



Full wwPDB EM Validation Report ⓘ

Nov 20, 2022 – 04:30 PM EST

PDB ID : 7UPH
EMDB ID : EMD-26666
Title : Structure of a ribosome with tethered subunits
Authors : Kim, D.S.; Watkins, A.; Bidstrup, E.; Lee, J.; Topkar, V.V.; Kofman, C.;
Schwarz, K.J.; Liu, Y.; Pintilie, G.; Roney, E.; Das, R.; Jewett, M.C.
Deposited on : 2022-04-15
Resolution : 4.18 Å(reported)
Based on initial model : 4YBB

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

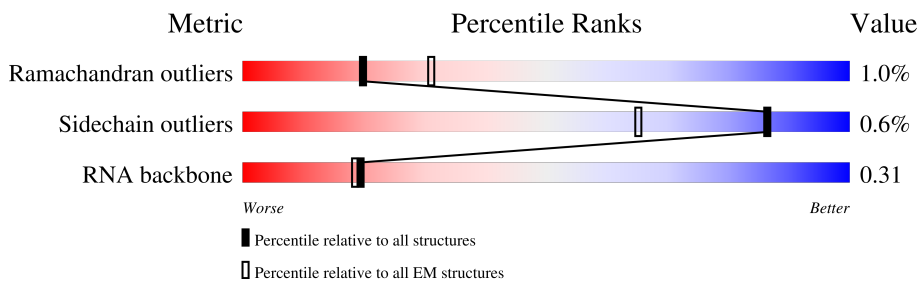
EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

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 4.18 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.





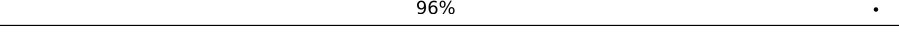
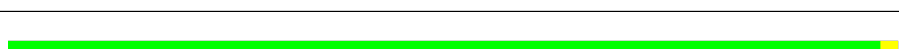

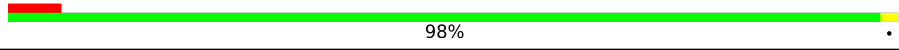
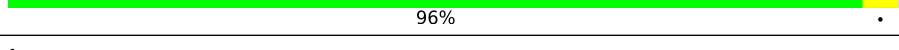
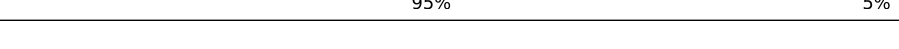

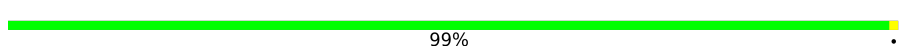
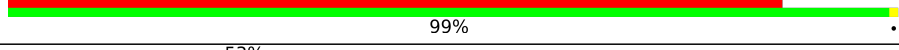
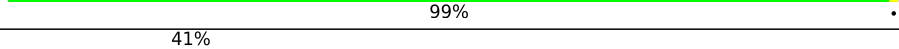
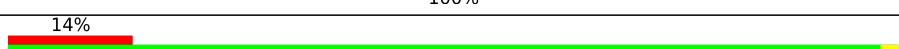
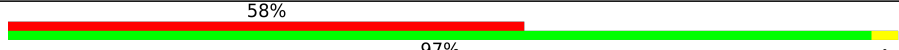
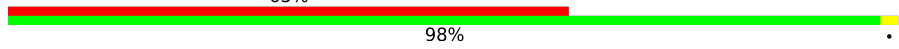
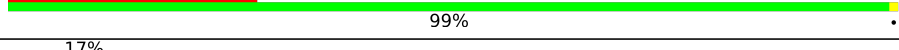
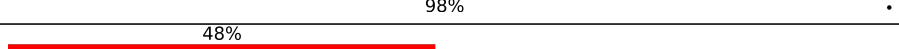

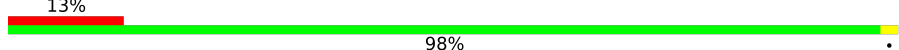
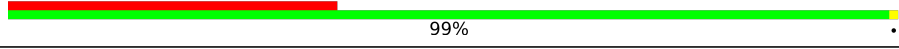
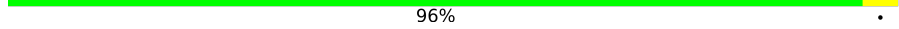



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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 $\leq 5\%$. 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	A	100	16% (Upper red bar) 99% (Green bar) 5% (Yellow bar) . (Grey bar)
2	B	88	48% (Upper red bar) 98% (Green bar) 5% (Yellow bar) . (Grey bar)
3	C	82	23% (Upper red bar) 95% (Green bar) 5% (Yellow bar)
4	D	80	44% (Upper red bar) 95% (Green bar) 5% (Yellow bar)
5	E	55	40% (Upper red bar) 98% (Green bar) . (Grey bar)
6	F	79	76% (Upper red bar) 99% (Green bar) . (Grey bar)
7	G	85	67% (Upper red bar) 100% (Green bar)
8	H	56	75% (Upper red bar) 96% (Green bar) . (Grey bar)

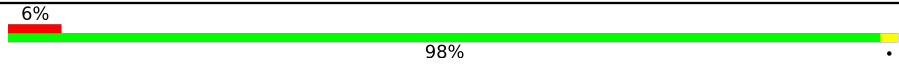
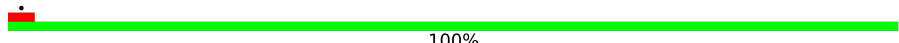
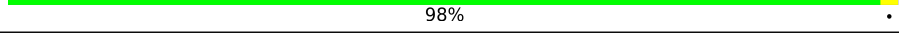
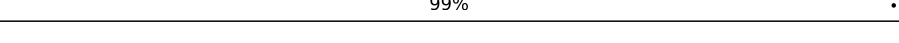
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Mol	Chain	Length	Quality of chain
9	I	4438	 63% 34%
10	J	118	 47% 47% 6%
11	K	271	 96%
12	L	209	 95%
13	M	201	 98%
14	N	177	 5% 98%
15	O	176	 6% 98%
16	R	142	 96%
17	S	122	 95% 5%
18	T	144	 99%
19	U	136	 95% 5%
20	V	120	 99%
21	W	224	 87% 99%
22	X	206	 53% 99%
23	Y	205	 41% 100%
24	Z	150	 14% 98%
25	a	100	 58% 97%
26	b	151	 63% 98%
27	c	129	 28% 99%
28	d	127	 17% 98%
29	e	98	 48% 97%
30	f	117	 42% 99%
31	g	123	 13% 98%
32	h	114	 37% 99%
33	i	56	96%

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Mol	Chain	Length	Quality of chain
34	j	50	 6% 98%
35	k	46	 96%
36	l	64	 100%
37	m	38	 100%
38	n	116	 98%
39	o	114	 7% 96%
40	p	117	 100%
41	q	103	 100%
42	r	110	 99%
43	s	93	 99%
44	t	102	 98%
45	u	94	 97%
46	v	75	 100%
47	w	77	 99%
48	x	62	 97%
49	y	58	 95% 5%

2 Entry composition [i](#)

There are 49 unique types of molecules in this entry. The entry contains 141080 atoms, of which 625 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 30S ribosomal protein S14.

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

- Molecule 2 is a protein called 30S ribosomal protein S15.

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

- Molecule 3 is a protein called 30S ribosomal protein S16.

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

- Molecule 4 is a protein called 30S ribosomal protein S17.

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

- Molecule 5 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
5	E	55	456	288	86	82	0	0

- Molecule 6 is a protein called 30S ribosomal protein S19.

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

- Molecule 7 is a protein called 30S ribosomal protein S20.

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

- Molecule 8 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	56	Total	C	N	O	S	0	0
			465	290	96	78	1		

- Molecule 9 is a RNA chain called Tethered rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace	
9	I	4438	Total	C	H	N	O	P	0	0
			95909	42519	625	17511	30816	4438		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	118	Total	C	N	O	P	0	0
			2529	1126	464	821	118		

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 21 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	W	224	Total	C	N	O	S	0	0
			1753	1109	315	321	8		

- Molecule 22 is a protein called 30S ribosomal protein S3.

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

- Molecule 23 is a protein called 30S ribosomal protein S4.

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

- Molecule 24 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Z	150	Total	C	N	O	S	0	0
			1105	687	211	201	6		

- Molecule 25 is a protein called 30S ribosomal protein S6.

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

- Molecule 26 is a protein called 30S ribosomal protein S7.

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

- Molecule 27 is a protein called 30S ribosomal protein S8.

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

- Molecule 28 is a protein called 30S ribosomal protein S9.

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

- Molecule 29 is a protein called 30S ribosomal protein S10.

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

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

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

- Molecule 31 is a protein called 30S ribosomal protein S12.

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

- Molecule 32 is a protein called 30S ribosomal protein S13.

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

- Molecule 33 is a protein called 50S ribosomal protein L32.

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

- Molecule 34 is a protein called 50S ribosomal protein L33.

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

- Molecule 35 is a protein called 50S ribosomal protein L34.

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

- Molecule 36 is a protein called 50S ribosomal protein L35.

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

- Molecule 37 is a protein called 50S ribosomal protein L36.

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

- Molecule 38 is a protein called 50S ribosomal protein L18.

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

- Molecule 39 is a protein called 50S ribosomal protein L19.

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

- Molecule 40 is a protein called 50S ribosomal protein L20.

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

- Molecule 41 is a protein called 50S ribosomal protein L21.

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

- Molecule 42 is a protein called 50S ribosomal protein L22.

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

- Molecule 43 is a protein called 50S ribosomal protein L23.

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

- Molecule 44 is a protein called 50S ribosomal protein L24.

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

- Molecule 45 is a protein called 50S ribosomal protein L25.

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

- Molecule 46 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	v	75	Total	C	N	O	S	0	0
			569	353	113	102	1		

- Molecule 47 is a protein called 50S ribosomal protein L28.

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

- Molecule 48 is a protein called 50S ribosomal protein L29.

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

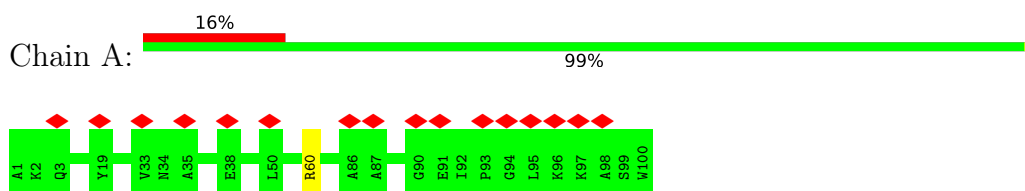
- Molecule 49 is a protein called 50S ribosomal protein L30.

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

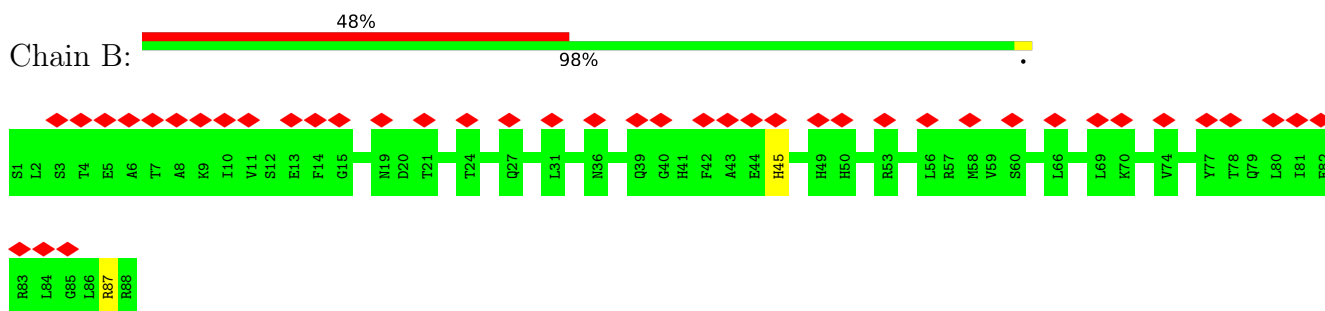
3 Residue-property plots [i](#)

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.

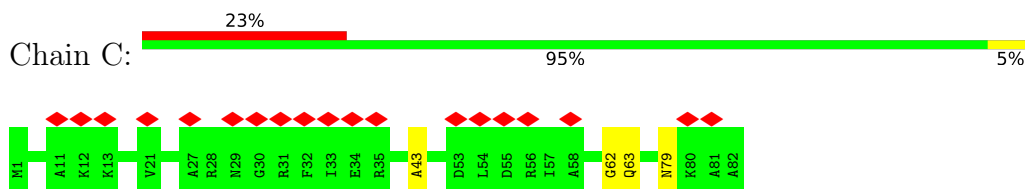
- Molecule 1: 30S ribosomal protein S14



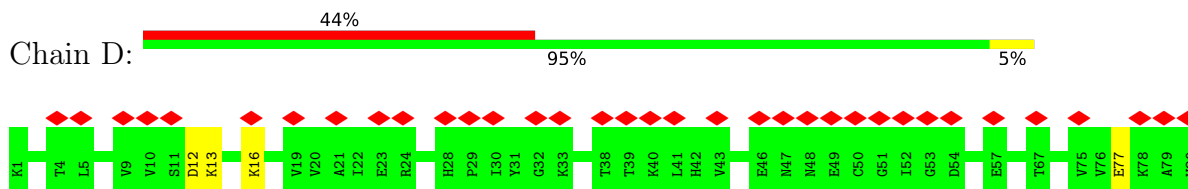
- Molecule 2: 30S ribosomal protein S15



- Molecule 3: 30S ribosomal protein S16

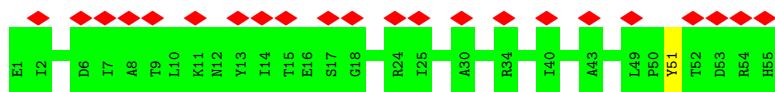


- Molecule 4: 30S ribosomal protein S17

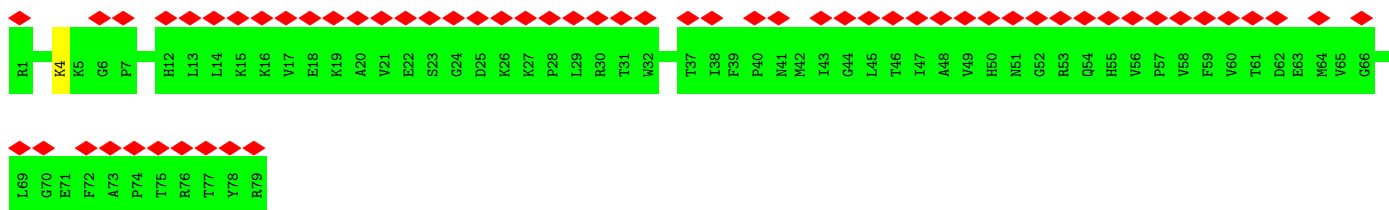
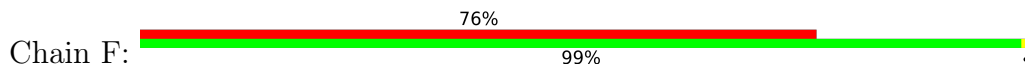


- Molecule 5: 30S ribosomal protein S18

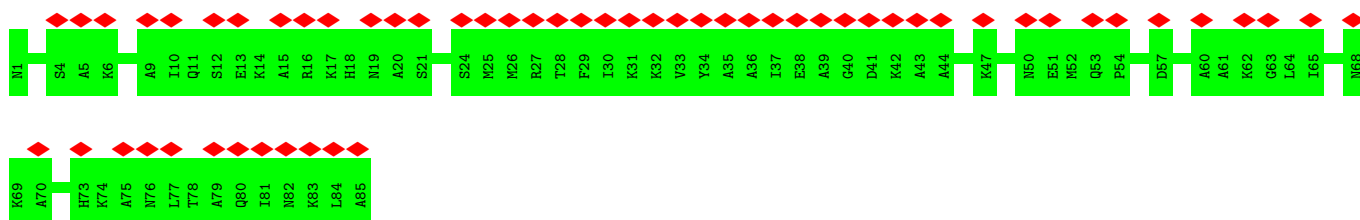




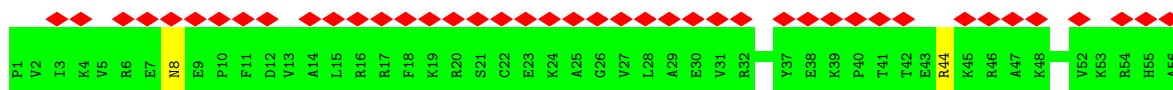
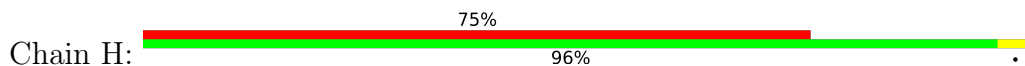
• Molecule 6: 30S ribosomal protein S19



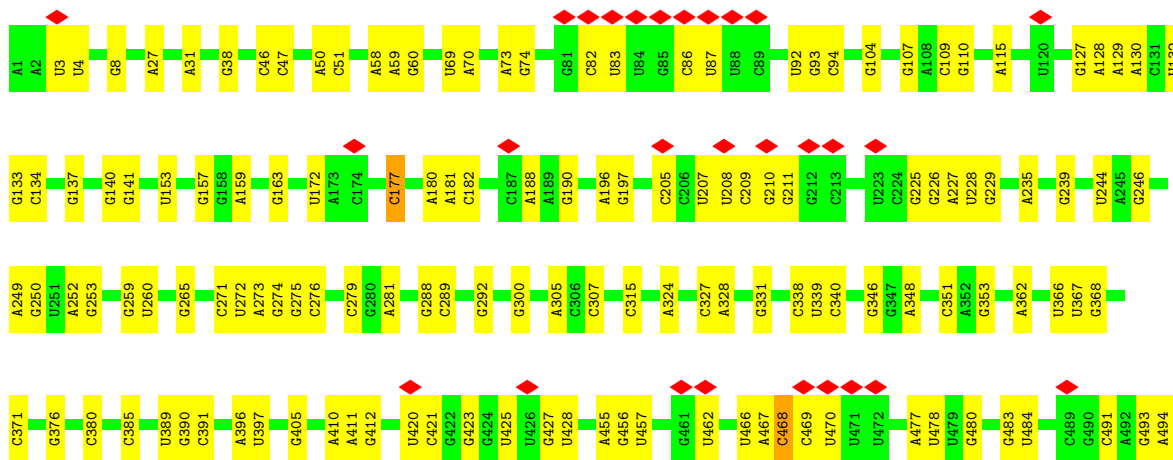
• Molecule 7: 30S ribosomal protein S20

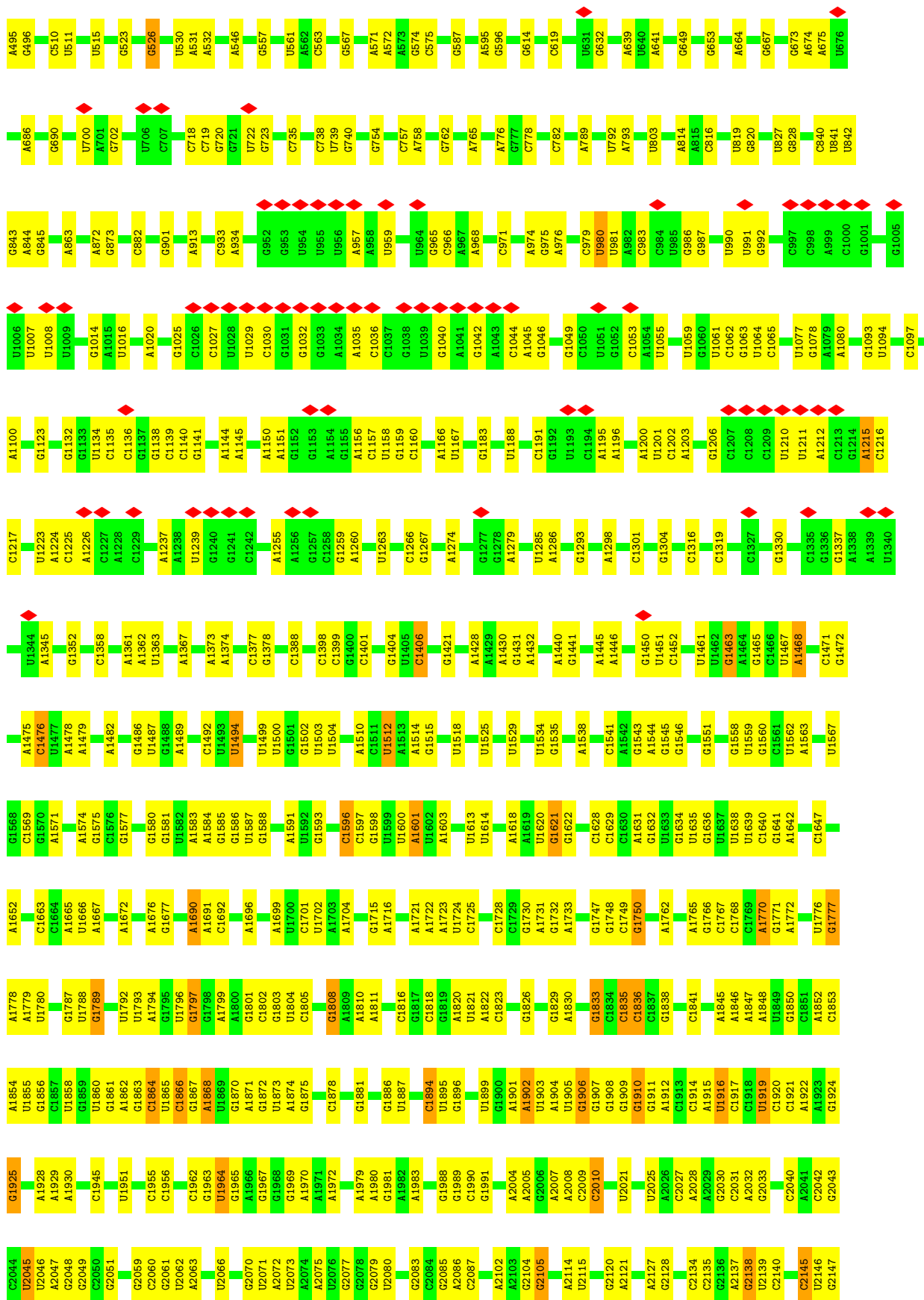


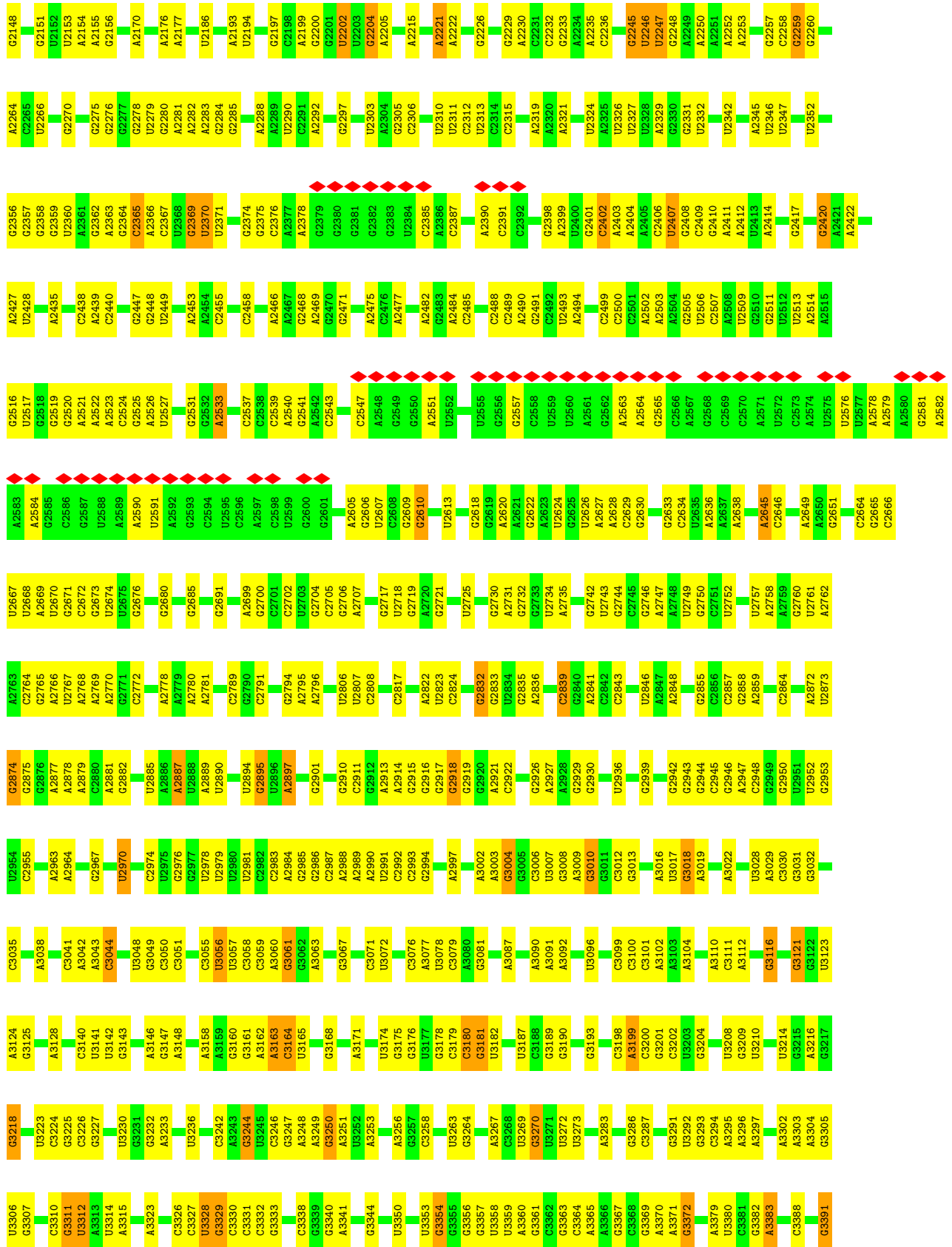
• Molecule 8: 30S ribosomal protein S21

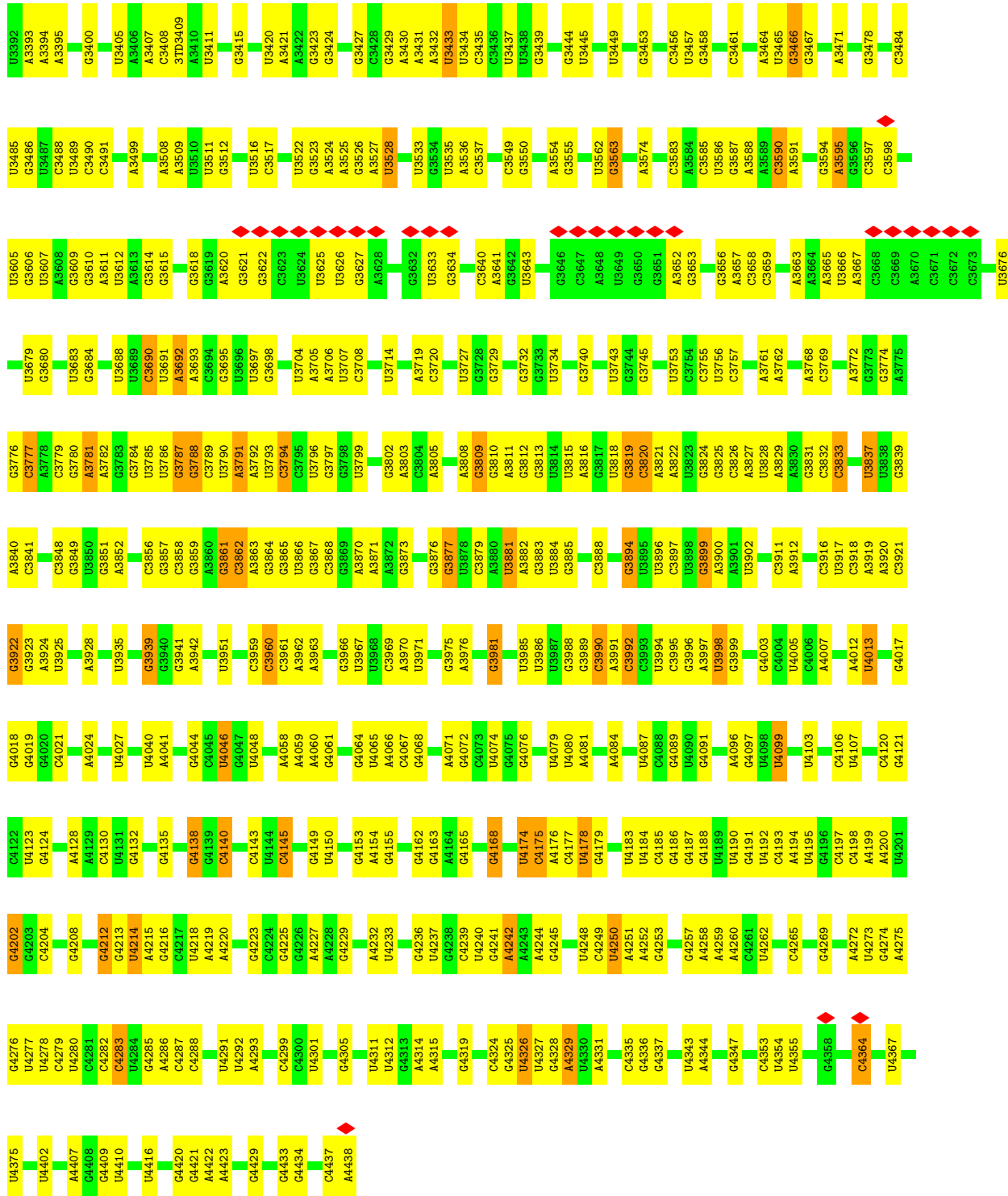


• Molecule 9: Tethered rRNA

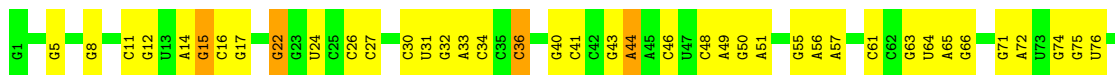


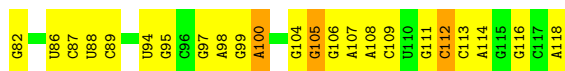






• Molecule 10: 5S rRNA

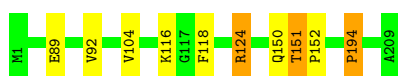




- Molecule 11: 50S ribosomal protein L2



- Molecule 12: 50S ribosomal protein L3



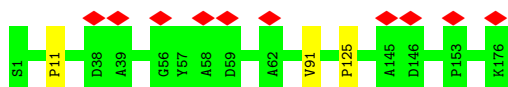
- Molecule 13: 50S ribosomal protein L4



- Molecule 14: 50S ribosomal protein L5



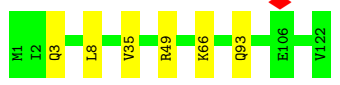
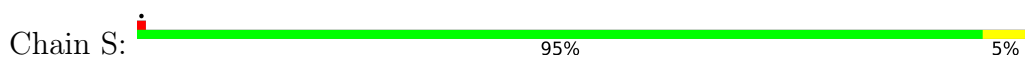
- Molecule 15: 50S ribosomal protein L6



- Molecule 16: 50S ribosomal protein L13



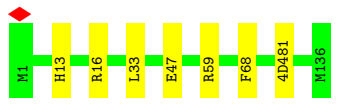
- Molecule 17: 50S ribosomal protein L14



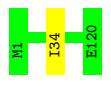
• Molecule 18: 50S ribosomal protein L15



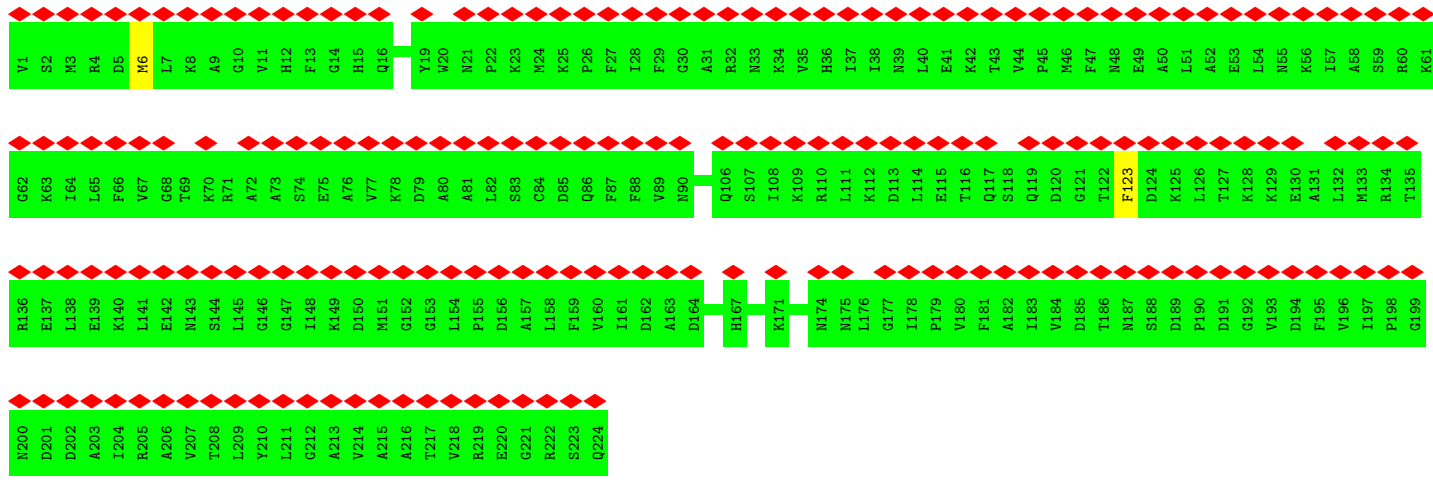
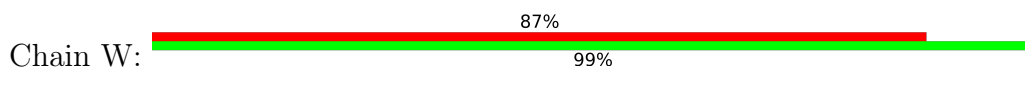
• Molecule 19: 50S ribosomal protein L16



• Molecule 20: 50S ribosomal protein L17

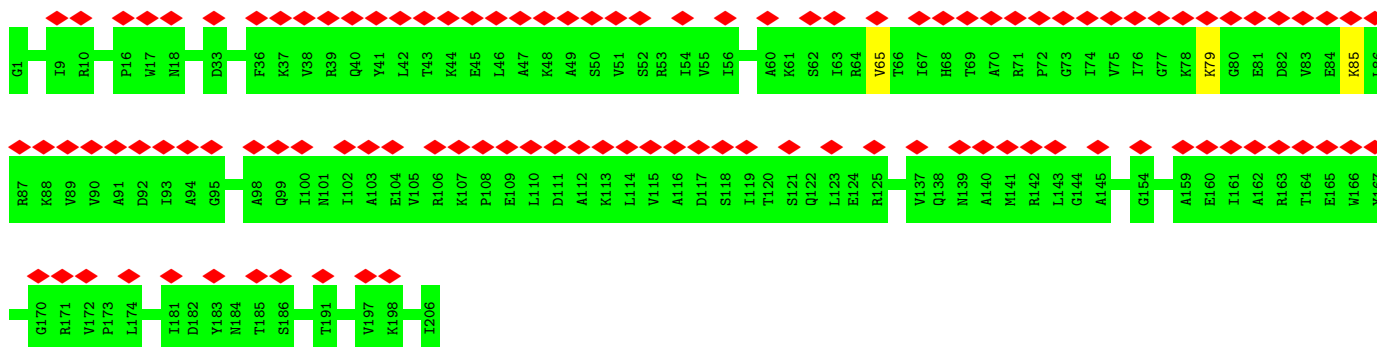


• Molecule 21: 30S ribosomal protein S2

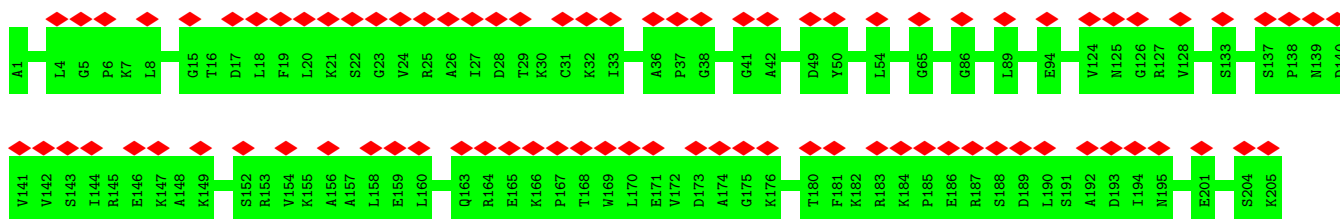
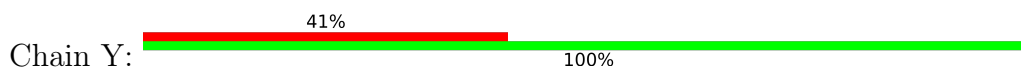


• Molecule 22: 30S ribosomal protein S3

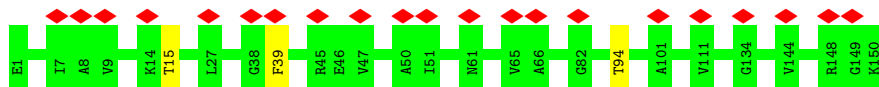




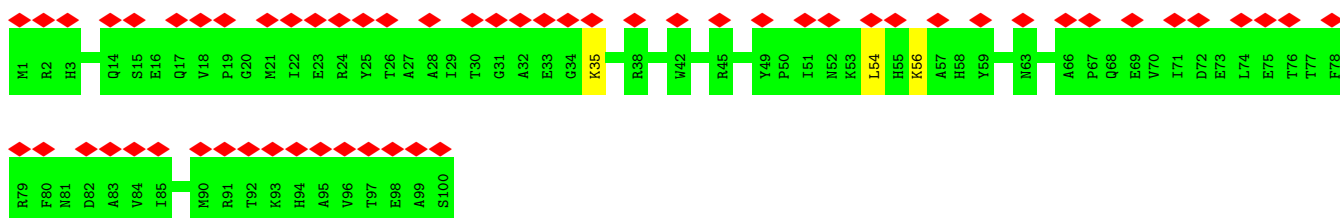
- Molecule 23: 30S ribosomal protein S4



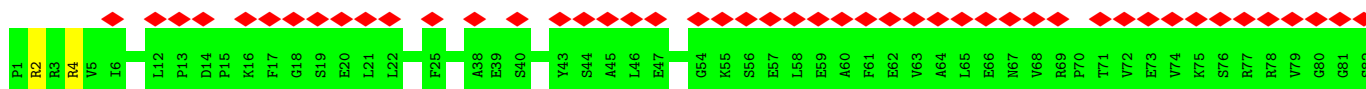
- Molecule 24: 30S ribosomal protein S5

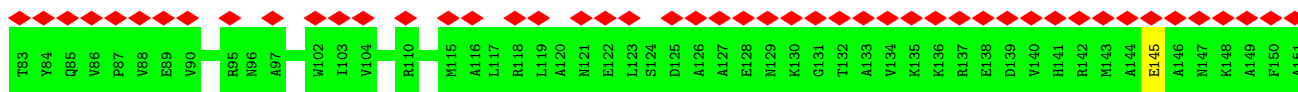


- Molecule 25: 30S ribosomal protein S6

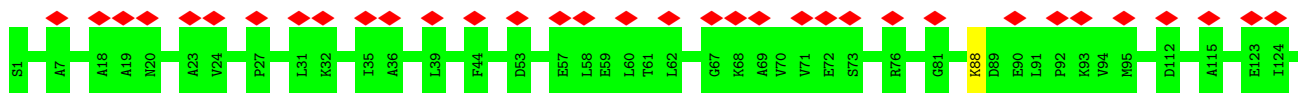


- Molecule 26: 30S ribosomal protein S7

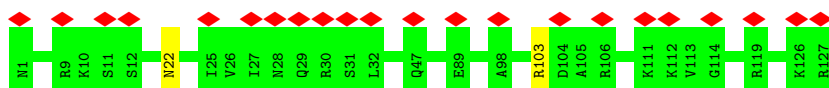




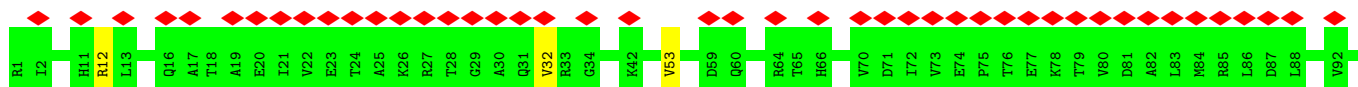
- Molecule 27: 30S ribosomal protein S8



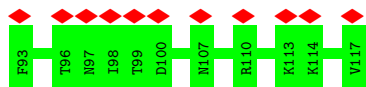
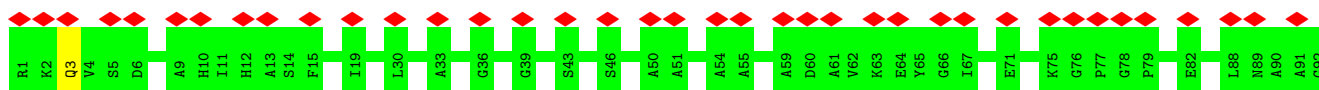
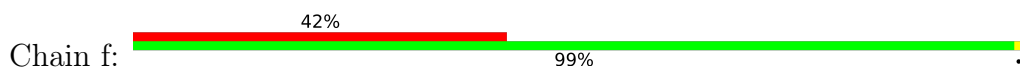
- Molecule 28: 30S ribosomal protein S9



- Molecule 29: 30S ribosomal protein S10

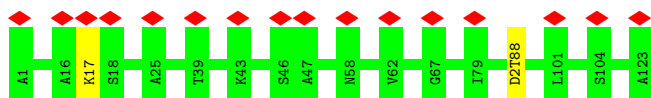


- Molecule 30: 30S ribosomal protein S11

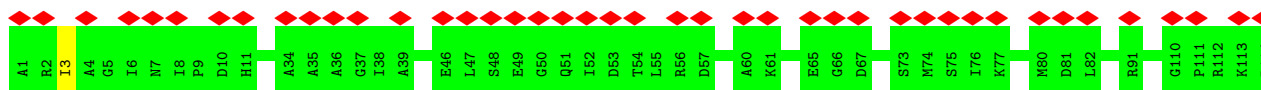


- Molecule 31: 30S ribosomal protein S12

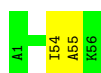




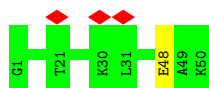
- Molecule 32: 30S ribosomal protein S13



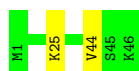
- Molecule 33: 50S ribosomal protein L32



- Molecule 34: 50S ribosomal protein L33



- Molecule 35: 50S ribosomal protein L34

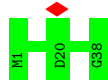


- Molecule 36: 50S ribosomal protein L35



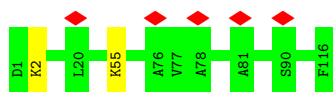
There are no outlier residues recorded for this chain.

- Molecule 37: 50S ribosomal protein L36

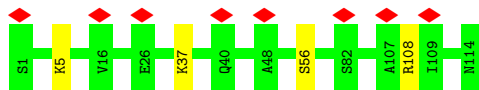


- Molecule 38: 50S ribosomal protein L18





- Molecule 39: 50S ribosomal protein L19



- Molecule 40: 50S ribosomal protein L20



There are no outlier residues recorded for this chain.

- Molecule 41: 50S ribosomal protein L21

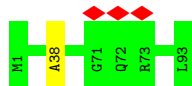


There are no outlier residues recorded for this chain.

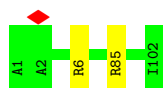
- Molecule 42: 50S ribosomal protein L22



- Molecule 43: 50S ribosomal protein L23

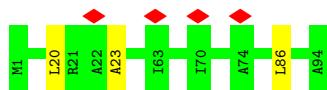


- Molecule 44: 50S ribosomal protein L24



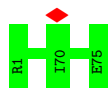
- Molecule 45: 50S ribosomal protein L25





- Molecule 46: 50S ribosomal protein L27

Chain v: 100%



- Molecule 47: 50S ribosomal protein L28

Chain w: 99%



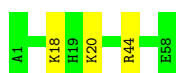
- Molecule 48: 50S ribosomal protein L29

Chain x: 97%



- Molecule 49: 50S ribosomal protein L30

Chain y: 95% 5%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	34852	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS TALOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.073	Depositor
Minimum map value	-0.210	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.058	Depositor
Recommended contour level	0.1	Depositor
Map size (\AA)	430.0, 430.0, 430.0	wwPDB
Map dimensions	500, 500, 500	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.86, 0.86, 0.86	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 4OC, 2MA, 5MC, MA6, 6MZ, 1MG, 2MG, OMG, G7M, 5MU, PSU, D2T, UR3, OMC, OMU, 4D4, 3TD

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	A	0.30	0/817	0.57	0/1088
2	B	0.27	0/722	0.61	0/964
3	C	0.55	2/659 (0.3%)	0.72	1/884 (0.1%)
4	D	0.30	0/658	0.62	0/881
5	E	0.27	0/463	0.63	0/621
6	F	0.26	0/653	0.51	0/877
7	G	0.28	0/671	0.52	0/888
8	H	0.25	0/472	0.63	1/627 (0.2%)
9	I	0.74	19/105898 (0.0%)	1.14	477/165194 (0.3%)
10	J	0.67	0/2828	1.35	25/4410 (0.6%)
11	K	0.68	5/2122 (0.2%)	0.96	7/2852 (0.2%)
12	L	0.53	1/1586 (0.1%)	0.80	3/2134 (0.1%)
13	M	0.38	0/1571	0.66	1/2113 (0.0%)
14	N	0.42	0/1435	0.68	0/1926
15	O	0.38	0/1343	0.69	0/1816
16	R	0.53	1/1152 (0.1%)	0.78	2/1551 (0.1%)
17	S	0.54	0/947	0.84	1/1268 (0.1%)
18	T	0.46	0/1062	0.88	3/1413 (0.2%)
19	U	0.48	1/1081 (0.1%)	0.77	4/1443 (0.3%)
20	V	0.43	0/973	0.79	0/1301
21	W	0.25	0/1784	0.47	0/2403
22	X	0.25	0/1652	0.51	0/2225
23	Y	0.26	0/1665	0.53	0/2227
24	Z	0.35	0/1118	0.64	1/1504 (0.1%)
25	a	0.28	0/835	0.56	0/1128
26	b	0.24	0/1196	0.53	0/1602
27	c	0.26	0/989	0.51	0/1326
28	d	0.25	0/1034	0.57	0/1375
29	e	0.26	0/797	0.57	0/1077
30	f	0.28	0/893	0.60	0/1205
31	g	0.29	0/960	0.59	0/1286

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	h	0.25	0/893	0.57	0/1193
33	i	0.36	0/450	0.66	0/599
34	j	0.28	0/416	0.63	0/554
35	k	0.39	0/380	0.75	0/498
36	l	0.38	0/513	0.69	0/676
37	m	0.33	0/303	0.72	0/397
38	n	0.35	0/902	0.68	0/1209
39	o	0.45	0/929	0.75	0/1242
40	p	0.45	0/960	0.71	0/1278
41	q	0.42	0/829	0.68	0/1107
42	r	0.38	0/864	0.63	0/1156
43	s	0.46	0/745	0.70	0/994
44	t	0.40	0/788	0.72	0/1051
45	u	0.35	0/766	0.69	2/1025 (0.2%)
46	v	0.42	0/576	0.72	0/762
47	w	0.43	0/635	0.72	1/848 (0.1%)
48	x	0.51	0/502	0.79	1/667 (0.1%)
49	y	0.35	0/453	0.73	0/605
All	All	0.66	29/151940 (0.0%)	1.05	530/227470 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
4	D	0	2
11	K	0	5
12	L	0	3
16	R	0	1
20	V	0	1
39	o	0	1
44	t	0	1
All	All	0	15

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	I	226	G	N3-C4	65.85	1.81	1.35
9	I	226	G	C2-N3	58.43	1.79	1.32
9	I	226	G	C6-N1	49.84	1.74	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	I	226	G	N1-C2	44.95	1.73	1.37
9	I	226	G	C5-C4	36.98	1.64	1.38
9	I	226	G	C5-C6	28.52	1.70	1.42
11	K	26	GLY	C-N	11.10	1.59	1.34
11	K	101	ARG	CZ-NH1	-10.04	1.20	1.33
3	C	62	GLY	C-N	9.32	1.55	1.34
3	C	63	GLN	N-CA	8.01	1.62	1.46
9	I	1770	A	N9-C4	-6.86	1.33	1.37
9	I	4277	U	C2-O2	-6.69	1.16	1.22
9	I	3163	A	C6-N1	-6.43	1.31	1.35
16	R	136	GLN	C-O	6.31	1.35	1.23
19	U	47	GLU	CD-OE1	5.95	1.32	1.25
11	K	101	ARG	NE-CZ	-5.92	1.25	1.33
9	I	2953	G	N9-C4	-5.87	1.33	1.38
11	K	101	ARG	CA-CB	5.82	1.66	1.53
11	K	65	ASP	CB-CG	-5.81	1.39	1.51
12	L	118	PHE	CE1-CZ	5.78	1.48	1.37
9	I	3003	A	N9-C4	-5.31	1.34	1.37
9	I	2645	A	N9-C4	-5.27	1.34	1.37
9	I	4277	U	N1-C2	-5.22	1.33	1.38
9	I	2331	G	N9-C4	-5.20	1.33	1.38
9	I	4064	G	N3-C4	-5.17	1.31	1.35
9	I	4212	G	N3-C4	-5.15	1.31	1.35
9	I	2331	G	N3-C4	-5.14	1.31	1.35
9	I	4064	G	N9-C4	-5.08	1.33	1.38
9	I	3372	G	N9-C4	-5.03	1.33	1.38

All (530) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	I	226	G	C2-N3-C4	28.85	126.33	111.90
9	I	226	G	N1-C2-N3	-26.39	108.06	123.90
9	I	226	G	N3-C4-C5	-22.26	117.47	128.60
9	I	3163	A	N9-C4-C5	-22.14	96.94	105.80
9	I	226	G	N3-C4-N9	20.28	138.17	126.00
9	I	3163	A	C8-N9-C4	18.45	113.18	105.80
9	I	226	G	N3-C2-N2	17.83	132.38	119.90
9	I	226	G	C5-C6-N1	15.34	119.17	111.50
9	I	226	G	C4-C5-N7	-14.91	104.83	110.80
18	T	115	GLU	OE1-CD-OE2	13.19	139.13	123.30
11	K	65	ASP	CB-CG-OD1	12.94	129.94	118.30
9	I	3163	A	C4-C5-N7	12.90	117.15	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	I	469	C	C6-N1-C2	-12.50	115.30	120.30
9	I	3163	A	N7-C8-N9	-11.87	107.87	113.80
9	I	3056	U	C5-C6-N1	-11.47	116.97	122.70
9	I	3595	A	O5'-P-OP1	-11.37	95.47	105.70
11	K	65	ASP	CB-CG-OD2	-11.25	108.17	118.30
3	C	62	GLY	C-N-CA	11.06	149.36	121.70
9	I	3788	G	N9-C4-C5	-10.34	101.26	105.40
9	I	3163	A	N3-C4-N9	10.34	135.67	127.40
9	I	226	G	N7-C8-N9	10.10	118.15	113.10
9	I	4064	G	N3-C2-N2	-9.78	113.06	119.90
9	I	4250	U	C5-C4-O4	-9.76	120.05	125.90
9	I	1906	G	N3-C4-N9	-9.51	120.29	126.00
9	I	4250	U	N3-C4-O4	9.32	125.92	119.40
9	I	2953	G	N3-C4-N9	-9.21	120.48	126.00
9	I	3788	G	C4-C5-N7	9.19	114.48	110.80
9	I	3781	A	N1-C6-N6	-9.19	113.09	118.60
9	I	3055	C	C6-N1-C2	9.17	123.97	120.30
9	I	4130	C	C6-N1-C2	9.08	123.93	120.30
9	I	3163	A	C5-C6-N1	9.08	122.24	117.70
9	I	3833	C	N1-C2-O2	9.08	124.35	118.90
9	I	2010	C	N3-C2-O2	-8.89	115.67	121.90
9	I	3056	U	C2-N3-C4	-8.86	121.68	127.00
9	I	3006	C	C2-N1-C1'	-8.77	109.15	118.80
9	I	3050	C	C6-N1-C2	-8.77	116.79	120.30
9	I	2610	G	C5-C6-O6	-8.66	123.40	128.60
18	T	115	GLU	CG-CD-OE1	-8.65	101.00	118.30
9	I	3788	G	C6-C5-N7	-8.62	125.23	130.40
9	I	3055	C	C5-C6-N1	-8.59	116.71	121.00
9	I	4019	G	C4-N9-C1'	-8.58	115.34	126.50
9	I	2331	G	N3-C4-N9	-8.57	120.86	126.00
9	I	2531	G	N3-C4-N9	-8.57	120.86	126.00
9	I	3787	G	N9-C1'-C2'	-8.52	102.62	112.00
9	I	4278	U	C2-N3-C4	-8.39	121.97	127.00
9	I	2331	G	N3-C2-N2	-8.36	114.05	119.90
9	I	3391	G	C4-N9-C1'	-8.33	115.67	126.50
9	I	4278	U	N3-C2-O2	-8.28	116.40	122.20
9	I	4064	G	N3-C4-N9	-8.25	121.05	126.00
9	I	272	U	P-O3'-C3'	8.14	129.47	119.70
9	I	4121	G	N3-C4-N9	-8.09	121.14	126.00
9	I	4121	G	C4-N9-C1'	-8.05	116.03	126.50
9	I	3981	G	N3-C4-N9	8.04	130.82	126.00
9	I	3809	G	C8-N9-C4	8.02	109.61	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	I	2953	G	N3-C4-C5	8.00	132.60	128.60
9	I	1770	A	C8-N9-C4	7.94	108.97	105.80
9	I	2145	C	C6-N1-C2	7.86	123.44	120.30
9	I	4178	U	C2-N1-C1'	-7.83	108.31	117.70
9	I	3787	G	N9-C4-C5	-7.81	102.28	105.40
9	I	4277	U	N1-C2-N3	7.81	119.58	114.90
11	K	101	ARG	NE-CZ-NH2	-7.80	116.40	120.30
9	I	3791	A	N1-C6-N6	7.80	123.28	118.60
9	I	3006	C	C6-N1-C1'	7.78	130.13	120.80
9	I	3819	G	N3-C4-N9	-7.77	121.34	126.00
9	I	2010	C	N1-C2-O2	7.75	123.55	118.90
9	I	3160	G	C4-N9-C1'	-7.70	116.50	126.50
9	I	1836	C	C2-N1-C1'	-7.64	110.40	118.80
9	I	1787	G	C5-C6-O6	-7.56	124.06	128.60
9	I	4121	G	C8-N9-C1'	7.55	136.81	127.00
9	I	1465	G	N7-C8-N9	7.54	116.87	113.10
9	I	2950	G	C4-N9-C1'	-7.47	116.79	126.50
9	I	3160	G	N3-C2-N2	-7.46	114.68	119.90
9	I	3787	G	C8-N9-C4	7.38	109.35	106.40
9	I	1916	U	C2-N3-C4	-7.36	122.58	127.00
9	I	3160	G	C6-C5-N7	7.35	134.81	130.40
9	I	1836	C	N1-C2-O2	-7.32	114.51	118.90
9	I	1910	G	N1-C6-O6	-7.31	115.51	119.90
9	I	3372	G	N3-C4-N9	-7.30	121.62	126.00
9	I	469	C	C2-N1-C1'	7.15	126.67	118.80
9	I	980	U	C2-N3-C4	-7.12	122.72	127.00
9	I	177	C	N3-C2-O2	-7.10	116.93	121.90
9	I	2362	G	C6-C5-N7	-7.10	126.14	130.40
9	I	3160	G	N3-C4-N9	-7.08	121.75	126.00
9	I	2362	G	N3-C4-N9	7.08	130.25	126.00
9	I	2331	G	C8-N9-C1'	7.04	136.15	127.00
9	I	3597	C	N1-C2-O2	-7.03	114.68	118.90
9	I	3160	G	C8-N9-C1'	6.99	136.09	127.00
9	I	2331	G	N9-C4-C5	6.99	108.19	105.40
9	I	2362	G	N9-C4-C5	-6.97	102.61	105.40
9	I	271	C	N1-C1'-C2'	-6.97	104.33	112.00
9	I	2407	U	C5-C4-O4	-6.97	121.72	125.90
9	I	2651	G	N3-C4-N9	6.96	130.17	126.00
9	I	2939	G	C8-N9-C4	6.94	109.17	106.40
9	I	3981	G	N9-C4-C5	-6.93	102.63	105.40
13	M	127	GLU	C-N-CA	6.93	139.03	121.70
9	I	3372	G	N3-C4-C5	6.92	132.06	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	I	4019	G	C8-N9-C1'	6.92	136.00	127.00
9	I	4128	A	N9-C4-C5	-6.91	103.04	105.80
11	K	100	ARG	CG-CD-NE	-6.88	97.35	111.80
10	J	17	G	N7-C8-N9	6.88	116.54	113.10
9	I	2918	G	N3-C4-N9	-6.86	121.88	126.00
9	I	2609	G	N9-C4-C5	-6.86	102.66	105.40
9	I	3163	A	C4-C5-C6	-6.85	113.57	117.00
9	I	3787	G	N3-C2-N2	6.85	124.70	119.90
9	I	3056	U	C4-C5-C6	6.84	123.81	119.70
9	I	2609	G	C4-C5-N7	6.83	113.53	110.80
9	I	1906	G	C8-N9-C1'	6.83	135.88	127.00
9	I	2970	U	C5-C4-O4	-6.81	121.81	125.90
9	I	2526	A	O4'-C1'-N9	6.81	113.65	108.20
9	I	4174	U	C2-N1-C1'	-6.80	109.54	117.70
9	I	470	U	C5-C6-N1	-6.80	119.30	122.70
9	I	4121	G	N3-C2-N2	-6.80	115.14	119.90
9	I	4278	U	C5-C6-N1	-6.74	119.33	122.70
16	R	32	LEU	CB-CG-CD2	-6.73	99.56	111.00
9	I	3367	G	N3-C2-N2	6.72	124.61	119.90
10	J	99	G	O5'-P-OP2	-6.70	99.67	105.70
9	I	3832	C	N3-C4-C5	6.70	124.58	121.90
9	I	2609	G	C5-C6-O6	-6.69	124.59	128.60
19	U	47	GLU	CG-CD-OE2	6.68	131.65	118.30
9	I	469	C	N3-C2-O2	-6.65	117.25	121.90
9	I	3809	G	N9-C4-C5	-6.65	102.74	105.40
9	I	2525	G	N3-C4-N9	6.64	129.98	126.00
9	I	3164	C	C4-C5-C6	6.63	120.71	117.40
9	I	1945	C	N3-C2-O2	-6.62	117.27	121.90
10	J	22	G	C4-C5-N7	6.60	113.44	110.80
9	I	226	G	N1-C6-O6	-6.59	115.94	119.90
9	I	1906	G	N9-C4-C5	6.59	108.04	105.40
9	I	3959	C	C2-N1-C1'	-6.57	111.57	118.80
9	I	3372	G	C4-N9-C1'	-6.56	117.97	126.50
9	I	3832	C	C6-N1-C2	6.56	122.92	120.30
10	J	26	C	C5-C6-N1	6.56	124.28	121.00
9	I	3899	G	N3-C4-N9	6.56	129.93	126.00
9	I	980	U	C5-C6-N1	-6.55	119.42	122.70
9	I	2331	G	C4-N9-C1'	-6.55	117.99	126.50
9	I	2895	G	N1-C6-O6	-6.54	115.97	119.90
9	I	1215	A	N9-C1'-C2'	-6.54	104.81	112.00
9	I	3163	A	C5-C6-N6	-6.54	118.47	123.70
9	I	3250	G	N3-C4-C5	6.53	131.87	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	J	63	G	N9-C4-C5	-6.53	102.79	105.40
9	I	3791	A	N9-C4-C5	-6.51	103.19	105.80
9	I	4239	C	N1-C2-O2	-6.50	115.00	118.90
9	I	2994	G	N7-C8-N9	6.48	116.34	113.10
9	I	4326	U	C6-N1-C2	6.48	124.89	121.00
9	I	2356	G	C4-N9-C1'	-6.48	118.08	126.50
9	I	3791	A	O4'-C1'-N9	-6.48	103.02	108.20
9	I	2140	C	C6-N1-C2	-6.47	117.71	120.30
9	I	2531	G	C8-N9-C1'	6.47	135.41	127.00
9	I	1787	G	N3-C4-N9	6.44	129.86	126.00
9	I	1797	G	C4-N9-C1'	-6.44	118.13	126.50
9	I	2918	G	C4-N9-C1'	-6.44	118.13	126.50
9	I	1910	G	C5-C6-O6	6.43	132.46	128.60
9	I	3218	G	N3-C2-N2	-6.43	115.40	119.90
9	I	4278	U	N1-C2-N3	6.40	118.74	114.90
9	I	2407	U	C6-N1-C1'	-6.39	112.26	121.20
9	I	2362	G	C8-N9-C1'	-6.37	118.72	127.00
9	I	3311	G	O4'-C1'-N9	6.36	113.28	108.20
9	I	1868	A	N9-C1'-C2'	-6.35	105.01	112.00
9	I	3755	C	C6-N1-C2	-6.35	117.76	120.30
9	I	1836	C	C6-N1-C1'	6.35	128.42	120.80
9	I	2402	C	C6-N1-C1'	6.34	128.41	120.80
9	I	3959	C	C5-C6-N1	-6.33	117.83	121.00
10	J	22	G	N9-C4-C5	-6.32	102.87	105.40
9	I	226	G	C5-C6-O6	-6.32	124.81	128.60
9	I	2134	C	C2-N1-C1'	-6.30	111.86	118.80
9	I	4174	U	P-O3'-C3'	6.30	127.27	119.70
11	K	100	ARG	NE-CZ-NH1	6.29	123.45	120.30
9	I	3690	C	C2-N3-C4	6.29	123.04	119.90
9	I	3981	G	C8-N9-C1'	-6.29	118.83	127.00
9	I	3788	G	N3-C4-N9	6.27	129.76	126.00
9	I	3597	C	C2-N1-C1'	-6.27	111.90	118.80
9	I	3528	U	C6-N1-C1'	-6.26	112.43	121.20
9	I	1836	C	N3-C4-N4	-6.25	113.62	118.00
9	I	3044	C	N3-C2-O2	-6.23	117.54	121.90
9	I	2839	C	C2-N1-C1'	-6.22	111.95	118.80
9	I	3788	G	N1-C6-O6	6.22	123.63	119.90
8	H	8	ASN	C-N-CA	-6.22	106.15	121.70
9	I	2531	G	C4-N9-C1'	-6.22	118.41	126.50
9	I	3528	U	C2-N1-C1'	6.22	125.16	117.70
9	I	2882	G	N3-C4-N9	6.21	129.72	126.00
9	I	3383	A	C8-N9-C4	-6.19	103.33	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	I	4329	A	C4-N9-C1'	-6.18	115.17	126.30
9	I	1586	G	C8-N9-C1'	-6.18	118.96	127.00
9	I	2488	C	N1-C2-O2	6.17	122.60	118.90
9	I	3391	G	C8-N9-C1'	6.17	135.03	127.00
9	I	3797	G	N3-C4-N9	-6.16	122.30	126.00
9	I	3899	G	C8-N9-C1'	-6.15	119.01	127.00
10	J	15	G	O5'-P-OP1	-6.14	100.17	105.70
9	I	1906	G	C4-N9-C1'	-6.14	118.51	126.50
9	I	3981	G	C6-C5-N7	-6.14	126.72	130.40
10	J	106	G	N7-C8-N9	6.14	116.17	113.10
9	I	3881	U	C5-C6-N1	6.13	125.77	122.70
9	I	2610	G	C4-C5-N7	6.13	113.25	110.80
9	I	2945	C	C6-N1-C2	-6.13	117.85	120.30
9	I	2420	G	C4-N9-C1'	-6.12	118.54	126.50
9	I	3071	C	N3-C2-O2	-6.12	117.61	121.90
9	I	2953	G	C4-N9-C1'	-6.12	118.54	126.50
9	I	3006	C	N3-C4-N4	-6.12	113.72	118.00
12	L	194	PRO	CA-N-CD	-6.12	102.94	111.50
9	I	3922	G	N3-C4-C5	-6.11	125.54	128.60
9	I	1906	G	N3-C4-C5	6.11	131.66	128.60
9	I	3372	G	C8-N9-C1'	6.11	134.94	127.00
9	I	2365	C	C6-N1-C1'	6.10	128.12	120.80
9	I	3391	G	C8-N9-C4	6.09	108.84	106.40
9	I	3121	G	C4-N9-C1'	6.08	134.41	126.50
9	I	1586	G	C4-N9-C1'	6.08	134.41	126.50
9	I	2918	G	C8-N9-C1'	6.08	134.91	127.00
9	I	3164	C	C5-C6-N1	-6.07	117.97	121.00
9	I	4178	U	C5-C6-N1	-6.07	119.67	122.70
9	I	3781	A	C5-C6-N6	6.06	128.55	123.70
9	I	3794	C	N3-C4-N4	-6.04	113.77	118.00
9	I	3894	G	N9-C1'-C2'	-6.04	105.35	112.00
9	I	2531	G	C6-C5-N7	6.03	134.02	130.40
9	I	4138	G	N3-C2-N2	-6.03	115.68	119.90
9	I	4242	A	N9-C1'-C2'	-6.02	105.37	112.00
9	I	4225	G	C5-C6-O6	6.01	132.21	128.60
9	I	3865	G	N9-C1'-C2'	-6.01	105.39	112.00
9	I	2365	C	C2-N1-C1'	-6.00	112.20	118.80
9	I	4324	C	O4'-C1'-N1	6.00	113.00	108.20
9	I	2531	G	N9-C4-C5	5.99	107.80	105.40
9	I	3995	C	C2-N1-C1'	-5.99	112.21	118.80
9	I	3787	G	C4-C5-N7	5.99	113.19	110.80
10	J	112	C	C6-N1-C1'	5.99	127.98	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	I	3004	G	C4-N9-C1'	-5.98	118.72	126.50
9	I	469	C	N1-C2-N3	5.98	123.39	119.20
9	I	2839	C	C6-N1-C1'	5.98	127.98	120.80
9	I	2259	G	N3-C4-N9	5.98	129.59	126.00
9	I	3837	U	N1-C2-O2	-5.97	118.62	122.80
9	I	4145	C	C6-N1-C2	5.96	122.69	120.30
9	I	1833	G	C4-N9-C1'	5.96	134.25	126.50
9	I	4130	C	C5-C6-N1	-5.96	118.02	121.00
12	L	116	LYS	C-N-CA	-5.96	109.78	122.30
9	I	3466	G	N3-C2-N2	-5.96	115.73	119.90
9	I	3121	G	C8-N9-C1'	-5.94	119.28	127.00
9	I	3819	G	C4-N9-C1'	-5.94	118.78	126.50
9	I	4329	A	C8-N9-C1'	5.94	138.39	127.70
9	I	2609	G	C8-N9-C4	5.93	108.77	106.40
9	I	1919	U	O4'-C1'-N1	5.92	112.93	108.20
9	I	1647	C	N1-C2-O2	5.91	122.44	118.90
9	I	1925	G	N9-C4-C5	-5.90	103.04	105.40
9	I	3116	G	N3-C4-N9	5.90	129.54	126.00
9	I	4324	C	C2-N3-C4	-5.90	116.95	119.90
9	I	2874	G	N3-C4-N9	5.89	129.54	126.00
9	I	2943	G	C4-N9-C1'	-5.88	118.85	126.50
9	I	3824	G	C8-N9-C4	-5.88	104.05	106.40
9	I	1797	G	N3-C4-N9	-5.86	122.48	126.00
9	I	3791	A	N9-C1'-C2'	-5.86	105.56	112.00
9	I	3123	U	N1-C2-N3	5.86	118.42	114.90
9	I	1916	U	C5-C6-N1	-5.85	119.77	122.70
9	I	3779	C	C2-N3-C4	-5.85	116.97	119.90
9	I	3819	G	N9-C4-C5	5.85	107.74	105.40
9	I	3864	G	N1-C6-O6	-5.85	116.39	119.90
9	I	1796	U	C2-N1-C1'	-5.84	110.69	117.70
9	I	3244	G	C8-N9-C4	5.83	108.73	106.40
9	I	4019	G	O4'-C1'-N9	5.82	112.85	108.20
9	I	4239	C	C2-N3-C4	-5.82	116.99	119.90
9	I	4178	U	C6-N1-C1'	5.81	129.34	121.20
9	I	2204	G	C4-N9-C1'	5.81	134.05	126.50
9	I	3597	C	C6-N1-C1'	5.81	127.77	120.80
9	I	3056	U	N1-C2-N3	5.81	118.38	114.90
9	I	3824	G	N3-C4-N9	-5.81	122.52	126.00
9	I	3819	G	C8-N9-C1'	5.80	134.54	127.00
9	I	3837	U	C2-N1-C1'	-5.80	110.73	117.70
9	I	1545	G	C4-N9-C1'	-5.79	118.97	126.50
9	I	2950	G	C8-N9-C1'	5.79	134.53	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	I	4202	G	C8-N9-C4	-5.78	104.09	106.40
9	I	1596	C	N3-C4-N4	-5.78	113.96	118.00
9	I	2369	G	C4-N9-C1'	5.77	134.01	126.50
9	I	1597	C	N3-C2-O2	-5.75	117.87	121.90
9	I	177	C	N1-C2-O2	5.75	122.35	118.90
9	I	3818	U	N3-C2-O2	-5.75	118.18	122.20
9	I	4202	G	N7-C8-N9	5.75	115.97	113.10
12	L	124	ARG	CA-CB-CG	-5.75	100.76	113.40
9	I	2362	G	C4-N9-C1'	5.74	133.97	126.50
9	I	2402	C	N1-C2-O2	-5.74	115.45	118.90
9	I	1906	G	C6-C5-N7	5.74	133.84	130.40
9	I	3010	G	C8-N9-C4	5.74	108.70	106.40
9	I	3848	C	C2-N1-C1'	5.74	125.11	118.80
11	K	101	ARG	N-CA-CB	-5.74	100.27	110.60
9	I	2942	G	N3-C4-C5	5.72	131.46	128.60
9	I	3061	G	N1-C6-O6	-5.72	116.47	119.90
9	I	3383	A	N7-C8-N9	5.71	116.66	113.80
48	x	5	LEU	CA-CB-CG	5.71	128.43	115.30
9	I	1803	G	C8-N9-C4	5.70	108.68	106.40
9	I	3794	C	C5-C4-N4	5.70	124.19	120.20
9	I	3056	U	N1-C2-O2	-5.70	118.81	122.80
9	I	1567	U	C5-C4-O4	-5.68	122.49	125.90
9	I	2983	C	C2-N1-C1'	-5.68	112.56	118.80
9	I	3391	G	N7-C8-N9	-5.67	110.26	113.10
9	I	4277	U	C6-N1-C2	-5.67	117.60	121.00
9	I	4064	G	N9-C4-C5	5.67	107.67	105.40
10	J	5	G	N9-C4-C5	-5.66	103.14	105.40
9	I	226	G	C6-C5-N7	5.66	133.80	130.40
9	I	4336	G	C8-N9-C4	5.66	108.66	106.40
9	I	1835	C	C6-N1-C2	5.66	122.56	120.30
9	I	3004	G	N3-C4-N9	-5.66	122.61	126.00
9	I	1468	A	N1-C6-N6	-5.65	115.21	118.60
9	I	1586	G	N3-C4-N9	5.65	129.39	126.00
9	I	3200	C	N1-C2-O2	5.64	122.28	118.90
9	I	1463	G	C8-N9-C4	5.63	108.65	106.40
9	I	4212	G	N9-C4-C5	5.63	107.65	105.40
10	J	26	C	C6-N1-C2	-5.63	118.05	120.30
10	J	63	G	C4-C5-N7	5.62	113.05	110.80
9	I	4278	U	C5-C4-O4	-5.62	122.53	125.90
9	I	1906	G	N3-C2-N2	-5.61	115.97	119.90
9	I	1465	G	C8-N9-C4	-5.61	104.16	106.40
9	I	2610	G	N1-C6-O6	5.61	123.26	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	I	3018	G	O4'-C1'-N9	5.61	112.69	108.20
9	I	3894	G	N3-C4-C5	5.61	131.40	128.60
9	I	1770	A	N3-C4-C5	5.61	130.72	126.80
10	J	17	G	C5-N7-C8	-5.60	101.50	104.30
9	I	3292	U	N1-C2-N3	5.60	118.26	114.90
9	I	4326	U	N3-C4-C5	5.60	117.96	114.60
9	I	271	C	C3'-C2'-C1'	-5.59	97.03	101.50
9	I	3959	C	C2-N3-C4	-5.59	117.11	119.90
9	I	3981	G	C4-N9-C1'	5.58	133.76	126.50
9	I	3180	C	C2-N1-C1'	-5.58	112.66	118.80
9	I	3755	C	N3-C2-O2	-5.58	118.00	121.90
9	I	4364	C	N1-C2-O2	5.58	122.25	118.90
9	I	2832	G	C4-N9-C1'	-5.58	119.25	126.50
9	I	1841	C	N1-C2-O2	-5.57	115.56	118.90
9	I	3121	G	N3-C4-N9	5.56	129.34	126.00
9	I	3692	A	O4'-C1'-N9	5.56	112.65	108.20
9	I	1833	G	C8-N9-C1'	-5.56	119.77	127.00
10	J	44	A	O4'-C1'-N9	5.55	112.64	108.20
9	I	1894	C	C4-C5-C6	5.55	120.17	117.40
9	I	2420	G	C8-N9-C4	5.55	108.62	106.40
9	I	1964	U	O4'-C1'-N1	-5.54	103.76	108.20
9	I	1690	A	C5-C6-N6	-5.54	119.27	123.70
9	I	1916	U	C2-N1-C1'	-5.54	111.05	117.70
9	I	3004	G	C8-N9-C1'	5.54	134.20	127.00
9	I	4121	G	N3-C4-C5	5.54	131.37	128.60
10	J	22	G	C6-C5-N7	-5.54	127.08	130.40
9	I	1797	G	N3-C4-C5	5.53	131.37	128.60
9	I	1494	U	C2-N1-C1'	-5.52	111.07	117.70
9	I	2897	A	C8-N9-C4	5.52	108.01	105.80
9	I	4188	G	C4-N9-C1'	-5.52	119.32	126.50
9	I	1494	U	C5-C6-N1	-5.52	119.94	122.70
9	I	1388	C	C4-C5-C6	5.51	120.15	117.40
9	I	3824	G	N9-C4-C5	5.51	107.60	105.40
9	I	3004	G	N3-C2-N2	-5.50	116.05	119.90
9	I	3244	G	C4-N9-C1'	-5.50	119.35	126.50
9	I	3354	G	N3-C4-N9	-5.50	122.70	126.00
9	I	1512	U	O4'-C1'-N1	5.49	112.59	108.20
9	I	3894	G	N3-C4-N9	-5.49	122.71	126.00
9	I	2531	G	N3-C4-C5	5.48	131.34	128.60
9	I	468	C	C4-C5-C6	-5.47	114.66	117.40
9	I	1789	G	N1-C6-O6	-5.47	116.62	119.90
9	I	2651	G	C8-N9-C1'	-5.47	119.89	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	I	3899	G	C4-N9-C1'	5.47	133.61	126.50
9	I	3861	G	C8-N9-C4	5.46	108.58	106.40
9	I	3922	G	N3-C4-N9	5.46	129.28	126.00
9	I	3292	U	C5-C4-O4	5.46	129.17	125.90
9	I	1647	C	N3-C2-O2	-5.45	118.08	121.90
9	I	3055	C	C4-C5-C6	5.44	120.12	117.40
9	I	2526	A	C4-N9-C1'	-5.44	116.52	126.30
9	I	2918	G	N3-C4-C5	5.43	131.32	128.60
9	I	3123	U	C2-N3-C4	-5.43	123.74	127.00
9	I	3123	U	C5-C6-N1	-5.43	119.98	122.70
9	I	2134	C	C6-N1-C1'	5.43	127.31	120.80
9	I	2953	G	C2-N3-C4	-5.42	109.19	111.90
9	I	4324	C	N1-C2-N3	5.42	122.99	119.20
9	I	2202	U	C5-C6-N1	-5.41	120.00	122.70
9	I	3200	C	N3-C2-O2	-5.41	118.12	121.90
9	I	1835	C	C5-C6-N1	-5.40	118.30	121.00
9	I	2942	G	C4-N9-C1'	-5.39	119.49	126.50
9	I	2080	U	C5-C6-N1	-5.39	120.01	122.70
19	U	47	GLU	CG-CD-OE1	-5.39	107.53	118.30
9	I	2942	G	N3-C4-N9	-5.38	122.77	126.00
9	I	2974	C	N1-C2-O2	-5.38	115.67	118.90
9	I	1796	U	C5-C6-N1	-5.38	120.01	122.70
9	I	2369	G	C8-N9-C1'	-5.38	120.01	127.00
9	I	3292	U	C5-C6-N1	-5.38	120.01	122.70
9	I	2839	C	O4'-C1'-N1	5.38	112.50	108.20
19	U	68	PHE	N-CA-C	-5.38	96.49	111.00
9	I	4347	G	C6-C5-N7	-5.37	127.18	130.40
9	I	2402	C	C2-N1-C1'	-5.36	112.90	118.80
9	I	4064	G	N3-C4-C5	5.36	131.28	128.60
9	I	2651	G	C4-N9-C1'	5.36	133.47	126.50
9	I	1808	G	C4-N9-C1'	-5.36	119.53	126.50
9	I	3116	G	C6-C5-N7	-5.36	127.19	130.40
10	J	57	A	N1-C6-N6	5.36	121.81	118.60
9	I	1768	C	C2-N1-C1'	-5.35	112.91	118.80
9	I	3833	C	C6-N1-C1'	-5.35	114.39	120.80
9	I	1545	G	C8-N9-C1'	5.34	133.95	127.00
9	I	4087	U	C5-C6-N1	-5.34	120.03	122.70
9	I	3590	C	C6-N1-C2	5.34	122.44	120.30
9	I	2362	G	C4-C5-N7	5.34	112.94	110.80
9	I	1601	A	C4-C5-C6	-5.34	114.33	117.00
9	I	3160	G	N1-C6-O6	-5.34	116.70	119.90
9	I	4121	G	C6-C5-N7	5.34	133.60	130.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	I	3832	C	N3-C4-N4	-5.33	114.27	118.00
9	I	4347	G	C4-N9-C1'	5.33	133.43	126.50
9	I	3018	G	C8-N9-C1'	5.33	133.93	127.00
9	I	3367	G	N1-C2-N2	-5.33	111.41	116.20
9	I	3202	C	C2-N3-C4	5.32	122.56	119.90
9	I	4168	G	O4'-C1'-N9	5.32	112.46	108.20
9	I	1797	G	C8-N9-C1'	5.32	133.92	127.00
9	I	2945	C	N3-C4-C5	-5.32	119.77	121.90
9	I	1836	C	C2-N3-C4	-5.32	117.24	119.90
9	I	2356	G	C8-N9-C1'	5.31	133.91	127.00
9	I	3202	C	N1-C2-O2	5.31	122.09	118.90
9	I	4188	G	N3-C4-N9	-5.31	122.82	126.00
10	J	100	A	C8-N9-C4	5.31	107.92	105.80
9	I	2953	G	C8-N9-C1'	5.30	133.89	127.00
9	I	4337	G	C4-N9-C1'	-5.30	119.61	126.50
17	S	8	LEU	CB-CG-CD2	-5.30	101.99	111.00
9	I	4175	C	O5'-P-OP1	5.29	117.05	110.70
47	w	28	PHE	C-N-CA	-5.29	108.46	121.70
9	I	3292	U	C2-N1-C1'	-5.29	111.35	117.70
9	I	3848	C	C6-N1-C1'	-5.29	114.45	120.80
9	I	3006	C	C5-C4-N4	5.29	123.90	120.20
9	I	4326	U	C5-C4-O4	-5.28	122.73	125.90
9	I	1787	G	C6-C5-N7	-5.28	127.23	130.40
9	I	2313	U	C5-C6-N1	-5.28	120.06	122.70
9	I	1865	U	N1-C1'-C2'	-5.28	106.19	112.00
10	J	57	A	C5-C6-N6	-5.28	119.48	123.70
9	I	2370	U	C2-N1-C1'	-5.28	111.37	117.70
9	I	3990	C	N3-C2-O2	-5.27	118.21	121.90
9	I	2531	G	C5-C6-O6	5.27	131.76	128.60
9	I	1621	G	N3-C4-N9	5.27	129.16	126.00
9	I	2943	G	C8-N9-C1'	5.27	133.85	127.00
9	I	4140	C	C6-N1-C2	-5.27	118.19	120.30
9	I	468	C	N1-C2-N3	-5.26	115.52	119.20
10	J	17	G	C4-C5-N7	5.26	112.91	110.80
16	R	32	LEU	CA-CB-CG	-5.26	103.21	115.30
9	I	1826	G	N3-C4-N9	-5.25	122.85	126.00
9	I	4225	G	N1-C6-O6	-5.25	116.75	119.90
9	I	4214	U	O4'-C1'-N1	5.25	112.40	108.20
9	I	3326	C	C2-N1-C1'	-5.25	113.03	118.80
9	I	2525	G	N3-C4-C5	-5.24	125.98	128.60
9	I	3478	G	N1-C6-O6	-5.24	116.75	119.90
9	I	3478	G	C5-C6-O6	5.24	131.75	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	I	3777	C	C6-N1-C1'	5.24	127.08	120.80
9	I	1925	G	C4-C5-N7	5.24	112.89	110.80
9	I	2953	G	C6-C5-N7	5.24	133.54	130.40
9	I	3981	G	C4-C5-N7	5.23	112.89	110.80
9	I	3819	G	C6-C5-N7	5.23	133.54	130.40
9	I	2887	A	O4'-C1'-N9	5.22	112.38	108.20
9	I	4130	C	C2-N1-C1'	-5.22	113.06	118.80
9	I	2407	U	C2-N1-C1'	5.21	123.95	117.70
9	I	3862	C	C6-N1-C2	5.21	122.38	120.30
9	I	1909	G	C8-N9-C4	-5.21	104.32	106.40
9	I	3810	G	C5-C6-O6	5.21	131.72	128.60
9	I	1476	C	C5-C6-N1	5.20	123.60	121.00
45	u	86	LEU	CA-CB-CG	-5.19	103.36	115.30
9	I	3969	C	C6-N1-C2	-5.19	118.22	120.30
9	I	1864	C	O4'-C1'-N1	-5.19	104.05	108.20
9	I	4337	G	N1-C6-O6	-5.18	116.79	119.90
10	J	36	C	C6-N1-C2	5.18	122.37	120.30
9	I	4013	U	C2-N1-C1'	-5.17	111.49	117.70
9	I	2533	A	C6-N1-C2	5.17	121.70	118.60
9	I	3797	G	C8-N9-C1'	5.17	133.72	127.00
9	I	4174	U	C5-C6-N1	-5.17	120.11	122.70
10	J	22	G	N1-C6-O6	5.17	123.00	119.90
9	I	3756	U	C5-C4-O4	-5.17	122.80	125.90
10	J	105	G	C6-N1-C2	-5.17	122.00	125.10
9	I	3230	U	N1-C2-O2	-5.17	119.19	122.80
9	I	4018	G	O4'-C1'-N9	5.16	112.33	108.20
9	I	3861	G	N9-C1'-C2'	-5.16	106.32	112.00
9	I	3876	G	C4-N9-C1'	5.16	133.21	126.50
9	I	2045	U	N3-C2-O2	-5.15	118.59	122.20
9	I	4121	G	N9-C4-C5	5.15	107.46	105.40
9	I	2105	G	O4'-C1'-N9	5.15	112.32	108.20
9	I	2983	C	N1-C2-O2	-5.15	115.81	118.90
9	I	2651	G	N3-C4-C5	-5.15	126.03	128.60
9	I	3199	A	C8-N9-C4	5.15	107.86	105.80
9	I	4188	G	C8-N9-C1'	5.14	133.69	127.00
9	I	3181	G	C8-N9-C4	5.14	108.46	106.40
9	I	2365	C	N1-C2-O2	-5.14	115.82	118.90
9	I	3160	G	C4-C5-N7	-5.14	108.75	110.80
11	K	32	LEU	CB-CG-CD2	5.14	119.73	111.00
9	I	2926	G	N1-C6-O6	5.13	122.98	119.90
9	I	3391	G	N9-C1'-C2'	-5.13	106.35	112.00
24	Z	39	PHE	CB-CG-CD1	5.13	124.39	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	I	2610	G	N9-C4-C5	-5.13	103.35	105.40
9	I	3820	C	O4'-C1'-N1	5.13	112.30	108.20
19	U	33	LEU	CA-CB-CG	5.13	127.09	115.30
9	I	3960	C	C6-N1-C2	5.12	122.35	120.30
9	I	4140	C	N3-C2-O2	-5.12	118.31	121.90
9	I	3753	U	C5-C6-N1	-5.12	120.14	122.70
9	I	1878	C	N1-C2-O2	-5.12	115.83	118.90
10	J	17	G	C6-C5-N7	-5.12	127.33	130.40
9	I	3797	G	C4-N9-C1'	-5.11	119.86	126.50
9	I	3328	U	N3-C4-O4	-5.11	115.82	119.40
9	I	1518	U	C5-C6-N1	-5.11	120.15	122.70
9	I	4347	G	C8-N9-C1'	-5.11	120.36	127.00
9	I	3788	G	C8-N9-C1'	-5.11	120.36	127.00
10	J	5	G	C4-C5-N7	5.11	112.84	110.80
9	I	3270	G	C8-N9-C1'	-5.10	120.36	127.00
9	I	2994	G	C5-N7-C8	-5.10	101.75	104.30
9	I	2138	G	N3-C2-N2	-5.09	116.33	119.90
10	J	15	G	N3-C4-N9	-5.09	122.94	126.00
9	I	3305	G	N1-C6-O6	-5.09	116.85	119.90
9	I	4019	G	N7-C8-N9	-5.09	110.56	113.10
9	I	2986	G	N3-C4-N9	-5.08	122.95	126.00
9	I	2221	A	N9-C4-C5	-5.08	103.77	105.80
9	I	4212	G	C8-N9-C4	-5.08	104.37	106.40
9	I	3160	G	N9-C1'-C2'	-5.08	106.41	112.00
9	I	4130	C	N3-C4-C5	5.08	123.93	121.90
9	I	4283	C	C6-N1-C1'	5.08	126.89	120.80
9	I	2342	U	C5-C6-N1	-5.07	120.17	122.70
9	I	3354	G	C4-N9-C1'	-5.07	119.91	126.50
9	I	3819	G	C4-C5-N7	-5.07	108.77	110.80
9	I	3995	C	C6-N1-C1'	5.07	126.88	120.80
9	I	3305	G	N1-C2-N2	-5.07	111.64	116.20
9	I	3877	G	N3-C4-C5	-5.07	126.07	128.60
9	I	4064	G	N1-C2-N2	5.06	120.76	116.20
9	I	3959	C	C6-N1-C2	5.06	122.33	120.30
9	I	1750	G	C2-N3-C4	-5.06	109.37	111.90
9	I	3484	C	N3-C2-O2	-5.06	118.36	121.90
45	u	20	LEU	CA-CB-CG	-5.05	103.68	115.30
9	I	1465	G	C4-N9-C1'	5.04	133.06	126.50
9	I	3018	G	C4-N9-C1'	-5.04	119.94	126.50
9	I	3312	U	C2-N1-C1'	-5.04	111.65	117.70
9	I	1777	G	N3-C2-N2	-5.04	116.37	119.90
9	I	3160	G	N1-C2-N2	5.04	120.73	116.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	I	1866	C	C6-N1-C2	5.04	122.31	120.30
9	I	2204	G	N7-C8-N9	5.03	115.62	113.10
9	I	2882	G	N9-C4-C5	-5.03	103.39	105.40
9	I	3837	U	C6-N1-C1'	5.03	128.25	121.20
9	I	1902	A	O4'-C1'-N9	-5.03	104.18	108.20
9	I	3864	G	C6-C5-N7	5.02	133.41	130.40
18	T	115	GLU	CB-CG-CD	5.02	127.77	114.20
9	I	3244	G	N3-C4-C5	5.02	131.11	128.60
9	I	1925	G	O4'-C1'-N9	-5.01	104.19	108.20
9	I	1909	G	N7-C8-N9	5.01	115.60	113.10
9	I	1621	G	N9-C4-C5	-5.00	103.40	105.40
9	I	2895	G	C5-C6-O6	5.00	131.60	128.60
9	I	385	C	N3-C2-O2	-5.00	118.40	121.90
9	I	3076	C	C2-N1-C1'	-5.00	113.30	118.80

There are no chirality outliers.

All (15) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	60	ARG	Sidechain
4	D	12	ASP	Peptide
4	D	13	LYS	Peptide
11	K	100	ARG	Peptide
11	K	101	ARG	Peptide
11	K	140	VAL	Peptide
11	K	63	ILE	Mainchain
11	K	81	GLU	Peptide
12	L	124	ARG	Sidechain
12	L	151	THR	Peptide
12	L	92	VAL	Peptide
16	R	71	ASP	Peptide
20	V	34	ILE	Peptide
39	o	108	ARG	Sidechain
44	t	85	ARG	Peptide

5.2 Too-close contacts

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	A	98/100 (98%)	90 (92%)	8 (8%)	0	100	100
2	B	86/88 (98%)	78 (91%)	6 (7%)	2 (2%)	6	37
3	C	80/82 (98%)	68 (85%)	10 (12%)	2 (2%)	5	35
4	D	78/80 (98%)	66 (85%)	10 (13%)	2 (3%)	5	35
5	E	53/55 (96%)	47 (89%)	5 (9%)	1 (2%)	8	41
6	F	77/79 (98%)	74 (96%)	2 (3%)	1 (1%)	12	48
7	G	83/85 (98%)	77 (93%)	6 (7%)	0	100	100
8	H	54/56 (96%)	51 (94%)	3 (6%)	0	100	100
11	K	269/271 (99%)	216 (80%)	52 (19%)	1 (0%)	34	71
12	L	207/209 (99%)	171 (83%)	30 (14%)	6 (3%)	4	33
13	M	199/201 (99%)	172 (86%)	25 (13%)	2 (1%)	15	53
14	N	175/177 (99%)	147 (84%)	27 (15%)	1 (1%)	25	64
15	O	174/176 (99%)	133 (76%)	38 (22%)	3 (2%)	9	44
16	R	140/142 (99%)	113 (81%)	24 (17%)	3 (2%)	7	39
17	S	120/122 (98%)	97 (81%)	20 (17%)	3 (2%)	5	35
18	T	142/144 (99%)	118 (83%)	23 (16%)	1 (1%)	22	62
19	U	133/136 (98%)	119 (90%)	14 (10%)	0	100	100
20	V	118/120 (98%)	100 (85%)	18 (15%)	0	100	100
21	W	222/224 (99%)	211 (95%)	10 (4%)	1 (0%)	29	68
22	X	204/206 (99%)	190 (93%)	12 (6%)	2 (1%)	15	53
23	Y	203/205 (99%)	200 (98%)	3 (2%)	0	100	100
24	Z	148/150 (99%)	127 (86%)	19 (13%)	2 (1%)	11	47
25	a	98/100 (98%)	85 (87%)	11 (11%)	2 (2%)	7	40
26	b	149/151 (99%)	143 (96%)	5 (3%)	1 (1%)	22	62
27	c	127/129 (98%)	116 (91%)	10 (8%)	1 (1%)	19	59

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	d	125/127 (98%)	118 (94%)	6 (5%)	1 (1%)	19	59
29	e	96/98 (98%)	81 (84%)	13 (14%)	2 (2%)	7	39
30	f	115/117 (98%)	94 (82%)	20 (17%)	1 (1%)	17	55
31	g	120/123 (98%)	107 (89%)	13 (11%)	0	100	100
32	h	112/114 (98%)	105 (94%)	6 (5%)	1 (1%)	17	55
33	i	54/56 (96%)	45 (83%)	7 (13%)	2 (4%)	3	28
34	j	48/50 (96%)	41 (85%)	6 (12%)	1 (2%)	7	39
35	k	44/46 (96%)	36 (82%)	7 (16%)	1 (2%)	6	37
36	l	62/64 (97%)	53 (86%)	9 (14%)	0	100	100
37	m	36/38 (95%)	31 (86%)	5 (14%)	0	100	100
38	n	114/116 (98%)	96 (84%)	18 (16%)	0	100	100
39	o	112/114 (98%)	93 (83%)	18 (16%)	1 (1%)	17	55
40	p	115/117 (98%)	97 (84%)	18 (16%)	0	100	100
41	q	101/103 (98%)	79 (78%)	22 (22%)	0	100	100
42	r	108/110 (98%)	94 (87%)	13 (12%)	1 (1%)	17	55
43	s	91/93 (98%)	71 (78%)	19 (21%)	1 (1%)	14	51
44	t	100/102 (98%)	72 (72%)	27 (27%)	1 (1%)	15	53
45	u	92/94 (98%)	80 (87%)	11 (12%)	1 (1%)	14	51
46	v	73/75 (97%)	65 (89%)	8 (11%)	0	100	100
47	w	75/77 (97%)	63 (84%)	12 (16%)	0	100	100
48	x	60/62 (97%)	49 (82%)	10 (17%)	1 (2%)	9	44
49	y	56/58 (97%)	46 (82%)	9 (16%)	1 (2%)	8	42
All	All	5346/5442 (98%)	4625 (86%)	668 (12%)	53 (1%)	20	53

All (53) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	43	ALA
11	K	101	ARG
12	L	104	VAL
15	O	91	VAL
16	R	81	ILE
18	T	111	ILE
22	X	65	VAL

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Mol	Chain	Res	Type
24	Z	94	THR
27	c	88	LYS
32	h	3	ILE
33	i	55	ALA
35	k	44	VAL
42	r	62	ASP
43	s	38	ALA
44	t	6	ARG
3	C	79	ASN
4	D	16	LYS
6	F	4	LYS
12	L	150	GLN
12	L	151	THR
17	S	35	VAL
21	W	123	PHE
24	Z	15	THR
25	a	56	LYS
26	b	145	GLU
28	d	22	ASN
29	e	53	VAL
30	f	3	GLN
2	B	45	HIS
14	N	175	PRO
25	a	54	LEU
33	i	54	ILE
39	o	56	SER
2	B	87	ARG
5	E	51	TYR
12	L	194	PRO
16	R	85	LYS
17	S	66	LYS
29	e	32	VAL
45	u	23	ALA
48	x	57	ASN
4	D	77	GLU
12	L	89	GLU
13	M	195	GLN
16	R	39	LYS
17	S	93	GLN
22	X	79	LYS
34	j	48	GLU
49	y	20	LYS

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Mol	Chain	Res	Type
13	M	83	VAL
12	L	152	PRO
15	O	11	PRO
15	O	125	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	83/83 (100%)	83 (100%)	0	100	100
2	B	76/76 (100%)	76 (100%)	0	100	100
3	C	65/65 (100%)	65 (100%)	0	100	100
4	D	74/74 (100%)	74 (100%)	0	100	100
5	E	48/48 (100%)	48 (100%)	0	100	100
6	F	70/70 (100%)	70 (100%)	0	100	100
7	G	65/65 (100%)	65 (100%)	0	100	100
8	H	48/48 (100%)	47 (98%)	1 (2%)	53	71
11	K	216/216 (100%)	213 (99%)	3 (1%)	67	80
12	L	164/164 (100%)	164 (100%)	0	100	100
13	M	165/165 (100%)	163 (99%)	2 (1%)	71	83
14	N	148/148 (100%)	146 (99%)	2 (1%)	67	80
15	O	137/137 (100%)	137 (100%)	0	100	100
16	R	116/116 (100%)	116 (100%)	0	100	100
17	S	103/103 (100%)	101 (98%)	2 (2%)	57	74
18	T	103/103 (100%)	103 (100%)	0	100	100
19	U	108/108 (100%)	105 (97%)	3 (3%)	43	65
20	V	100/100 (100%)	100 (100%)	0	100	100
21	W	186/186 (100%)	185 (100%)	1 (0%)	88	93
22	X	170/170 (100%)	169 (99%)	1 (1%)	86	92

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
23	Y	172/172 (100%)	172 (100%)	0	100	100
24	Z	113/113 (100%)	113 (100%)	0	100	100
25	a	87/87 (100%)	86 (99%)	1 (1%)	73	84
26	b	124/124 (100%)	122 (98%)	2 (2%)	62	78
27	c	104/104 (100%)	104 (100%)	0	100	100
28	d	105/105 (100%)	104 (99%)	1 (1%)	76	86
29	e	86/86 (100%)	85 (99%)	1 (1%)	71	83
30	f	90/90 (100%)	90 (100%)	0	100	100
31	g	102/102 (100%)	101 (99%)	1 (1%)	76	86
32	h	92/92 (100%)	92 (100%)	0	100	100
33	i	47/47 (100%)	47 (100%)	0	100	100
34	j	45/45 (100%)	45 (100%)	0	100	100
35	k	38/38 (100%)	37 (97%)	1 (3%)	46	66
36	l	51/51 (100%)	51 (100%)	0	100	100
37	m	34/34 (100%)	34 (100%)	0	100	100
38	n	86/86 (100%)	84 (98%)	2 (2%)	50	69
39	o	99/99 (100%)	97 (98%)	2 (2%)	55	73
40	p	89/89 (100%)	89 (100%)	0	100	100
41	q	84/84 (100%)	84 (100%)	0	100	100
42	r	93/93 (100%)	93 (100%)	0	100	100
43	s	80/80 (100%)	80 (100%)	0	100	100
44	t	83/83 (100%)	83 (100%)	0	100	100
45	u	78/78 (100%)	78 (100%)	0	100	100
46	v	56/57 (98%)	56 (100%)	0	100	100
47	w	67/67 (100%)	67 (100%)	0	100	100
48	x	54/54 (100%)	54 (100%)	0	100	100
49	y	48/48 (100%)	46 (96%)	2 (4%)	30	55
All	All	4452/4453 (100%)	4424 (99%)	28 (1%)	86	92

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

Mol	Chain	Res	Type
8	H	44	ARG

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Mol	Chain	Res	Type
11	K	51	ARG
11	K	101	ARG
11	K	202	ARG
13	M	57	LYS
13	M	139	LYS
14	N	79	ARG
14	N	111	ARG
17	S	3	GLN
17	S	49	ARG
19	U	13	HIS
19	U	16	ARG
19	U	59	ARG
21	W	6	MET
22	X	85	LYS
25	a	35	LYS
26	b	2	ARG
26	b	4	ARG
28	d	103	ARG
29	e	12	ARG
31	g	17	LYS
35	k	25	LYS
38	n	2	LYS
38	n	55	LYS
39	o	5	LYS
39	o	37	LYS
49	y	18	LYS
49	y	44	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (65) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
2	B	34	GLN
3	C	26	ASN
6	F	55	HIS
11	K	36	ASN
11	K	69	ASN
11	K	127	ASN
11	K	162	GLN
11	K	231	HIS
11	K	250	GLN
12	L	42	ASN

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Mol	Chain	Res	Type
12	L	173	GLN
13	M	62	GLN
15	O	44	HIS
15	O	63	GLN
15	O	110	HIS
15	O	114	HIS
15	O	115	GLN
15	O	138	GLN
16	R	86	GLN
17	S	3	GLN
17	S	29	HIS
17	S	90	ASN
18	T	99	ASN
19	U	45	GLN
20	V	9	GLN
20	V	16	HIS
20	V	23	ASN
20	V	81	ASN
21	W	39	ASN
21	W	48	ASN
21	W	117	GLN
21	W	174	ASN
22	X	2	GLN
23	Y	115	GLN
23	Y	119	HIS
24	Z	126	ASN
24	Z	139	ASN
25	a	3	HIS
25	a	11	HIS
25	a	68	GLN
27	c	17	GLN
28	d	72	GLN
28	d	78	HIS
28	d	107	GLN
29	e	54	ASN
30	f	26	GLN
31	g	71	HIS
32	h	51	GLN
32	h	90	HIS
33	i	37	HIS
33	i	41	HIS
34	j	43	HIS

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Mol	Chain	Res	Type
37	m	35	GLN
39	o	2	ASN
39	o	9	GLN
41	q	66	HIS
42	r	57	ASN
43	s	48	GLN
44	t	68	ASN
45	u	51	GLN
46	v	66	ASN
48	x	26	ASN
48	x	37	GLN
48	x	57	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
10	J	117/118 (99%)	54 (46%)	2 (1%)
9	I	4428/4438 (99%)	1489 (33%)	119 (2%)
All	All	4545/4556 (99%)	1543 (33%)	121 (2%)

All (1543) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
9	I	3	U
9	I	4	U
9	I	8	G
9	I	27	A
9	I	31	A
9	I	38	G
9	I	46	C
9	I	47	C
9	I	50	A
9	I	51	C
9	I	58	A
9	I	59	A
9	I	60	G
9	I	69	U
9	I	70	A
9	I	73	A
9	I	74	G
9	I	82	C

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Mol	Chain	Res	Type
9	I	83	U
9	I	86	C
9	I	87	U
9	I	92	U
9	I	93	G
9	I	94	C
9	I	104	G
9	I	107	G
9	I	109	C
9	I	110	G
9	I	115	A
9	I	127	G
9	I	128	A
9	I	129	A
9	I	130	A
9	I	133	G
9	I	134	C
9	I	137	G
9	I	140	G
9	I	141	G
9	I	153	U
9	I	157	G
9	I	159	A
9	I	163	G
9	I	172	U
9	I	177	C
9	I	180	A
9	I	181	A
9	I	182	C
9	I	188	A
9	I	190	G
9	I	197	G
9	I	205	C
9	I	207	U
9	I	208	U
9	I	209	C
9	I	210	G
9	I	211	G
9	I	225	G
9	I	227	A
9	I	228	U
9	I	229	G

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Mol	Chain	Res	Type
9	I	235	A
9	I	239	G
9	I	244	U
9	I	246	G
9	I	249	A
9	I	250	G
9	I	252	A
9	I	253	G
9	I	259	G
9	I	260	U
9	I	265	G
9	I	273	A
9	I	274	G
9	I	275	G
9	I	276	C
9	I	279	C
9	I	281	A
9	I	288	G
9	I	289	C
9	I	292	G
9	I	300	G
9	I	305	A
9	I	307	C
9	I	315	C
9	I	324	A
9	I	327	C
9	I	328	A
9	I	331	G
9	I	338	C
9	I	339	U
9	I	340	C
9	I	346	G
9	I	348	A
9	I	351	C
9	I	353	G
9	I	362	A
9	I	366	U
9	I	367	U
9	I	368	G
9	I	371	C
9	I	376	G
9	I	380	C

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Mol	Chain	Res	Type
9	I	389	U
9	I	390	G
9	I	391	C
9	I	396	A
9	I	397	U
9	I	405	G
9	I	410	A
9	I	411	A
9	I	412	G
9	I	420	U
9	I	421	C
9	I	423	G
9	I	425	U
9	I	428	U
9	I	455	A
9	I	456	G
9	I	457	U
9	I	462	U
9	I	466	U
9	I	467	A
9	I	468	C
9	I	477	A
9	I	478	U
9	I	480	G
9	I	483	G
9	I	484	U
9	I	491	C
9	I	493	G
9	I	494	A
9	I	495	A
9	I	496	G
9	I	510	C
9	I	511	U
9	I	523	G
9	I	526	G7M
9	I	530	U
9	I	531	A
9	I	532	A
9	I	546	A
9	I	557	G
9	I	561	U
9	I	563	C

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Mol	Chain	Res	Type
9	I	567	G
9	I	571	A
9	I	572	A
9	I	574	G
9	I	575	C
9	I	587	G
9	I	595	A
9	I	596	G
9	I	614	G
9	I	619	C
9	I	632	G
9	I	639	A
9	I	641	A
9	I	649	G
9	I	653	G
9	I	664	A
9	I	667	G
9	I	674	A
9	I	675	A
9	I	686	A
9	I	690	G
9	I	700	U
9	I	702	G
9	I	718	C
9	I	720	G
9	I	722	U
9	I	723	G
9	I	735	C
9	I	738	C
9	I	739	U
9	I	740	G
9	I	754	G
9	I	758	A
9	I	762	G
9	I	765	A
9	I	776	A
9	I	778	C
9	I	782	C
9	I	789	A
9	I	792	U
9	I	793	A
9	I	803	U

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Mol	Chain	Res	Type
9	I	814	A
9	I	816	C
9	I	820	G
9	I	827	U
9	I	828	G
9	I	840	C
9	I	841	U
9	I	842	U
9	I	843	G
9	I	844	A
9	I	845	G
9	I	863	A
9	I	872	A
9	I	873	G
9	I	882	C
9	I	901	G
9	I	913	A
9	I	933	C
9	I	934	A
9	I	957	A
9	I	959	U
9	I	968	A
9	I	971	C
9	I	974	A
9	I	975	G
9	I	976	A
9	I	979	C
9	I	980	U
9	I	981	U
9	I	983	C
9	I	986	G
9	I	987	G
9	I	991	U
9	I	992	G
9	I	1007	U
9	I	1008	U
9	I	1014	G
9	I	1016	U
9	I	1020	A
9	I	1025	G
9	I	1027	C
9	I	1029	U

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Mol	Chain	Res	Type
9	I	1030	C
9	I	1032	G
9	I	1035	A
9	I	1036	C
9	I	1040	G
9	I	1042	G
9	I	1044	C
9	I	1045	A
9	I	1046	G
9	I	1049	G
9	I	1053	C
9	I	1055	U
9	I	1059	U
9	I	1061	U
9	I	1062	C
9	I	1063	G
9	I	1064	U
9	I	1065	C
9	I	1077	U
9	I	1078	G
9	I	1080	A
9	I	1093	G
9	I	1094	U
9	I	1097	C
9	I	1100	A
9	I	1123	G
9	I	1132	G
9	I	1134	U
9	I	1135	C
9	I	1136	C
9	I	1138	G
9	I	1139	C
9	I	1140	C
9	I	1141	G
9	I	1144	A
9	I	1145	A
9	I	1150	A
9	I	1151	A
9	I	1157	C
9	I	1158	U
9	I	1159	G
9	I	1160	C

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Mol	Chain	Res	Type
9	I	1166	A
9	I	1167	U
9	I	1183	G
9	I	1188	U
9	I	1191	C
9	I	1195	A
9	I	1196	A
9	I	1200	A
9	I	1201	U
9	I	1202	C
9	I	1203	A
9	I	1211	U
9	I	1212	A
9	I	1216	C
9	I	1217	C
9	I	1223	U
9	I	1224	A
9	I	1225	C
9	I	1226	A
9	I	1237	A
9	I	1239	U
9	I	1255	A
9	I	1260	A
9	I	1263	U
9	I	1267	G
9	I	1274	A
9	I	1279	A
9	I	1285	U
9	I	1286	A
9	I	1293	G
9	I	1298	A
9	I	1301	C
9	I	1304	G
9	I	1316	C
9	I	1319	C
9	I	1330	G
9	I	1337	G
9	I	1345	A
9	I	1352	G
9	I	1358	C
9	I	1361	A
9	I	1362	A

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Mol	Chain	Res	Type
9	I	1363	U
9	I	1367	A
9	I	1373	A
9	I	1374	A
9	I	1377	C
9	I	1378	G
9	I	1398	C
9	I	1399	C
9	I	1404	G
9	I	1406	5MC
9	I	1421	G
9	I	1428	A
9	I	1430	A
9	I	1431	G
9	I	1432	A
9	I	1440	A
9	I	1441	G
9	I	1446	A
9	I	1450	G
9	I	1451	U
9	I	1452	C
9	I	1461	U
9	I	1463	G
9	I	1467	U
9	I	1468	A
9	I	1471	C
9	I	1472	G
9	I	1475	A
9	I	1476	C
9	I	1478	A
9	I	1479	A
9	I	1482	A
9	I	1487	U
9	I	1489	A
9	I	1492	C
9	I	1494	U
9	I	1499	U
9	I	1500	U
9	I	1502	G
9	I	1503	U
9	I	1504	U
9	I	1510	A

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Mol	Chain	Res	Type
9	I	1512	U
9	I	1514	A
9	I	1515	G
9	I	1525	U
9	I	1529	U
9	I	1534	U
9	I	1535	G
9	I	1538	A
9	I	1541	C
9	I	1543	G
9	I	1544	A
9	I	1546	G
9	I	1551	G
9	I	1558	G
9	I	1559	U
9	I	1560	G
9	I	1562	U
9	I	1563	A
9	I	1569	C
9	I	1571	A
9	I	1574	A
9	I	1575	G
9	I	1577	G
9	I	1580	G
9	I	1581	G
9	I	1583	A
9	I	1584	A
9	I	1585	G
9	I	1587	U
9	I	1588	G
9	I	1591	A
9	I	1593	G
9	I	1596	C
9	I	1598	G
9	I	1600	U
9	I	1601	A
9	I	1603	A
9	I	1613	U
9	I	1614	U
9	I	1618	A
9	I	1620	U
9	I	1621	G

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Mol	Chain	Res	Type
9	I	1622	G
9	I	1628	C
9	I	1629	C
9	I	1631	A
9	I	1632	G
9	I	1634	G
9	I	1635	U
9	I	1636	G
9	I	1638	U
9	I	1639	U
9	I	1640	C
9	I	1641	G
9	I	1642	A
9	I	1652	A
9	I	1663	C
9	I	1665	A
9	I	1666	U
9	I	1667	A
9	I	1672	A
9	I	1676	A
9	I	1677	G
9	I	1691	A
9	I	1692	C
9	I	1696	A
9	I	1699	A
9	I	1701	C
9	I	1702	U
9	I	1704	A
9	I	1715	G
9	I	1716	A
9	I	1721	A
9	I	1722	A
9	I	1723	A
9	I	1724	U
9	I	1725	C
9	I	1728	C
9	I	1730	G
9	I	1731	A
9	I	1732	G
9	I	1733	A
9	I	1747	G
9	I	1748	G

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Mol	Chain	Res	Type
9	I	1749	C
9	I	1750	G
9	I	1762	A
9	I	1765	A
9	I	1766	G
9	I	1767	C
9	I	1770	A
9	I	1771	G
9	I	1772	A
9	I	1776	U
9	I	1777	G
9	I	1778	A
9	I	1779	A
9	I	1780	U
9	I	1788	U
9	I	1789	G
9	I	1792	U
9	I	1793	U
9	I	1794	A
9	I	1797	G
9	I	1799	A
9	I	1801	G
9	I	1802	C
9	I	1804	U
9	I	1805	C
9	I	1808	G
9	I	1810	A
9	I	1811	A
9	I	1816	C
9	I	1818	C
9	I	1821	U
9	I	1822	A
9	I	1823	C
9	I	1829	G
9	I	1830	A
9	I	1833	G
9	I	1835	C
9	I	1836	C
9	I	1838	G
9	I	1845	A
9	I	1847	A
9	I	1848	A

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Mol	Chain	Res	Type
9	I	1850	G
9	I	1852	A
9	I	1853	C
9	I	1854	A
9	I	1855	U
9	I	1856	G
9	I	1858	U
9	I	1860	U
9	I	1861	G
9	I	1862	A
9	I	1863	G
9	I	1864	C
9	I	1866	C
9	I	1867	G
9	I	1868	A
9	I	1870	G
9	I	1871	A
9	I	1872	G
9	I	1873	U
9	I	1874	A
9	I	1875	G
9	I	1881	G
9	I	1886	G
9	I	1887	U
9	I	1894	C
9	I	1895	U
9	I	1896	G
9	I	1899	U
9	I	1901	A
9	I	1902	A
9	I	1903	U
9	I	1904	A
9	I	1905	U
9	I	1906	G
9	I	1907	G
9	I	1908	G
9	I	1910	G
9	I	1911	G
9	I	1912	A
9	I	1914	C
9	I	1915	A
9	I	1916	U

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Mol	Chain	Res	Type
9	I	1917	C
9	I	1919	U
9	I	1920	C
9	I	1921	C
9	I	1922	A
9	I	1924	G
9	I	1925	G
9	I	1928	A
9	I	1929	A
9	I	1930	A
9	I	1951	U
9	I	1955	C
9	I	1956	C
9	I	1962	C
9	I	1963	G
9	I	1965	G
9	I	1967	G
9	I	1970	A
9	I	1972	A
9	I	1979	A
9	I	1980	A
9	I	1981	G
9	I	1983	A
9	I	1988	G
9	I	1989	G
9	I	1990	C
9	I	1991	G
9	I	2004	A
9	I	2005	A
9	I	2008	A
9	I	2009	C
9	I	2010	C
9	I	2021	U
9	I	2025	U
9	I	2027	C
9	I	2028	A
9	I	2030	G
9	I	2031	C
9	I	2032	A
9	I	2033	G
9	I	2040	C
9	I	2043	G

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Mol	Chain	Res	Type
9	I	2045	U
9	I	2046	U
9	I	2047	A
9	I	2048	G
9	I	2049	G
9	I	2051	G
9	I	2059	G
9	I	2060	C
9	I	2061	G
9	I	2062	U
9	I	2063	A
9	I	2066	U
9	I	2070	G
9	I	2071	U
9	I	2072	A
9	I	2073	U
9	I	2075	A
9	I	2077	G
9	I	2079	G
9	I	2083	G
9	I	2086	A
9	I	2087	C
9	I	2102	A
9	I	2104	G
9	I	2105	G
9	I	2114	A
9	I	2115	U
9	I	2120	G
9	I	2121	A
9	I	2127	A
9	I	2128	G
9	I	2135	C
9	I	2137	A
9	I	2138	G
9	I	2139	U
9	I	2145	C
9	I	2146	U
9	I	2147	G
9	I	2148	G
9	I	2151	G
9	I	2153	U
9	I	2154	A

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Mol	Chain	Res	Type
9	I	2155	A
9	I	2156	G
9	I	2170	A
9	I	2176	A
9	I	2177	A
9	I	2186	U
9	I	2193	A
9	I	2194	U
9	I	2197	G
9	I	2199	A
9	I	2200	G
9	I	2202	U
9	I	2204	G
9	I	2205	A
9	I	2215	A
9	I	2221	A
9	I	2222	A
9	I	2226	G
9	I	2229	G
9	I	2230	A
9	I	2232	C
9	I	2233	G
9	I	2235	A
9	I	2236	C
9	I	2245	1MG
9	I	2246	PSU
9	I	2247	5MU
9	I	2248	G
9	I	2250	A
9	I	2252	A
9	I	2253	A
9	I	2257	G
9	I	2258	C
9	I	2259	G
9	I	2260	G
9	I	2264	A
9	I	2266	U
9	I	2270	G
9	I	2275	G
9	I	2276	G
9	I	2278	G
9	I	2279	U

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Mol	Chain	Res	Type
9	I	2280	G
9	I	2281	A
9	I	2282	A
9	I	2283	A
9	I	2284	G
9	I	2285	G
9	I	2288	A
9	I	2290	U
9	I	2292	A
9	I	2297	G
9	I	2303	U
9	I	2305	G
9	I	2306	C
9	I	2310	U
9	I	2311	U
9	I	2312	C
9	I	2315	C
9	I	2319	A
9	I	2321	A
9	I	2324	U
9	I	2326	U
9	I	2327	U
9	I	2329	A
9	I	2332	U
9	I	2345	A
9	I	2346	U
9	I	2347	U
9	I	2352	U
9	I	2357	G
9	I	2358	G
9	I	2359	G
9	I	2360	U
9	I	2364	G
9	I	2365	C
9	I	2366	A
9	I	2367	C
9	I	2369	G
9	I	2370	U
9	I	2371	U
9	I	2374	G
9	I	2375	G
9	I	2376	C

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Mol	Chain	Res	Type
9	I	2378	A
9	I	2385	C
9	I	2387	C
9	I	2390	A
9	I	2391	C
9	I	2398	G
9	I	2399	A
9	I	2401	G
9	I	2402	C
9	I	2403	A
9	I	2404	A
9	I	2406	C
9	I	2407	U
9	I	2408	G
9	I	2409	C
9	I	2410	G
9	I	2411	A
9	I	2412	A
9	I	2414	A
9	I	2417	G
9	I	2420	G
9	I	2422	A
9	I	2427	A
9	I	2428	U
9	I	2435	A
9	I	2439	A
9	I	2440	C
9	I	2447	G
9	I	2448	G
9	I	2453	A
9	I	2455	C
9	I	2458	C
9	I	2466	A
9	I	2468	G
9	I	2469	A
9	I	2471	G
9	I	2475	A
9	I	2477	A
9	I	2482	A
9	I	2485	C
9	I	2489	C
9	I	2490	A

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Mol	Chain	Res	Type
9	I	2491	G
9	I	2493	U
9	I	2494	A
9	I	2499	C
9	I	2500	C
9	I	2502	A
9	I	2503	A
9	I	2506	U
9	I	2507	C
9	I	2509	U
9	I	2511	G
9	I	2513	U
9	I	2514	A
9	I	2516	G
9	I	2517	U
9	I	2519	G
9	I	2520	G
9	I	2521	A
9	I	2522	A
9	I	2523	A
9	I	2524	C
9	I	2527	U
9	I	2533	A
9	I	2537	C
9	I	2539	C
9	I	2540	A
9	I	2541	G
9	I	2543	C
9	I	2547	C
9	I	2551	A
9	I	2557	G
9	I	2563	A
9	I	2564	A
9	I	2565	G
9	I	2576	U
9	I	2578	A
9	I	2579	A
9	I	2581	G
9	I	2582	A
9	I	2584	A
9	I	2591	U
9	I	2605	A

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Mol	Chain	Res	Type
9	I	2606	G
9	I	2607	U
9	I	2610	G
9	I	2613	U
9	I	2618	G
9	I	2620	A
9	I	2622	G
9	I	2624	U
9	I	2626	U
9	I	2627	A
9	I	2628	A
9	I	2629	C
9	I	2630	G
9	I	2633	G
9	I	2634	C
9	I	2636	A
9	I	2638	A
9	I	2645	A
9	I	2646	C
9	I	2649	A
9	I	2664	C
9	I	2665	G
9	I	2666	C
9	I	2667	U
9	I	2668	U
9	I	2669	A
9	I	2670	U
9	I	2671	G
9	I	2672	C
9	I	2673	G
9	I	2674	U
9	I	2676	G
9	I	2680	G
9	I	2685	G
9	I	2691	G
9	I	2699	A
9	I	2700	G
9	I	2702	C
9	I	2704	G
9	I	2705	C
9	I	2706	G
9	I	2707	A

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Mol	Chain	Res	Type
9	I	2717	G
9	I	2718	U
9	I	2719	G
9	I	2721	G
9	I	2725	U
9	I	2730	G
9	I	2731	A
9	I	2732	G
9	I	2735	A
9	I	2742	G
9	I	2744	G
9	I	2746	G
9	I	2747	A
9	I	2749	U
9	I	2750	G
9	I	2752	U
9	I	2758	A
9	I	2760	G
9	I	2761	U
9	I	2762	A
9	I	2764	C
9	I	2765	G
9	I	2766	A
9	I	2767	U
9	I	2768	A
9	I	2770	A
9	I	2772	C
9	I	2778	A
9	I	2780	A
9	I	2781	A
9	I	2789	C
9	I	2791	C
9	I	2794	G
9	I	2795	A
9	I	2796	A
9	I	2806	U
9	I	2808	C
9	I	2817	C
9	I	2822	A
9	I	2823	U
9	I	2824	C
9	I	2833	G

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Mol	Chain	Res	Type
9	I	2835	G
9	I	2836	A
9	I	2839	C
9	I	2841	A
9	I	2843	C
9	I	2846	U
9	I	2848	A
9	I	2855	G
9	I	2857	C
9	I	2858	G
9	I	2859	A
9	I	2864	C
9	I	2872	A
9	I	2873	U
9	I	2874	G
9	I	2875	G
9	I	2877	A
9	I	2878	A
9	I	2879	A
9	I	2881	A
9	I	2885	U
9	I	2887	A
9	I	2889	A
9	I	2890	U
9	I	2894	U
9	I	2895	G
9	I	2897	A
9	I	2901	G
9	I	2910	G
9	I	2911	C
9	I	2913	A
9	I	2914	A
9	I	2915	G
9	I	2916	G
9	I	2917	G
9	I	2918	G
9	I	2919	G
9	I	2921	A
9	I	2922	C
9	I	2927	A
9	I	2929	G
9	I	2930	G

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Mol	Chain	Res	Type
9	I	2936	U
9	I	2944	G
9	I	2946	G
9	I	2947	A
9	I	2948	C
9	I	2952	U
9	I	2955	C
9	I	2963	A
9	I	2964	A
9	I	2967	G
9	I	2970	U
9	I	2976	G
9	I	2978	U
9	I	2979	U
9	I	2981	U
9	I	2984	A
9	I	2985	G
9	I	2987	C
9	I	2988	A
9	I	2989	A
9	I	2990	A
9	I	2991	U
9	I	2992	C
9	I	2993	C
9	I	2997	A
9	I	3002	A
9	I	3004	G
9	I	3007	U
9	I	3008	G
9	I	3009	A
9	I	3010	G
9	I	3012	C
9	I	3013	G
9	I	3016	A
9	I	3017	U
9	I	3018	G
9	I	3019	A
9	I	3022	A
9	I	3028	U
9	I	3029	A
9	I	3030	C
9	I	3031	G

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Mol	Chain	Res	Type
9	I	3032	G
9	I	3035	C
9	I	3038	A
9	I	3041	C
9	I	3042	A
9	I	3043	A
9	I	3044	C
9	I	3048	U
9	I	3049	G
9	I	3051	C
9	I	3056	U
9	I	3057	U
9	I	3058	C
9	I	3059	C
9	I	3060	A
9	I	3061	G
9	I	3063	A
9	I	3067	G
9	I	3072	U
9	I	3077	A
9	I	3078	U
9	I	3079	C
9	I	3081	G
9	I	3087	A
9	I	3090	A
9	I	3091	A
9	I	3092	A
9	I	3096	U
9	I	3099	C
9	I	3100	C
9	I	3101	C
9	I	3102	A
9	I	3104	A
9	I	3110	A
9	I	3111	C
9	I	3116	G
9	I	3121	G
9	I	3124	A
9	I	3125	G
9	I	3128	A
9	I	3140	C
9	I	3141	U

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Mol	Chain	Res	Type
9	I	3142	U
9	I	3143	G
9	I	3146	A
9	I	3147	G
9	I	3148	A
9	I	3158	A
9	I	3161	G
9	I	3162	A
9	I	3164	C
9	I	3165	U
9	I	3168	G
9	I	3171	A
9	I	3174	U
9	I	3176	G
9	I	3178	G
9	I	3179	C
9	I	3180	C
9	I	3181	G
9	I	3182	U
9	I	3187	U
9	I	3189	G
9	I	3190	G
9	I	3193	G
9	I	3198	C
9	I	3199	A
9	I	3201	G
9	I	3204	G
9	I	3208	U
9	I	3209	G
9	I	3210	U
9	I	3214	U
9	I	3216	A
9	I	3218	G
9	I	3223	U
9	I	3224	C
9	I	3225	G
9	I	3226	C
9	I	3227	G
9	I	3232	G
9	I	3233	A
9	I	3236	U
9	I	3242	C

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Mol	Chain	Res	Type
9	I	3244	G
9	I	3246	C
9	I	3247	G
9	I	3248	A
9	I	3249	A
9	I	3250	G
9	I	3251	A
9	I	3253	A
9	I	3256	A
9	I	3258	C
9	I	3263	U
9	I	3264	G
9	I	3267	A
9	I	3269	U
9	I	3270	G
9	I	3272	U
9	I	3273	U
9	I	3283	A
9	I	3286	G
9	I	3287	C
9	I	3291	G
9	I	3293	G
9	I	3294	C
9	I	3295	A
9	I	3296	A
9	I	3297	A
9	I	3302	A
9	I	3303	A
9	I	3304	A
9	I	3306	U
9	I	3307	G
9	I	3310	C
9	I	3311	G
9	I	3312	U
9	I	3314	U
9	I	3315	A
9	I	3323	A
9	I	3328	U
9	I	3329	2MG
9	I	3330	C
9	I	3331	C
9	I	3332	C

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Mol	Chain	Res	Type
9	I	3333	G
9	I	3338	C
9	I	3340	G
9	I	3341	A
9	I	3344	G
9	I	3350	U
9	I	3353	U
9	I	3354	G
9	I	3356	G
9	I	3357	G
9	I	3358	U
9	I	3359	U
9	I	3360	A
9	I	3361	G
9	I	3363	G
9	I	3364	C
9	I	3365	A
9	I	3369	G
9	I	3370	A
9	I	3371	A
9	I	3372	G
9	I	3379	A
9	I	3380	U
9	I	3382	G
9	I	3383	A
9	I	3388	C
9	I	3391	G
9	I	3393	A
9	I	3394	A
9	I	3395	A
9	I	3400	G
9	I	3408	C
9	I	3415	G
9	I	3420	U
9	I	3421	A
9	I	3423	G
9	I	3424	G
9	I	3427	G
9	I	3429	G
9	I	3430	A
9	I	3431	A
9	I	3432	A

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Mol	Chain	Res	Type
9	I	3433	5MU
9	I	3434	U
9	I	3435	C
9	I	3437	U
9	I	3439	G
9	I	3444	G
9	I	3445	U
9	I	3449	U
9	I	3453	G
9	I	3457	U
9	I	3458	G
9	I	3461	C
9	I	3464	A
9	I	3465	U
9	I	3466	G
9	I	3467	G
9	I	3471	A
9	I	3485	U
9	I	3486	G
9	I	3488	C
9	I	3489	U
9	I	3490	C
9	I	3491	C
9	I	3499	A
9	I	3508	A
9	I	3509	A
9	I	3511	U
9	I	3512	G
9	I	3516	U
9	I	3517	C
9	I	3522	U
9	I	3523	G
9	I	3525	A
9	I	3526	G
9	I	3527	A
9	I	3528	U
9	I	3533	U
9	I	3535	U
9	I	3536	A
9	I	3537	C
9	I	3549	C
9	I	3550	G

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Mol	Chain	Res	Type
9	I	3554	A
9	I	3555	G
9	I	3562	U
9	I	3563	G7M
9	I	3574	A
9	I	3583	C
9	I	3585	C
9	I	3586	U
9	I	3587	G
9	I	3588	A
9	I	3590	C
9	I	3591	A
9	I	3594	G
9	I	3595	A
9	I	3598	C
9	I	3605	U
9	I	3606	G
9	I	3607	U
9	I	3609	G
9	I	3610	G
9	I	3611	A
9	I	3612	U
9	I	3614	G
9	I	3615	G
9	I	3618	G
9	I	3620	A
9	I	3622	G
9	I	3625	U
9	I	3626	U
9	I	3627	G
9	I	3633	U
9	I	3634	G
9	I	3640	C
9	I	3641	A
9	I	3643	U
9	I	3652	A
9	I	3653	G
9	I	3657	A
9	I	3658	C
9	I	3659	C
9	I	3663	A
9	I	3665	A

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Mol	Chain	Res	Type
9	I	3666	U
9	I	3667	A
9	I	3676	U
9	I	3680	G
9	I	3683	U
9	I	3684	G
9	I	3688	U
9	I	3690	C
9	I	3691	U
9	I	3692	A
9	I	3693	A
9	I	3695	G
9	I	3697	U
9	I	3698	G
9	I	3704	U
9	I	3705	A
9	I	3706	A
9	I	3707	U
9	I	3708	C
9	I	3714	U
9	I	3719	A
9	I	3720	C
9	I	3727	U
9	I	3729	G
9	I	3732	G
9	I	3734	U
9	I	3740	G
9	I	3743	U
9	I	3757	C
9	I	3761	A
9	I	3762	A
9	I	3769	C
9	I	3772	A
9	I	3774	G
9	I	3776	G
9	I	3777	C
9	I	3781	A
9	I	3782	A
9	I	3784	G
9	I	3785	U
9	I	3786	U
9	I	3787	G

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Mol	Chain	Res	Type
9	I	3788	G
9	I	3789	C
9	I	3790	U
9	I	3791	A
9	I	3792	A
9	I	3793	U
9	I	3794	C
9	I	3796	U
9	I	3799	U
9	I	3802	G
9	I	3803	A
9	I	3805	A
9	I	3809	G
9	I	3811	A
9	I	3812	G
9	I	3813	G
9	I	3816	A
9	I	3819	G
9	I	3820	C
9	I	3821	A
9	I	3822	A
9	I	3825	G
9	I	3826	C
9	I	3827	A
9	I	3828	U
9	I	3829	A
9	I	3831	G
9	I	3833	C
9	I	3837	U
9	I	3839	G
9	I	3840	A
9	I	3841	C
9	I	3849	G
9	I	3851	G
9	I	3852	A
9	I	3856	C
9	I	3857	G
9	I	3858	C
9	I	3859	G
9	I	3861	G
9	I	3862	C
9	I	3863	A

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Mol	Chain	Res	Type
9	I	3866	U
9	I	3867	G
9	I	3868	C
9	I	3870	A
9	I	3871	A
9	I	3873	G
9	I	3877	G
9	I	3879	C
9	I	3881	U
9	I	3882	A
9	I	3883	G
9	I	3884	U
9	I	3885	G
9	I	3888	C
9	I	3894	G
9	I	3896	U
9	I	3897	C
9	I	3899	G
9	I	3900	A
9	I	3902	U
9	I	3911	C
9	I	3912	A
9	I	3916	C
9	I	3917	U
9	I	3918	C
9	I	3919	A
9	I	3920	A
9	I	3922	G
9	I	3923	G
9	I	3924	A
9	I	3925	U
9	I	3928	A
9	I	3935	U
9	I	3939	2MG
9	I	3941	G
9	I	3942	A
9	I	3960	C
9	I	3961	C
9	I	3962	A
9	I	3963	A
9	I	3966	G
9	I	3967	U

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Mol	Chain	Res	Type
9	I	3970	A
9	I	3971	U
9	I	3976	A
9	I	3981	G
9	I	3985	U
9	I	3986	U
9	I	3988	G
9	I	3990	C
9	I	3991	A
9	I	3992	OMC
9	I	3994	U
9	I	3996	G
9	I	3998	PSU
9	I	3999	G
9	I	4003	G
9	I	4005	U
9	I	4007	A
9	I	4012	A
9	I	4013	U
9	I	4017	G
9	I	4021	C
9	I	4024	A
9	I	4027	U
9	I	4041	A
9	I	4044	G
9	I	4046	OMU
9	I	4048	U
9	I	4058	A
9	I	4059	A
9	I	4060	A
9	I	4061	G
9	I	4065	U
9	I	4066	A
9	I	4067	C
9	I	4068	G
9	I	4072	G
9	I	4076	G
9	I	4079	U
9	I	4080	U
9	I	4081	A
9	I	4084	A
9	I	4089	G

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Mol	Chain	Res	Type
9	I	4091	G
9	I	4097	G
9	I	4099	PSU
9	I	4103	U
9	I	4106	C
9	I	4107	U
9	I	4120	C
9	I	4123	U
9	I	4124	G
9	I	4132	G
9	I	4135	G
9	I	4138	G
9	I	4140	C
9	I	4143	C
9	I	4145	C
9	I	4149	G
9	I	4150	U
9	I	4153	G
9	I	4154	A
9	I	4155	G
9	I	4162	G
9	I	4163	G
9	I	4165	G
9	I	4168	G
9	I	4175	C
9	I	4176	A
9	I	4177	C
9	I	4178	U
9	I	4179	G
9	I	4183	U
9	I	4184	U
9	I	4185	C
9	I	4186	G
9	I	4187	G
9	I	4190	U
9	I	4191	G
9	I	4192	U
9	I	4193	C
9	I	4194	A
9	I	4195	U
9	I	4197	C
9	I	4198	C

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Mol	Chain	Res	Type
9	I	4199	A
9	I	4200	A
9	I	4202	G
9	I	4204	C
9	I	4208	G
9	I	4212	G
9	I	4213	G
9	I	4215	A
9	I	4216	G
9	I	4218	U
9	I	4219	A
9	I	4220	A
9	I	4223	G
9	I	4227	A
9	I	4229	G
9	I	4232	A
9	I	4233	U
9	I	4236	G
9	I	4237	U
9	I	4240	U
9	I	4241	G
9	I	4242	A
9	I	4244	A
9	I	4245	G
9	I	4248	U
9	I	4249	C
9	I	4250	U
9	I	4251	A
9	I	4252	A
9	I	4253	G
9	I	4257	G
9	I	4258	A
9	I	4259	A
9	I	4260	A
9	I	4262	U
9	I	4265	C
9	I	4269	G
9	I	4272	A
9	I	4273	U
9	I	4274	G
9	I	4275	A
9	I	4276	G

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Mol	Chain	Res	Type
9	I	4279	C
9	I	4280	U
9	I	4282	C
9	I	4283	C
9	I	4285	G
9	I	4286	A
9	I	4287	C
9	I	4288	C
9	I	4291	U
9	I	4292	U
9	I	4293	A
9	I	4299	C
9	I	4301	U
9	I	4305	G
9	I	4311	U
9	I	4312	U
9	I	4314	A
9	I	4315	A
9	I	4319	G
9	I	4326	U
9	I	4327	U
9	I	4328	G
9	I	4329	A
9	I	4331	A
9	I	4335	C
9	I	4343	U
9	I	4344	A
9	I	4353	C
9	I	4354	U
9	I	4355	U
9	I	4364	C
9	I	4367	U
9	I	4375	U
9	I	4407	A
9	I	4409	G
9	I	4410	U
9	I	4416	U
9	I	4421	G
9	I	4429	G
9	I	4433	G
9	I	4434	G
9	I	4437	C

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Mol	Chain	Res	Type
9	I	4438	A
10	J	8	G
10	J	11	C
10	J	12	G
10	J	14	A
10	J	15	G
10	J	16	C
10	J	22	G
10	J	24	U
10	J	27	C
10	J	30	C
10	J	31	U
10	J	32	G
10	J	33	A
10	J	34	C
10	J	36	C
10	J	40	G
10	J	41	C
10	J	43	G
10	J	44	A
10	J	46	C
10	J	48	C
10	J	49	A
10	J	50	G
10	J	51	A
10	J	55	G
10	J	56	A
10	J	61	C
10	J	64	U
10	J	65	A
10	J	66	G
10	J	72	A
10	J	74	G
10	J	75	G
10	J	76	U
10	J	82	G
10	J	86	U
10	J	87	C
10	J	88	U
10	J	89	C
10	J	95	G
10	J	97	G

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Mol	Chain	Res	Type
10	J	98	A
10	J	100	A
10	J	104	G
10	J	105	G
10	J	107	A
10	J	108	A
10	J	109	C
10	J	111	G
10	J	112	C
10	J	113	C
10	J	114	A
10	J	116	G
10	J	118	A

All (121) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
9	I	3	U
9	I	132	U
9	I	196	A
9	I	208	U
9	I	227	A
9	I	228	U
9	I	249	A
9	I	252	A
9	I	273	A
9	I	390	G
9	I	410	A
9	I	427	G
9	I	571	A
9	I	673	G
9	I	719	C
9	I	757	C
9	I	819	U
9	I	990	U
9	I	1077	U
9	I	1138	G
9	I	1156	A
9	I	1210	U
9	I	1215	A
9	I	1259	G
9	I	1266	C

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Mol	Chain	Res	Type
9	I	1445	A
9	I	1475	A
9	I	1476	C
9	I	1486	G
9	I	1499	U
9	I	1584	A
9	I	1600	U
9	I	1690	A
9	I	1723	A
9	I	1770	A
9	I	1771	G
9	I	1777	G
9	I	1820	A
9	I	1829	G
9	I	1835	C
9	I	1846	A
9	I	1904	A
9	I	1928	A
9	I	1964	U
9	I	1969	G
9	I	1979	A
9	I	2007	A
9	I	2042	C
9	I	2085	G
9	I	2104	G
9	I	2127	A
9	I	2138	G
9	I	2147	G
9	I	2247	5MU
9	I	2280	G
9	I	2284	G
9	I	2357	G
9	I	2363	A
9	I	2403	A
9	I	2438	C
9	I	2484	A
9	I	2505	G
9	I	2578	A
9	I	2590	A
9	I	2718	U
9	I	2734	U
9	I	2743	U

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Mol	Chain	Res	Type
9	I	2757	U
9	I	2769	A
9	I	2807	U
9	I	2822	A
9	I	2832	G
9	I	2873	U
9	I	2877	A
9	I	3058	C
9	I	3060	A
9	I	3163	A
9	I	3175	G
9	I	3181	G
9	I	3225	G
9	I	3250	G
9	I	3310	C
9	I	3327	C
9	I	3360	A
9	I	3407	A
9	I	3488	C
9	I	3594	G
9	I	3621	G
9	I	3640	C
9	I	3656	G
9	I	3679	U
9	I	3692	A
9	I	3705	A
9	I	3719	A
9	I	3761	A
9	I	3768	A
9	I	3780	G
9	I	3808	A
9	I	3815	U
9	I	3820	C
9	I	3840	A
9	I	3883	G
9	I	3919	A
9	I	3921	C
9	I	3975	G
9	I	3989	G
9	I	4040	U
9	I	4058	A
9	I	4071	A

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Mol	Chain	Res	Type
9	I	4096	A
9	I	4174	U
9	I	4177	C
9	I	4214	U
9	I	4244	A
9	I	4249	C
9	I	4250	U
9	I	4291	U
9	I	4314	A
9	I	4325	G
10	J	71	G
10	J	94	U

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

35 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	UR3	I	4402	9	19,22,23	2.81	8 (42%)	26,32,35	1.32	3 (11%)
9	6MZ	I	3112	9	18,25,26	1.93	3 (16%)	16,36,39	1.96	3 (18%)
9	5MC	I	966	9	18,22,23	3.89	8 (44%)	26,32,35	0.99	1 (3%)
9	2MG	I	965	9	18,26,27	2.67	6 (33%)	16,38,41	1.35	3 (18%)
9	PSU	I	515	9	18,21,22	4.41	8 (44%)	22,30,33	2.01	6 (27%)
9	OMC	I	3992	9	19,22,23	3.33	8 (42%)	26,31,34	0.80	0
9	PSU	I	2246	9	18,21,22	4.44	8 (44%)	22,30,33	2.33	6 (27%)
9	2MG	I	1206	9	18,26,27	2.65	6 (33%)	16,38,41	1.39	3 (18%)
9	4OC	I	1401	9	20,23,24	3.14	8 (40%)	26,32,35	0.84	0
9	OMG	I	3745	9	18,26,27	2.71	8 (44%)	19,38,41	1.49	4 (21%)
9	3TD	I	3409	9	18,22,23	4.06	6 (33%)	22,32,35	1.58	2 (9%)
9	6MZ	I	3524	9	18,25,26	1.87	3 (16%)	16,36,39	2.32	3 (18%)
9	OMU	I	4046	9	19,22,23	2.82	6 (31%)	26,31,34	1.72	4 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	PSU	I	3951	9	18,21,22	4.17	8 (44%)	22,30,33	2.36	6 (27%)
9	5MU	I	2247	9	19,22,23	4.59	6 (31%)	28,32,35	3.80	10 (35%)
9	2MA	I	3997	9	17,25,26	2.55	5 (29%)	17,37,40	1.27	2 (11%)
9	PSU	I	3411	9	18,21,22	4.44	8 (44%)	22,30,33	1.79	6 (27%)
9	2MG	I	3329	9	18,26,27	2.56	7 (38%)	16,38,41	1.42	3 (18%)
9	1MG	I	2245	9	18,26,27	2.49	5 (27%)	19,39,42	1.32	2 (10%)
9	5MU	I	3433	9	19,22,23	4.55	6 (31%)	28,32,35	3.86	10 (35%)
9	PSU	I	3998	9	18,21,22	4.34	9 (50%)	22,30,33	2.03	5 (22%)
9	5MC	I	3456	9	18,22,23	3.65	8 (44%)	26,32,35	1.14	1 (3%)
9	5MC	I	1406	9	18,22,23	3.74	8 (44%)	26,32,35	1.01	1 (3%)
9	2MG	I	3939	9	18,26,27	2.43	7 (38%)	16,38,41	1.63	4 (25%)
9	2MG	I	4420	9	18,26,27	2.61	7 (38%)	16,38,41	1.41	3 (18%)
9	MA6	I	4422	9	19,26,27	1.03	2 (10%)	18,38,41	5.68	3 (16%)
31	D2T	g	88	31	7,9,10	1.10	0	6,11,13	2.39	2 (33%)
9	PSU	I	2449	9	18,21,22	4.20	8 (44%)	22,30,33	2.06	5 (22%)
19	4D4	U	81	19	9,11,12	2.62	3 (33%)	8,13,15	0.76	0
9	PSU	I	3405	9	18,21,22	4.41	8 (44%)	22,30,33	1.97	5 (22%)
9	PSU	I	4099	9	18,21,22	4.23	9 (50%)	22,30,33	1.92	6 (27%)
9	G7M	I	3563	9	20,26,27	2.61	7 (35%)	17,39,42	1.12	1 (5%)
9	PSU	I	4074	9	18,21,22	4.22	9 (50%)	22,30,33	2.02	5 (22%)
9	G7M	I	526	9	20,26,27	2.77	8 (40%)	17,39,42	1.07	1 (5%)
9	MA6	I	4423	9	19,26,27	1.01	2 (10%)	18,38,41	5.72	3 (16%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	UR3	I	4402	9	-	4/7/25/26	0/2/2/2
9	6MZ	I	3112	9	-	4/5/27/28	0/3/3/3
9	5MC	I	966	9	-	1/7/25/26	0/2/2/2
9	2MG	I	965	9	-	2/5/27/28	0/3/3/3
9	PSU	I	515	9	-	0/7/25/26	0/2/2/2
9	OMC	I	3992	9	-	4/9/27/28	0/2/2/2
9	PSU	I	2246	9	-	2/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	2MG	I	1206	9	-	1/5/27/28	0/3/3/3
9	4OC	I	1401	9	-	1/9/29/30	0/2/2/2
9	OMG	I	3745	9	-	0/5/27/28	0/3/3/3
9	3TD	I	3409	9	-	1/7/25/26	0/2/2/2
9	6MZ	I	3524	9	-	3/5/27/28	0/3/3/3
9	OMU	I	4046	9	-	4/9/27/28	0/2/2/2
9	PSU	I	3951	9	-	2/7/25/26	0/2/2/2
9	5MU	I	2247	9	-	2/7/25/26	0/2/2/2
9	2MA	I	3997	9	-	2/3/25/26	0/3/3/3
9	PSU	I	3411	9	-	1/7/25/26	0/2/2/2
9	2MG	I	3329	9	-	1/5/27/28	0/3/3/3
9	1MG	I	2245	9	-	2/3/25/26	0/3/3/3
9	5MU	I	3433	9	-	1/7/25/26	0/2/2/2
9	PSU	I	3998	9	-	2/7/25/26	0/2/2/2
9	5MC	I	3456	9	-	4/7/25/26	0/2/2/2
9	5MC	I	1406	9	-	4/7/25/26	0/2/2/2
9	2MG	I	3939	9	-	2/5/27/28	0/3/3/3
9	2MG	I	4420	9	-	2/5/27/28	0/3/3/3
9	MA6	I	4422	9	-	4/7/29/30	0/3/3/3
31	D2T	g	88	31	-	3/7/12/14	-
9	PSU	I	2449	9	-	2/7/25/26	0/2/2/2
19	4D4	U	81	19	-	3/11/12/14	-
9	PSU	I	3405	9	-	0/7/25/26	0/2/2/2
9	PSU	I	4099	9	-	5/7/25/26	0/2/2/2
9	G7M	I	3563	9	-	2/3/25/26	0/3/3/3
9	PSU	I	4074	9	-	3/7/25/26	0/2/2/2
9	G7M	I	526	9	-	3/3/25/26	0/3/3/3
9	MA6	I	4423	9	-	1/7/29/30	0/3/3/3

All (226) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	I	3409	3TD	C6-C5	11.90	1.49	1.35
9	I	3411	PSU	C6-C5	11.68	1.48	1.35
9	I	2246	PSU	C6-C5	11.59	1.48	1.35
9	I	515	PSU	C6-C5	11.36	1.48	1.35
9	I	3405	PSU	C6-C5	11.36	1.48	1.35
9	I	3998	PSU	C6-C5	11.00	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	I	4074	PSU	C6-C5	10.84	1.47	1.35
9	I	3951	PSU	C6-C5	10.63	1.47	1.35
9	I	4099	PSU	C6-C5	10.63	1.47	1.35
9	I	2449	PSU	C6-C5	10.61	1.47	1.35
9	I	2247	5MU	C6-N1	10.33	1.55	1.38
9	I	2247	5MU	C2-N1	10.24	1.54	1.38
9	I	3433	5MU	C6-N1	10.12	1.55	1.38
9	I	3433	5MU	C2-N1	9.97	1.54	1.38
9	I	966	5MC	C6-C5	9.79	1.50	1.34
9	I	2246	PSU	C2-N1	9.70	1.49	1.36
9	I	3405	PSU	C2-N1	9.64	1.49	1.36
9	I	3411	PSU	C2-N1	9.54	1.49	1.36
9	I	3998	PSU	C2-N1	9.51	1.49	1.36
9	I	515	PSU	C2-N1	9.49	1.49	1.36
9	I	2449	PSU	C2-N1	9.39	1.49	1.36
9	I	1406	5MC	C6-C5	9.34	1.49	1.34
9	I	4099	PSU	C2-N1	9.26	1.49	1.36
9	I	3456	5MC	C6-C5	9.19	1.49	1.34
9	I	3951	PSU	C2-N1	9.15	1.49	1.36
9	I	3433	5MU	C4-C5	9.13	1.59	1.44
9	I	4074	PSU	C2-N1	9.01	1.48	1.36
9	I	2247	5MU	C4-C5	8.97	1.59	1.44
9	I	3409	3TD	C2-N1	8.89	1.48	1.37
9	I	3997	2MA	C2-N3	8.13	1.48	1.31
9	I	2246	PSU	C2-N3	7.80	1.50	1.37
9	I	515	PSU	C2-N3	7.77	1.50	1.37
9	I	3405	PSU	C2-N3	7.69	1.50	1.37
9	I	3998	PSU	C2-N3	7.68	1.50	1.37
9	I	3433	5MU	C4-N3	-7.61	1.24	1.38
9	I	3411	PSU	C2-N3	7.56	1.50	1.37
9	I	2247	5MU	C4-N3	-7.55	1.24	1.38
9	I	966	5MC	C4-N3	7.41	1.46	1.34
9	I	4099	PSU	C2-N3	7.35	1.50	1.37
9	I	2449	PSU	C2-N3	7.35	1.50	1.37
9	I	4074	PSU	C2-N3	7.34	1.50	1.37
9	I	4402	UR3	C2-N1	7.33	1.49	1.38
9	I	3951	PSU	C2-N3	7.27	1.50	1.37
9	I	1406	5MC	C4-N3	7.21	1.46	1.34
9	I	1401	4OC	C4-N3	7.09	1.45	1.32
9	I	3456	5MC	C4-N3	7.07	1.46	1.34
9	I	3112	6MZ	C6-N6	6.91	1.46	1.35
9	I	4046	OMU	C2-N1	6.61	1.49	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	I	966	5MC	C2-N3	6.58	1.49	1.36
9	I	3992	OMC	C6-C5	6.48	1.50	1.35
9	I	526	G7M	C2-N2	6.45	1.49	1.34
9	I	3524	6MZ	C6-N6	6.39	1.45	1.35
9	I	2247	5MU	C6-C5	6.39	1.45	1.34
19	U	81	4D4	CZ-NE	6.34	1.45	1.33
9	I	4046	OMU	C2-N3	6.31	1.49	1.38
9	I	3992	OMC	C2-N3	6.31	1.49	1.36
9	I	1406	5MC	C2-N3	6.30	1.49	1.36
9	I	3456	5MC	C2-N3	6.30	1.49	1.36
9	I	3433	5MU	C6-C5	6.26	1.44	1.34
9	I	4402	UR3	C6-C5	6.22	1.49	1.35
9	I	1401	4OC	C6-C5	6.19	1.49	1.35
9	I	3563	G7M	C2-N2	6.12	1.48	1.34
9	I	1401	4OC	C2-N3	6.11	1.48	1.36
9	I	1206	2MG	C2-N2	5.96	1.46	1.33
9	I	965	2MG	C2-N2	5.96	1.46	1.33
9	I	3992	OMC	C4-N4	5.95	1.48	1.33
9	I	3409	3TD	C6-N1	5.94	1.46	1.36
9	I	4420	2MG	C2-N2	5.92	1.46	1.33
9	I	3992	OMC	C4-N3	5.91	1.46	1.34
9	I	2245	1MG	C2-N2	5.88	1.44	1.34
9	I	3329	2MG	C2-N2	5.81	1.46	1.33
9	I	3405	PSU	C6-N1	5.73	1.45	1.36
9	I	3411	PSU	C6-N1	5.71	1.45	1.36
9	I	2245	1MG	C2-N3	5.70	1.44	1.34
9	I	3563	G7M	C2-N3	5.69	1.47	1.33
9	I	4046	OMU	C6-C5	5.67	1.48	1.35
9	I	526	G7M	C2-N3	5.67	1.47	1.33
9	I	966	5MC	C6-N1	5.58	1.47	1.38
9	I	3998	PSU	C6-N1	5.56	1.45	1.36
9	I	4099	PSU	C6-N1	5.51	1.45	1.36
9	I	3745	OMG	C4-N3	5.50	1.50	1.37
9	I	515	PSU	C6-N1	5.44	1.45	1.36
9	I	3939	2MG	C2-N2	5.41	1.45	1.33
9	I	965	2MG	C2-N1	5.40	1.45	1.36
9	I	3745	OMG	C2-N3	5.36	1.46	1.33
9	I	4074	PSU	C6-N1	5.33	1.45	1.36
9	I	2246	PSU	C6-N1	5.32	1.45	1.36
9	I	1206	2MG	C2-N1	5.26	1.45	1.36
9	I	4402	UR3	C2-N3	5.22	1.49	1.39
9	I	3951	PSU	C6-N1	5.22	1.44	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	I	1206	2MG	C4-N3	5.22	1.50	1.37
9	I	2449	PSU	C6-N1	5.19	1.44	1.36
9	I	1406	5MC	C6-N1	5.18	1.46	1.38
9	I	4420	2MG	C4-N3	5.16	1.49	1.37
9	I	965	2MG	C4-N3	5.11	1.49	1.37
9	I	526	G7M	C4-N3	5.06	1.49	1.37
9	I	3745	OMG	C2-N2	5.03	1.46	1.34
9	I	3329	2MG	C2-N1	4.99	1.44	1.36
9	I	4420	2MG	C2-N1	4.98	1.44	1.36
9	I	3329	2MG	C4-N3	4.86	1.49	1.37
9	I	3992	OMC	C2-N1	4.83	1.50	1.40
9	I	3456	5MC	C6-N1	4.76	1.46	1.38
9	I	3563	G7M	C4-N3	4.75	1.48	1.37
9	I	3939	2MG	C2-N1	4.66	1.44	1.36
9	I	3939	2MG	C4-N3	4.55	1.48	1.37
9	I	1401	4OC	C4-N4	4.53	1.45	1.35
9	I	2245	1MG	C4-N3	4.47	1.48	1.37
9	I	3409	3TD	C2-N3	4.45	1.48	1.38
9	I	526	G7M	C6-N1	4.40	1.44	1.37
9	I	966	5MC	C2-N1	4.34	1.49	1.40
9	I	966	5MC	C4-N4	4.22	1.45	1.34
9	I	3997	2MA	C4-N3	4.21	1.47	1.37
9	I	1406	5MC	C4-N4	4.14	1.44	1.34
9	I	1401	4OC	C2-N1	4.13	1.48	1.40
9	I	1406	5MC	C2-N1	4.11	1.48	1.40
9	I	515	PSU	C4-N3	4.10	1.46	1.38
9	I	3456	5MC	C4-N4	4.07	1.44	1.34
9	I	3405	PSU	C4-N3	3.84	1.46	1.38
9	I	3998	PSU	C4-N3	3.84	1.46	1.38
9	I	965	2MG	C6-N1	3.83	1.43	1.37
9	I	1401	4OC	C5-C4	3.83	1.49	1.40
9	I	3563	G7M	C6-N1	3.82	1.43	1.37
9	I	4099	PSU	C4-N3	3.78	1.45	1.38
9	I	3992	OMC	C6-N1	3.77	1.47	1.38
9	I	3456	5MC	C2-N1	3.77	1.48	1.40
9	I	3411	PSU	C4-N3	3.77	1.45	1.38
9	I	1206	2MG	C6-N1	3.74	1.43	1.37
9	I	4420	2MG	C6-N1	3.73	1.43	1.37
9	I	2449	PSU	C4-N3	3.66	1.45	1.38
9	I	4074	PSU	C4-N3	3.64	1.45	1.38
9	I	2246	PSU	C4-N3	3.58	1.45	1.38
9	I	3951	PSU	C4-N3	3.42	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	I	3745	OMG	C5-C6	3.40	1.54	1.47
9	I	1206	2MG	C5-C6	3.40	1.54	1.47
9	I	965	2MG	C5-C6	3.37	1.54	1.47
9	I	4046	OMU	C4-N3	3.36	1.44	1.38
9	I	3745	OMG	C5-C4	-3.35	1.34	1.43
9	I	526	G7M	C5-C6	3.34	1.54	1.45
9	I	3745	OMG	C6-N1	3.34	1.42	1.37
19	U	81	4D4	CZ-NH2	3.32	1.45	1.32
9	I	3939	2MG	C6-N1	3.31	1.42	1.37
9	I	3992	OMC	O2-C2	-3.29	1.17	1.23
9	I	3329	2MG	C6-N1	3.28	1.42	1.37
9	I	1401	4OC	C6-N1	3.14	1.45	1.38
9	I	4420	2MG	C5-C6	3.13	1.53	1.47
9	I	526	G7M	C2-N1	3.08	1.45	1.37
9	I	3939	2MG	C5-C4	-3.05	1.35	1.43
9	I	4402	UR3	C6-N1	3.05	1.45	1.38
9	I	3329	2MG	C5-C6	3.03	1.53	1.47
9	I	3563	G7M	C5-C6	3.01	1.53	1.45
9	I	3524	6MZ	C5-C4	-2.94	1.33	1.40
9	I	2245	1MG	C5-C4	-2.93	1.35	1.43
9	I	3409	3TD	C4-N3	2.87	1.46	1.40
9	I	3329	2MG	C5-C4	-2.83	1.35	1.43
9	I	3951	PSU	O4'-C1'	-2.80	1.40	1.43
9	I	4423	MA6	C5-C4	-2.79	1.33	1.40
9	I	3992	OMC	C5-C4	2.74	1.49	1.42
9	I	4422	MA6	C5-C4	-2.73	1.33	1.40
9	I	4046	OMU	O4-C4	-2.72	1.19	1.24
9	I	4046	OMU	O2-C2	-2.70	1.18	1.23
9	I	3112	6MZ	C5-C4	-2.70	1.33	1.40
9	I	3997	2MA	C2-N1	2.69	1.44	1.36
9	I	3563	G7M	C2-N1	2.64	1.44	1.37
9	I	3745	OMG	O6-C6	-2.63	1.18	1.23
9	I	4420	2MG	C5-C4	-2.63	1.36	1.43
9	I	1401	4OC	O2-C2	-2.62	1.18	1.23
9	I	3411	PSU	C1'-C5	2.56	1.56	1.50
9	I	3939	2MG	C5-C6	2.54	1.52	1.47
9	I	3563	G7M	O6-C6	-2.53	1.18	1.23
9	I	515	PSU	C1'-C5	2.52	1.56	1.50
9	I	3456	5MC	O2-C2	-2.51	1.19	1.23
9	I	3997	2MA	C6-N1	2.48	1.43	1.38
9	I	965	2MG	C5-C4	-2.44	1.36	1.43
9	I	4099	PSU	O4-C4	-2.43	1.19	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	I	2246	PSU	O4'-C1'	-2.43	1.40	1.43
9	I	4074	PSU	O2-C2	-2.42	1.18	1.23
9	I	2245	1MG	O6-C6	-2.39	1.17	1.22
9	I	3951	PSU	O2-C2	-2.39	1.18	1.23
9	I	4074	PSU	O4-C4	-2.39	1.19	1.23
9	I	4099	PSU	O2-C2	-2.37	1.18	1.23
9	I	3951	PSU	O4-C4	-2.35	1.19	1.23
9	I	4099	PSU	C1'-C5	2.35	1.55	1.50
9	I	3745	OMG	C2-N1	2.34	1.43	1.37
9	I	2449	PSU	O2-C2	-2.34	1.18	1.23
9	I	3939	2MG	O6-C6	-2.34	1.18	1.23
9	I	2246	PSU	O2-C2	-2.31	1.18	1.23
9	I	2449	PSU	O4-C4	-2.30	1.19	1.23
9	I	3405	PSU	O4-C4	-2.29	1.19	1.23
9	I	1206	2MG	C5-C4	-2.28	1.37	1.43
9	I	4402	UR3	C5-C4	2.25	1.49	1.43
9	I	1406	5MC	CM5-C5	2.24	1.56	1.50
9	I	3112	6MZ	C2-N3	2.21	1.35	1.32
9	I	3998	PSU	C1'-C5	2.21	1.55	1.50
9	I	4402	UR3	O4-C4	-2.20	1.18	1.23
9	I	4422	MA6	C2-N3	2.20	1.35	1.32
9	I	3998	PSU	O4'-C1'	-2.20	1.40	1.43
19	U	81	4D4	CZ-NH1	-2.20	1.25	1.34
9	I	966	5MC	CM5-C5	2.20	1.56	1.50
9	I	3998	PSU	O4-C4	-2.20	1.19	1.23
9	I	1406	5MC	O2-C2	-2.19	1.19	1.23
9	I	3997	2MA	C5-C4	-2.18	1.37	1.43
9	I	3411	PSU	O4-C4	-2.17	1.19	1.23
9	I	515	PSU	O2-C2	-2.17	1.18	1.23
9	I	3524	6MZ	C2-N3	2.16	1.35	1.32
9	I	526	G7M	O6-C6	-2.16	1.18	1.23
9	I	966	5MC	O2-C2	-2.14	1.19	1.23
9	I	4402	UR3	O2-C2	-2.14	1.18	1.22
9	I	3456	5MC	CM5-C5	2.13	1.56	1.50
9	I	515	PSU	O4-C4	-2.13	1.19	1.23
9	I	3433	5MU	O2-C2	-2.13	1.19	1.23
9	I	3998	PSU	O2-C2	-2.13	1.18	1.23
9	I	3409	3TD	O4-C4	-2.13	1.18	1.23
9	I	3329	2MG	O6-C6	-2.12	1.19	1.23
9	I	4074	PSU	O4'-C1'	-2.11	1.40	1.43
9	I	3405	PSU	C1'-C5	2.11	1.55	1.50
9	I	526	G7M	C8-N7	2.10	1.37	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	I	4423	MA6	C2-N3	2.10	1.35	1.32
9	I	2247	5MU	O2-C2	-2.10	1.19	1.23
9	I	4074	PSU	C1'-C5	2.10	1.55	1.50
9	I	4402	UR3	C4-N3	2.10	1.45	1.40
9	I	3405	PSU	O2-C2	-2.07	1.19	1.23
9	I	4099	PSU	O4'-C1'	-2.07	1.41	1.43
9	I	2246	PSU	C1'-C5	2.06	1.54	1.50
9	I	3411	PSU	O2-C2	-2.04	1.19	1.23
9	I	4420	2MG	O6-C6	-2.02	1.19	1.23
9	I	2449	PSU	C1'-C5	2.01	1.54	1.50

All (122) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	I	4422	MA6	N1-C6-N6	-20.72	95.25	117.06
9	I	4423	MA6	N1-C6-N6	-20.62	95.36	117.06
9	I	3433	5MU	C5-C4-N3	12.58	126.05	115.31
9	I	2247	5MU	C5-C4-N3	12.36	125.86	115.31
9	I	3433	5MU	C5-C6-N1	-11.53	111.48	123.34
9	I	4423	MA6	C1'-N9-C4	-11.29	106.80	126.64
9	I	2247	5MU	C5-C6-N1	-10.98	112.04	123.34
9	I	4422	MA6	C1'-N9-C4	-10.86	107.56	126.64
9	I	3524	6MZ	C9-N6-C6	-5.97	117.73	122.87
9	I	3524	6MZ	N3-C2-N1	-5.64	119.86	128.68
9	I	3951	PSU	C6-C5-C4	5.62	122.13	118.20
9	I	4423	MA6	N3-C2-N1	-5.52	120.05	128.68
9	I	2246	PSU	N1-C2-N3	5.45	121.31	115.13
9	I	4046	OMU	C4-N3-C2	-5.43	119.42	126.58
9	I	2246	PSU	C6-C5-C4	5.42	121.99	118.20
9	I	4422	MA6	N3-C2-N1	-5.41	120.22	128.68
9	I	2246	PSU	C4-N3-C2	-5.36	118.61	126.34
9	I	3112	6MZ	N3-C2-N1	-5.34	120.34	128.68
9	I	2247	5MU	C4-N3-C2	-5.29	120.51	127.35
9	I	3951	PSU	C4-N3-C2	-5.27	118.75	126.34
9	I	3433	5MU	C4-N3-C2	-5.26	120.54	127.35
9	I	3951	PSU	N1-C2-N3	5.17	120.99	115.13
9	I	4099	PSU	C4-N3-C2	-5.10	118.98	126.34
9	I	3409	3TD	N1-C2-N3	4.98	120.07	116.14
9	I	4074	PSU	C4-N3-C2	-4.88	119.30	126.34
9	I	3998	PSU	C4-N3-C2	-4.88	119.31	126.34
9	I	2247	5MU	O4-C4-C5	-4.86	119.26	124.90
9	I	2449	PSU	C4-N3-C2	-4.77	119.47	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	I	515	PSU	C4-N3-C2	-4.73	119.53	126.34
9	I	4074	PSU	N1-C2-N3	4.67	120.42	115.13
9	I	2449	PSU	N1-C2-N3	4.66	120.41	115.13
9	I	3405	PSU	C4-N3-C2	-4.64	119.65	126.34
9	I	3433	5MU	O4-C4-C5	-4.62	119.55	124.90
9	I	2449	PSU	C6-C5-C4	4.60	121.42	118.20
9	I	4402	UR3	C4-N3-C2	-4.59	120.24	124.56
9	I	515	PSU	N1-C2-N3	4.57	120.31	115.13
9	I	3998	PSU	N1-C2-N3	4.55	120.29	115.13
9	I	2247	5MU	N3-C2-N1	4.53	120.90	114.89
9	I	3456	5MC	C5-C6-N1	-4.30	118.92	123.34
9	I	3433	5MU	C5M-C5-C6	-4.27	117.14	122.85
9	I	3405	PSU	N1-C2-N3	4.24	119.93	115.13
9	I	2247	5MU	C5M-C5-C6	-4.21	117.23	122.85
9	I	4099	PSU	N1-C2-N3	4.21	119.90	115.13
9	I	3411	PSU	C4-N3-C2	-4.14	120.37	126.34
31	g	88	D2T	CB1-SB-CB	4.12	109.90	102.44
9	I	3433	5MU	N3-C2-N1	4.11	120.34	114.89
9	I	3405	PSU	C6-C5-C4	4.08	121.05	118.20
9	I	3411	PSU	N1-C2-N3	4.05	119.72	115.13
9	I	3939	2MG	C5-C6-N1	4.02	121.05	113.95
9	I	3998	PSU	C6-C5-C4	4.02	121.01	118.20
9	I	3409	3TD	C4-N3-C2	-3.97	120.30	124.61
9	I	3112	6MZ	C9-N6-C6	-3.95	119.47	122.87
9	I	3563	G7M	C2-N1-C6	-3.94	117.85	125.10
9	I	2245	1MG	C5-C6-N1	3.90	119.76	113.90
9	I	3433	5MU	C5M-C5-C4	3.82	122.97	118.77
9	I	4046	OMU	C5-C4-N3	3.73	120.42	114.84
9	I	4420	2MG	C5-C6-N1	3.69	120.46	113.95
9	I	3329	2MG	C5-C6-N1	3.65	120.40	113.95
9	I	2247	5MU	C5M-C5-C4	3.65	122.78	118.77
9	I	3112	6MZ	C2-N1-C6	3.64	119.71	116.59
9	I	515	PSU	C6-C5-C4	3.49	120.64	118.20
9	I	966	5MC	C5-C6-N1	-3.48	119.76	123.34
9	I	1206	2MG	C5-C6-N1	3.47	120.08	113.95
9	I	4074	PSU	C6-C5-C4	3.46	120.62	118.20
9	I	3745	OMG	C5-C6-N1	3.46	120.06	113.95
9	I	3524	6MZ	C2-N1-C6	3.42	119.52	116.59
9	I	965	2MG	C5-C6-N1	3.39	119.93	113.95
9	I	4046	OMU	N3-C2-N1	3.37	119.36	114.89
9	I	3997	2MA	C5-C6-N1	3.27	119.66	114.02
9	I	1406	5MC	C5-C6-N1	-3.26	119.98	123.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	I	3745	OMG	C2-N1-C6	-3.26	119.10	125.10
31	g	88	D2T	OD2-CG-CB	3.20	120.07	113.15
9	I	3411	PSU	C6-N1-C2	-3.20	119.41	122.68
9	I	3939	2MG	O6-C6-C5	-3.16	118.21	124.37
9	I	2449	PSU	C6-N1-C2	-3.15	119.47	122.68
9	I	3998	PSU	C6-N1-C2	-3.12	119.49	122.68
9	I	3951	PSU	C6-N1-C2	-3.09	119.52	122.68
9	I	515	PSU	O2-C2-N1	-3.09	119.39	122.79
9	I	2246	PSU	C6-N1-C2	-3.08	119.53	122.68
9	I	515	PSU	C6-N1-C2	-3.08	119.54	122.68
9	I	4074	PSU	C6-N1-C2	-3.03	119.59	122.68
9	I	526	G7M	C2-N1-C6	-2.99	119.59	125.10
9	I	3433	5MU	O4-C4-N3	-2.98	114.40	120.12
9	I	3433	5MU	O2-C2-N1	-2.97	118.83	122.79
9	I	4046	OMU	O4-C4-C5	-2.92	120.02	125.16
9	I	3329	2MG	C8-N7-C5	2.90	108.51	102.99
9	I	3405	PSU	C6-N1-C2	-2.85	119.77	122.68
9	I	4074	PSU	O2-C2-N1	-2.84	119.66	122.79
9	I	3411	PSU	C6-C5-C4	2.84	120.19	118.20
9	I	965	2MG	C8-N7-C5	2.81	108.34	102.99
9	I	2246	PSU	O2-C2-N1	-2.77	119.74	122.79
9	I	4420	2MG	C8-N7-C5	2.76	108.25	102.99
9	I	2247	5MU	O4-C4-N3	-2.73	114.88	120.12
9	I	4099	PSU	C6-C5-C4	2.73	120.11	118.20
9	I	1206	2MG	C8-N7-C5	2.73	108.19	102.99
9	I	3745	OMG	C8-N7-C5	2.73	108.19	102.99
9	I	4402	UR3	C6-N1-C2	-2.71	119.36	121.79
9	I	2247	5MU	O2-C2-N1	-2.67	119.23	122.79
9	I	3997	2MA	C8-N7-C5	2.63	107.99	102.99
9	I	2245	1MG	O6-C6-C5	-2.62	119.55	124.19
9	I	3951	PSU	O2-C2-N1	-2.59	119.94	122.79
9	I	4099	PSU	C6-N1-C2	-2.58	120.05	122.68
9	I	3939	2MG	CM2-N2-C2	-2.49	118.35	123.86
9	I	4420	2MG	O6-C6-C5	-2.48	119.54	124.37
9	I	3939	2MG	C8-N7-C5	2.38	107.53	102.99
9	I	515	PSU	O4'-C1'-C2'	2.36	108.47	105.14
9	I	2247	5MU	C6-C5-C4	2.35	120.00	118.03
9	I	3329	2MG	O6-C6-C5	-2.34	119.81	124.37
9	I	4099	PSU	O2-C2-N1	-2.33	120.23	122.79
9	I	3998	PSU	O2-C2-N1	-2.32	120.23	122.79
9	I	3411	PSU	O4'-C1'-C2'	2.31	108.40	105.14
9	I	1206	2MG	O6-C6-C5	-2.30	119.89	124.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	I	3405	PSU	O2-C2-N1	-2.29	120.27	122.79
9	I	3433	5MU	C6-C5-C4	2.22	119.89	118.03
9	I	965	2MG	O6-C6-C5	-2.19	120.09	124.37
9	I	2449	PSU	O2-C2-N1	-2.11	120.46	122.79
9	I	3745	OMG	O6-C6-C5	-2.10	120.27	124.37
9	I	4402	UR3	C1'-N1-C2	2.09	120.52	116.99
9	I	3951	PSU	C5-C6-N1	-2.03	119.06	122.11
9	I	3411	PSU	O2-C2-N1	-2.03	120.56	122.79
9	I	2246	PSU	C5-C6-N1	-2.02	119.07	122.11
9	I	4099	PSU	O4'-C1'-C2'	2.02	107.99	105.14

There are no chirality outliers.

All (78) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
19	U	81	4D4	O-C-CA-CB
19	U	81	4D4	N-CA-CB-CG
19	U	81	4D4	NE-CD-CG-CB
31	g	88	D2T	CA-CB-SB-CB1
31	g	88	D2T	CG-CB-SB-CB1
9	I	1401	4OC	C1'-C2'-O2'-CM2
9	I	1406	5MC	O4'-C4'-C5'-O5'
9	I	2247	5MU	C3'-C4'-C5'-O5'
9	I	3112	6MZ	C5-C6-N6-C9
9	I	3112	6MZ	N1-C6-N6-C9
9	I	3112	6MZ	C3'-C4'-C5'-O5'
9	I	3524	6MZ	O4'-C4'-C5'-O5'
9	I	3524	6MZ	C3'-C4'-C5'-O5'
9	I	3939	2MG	C3'-C4'-C5'-O5'
9	I	3998	PSU	C3'-C4'-C5'-O5'
9	I	3998	PSU	O4'-C4'-C5'-O5'
9	I	4046	OMU	O4'-C4'-C5'-O5'
9	I	4074	PSU	C2'-C1'-C5-C4
9	I	4099	PSU	C2'-C1'-C5-C4
9	I	4099	PSU	C2'-C1'-C5-C6
9	I	4099	PSU	C3'-C4'-C5'-O5'
9	I	1406	5MC	C3'-C4'-C5'-O5'
9	I	2246	PSU	O4'-C4'-C5'-O5'
9	I	3939	2MG	O4'-C4'-C5'-O5'
9	I	3951	PSU	O4'-C4'-C5'-O5'
9	I	4046	OMU	C3'-C4'-C5'-O5'
9	I	4099	PSU	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
9	I	2246	PSU	C3'-C4'-C5'-O5'
9	I	3112	6MZ	O4'-C4'-C5'-O5'
9	I	3951	PSU	C3'-C4'-C5'-O5'
9	I	3997	2MA	O4'-C4'-C5'-O5'
9	I	4402	UR3	C2'-C1'-N1-C6
9	I	2247	5MU	O4'-C4'-C5'-O5'
9	I	3456	5MC	O4'-C4'-C5'-O5'
9	I	4402	UR3	C2'-C1'-N1-C2
9	I	3992	OMC	C2'-C1'-N1-C2
9	I	965	2MG	O4'-C4'-C5'-O5'
9	I	3456	5MC	C3'-C4'-C5'-O5'
9	I	3524	6MZ	N1-C6-N6-C9
9	I	4422	MA6	C5-C6-N6-C10
9	I	526	G7M	C3'-C4'-C5'-O5'
9	I	2449	PSU	O4'-C4'-C5'-O5'
9	I	3992	OMC	C2'-C1'-N1-C6
9	I	965	2MG	C3'-C4'-C5'-O5'
9	I	4402	UR3	O4'-C1'-N1-C6
9	I	3992	OMC	C4'-C5'-O5'-P
9	I	4402	UR3	O4'-C1'-N1-C2
9	I	526	G7M	C4'-C5'-O5'-P
9	I	2245	1MG	O4'-C4'-C5'-O5'
9	I	4422	MA6	C5-C6-N6-C9
9	I	526	G7M	O4'-C4'-C5'-O5'
9	I	4420	2MG	O4'-C4'-C5'-O5'
9	I	1406	5MC	C2'-C1'-N1-C2
9	I	3563	G7M	C4'-C5'-O5'-P
9	I	4099	PSU	C4'-C5'-O5'-P
9	I	4423	MA6	C4'-C5'-O5'-P
9	I	1406	5MC	C2'-C1'-N1-C6
9	I	966	5MC	C4'-C5'-O5'-P
9	I	3409	3TD	O4'-C1'-C5-C4
9	I	3411	PSU	O4'-C1'-C5-C4
9	I	4074	PSU	O4'-C1'-C5-C4
9	I	4046	OMU	C2'-C1'-N1-C2
9	I	4046	OMU	C2'-C1'-N1-C6
9	I	3329	2MG	O4'-C4'-C5'-O5'
9	I	3997	2MA	C3'-C4'-C5'-O5'
9	I	3456	5MC	C2'-C1'-N1-C6
9	I	1206	2MG	O4'-C4'-C5'-O5'
9	I	2449	PSU	C3'-C4'-C5'-O5'
31	g	88	D2T	SB-CB-CG-OD2

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Mol	Chain	Res	Type	Atoms
9	I	3456	5MC	O4'-C1'-N1-C6
9	I	2245	1MG	C3'-C4'-C5'-O5'
9	I	4422	MA6	O4'-C4'-C5'-O5'
9	I	4074	PSU	O4'-C1'-C5-C6
9	I	3433	5MU	C2'-C1'-N1-C2
9	I	3563	G7M	O4'-C4'-C5'-O5'
9	I	3992	OMC	O4'-C4'-C5'-O5'
9	I	4420	2MG	C3'-C4'-C5'-O5'
9	I	4422	MA6	C3'-C4'-C5'-O5'

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](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
9	I	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	I	1500:U	O3'	1501:G	P	17.28
1	I	2385:C	O3'	2386:A	P	15.64

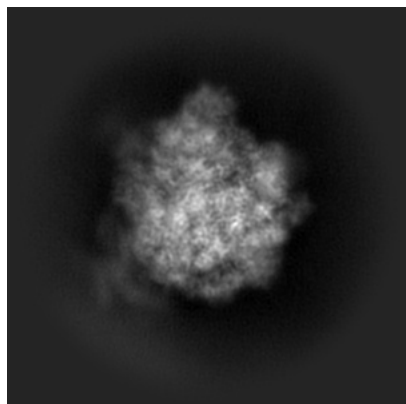
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-26666. These allow visual inspection of the internal detail of the map and identification of artifacts.

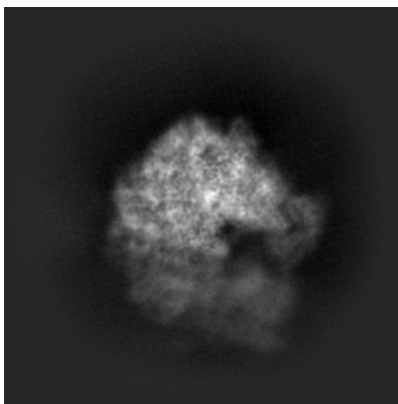
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

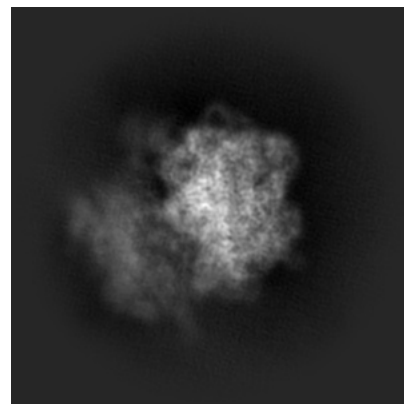
6.1.1 Primary map



X

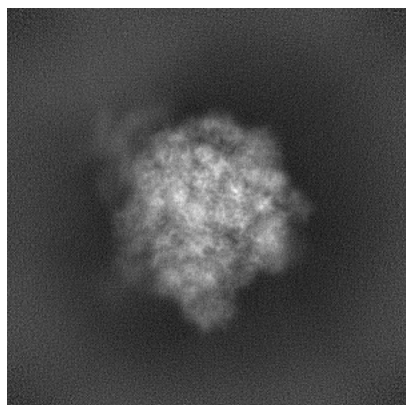


Y

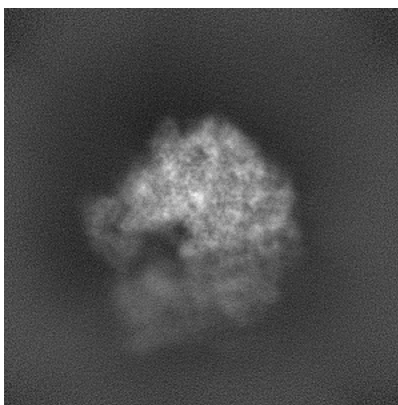


Z

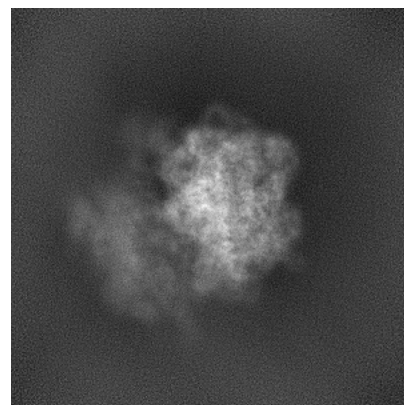
6.1.2 Raw map



X



Y

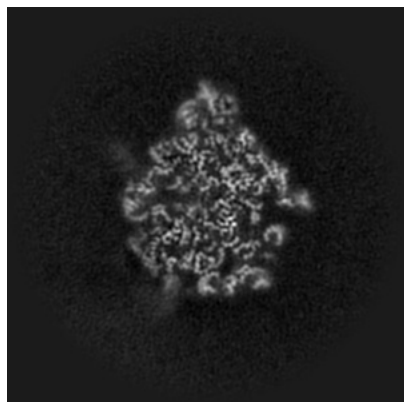


Z

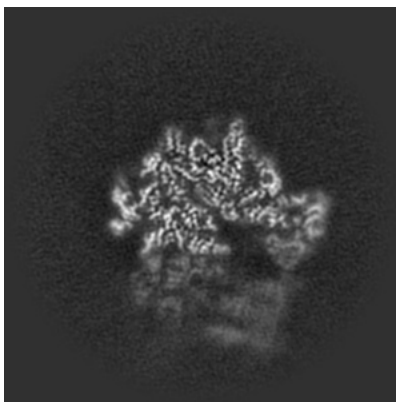
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

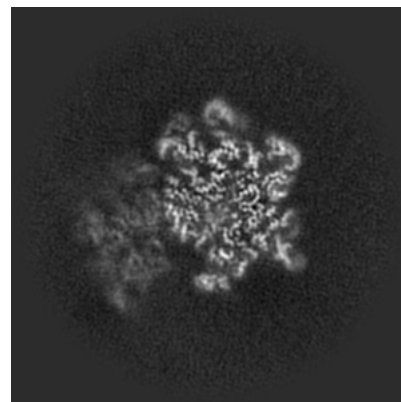
6.2.1 Primary map



X Index: 250

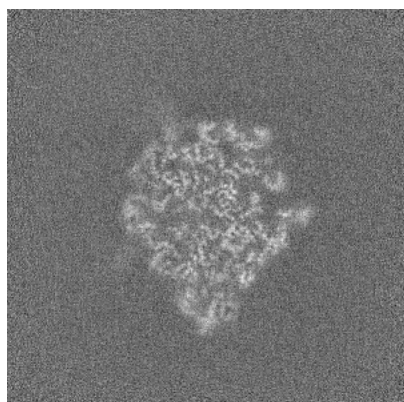


Y Index: 250

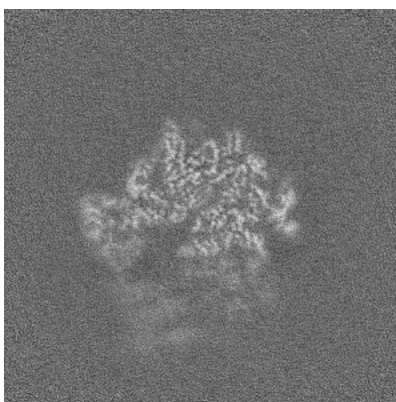


Z Index: 250

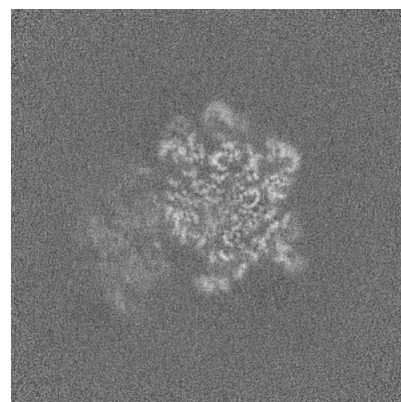
6.2.2 Raw map



X Index: 250



Y Index: 250

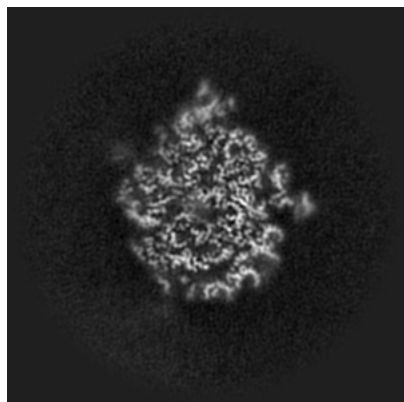


Z Index: 250

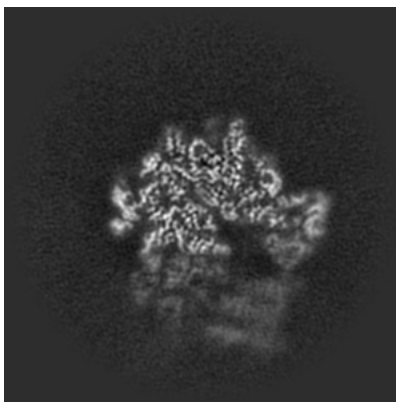
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

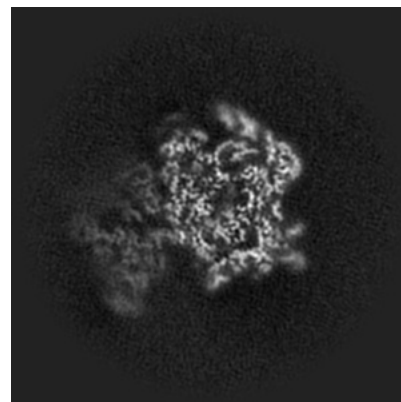
6.3.1 Primary map



X Index: 259

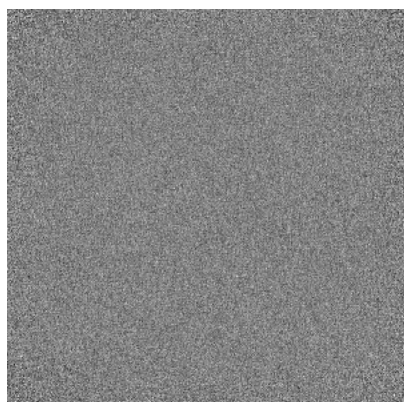


Y Index: 249

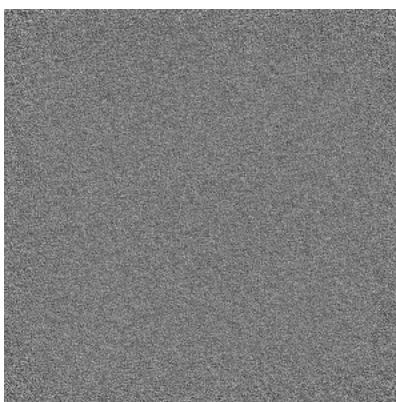


Z Index: 239

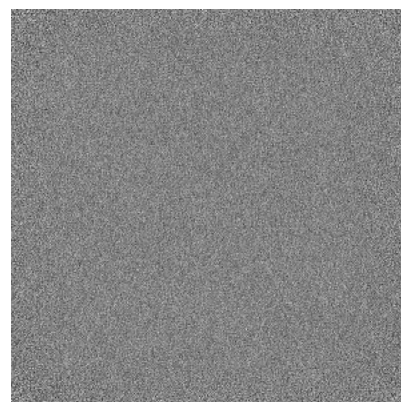
6.3.2 Raw map



X Index: 0



Y Index: 0

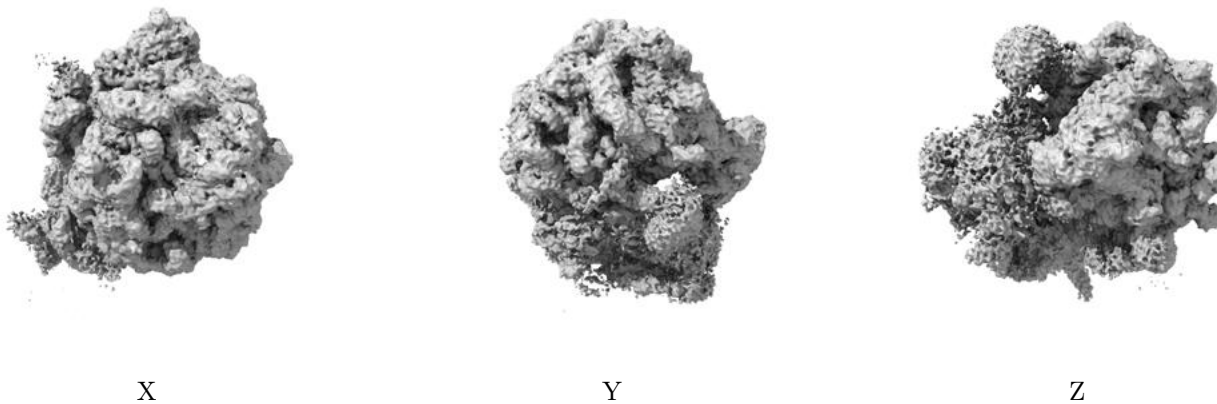


Z Index: 0

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

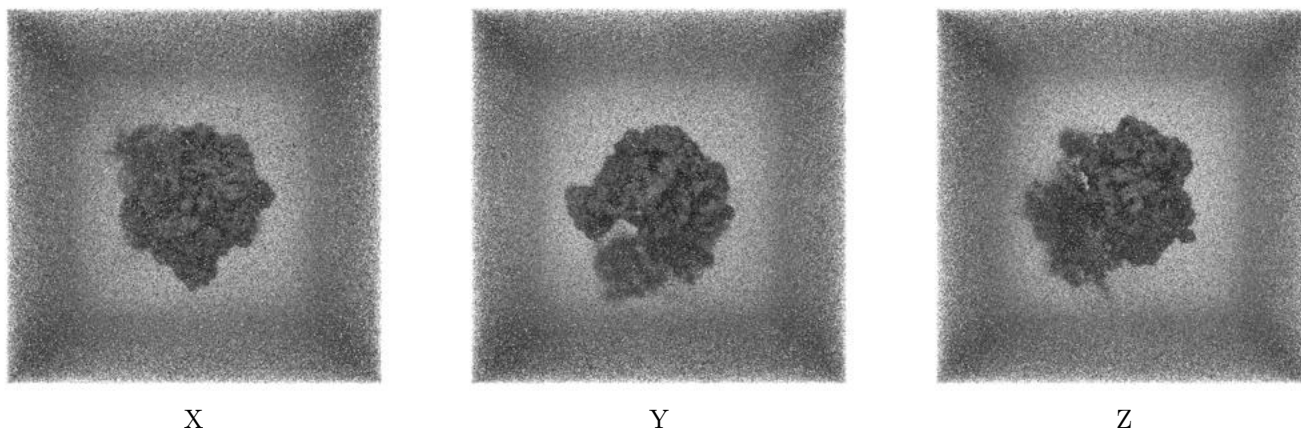
6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map



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.

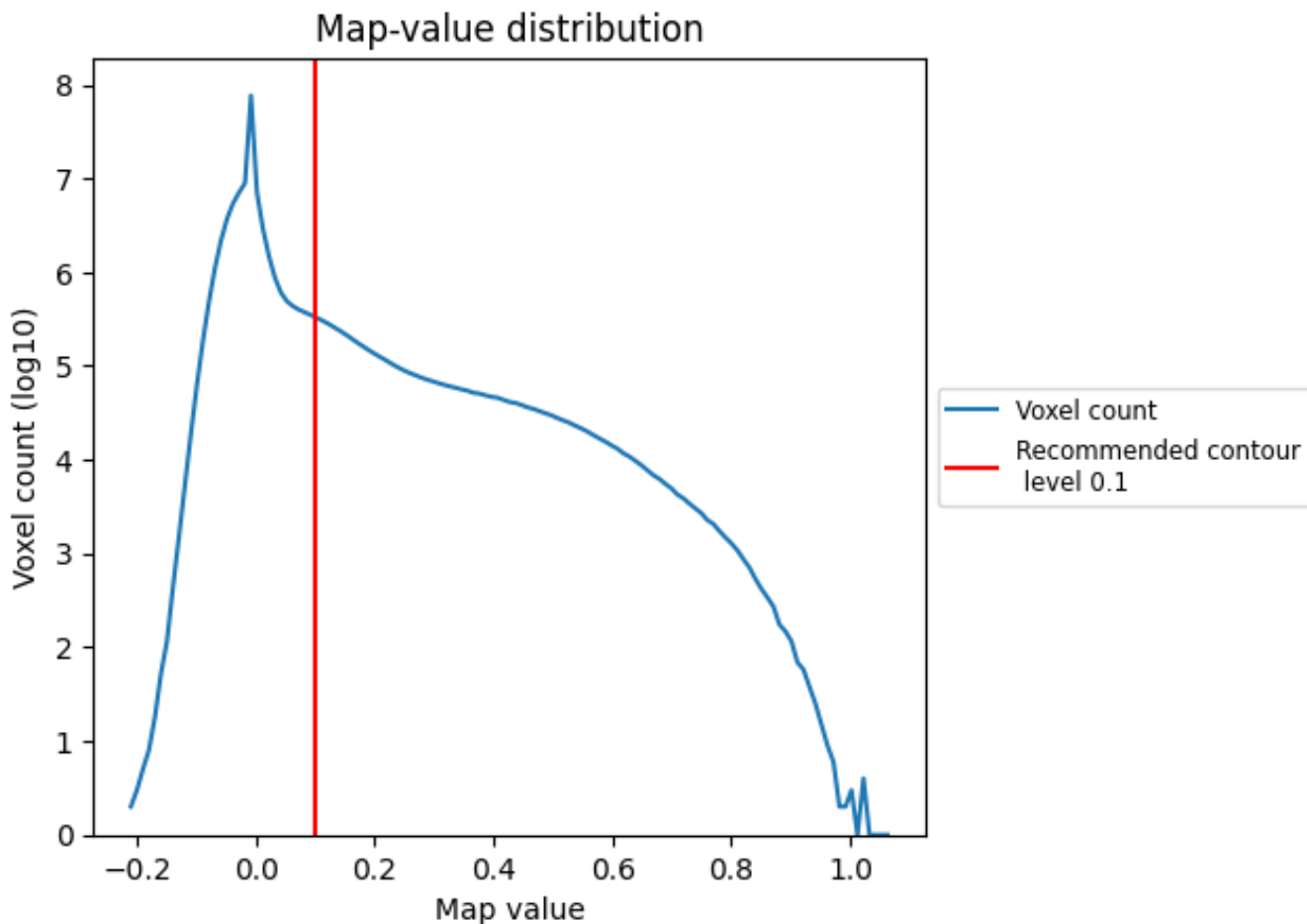
6.5 Mask visualisation [i](#)

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

7 Map analysis [i](#)

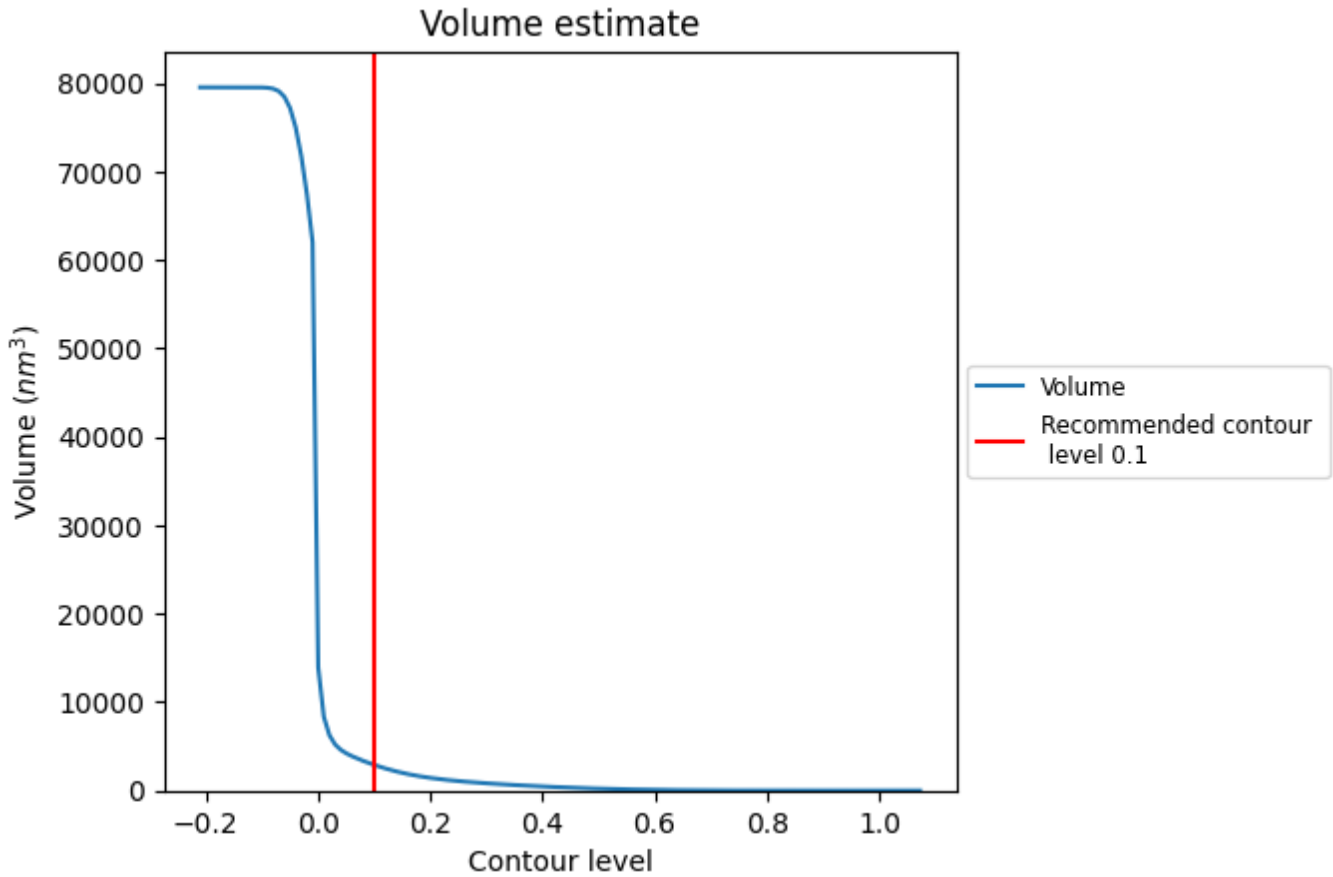
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

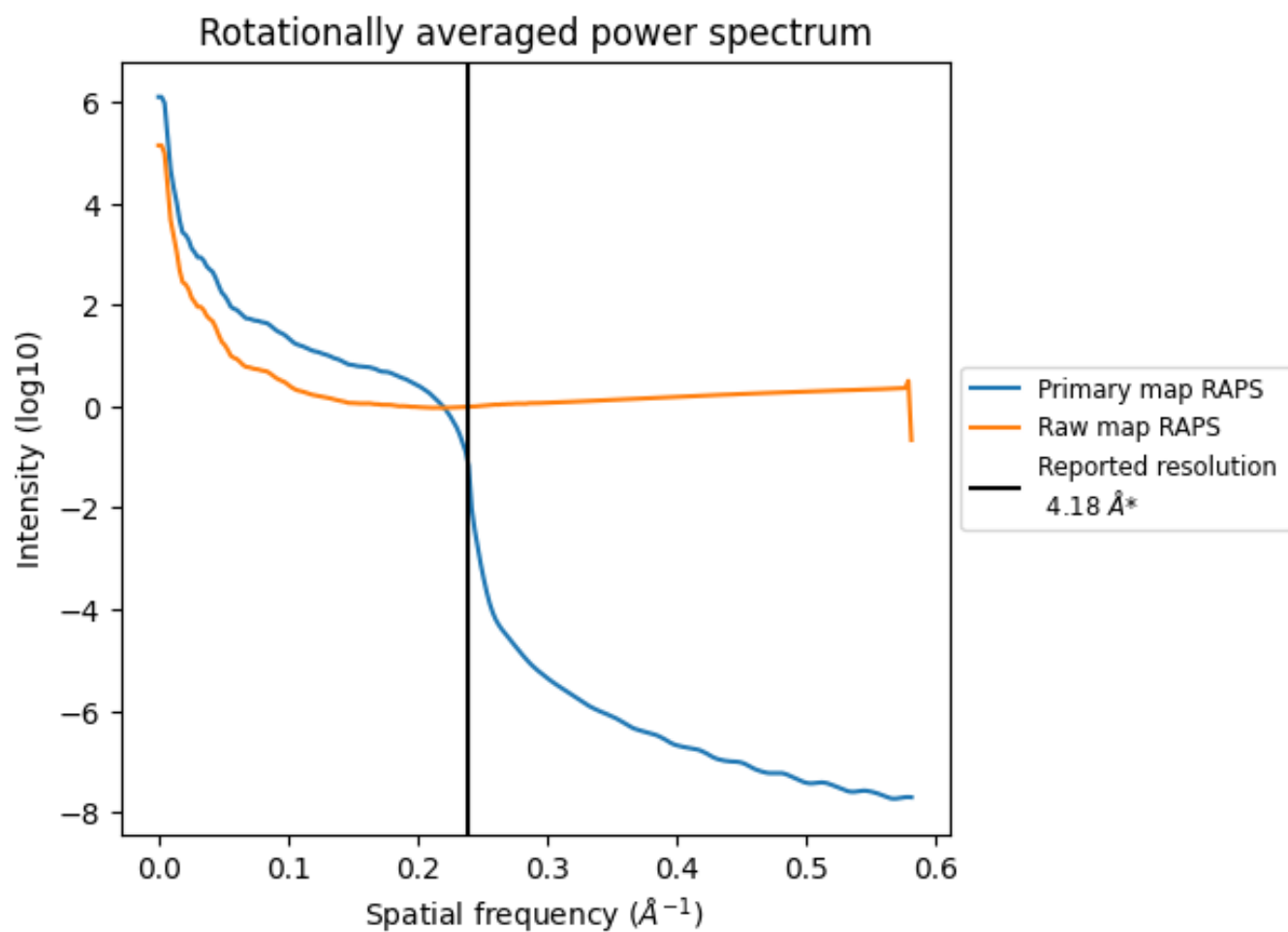
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2909 nm³; this corresponds to an approximate mass of 2628 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

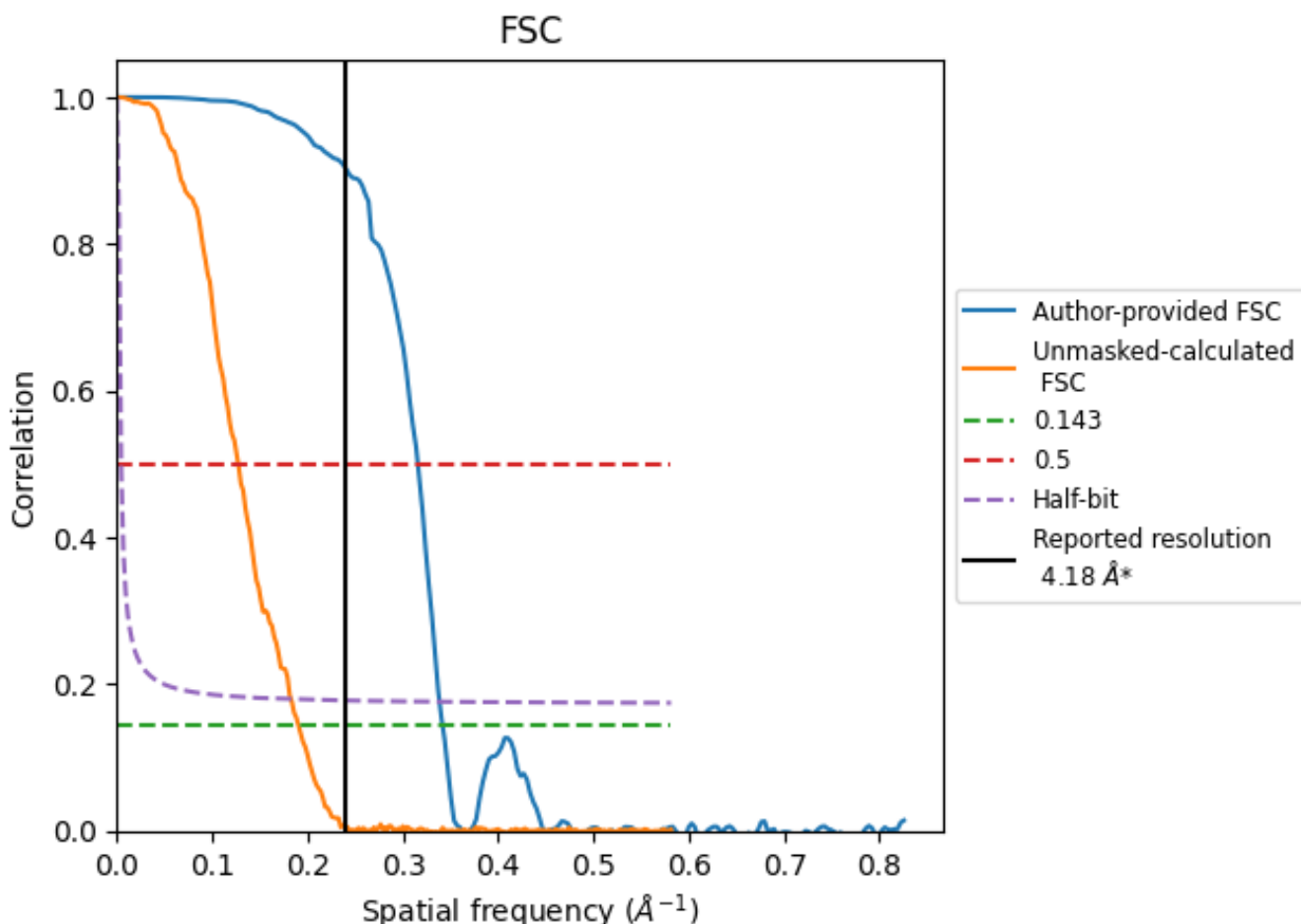


*Reported resolution corresponds to spatial frequency of 0.239 Å⁻¹

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 0.239 Å⁻¹

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.18	-	-
Author-provided FSC curve	2.93	3.17	2.96
Unmasked-calculated*	5.24	7.85	5.47

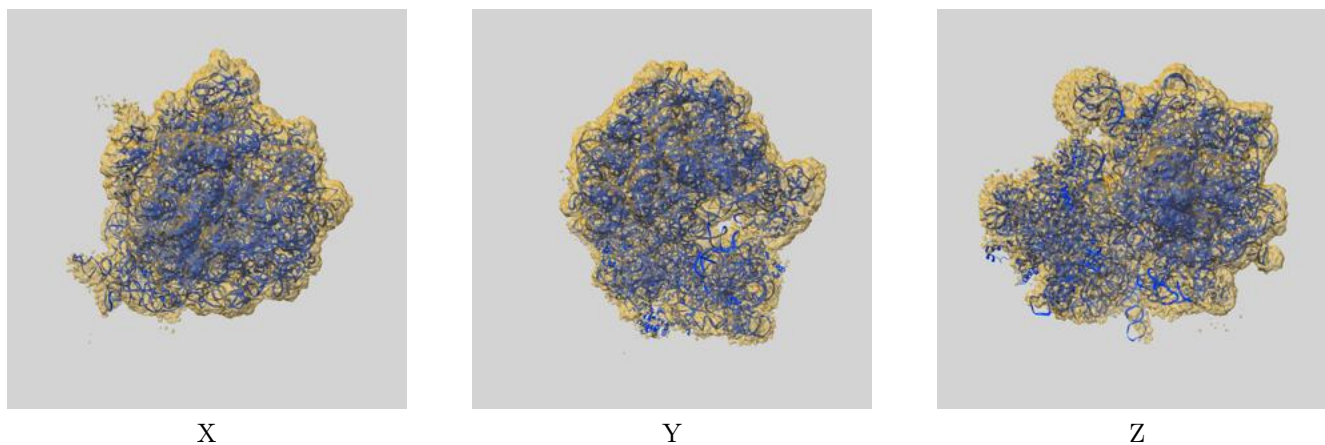
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 2.93 differs from the reported value 4.18 by more than 10 %

The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 5.24 differs from the reported value 4.18 by more than 10 %

9 Map-model fit [i](#)

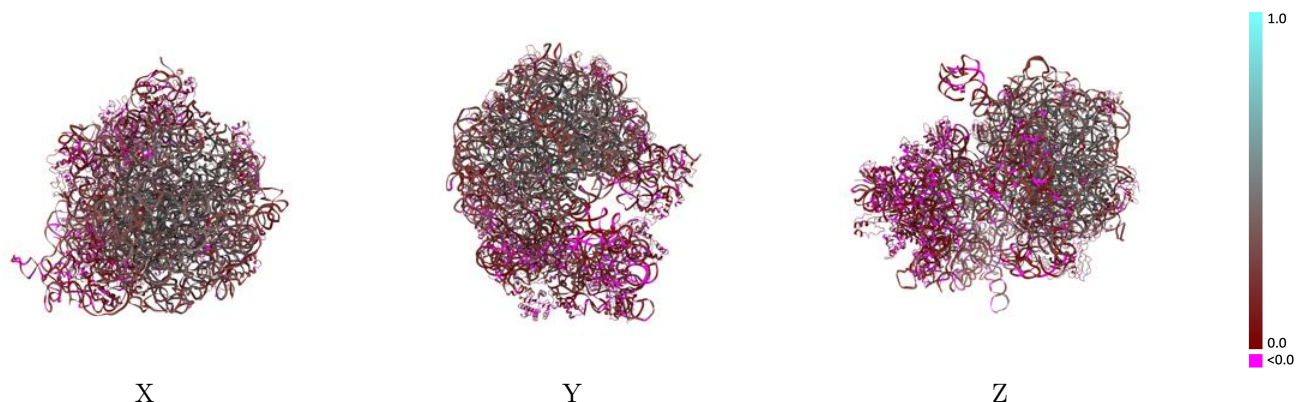
This section contains information regarding the fit between EMDB map EMD-26666 and PDB model 7UPH. Per-residue inclusion information can be found in section 3 on page 13.

9.1 Map-model overlay [i](#)



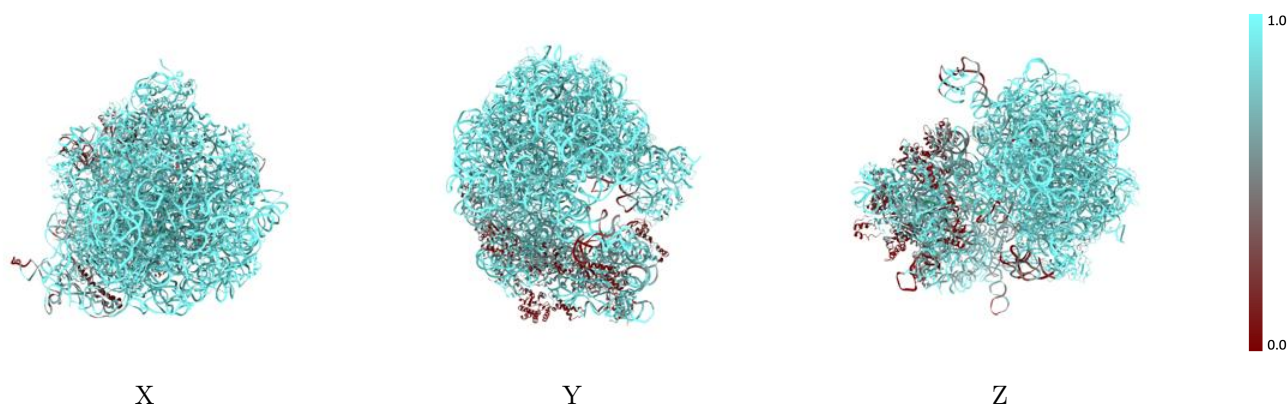
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



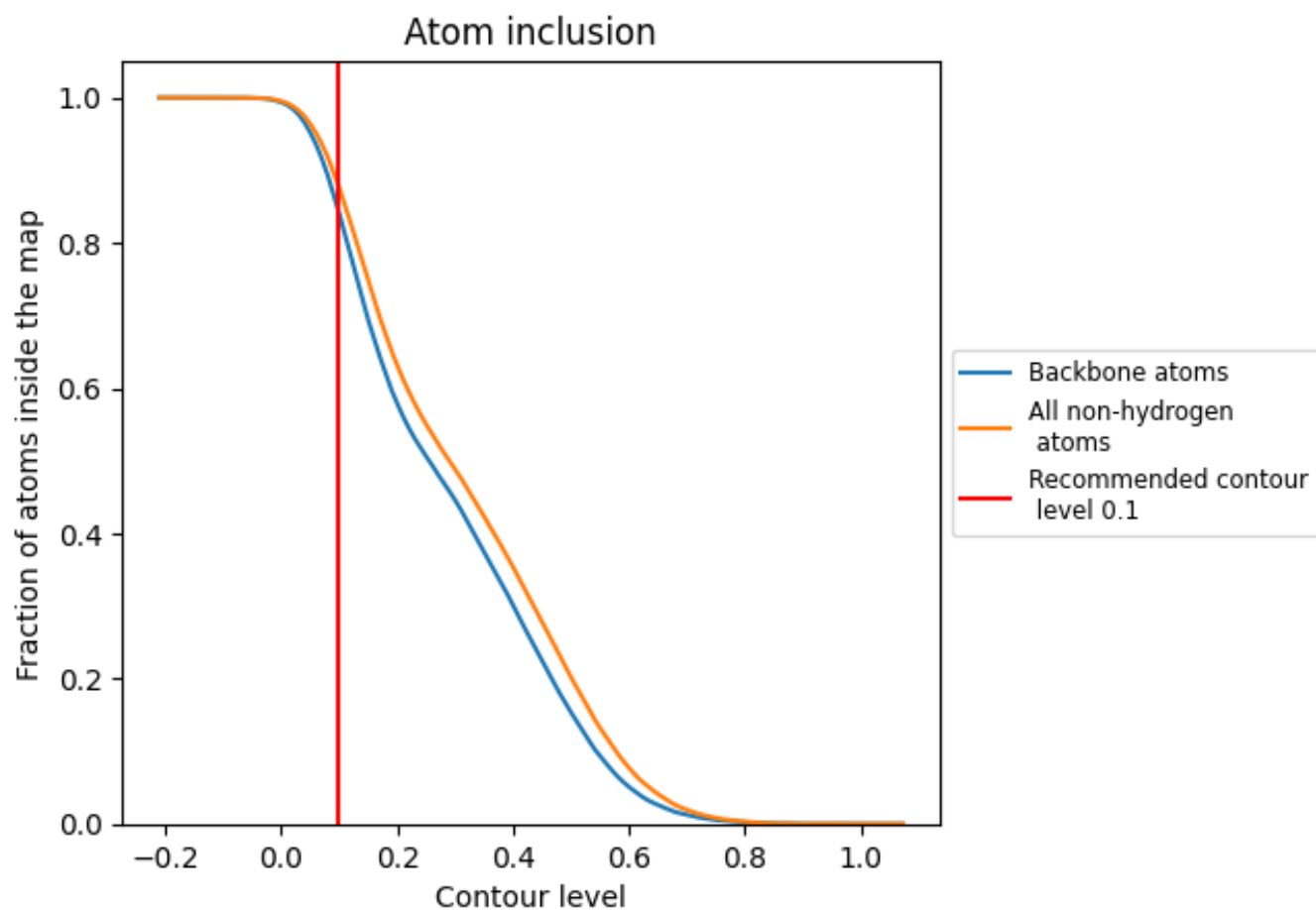
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.1).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 88% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary































The table lists the average atom inclusion at the recommended contour level (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8766	 0.2400
A	 0.7610	 0.0710
B	 0.4928	 0.1220
C	 0.7033	 0.1010
D	 0.4992	 0.1100
E	 0.5423	 0.1030
F	 0.2235	 0.0820
G	 0.2723	 0.0490
H	 0.2072	 0.0660
I	 0.9286	 0.2690
J	 0.9838	 0.1870
K	 0.9673	 0.2620
L	 0.9720	 0.2320
M	 0.9855	 0.2770
N	 0.9032	 0.1100
O	 0.9244	 0.1440
R	 0.9800	 0.2660
S	 0.9102	 0.1770
T	 0.9766	 0.2820
U	 0.9751	 0.2430
V	 0.9653	 0.2620
W	 0.1533	 0.0940
X	 0.4003	 0.0950
Y	 0.4906	 0.0880
Z	 0.7221	 0.1790
a	 0.3731	 0.1020
b	 0.3677	 0.1200
c	 0.6365	 0.1640
d	 0.7365	 0.0920
e	 0.4961	 0.1210
f	 0.4701	 0.0950
g	 0.7476	 0.2300
h	 0.5411	 0.1190
i	 0.9860	 0.3590
j	 0.8653	 0.1050



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Chain	Atom inclusion	Q-score
k	 0.9915	 0.4020
l	 0.9878	 0.3730
m	 0.9110	 0.1150
n	 0.9293	 0.1460
o	 0.8480	 0.1160
p	 0.9780	 0.2860
q	 0.9774	 0.2520
r	 0.9904	 0.3640
s	 0.9502	 0.2180
t	 0.9596	 0.1780
u	 0.9377	 0.1380
v	 0.9297	 0.1640
w	 0.9767	 0.2910
x	 0.9959	 0.2010
y	 0.9954	 0.2680