7	A	2498	OMC	O4'-C4'-C5'-O5'
7	A	2503	2MA	O4'-C4'-C5'-O5'
7	A	2504	PSU	C3'-C4'-C5'-O5'
55	w	8	4SU	C3'-C4'-C5'-O5'
55	w	46	G7M	C3'-C4'-C5'-O5'
55	w	54	5MU	C3'-C4'-C5'-O5'
7	A	747	5MC	O4'-C4'-C5'-O5'
7	A	1835	2MG	C3'-C4'-C5'-O5'
7	A	2445	2MG	O4'-C4'-C5'-O5'
7	A	2498	OMC	C3'-C4'-C5'-O5'
33	a	1498	UR3	O4'-C4'-C5'-O5'
55	w	54	5MU	O4'-C4'-C5'-O5'
55	w	37	MIA	N1-C6-N6-C12
7	A	2552	OMU	O4'-C1'-N1-C6
7	A	1835	2MG	O4'-C4'-C5'-O5'
7	A	2552	OMU	C3'-C4'-C5'-O5'
33	a	1498	UR3	C3'-C4'-C5'-O5'
7	A	2030	6MZ	O4'-C4'-C5'-O5'
7	A	2552	OMU	O4'-C4'-C5'-O5'
7	A	2604	PSU	O4'-C4'-C5'-O5'
33	a	527	G7M	O4'-C4'-C5'-O5'
55	w	55	PSU	O4'-C4'-C5'-O5'
33	a	1519	MA6	C5-C6-N6-C10
55	w	55	PSU	C3'-C4'-C5'-O5'
7	A	2030	6MZ	C4'-C5'-O5'-P
55	w	37	MIA	C4'-C5'-O5'-P

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Mol	Chain	Res	Type	Atoms
7	A	2503	2MA	C3'-C4'-C5'-O5'
7	A	2552	OMU	C1'-C2'-O2'-CM2
7	A	1962	5MC	O4'-C1'-N1-C2
55	w	46	G7M	C4'-C5'-O5'-P
33	a	527	G7M	C4'-C5'-O5'-P
33	a	1519	MA6	C4'-C5'-O5'-P
7	A	1962	5MC	O4'-C1'-N1-C6
7	A	747	5MC	C4'-C5'-O5'-P
55	w	54	5MU	C4'-C5'-O5'-P
7	A	746	PSU	O4'-C1'-C5-C4
55	w	55	PSU	O4'-C1'-C5-C4
7	A	1618	6MZ	C5-C6-N6-C9
7	A	2030	6MZ	C5-C6-N6-C9
7	A	746	PSU	O4'-C1'-C5-C6
7	A	2498	OMC	C2'-C1'-N1-C2
7	A	1618	6MZ	C3'-C4'-C5'-O5'
7	A	2069	G7M	O4'-C4'-C5'-O5'
7	A	2498	OMC	C2'-C1'-N1-C6

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 358 ligands modelled in this entry, 358 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

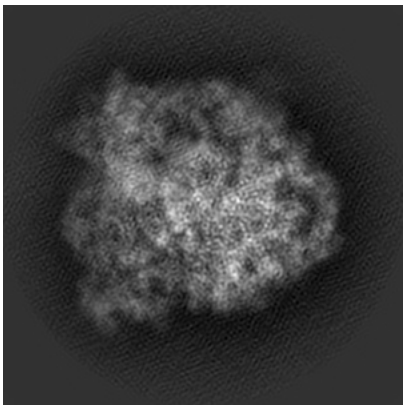
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-10908. These allow visual inspection of the internal detail of the map and identification of artifacts.

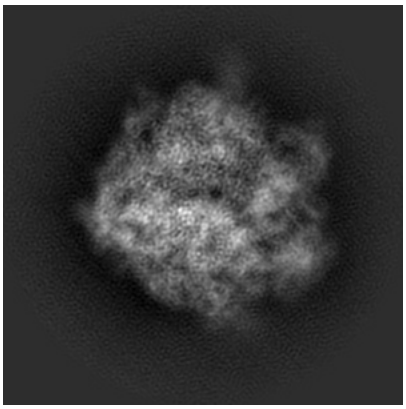
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

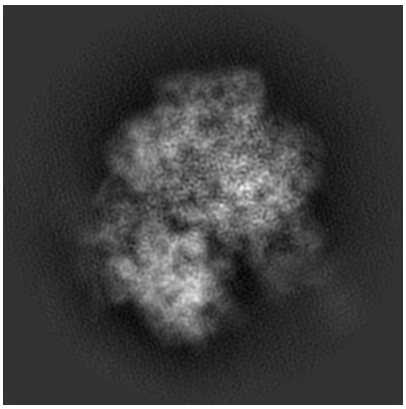
6.1.1 Primary map



X

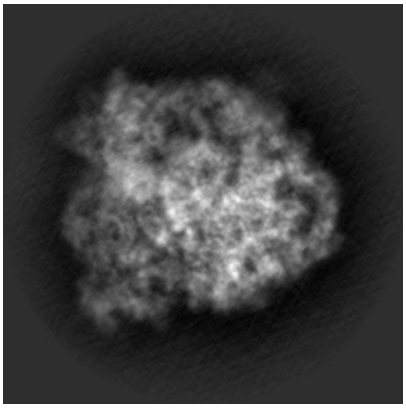


Y

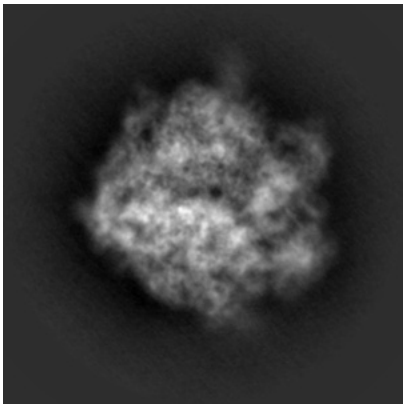


Z

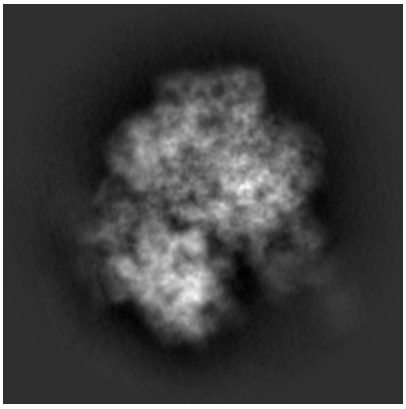
6.1.2 Raw map



X



Y

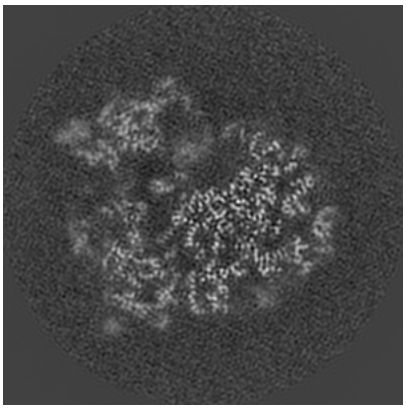


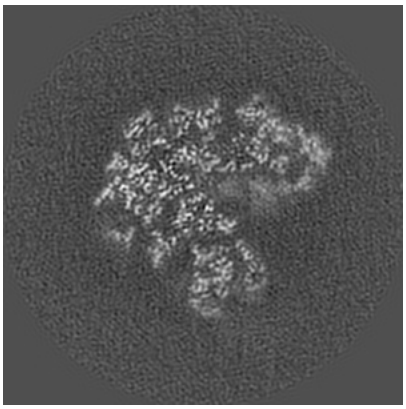
Z

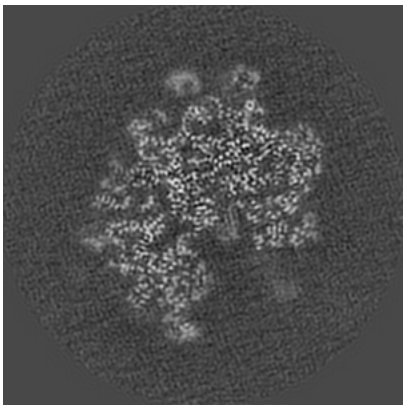
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

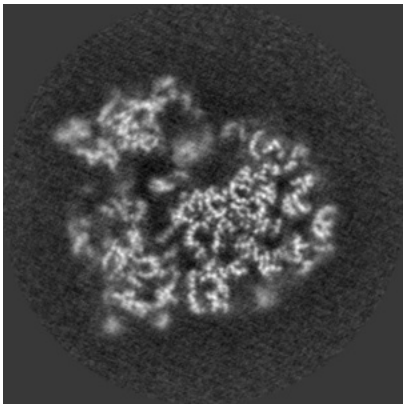
6.2.1 Primary map

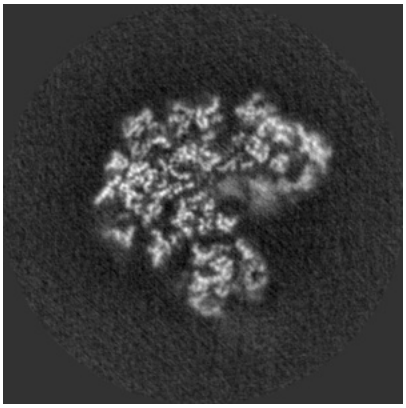

X Index: 162

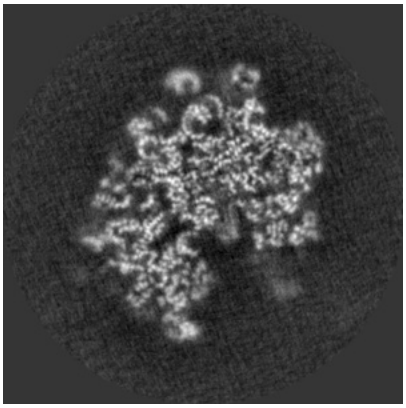

Y Index: 162


Z Index: 162

6.2.2 Raw map


X Index: 162

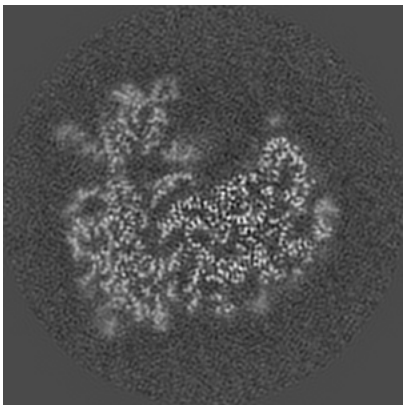

Y Index: 162

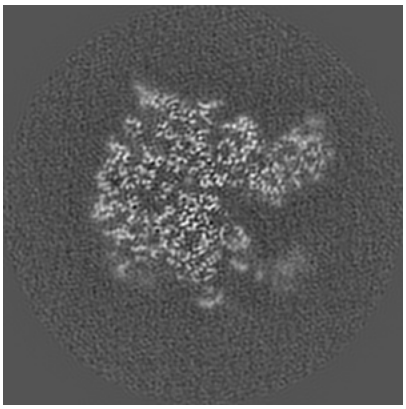

Z Index: 162

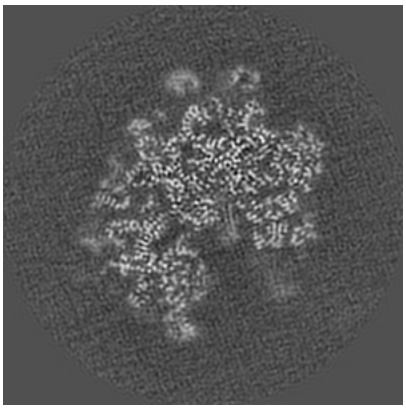
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

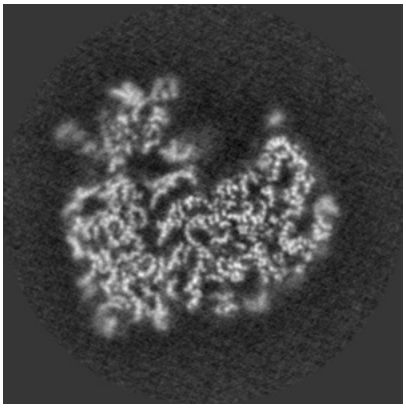
6.3.1 Primary map

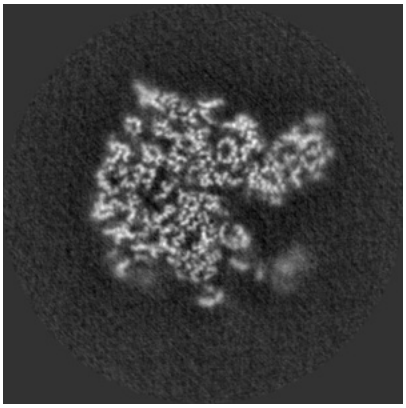

X Index: 156

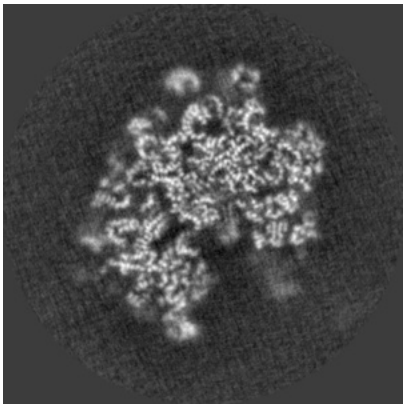

Y Index: 180


Z Index: 163

6.3.2 Raw map


X Index: 155

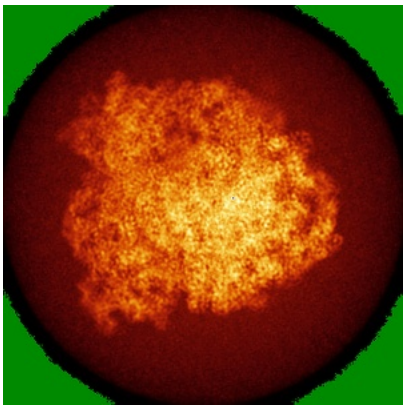

Y Index: 180

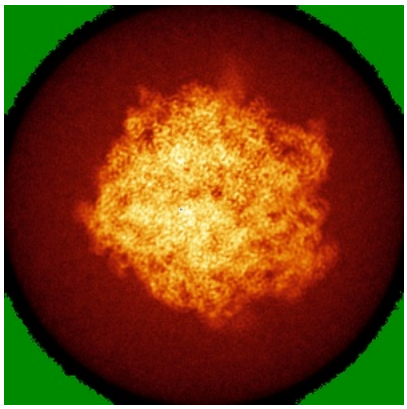

Z Index: 163

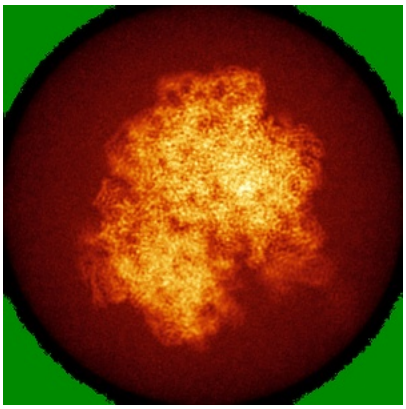
The images above show the largest variance slices of the map in three orthogonal directions.

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

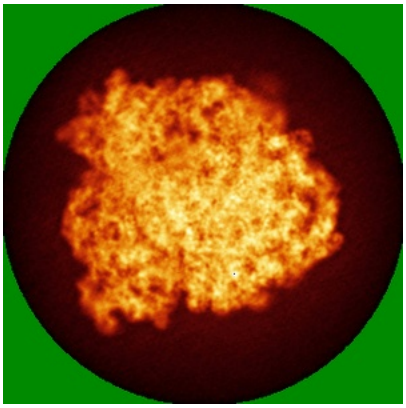
6.4.1 Primary map

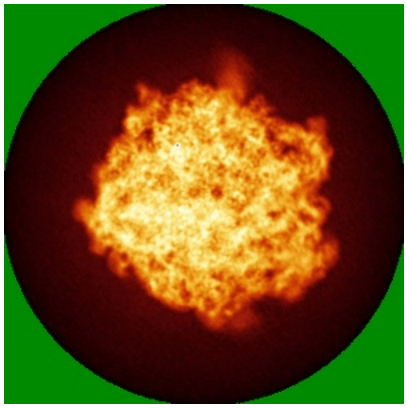

X

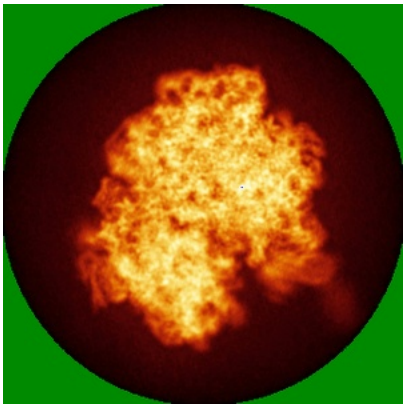

Y


Z

6.4.2 Raw map


X

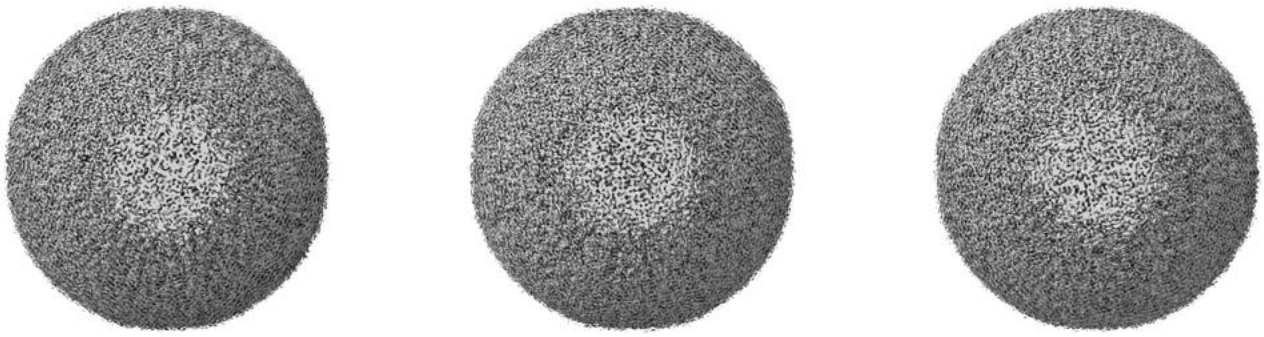

Y


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)

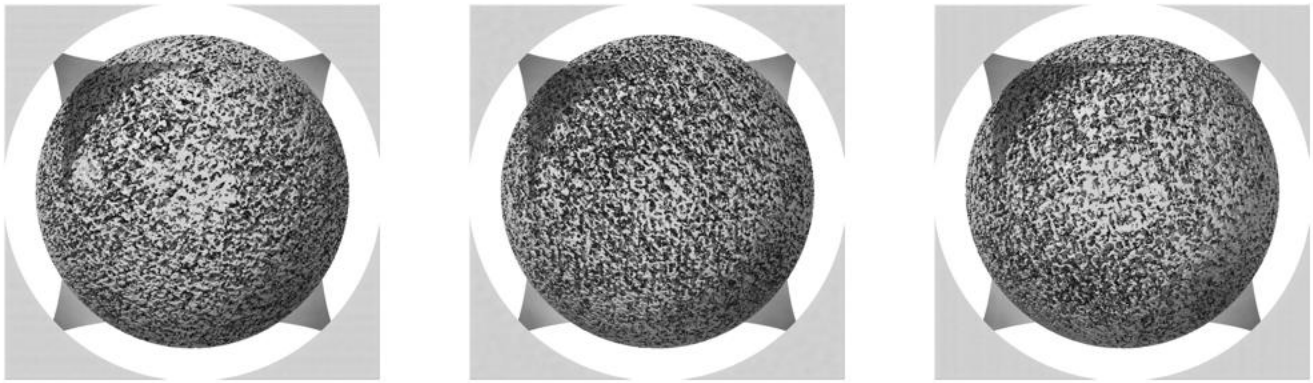
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.015. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

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

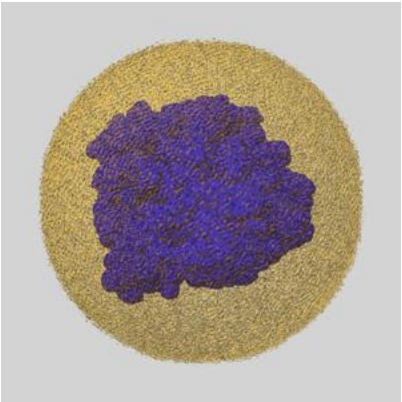
6.6 Mask visualisation (i)

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

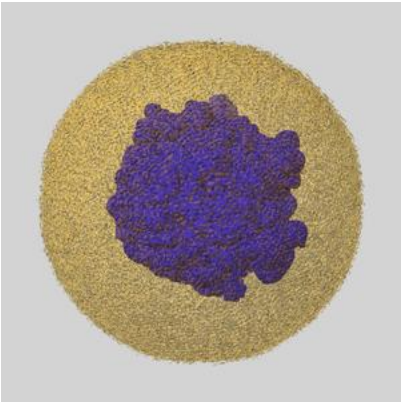
A mask typically either:

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

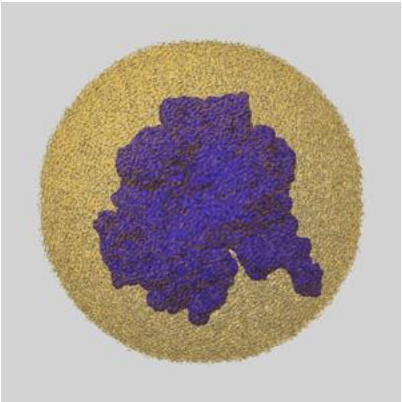
6.6.1 emd_10908_msk_1.map (i)



X



Y

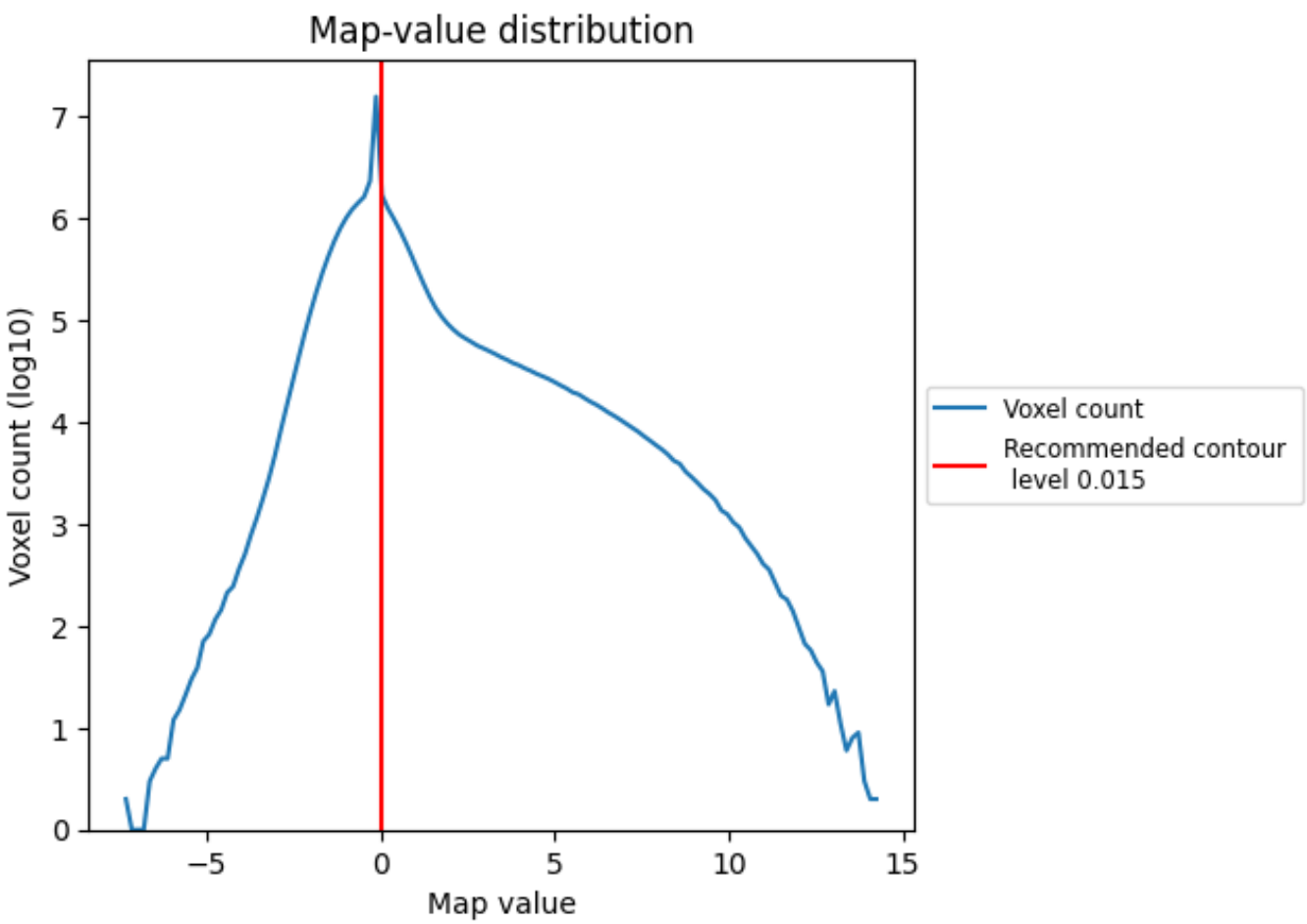


Z

7 Map analysis (i)

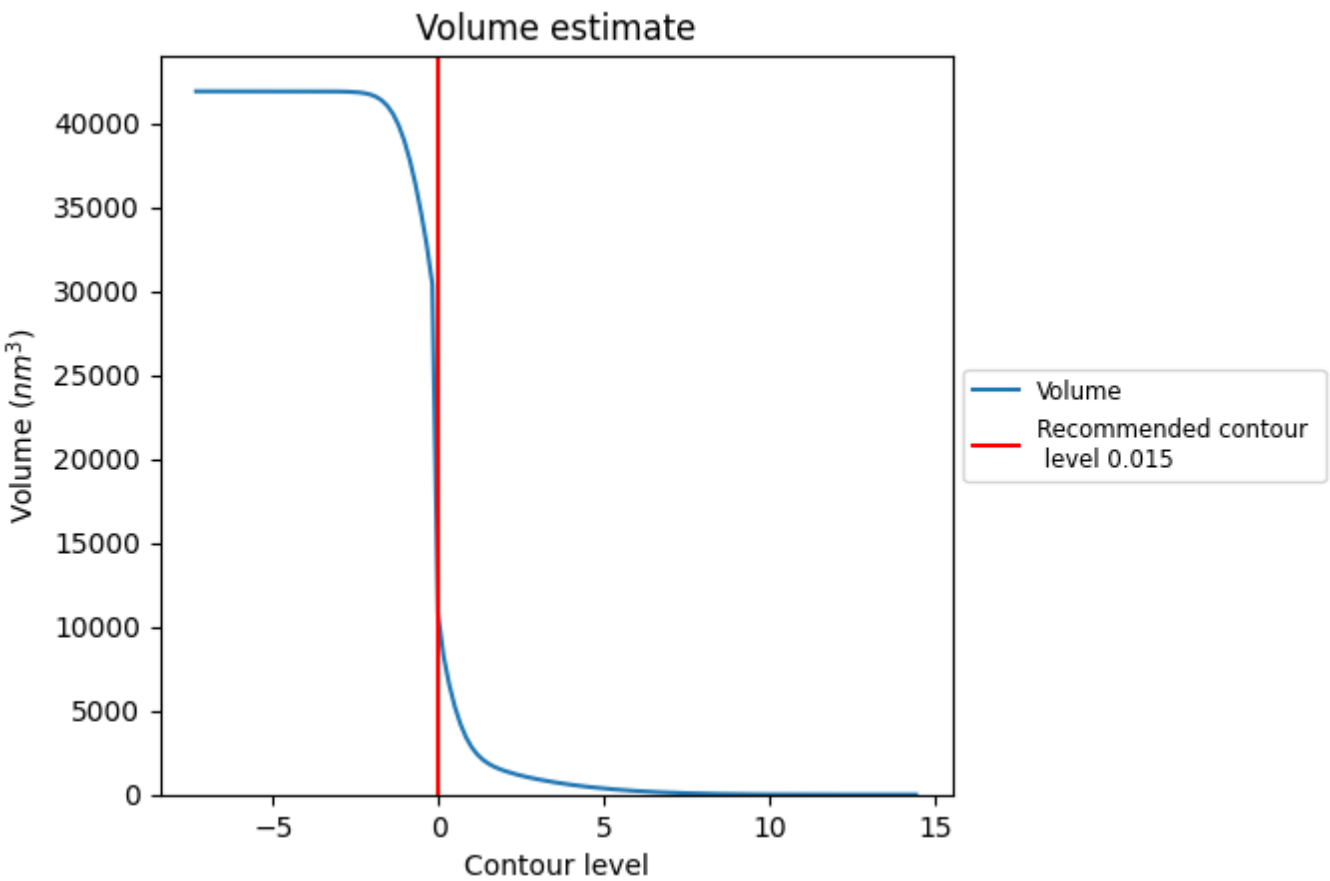
This section contains the results of statistical analysis of the map.

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.

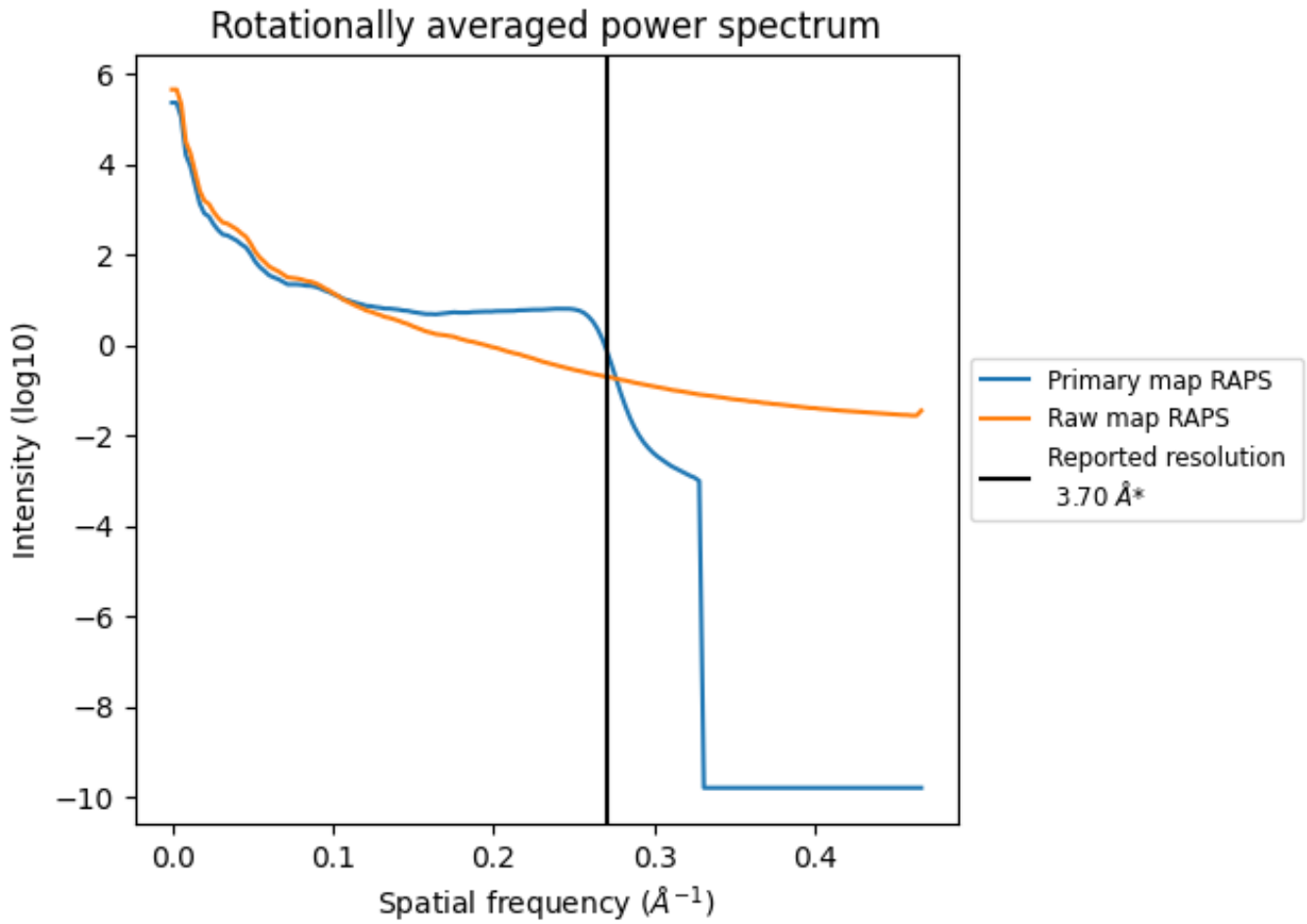
7.2 Volume estimate (i)



The volume at the recommended contour level is 10367 nm^3; this corresponds to an approximate mass of 9365 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

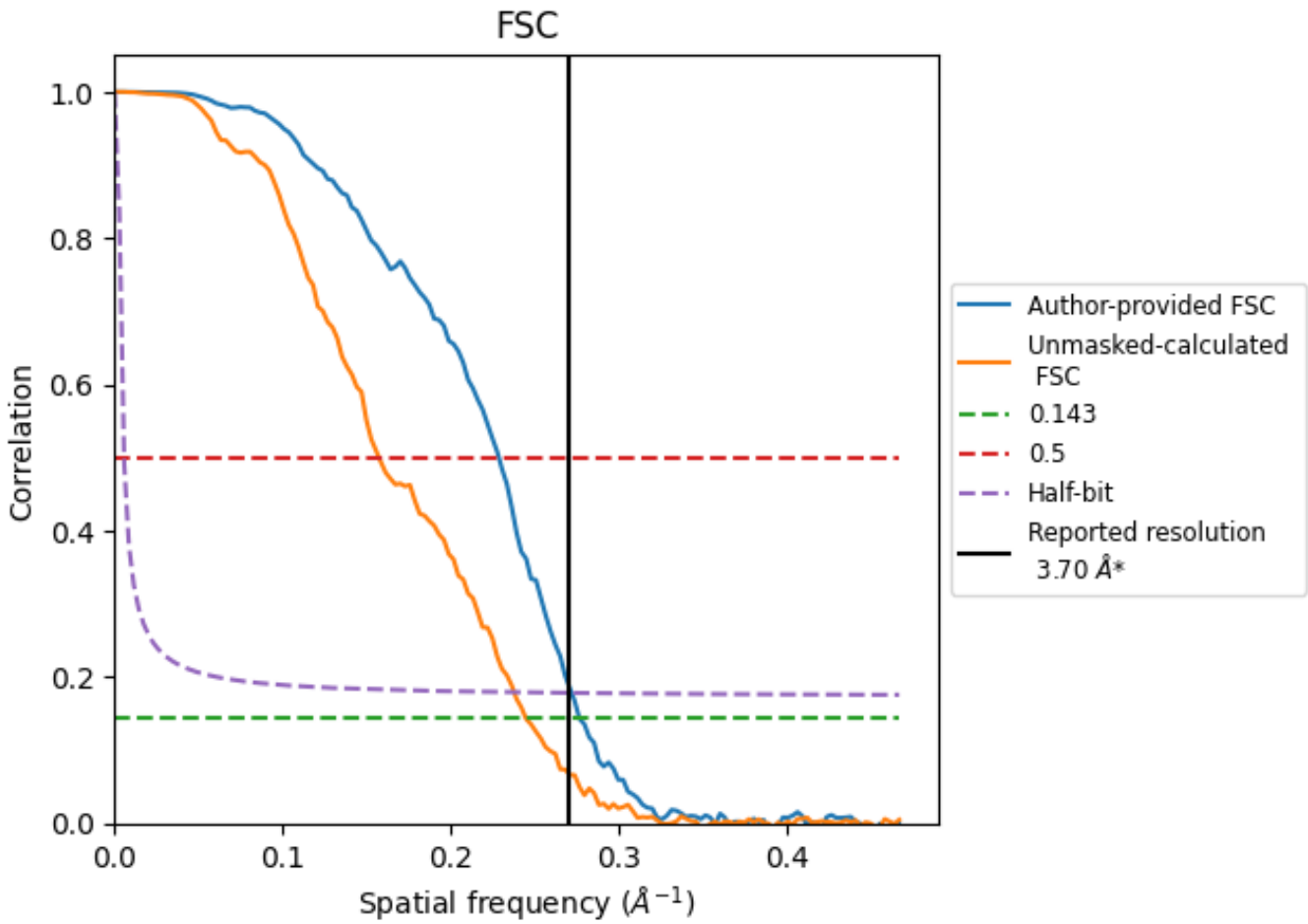


*Reported resolution corresponds to spatial frequency of 0.270 Å^{-1}

8 Fourier-Shell correlation (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 0.270 Å^{-1}

8.2 Resolution estimates (i)

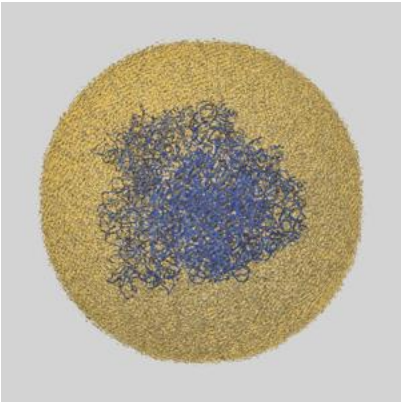
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	3.62	4.38	3.68
Unmasked-calculated*	4.09	6.37	4.21

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.09 differs from the reported value 3.7 by more than 10 %

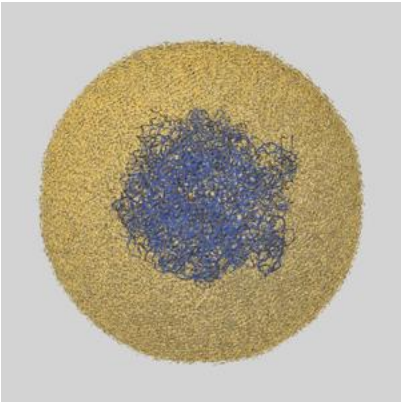
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-10908 and PDB model 6YSU. Per-residue inclusion information can be found in section 3 on page 15.

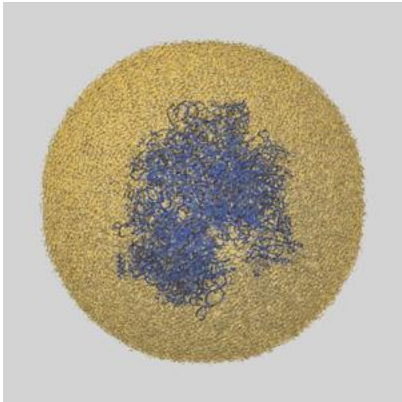
9.1 Map-model overlay (i)



X



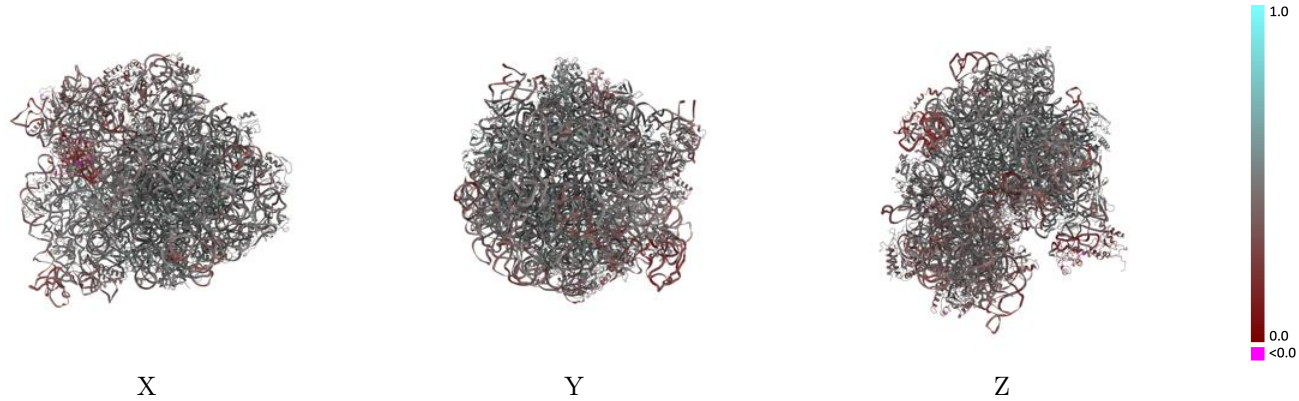
Y



Z

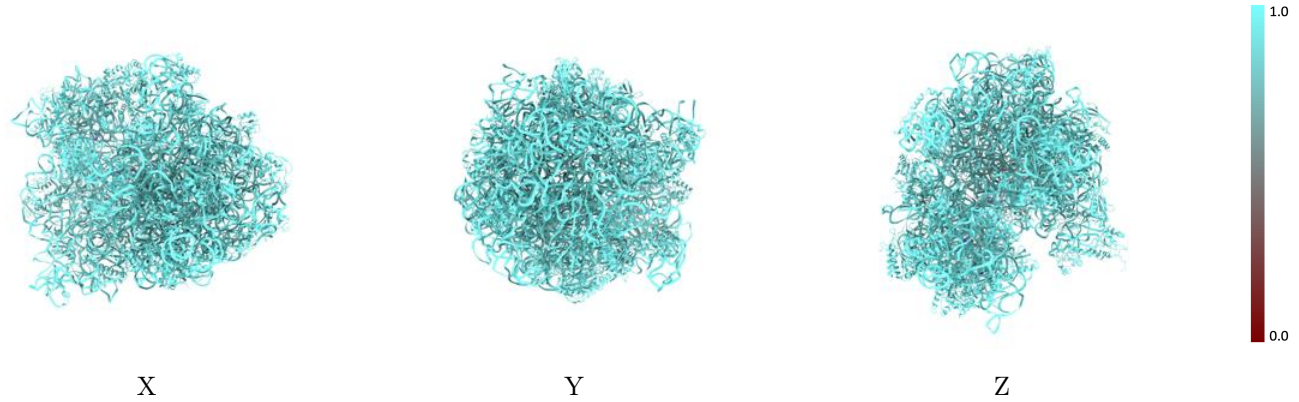
The images above show the 3D surface view of the map at the recommended contour level 0.015 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



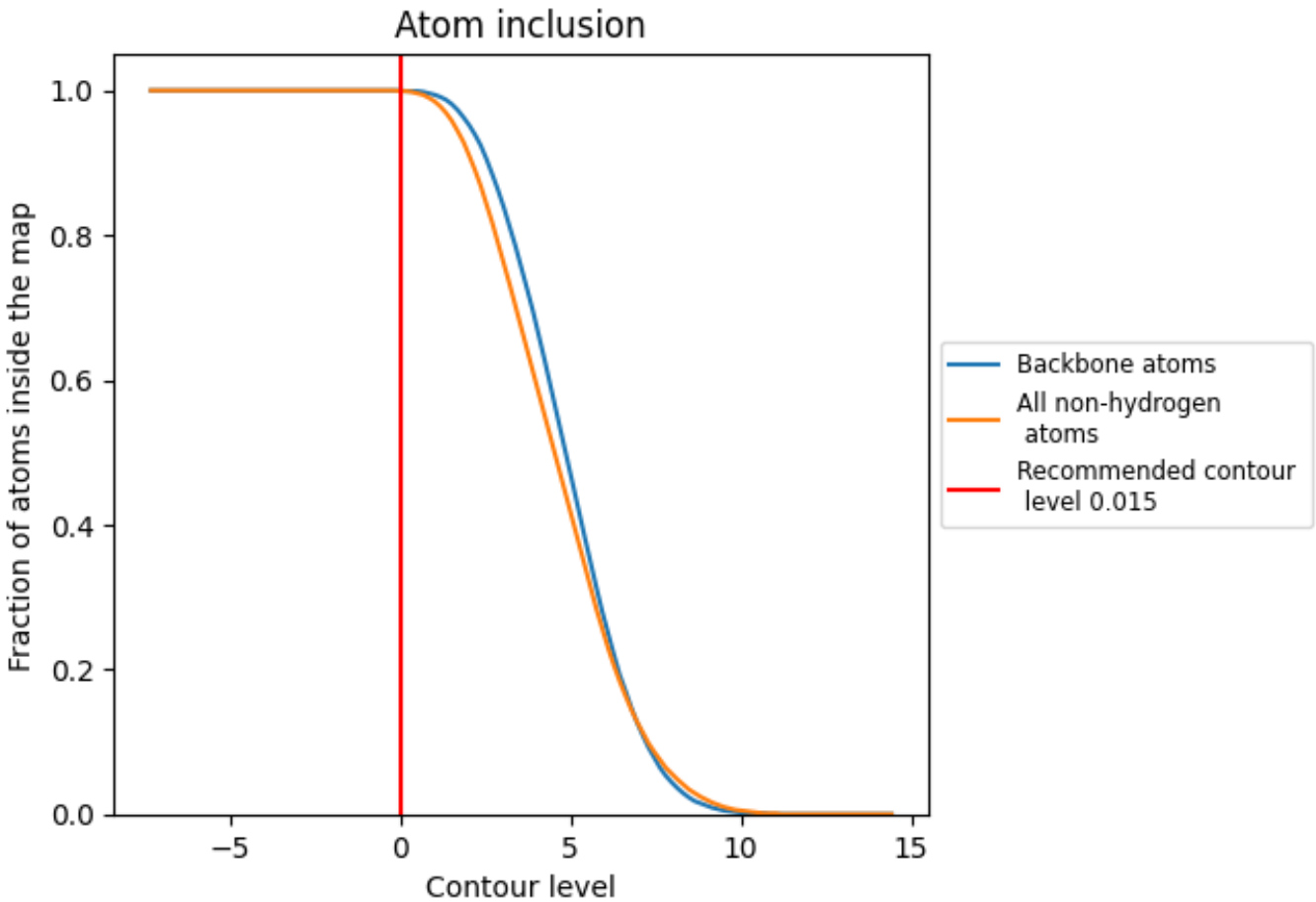
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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)



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 (0.015).

9.4 Atom inclusion (i)



At the recommended contour level, 100% of all backbone atoms, 100% 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 (0.015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9990	0.4460
0	1.0000	0.5050
1	0.9950	0.4970
2	0.9970	0.5250
3	0.9980	0.5170
4	1.0000	0.5120
5	1.0000	0.2850
A	1.0000	0.4500
B	1.0000	0.4160
C	0.9980	0.5170
D	0.9990	0.5070
E	1.0000	0.4880
F	1.0000	0.3980
G	1.0000	0.4570
H	0.9980	0.3960
I	0.9970	0.2800
J	0.9980	0.5100
K	0.9990	0.5110
L	0.9970	0.4980
M	0.9970	0.5030
N	0.9990	0.5050
O	1.0000	0.4360
P	1.0000	0.5050
Q	1.0000	0.5010
R	1.0000	0.5000
S	0.9980	0.5050
T	1.0000	0.4930
U	0.9990	0.4640
V	0.9990	0.4740
W	1.0000	0.5200
X	0.9950	0.4990
Y	1.0000	0.4320
Z	1.0000	0.4980
a	1.0000	0.4270
b	0.9960	0.4300

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Chain	Atom inclusion	Q-score
c	0.9980	0.4500
d	0.9990	0.4480
e	0.9980	0.4820
f	0.9990	0.4410
g	0.9990	0.3910
h	0.9990	0.4810
i	0.9980	0.4130
j	0.9960	0.4000
k	0.9980	0.4630
l	0.9980	0.4920
m	1.0000	0.4030
n	1.0000	0.4340
o	1.0000	0.4570
p	1.0000	0.4610
q	0.9980	0.4560
r	1.0000	0.4780
s	1.0000	0.4230
t	0.9990	0.4400
u	1.0000	0.4180
v	1.0000	0.4260
w	0.9950	0.3300
x	1.0000	0.4530
y	0.9880	0.4320