Full wwPDB EM Validation Report (i)

Apr 17, 2024 – 05:30 pm BST

PDB ID	:	5LZF
EMDB ID	:	EMD-4126
Title	:	Structure of the 70S ribosome with fMetSec-tRNASec in the hybrid pre-translocation state (H)
Authors	:	Fischer, N.; Neumann, P.; Bock, L.V.; Maracci, C.; Wang, Z.; Paleskava, A.; Konevega, A.L.; Schroeder, G.F.; Grubmueller, H.; Ficner, R.; Rodnina, M.V.; Stark, H.
Deposited on	:	2016-09-29
Resolution	:	4.60 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

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

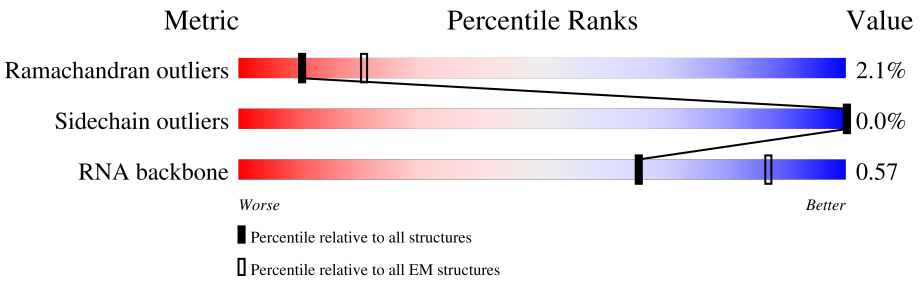
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.60 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	a	1539	68% 28%
2	b	218	37% 95%
3	c	206	15% 99%
4	d	205	25% 100%
5	e	157	11% 96%
6	f	100	9% 94% 5%
7	g	151	30% 97%
8	h	129	13% 98%

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Mol	Chain	Length	Quality of chain
9	i	127	20% 98%
10	j	98	31% 96%
11	k	116	9% 97%
12	l	123	11% 94% 5%
13	m	114	25% 97%
14	n	100	21% 99%
15	o	88	10% 95% 5%
16	p	82	21% 99%
17	q	80	12% 99%
18	r	65	12% 92% 8%
19	s	86	33% 94% 5%
20	t	85	15% 100%
21	u	65	29% 92% 8%
22	v	77	5% 48% 27% 25%
23	x	48	48% 29% 38% 31%
24	y	95	11% 53% 33% 15%
25	A	2903	69% 27%
26	B	120	73% 26%
27	C	271	7% 98%
28	D	209	8% 98%
29	E	201	11% 99%
30	F	177	19% 97%
31	G	176	9% 97%
32	I	141	86% 95% 5%
33	H	149	81% 97%

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Mol	Chain	Length	Quality of chain
34	J	142	5% 99%
35	K	122	7% 97%
36	L	143	10% 97%
37	M	136	7% 97%
38	N	120	8% 99%
39	O	116	9% 100%
40	P	114	9% 99%
41	Q	117	100%
42	R	103	10% 99%
43	S	110	98%
44	T	93	9% 99%
45	U	102	9% 98%
46	V	94	6% 100%
47	W	75	8% 100%
48	X	77	6% 99%
49	Y	63	97%
50	Z	58	14% 100%
51	0	56	9% 100%
52	1	50	20% 98%
53	2	46	9% 96%
54	3	64	9% 98%
55	4	38	13% 97%
56	6	66	35% 94% 6%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	G7M	a	527	X	-	-	-
25	G7M	A	2069	X	-	-	-

2 Entry composition (i)

There are 57 unique types of molecules in this entry. The entry contains 148005 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	a	1539	33029	14738	6052	10700	1539	0	0

- Molecule 2 is a protein called 30S ribosomal protein S2.

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

- Molecule 3 is a protein called 30S ribosomal protein S3.

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

- Molecule 4 is a protein called 30S ribosomal protein S4.

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

- Molecule 5 is a protein called 30S ribosomal protein S5.

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

- Molecule 6 is a protein called 30S ribosomal protein S6.

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

- Molecule 7 is a protein called 30S ribosomal protein S7.

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

- Molecule 8 is a protein called 30S ribosomal protein S8.

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

- Molecule 9 is a protein called 30S ribosomal protein S9.

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

- Molecule 10 is a protein called 30S ribosomal protein S10.

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

- Molecule 11 is a protein called 30S ribosomal protein S11.

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

- Molecule 12 is a protein called 30S ribosomal protein S12.

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

- Molecule 13 is a protein called 30S ribosomal protein S13.

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

- Molecule 14 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	n	100	794	495	164	132	3	0	0

- Molecule 15 is a protein called 30S ribosomal protein S15.

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

- Molecule 16 is a protein called 30S ribosomal protein S16.

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

- Molecule 17 is a protein called 30S ribosomal protein S17.

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

- Molecule 18 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
18	r	65	505	317	96	92	0	0

- Molecule 19 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	s	86	687	438	131	116	2	0	0

- Molecule 20 is a protein called 30S ribosomal protein S20.

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

- Molecule 21 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	u	65	496	307	100	88	1	0	0

- Molecule 22 is a RNA chain called tRNAfMet.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	N	O	P	S		
22	v	77	1643	733	297	535	77	1	0	0

- Molecule 23 is a RNA chain called SECIS mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
23	x	48	1025	457	183	337	48	0	0

- Molecule 24 is a RNA chain called fMetSec-tRNASec.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
24	y	95	2031	907	357	672	95	0	0

- Molecule 25 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
25	A	2900	62275	27788	11459	20128	2900	0	0

- Molecule 26 is a RNA chain called 5S ribosomal RNA.

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

- Molecule 27 is a protein called 50S ribosomal protein L2.

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

- Molecule 28 is a protein called 50S ribosomal protein L3.

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

- Molecule 29 is a protein called 50S ribosomal protein L4.

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

- Molecule 30 is a protein called 50S ribosomal protein L5.

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

- Molecule 31 is a protein called 50S ribosomal protein L6.

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

- Molecule 32 is a protein called 50S ribosomal protein L11.

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

- Molecule 33 is a protein called 50S ribosomal protein L9.

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

- Molecule 34 is a protein called 50S ribosomal protein L13.

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

- Molecule 35 is a protein called 50S ribosomal protein L14.

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

- Molecule 36 is a protein called 50S ribosomal protein L15.

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

- Molecule 37 is a protein called 50S ribosomal protein L16.

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

- Molecule 38 is a protein called 50S ribosomal protein L17.

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

- Molecule 39 is a protein called 50S ribosomal protein L18.

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

- Molecule 40 is a protein called 50S ribosomal protein L19.

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

- Molecule 41 is a protein called 50S ribosomal protein L20.

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

- Molecule 42 is a protein called 50S ribosomal protein L21.

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

- Molecule 43 is a protein called 50S ribosomal protein L22.

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

- Molecule 44 is a protein called 50S ribosomal protein L23.

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

- Molecule 45 is a protein called 50S ribosomal protein L24.

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

- Molecule 46 is a protein called 50S ribosomal protein L25.

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

- Molecule 47 is a protein called 50S ribosomal protein L27.

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

- Molecule 48 is a protein called 50S ribosomal protein L28.

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

- Molecule 49 is a protein called 50S ribosomal protein L29.

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

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

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

- Molecule 51 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
51	0	56	444	269	94	80	1	0	0

- Molecule 52 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
52	1	50	410	263	75	72	0	0

- Molecule 53 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
53	2	46	377	228	90	57	2	0	0

- Molecule 54 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
54	3	64	504	323	105	74	2	0	0

- Molecule 55 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
55	4	38	302	185	65	48	4	0	0

- Molecule 56 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
56	6	66	523	323	99	95	6	0	0

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

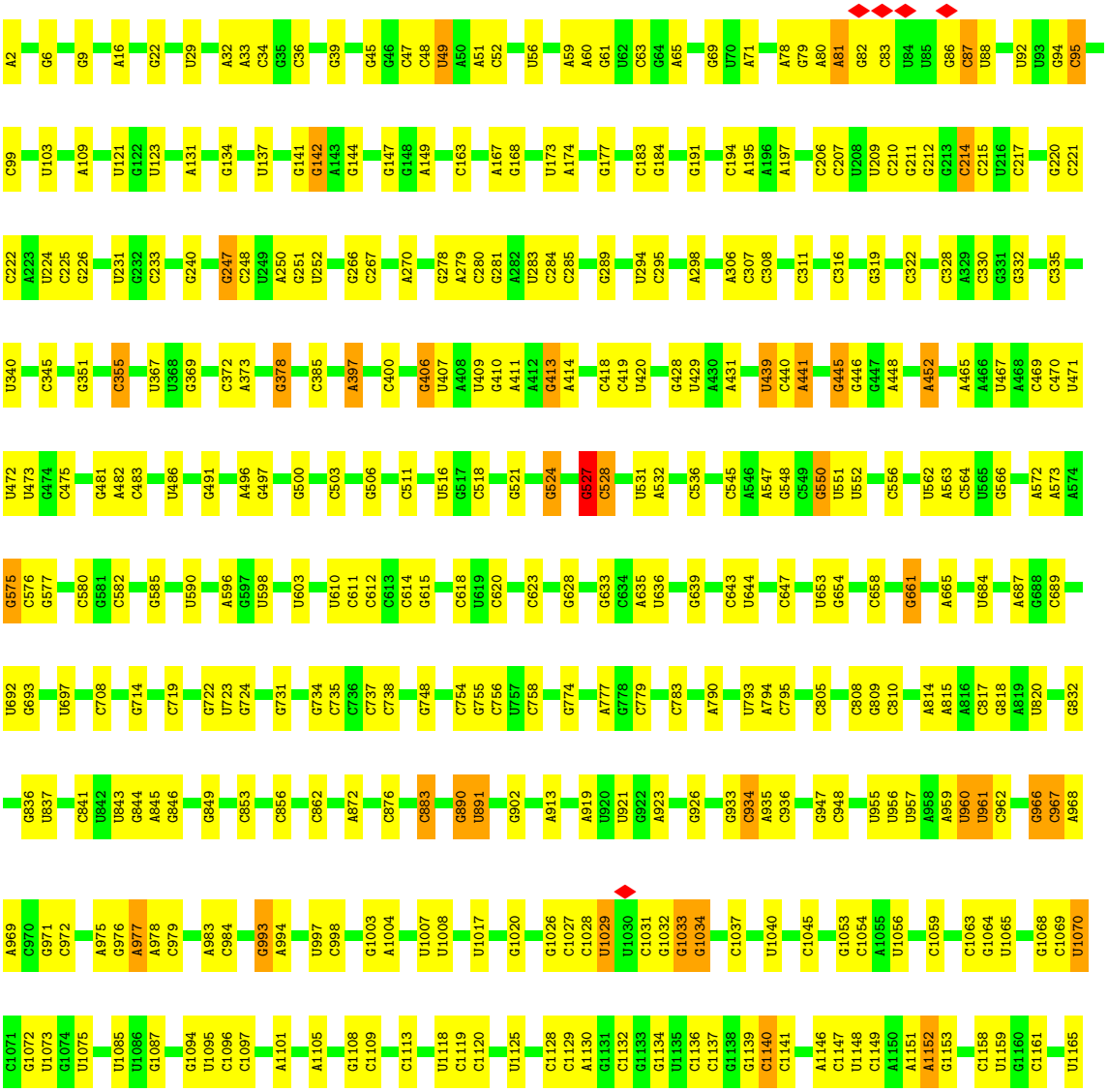
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
57	4	1	1	1	0
			Total	Zn	
57	6	1	1	1	0

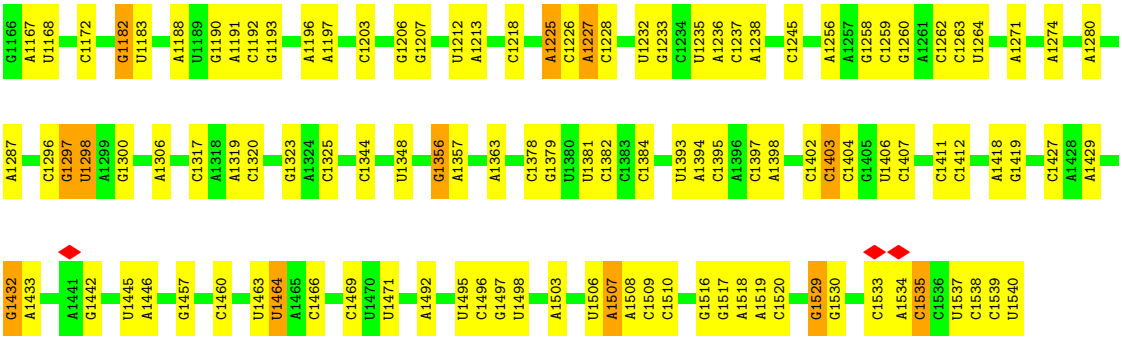
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: 16S ribosomal RNA

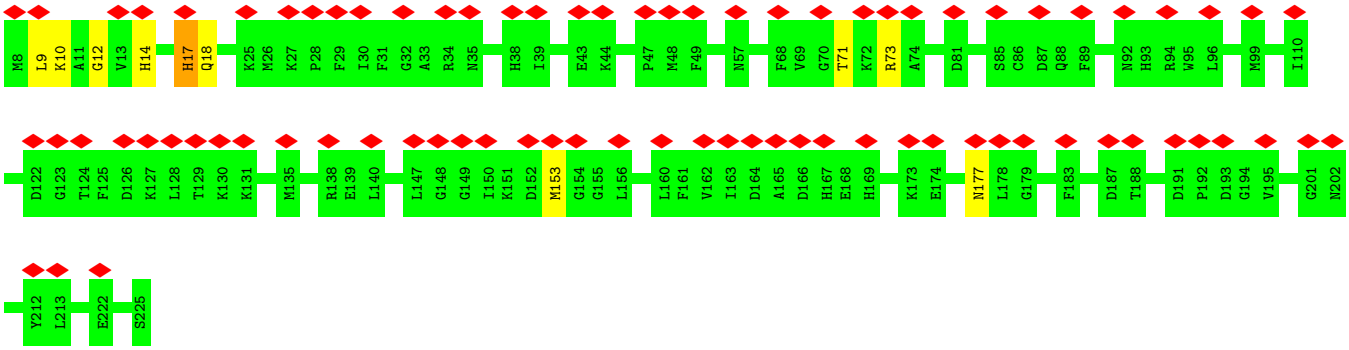
Chain a: 68% 28%





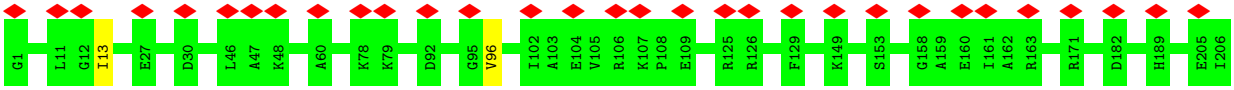
- Molecule 2: 30S ribosomal protein S2

Chain b: 37% 95%



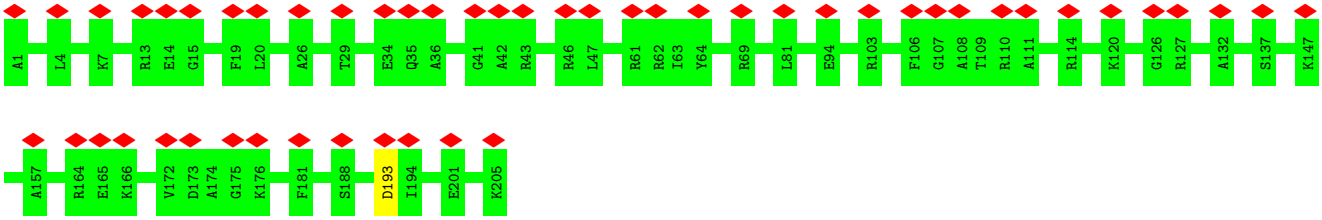
- Molecule 3: 30S ribosomal protein S3

Chain c: 15% 99%



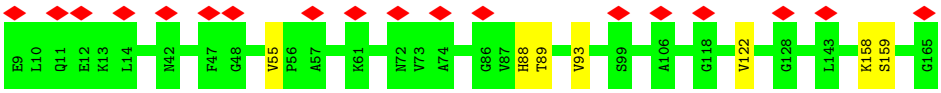
- Molecule 4: 30S ribosomal protein S4

Chain d: 25% 100%



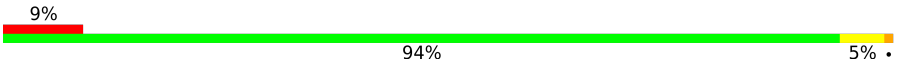
- Molecule 5: 30S ribosomal protein S5

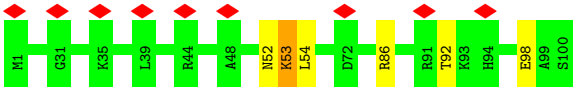
Chain e: 11% 96%



• Molecule 6: 30S ribosomal protein S6

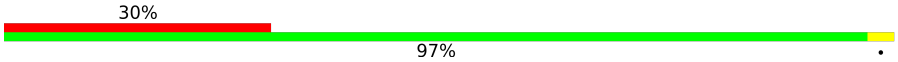
Chain f:

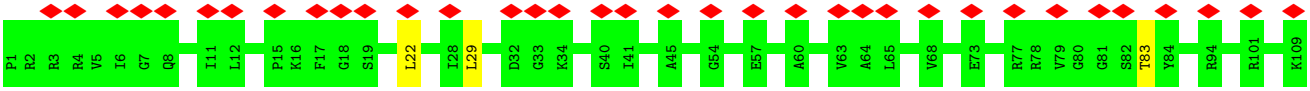


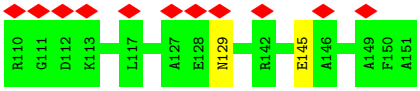


• Molecule 7: 30S ribosomal protein S7

Chain g:

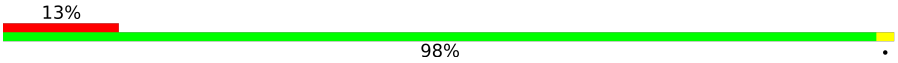


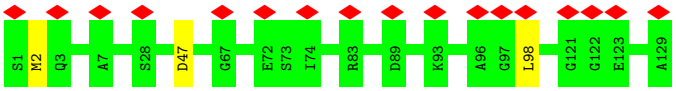




• Molecule 8: 30S ribosomal protein S8

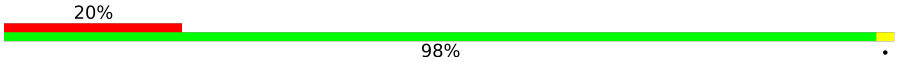
Chain h:

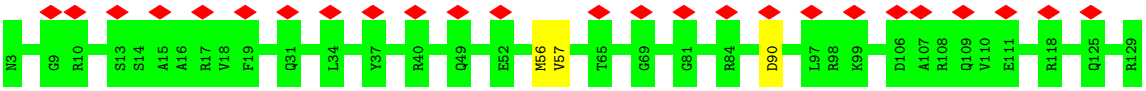




• Molecule 9: 30S ribosomal protein S9

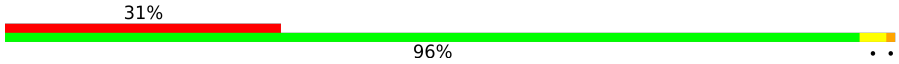
Chain i:

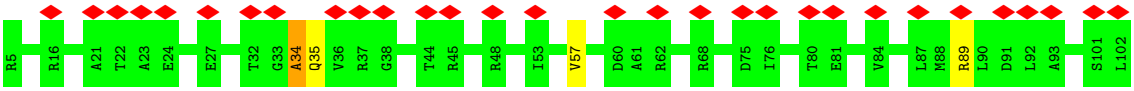




• Molecule 10: 30S ribosomal protein S10

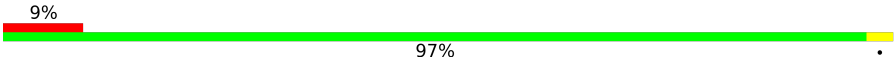
Chain j:

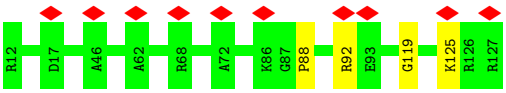




• Molecule 11: 30S ribosomal protein S11

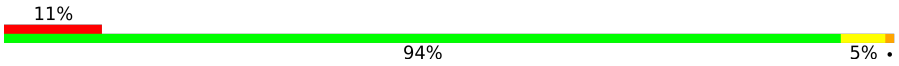
Chain k:

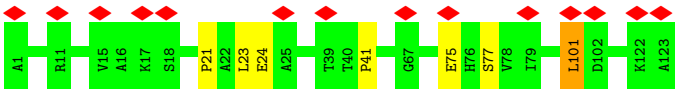




• Molecule 12: 30S ribosomal protein S12

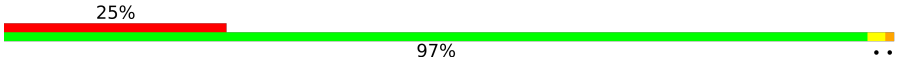
Chain l:

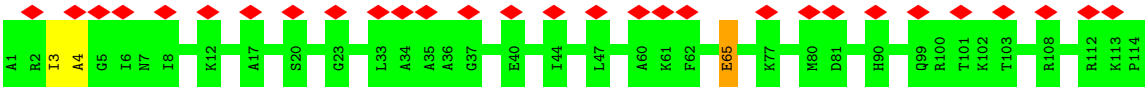




• Molecule 13: 30S ribosomal protein S13

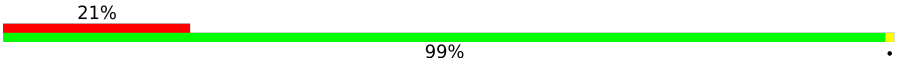
Chain m:

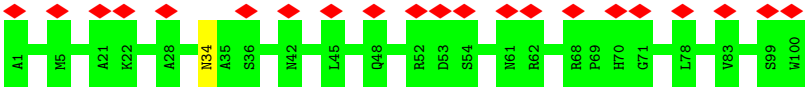




• Molecule 14: 30S ribosomal protein S14

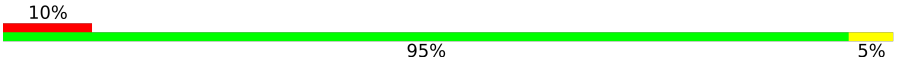
Chain n:

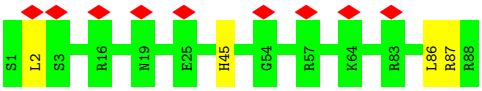




• Molecule 15: 30S ribosomal protein S15

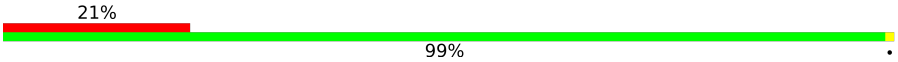
Chain o:

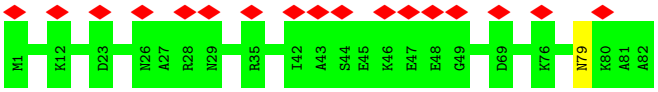




• Molecule 16: 30S ribosomal protein S16

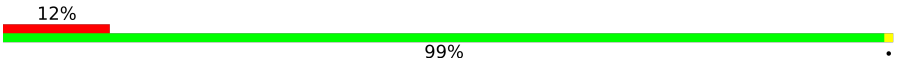
Chain p:





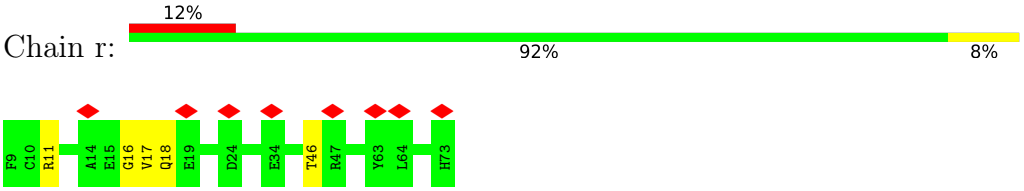
• Molecule 17: 30S ribosomal protein S17

Chain q:



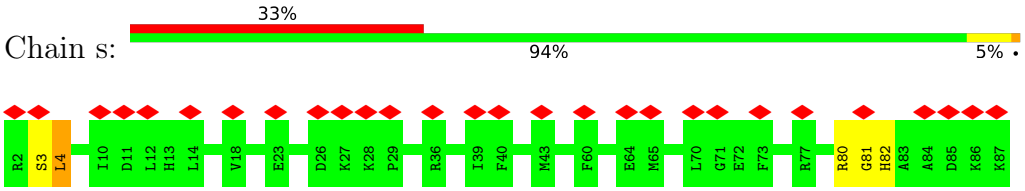
• Molecule 18: 30S ribosomal protein S18

Chain r:



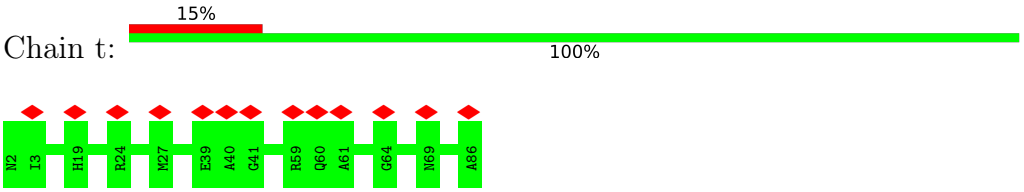
• Molecule 19: 30S ribosomal protein S19

Chain s:



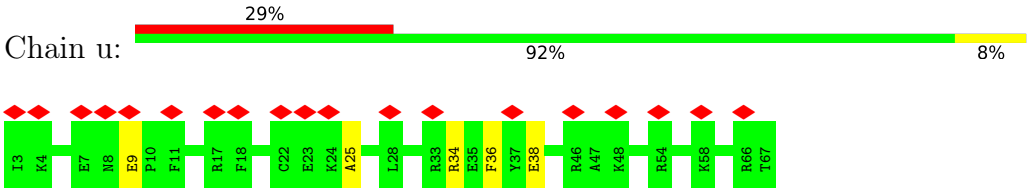
• Molecule 20: 30S ribosomal protein S20

Chain t:



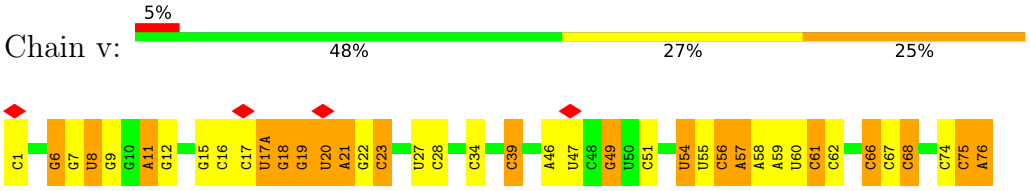
• Molecule 21: 30S ribosomal protein S21

Chain u:



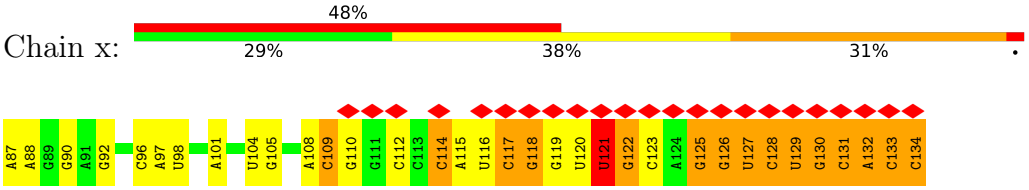
• Molecule 22: tRNAfMet

Chain v:



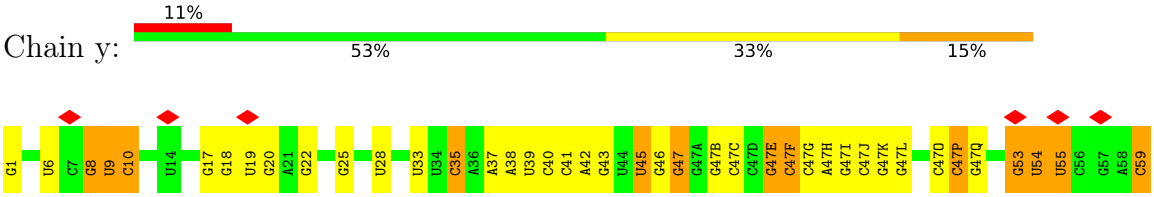
• Molecule 23: SECIS mRNA

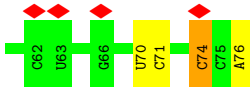
Chain x:



• Molecule 24: fMetSec-tRNASec

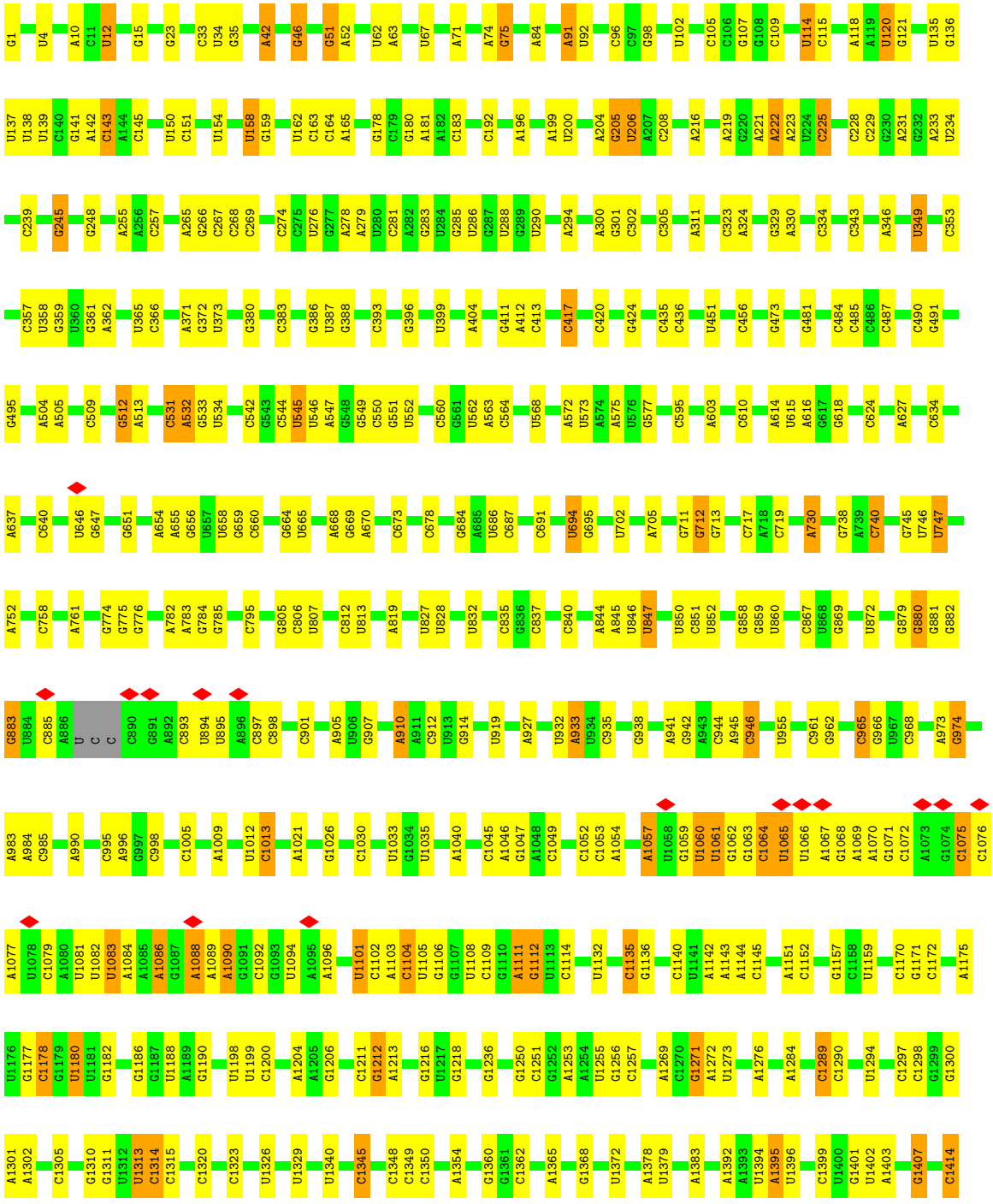
Chain y:

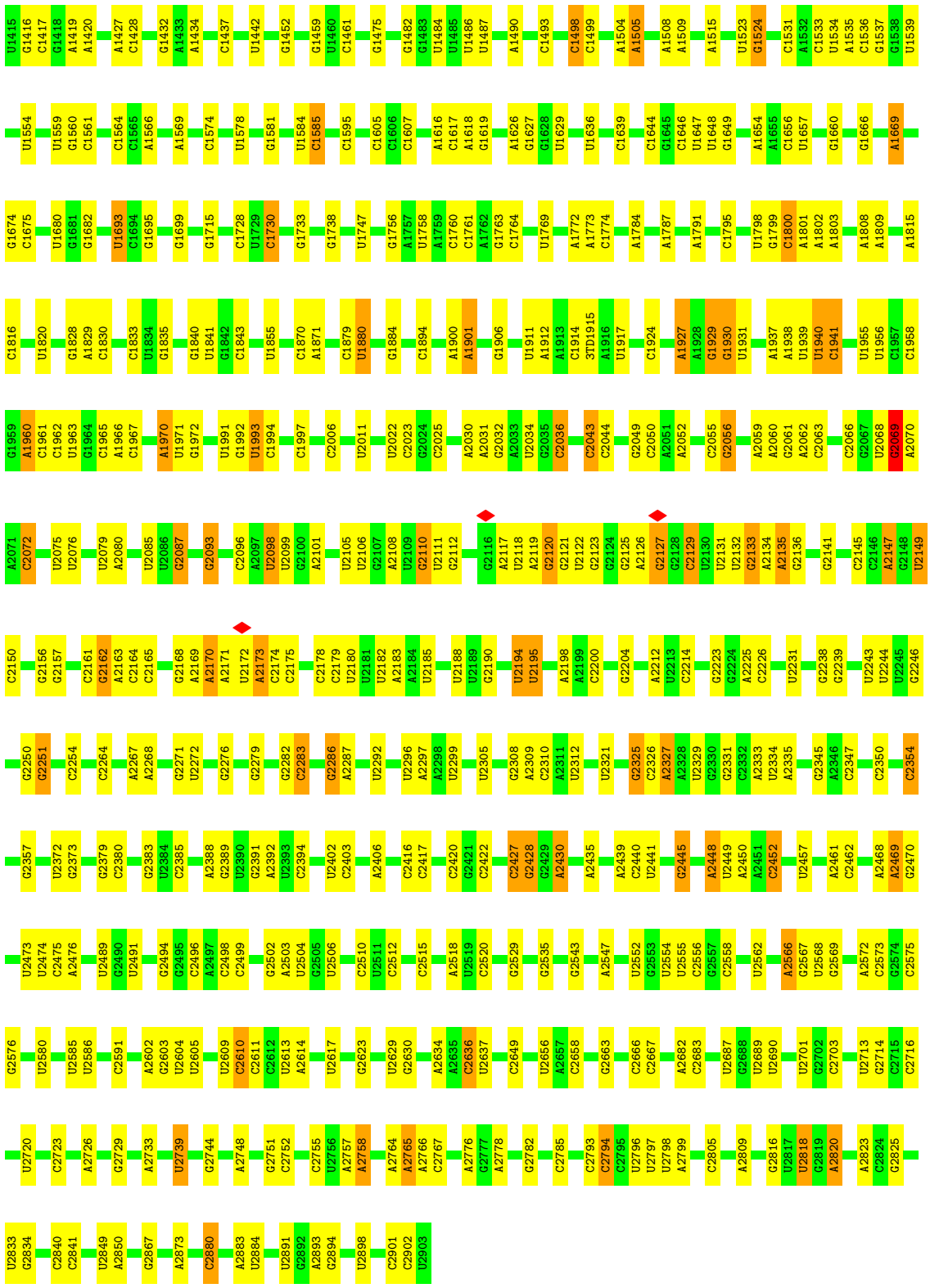




• Molecule 25: 23S ribosomal RNA

Chain A:



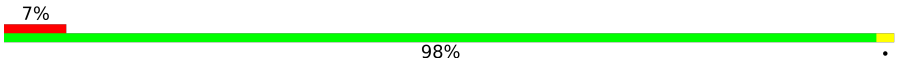


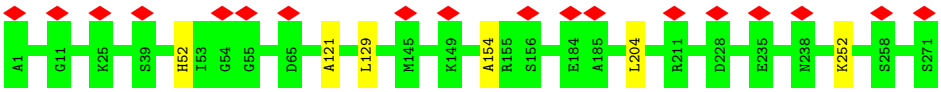
- Molecule 26: 5S ribosomal RNA

Chain B: 73% 26%

• Molecule 27: 50S ribosomal protein L2

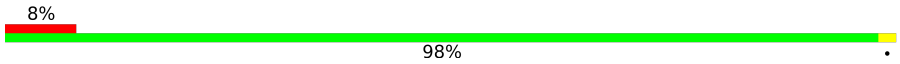
Chain C:

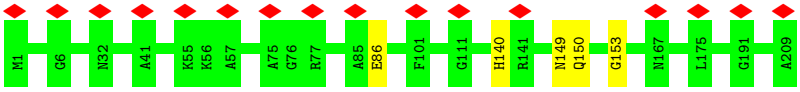




• Molecule 28: 50S ribosomal protein L3

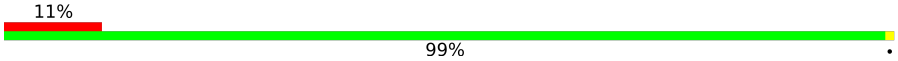
Chain D:

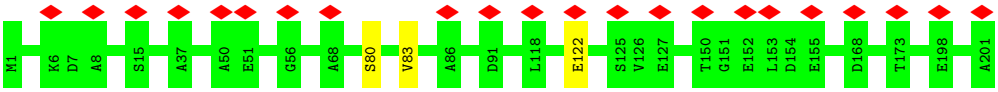




• Molecule 29: 50S ribosomal protein L4

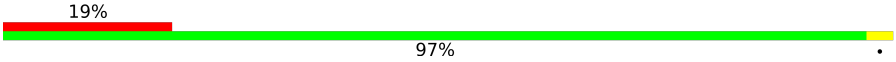
Chain E:

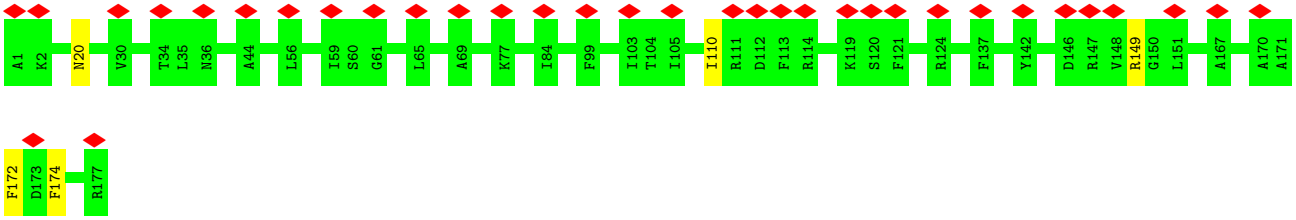




• Molecule 30: 50S ribosomal protein L5

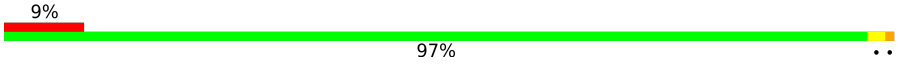
Chain F:





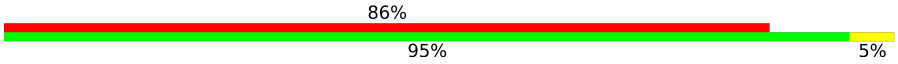
• Molecule 31: 50S ribosomal protein L6

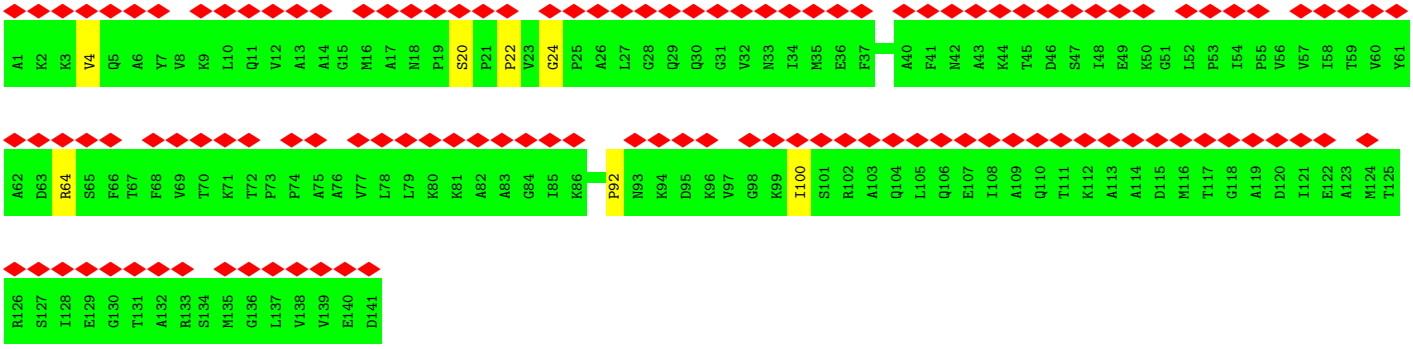
Chain G:



• Molecule 32: 50S ribosomal protein L11

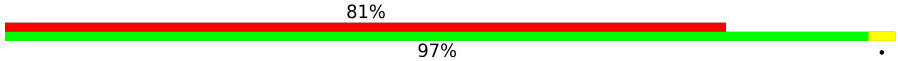
Chain I:





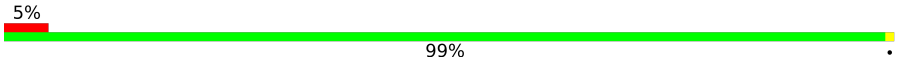
- Molecule 33: 50S ribosomal protein L9

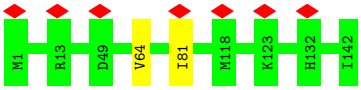
Chain H:



- Molecule 34: 50S ribosomal protein L13

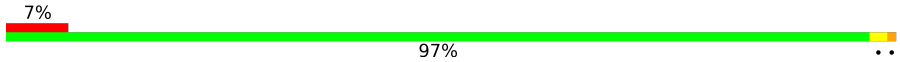
Chain J:

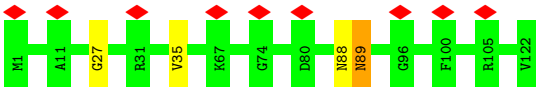




- Molecule 35: 50S ribosomal protein L14

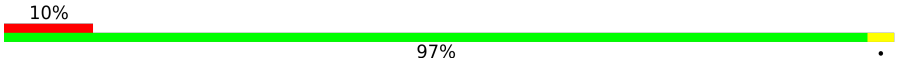
Chain K:

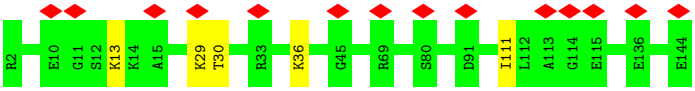




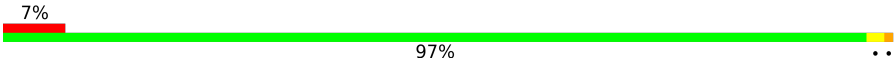
- Molecule 36: 50S ribosomal protein L15

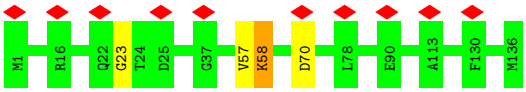
Chain L:



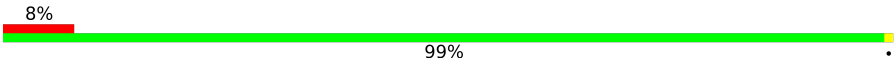


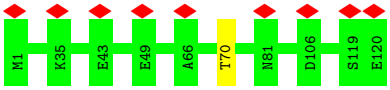
- Molecule 37: 50S ribosomal protein L16

Chain M: 

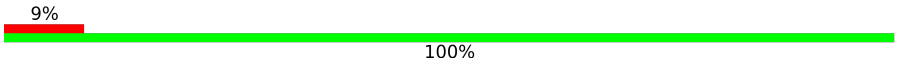


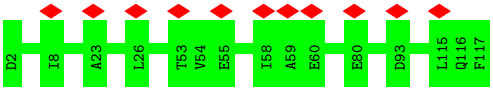
• Molecule 38: 50S ribosomal protein L17

Chain N: 

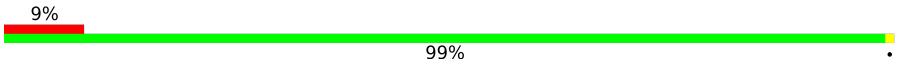


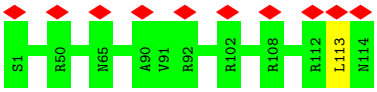
• Molecule 39: 50S ribosomal protein L18

Chain O: 

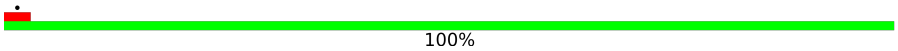


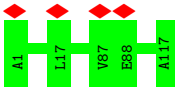
• Molecule 40: 50S ribosomal protein L19

Chain P: 

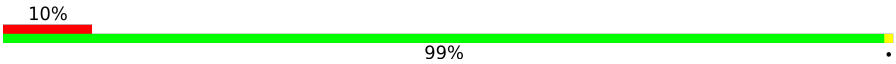


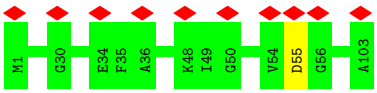
• Molecule 41: 50S ribosomal protein L20

Chain Q: 

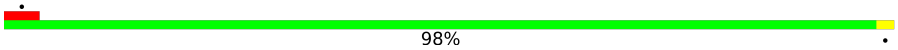


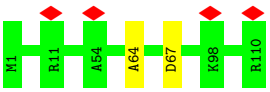
• Molecule 42: 50S ribosomal protein L21

Chain R: 



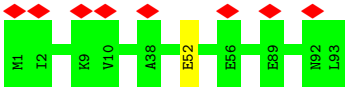
• Molecule 43: 50S ribosomal protein L22

Chain S: 



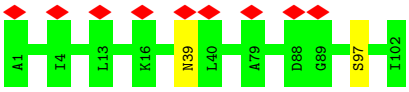
• Molecule 44: 50S ribosomal protein L23

Chain T: 9% 99%



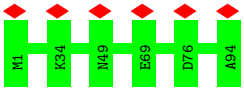
• Molecule 45: 50S ribosomal protein L24

Chain U: 9% 98%



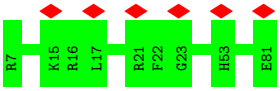
• Molecule 46: 50S ribosomal protein L25

Chain V: 6% 100%



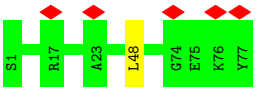
• Molecule 47: 50S ribosomal protein L27

Chain W: 8% 100%



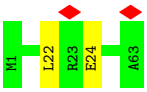
• Molecule 48: 50S ribosomal protein L28

Chain X: 6% 99%



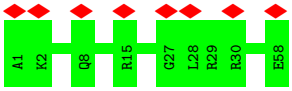
• Molecule 49: 50S ribosomal protein L29

Chain Y: 97%



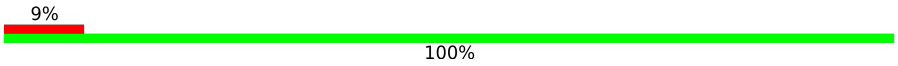
• Molecule 50: 50S ribosomal protein L30

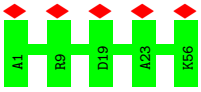
Chain Z: 14% 100%



• Molecule 51: 50S ribosomal protein L32

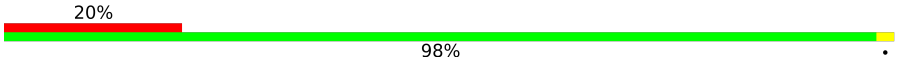
Chain 0:

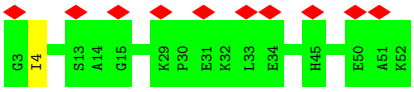




• Molecule 52: 50S ribosomal protein L33

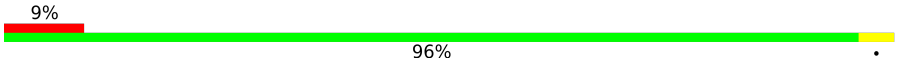
Chain 1:

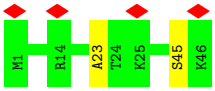




• Molecule 53: 50S ribosomal protein L34

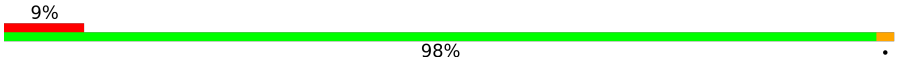
Chain 2:

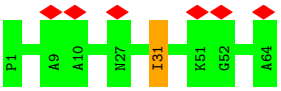




• Molecule 54: 50S ribosomal protein L35

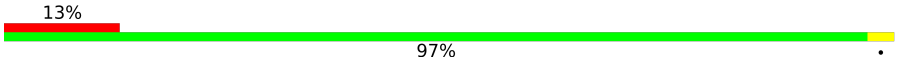
Chain 3:

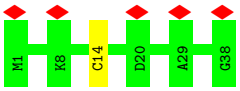




• Molecule 55: 50S ribosomal protein L36

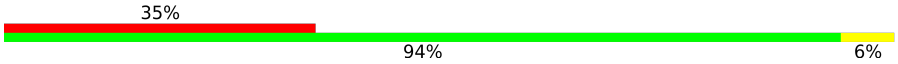
Chain 4:

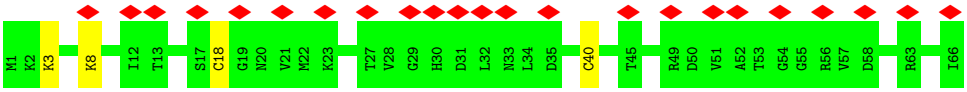




• Molecule 56: 50S ribosomal protein L31

Chain 6:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	19868	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY; Local CTF correction, after MSA based classification and averaging of local power spectra	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	30	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	2600	Depositor
Magnification	59000	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	2.225	Depositor
Minimum map value	-1.150	Depositor
Average map value	0.020	Depositor
Map value standard deviation	0.199	Depositor
Recommended contour level	0.4	Depositor
Map size (Å)	315.52, 315.52, 315.52	wwPDB
Map dimensions	272, 272, 272	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.16, 1.16, 1.16	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: OMC, 4OC, PSU, 5MU, 1MG, 6IA, ZN, 2MG, 5MC, 4SU, 6MZ, H2U, OMG, 2MA, MA6, G7M, 3TD, UR3, OMU

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	0.57	2/36701 (0.0%)	1.39	573/57246 (1.0%)
2	b	0.42	0/1736	0.70	0/2338
3	c	0.35	0/1652	0.59	0/2225
4	d	0.38	0/1665	0.61	0/2227
5	e	0.43	1/1170 (0.1%)	0.74	0/1573
6	f	0.40	0/836	0.75	1/1128 (0.1%)
7	g	0.34	0/1196	0.62	1/1602 (0.1%)
8	h	0.35	0/989	0.65	1/1326 (0.1%)
9	i	0.36	0/1034	0.68	0/1375
10	j	0.35	0/797	0.72	0/1077
11	k	0.37	0/886	0.69	0/1195
12	l	0.40	0/969	0.72	1/1300 (0.1%)
13	m	0.38	0/893	0.72	2/1193 (0.2%)
14	n	0.39	0/806	0.61	0/1074
15	o	0.34	0/722	0.59	1/964 (0.1%)
16	p	0.41	0/659	0.66	0/884
17	q	0.46	0/658	0.80	0/881
18	r	0.35	0/512	0.63	0/689
19	s	0.46	0/703	0.85	2/944 (0.2%)
20	t	0.40	0/671	0.59	0/888
21	u	0.53	1/501 (0.2%)	0.76	0/668
22	v	0.91	3/1746 (0.2%)	2.04	87/2721 (3.2%)
23	x	0.88	2/1145 (0.2%)	1.88	49/1781 (2.8%)
24	y	0.67	1/2168 (0.0%)	1.59	54/3375 (1.6%)
25	A	0.56	10/69173 (0.0%)	1.32	813/107908 (0.8%)
26	B	0.57	1/2873 (0.0%)	1.39	54/4478 (1.2%)
27	C	0.36	0/2122	0.68	1/2852 (0.0%)
28	D	0.38	0/1586	0.66	0/2134
29	E	0.38	0/1571	0.63	0/2113
30	F	0.42	0/1435	0.74	1/1926 (0.1%)
31	G	0.36	0/1343	0.62	1/1816 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	I	0.43	0/1046	0.74	1/1410 (0.1%)
33	H	0.36	0/1122	0.63	0/1515
34	J	0.39	0/1152	0.61	0/1551
35	K	0.40	0/948	0.66	0/1268
36	L	0.38	0/1054	0.68	0/1403
37	M	0.40	0/1093	0.68	1/1460 (0.1%)
38	N	0.38	0/974	0.64	0/1301
39	O	0.43	0/902	0.61	0/1209
40	P	0.36	0/929	0.66	1/1242 (0.1%)
41	Q	0.43	0/960	0.57	0/1278
42	R	0.36	0/829	0.70	0/1107
43	S	0.35	0/864	0.59	0/1156
44	T	0.36	0/745	0.64	0/994
45	U	0.39	0/788	0.70	0/1051
46	V	0.40	0/766	0.67	0/1025
47	W	0.35	0/582	0.57	0/769
48	X	0.34	0/635	0.60	1/848 (0.1%)
49	Y	0.38	0/510	0.64	0/677
50	Z	0.35	0/453	0.61	0/605
51	0	0.33	0/450	0.63	0/599
52	1	0.39	0/417	0.75	0/554
53	2	0.35	0/380	0.60	0/498
54	3	0.40	0/513	0.68	1/676 (0.1%)
55	4	0.52	0/303	0.91	1/397 (0.3%)
56	6	0.51	0/532	0.98	1/709 (0.1%)
All	All	0.53	21/159865 (0.0%)	1.23	1649/239203 (0.7%)

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	2	1
2	b	0	4
5	e	0	1
6	f	0	1
9	i	0	1
10	j	0	1
13	m	0	1
18	r	0	1
23	x	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
25	A	2	0
31	G	0	1
33	H	0	1
35	K	0	2
36	L	0	1
37	M	0	1
43	S	0	1
49	Y	0	1
All	All	4	20

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	v	61	C	N1-C6	-10.77	1.30	1.37
23	x	87	A	OP3-P	-10.64	1.48	1.61
26	B	1	U	OP3-P	-10.60	1.48	1.61
24	y	1	G	OP3-P	-10.59	1.48	1.61
25	A	1	G	OP3-P	-10.51	1.48	1.61
1	a	2	A	OP3-P	-10.48	1.48	1.61
22	v	61	C	C4-C5	-7.70	1.36	1.43
25	A	2439	A	N9-C4	6.50	1.41	1.37
5	e	55	VAL	C-N	6.18	1.46	1.34
22	v	58	A	N9-C4	6.17	1.41	1.37
25	A	2156	G	N7-C5	-5.97	1.35	1.39
25	A	1111	A	O3'-P	5.93	1.68	1.61
21	u	9	GLU	C-N	5.87	1.45	1.34
25	A	359	G	C6-N1	5.74	1.43	1.39
25	A	933	A	N9-C4	5.70	1.41	1.37
25	A	1086	A	C2-N3	-5.58	1.28	1.33
25	A	2448	A	N9-C4	-5.36	1.34	1.37
23	x	125	G	O3'-P	5.24	1.67	1.61
25	A	984	A	N9-C4	-5.14	1.34	1.37
1	a	496	A	N9-C4	5.07	1.40	1.37
25	A	1313	U	N1-C2	5.00	1.43	1.38

All (1649) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	v	61	C	C6-N1-C2	-17.40	113.34	120.30
22	v	61	C	N3-C4-C5	-15.90	115.54	121.90
24	y	35	C	C5-C6-N1	15.50	128.75	121.00
24	y	74	C	N1-C2-O2	14.94	127.87	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	a	419	C	C6-N1-C2	-14.23	114.61	120.30
25	A	2072	C	C5-C6-N1	13.52	127.76	121.00
22	v	56	C	N1-C2-O2	13.50	127.00	118.90
22	v	56	C	C6-N1-C2	-13.30	114.98	120.30
1	a	322	C	C6-N1-C2	-13.20	115.02	120.30
24	y	74	C	N3-C2-O2	-12.75	112.97	121.90
22	v	61	C	N3-C4-N4	12.65	126.86	118.00
23	x	121	U	C5-C6-N1	12.41	128.91	122.70
25	A	2072	C	C6-N1-C2	-12.25	115.40	120.30
25	A	281	C	C6-N1-C2	-12.25	115.40	120.30
25	A	542	C	N3-C2-O2	-12.17	113.38	121.90
23	x	133	C	N1-C2-O2	12.10	126.16	118.90
22	v	56	C	N3-C2-O2	-12.05	113.46	121.90
25	A	1313	U	N3-C2-O2	-12.02	113.78	122.20
25	A	1313	U	N1-C2-O2	11.99	131.19	122.80
22	v	74	C	C6-N1-C2	-11.83	115.57	120.30
24	y	35	C	C6-N1-C2	-11.70	115.62	120.30
25	A	2179	C	C6-N1-C2	-11.69	115.62	120.30
1	a	754	C	N1-C2-O2	11.68	125.91	118.90
1	a	1141	C	C6-N1-C2	-11.63	115.65	120.30
23	x	121	U	N3-C2-O2	-11.05	114.46	122.20
25	A	135	U	N3-C2-O2	-11.04	114.47	122.20
25	A	2179	C	C5-C6-N1	11.04	126.52	121.00
25	A	1294	U	N3-C2-O2	-11.03	114.48	122.20
1	a	206	C	N1-C2-O2	-10.98	112.31	118.90
25	A	1313	U	C2-N1-C1'	10.90	130.78	117.70
25	A	62	U	N1-C2-O2	10.87	130.41	122.80
1	a	340	U	N3-C2-O2	-10.77	114.66	122.20
23	x	121	U	C6-N1-C2	-10.74	114.55	121.00
26	B	4	C	C5-C6-N1	10.73	126.36	121.00
22	v	61	C	C5-C6-N1	10.54	126.27	121.00
25	A	359	G	N3-C2-N2	-10.53	112.53	119.90
25	A	1088	A	C2-N3-C4	10.44	115.82	110.60
25	A	1081	U	N1-C2-O2	10.33	130.03	122.80
25	A	143	C	C6-N1-C2	-10.26	116.19	120.30
25	A	1843	C	C6-N1-C2	-10.22	116.21	120.30
23	x	133	C	N3-C2-O2	-10.21	114.75	121.90
25	A	281	C	N1-C2-O2	10.21	125.03	118.90
1	a	1306	A	N7-C8-N9	10.20	118.90	113.80
25	A	1170	C	C6-N1-C2	-10.18	116.23	120.30
25	A	2267	A	C2-N3-C4	10.13	115.67	110.60
25	A	546	U	N3-C2-O2	-10.12	115.11	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	v	61	C	N1-C2-O2	10.11	124.97	118.90
22	v	56	C	C5-C6-N1	10.06	126.03	121.00
25	A	2072	C	C2-N1-C1'	10.03	129.83	118.80
1	a	1427	C	C6-N1-C2	-10.02	116.29	120.30
1	a	1158	C	N1-C2-O2	10.02	124.91	118.90
22	v	61	C	C2-N1-C1'	10.01	129.81	118.80
25	A	2150	C	N1-C2-N3	10.00	126.20	119.20
25	A	62	U	C2-N1-C1'	9.95	129.64	117.70
24	y	74	C	C2-N1-C1'	9.94	129.73	118.80
1	a	78	A	N1-C2-N3	-9.93	124.34	129.30
25	A	2150	C	C2-N3-C4	-9.92	114.94	119.90
22	v	68	C	C6-N1-C2	-9.91	116.34	120.30
25	A	850	U	N1-C2-O2	9.90	129.73	122.80
22	v	61	C	O4'-C1'-N1	9.88	116.10	108.20
25	A	62	U	N3-C2-O2	-9.87	115.29	122.20
1	a	735	C	C6-N1-C2	-9.87	116.35	120.30
26	B	4	C	C6-N1-C2	-9.82	116.37	120.30
1	a	735	C	C5-C6-N1	9.81	125.91	121.00
22	v	58	A	C2-N3-C4	9.79	115.50	110.60
1	a	1141	C	N3-C2-O2	-9.79	115.05	121.90
25	A	305	C	C5-C6-N1	9.76	125.88	121.00
1	a	1134	G	N1-C6-O6	-9.71	114.08	119.90
23	x	125	G	N9-C1'-C2'	-9.70	101.33	112.00
1	a	1146	A	N1-C6-N6	-9.69	112.78	118.60
25	A	1830	C	C6-N1-C2	-9.67	116.43	120.30
25	A	1081	U	N3-C2-O2	-9.67	115.43	122.20
26	B	26	C	N1-C2-O2	9.63	124.68	118.90
1	a	332	G	N1-C6-O6	-9.59	114.15	119.90
25	A	691	C	C6-N1-C2	-9.59	116.47	120.30
1	a	1382	C	C6-N1-C2	-9.58	116.47	120.30
22	v	68	C	C5-C6-N1	9.57	125.78	121.00
1	a	1007	U	N3-C2-O2	-9.56	115.50	122.20
24	y	74	C	C6-N1-C2	-9.54	116.49	120.30
1	a	979	C	C6-N1-C2	-9.52	116.49	120.30
1	a	1263	C	C5-C6-N1	9.51	125.75	121.00
1	a	658	C	N1-C2-O2	9.50	124.60	118.90
26	B	12	C	C6-N1-C2	-9.46	116.52	120.30
26	B	30	C	C6-N1-C2	-9.44	116.53	120.30
22	v	74	C	C5-C6-N1	9.42	125.71	121.00
25	A	2117	A	C5-C6-N6	-9.39	116.19	123.70
1	a	1469	C	N1-C2-O2	9.36	124.52	118.90
22	v	19	G	O4'-C1'-N9	-9.35	100.72	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	a	580	C	C5-C6-N1	9.35	125.67	121.00
1	a	754	C	C2-N1-C1'	9.30	129.03	118.80
25	A	143	C	C5-C6-N1	9.30	125.65	121.00
1	a	215	C	C2-N1-C1'	9.29	129.02	118.80
25	A	1774	C	N3-C2-O2	-9.29	115.40	121.90
25	A	2110	G	C5-C6-O6	9.28	134.17	128.60
25	A	990	A	N1-C6-N6	-9.26	113.05	118.60
25	A	2751	G	C2-N3-C4	9.24	116.52	111.90
25	A	120	U	C5-C4-O4	-9.23	120.36	125.90
22	v	51	C	C5-C6-N1	9.23	125.61	121.00
13	m	65	GLU	N-CA-CB	-9.22	94.00	110.60
1	a	1075	U	N3-C2-O2	-9.22	115.75	122.20
22	v	51	C	C6-N1-C2	-9.21	116.61	120.30
23	x	117	C	N1-C2-O2	9.21	124.43	118.90
1	a	1382	C	N1-C2-O2	9.19	124.41	118.90
25	A	795	C	C6-N1-C2	-9.17	116.63	120.30
25	A	135	U	N1-C2-O2	9.14	129.20	122.80
25	A	1956	U	N3-C2-O2	-9.14	115.80	122.20
22	v	61	C	C4-C5-C6	9.12	121.96	117.40
23	x	117	C	C2-N1-C1'	9.12	128.83	118.80
23	x	121	U	N1-C1'-C2'	-9.11	101.98	112.00
1	a	470	C	C5-C6-N1	9.10	125.55	121.00
25	A	998	C	C5-C6-N1	9.07	125.54	121.00
25	A	1993	U	N3-C2-O2	-9.06	115.86	122.20
1	a	1306	A	C8-N9-C4	-9.02	102.19	105.80
1	a	1382	C	N3-C2-O2	-9.01	115.59	121.90
25	A	2292	U	C5-C6-N1	9.00	127.20	122.70
1	a	1158	C	N3-C2-O2	-8.98	115.61	121.90
25	A	2683	C	N1-C2-O2	8.97	124.28	118.90
1	a	141	G	N3-C2-N2	-8.96	113.63	119.90
1	a	1027	C	C5-C6-N1	8.95	125.47	121.00
25	A	281	C	C5-C6-N1	8.95	125.47	121.00
1	a	1225	A	N9-C4-C5	-8.91	102.24	105.80
25	A	1843	C	C5-C6-N1	8.91	125.45	121.00
1	a	397	A	C2-N3-C4	8.90	115.05	110.60
25	A	2110	G	N3-C4-N9	-8.90	120.66	126.00
1	a	322	C	C5-C6-N1	8.89	125.44	121.00
25	A	610	C	C6-N1-C2	-8.86	116.75	120.30
1	a	1158	C	C2-N1-C1'	8.86	128.55	118.80
1	a	1245	C	C5-C6-N1	8.84	125.42	121.00
1	a	215	C	N1-C2-O2	8.81	124.19	118.90
25	A	2805	C	C6-N1-C2	-8.75	116.80	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	a	78	A	N9-C4-C5	-8.73	102.31	105.80
24	y	47(O)	C	C5-C6-N1	8.72	125.36	121.00
25	A	281	C	N3-C2-O2	-8.72	115.80	121.90
25	A	1348	C	N1-C2-O2	8.72	124.13	118.90
25	A	669	G	N3-C4-C5	-8.70	124.25	128.60
25	A	946	C	C6-N1-C2	-8.70	116.82	120.30
1	a	1497	G	C2-N3-C4	8.70	116.25	111.90
22	v	1	C	C2-N3-C4	8.69	124.24	119.90
25	A	288	U	N3-C2-O2	-8.68	116.13	122.20
1	a	1263	C	C6-N1-C2	-8.67	116.83	120.30
1	a	87	C	C6-N1-C2	-8.65	116.84	120.30
1	a	603	U	N3-C2-O2	-8.65	116.14	122.20
25	A	2439	A	C2-N3-C4	8.64	114.92	110.60
24	y	47(O)	C	C6-N1-C2	-8.63	116.85	120.30
22	v	75	C	N1-C2-O2	8.63	124.08	118.90
23	x	121	U	N1-C2-O2	8.62	128.84	122.80
25	A	1498	C	C2-N1-C1'	8.62	128.29	118.80
1	a	993	G	N3-C4-N9	8.62	131.17	126.00
25	A	1956	U	N1-C2-O2	8.62	128.83	122.80
1	a	322	C	N3-C2-O2	-8.60	115.88	121.90
1	a	1384	C	N1-C2-O2	8.60	124.06	118.90
25	A	120	U	N3-C4-O4	8.60	125.42	119.40
22	v	18	G	O5'-P-OP2	-8.57	97.99	105.70
25	A	795	C	C5-C6-N1	8.57	125.28	121.00
25	A	1101	U	N3-C2-O2	-8.54	116.22	122.20
22	v	19	G	N1-C6-O6	-8.54	114.78	119.90
1	a	618	C	N1-C2-O2	8.53	124.02	118.90
25	A	850	U	N3-C2-O2	-8.53	116.23	122.20
22	v	60	U	C5-C6-N1	8.53	126.96	122.70
1	a	307	C	N1-C2-O2	8.52	124.01	118.90
22	v	61	C	N3-C2-O2	-8.50	115.95	121.90
1	a	1134	G	C6-C5-N7	8.50	135.50	130.40
25	A	2617	U	N3-C2-O2	-8.46	116.28	122.20
25	A	305	C	C6-N1-C2	-8.41	116.94	120.30
25	A	542	C	N3-C4-N4	-8.41	112.11	118.00
23	x	117	C	O5'-P-OP1	-8.41	98.13	105.70
25	A	2200	C	C5-C6-N1	8.41	125.20	121.00
1	a	419	C	O4'-C1'-N1	8.40	114.92	108.20
25	A	1830	C	C2-N1-C1'	8.40	128.04	118.80
25	A	546	U	N1-C2-O2	8.39	128.67	122.80
25	A	257	C	N1-C2-O2	8.36	123.92	118.90
26	B	70	C	C6-N1-C2	-8.35	116.96	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	A	2226	C	N1-C2-O2	8.35	123.91	118.90
1	a	340	U	N1-C2-O2	8.31	128.62	122.80
25	A	137	U	N3-C2-O2	-8.31	116.38	122.20
25	A	2474	U	N3-C2-O2	-8.31	116.38	122.20
1	a	206	C	C2-N3-C4	-8.31	115.75	119.90
1	a	891	U	C5-C6-N1	8.29	126.85	122.70
25	A	545	U	N1-C1'-C2'	-8.29	102.88	112.00
25	A	2179	C	N3-C2-O2	-8.28	116.10	121.90
25	A	1680	U	C6-N1-C2	-8.28	116.03	121.00
25	A	1656	C	C6-N1-C2	-8.27	116.99	120.30
25	A	542	C	N1-C2-O2	8.26	123.86	118.90
25	A	2473	U	N3-C2-O2	-8.22	116.44	122.20
25	A	2884	U	N3-C2-O2	-8.22	116.44	122.20
22	v	61	C	P-O3'-C3'	8.22	129.56	119.70
25	A	1170	C	C5-C6-N1	8.21	125.11	121.00
25	A	359	G	C6-N1-C2	-8.20	120.18	125.10
1	a	103	U	N3-C2-O2	-8.19	116.47	122.20
25	A	2720	U	N1-C2-O2	8.19	128.53	122.80
24	y	59	C	N1-C2-O2	8.17	123.80	118.90
25	A	2720	U	N3-C2-O2	-8.17	116.48	122.20
25	A	542	C	C5-C4-N4	8.16	125.91	120.20
1	a	548	G	N9-C4-C5	-8.15	102.14	105.40
25	A	2179	C	N1-C2-O2	8.12	123.77	118.90
26	B	26	C	N3-C2-O2	-8.11	116.22	121.90
1	a	1119	C	C6-N1-C2	-8.10	117.06	120.30
22	v	23	C	C6-N1-C2	-8.09	117.06	120.30
25	A	998	C	C6-N1-C2	-8.09	117.06	120.30
25	A	2666	C	N1-C2-O2	8.09	123.75	118.90
1	a	215	C	C5-C6-N1	8.08	125.04	121.00
1	a	598	U	N3-C2-O2	-8.07	116.55	122.20
24	y	47(P)	C	N1-C2-O2	8.06	123.74	118.90
25	A	2473	U	N1-C2-O2	8.06	128.44	122.80
25	A	1803	A	N1-C2-N3	8.05	133.33	129.30
25	A	2649	C	C5-C6-N1	8.05	125.03	121.00
25	A	1799	G	C5-C6-O6	-8.05	123.77	128.60
25	A	154	U	C5-C6-N1	8.05	126.72	122.70
1	a	16	A	C6-N1-C2	8.04	123.42	118.60
25	A	2063	C	N3-C2-O2	-8.03	116.28	121.90
24	y	47(P)	C	C2-N1-C1'	8.03	127.63	118.80
1	a	440	C	C6-N1-C2	-8.03	117.09	120.30
1	a	979	C	N3-C2-O2	-8.02	116.29	121.90
1	a	1134	G	N3-C4-N9	-8.01	121.19	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	a	754	C	C6-N1-C1'	-7.99	111.21	120.80
25	A	691	C	C5-C6-N1	7.98	124.99	121.00
1	a	420	U	N3-C2-O2	-7.97	116.62	122.20
25	A	2110	G	N1-C6-O6	-7.97	115.12	119.90
25	A	2555	U	C5-C6-N1	7.96	126.68	122.70
1	a	252	U	N3-C2-O2	-7.95	116.63	122.20
1	a	1406	U	N3-C2-O2	-7.95	116.63	122.20
1	a	221	C	C6-N1-C2	-7.95	117.12	120.30
25	A	560	C	C5-C6-N1	7.94	124.97	121.00
1	a	1182	G	OP2-P-O3'	7.93	122.64	105.20
23	x	118	G	OP1-P-OP2	-7.92	107.72	119.60
25	A	154	U	C5-C4-O4	-7.91	121.15	125.90
25	A	1927	A	N7-C8-N9	7.90	117.75	113.80
25	A	1101	U	N1-C2-O2	7.90	128.33	122.80
1	a	1096	C	C6-N1-C2	-7.90	117.14	120.30
25	A	2462	C	C5-C6-N1	7.89	124.95	121.00
25	A	67	U	N3-C4-O4	7.88	124.92	119.40
22	v	18	G	C8-N9-C4	-7.88	103.25	106.40
24	y	47(C)	C	C5-C6-N1	7.86	124.93	121.00
25	A	965	C	C5-C6-N1	7.86	124.93	121.00
1	a	207	C	N3-C2-O2	-7.85	116.40	121.90
25	A	933	A	C2-N3-C4	7.85	114.52	110.60
26	B	12	C	N3-C2-O2	-7.84	116.41	121.90
25	A	1680	U	N3-C2-O2	-7.82	116.73	122.20
1	a	168	G	N9-C4-C5	-7.82	102.27	105.40
22	v	56	C	C2-N1-C1'	7.81	127.39	118.80
23	x	127	U	P-O3'-C3'	7.81	129.07	119.70
23	x	118	G	O5'-P-OP2	7.80	120.06	110.70
1	a	1463	U	N3-C2-O2	-7.80	116.74	122.20
25	A	1595	C	C5-C6-N1	7.79	124.89	121.00
25	A	1993	U	N1-C2-O2	7.76	128.24	122.80
1	a	1496	C	C6-N1-C2	-7.75	117.20	120.30
25	A	1114	C	C5-C6-N1	7.75	124.87	121.00
1	a	1158	C	C6-N1-C2	-7.74	117.20	120.30
25	A	136	G	N1-C6-O6	-7.74	115.26	119.90
22	v	61	C	C2-N3-C4	7.73	123.77	119.90
25	A	883	G	N7-C8-N9	7.73	116.97	113.10
1	a	1109	C	N1-C2-O2	7.73	123.54	118.90
25	A	550	C	C5-C6-N1	7.71	124.86	121.00
1	a	936	C	C6-N1-C2	-7.70	117.22	120.30
1	a	923	A	N7-C8-N9	7.69	117.64	113.80
1	a	735	C	C2-N1-C1'	7.68	127.25	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	A	1348	C	C6-N1-C2	-7.67	117.23	120.30
25	A	1075	C	C2-N3-C4	7.66	123.73	119.90
25	A	1092	C	C6-N1-C2	-7.66	117.23	120.30
25	A	2649	C	C6-N1-C2	-7.66	117.23	120.30
1	a	979	C	N1-C2-O2	7.66	123.50	118.90
25	A	813	U	N3-C2-O2	-7.64	116.85	122.20
1	a	737	C	C5-C6-N1	7.64	124.82	121.00
23	x	126	G	P-O3'-C3'	7.64	128.87	119.70
1	a	1119	C	C5-C6-N1	7.63	124.82	121.00
24	y	35	C	N3-C4-N4	7.62	123.34	118.00
25	A	1057	A	N9-C4-C5	-7.62	102.75	105.80
1	a	580	C	C6-N1-C2	-7.62	117.25	120.30
25	A	946	C	C5-C6-N1	7.62	124.81	121.00
22	v	56	C	P-O3'-C3'	7.62	128.84	119.70
25	A	1053	C	C5-C6-N1	7.61	124.81	121.00
25	A	33	C	C6-N1-C2	-7.61	117.26	120.30
22	v	39	C	C2-N1-C1'	7.60	127.16	118.80
23	x	127	U	O4'-C1'-N1	7.59	114.28	108.20
25	A	2075	U	C5-C4-O4	-7.59	121.34	125.90
1	a	1258	G	N3-C2-N2	-7.59	114.59	119.90
25	A	2063	C	C6-N1-C2	-7.59	117.27	120.30
1	a	1245	C	C6-N1-C2	-7.58	117.27	120.30
25	A	2566	A	OP2-P-O3'	7.58	121.87	105.20
25	A	358	U	N3-C2-O2	-7.56	116.91	122.20
22	v	17	C	P-O3'-C3'	7.55	128.76	119.70
25	A	2840	C	C5-C6-N1	7.55	124.77	121.00
1	a	491	G	N3-C4-N9	7.54	130.52	126.00
25	A	1159	U	N3-C2-O2	-7.54	116.92	122.20
25	A	1053	C	C6-N1-C2	-7.53	117.29	120.30
25	A	154	U	C2-N1-C1'	7.52	126.73	117.70
1	a	1404	C	C6-N1-C2	-7.52	117.29	120.30
24	y	47(E)	G	C5-N7-C8	7.52	108.06	104.30
25	A	2179	C	C2-N3-C4	7.52	123.66	119.90
24	y	47(C)	C	C6-N1-C2	-7.51	117.30	120.30
25	A	2884	U	N1-C2-O2	7.51	128.06	122.80
1	a	491	G	N9-C4-C5	-7.50	102.40	105.40
1	a	1395	C	N1-C2-O2	7.50	123.40	118.90
25	A	283	G	N3-C2-N2	-7.50	114.65	119.90
25	A	2450	A	C6-N1-C2	7.49	123.09	118.60
25	A	2099	U	C5-C6-N1	7.48	126.44	122.70
1	a	1263	C	C2-N1-C1'	7.47	127.02	118.80
1	a	611	C	N1-C2-O2	7.47	123.38	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	A	1585	C	N1-C2-O2	7.47	123.38	118.90
25	A	2200	C	C6-N1-C2	-7.47	117.31	120.30
25	A	1294	U	N1-C2-O2	7.46	128.02	122.80
25	A	2474	U	N1-C2-O2	7.46	128.02	122.80
25	A	2666	C	N3-C2-O2	-7.44	116.69	121.90
25	A	551	G	C2-N3-C4	-7.43	108.18	111.90
25	A	1349	C	C6-N1-C2	-7.43	117.33	120.30
1	a	168	G	N1-C6-O6	7.43	124.36	119.90
25	A	669	G	C4-N9-C1'	7.43	136.16	126.50
25	A	2175	C	N1-C2-O2	7.43	123.36	118.90
1	a	1538	C	N1-C2-O2	-7.42	114.44	118.90
25	A	1111	A	P-O3'-C3'	7.42	128.60	119.70
23	x	122	G	C5-N7-C8	7.42	108.01	104.30
25	A	1929	G	C8-N9-C4	-7.42	103.43	106.40
1	a	754	C	N3-C2-O2	-7.41	116.71	121.90
1	a	1384	C	C2-N1-C1'	7.41	126.95	118.80
1	a	1003	G	N1-C6-O6	-7.40	115.46	119.90
22	v	60	U	C6-N1-C2	-7.40	116.56	121.00
1	a	87	C	N3-C4-C5	-7.39	118.94	121.90
25	A	1114	C	C6-N1-C2	-7.39	117.34	120.30
1	a	618	C	N3-C2-O2	-7.38	116.73	121.90
22	v	18	G	N3-C4-N9	-7.37	121.58	126.00
22	v	17(A)	U	OP1-P-O3'	7.37	121.42	105.20
1	a	224	U	N3-C2-O2	-7.37	117.04	122.20
25	A	550	C	C6-N1-C2	-7.35	117.36	120.30
25	A	2117	A	N1-C6-N6	7.34	123.00	118.60
1	a	431	A	N1-C6-N6	-7.34	114.20	118.60
55	4	14	CYS	CA-CB-SG	7.33	127.20	114.00
25	A	2462	C	C6-N1-C2	-7.33	117.37	120.30
25	A	1803	A	N7-C8-N9	7.33	117.46	113.80
1	a	1406	U	N1-C2-O2	7.32	127.92	122.80
1	a	217	C	C6-N1-C2	-7.31	117.38	120.30
25	A	2558	C	C5-C6-N1	7.31	124.66	121.00
1	a	1227	A	C5-C6-N6	-7.31	117.85	123.70
25	A	274	C	N3-C2-O2	-7.31	116.78	121.90
25	A	2150	C	C6-N1-C1'	7.31	129.57	120.80
25	A	898	C	C6-N1-C2	-7.30	117.38	120.30
25	A	67	U	C5-C4-O4	-7.30	121.52	125.90
25	A	1052	C	C5-C6-N1	7.29	124.65	121.00
25	A	1171	G	N3-C4-N9	-7.29	121.63	126.00
1	a	406	G	C6-C5-N7	-7.28	126.03	130.40
25	A	832	U	N3-C2-O2	-7.27	117.11	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	A	1348	C	N3-C2-O2	-7.27	116.81	121.90
1	a	82	G	N1-C6-O6	-7.26	115.54	119.90
1	a	1225	A	C4-C5-N7	7.25	114.33	110.70
25	A	257	C	N3-C2-O2	-7.25	116.82	121.90
1	a	1134	G	C5-C6-O6	7.25	132.95	128.60
25	A	2267	A	N1-C6-N6	-7.25	114.25	118.60
1	a	406	G	N9-C4-C5	-7.24	102.50	105.40
25	A	359	G	C2-N3-C4	7.24	115.52	111.90
1	a	496	A	C2-N3-C4	7.24	114.22	110.60
25	A	2150	C	N1-C2-O2	-7.24	114.56	118.90
25	A	2610	C	P-O3'-C3'	7.23	128.37	119.70
25	A	1803	A	C2-N3-C4	-7.23	106.99	110.60
1	a	1120	C	C6-N1-C2	-7.22	117.41	120.30
1	a	406	G	N3-C4-N9	7.22	130.33	126.00
25	A	278	A	C2-N3-C4	7.21	114.21	110.60
25	A	1314	C	C6-N1-C2	-7.21	117.41	120.30
1	a	141	G	C2-N3-C4	7.21	115.51	111.90
25	A	552	U	N3-C2-O2	-7.20	117.16	122.20
25	A	2427	C	OP1-P-O3'	7.19	121.01	105.20
25	A	2752	C	N1-C2-O2	7.18	123.21	118.90
1	a	16	A	N1-C2-N3	-7.18	125.71	129.30
25	A	420	C	C2-N1-C1'	7.17	126.69	118.80
25	A	2723	C	C6-N1-C2	-7.17	117.43	120.30
25	A	1994	C	C6-N1-C2	-7.17	117.43	120.30
25	A	2379	G	N9-C4-C5	-7.17	102.53	105.40
25	A	2072	C	N1-C2-O2	7.16	123.20	118.90
22	v	18	G	C8-N9-C1'	7.16	136.31	127.00
25	A	1052	C	C6-N1-C2	-7.15	117.44	120.30
1	a	737	C	C6-N1-C2	-7.15	117.44	120.30
1	a	1152	A	N9-C4-C5	-7.15	102.94	105.80
25	A	1800	C	C5-C6-N1	7.15	124.57	121.00
1	a	470	C	C6-N1-C2	-7.14	117.44	120.30
1	a	56	U	C5-C6-N1	7.14	126.27	122.70
25	A	1082	U	N3-C2-O2	-7.14	117.20	122.20
26	B	31	C	C6-N1-C2	-7.12	117.45	120.30
1	a	962	C	N1-C2-O2	7.12	123.17	118.90
1	a	1134	G	N9-C4-C5	7.12	108.25	105.40
24	y	6	U	N3-C2-O2	-7.12	117.21	122.20
25	A	2898	U	C5-C6-N1	7.12	126.26	122.70
25	A	1362	C	C5-C6-N1	7.12	124.56	121.00
1	a	1379	G	N1-C6-O6	-7.12	115.63	119.90
25	A	91	A	P-O3'-C3'	7.11	128.24	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	a	142	G	C2-N3-C4	7.11	115.45	111.90
23	x	109	C	N1-C2-O2	7.11	123.16	118.90
1	a	1033	G	N3-C4-N9	7.10	130.26	126.00
25	A	2185	U	N3-C2-O2	-7.10	117.23	122.20
26	B	60	C	C5-C6-N1	7.10	124.55	121.00
25	A	2765	A	C2-N3-C4	7.10	114.15	110.60
25	A	551	G	C5-C6-N1	-7.09	107.95	111.50
25	A	1092	C	C5-C6-N1	7.09	124.54	121.00
25	A	1103	A	OP1-P-O3'	7.08	120.78	105.20
1	a	1469	C	N3-C2-O2	-7.08	116.94	121.90
25	A	274	C	C6-N1-C2	-7.07	117.47	120.30
1	a	805	C	C2-N1-C1'	7.07	126.58	118.80
25	A	2194	U	C5-C6-N1	7.07	126.23	122.70
22	v	58	A	C8-N9-C4	-7.06	102.98	105.80
1	a	1259	C	C6-N1-C2	-7.05	117.48	120.30
25	A	2101	A	N7-C8-N9	7.05	117.33	113.80
1	a	1113	C	C2-N1-C1'	7.05	126.55	118.80
25	A	1970	A	N1-C6-N6	-7.05	114.37	118.60
37	M	58	LYS	N-CA-CB	-7.05	97.91	110.60
25	A	1539	U	C5-C6-N1	7.05	126.22	122.70
1	a	1538	C	C2-N3-C4	-7.04	116.38	119.90
1	a	580	C	C2-N1-C1'	7.04	126.55	118.80
26	B	42	C	N1-C2-O2	7.04	123.13	118.90
25	A	2135	A	P-O3'-C3'	7.04	128.15	119.70
1	a	610	U	N3-C2-O2	-7.04	117.27	122.20
1	a	1033	G	C6-C5-N7	-7.04	126.18	130.40
25	A	1102	C	C6-N1-C2	-7.04	117.48	120.30
1	a	1510	C	C6-N1-C2	-7.03	117.49	120.30
24	y	47(E)	G	O4'-C1'-N9	7.03	113.83	108.20
25	A	669	G	C2-N3-C4	7.03	115.41	111.90
1	a	215	C	C6-N1-C1'	-7.02	112.38	120.80
1	a	658	C	N3-C2-O2	-7.01	116.99	121.90
25	A	2758	A	N1-C6-N6	-7.00	114.40	118.60
25	A	2120	G	N3-C4-C5	-7.00	125.10	128.60
1	a	1027	C	C6-N1-C2	-7.00	117.50	120.30
1	a	1075	U	N1-C2-O2	6.99	127.70	122.80
1	a	1296	C	C6-N1-C2	-6.99	117.50	120.30
1	a	322	C	N1-C2-O2	6.98	123.09	118.90
25	A	2568	U	C5-C6-N1	6.98	126.19	122.70
23	x	117	C	C6-N1-C1'	-6.98	112.43	120.80
1	a	1344	C	C6-N1-C2	-6.98	117.51	120.30
1	a	284	C	C6-N1-C2	-6.97	117.51	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	a	307	C	N3-C2-O2	-6.97	117.02	121.90
1	a	1325	C	C6-N1-C2	-6.96	117.52	120.30
1	a	556	C	C5-C6-N1	6.96	124.48	121.00
25	A	302	C	C5-C6-N1	6.96	124.48	121.00
25	A	669	G	N3-C4-N9	6.96	130.18	126.00
25	A	1362	C	C6-N1-C2	-6.96	117.52	120.30
26	B	97	C	C2-N1-C1'	6.95	126.45	118.80
1	a	1235	U	C5-C6-N1	6.95	126.17	122.70
22	v	75	C	N3-C2-O2	-6.95	117.04	121.90
1	a	1412	C	C6-N1-C2	-6.93	117.53	120.30
1	a	550	G	C4-C5-N7	6.93	113.57	110.80
25	A	2417	C	C6-N1-C2	-6.93	117.53	120.30
25	A	305	C	N1-C2-O2	6.92	123.05	118.90
25	A	1314	C	C5-C6-N1	6.92	124.46	121.00
25	A	1152	C	C6-N1-C2	-6.92	117.53	120.30
1	a	1393	U	N3-C2-O2	-6.91	117.36	122.20
25	A	143	C	N1-C2-O2	6.91	123.04	118.90
25	A	1730	C	C6-N1-C2	-6.91	117.54	120.30
25	A	2782	G	C6-C5-N7	-6.90	126.26	130.40
25	A	2076	U	N1-C2-O2	6.89	127.63	122.80
26	B	12	C	N1-C2-O2	6.89	123.03	118.90
25	A	1314	C	C2-N1-C1'	6.89	126.38	118.80
1	a	207	C	C6-N1-C2	-6.88	117.55	120.30
1	a	355	C	C5-C6-N1	6.87	124.43	121.00
25	A	2751	G	N3-C4-C5	-6.87	125.17	128.60
1	a	552	U	C5-C6-N1	6.86	126.13	122.70
25	A	610	C	C2-N1-C1'	6.86	126.35	118.80
25	A	62	U	C5-C6-N1	6.86	126.13	122.70
25	A	1656	C	C5-C6-N1	6.86	124.43	121.00
1	a	294	U	C5-C6-N1	6.85	126.12	122.70
1	a	168	G	C6-C5-N7	-6.84	126.29	130.40
25	A	302	C	C6-N1-C2	-6.84	117.56	120.30
25	A	183	C	N3-C2-O2	-6.83	117.12	121.90
25	A	1188	U	N1-C2-O2	6.83	127.58	122.80
1	a	1227	A	N1-C6-N6	6.83	122.69	118.60
26	B	45	A	C5-C6-N1	6.83	121.11	117.70
25	A	2076	U	N3-C2-O2	-6.82	117.42	122.20
25	A	2379	G	N1-C6-O6	6.82	123.99	119.90
25	A	357	C	C6-N1-C2	-6.82	117.57	120.30
25	A	872	U	C5-C6-N1	6.82	126.11	122.70
25	A	222	A	O4'-C1'-N9	-6.82	102.75	108.20
25	A	2452	C	N3-C2-O2	-6.82	117.13	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	206	U	C5-C6-N1	6.82	126.11	122.70
25	A	2379	G	C6-C5-N7	-6.82	126.31	130.40
56	6	18	CYS	CA-CB-SG	-6.82	101.73	114.00
22	v	39	C	C5-C6-N1	6.81	124.41	121.00
25	A	154	U	N3-C4-O4	6.80	124.16	119.40
1	a	722	G	C2-N3-C4	6.80	115.30	111.90
1	a	1003	G	C5-C6-O6	6.80	132.68	128.60
25	A	2818	U	N1-C2-O2	6.80	127.56	122.80
25	A	2127	G	N1-C2-N2	-6.80	110.08	116.20
1	a	63	C	C5-C6-N1	6.79	124.40	121.00
25	A	546	U	C6-N1-C2	-6.79	116.93	121.00
25	A	1960	A	N9-C4-C5	-6.78	103.09	105.80
1	a	1296	C	C5-C6-N1	6.77	124.39	121.00
1	a	1087	G	N9-C4-C5	-6.77	102.69	105.40
25	A	2617	U	N1-C2-O2	6.77	127.54	122.80
1	a	883	C	C5-C6-N1	6.76	124.38	121.00
25	A	2170	A	C5-C6-N6	-6.76	118.29	123.70
1	a	1003	G	N3-C2-N2	-6.76	115.17	119.90
1	a	612	C	C6-N1-C2	-6.76	117.60	120.30
25	A	2044	C	C6-N1-C2	-6.75	117.60	120.30
25	A	2448	A	C2-N3-C4	-6.75	107.22	110.60
25	A	2075	U	N3-C4-O4	6.74	124.12	119.40
1	a	756	C	N1-C2-O2	6.74	122.94	118.90
25	A	1140	C	C2-N1-C1'	6.74	126.21	118.80
22	v	23	C	C5-C6-N1	6.74	124.37	121.00
1	a	284	C	C5-C6-N1	6.73	124.37	121.00
1	a	506	G	N9-C4-C5	-6.73	102.71	105.40
25	A	359	G	N1-C2-N2	6.72	122.25	116.20
25	A	840	C	C5-C6-N1	6.72	124.36	121.00
25	A	2515	C	C5-C6-N1	6.72	124.36	121.00
26	B	26	C	C6-N1-C2	-6.72	117.61	120.30
1	a	322	C	N3-C4-C5	-6.72	119.21	121.90
1	a	1427	C	C5-C6-N1	6.72	124.36	121.00
1	a	1232	U	N3-C2-O2	-6.71	117.50	122.20
1	a	548	G	C4-C5-N7	6.71	113.48	110.80
1	a	1109	C	N3-C2-O2	-6.71	117.20	121.90
22	v	75	C	C2-N1-C1'	6.71	126.18	118.80
1	a	808	C	C6-N1-C2	-6.71	117.62	120.30
1	a	977	A	C2-N3-C4	6.71	113.95	110.60
1	a	220	G	C5-C6-O6	-6.70	124.58	128.60
1	a	1259	C	C5-C6-N1	6.70	124.35	121.00
25	A	2782	G	N9-C4-C5	-6.69	102.72	105.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	2840	C	C6-N1-C2	-6.69	117.62	120.30
1	a	240	G	N9-C4-C5	-6.69	102.72	105.40
25	A	2794	C	C5-C6-N1	6.69	124.35	121.00
1	a	1134	G	C8-N9-C1'	6.69	135.70	127.00
1	a	332	G	C6-C5-N7	6.69	134.41	130.40
25	A	837	C	N3-C2-O2	-6.68	117.22	121.90
1	a	934	C	O4'-C1'-N1	-6.68	102.86	108.20
1	a	961	U	N1-C2-O2	6.68	127.48	122.80
25	A	1057	A	N1-C2-N3	-6.68	125.96	129.30
25	A	658	U	C5-C6-N1	6.67	126.04	122.70
1	a	491	G	C4-C5-N7	6.67	113.47	110.80
25	A	33	C	C5-C6-N1	6.67	124.33	121.00
25	A	2226	C	N3-C2-O2	-6.67	117.23	121.90
24	y	10	C	C5-C6-N1	6.67	124.33	121.00
1	a	78	A	C4-C5-N7	6.66	114.03	110.70
1	a	1119	C	C2-N1-C1'	6.66	126.13	118.80
1	a	527	G7M	P-O3'-C3'	6.66	127.69	119.70
1	a	1357	A	C8-N9-C4	-6.66	103.14	105.80
25	A	1830	C	C5-C6-N1	6.65	124.33	121.00
25	A	1088	A	N1-C6-N6	-6.65	114.61	118.60
25	A	1774	C	C6-N1-C2	-6.65	117.64	120.30
25	A	1669	A	C2-N3-C4	6.64	113.92	110.60
25	A	2683	C	N3-C2-O2	-6.64	117.25	121.90
25	A	2751	G	N1-C6-O6	-6.64	115.92	119.90
1	a	406	G	C8-N9-C1'	-6.64	118.37	127.00
1	a	1113	C	N1-C2-O2	6.64	122.88	118.90
25	A	542	C	C6-N1-C2	-6.63	117.65	120.30
25	A	2782	G	C4-C5-N7	6.63	113.45	110.80
1	a	984	C	C6-N1-C2	-6.63	117.65	120.30
1	a	1507	A	P-O3'-C3'	6.63	127.65	119.70
1	a	978	A	N1-C6-N6	-6.62	114.63	118.60
25	A	1675	C	N1-C2-O2	6.62	122.87	118.90
25	A	2254	C	N1-C2-O2	6.62	122.87	118.90
25	A	1088	A	N1-C2-N3	-6.61	125.99	129.30
25	A	687	C	N1-C2-O2	6.61	122.87	118.90
25	A	343	C	N1-C2-O2	6.61	122.87	118.90
25	A	2282	G	N9-C4-C5	6.61	108.04	105.40
25	A	544	C	C6-N1-C2	-6.61	117.66	120.30
1	a	1003	G	N9-C4-C5	6.60	108.04	105.40
25	A	2006	C	C2-N1-C1'	6.60	126.06	118.80
22	v	57	A	N3-C4-N9	-6.60	122.12	127.40
25	A	1298	C	C6-N1-C2	-6.59	117.66	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	A	1774	C	N1-C2-O2	6.59	122.85	118.90
25	A	383	C	N1-C2-O2	6.58	122.85	118.90
25	A	2794	C	N1-C2-O2	6.58	122.85	118.90
22	v	57	A	C6-C5-N7	6.58	136.91	132.30
1	a	225	C	C6-N1-C2	-6.58	117.67	120.30
1	a	439	U	N1-C2-O2	6.58	127.40	122.80
1	a	1072	G	C6-C5-N7	-6.58	126.45	130.40
24	y	47(E)	G	C4-C5-N7	-6.57	108.17	110.80
25	A	281	C	C2-N3-C4	6.57	123.19	119.90
25	A	420	C	C5-C6-N1	6.57	124.28	121.00
1	a	1384	C	C5-C6-N1	6.57	124.28	121.00
25	A	618	G	N3-C4-C5	-6.57	125.32	128.60
25	A	1313	U	C6-N1-C1'	-6.57	112.01	121.20
1	a	783	C	C6-N1-C2	-6.56	117.67	120.30
1	a	142	G	N1-C6-O6	-6.56	115.96	119.90
1	a	491	G	C5-C6-O6	-6.56	124.66	128.60
25	A	359	G	C5-C6-O6	-6.56	124.67	128.60
1	a	295	C	C2-N1-C1'	6.56	126.01	118.80
25	A	183	C	N1-C2-O2	6.55	122.83	118.90
22	v	66	C	N1-C2-O2	6.55	122.83	118.90
25	A	2430	A	C2-N3-C4	6.54	113.87	110.60
25	A	550	C	C2-N1-C1'	6.54	126.00	118.80
25	A	2175	C	N3-C2-O2	-6.54	117.32	121.90
23	x	133	C	P-O3'-C3'	6.54	127.55	119.70
25	A	1290	C	C5-C6-N1	6.54	124.27	121.00
25	A	2416	C	C5-C6-N1	6.54	124.27	121.00
22	v	58	A	N3-C4-C5	-6.53	122.23	126.80
24	y	35	C	C2-N3-C4	6.53	123.16	119.90
25	A	290	U	C5-C6-N1	6.53	125.96	122.70
1	a	29	U	N3-C2-O2	-6.52	117.63	122.20
25	A	1402	U	N3-C2-O2	-6.52	117.63	122.20
25	A	1564	C	C5-C6-N1	6.52	124.26	121.00
22	v	39	C	C6-N1-C2	-6.52	117.69	120.30
25	A	12	U	N3-C2-O2	-6.52	117.64	122.20
25	A	1585	C	N3-C2-O2	-6.51	117.34	121.90
1	a	837	U	N1-C2-O2	6.51	127.36	122.80
1	a	563	A	N9-C4-C5	-6.51	103.20	105.80
26	B	31	C	C2-N1-C1'	6.51	125.96	118.80
1	a	993	G	N3-C4-C5	-6.49	125.35	128.60
1	a	1008	U	C5-C6-N1	6.49	125.95	122.70
1	a	1182	G	P-O3'-C3'	6.49	127.49	119.70
23	x	134	C	N1-C2-O2	6.49	122.79	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	1880	U	N3-C2-O2	-6.49	117.66	122.20
25	A	1200	C	C6-N1-C2	-6.49	117.71	120.30
25	A	806	C	C6-N1-C2	-6.48	117.71	120.30
26	B	31	C	N1-C2-O2	6.48	122.79	118.90
1	a	644	U	N3-C2-O2	-6.48	117.67	122.20
25	A	105	C	C6-N1-C2	-6.48	117.71	120.30
1	a	550	G	C6-C5-N7	-6.47	126.52	130.40
1	a	295	C	N1-C2-O2	6.47	122.78	118.90
25	A	1958	C	C6-N1-C2	-6.46	117.71	120.30
23	x	129	U	C5'-C4'-C3'	6.46	126.34	116.00
25	A	2805	C	C5-C6-N1	6.46	124.23	121.00
1	a	1442	G	C2-N3-C4	6.45	115.13	111.90
25	A	1108	U	C5-C6-N1	6.45	125.93	122.70
1	a	610	U	N1-C2-O2	6.45	127.32	122.80
1	a	841	C	C6-N1-C2	-6.45	117.72	120.30
1	a	536	C	C5-C6-N1	6.45	124.22	121.00
1	a	1225	A	N1-C2-N3	-6.44	126.08	129.30
25	A	2282	G	N3-C4-N9	-6.44	122.14	126.00
1	a	335	C	C6-N1-C2	-6.44	117.72	120.30
25	A	1505	A	N9-C4-C5	-6.44	103.22	105.80
25	A	2069	G7M	P-O3'-C3'	6.44	127.42	119.70
23	x	128	C	C3'-C2'-C1'	6.43	106.65	101.50
1	a	837	U	N3-C2-O2	-6.43	117.70	122.20
1	a	503	C	C6-N1-C2	-6.43	117.73	120.30
25	A	1313	U	C6-N1-C2	-6.43	117.14	121.00
26	B	97	C	C6-N1-C2	-6.43	117.73	120.30
25	A	1135	C	OP1-P-O3'	6.42	119.33	105.20
1	a	1442	G	N3-C4-C5	-6.42	125.39	128.60
25	A	2079	U	N3-C2-O2	-6.42	117.70	122.20
26	B	31	C	N3-C2-O2	-6.42	117.41	121.90
1	a	563	A	N3-C4-N9	6.42	132.53	127.40
25	A	2667	C	N1-C2-O2	6.42	122.75	118.90
25	A	532	A	C2-N3-C4	6.42	113.81	110.60
25	A	2841	C	C6-N1-C2	-6.42	117.73	120.30
25	A	2093	G	C5-N7-C8	6.42	107.51	104.30
25	A	2752	C	N3-C2-O2	-6.42	117.41	121.90
25	A	2267	A	N1-C2-N3	-6.41	126.09	129.30
25	A	2063	C	N1-C2-O2	6.41	122.75	118.90
22	v	17(A)	U	P-O3'-C3'	6.39	127.37	119.70
24	y	47(E)	G	P-O3'-C3'	6.39	127.37	119.70
1	a	285	C	C6-N1-C2	-6.39	117.74	120.30
1	a	1037	C	C6-N1-C2	-6.39	117.75	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	a	1384	C	C6-N1-C2	-6.38	117.75	120.30
25	A	1326	U	N1-C2-O2	6.38	127.27	122.80
25	A	1574	C	C6-N1-C2	-6.38	117.75	120.30
25	A	1927	A	C8-N9-C4	-6.38	103.25	105.80
1	a	439	U	N3-C2-O2	-6.38	117.73	122.20
1	a	491	G	C6-C5-N7	-6.37	126.58	130.40
24	y	35	C	C4-C5-C6	-6.37	114.21	117.40
1	a	1192	C	N3-C4-C5	6.37	124.45	121.90
25	A	2452	C	N1-C2-O2	6.37	122.72	118.90
25	A	1082	U	N1-C2-O2	6.37	127.26	122.80
25	A	2105	U	C5-C6-N1	6.37	125.88	122.70
25	A	1257	C	C6-N1-C2	-6.37	117.75	120.30
1	a	1203	C	N1-C2-O2	6.36	122.72	118.90
25	A	1081	U	N3-C4-C5	6.36	118.42	114.60
1	a	962	C	C2-N1-C1'	6.35	125.79	118.80
23	x	130	G	N9-C1'-C2'	-6.34	105.02	112.00
1	a	1496	C	C2-N1-C1'	6.34	125.78	118.80
25	A	2267	A	C5-C6-N1	6.34	120.87	117.70
25	A	2379	G	N3-C4-N9	6.34	129.80	126.00
25	A	2841	C	C5-C6-N1	6.34	124.17	121.00
25	A	1605	C	N1-C2-O2	6.34	122.70	118.90
25	A	660	C	C5-C6-N1	6.33	124.17	121.00
25	A	837	C	C6-N1-C2	-6.33	117.77	120.30
25	A	1644	C	N3-C2-O2	-6.33	117.47	121.90
25	A	2076	U	C2-N1-C1'	6.33	125.30	117.70
1	a	890	G	P-O3'-C3'	6.33	127.30	119.70
24	y	47(P)	C	C6-N1-C2	-6.33	117.77	120.30
25	A	1605	C	N3-C2-O2	-6.33	117.47	121.90
25	A	1730	C	C6-N1-C1'	6.33	128.39	120.80
1	a	1087	G	C6-C5-N7	-6.33	126.60	130.40
22	v	49	G	N3-C4-N9	6.33	129.80	126.00
25	A	610	C	C5-C6-N1	6.33	124.16	121.00
25	A	62	U	C6-N1-C2	-6.32	117.21	121.00
25	A	1159	U	N1-C2-O2	6.32	127.22	122.80
25	A	912	C	C2-N1-C1'	6.32	125.75	118.80
25	A	1198	U	N3-C2-O2	-6.32	117.78	122.20
1	a	506	G	C4-C5-N7	6.32	113.33	110.80
25	A	2185	U	N1-C2-O2	6.32	127.22	122.80
24	y	47(F)	C	P-O3'-C3'	6.31	127.27	119.70
25	A	158	U	N1-C2-O2	6.31	127.22	122.80
1	a	168	G	C4-C5-N7	6.31	113.32	110.80
1	a	177	G	C2-N3-C4	6.31	115.05	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	x	114	C	C5-C4-N4	-6.31	115.78	120.20
1	a	419	C	C6-N1-C1'	6.31	128.37	120.80
1	a	748	G	N9-C4-C5	-6.30	102.88	105.40
25	A	2898	U	C5-C4-O4	-6.30	122.12	125.90
1	a	217	C	C5-C6-N1	6.30	124.15	121.00
25	A	1345	C	C6-N1-C2	-6.30	117.78	120.30
25	A	2120	G	C2-N3-C4	6.30	115.05	111.90
25	A	2226	C	C6-N1-C2	-6.30	117.78	120.30
1	a	1087	G	C4-C5-N7	6.30	113.32	110.80
24	y	40	C	N1-C2-O2	6.30	122.68	118.90
24	y	74	C	C5-C6-N1	6.30	124.15	121.00
25	A	435	C	N1-C2-O2	6.30	122.68	118.90
1	a	692	U	C6-N1-C2	-6.29	117.23	121.00
24	y	47(P)	C	N3-C2-O2	-6.29	117.50	121.90
1	a	1134	G	C4-N9-C1'	-6.28	118.34	126.50
22	v	68	C	C2-N1-C1'	6.28	125.70	118.80
25	A	484	C	C6-N1-C2	-6.28	117.79	120.30
25	A	2379	G	C4-C5-N7	6.28	113.31	110.80
26	B	42	C	N3-C2-O2	-6.27	117.51	121.90
25	A	2150	C	C2-N1-C1'	-6.27	111.91	118.80
24	y	53	G	N9-C4-C5	-6.26	102.90	105.40
1	a	1463	U	N1-C2-O2	6.26	127.18	122.80
25	A	2036	C	C6-N1-C2	-6.25	117.80	120.30
25	A	305	C	C2-N1-C1'	6.25	125.67	118.80
23	x	117	C	OP1-P-O3'	6.25	118.94	105.20
25	A	1760	C	C5-C6-N1	6.25	124.12	121.00
1	a	1460	C	C5-C6-N1	6.25	124.12	121.00
24	y	6	U	N1-C2-O2	6.25	127.17	122.80
1	a	550	G	N1-C6-O6	6.24	123.65	119.90
1	a	979	C	C5-C6-N1	6.24	124.12	121.00
25	A	1049	C	C6-N1-C2	-6.24	117.80	120.30
1	a	1119	C	N1-C2-O2	6.23	122.64	118.90
19	s	4	LEU	CB-CG-CD1	-6.23	100.41	111.00
25	A	2818	U	N3-C2-O2	-6.23	117.84	122.20
25	A	208	C	C5-C6-N1	6.22	124.11	121.00
25	A	1798	U	N3-C2-O2	-6.22	117.84	122.20
1	a	972	C	C6-N1-C2	-6.22	117.81	120.30
1	a	1357	A	N7-C8-N9	6.22	116.91	113.80
1	a	407	U	N3-C2-O2	-6.22	117.84	122.20
1	a	1105	A	N9-C4-C5	-6.22	103.31	105.80
23	x	105	G	C5-C6-O6	-6.22	124.87	128.60
25	A	2101	A	C8-N9-C4	-6.22	103.31	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	v	21	A	C5-C6-N6	-6.21	118.74	123.70
25	A	1021	A	C2-N3-C4	6.20	113.70	110.60
24	y	71	C	N1-C2-O2	6.20	122.62	118.90
1	a	34	C	C5-C6-N1	6.20	124.10	121.00
25	A	912	C	C6-N1-C2	-6.20	117.82	120.30
25	A	1841	U	N3-C2-O2	-6.20	117.86	122.20
1	a	63	C	C6-N1-C2	-6.20	117.82	120.30
25	A	399	U	N3-C2-O2	-6.19	117.86	122.20
25	A	1323	C	N1-C2-O2	6.19	122.61	118.90
1	a	644	U	N1-C2-O2	6.19	127.13	122.80
1	a	1097	C	C2-N1-C1'	6.19	125.61	118.80
24	y	35	C	C5-C4-N4	-6.18	115.87	120.20
25	A	1644	C	N1-C2-O2	6.18	122.61	118.90
25	A	2179	C	N3-C4-C5	-6.18	119.43	121.90
25	A	1561	C	C5-C6-N1	6.18	124.09	121.00
25	A	1005	C	C6-N1-C2	-6.18	117.83	120.30
1	a	441	A	C2-N3-C4	6.17	113.69	110.60
25	A	1901	A	O5'-P-OP2	-6.17	100.14	105.70
1	a	737	C	C2-N1-C1'	6.17	125.59	118.80
24	y	53	G	C4-C5-N7	6.17	113.27	110.80
26	B	28	C	C6-N1-C2	-6.17	117.83	120.30
1	a	1097	C	N1-C2-O2	6.17	122.60	118.90
24	y	41	C	C6-N1-C2	-6.17	117.83	120.30
22	v	76	A	C4-C5-N7	6.17	113.78	110.70
25	A	1103	A	C4-C5-N7	6.17	113.78	110.70
25	A	1106	G	C2-N3-C4	6.17	114.98	111.90
1	a	1379	G	N9-C4-C5	6.17	107.87	105.40
25	A	349	U	N1-C2-O2	6.17	127.12	122.80
25	A	2188	U	C5-C6-N1	6.16	125.78	122.70
25	A	2555	U	C6-N1-C2	-6.16	117.30	121.00
1	a	623	C	C6-N1-C2	-6.15	117.84	120.30
1	a	1140	C	C6-N1-C2	-6.15	117.84	120.30
26	B	47	C	N1-C2-O2	6.14	122.59	118.90
25	A	1348	C	C5-C6-N1	6.14	124.07	121.00
26	B	4	C	C2-N3-C4	6.14	122.97	119.90
25	A	618	G	C2-N3-C4	6.14	114.97	111.90
25	A	1924	C	C5-C6-N1	6.14	124.07	121.00
1	a	49	U	N1-C2-O2	-6.14	118.50	122.80
1	a	1298	U	C5-C4-O4	-6.14	122.22	125.90
24	y	10	C	C2-N1-C1'	6.13	125.55	118.80
1	a	168	G	C5-C6-O6	-6.13	124.92	128.60
25	A	1313	U	C5-C6-N1	6.13	125.76	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	a	322	C	C2-N1-C1'	6.13	125.54	118.80
25	A	2170	A	C4-C5-N7	6.12	113.76	110.70
25	A	910	A	N1-C6-N6	-6.12	114.93	118.60
1	a	1225	A	N3-C4-N9	6.11	132.29	127.40
25	A	1290	C	C6-N1-C2	-6.11	117.86	120.30
25	A	1803	A	C8-N9-C4	-6.11	103.36	105.80
25	A	274	C	N1-C2-O2	6.10	122.56	118.90
1	a	270	A	N9-C4-C5	-6.10	103.36	105.80
1	a	1258	G	N9-C4-C5	6.10	107.84	105.40
25	A	420	C	C6-N1-C2	-6.10	117.86	120.30
25	A	225	C	C6-N1-C2	-6.10	117.86	120.30
25	A	234	U	N3-C2-O2	-6.10	117.93	122.20
25	A	151	C	C6-N1-C2	-6.09	117.86	120.30
25	A	2379	G	C5-C6-O6	-6.09	124.94	128.60
25	A	2417	C	C5-C6-N1	6.09	124.05	121.00
24	y	39	U	C5-C4-O4	-6.09	122.25	125.90
25	A	234	U	N1-C2-O2	6.09	127.06	122.80
1	a	168	G	N3-C4-N9	6.09	129.65	126.00
25	A	893	C	C5-C6-N1	6.09	124.04	121.00
25	A	1498	C	C6-N1-C1'	-6.09	113.50	120.80
25	A	2820	A	OP1-P-O3'	6.09	118.59	105.20
1	a	307	C	C6-N1-C2	-6.08	117.87	120.30
1	a	316	C	C6-N1-C2	-6.08	117.87	120.30
1	a	87	C	C2-N3-C4	6.08	122.94	119.90
25	A	2173	A	N1-C6-N6	-6.08	114.95	118.60
25	A	1798	U	N1-C2-O2	6.08	127.05	122.80
1	a	233	C	C6-N1-C2	-6.07	117.87	120.30
1	a	1432	G	P-O3'-C3'	6.07	126.99	119.70
25	A	1060	U	OP1-P-O3'	6.07	118.55	105.20
1	a	103	U	N1-C2-O2	6.07	127.05	122.80
1	a	1382	C	C5-C6-N1	6.07	124.03	121.00
1	a	805	C	N1-C2-O2	6.07	122.54	118.90
25	A	1830	C	N1-C2-O2	6.06	122.54	118.90
1	a	141	G	N1-C2-N2	6.06	121.66	116.20
1	a	163	C	C6-N1-C2	-6.06	117.88	120.30
1	a	332	G	C5-C6-O6	6.06	132.24	128.60
25	A	2099	U	C6-N1-C2	-6.06	117.36	121.00
1	a	853	C	C5-C6-N1	6.06	124.03	121.00
1	a	1045	C	N1-C2-O2	6.06	122.53	118.90
25	A	283	G	C6-N1-C2	-6.06	121.47	125.10
22	v	28	C	N1-C2-O2	6.05	122.53	118.90
1	a	1017	U	C2-N1-C1'	6.05	124.96	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	A	2072	C	N3-C4-N4	6.05	122.23	118.00
1	a	1225	A	C6-C5-N7	-6.05	128.07	132.30
1	a	647	C	C6-N1-C2	-6.04	117.88	120.30
23	x	117	C	N3-C2-O2	-6.04	117.67	121.90
25	A	2723	C	C5-C6-N1	6.04	124.02	121.00
1	a	1497	G	C5-C6-N1	6.04	114.52	111.50
25	A	1795	C	C5-C6-N1	6.04	124.02	121.00
1	a	1412	C	C5-C6-N1	6.04	124.02	121.00
26	B	97	C	N1-C2-O2	6.04	122.52	118.90
1	a	883	C	C6-N1-C2	-6.03	117.89	120.30
25	A	399	U	N1-C2-O2	6.03	127.02	122.80
1	a	1203	C	C5-C6-N1	6.03	124.02	121.00
1	a	603	U	N1-C2-N3	6.03	118.52	114.90
25	A	145	C	C5-C6-N1	6.02	124.01	121.00
25	A	2439	A	N3-C4-N9	6.02	132.22	127.40
23	x	117	C	OP2-P-O3'	-6.02	91.95	105.20
25	A	669	G	C8-N9-C1'	-6.02	119.18	127.00
25	A	205	G	OP2-P-O3'	6.02	118.44	105.20
25	A	413	C	C6-N1-C2	-6.01	117.89	120.30
22	v	51	C	N1-C2-O2	6.01	122.51	118.90
1	a	548	G	C5-C6-O6	-6.01	125.00	128.60
1	a	1073	U	C5-C6-N1	6.01	125.70	122.70
25	A	1940	U	P-O3'-C3'	6.01	126.91	119.70
25	A	946	C	C2-N1-C1'	6.00	125.41	118.80
25	A	158	U	N3-C2-O2	-6.00	118.00	122.20
1	a	1496	C	N1-C2-O2	6.00	122.50	118.90
26	B	3	C	C2-N1-C1'	6.00	125.40	118.80
23	x	125	G	C3'-C2'-C1'	6.00	106.30	101.50
25	A	2043	C	C2-N1-C1'	5.99	125.39	118.80
25	A	2510	C	C6-N1-C2	-5.99	117.90	120.30
25	A	1803	A	C5-N7-C8	-5.99	100.91	103.90
25	A	1760	C	N1-C2-O2	5.99	122.49	118.90
1	a	419	C	N3-C2-O2	-5.98	117.71	121.90
1	a	406	G	C4-N9-C1'	5.98	134.28	126.50
25	A	2515	C	C6-N1-C2	-5.98	117.91	120.30
1	a	483	C	C6-N1-C2	-5.98	117.91	120.30
1	a	1165	U	N3-C2-O2	-5.98	118.01	122.20
25	A	1760	C	C6-N1-C2	-5.98	117.91	120.30
1	a	99	C	C6-N1-C2	-5.97	117.91	120.30
25	A	2110	G	N3-C4-C5	5.97	131.59	128.60
25	A	1675	C	N3-C2-O2	-5.97	117.72	121.90
25	A	998	C	N1-C2-O2	5.97	122.48	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	A	2751	G	C8-N9-C4	-5.96	104.01	106.40
25	A	359	G	C5-C6-N1	5.96	114.48	111.50
25	A	1140	C	C6-N1-C2	-5.95	117.92	120.30
25	A	2658	C	C6-N1-C2	-5.95	117.92	120.30
1	a	141	G	C6-N1-C2	-5.94	121.53	125.10
1	a	947	G	C8-N9-C4	-5.94	104.02	106.40
22	v	28	C	C6-N1-C2	-5.94	117.92	120.30
25	A	2271	G	C5-C6-O6	-5.94	125.04	128.60
1	a	1075	U	C6-N1-C2	-5.94	117.44	121.00
25	A	1298	C	C5-C6-N1	5.94	123.97	121.00
1	a	248	C	N1-C2-O2	5.94	122.46	118.90
25	A	990	A	C2-N3-C4	5.94	113.57	110.60
25	A	2687	U	C5-C6-N1	5.94	125.67	122.70
1	a	661	G	N9-C4-C5	-5.93	103.03	105.40
1	a	240	G	C4-C5-N7	5.93	113.17	110.80
1	a	400	C	C5-C6-N1	5.93	123.97	121.00
1	a	141	G	N9-C4-C5	5.93	107.77	105.40
22	v	67	C	C6-N1-C2	-5.93	117.93	120.30
31	G	118	ALA	N-CA-CB	-5.93	101.80	110.10
1	a	214	C	C6-N1-C2	-5.93	117.93	120.30
1	a	420	U	N1-C2-O2	5.92	126.95	122.80
1	a	575	G	N3-C2-N2	-5.92	115.75	119.90
25	A	1941	C	N1-C2-O2	5.92	122.45	118.90
26	B	26	C	C2-N1-C1'	5.92	125.31	118.80
1	a	961	U	O5'-P-OP1	-5.92	100.38	105.70
25	A	2439	A	N3-C4-C5	-5.91	122.66	126.80
1	a	87	C	C5-C6-N1	5.91	123.96	121.00
24	y	40	C	C2-N1-C1'	5.91	125.30	118.80
25	A	738	G	N9-C4-C5	5.91	107.76	105.40
25	A	935	C	C2-N1-C1'	5.91	125.30	118.80
1	a	1497	G	N3-C4-C5	-5.91	125.65	128.60
25	A	46	G	N9-C4-C5	-5.91	103.04	105.40
1	a	960	U	N1-C2-O2	5.90	126.93	122.80
30	F	172	PHE	C-N-CA	5.90	136.46	121.70
1	a	947	G	N7-C8-N9	5.90	116.05	113.10
1	a	1096	C	C5-C6-N1	5.90	123.95	121.00
1	a	222	C	C6-N1-C2	-5.89	117.94	120.30
1	a	550	G	N9-C4-C5	-5.89	103.04	105.40
25	A	2254	C	N3-C2-O2	-5.89	117.77	121.90
26	B	60	C	C6-N1-C2	-5.89	117.94	120.30
1	a	1319	A	O4'-C1'-N9	-5.89	103.49	108.20
25	A	2079	U	N1-C2-O2	5.89	126.92	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	s	81	GLY	C-N-CA	5.88	136.41	121.70
24	y	74	C	C6-N1-C1'	-5.88	113.74	120.80
1	a	506	G	N3-C4-N9	5.88	129.53	126.00
1	a	551	U	C5-C6-N1	5.88	125.64	122.70
25	A	624	C	C6-N1-C2	-5.88	117.95	120.30
25	A	634	C	C6-N1-C2	-5.88	117.95	120.30
1	a	563	A	C2-N3-C4	5.88	113.54	110.60
25	A	62	U	C6-N1-C1'	-5.87	112.98	121.20
25	A	2127	G	N3-C2-N2	5.87	124.01	119.90
25	A	2329	U	C5-C6-N1	5.87	125.64	122.70
25	A	2117	A	C5-C6-N1	5.87	120.64	117.70
1	a	548	G	N1-C6-O6	5.87	123.42	119.90
1	a	692	U	N3-C2-O2	-5.87	118.09	122.20
1	a	1075	U	C5-C6-N1	5.87	125.63	122.70
25	A	145	C	C6-N1-C2	-5.86	117.95	120.30
25	A	2755	C	N3-C4-C5	5.86	124.25	121.90
1	a	636	U	C5-C6-N1	5.86	125.63	122.70
26	B	30	C	N3-C2-O2	-5.86	117.80	121.90
26	B	45	A	C5-C6-N6	-5.86	119.01	123.70
25	A	965	C	C6-N1-C2	-5.86	117.96	120.30
1	a	1070	U	N1-C2-O2	5.86	126.90	122.80
25	A	712	G	N3-C4-C5	-5.85	125.67	128.60
1	a	961	U	N3-C2-O2	-5.85	118.10	122.20
1	a	598	U	N1-C2-O2	5.85	126.90	122.80
1	a	1306	A	C5-N7-C8	-5.85	100.97	103.90
25	A	634	C	C5-C6-N1	5.85	123.92	121.00
25	A	1090	A	C4-C5-N7	5.85	113.62	110.70
1	a	503	C	C5-C6-N1	5.84	123.92	121.00
25	A	1993	U	C2-N1-C1'	5.84	124.71	117.70
1	a	355	C	C6-N1-C2	-5.84	117.96	120.30
1	a	1510	C	C2-N1-C1'	5.84	125.23	118.80
1	a	207	C	N1-C2-O2	5.84	122.40	118.90
1	a	1466	C	N3-C2-O2	-5.84	117.81	121.90
25	A	2785	C	C6-N1-C2	-5.84	117.97	120.30
1	a	1510	C	C5-C6-N1	5.84	123.92	121.00
22	v	23	C	C2-N1-C1'	5.84	125.22	118.80
25	A	353	C	C5-C6-N1	5.84	123.92	121.00
23	x	121	U	C3'-C2'-C1'	5.83	106.17	101.50
25	A	84	A	C5-N7-C8	5.83	106.81	103.90
25	A	1057	A	C6-N1-C2	5.83	122.10	118.60
25	A	2150	C	C6-N1-C2	-5.83	117.97	120.30
26	B	38	C	N1-C2-O2	5.83	122.40	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	a	428	G	OP1-P-O3'	5.83	118.02	105.20
1	a	1149	C	C6-N1-C2	-5.83	117.97	120.30
25	A	2793	C	N3-C2-O2	-5.82	117.82	121.90
25	A	944	C	N3-C2-O2	-5.82	117.82	121.90
1	a	628	G	N1-C6-O6	-5.82	116.41	119.90
1	a	1152	A	N1-C6-N6	5.82	122.09	118.60
25	A	1103	A	N9-C4-C5	-5.82	103.47	105.80
25	A	2006	C	N1-C2-O2	5.82	122.39	118.90
1	a	506	G	C6-C5-N7	-5.82	126.91	130.40
25	A	2416	C	C6-N1-C2	-5.82	117.97	120.30
1	a	1190	G	P-O3'-C3'	5.81	126.67	119.70
25	A	919	U	N1-C2-O2	5.81	126.87	122.80
25	A	2129	C	N3-C2-O2	-5.81	117.83	121.90
1	a	1152	A	C4-C5-N7	5.81	113.61	110.70
25	A	512	G	OP2-P-O3'	5.81	117.98	105.20
1	a	231	U	N3-C2-O2	-5.80	118.14	122.20
1	a	1140	C	C2-N1-C1'	5.80	125.19	118.80
25	A	2794	C	C6-N1-C2	-5.80	117.98	120.30
1	a	294	U	N3-C4-O4	5.80	123.46	119.40
25	A	2794	C	C2-N1-C1'	5.80	125.18	118.80
25	A	1461	C	C5-C6-N1	5.79	123.90	121.00
25	A	2098	U	C2-N1-C1'	5.79	124.65	117.70
23	x	125	G	C4'-C3'-O3'	5.79	124.58	113.00
1	a	240	G	N1-C6-O6	5.79	123.37	119.90
1	a	1237	C	C5-C6-N1	5.79	123.89	121.00
25	A	2499	C	N1-C2-O2	5.79	122.37	118.90
25	A	1326	U	N3-C2-O2	-5.78	118.15	122.20
25	A	2044	C	C5-C6-N1	5.78	123.89	121.00
25	A	2496	C	N1-C2-O2	5.78	122.37	118.90
25	A	12	U	N1-C2-O2	5.78	126.84	122.80
25	A	1065	U	C6-N1-C2	-5.77	117.54	121.00
25	A	1145	C	C6-N1-C2	-5.77	117.99	120.30
1	a	1379	G	N3-C2-N2	-5.77	115.86	119.90
25	A	1855	U	N3-C2-O2	-5.77	118.16	122.20
25	A	2006	C	C6-N1-C2	-5.77	117.99	120.30
25	A	852	U	C5-C6-N1	5.77	125.58	122.70
25	A	2701	U	C5-C6-N1	5.77	125.58	122.70
1	a	1403	C	N1-C2-O2	5.76	122.36	118.90
22	v	56	C	C3'-C2'-C1'	5.76	106.11	101.50
1	a	1017	U	C5-C6-N1	5.76	125.58	122.70
24	y	10	C	C6-N1-C2	-5.76	118.00	120.30
25	A	1289	C	C6-N1-C2	-5.76	118.00	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	a	735	C	N1-C2-O2	5.76	122.36	118.90
25	A	2185	U	C6-N1-C2	-5.76	117.55	121.00
25	A	2147	A	O4'-C1'-N9	5.75	112.80	108.20
25	A	2767	C	C6-N1-C2	-5.75	118.00	120.30
25	A	1171	G	N3-C4-C5	5.75	131.47	128.60
25	A	1340	U	N3-C2-O2	-5.74	118.18	122.20
25	A	2056	G	C4-C5-N7	5.74	113.10	110.80
25	A	1505	A	N1-C6-N6	5.74	122.04	118.60
1	a	1442	G	N3-C4-N9	5.74	129.44	126.00
25	A	1531	C	C6-N1-C2	-5.74	118.00	120.30
25	A	2496	C	N3-C2-O2	-5.74	117.88	121.90
26	B	8	C	C6-N1-C2	-5.74	118.00	120.30
22	v	76	A	C5-C6-N6	-5.73	119.11	123.70
25	A	1188	U	N3-C2-O2	-5.73	118.19	122.20
25	A	1799	G	C4-C5-N7	5.73	113.09	110.80
1	a	406	G	N1-C6-O6	5.73	123.34	119.90
25	A	712	G	N3-C4-N9	5.73	129.44	126.00
25	A	1800	C	C6-N1-C2	-5.73	118.01	120.30
25	A	2226	C	C5-C6-N1	5.73	123.86	121.00
22	v	34	C	C5-C6-N1	5.73	123.86	121.00
25	A	42	A	N9-C4-C5	-5.73	103.51	105.80
25	A	2782	G	N1-C6-O6	5.73	123.34	119.90
1	a	1070	U	N3-C2-O2	-5.73	118.19	122.20
1	a	1134	G	C4-C5-N7	-5.73	108.51	110.80
25	A	484	C	C5-C6-N1	5.73	123.86	121.00
1	a	252	U	N1-C2-O2	5.72	126.81	122.80
24	y	47(E)	G	N7-C8-N9	-5.72	110.24	113.10
25	A	758	C	C6-N1-C2	-5.72	118.01	120.30
25	A	2739	U	N3-C2-O2	-5.72	118.19	122.20
1	a	590	U	N3-C2-O2	-5.72	118.19	122.20
25	A	1680	U	N1-C2-N3	5.72	118.33	114.90
25	A	2283	C	N3-C2-O2	-5.72	117.90	121.90
1	a	748	G	C4-C5-N7	5.72	113.09	110.80
1	a	1146	A	C5-C6-N6	5.72	128.28	123.70
25	A	2556	C	N1-C2-O2	5.72	122.33	118.90
1	a	1404	C	C2-N1-C1'	5.71	125.09	118.80
25	A	396	G	N7-C8-N9	5.71	115.96	113.10
25	A	867	C	N1-C2-O2	5.71	122.33	118.90
25	A	935	C	C5-C6-N1	5.71	123.86	121.00
25	A	2428	G	OP1-P-OP2	-5.71	111.03	119.60
1	a	1411	C	C5-C6-N1	5.71	123.86	121.00
25	A	1524	G	N7-C8-N9	5.71	115.95	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	a	853	C	C6-N1-C2	-5.71	118.02	120.30
1	a	876	C	C6-N1-C2	-5.71	118.02	120.30
25	A	2610	C	OP2-P-O3'	5.71	117.76	105.20
25	A	2085	U	N3-C2-O2	-5.71	118.20	122.20
26	B	37	C	N1-C2-O2	5.71	122.32	118.90
1	a	948	C	C6-N1-C2	-5.70	118.02	120.30
26	B	4	C	OP1-P-OP2	-5.70	111.04	119.60
1	a	471	U	C5-C6-N1	5.70	125.55	122.70
25	A	136	G	C6-C5-N7	5.70	133.82	130.40
25	A	158	U	P-O3'-C3'	5.70	126.54	119.70
25	A	935	C	C6-N1-C2	-5.70	118.02	120.30
1	a	385	C	C6-N1-C2	-5.69	118.02	120.30
1	a	611	C	N3-C2-O2	-5.69	117.92	121.90
25	A	807	U	N3-C2-O2	-5.69	118.22	122.20
1	a	1140	C	C5-C6-N1	5.69	123.84	121.00
25	A	109	C	C5-C6-N1	5.69	123.84	121.00
26	B	3	C	OP1-P-O3'	5.68	117.70	105.20
25	A	290	U	C6-N1-C2	-5.68	117.59	121.00
25	A	358	U	N1-C2-O2	5.68	126.78	122.80
25	A	2072	C	C2-N3-C4	5.68	122.74	119.90
25	A	740	C	C5-C6-N1	5.68	123.84	121.00
22	v	27	U	N3-C2-O2	-5.68	118.22	122.20
25	A	2110	G	C6-C5-N7	5.68	133.81	130.40
15	o	86	LEU	CA-CB-CG	5.67	128.35	115.30
25	A	417	C	C6-N1-C2	-5.67	118.03	120.30
1	a	1034	G	C5-C6-O6	-5.67	125.20	128.60
25	A	2816	G	N3-C2-N2	-5.67	115.93	119.90
26	B	37	C	N3-C2-O2	-5.67	117.93	121.90
1	a	52	C	C6-N1-C2	-5.67	118.03	120.30
25	A	919	U	N3-C2-O2	-5.67	118.23	122.20
25	A	2162	G	P-O3'-C3'	5.67	126.50	119.70
22	v	11	A	O5'-P-OP1	5.66	117.50	110.70
25	A	420	C	N1-C2-O2	5.66	122.30	118.90
1	a	620	C	N1-C2-O2	5.66	122.30	118.90
1	a	697	U	N3-C2-O2	-5.66	118.24	122.20
25	A	1484	U	C5-C4-O4	-5.66	122.50	125.90
1	a	1059	C	C6-N1-C2	-5.66	118.04	120.30
23	x	92	G	N1-C2-N2	-5.66	111.11	116.20
23	x	128	C	N1-C2-O2	-5.66	115.51	118.90
1	a	248	C	C2-N1-C1'	5.65	125.02	118.80
1	a	647	C	C5-C6-N1	5.65	123.83	121.00
1	a	960	U	P-O3'-C3'	5.65	126.48	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	A	694	U	C5-C6-N1	5.65	125.53	122.70
25	A	2898	U	N3-C4-O4	5.65	123.36	119.40
26	B	111	U	N3-C2-O2	-5.65	118.25	122.20
25	A	974	G	N3-C4-N9	5.64	129.39	126.00
25	A	1880	U	N1-C2-O2	5.64	126.75	122.80
25	A	2162	G	C4-N9-C1'	-5.64	119.16	126.50
25	A	2264	C	C2-N3-C4	-5.64	117.08	119.90
1	a	445	G	N3-C4-N9	5.64	129.38	126.00
25	A	383	C	N3-C2-O2	-5.64	117.95	121.90
1	a	419	C	C5-C6-N1	5.64	123.82	121.00
1	a	1225	A	C8-N9-C1'	-5.64	117.55	127.70
25	A	2636	C	C5-C6-N1	5.64	123.82	121.00
1	a	1045	C	C5-C6-N1	5.63	123.82	121.00
25	A	595	C	C5-C6-N1	5.63	123.82	121.00
1	a	1125	U	N1-C2-N3	5.63	118.28	114.90
23	x	101	A	N1-C2-N3	-5.63	126.48	129.30
25	A	512	G	P-O3'-C3'	5.63	126.45	119.70
1	a	979	C	C2-N1-C1'	5.63	124.99	118.80
25	A	1061	U	OP1-P-OP2	-5.62	111.16	119.60
25	A	1310	G	OP2-P-O3'	5.62	117.57	105.20
1	a	506	G	C5-C6-O6	-5.62	125.23	128.60
25	A	1761	C	N1-C2-O2	5.62	122.27	118.90
25	A	151	C	C5-C6-N1	5.62	123.81	121.00
25	A	2420	C	C5-C6-N1	5.62	123.81	121.00
1	a	452	A	N1-C2-N3	-5.62	126.49	129.30
25	A	1894	C	N1-C2-O2	5.62	122.27	118.90
1	a	142	G	N3-C4-C5	-5.61	125.79	128.60
1	a	891	U	C6-N1-C2	-5.61	117.63	121.00
25	A	837	C	N1-C2-O2	5.61	122.27	118.90
25	A	2117	A	C4-C5-N7	5.61	113.51	110.70
1	a	1128	C	N1-C2-O2	5.61	122.27	118.90
1	a	1148	U	N3-C2-O2	-5.61	118.27	122.20
1	a	998	C	C6-N1-C2	-5.61	118.06	120.30
1	a	1469	C	N3-C4-N4	-5.61	114.08	118.00
25	A	1030	C	C5-C6-N1	5.60	123.80	121.00
25	A	1157	G	N3-C4-N9	5.60	129.36	126.00
25	A	2884	U	C2-N1-C1'	5.60	124.42	117.70
25	A	143	C	N3-C2-O2	-5.60	117.98	121.90
25	A	1049	C	C5-C6-N1	5.60	123.80	121.00
25	A	435	C	N3-C2-O2	-5.60	117.98	121.90
25	A	1693	U	O4'-C1'-N1	-5.60	103.72	108.20
1	a	684	U	N3-C2-O2	-5.60	118.28	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	A	847	U	N3-C2-O2	-5.60	118.28	122.20
25	A	1595	C	C6-N1-C2	-5.60	118.06	120.30
25	A	1057	A	C4-C5-N7	5.59	113.50	110.70
25	A	1212	G	P-O3'-C3'	5.59	126.41	119.70
1	a	623	C	C2-N1-C1'	5.59	124.95	118.80
24	y	45	U	O5'-P-OP2	-5.59	100.67	105.70
1	a	689	C	C5-C6-N1	5.59	123.80	121.00
1	a	998	C	N3-C2-O2	-5.59	117.99	121.90
1	a	1263	C	N1-C2-O2	5.59	122.25	118.90
25	A	46	G	C4-C5-N7	5.59	113.04	110.80
25	A	1830	C	N3-C2-O2	-5.59	117.99	121.90
1	a	997	U	N3-C2-O2	-5.59	118.29	122.20
25	A	1271	G	C8-N9-C4	-5.59	104.16	106.40
25	A	665	U	C5-C6-N1	5.59	125.49	122.70
25	A	2489	U	C5-C4-O4	-5.59	122.55	125.90
1	a	661	G	N3-C4-N9	5.58	129.35	126.00
25	A	62	U	C2-N3-C4	5.58	130.35	127.00
25	A	1216	G	O4'-C1'-N9	5.58	112.67	108.20
1	a	563	A	N1-C2-N3	-5.58	126.51	129.30
25	A	835	C	C6-N1-C2	-5.58	118.07	120.30
25	A	1354	A	N7-C8-N9	5.58	116.59	113.80
25	A	1407	G	C4-C5-N7	5.58	113.03	110.80
25	A	1505	A	C4-C5-N7	5.58	113.49	110.70
25	A	2558	C	C6-N1-C2	-5.58	118.07	120.30
1	a	1264	U	N3-C2-O2	-5.57	118.30	122.20
25	A	2562	U	N3-C2-O2	-5.57	118.30	122.20
1	a	983	A	N3-C4-C5	-5.57	122.90	126.80
1	a	1356	G	C4-C5-N7	5.57	113.03	110.80
1	a	1109	C	C6-N1-C2	-5.57	118.07	120.30
23	x	133	C	C6-N1-C2	-5.57	118.07	120.30
25	A	1395	A	O4'-C1'-N9	5.57	112.65	108.20
25	A	2271	G	N1-C6-O6	5.57	123.24	119.90
1	a	109	A	N7-C8-N9	5.56	116.58	113.80
25	A	2179	C	C2-N1-C1'	5.56	124.92	118.80
1	a	1113	C	C6-N1-C2	-5.56	118.08	120.30
25	A	2036	C	C5-C6-N1	5.56	123.78	121.00
25	A	2156	G	C4-C5-C6	5.56	122.14	118.80
25	A	2282	G	C6-C5-N7	5.56	133.74	130.40
54	3	31	ILE	CG1-CB-CG2	-5.56	99.18	111.40
1	a	1271	A	N9-C4-C5	-5.55	103.58	105.80
26	B	4	C	O5'-P-OP1	5.55	117.36	110.70
24	y	43	G	N9-C4-C5	-5.55	103.18	105.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	y	47	G	N7-C8-N9	5.55	115.88	113.10
25	A	1178	C	C6-N1-C2	-5.55	118.08	120.30
1	a	1395	C	N3-C2-O2	-5.54	118.02	121.90
25	A	4	U	C5-C6-N1	5.54	125.47	122.70
25	A	1199	U	C5-C6-N1	5.54	125.47	122.70
23	x	125	G	C4-N9-C1'	-5.54	119.30	126.50
24	y	47(P)	C	C5-C6-N1	5.54	123.77	121.00
25	A	485	C	N1-C2-O2	5.54	122.22	118.90
1	a	654	G	N9-C4-C5	-5.54	103.18	105.40
1	a	551	U	C5-C4-O4	-5.54	122.58	125.90
22	v	11	A	N1-C2-N3	-5.54	126.53	129.30
25	A	2666	C	C6-N1-C2	-5.54	118.08	120.30
25	A	1879	C	C5-C6-N1	5.54	123.77	121.00
1	a	123	U	C5-C6-N1	5.53	125.47	122.70
25	A	143	C	C2-N3-C4	5.53	122.67	119.90
26	B	12	C	C5-C6-N1	5.53	123.77	121.00
1	a	418	C	C6-N1-C2	-5.53	118.09	120.30
25	A	933	A	N3-C4-C5	-5.53	122.93	126.80
25	A	2901	C	N1-C2-O2	5.52	122.21	118.90
1	a	1384	C	N3-C2-O2	-5.52	118.04	121.90
24	y	40	C	C5-C6-N1	5.52	123.76	121.00
25	A	1442	U	C5-C6-N1	5.52	125.46	122.70
1	a	1225	A	N1-C6-N6	5.52	121.91	118.60
25	A	883	G	C8-N9-C4	-5.52	104.19	106.40
25	A	2901	C	C2-N1-C1'	5.52	124.87	118.80
25	A	2462	C	C2-N1-C1'	5.52	124.87	118.80
25	A	2703	C	C6-N1-C2	-5.52	118.09	120.30
1	a	1161	C	N1-C2-O2	5.51	122.21	118.90
1	a	891	U	N3-C2-O2	-5.51	118.34	122.20
25	A	362	A	C2-N3-C4	5.51	113.36	110.60
25	A	531	C	C6-N1-C2	5.51	122.50	120.30
1	a	446	G	N3-C4-N9	5.51	129.31	126.00
1	a	684	U	N1-C2-N3	5.51	118.20	114.90
1	a	1535	C	N1-C2-O2	5.51	122.20	118.90
23	x	132	A	C3'-C2'-C1'	5.50	105.90	101.50
25	A	2120	G	N3-C4-N9	5.50	129.30	126.00
25	A	2327	A	O5'-P-OP2	-5.50	100.75	105.70
1	a	56	U	C5-C4-O4	-5.49	122.60	125.90
1	a	923	A	C6-C5-N7	-5.49	128.46	132.30
25	A	1090	A	N9-C4-C5	-5.49	103.60	105.80
1	a	1218	C	O5'-P-OP2	-5.49	100.76	105.70
25	A	974	G	N3-C4-C5	-5.49	125.85	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	A	2372	U	N3-C2-O2	-5.49	118.36	122.20
23	x	92	G	C5-C6-O6	5.49	131.89	128.60
25	A	305	C	C2-N3-C4	5.49	122.64	119.90
1	a	580	C	N3-C4-N4	5.49	121.84	118.00
1	a	708	C	C5-C6-N1	5.49	123.74	121.00
1	a	1147	C	N1-C2-O2	5.49	122.19	118.90
25	A	2098	U	N3-C2-O2	-5.49	118.36	122.20
1	a	1158	C	C6-N1-C1'	-5.48	114.22	120.80
25	A	1005	C	C2-N1-C1'	5.48	124.83	118.80
27	C	129	LEU	CA-CB-CG	5.48	127.90	115.30
1	a	1040	U	C5-C6-N1	5.48	125.44	122.70
25	A	281	C	C2-N1-C1'	5.48	124.83	118.80
25	A	2325	G	N9-C4-C5	-5.48	103.21	105.40
25	A	349	U	N3-C2-O2	-5.48	118.37	122.20
1	a	1464	U	N1-C2-N3	5.47	118.19	114.90
25	A	1533	C	C6-N1-C2	-5.47	118.11	120.30
25	A	301	G	O4'-C1'-N9	5.47	112.58	108.20
25	A	2286	G	P-O3'-C3'	5.47	126.27	119.70
1	a	206	C	N1-C2-N3	5.47	123.03	119.20
22	v	1	C	N1-C2-O2	5.47	122.18	118.90
25	A	2194	U	P-O3'-C3'	5.46	126.26	119.70
1	a	1537	U	C5-C6-N1	5.46	125.43	122.70
25	A	2098	U	N1-C2-O2	5.46	126.62	122.80
25	A	532	A	N3-C4-N9	5.46	131.77	127.40
25	A	1561	C	C6-N1-C2	-5.46	118.12	120.30
1	a	921	U	C5-C6-N1	5.45	125.43	122.70
25	A	550	C	N1-C2-O2	5.45	122.17	118.90
25	A	1799	G	N9-C4-C5	-5.45	103.22	105.40
25	A	1486	U	N3-C2-O2	-5.45	118.39	122.20
25	A	832	U	N1-C2-N3	5.44	118.16	114.90
25	A	1269	A	N9-C4-C5	-5.44	103.62	105.80
25	A	205	G	O4'-C1'-N9	5.44	112.55	108.20
1	a	496	A	N3-C4-C5	-5.44	122.99	126.80
25	A	2299	U	C5-C6-N1	5.44	125.42	122.70
1	a	722	G	N3-C4-C5	-5.44	125.88	128.60
25	A	2162	G	C8-N9-C4	5.44	108.57	106.40
7	g	22	LEU	CA-CB-CG	5.43	127.80	115.30
25	A	269	C	C6-N1-C2	-5.43	118.13	120.30
25	A	1747	U	C5-C6-N1	5.43	125.42	122.70
1	a	448	A	C2-N3-C4	5.43	113.32	110.60
24	y	35	C	N1-C2-O2	5.43	122.16	118.90
25	A	546	U	C2-N1-C1'	5.43	124.22	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	A	286	U	C5-C6-N1	5.43	125.41	122.70
25	A	2093	G	N7-C8-N9	-5.43	110.39	113.10
1	a	78	A	N3-C4-N9	5.42	131.74	127.40
24	y	8	G	O4'-C1'-N9	5.42	112.54	108.20
25	A	115	C	C6-N1-C2	-5.42	118.13	120.30
1	a	955	U	N1-C2-O2	5.42	126.59	122.80
25	A	867	C	N3-C2-O2	-5.42	118.11	121.90
25	A	1372	U	N3-C2-O2	-5.42	118.41	122.20
26	B	4	C	N1-C2-O2	5.42	122.15	118.90
26	B	12	C	O5'-P-OP2	5.42	117.20	110.70
25	A	51	G	P-O3'-C3'	5.42	126.20	119.70
25	A	560	C	C6-N1-C2	-5.41	118.14	120.30
25	A	495	G	N3-C4-N9	5.41	129.25	126.00
22	v	18	G	N7-C8-N9	5.41	115.80	113.10
24	y	40	C	C6-N1-C2	-5.41	118.14	120.30
25	A	2195	U	O4'-C1'-N1	5.41	112.53	108.20
22	v	60	U	O5'-P-OP1	5.41	117.19	110.70
1	a	142	G	C8-N9-C4	-5.41	104.24	106.40
1	a	993	G	C2-N3-C4	5.41	114.60	111.90
22	v	66	C	C2-N1-C1'	5.41	124.75	118.80
25	A	2185	U	C5-C6-N1	5.41	125.40	122.70
25	A	2243	U	N3-C2-O2	-5.41	118.42	122.20
1	a	33	A	N7-C8-N9	5.40	116.50	113.80
1	a	1297	G	P-O3'-C3'	5.40	126.18	119.70
25	A	738	G	N1-C6-O6	-5.40	116.66	119.90
25	A	1929	G	C2-N3-C4	5.40	114.60	111.90
25	A	2141	G	C2-N3-C4	-5.40	109.20	111.90
1	a	1118	U	C5-C6-N1	5.40	125.40	122.70
25	A	417	C	C5-C6-N1	5.40	123.70	121.00
25	A	1498	C	C6-N1-C2	-5.40	118.14	120.30
1	a	580	C	N1-C2-O2	5.40	122.14	118.90
1	a	524	G	C4-C5-N7	5.39	112.96	110.80
25	A	365	U	C5-C4-O4	-5.39	122.66	125.90
25	A	966	G	N9-C4-C5	-5.39	103.24	105.40
25	A	968	C	C6-N1-C2	-5.39	118.14	120.30
1	a	1029	U	C5-C6-N1	5.39	125.39	122.70
25	A	393	C	C6-N1-C2	-5.39	118.14	120.30
25	A	730	A	N9-C4-C5	-5.39	103.64	105.80
25	A	2739	U	N1-C2-O2	5.39	126.57	122.80
25	A	1399	C	C5-C6-N1	5.39	123.69	121.00
1	a	1460	C	C6-N1-C2	-5.39	118.14	120.30
6	f	53	LYS	N-CA-CB	5.39	120.30	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	x	134	C	N3-C2-O2	-5.38	118.13	121.90
25	A	1088	A	C5-C6-N1	5.38	120.39	117.70
1	a	1072	G	N3-C4-N9	5.38	129.23	126.00
25	A	687	C	N3-C2-O2	-5.38	118.13	121.90
25	A	1956	U	C5-C4-O4	5.38	129.13	125.90
1	a	1348	U	N1-C2-O2	5.38	126.57	122.80
1	a	472	U	N3-C2-O2	-5.38	118.44	122.20
1	a	524	G	N9-C4-C5	-5.38	103.25	105.40
25	A	2264	C	O4'-C1'-N1	5.38	112.50	108.20
1	a	56	U	N3-C4-O4	5.38	123.16	119.40
1	a	1040	U	C5-C4-O4	-5.38	122.67	125.90
25	A	1498	C	C5-C6-N1	5.38	123.69	121.00
1	a	378	G	C8-N9-C4	-5.37	104.25	106.40
1	a	137	U	N3-C2-O2	-5.37	118.44	122.20
1	a	614	C	C5-C6-N1	5.37	123.69	121.00
1	a	1140	C	N1-C2-O2	5.37	122.12	118.90
25	A	2072	C	C6-N1-C1'	-5.37	114.36	120.80
25	A	2901	C	C6-N1-C2	-5.37	118.15	120.30
1	a	1262	C	N1-C2-O2	5.37	122.12	118.90
25	A	912	C	C5-C6-N1	5.36	123.68	121.00
25	A	1349	C	N1-C2-O2	5.36	122.12	118.90
25	A	283	G	N9-C4-C5	5.36	107.54	105.40
1	a	856	C	C6-N1-C2	-5.36	118.16	120.30
25	A	1104	C	C6-N1-C2	-5.36	118.16	120.30
25	A	2902	C	C6-N1-C2	-5.36	118.16	120.30
1	a	99	C	C5-C6-N1	5.36	123.68	121.00
1	a	957	U	N3-C2-O2	-5.36	118.45	122.20
25	A	305	C	N3-C4-N4	5.36	121.75	118.00
25	A	1083	U	C6-N1-C2	-5.36	117.79	121.00
25	A	1629	U	N3-C2-O2	-5.35	118.45	122.20
25	A	2428	G	OP1-P-O3'	5.35	116.98	105.20
1	a	215	C	C2-N3-C4	5.35	122.58	119.90
25	A	2226	C	C2-N1-C1'	5.35	124.69	118.80
25	A	2755	C	N1-C2-O2	5.35	122.11	118.90
25	A	143	C	C2-N1-C1'	5.35	124.69	118.80
1	a	1325	C	C5-C6-N1	5.35	123.67	121.00
25	A	2093	G	C4-C5-N7	-5.35	108.66	110.80
1	a	59	A	C2-N3-C4	5.35	113.27	110.60
1	a	446	G	C4-C5-N7	5.34	112.94	110.80
1	a	719	C	N1-C2-O2	5.34	122.11	118.90
25	A	141	G	N3-C4-C5	-5.34	125.93	128.60
25	A	1064	C	C4-C5-C6	5.34	120.07	117.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	v	11	A	N9-C4-C5	-5.34	103.66	105.80
25	A	268	C	C6-N1-C2	-5.34	118.16	120.30
25	A	2591	C	C6-N1-C2	-5.34	118.16	120.30
1	a	500	G	C6-C5-N7	-5.34	127.20	130.40
1	a	1027	C	C2-N3-C4	5.34	122.57	119.90
1	a	1225	A	C4-N9-C1'	5.34	135.91	126.30
25	A	944	C	N1-C2-O2	5.34	122.10	118.90
25	A	366	C	C5-C6-N1	5.33	123.67	121.00
25	A	678	C	C6-N1-C2	-5.33	118.17	120.30
1	a	661	G	C4-C5-N7	5.33	112.93	110.80
22	v	76	A	C5-N7-C8	-5.33	101.23	103.90
1	a	1529	G	N9-C4-C5	-5.33	103.27	105.40
25	A	2175	C	N3-C4-N4	-5.33	114.27	118.00
22	v	23	C	N1-C2-O2	5.33	122.10	118.90
25	A	353	C	C6-N1-C2	-5.33	118.17	120.30
1	a	491	G	N1-C6-O6	5.33	123.10	119.90
1	a	862	C	C2-N1-C1'	5.33	124.66	118.80
1	a	177	G	N3-C4-N9	5.33	129.19	126.00
23	x	117	C	C5-C6-N1	5.33	123.66	121.00
25	A	84	A	N7-C8-N9	-5.33	111.14	113.80
25	A	1315	C	N1-C2-O2	5.32	122.09	118.90
25	A	2448	A	N3-C4-C5	5.32	130.52	126.80
23	x	125	G	N1-C2-N2	5.32	120.98	116.20
1	a	714	G	N7-C8-N9	5.31	115.76	113.10
1	a	1497	G	N1-C6-O6	-5.31	116.71	119.90
25	A	436	C	N3-C2-O2	-5.31	118.18	121.90
25	A	901	C	N1-C2-O2	5.31	122.09	118.90
1	a	308	C	C5-C6-N1	5.31	123.66	121.00
24	y	28	U	C5-C6-N1	5.31	125.35	122.70
25	A	396	G	C6-C5-N7	-5.31	127.22	130.40
25	A	2782	G	C8-N9-C1'	-5.31	120.10	127.00
25	A	164	C	C6-N1-C2	-5.31	118.18	120.30
1	a	207	C	C5-C4-N4	5.30	123.91	120.20
25	A	154	U	C6-N1-C1'	-5.30	113.78	121.20
25	A	2469	A	C2-N3-C4	5.30	113.25	110.60
1	a	95	C	N1-C2-O2	5.30	122.08	118.90
25	A	860	U	N3-C2-O2	-5.30	118.49	122.20
22	v	75	C	C5'-C4'-O4'	5.30	115.46	109.10
1	a	1235	U	N3-C4-O4	5.29	123.11	119.40
25	A	1728	C	C6-N1-C2	-5.29	118.18	120.30
25	A	2156	G	C5-N7-C8	5.29	106.95	104.30
1	a	1007	U	C6-N1-C2	-5.29	117.83	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	A	912	C	N1-C2-O2	5.29	122.08	118.90
25	A	2656	U	N1-C2-O2	5.29	126.50	122.80
1	a	1072	G	C4-N9-C1'	5.29	133.38	126.50
25	A	208	C	C6-N1-C2	-5.29	118.19	120.30
1	a	1471	U	C2-N1-C1'	5.29	124.04	117.70
1	a	1509	C	C5-C6-N1	5.29	123.64	121.00
24	y	71	C	C2-N1-C1'	5.28	124.61	118.80
25	A	2575	C	C6-N1-C2	-5.28	118.19	120.30
1	a	582	C	N1-C2-O2	5.28	122.07	118.90
25	A	545	U	C3'-C2'-C1'	5.28	105.72	101.50
22	v	74	C	O4'-C1'-N1	5.28	112.42	108.20
25	A	2195	U	N3-C2-O2	-5.28	118.50	122.20
1	a	585	G	C5-C6-O6	-5.28	125.43	128.60
1	a	738	C	C2-N1-C1'	5.28	124.61	118.80
25	A	417	C	C2-N1-C1'	5.28	124.61	118.80
25	A	851	C	C6-N1-C2	-5.28	118.19	120.30
25	A	487	C	N1-C2-O2	5.28	122.07	118.90
1	a	311	C	C6-N1-C2	-5.27	118.19	120.30
1	a	654	G	C6-C5-N7	-5.27	127.24	130.40
1	a	194	C	C6-N1-C2	-5.27	118.19	120.30
1	a	993	G	C4-N9-C1'	5.27	133.35	126.50
22	v	74	C	N3-C2-O2	-5.27	118.21	121.90
25	A	245	G	C4-C5-N7	5.27	112.91	110.80
1	a	1161	C	C6-N1-C2	-5.27	118.19	120.30
26	B	70	C	C2-N1-C1'	5.27	124.59	118.80
25	A	75	G	C2-N3-C4	5.27	114.53	111.90
25	A	1799	G	N1-C6-O6	5.27	123.06	119.90
25	A	1914	C	N1-C2-O2	5.26	122.06	118.90
1	a	419	C	N1-C2-N3	5.26	122.88	119.20
1	a	1495	U	N3-C2-O2	-5.26	118.52	122.20
26	B	40	U	C5-C4-O4	-5.26	122.74	125.90
1	a	956	U	N3-C2-O2	-5.26	118.52	122.20
1	a	891	U	N1-C2-O2	5.26	126.48	122.80
25	A	2214	C	N1-C2-O2	5.26	122.06	118.90
1	a	81	A	C2-N3-C4	5.26	113.23	110.60
1	a	618	C	C6-N1-C2	-5.26	118.20	120.30
25	A	2380	C	C6-N1-C2	-5.26	118.20	120.30
25	A	1533	C	N3-C2-O2	-5.25	118.22	121.90
1	a	923	A	C5-N7-C8	-5.25	101.27	103.90
25	A	278	A	N3-C4-C5	-5.25	123.12	126.80
1	a	78	A	C6-N1-C2	5.25	121.75	118.60
25	A	1407	G	N9-C4-C5	-5.25	103.30	105.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	a	473	U	N3-C2-O2	-5.25	118.53	122.20
25	A	984	A	OP1-P-O3'	5.25	116.75	105.20
25	A	137	U	N1-C2-O2	5.25	126.47	122.80
25	A	1323	C	N3-C2-O2	-5.25	118.23	121.90
22	v	6	G	N9-C4-C5	5.24	107.50	105.40
25	A	2512	C	C6-N1-C2	-5.24	118.20	120.30
40	P	113	LEU	CA-CB-CG	5.24	127.36	115.30
25	A	1930	G	P-O3'-C3'	5.24	125.99	119.70
1	a	1072	G	N1-C6-O6	5.24	123.04	119.90
25	A	1290	C	C2-N1-C1'	5.24	124.56	118.80
25	A	1636	U	C5-C6-N1	5.24	125.32	122.70
1	a	36	C	N1-C2-O2	5.24	122.04	118.90
1	a	697	U	N1-C2-O2	5.24	126.47	122.80
1	a	1153	G	N1-C6-O6	-5.24	116.76	119.90
22	v	19	G	C5-C6-O6	5.24	131.74	128.60
25	A	850	U	C2-N3-C4	5.24	130.14	127.00
25	A	2898	U	C2-N1-C1'	5.24	123.98	117.70
26	B	28	C	C5-C6-N1	5.24	123.62	121.00
1	a	919	A	C2-N3-C4	-5.24	107.98	110.60
1	a	1197	A	N9-C4-C5	-5.24	103.71	105.80
25	A	860	U	N1-C2-O2	5.24	126.46	122.80
25	A	867	C	C6-N1-C2	-5.23	118.21	120.30
25	A	2170	A	C5-N7-C8	-5.23	101.28	103.90
23	x	122	G	C8-N9-C1'	-5.23	120.20	127.00
24	y	46	G	O4'-C1'-N9	5.23	112.39	108.20
25	A	927	A	C5-C6-N6	-5.23	119.52	123.70
25	A	1180	U	N1-C2-O2	5.23	126.46	122.80
25	A	2098	U	C5-C6-N1	5.23	125.31	122.70
26	B	97	C	C5-C6-N1	5.23	123.61	121.00
22	v	58	A	N1-C6-N6	-5.22	115.47	118.60
23	x	130	G	N7-C8-N9	5.22	115.71	113.10
25	A	2757	A	C2-N3-C4	5.22	113.21	110.60
25	A	2782	G	N3-C4-N9	5.22	129.13	126.00
25	A	495	G	C5-C6-O6	-5.22	125.47	128.60
26	B	38	C	C2-N1-C1'	5.22	124.55	118.80
25	A	2448	A	N3-C4-N9	-5.22	123.22	127.40
1	a	445	G	N9-C4-C5	-5.22	103.31	105.40
25	A	1843	C	C2-N1-C1'	5.22	124.54	118.80
26	B	111	U	N1-C2-O2	5.22	126.45	122.80
1	a	413	G	C2-N3-C4	5.22	114.51	111.90
26	B	47	C	N3-C2-O2	-5.22	118.25	121.90
1	a	1161	C	N3-C2-O2	-5.22	118.25	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	a	1007	U	N1-C2-O2	5.21	126.45	122.80
23	x	117	C	P-O3'-C3'	5.21	125.96	119.70
1	a	397	A	N3-C4-N9	5.21	131.57	127.40
23	x	122	G	N7-C8-N9	-5.21	110.50	113.10
1	a	446	G	N9-C4-C5	-5.21	103.32	105.40
25	A	1348	C	C2-N1-C1'	5.21	124.53	118.80
25	A	1669	A	N3-C4-N9	5.21	131.57	127.40
1	a	446	G	C6-C5-N7	-5.20	127.28	130.40
23	x	105	G	N1-C6-O6	5.20	123.02	119.90
25	A	2556	C	N3-C2-O2	-5.20	118.26	121.90
25	A	436	C	C6-N1-C2	-5.20	118.22	120.30
25	A	852	U	N3-C4-O4	5.20	123.04	119.40
25	A	2244	U	N3-C2-O2	-5.20	118.56	122.20
1	a	1356	G	N9-C4-C5	-5.20	103.32	105.40
1	a	1466	C	C6-N1-C2	-5.20	118.22	120.30
25	A	717	C	N3-C2-O2	-5.20	118.26	121.90
1	a	661	G	C6-C5-N7	-5.20	127.28	130.40
22	v	12	G	O4'-C1'-N9	5.20	112.36	108.20
25	A	2056	G	C6-C5-N7	-5.20	127.28	130.40
13	m	65	GLU	CA-CB-CG	5.19	124.82	113.40
25	A	2179	C	C5-C4-N4	5.19	123.83	120.20
25	A	544	C	C5-C6-N1	5.19	123.59	121.00
25	A	1533	C	N1-C2-O2	5.19	122.01	118.90
25	A	1639	C	N1-C2-O2	5.19	122.01	118.90
1	a	252	U	C6-N1-C2	-5.19	117.89	121.00
1	a	585	G	C4-C5-N7	5.19	112.88	110.80
8	h	98	LEU	CA-CB-CG	5.19	127.23	115.30
1	a	959	A	N7-C8-N9	5.18	116.39	113.80
25	A	942	G	N1-C6-O6	-5.18	116.79	119.90
25	A	1350	C	C2-N1-C1'	5.18	124.50	118.80
25	A	1013	C	C6-N1-C2	-5.18	118.23	120.30
26	B	48	U	N3-C2-O2	-5.18	118.57	122.20
25	A	192	C	C6-N1-C2	-5.18	118.23	120.30
25	A	546	U	C5-C6-N1	5.18	125.29	122.70
25	A	2117	A	C6-C5-N7	-5.18	128.67	132.30
25	A	2133	G	C2-N3-C4	5.18	114.49	111.90
1	a	1509	C	C6-N1-C2	-5.18	118.23	120.30
25	A	413	C	C5-C6-N1	5.18	123.59	121.00
25	A	1399	C	C6-N1-C2	-5.18	118.23	120.30
1	a	548	G	C8-N9-C4	5.17	108.47	106.40
1	a	639	G	N9-C4-C5	-5.17	103.33	105.40
1	a	1069	C	O4'-C1'-N1	5.17	112.34	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	a	1087	G	N1-C6-O6	5.17	123.00	119.90
25	A	1323	C	C6-N1-C2	-5.17	118.23	120.30
1	a	1496	C	N3-C2-O2	-5.17	118.28	121.90
25	A	278	A	N3-C4-N9	5.17	131.54	127.40
25	A	396	G	C4-C5-N7	5.17	112.87	110.80
22	v	51	C	C2-N1-C1'	5.17	124.48	118.80
24	y	47(P)	C	C6-N1-C1'	-5.17	114.60	120.80
25	A	225	C	N3-C2-O2	-5.17	118.28	121.90
1	a	528	C	C6-N1-C2	-5.17	118.23	120.30
25	A	717	C	N1-C2-O2	5.16	122.00	118.90
1	a	92	U	N1-C2-N3	5.16	118.00	114.90
25	A	1030	C	C6-N1-C2	-5.16	118.24	120.30
1	a	294	U	C5-C4-O4	-5.16	122.81	125.90
25	A	1487	U	N1-C2-O2	5.16	126.41	122.80
1	a	921	U	C6-N1-C2	-5.16	117.91	121.00
25	A	712	G	C2-N3-C4	5.15	114.48	111.90
25	A	640	C	C5-C6-N1	5.15	123.58	121.00
1	a	643	C	C6-N1-C2	-5.15	118.24	120.30
24	y	10	C	N1-C2-O2	5.15	121.99	118.90
25	A	1795	C	C6-N1-C2	-5.15	118.24	120.30
1	a	469	C	N1-C2-O2	5.14	121.99	118.90
1	a	1172	C	C6-N1-C2	-5.14	118.24	120.30
25	A	2066	C	C6-N1-C2	-5.14	118.24	120.30
25	A	2420	C	C6-N1-C2	-5.14	118.24	120.30
26	B	47	C	C6-N1-C2	-5.14	118.24	120.30
24	y	70	U	N3-C2-O2	-5.14	118.60	122.20
1	a	1033	G	C4-C5-N7	5.14	112.86	110.80
25	A	1787	A	N9-C4-C5	-5.14	103.75	105.80
25	A	2440	C	C6-N1-C2	-5.14	118.25	120.30
26	B	15	A	C6-N1-C2	5.14	121.68	118.60
1	a	1356	G	C6-C5-N7	-5.14	127.32	130.40
25	A	114	U	N1-C2-O2	5.14	126.40	122.80
25	A	2796	U	N3-C2-O2	-5.14	118.60	122.20
22	v	57	A	N7-C8-N9	-5.13	111.23	113.80
25	A	882	G	O4'-C1'-N9	5.13	112.31	108.20
22	v	34	C	N1-C2-O2	5.13	121.98	118.90
25	A	552	U	N1-C2-O2	5.13	126.39	122.80
25	A	673	C	C6-N1-C2	-5.13	118.25	120.30
25	A	1171	G	N3-C2-N2	-5.13	116.31	119.90
1	a	506	G	N1-C6-O6	5.13	122.98	119.90
25	A	2667	C	N3-C2-O2	-5.13	118.31	121.90
1	a	45	G	N3-C4-N9	5.13	129.08	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	A	758	C	N3-C2-O2	-5.13	118.31	121.90
25	A	1830	C	C6-N1-C1'	-5.13	114.65	120.80
1	a	805	C	C5-C6-N1	5.12	123.56	121.00
25	A	551	G	C6-N1-C2	5.12	128.17	125.10
26	B	3	C	C5-C6-N1	5.12	123.56	121.00
1	a	167	A	N9-C4-C5	-5.12	103.75	105.80
1	a	738	C	C5-C6-N1	5.12	123.56	121.00
1	a	1007	U	N1-C2-N3	5.12	117.97	114.90
25	A	1531	C	C5-C6-N1	5.12	123.56	121.00
1	a	283	U	N3-C2-O2	-5.12	118.62	122.20
25	A	2276	G	N3-C2-N2	-5.12	116.32	119.90
26	B	30	C	N1-C2-O2	5.12	121.97	118.90
1	a	295	C	C6-N1-C2	-5.12	118.25	120.30
1	a	1227	A	N9-C4-C5	-5.12	103.75	105.80
1	a	748	G	C6-C5-N7	-5.12	127.33	130.40
25	A	2011	U	N3-C2-O2	-5.12	118.62	122.20
25	A	1108	U	N1-C2-O2	5.11	126.38	122.80
1	a	409	U	N1-C2-O2	5.11	126.38	122.80
1	a	419	C	C5-C4-N4	5.11	123.78	120.20
1	a	983	A	C8-N9-C4	-5.11	103.76	105.80
1	a	1125	U	C6-N1-C2	-5.11	117.94	121.00
22	v	57	A	N9-C4-C5	5.11	107.84	105.80
25	A	114	U	N3-C2-O2	-5.11	118.62	122.20
25	A	1657	U	N3-C2-O2	-5.11	118.63	122.20
25	A	568	U	N3-C2-O2	-5.10	118.63	122.20
24	y	9	U	OP2-P-O3'	5.10	116.42	105.20
25	A	1461	C	C6-N1-C2	-5.10	118.26	120.30
25	A	2354	C	C6-N1-C2	-5.10	118.26	120.30
1	a	620	C	N3-C2-O2	-5.10	118.33	121.90
1	a	1203	C	C2-N1-C1'	5.10	124.41	118.80
22	v	39	C	N1-C2-O2	5.10	121.96	118.90
1	a	240	G	C5-C6-O6	-5.10	125.54	128.60
1	a	795	C	C6-N1-C2	-5.10	118.26	120.30
1	a	805	C	N3-C4-N4	5.10	121.57	118.00
1	a	1537	U	C6-N1-C2	-5.10	117.94	121.00
25	A	1297	C	C6-N1-C2	-5.10	118.26	120.30
23	x	92	G	N3-C2-N2	5.09	123.47	119.90
25	A	534	U	C5-C6-N1	5.09	125.25	122.70
1	a	1228	C	C2-N1-C1'	5.09	124.40	118.80
1	a	418	C	C5-C6-N1	5.09	123.54	121.00
1	a	1274	A	C2-N3-C4	5.09	113.14	110.60
25	A	2149	U	C5-C6-N1	5.09	125.25	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	A	2243	U	N1-C2-O2	5.09	126.36	122.80
1	a	1129	C	C6-N1-C2	-5.09	118.27	120.30
25	A	2110	G	N9-C4-C5	5.09	107.44	105.40
1	a	1064	G	C5-C6-O6	-5.08	125.55	128.60
1	a	475	C	C6-N1-C2	-5.08	118.27	120.30
1	a	137	U	N1-C2-O2	5.08	126.36	122.80
25	A	2637	U	C5-C6-N1	5.08	125.24	122.70
1	a	215	C	C5-C4-N4	-5.08	116.64	120.20
1	a	1151	A	C5-C6-N6	-5.08	119.64	123.70
1	a	247	G	N9-C4-C5	-5.07	103.37	105.40
1	a	295	C	C5-C6-N1	5.07	123.54	121.00
25	A	366	C	C6-N1-C2	-5.07	118.27	120.30
25	A	373	U	N3-C2-O2	-5.07	118.65	122.20
25	A	1349	C	C5-C6-N1	5.07	123.54	121.00
25	A	1772	A	N7-C8-N9	5.07	116.34	113.80
25	A	2880	C	N3-C4-C5	5.07	123.93	121.90
1	a	810	C	C2-N1-C1'	5.07	124.38	118.80
25	A	1035	U	N3-C2-O2	-5.07	118.65	122.20
48	X	48	LEU	CA-CB-CG	5.07	126.96	115.30
25	A	2591	C	C5-C6-N1	5.07	123.53	121.00
1	a	220	G	N1-C6-O6	5.07	122.94	119.90
25	A	136	G	C5-C6-O6	5.07	131.64	128.60
25	A	288	U	N1-C2-N3	5.07	117.94	114.90
1	a	445	G	C6-C5-N7	-5.07	127.36	130.40
1	a	962	C	N3-C2-O2	-5.07	118.36	121.90
22	v	28	C	N3-C2-O2	-5.07	118.35	121.90
25	A	1666	G	N3-C2-N2	-5.07	116.35	119.90
23	x	131	C	O4'-C1'-N1	5.06	112.25	108.20
25	A	1585	C	C6-N1-C2	-5.06	118.28	120.30
22	v	34	C	C2-N3-C4	5.06	122.43	119.90
25	A	2389	G	C4-C5-N7	5.06	112.82	110.80
25	A	1657	U	N1-C2-O2	5.06	126.34	122.80
1	a	1235	U	C5-C4-O4	-5.06	122.87	125.90
25	A	75	G	N3-C4-C5	-5.06	126.07	128.60
1	a	452	A	N9-C4-C5	-5.05	103.78	105.80
1	a	779	C	C6-N1-C2	-5.05	118.28	120.30
25	A	1112	G	C5'-C4'-C3'	5.05	124.08	116.00
25	A	2461	A	N9-C4-C5	-5.05	103.78	105.80
25	A	2562	U	N1-C2-O2	5.05	126.33	122.80
1	a	503	C	C2-N1-C1'	5.05	124.35	118.80
25	A	933	A	N3-C4-N9	5.05	131.44	127.40
1	a	1130	A	C5-C6-N6	-5.05	119.66	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	A	46	G	C6-C5-N7	-5.05	127.37	130.40
25	A	2473	U	C2-N1-C1'	5.05	123.75	117.70
1	a	177	G	N3-C4-C5	-5.04	126.08	128.60
25	A	669	G	C8-N9-C4	-5.04	104.38	106.40
22	v	11	A	C4-C5-N7	5.04	113.22	110.70
25	A	1092	C	N1-C2-O2	5.04	121.92	118.90
25	A	2272	U	C6-N1-C2	-5.04	117.97	121.00
26	B	28	C	C2-N1-C1'	5.04	124.34	118.80
1	a	1068	G	C5-N7-C8	5.04	106.82	104.30
25	A	880	G	P-O3'-C3'	5.04	125.75	119.70
25	A	1840	G	C6-C5-N7	-5.04	127.38	130.40
25	A	1314	C	N1-C2-O2	5.04	121.92	118.90
1	a	635	A	C6-N1-C2	5.03	121.62	118.60
1	a	993	G	C8-N9-C1'	-5.03	120.46	127.00
1	a	1188	A	N7-C8-N9	5.03	116.32	113.80
25	A	1103	A	N3-C4-N9	5.03	131.43	127.40
25	A	1350	C	C6-N1-C2	-5.03	118.29	120.30
25	A	1417	C	N1-C2-O2	5.03	121.92	118.90
25	A	2649	C	C2-N1-C1'	5.03	124.34	118.80
12	l	101	LEU	CA-CB-CG	5.03	126.87	115.30
1	a	758	C	OP2-P-O3'	5.03	116.26	105.20
25	A	719	C	C6-N1-C2	-5.03	118.29	120.30
25	A	1090	A	N1-C2-N3	-5.03	126.79	129.30
1	a	420	U	C6-N1-C2	-5.03	117.98	121.00
25	A	1350	C	N1-C2-O2	5.02	121.92	118.90
25	A	2231	U	C5-C6-N1	5.02	125.21	122.70
1	a	397	A	N3-C4-C5	-5.02	123.29	126.80
1	a	719	C	N3-C2-O2	-5.02	118.39	121.90
25	A	2025	C	C5-C6-N1	5.02	123.51	121.00
25	A	2292	U	C6-N1-C2	-5.02	117.99	121.00
32	I	100	ILE	CG1-CB-CG2	-5.02	100.36	111.40
25	A	2799	A	N1-C2-N3	-5.02	126.79	129.30
25	A	1414	C	C5-C6-N1	5.02	123.51	121.00
25	A	150	U	C5-C6-N1	5.01	125.21	122.70
25	A	711	G	N3-C4-C5	-5.01	126.09	128.60
25	A	840	C	C6-N1-C2	-5.01	118.30	120.30
25	A	2087	G	N7-C8-N9	5.01	115.61	113.10
22	v	49	G	N3-C4-C5	-5.01	126.09	128.60
25	A	2394	C	N1-C2-O2	5.01	121.91	118.90
25	A	353	C	N1-C2-O2	5.01	121.91	118.90
25	A	2170	A	C5-C6-N1	5.01	120.21	117.70
25	A	2254	C	C6-N1-C2	-5.01	118.30	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	A	1109	C	C5-C6-N1	5.01	123.50	121.00
25	A	1276	A	N9-C4-C5	-5.01	103.80	105.80
25	A	1487	U	N3-C2-O2	-5.01	118.69	122.20
25	A	1320	C	N3-C4-N4	5.00	121.50	118.00
26	B	10	G	C2-N3-C4	5.00	114.40	111.90
25	A	396	G	C5-N7-C8	-5.00	101.80	104.30
25	A	717	C	C6-N1-C2	-5.00	118.30	120.30

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	a	527	G7M	C4',C3'
25	A	2069	G7M	C4',C3'

All (20) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
31	G	117	PRO	Peptide
33	H	8	LYS	Peptide
35	K	88	ASN	Mainchain
35	K	89	ASN	Mainchain
36	L	13	LYS	Peptide
37	M	57	VAL	Peptide
43	S	64	ALA	Mainchain
49	Y	24	GLU	Mainchain
1	a	60	A	Sidechain
2	b	10	LYS	Peptide
2	b	12	GLY	Peptide
2	b	17	HIS	Peptide
2	b	73	ARG	Mainchain
5	e	88	HIS	Peptide
6	f	52	ASN	Mainchain
9	i	56	MET	Peptide
10	j	34	ALA	Mainchain
13	m	3	ILE	Mainchain
18	r	16	GLY	Peptide
23	x	121	U	Sidechain

5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	b	216/218 (99%)	189 (88%)	20 (9%)	7 (3%)	4	30
3	c	204/206 (99%)	197 (97%)	5 (2%)	2 (1%)	15	54
4	d	203/205 (99%)	188 (93%)	14 (7%)	1 (0%)	29	68
5	e	155/157 (99%)	134 (86%)	16 (10%)	5 (3%)	4	30
6	f	98/100 (98%)	86 (88%)	7 (7%)	5 (5%)	2	22
7	g	149/151 (99%)	131 (88%)	14 (9%)	4 (3%)	5	34
8	h	127/129 (98%)	116 (91%)	9 (7%)	2 (2%)	9	45
9	i	125/127 (98%)	105 (84%)	18 (14%)	2 (2%)	9	45
10	j	96/98 (98%)	85 (88%)	7 (7%)	4 (4%)	3	25
11	k	114/116 (98%)	99 (87%)	11 (10%)	4 (4%)	3	28
12	l	121/123 (98%)	103 (85%)	11 (9%)	7 (6%)	1	20
13	m	112/114 (98%)	101 (90%)	9 (8%)	2 (2%)	8	42
14	n	98/100 (98%)	88 (90%)	10 (10%)	0	100	100
15	o	86/88 (98%)	77 (90%)	6 (7%)	3 (4%)	3	28
16	p	80/82 (98%)	73 (91%)	6 (8%)	1 (1%)	12	48
17	q	78/80 (98%)	68 (87%)	9 (12%)	1 (1%)	12	48
18	r	63/65 (97%)	56 (89%)	3 (5%)	4 (6%)	1	19
19	s	84/86 (98%)	76 (90%)	4 (5%)	4 (5%)	2	23
20	t	83/85 (98%)	80 (96%)	3 (4%)	0	100	100
21	u	63/65 (97%)	53 (84%)	6 (10%)	4 (6%)	1	19
27	C	269/271 (99%)	242 (90%)	22 (8%)	5 (2%)	8	40
28	D	207/209 (99%)	192 (93%)	10 (5%)	5 (2%)	6	36
29	E	199/201 (99%)	188 (94%)	8 (4%)	3 (2%)	10	46
30	F	175/177 (99%)	155 (89%)	16 (9%)	4 (2%)	6	37
31	G	174/176 (99%)	161 (92%)	9 (5%)	4 (2%)	6	37

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
32	I	139/141 (99%)	120 (86%)	13 (9%)	6 (4%)	2	25
33	H	147/149 (99%)	130 (88%)	14 (10%)	3 (2%)	7	40
34	J	140/142 (99%)	132 (94%)	6 (4%)	2 (1%)	11	47
35	K	120/122 (98%)	108 (90%)	9 (8%)	3 (2%)	5	35
36	L	141/143 (99%)	129 (92%)	8 (6%)	4 (3%)	5	33
37	M	134/136 (98%)	123 (92%)	8 (6%)	3 (2%)	6	37
38	N	118/120 (98%)	107 (91%)	10 (8%)	1 (1%)	19	60
39	O	114/116 (98%)	106 (93%)	8 (7%)	0	100	100
40	P	112/114 (98%)	103 (92%)	9 (8%)	0	100	100
41	Q	115/117 (98%)	109 (95%)	6 (5%)	0	100	100
42	R	101/103 (98%)	91 (90%)	9 (9%)	1 (1%)	15	54
43	S	108/110 (98%)	101 (94%)	6 (6%)	1 (1%)	17	56
44	T	91/93 (98%)	83 (91%)	7 (8%)	1 (1%)	14	52
45	U	100/102 (98%)	90 (90%)	8 (8%)	2 (2%)	7	40
46	V	92/94 (98%)	87 (95%)	5 (5%)	0	100	100
47	W	73/75 (97%)	69 (94%)	4 (6%)	0	100	100
48	X	75/77 (97%)	72 (96%)	3 (4%)	0	100	100
49	Y	61/63 (97%)	58 (95%)	2 (3%)	1 (2%)	9	45
50	Z	56/58 (97%)	51 (91%)	5 (9%)	0	100	100
51	0	54/56 (96%)	52 (96%)	2 (4%)	0	100	100
52	1	48/50 (96%)	46 (96%)	1 (2%)	1 (2%)	7	38
53	2	44/46 (96%)	41 (93%)	1 (2%)	2 (4%)	2	24
54	3	62/64 (97%)	59 (95%)	2 (3%)	1 (2%)	9	45
55	4	36/38 (95%)	33 (92%)	3 (8%)	0	100	100
56	6	64/66 (97%)	56 (88%)	5 (8%)	3 (5%)	2	24
All	All	5724/5824 (98%)	5199 (91%)	407 (7%)	118 (2%)	10	38

All (118) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	b	18	GLN
5	e	89	THR
5	e	93	VAL

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Mol	Chain	Res	Type
6	f	53	LYS
6	f	54	LEU
9	i	57	VAL
9	i	90	ASP
13	m	65	GLU
16	p	79	ASN
17	q	51	GLU
18	r	17	VAL
19	s	82	HIS
21	u	25	ALA
27	C	204	LEU
29	E	83	VAL
30	F	149	ARG
30	F	174	PHE
31	G	118	ALA
33	H	3	VAL
33	H	9	VAL
34	J	81	ILE
36	L	36	LYS
37	M	58	LYS
37	M	70	ASP
52	1	4	ILE
2	b	14	HIS
6	f	86	ARG
7	g	29	LEU
7	g	129	ASN
7	g	145	GLU
10	j	57	VAL
11	k	88	PRO
11	k	119	GLY
12	l	75	GLU
12	l	101	LEU
18	r	11	ARG
19	s	80	ARG
21	u	38	GLU
28	D	150	GLN
29	E	122	GLU
31	G	46	ASP
32	I	4	VAL
32	I	24	GLY
32	I	64	ARG
35	K	27	GLY

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Mol	Chain	Res	Type
35	K	35	VAL
36	L	30	THR
36	L	111	ILE
37	M	23	GLY
44	T	52	GLU
49	Y	22	LEU
56	6	40	CYS
2	b	17	HIS
5	e	122	VAL
7	g	83	THR
8	h	2	MET
10	j	34	ALA
10	j	35	GLN
12	l	24	GLU
13	m	4	ALA
15	o	2	LEU
15	o	45	HIS
18	r	46	THR
27	C	52	HIS
27	C	121	ALA
28	D	86	GLU
28	D	140	HIS
30	F	20	ASN
36	L	29	LYS
38	N	70	THR
43	S	67	ASP
45	U	39	ASN
53	2	23	ALA
53	2	45	SER
56	6	3	LYS
56	6	8	LYS
2	b	177	ASN
4	d	193	ASP
5	e	158	LYS
5	e	159	SER
6	f	92	THR
6	f	98	GLU
8	h	47	ASP
11	k	92	ARG
11	k	125	LYS
12	l	23	LEU
15	o	87	ARG

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Mol	Chain	Res	Type
18	r	18	GLN
19	s	4	LEU
21	u	34	ARG
28	D	149	ASN
29	E	80	SER
32	I	20	SER
33	H	11	ASN
42	R	55	ASP
45	U	97	SER
10	j	89	ARG
12	l	21	PRO
12	l	77	SER
31	G	109	SER
32	I	22	PRO
35	K	89	ASN
2	b	9	LEU
2	b	71	THR
2	b	153	MET
3	c	96	VAL
19	s	3	SER
21	u	36	PHE
27	C	154	ALA
27	C	252	LYS
30	F	110	ILE
31	G	108	PHE
32	I	92	PRO
54	3	31	ILE
3	c	13	ILE
12	l	41	PRO
28	D	153	GLY
34	J	64	VAL

5.3.2 Protein sidechains (i)

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

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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	b	180/180 (100%)	180 (100%)	0	100	100
3	c	170/170 (100%)	170 (100%)	0	100	100
4	d	172/172 (100%)	172 (100%)	0	100	100
5	e	119/119 (100%)	119 (100%)	0	100	100
6	f	87/87 (100%)	87 (100%)	0	100	100
7	g	124/124 (100%)	124 (100%)	0	100	100
8	h	104/104 (100%)	104 (100%)	0	100	100
9	i	105/105 (100%)	105 (100%)	0	100	100
10	j	86/86 (100%)	86 (100%)	0	100	100
11	k	89/89 (100%)	89 (100%)	0	100	100
12	l	103/103 (100%)	103 (100%)	0	100	100
13	m	92/92 (100%)	92 (100%)	0	100	100
14	n	79/83 (95%)	78 (99%)	1 (1%)	69	82
15	o	76/76 (100%)	76 (100%)	0	100	100
16	p	65/65 (100%)	65 (100%)	0	100	100
17	q	74/74 (100%)	74 (100%)	0	100	100
18	r	48/56 (86%)	48 (100%)	0	100	100
19	s	74/74 (100%)	74 (100%)	0	100	100
20	t	65/65 (100%)	65 (100%)	0	100	100
21	u	44/55 (80%)	44 (100%)	0	100	100
27	C	216/216 (100%)	216 (100%)	0	100	100
28	D	164/164 (100%)	164 (100%)	0	100	100
29	E	165/165 (100%)	165 (100%)	0	100	100
30	F	148/148 (100%)	148 (100%)	0	100	100
31	G	137/137 (100%)	137 (100%)	0	100	100
32	I	109/109 (100%)	109 (100%)	0	100	100
33	H	114/114 (100%)	114 (100%)	0	100	100
34	J	116/116 (100%)	116 (100%)	0	100	100
35	K	103/103 (100%)	103 (100%)	0	100	100
36	L	102/102 (100%)	102 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
37	M	109/109 (100%)	109 (100%)	0	100	100
38	N	100/100 (100%)	100 (100%)	0	100	100
39	O	86/86 (100%)	86 (100%)	0	100	100
40	P	99/99 (100%)	99 (100%)	0	100	100
41	Q	89/89 (100%)	89 (100%)	0	100	100
42	R	84/84 (100%)	84 (100%)	0	100	100
43	S	93/93 (100%)	93 (100%)	0	100	100
44	T	80/80 (100%)	80 (100%)	0	100	100
45	U	83/83 (100%)	83 (100%)	0	100	100
46	V	78/78 (100%)	78 (100%)	0	100	100
47	W	57/57 (100%)	57 (100%)	0	100	100
48	X	67/67 (100%)	67 (100%)	0	100	100
49	Y	55/55 (100%)	55 (100%)	0	100	100
50	Z	48/48 (100%)	48 (100%)	0	100	100
51	0	47/47 (100%)	47 (100%)	0	100	100
52	1	45/45 (100%)	45 (100%)	0	100	100
53	2	38/38 (100%)	38 (100%)	0	100	100
54	3	51/51 (100%)	51 (100%)	0	100	100
55	4	34/34 (100%)	34 (100%)	0	100	100
56	6	59/59 (100%)	59 (100%)	0	100	100
All	All	4732/4755 (100%)	4731 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
14	n	34	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
2	b	17	HIS
3	c	5	HIS
7	g	129	ASN
8	h	3	GLN

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Mol	Chain	Res	Type
8	h	15	ASN
9	i	125	GLN
10	j	58	ASN
16	p	18	GLN
16	p	59	HIS
17	q	44	HIS
27	C	85	ASN
30	F	80	GLN
38	N	62	ASN
39	O	98	GLN
46	V	87	GLN
48	X	15	ASN
50	Z	19	HIS
55	4	35	GLN
55	4	37	GLN
56	6	41	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	a	1535/1539 (99%)	238 (15%)	0
22	v	76/77 (98%)	28 (36%)	0
23	x	47/48 (97%)	30 (63%)	0
24	y	93/95 (97%)	31 (33%)	0
25	A	2894/2903 (99%)	569 (19%)	25 (0%)
26	B	119/120 (99%)	11 (9%)	1 (0%)
All	All	4764/4782 (99%)	907 (19%)	26 (0%)

All (907) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	a	6	G
1	a	9	G
1	a	22	G
1	a	32	A
1	a	39	G
1	a	47	C
1	a	48	C
1	a	49	U
1	a	51	A
1	a	61	G

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Mol	Chain	Res	Type
1	a	65	A
1	a	69	G
1	a	71	A
1	a	79	G
1	a	80	A
1	a	81	A
1	a	83	C
1	a	86	G
1	a	87	C
1	a	88	U
1	a	94	G
1	a	95	C
1	a	121	U
1	a	131	A
1	a	134	G
1	a	142	G
1	a	144	G
1	a	147	G
1	a	149	A
1	a	173	U
1	a	174	A
1	a	183	C
1	a	184	G
1	a	191	G
1	a	195	A
1	a	197	A
1	a	209	U
1	a	210	C
1	a	211	G
1	a	212	G
1	a	214	C
1	a	226	G
1	a	247	G
1	a	250	A
1	a	251	G
1	a	266	G
1	a	267	C
1	a	278	G
1	a	279	A
1	a	280	C
1	a	281	G
1	a	289	G

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Mol	Chain	Res	Type
1	a	298	A
1	a	306	A
1	a	319	G
1	a	328	C
1	a	330	C
1	a	345	C
1	a	351	G
1	a	355	C
1	a	367	U
1	a	369	G
1	a	372	C
1	a	373	A
1	a	378	G
1	a	397	A
1	a	406	G
1	a	410	G
1	a	411	A
1	a	413	G
1	a	414	A
1	a	429	U
1	a	439	U
1	a	441	A
1	a	445	G
1	a	452	A
1	a	465	A
1	a	467	U
1	a	481	G
1	a	482	A
1	a	486	U
1	a	497	G
1	a	511	C
1	a	518	C
1	a	521	G
1	a	524	G
1	a	527	G7M
1	a	528	C
1	a	531	U
1	a	532	A
1	a	545	C
1	a	547	A
1	a	550	G
1	a	562	U

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Mol	Chain	Res	Type
1	a	564	C
1	a	566	G
1	a	572	A
1	a	573	A
1	a	575	G
1	a	576	C
1	a	577	G
1	a	596	A
1	a	615	G
1	a	633	G
1	a	653	U
1	a	661	G
1	a	665	A
1	a	687	A
1	a	693	G
1	a	723	U
1	a	724	G
1	a	731	G
1	a	734	G
1	a	755	G
1	a	774	G
1	a	777	A
1	a	790	A
1	a	793	U
1	a	794	A
1	a	809	G
1	a	814	A
1	a	815	A
1	a	817	C
1	a	818	G
1	a	820	U
1	a	832	G
1	a	836	G
1	a	843	U
1	a	844	G
1	a	845	A
1	a	846	G
1	a	849	G
1	a	872	A
1	a	883	C
1	a	890	G
1	a	891	U

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Mol	Chain	Res	Type
1	a	902	G
1	a	913	A
1	a	926	G
1	a	933	G
1	a	934	C
1	a	935	A
1	a	960	U
1	a	961	U
1	a	966	2MG
1	a	967	5MC
1	a	968	A
1	a	969	A
1	a	971	G
1	a	975	A
1	a	976	G
1	a	977	A
1	a	993	G
1	a	994	A
1	a	1004	A
1	a	1020	G
1	a	1026	G
1	a	1028	C
1	a	1029	U
1	a	1031	C
1	a	1032	G
1	a	1033	G
1	a	1034	G
1	a	1053	G
1	a	1054	C
1	a	1056	U
1	a	1063	C
1	a	1065	U
1	a	1070	U
1	a	1085	U
1	a	1094	G
1	a	1095	U
1	a	1101	A
1	a	1108	G
1	a	1132	C
1	a	1136	C
1	a	1137	C
1	a	1139	G

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Mol	Chain	Res	Type
1	a	1140	C
1	a	1152	A
1	a	1159	U
1	a	1167	A
1	a	1168	U
1	a	1182	G
1	a	1183	U
1	a	1191	A
1	a	1193	G
1	a	1196	A
1	a	1206	G
1	a	1212	U
1	a	1213	A
1	a	1225	A
1	a	1226	C
1	a	1227	A
1	a	1233	G
1	a	1236	A
1	a	1238	A
1	a	1256	A
1	a	1260	G
1	a	1280	A
1	a	1287	A
1	a	1297	G
1	a	1298	U
1	a	1300	G
1	a	1317	C
1	a	1320	C
1	a	1323	G
1	a	1356	G
1	a	1363	A
1	a	1378	C
1	a	1381	U
1	a	1394	A
1	a	1397	C
1	a	1398	A
1	a	1403	C
1	a	1418	A
1	a	1419	G
1	a	1429	A
1	a	1432	G
1	a	1433	A

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Mol	Chain	Res	Type
1	a	1445	U
1	a	1446	A
1	a	1457	G
1	a	1464	U
1	a	1492	A
1	a	1503	A
1	a	1506	U
1	a	1507	A
1	a	1508	A
1	a	1517	G
1	a	1520	C
1	a	1529	G
1	a	1530	G
1	a	1533	C
1	a	1534	A
1	a	1535	C
1	a	1539	C
1	a	1540	U
22	v	6	G
22	v	7	G
22	v	8	4SU
22	v	9	G
22	v	11	A
22	v	15	G
22	v	16	C
22	v	17(A)	U
22	v	18	G
22	v	19	G
22	v	20	H2U
22	v	21	A
22	v	22	G
22	v	23	C
22	v	39	C
22	v	46	A
22	v	47	U
22	v	49	G
22	v	54	5MU
22	v	56	C
22	v	57	A
22	v	59	A
22	v	61	C
22	v	62	C

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Mol	Chain	Res	Type
22	v	66	C
22	v	68	C
22	v	75	C
22	v	76	A
23	x	88	A
23	x	90	G
23	x	96	C
23	x	97	A
23	x	98	U
23	x	104	U
23	x	108	A
23	x	109	C
23	x	110	G
23	x	112	C
23	x	114	C
23	x	115	A
23	x	116	U
23	x	117	C
23	x	118	G
23	x	119	G
23	x	120	U
23	x	121	U
23	x	122	G
23	x	123	C
23	x	125	G
23	x	126	G
23	x	127	U
23	x	128	C
23	x	129	U
23	x	130	G
23	x	131	C
23	x	132	A
23	x	133	C
23	x	134	C
24	y	8	G
24	y	9	U
24	y	10	C
24	y	17	G
24	y	18	G
24	y	20	G
24	y	22	G
24	y	25	G

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Mol	Chain	Res	Type
24	y	33	U
24	y	35	C
24	y	38	A
24	y	42	A
24	y	45	U
24	y	47	G
24	y	47(B)	G
24	y	47(E)	G
24	y	47(F)	C
24	y	47(G)	C
24	y	47(H)	A
24	y	47(I)	G
24	y	47(J)	C
24	y	47(K)	G
24	y	47(L)	G
24	y	47(P)	C
24	y	47(Q)	G
24	y	53	G
24	y	54	5MU
24	y	55	PSU
24	y	59	C
24	y	74	C
24	y	76	A
25	A	10	A
25	A	12	U
25	A	15	G
25	A	23	G
25	A	34	U
25	A	35	G
25	A	42	A
25	A	46	G
25	A	51	G
25	A	52	A
25	A	63	A
25	A	71	A
25	A	74	A
25	A	75	G
25	A	92	U
25	A	96	C
25	A	98	G
25	A	102	U
25	A	107	G

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Mol	Chain	Res	Type
25	A	114	U
25	A	118	A
25	A	120	U
25	A	121	G
25	A	138	U
25	A	139	U
25	A	142	A
25	A	143	C
25	A	158	U
25	A	159	G
25	A	162	U
25	A	163	C
25	A	165	A
25	A	178	G
25	A	180	G
25	A	181	A
25	A	196	A
25	A	199	A
25	A	200	U
25	A	204	A
25	A	205	G
25	A	206	U
25	A	216	A
25	A	219	A
25	A	221	A
25	A	222	A
25	A	223	A
25	A	225	C
25	A	228	C
25	A	229	C
25	A	231	A
25	A	233	A
25	A	239	C
25	A	245	G
25	A	248	G
25	A	255	A
25	A	265	A
25	A	266	G
25	A	267	C
25	A	276	U
25	A	279	A
25	A	285	G

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Mol	Chain	Res	Type
25	A	294	A
25	A	300	A
25	A	311	A
25	A	323	C
25	A	324	A
25	A	329	G
25	A	330	A
25	A	334	C
25	A	346	A
25	A	349	U
25	A	361	G
25	A	371	A
25	A	372	G
25	A	380	G
25	A	386	G
25	A	387	U
25	A	388	G
25	A	404	A
25	A	411	G
25	A	412	A
25	A	417	C
25	A	424	G
25	A	451	U
25	A	456	C
25	A	473	G
25	A	481	G
25	A	490	C
25	A	491	G
25	A	504	A
25	A	505	A
25	A	509	C
25	A	513	A
25	A	531	C
25	A	532	A
25	A	533	G
25	A	545	U
25	A	547	A
25	A	549	G
25	A	562	U
25	A	563	A
25	A	564	C
25	A	572	A

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Mol	Chain	Res	Type
25	A	573	U
25	A	575	A
25	A	577	G
25	A	603	A
25	A	614	A
25	A	615	U
25	A	616	A
25	A	627	A
25	A	637	A
25	A	646	U
25	A	647	G
25	A	651	G
25	A	654	A
25	A	655	A
25	A	656	G
25	A	659	G
25	A	664	G
25	A	668	A
25	A	670	A
25	A	684	G
25	A	686	U
25	A	694	U
25	A	695	G
25	A	702	U
25	A	705	A
25	A	712	G
25	A	713	G
25	A	730	A
25	A	740	C
25	A	747	5MU
25	A	752	A
25	A	761	A
25	A	775	G
25	A	776	G
25	A	782	A
25	A	783	A
25	A	784	G
25	A	785	G
25	A	805	G
25	A	812	C
25	A	819	A
25	A	827	U

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Mol	Chain	Res	Type
25	A	828	U
25	A	844	A
25	A	845	A
25	A	846	U
25	A	847	U
25	A	858	G
25	A	859	G
25	A	869	G
25	A	879	G
25	A	881	G
25	A	883	G
25	A	885	C
25	A	894	U
25	A	895	U
25	A	897	C
25	A	905	A
25	A	907	G
25	A	910	A
25	A	914	G
25	A	932	U
25	A	933	A
25	A	938	G
25	A	941	A
25	A	945	A
25	A	946	C
25	A	961	C
25	A	962	G
25	A	965	C
25	A	973	A
25	A	974	G
25	A	983	A
25	A	985	C
25	A	995	C
25	A	996	A
25	A	1009	A
25	A	1012	U
25	A	1013	C
25	A	1026	G
25	A	1033	U
25	A	1040	A
25	A	1045	C
25	A	1046	A

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Mol	Chain	Res	Type
25	A	1047	G
25	A	1054	A
25	A	1057	A
25	A	1059	G
25	A	1060	U
25	A	1061	U
25	A	1062	G
25	A	1063	G
25	A	1064	C
25	A	1065	U
25	A	1066	U
25	A	1067	A
25	A	1068	G
25	A	1069	A
25	A	1070	A
25	A	1071	G
25	A	1072	C
25	A	1075	C
25	A	1076	C
25	A	1077	A
25	A	1079	C
25	A	1083	U
25	A	1084	A
25	A	1086	A
25	A	1088	A
25	A	1089	A
25	A	1090	A
25	A	1094	U
25	A	1096	A
25	A	1101	U
25	A	1104	C
25	A	1105	U
25	A	1111	A
25	A	1112	G
25	A	1132	U
25	A	1135	C
25	A	1136	G
25	A	1142	A
25	A	1143	A
25	A	1144	A
25	A	1151	A
25	A	1172	C

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Mol	Chain	Res	Type
25	A	1175	A
25	A	1177	G
25	A	1178	C
25	A	1180	U
25	A	1186	G
25	A	1204	A
25	A	1206	G
25	A	1211	C
25	A	1212	G
25	A	1213	A
25	A	1218	G
25	A	1236	G
25	A	1250	G
25	A	1251	C
25	A	1253	A
25	A	1255	U
25	A	1256	G
25	A	1271	G
25	A	1272	A
25	A	1273	U
25	A	1284	A
25	A	1289	C
25	A	1300	G
25	A	1301	A
25	A	1302	A
25	A	1305	C
25	A	1311	G
25	A	1313	U
25	A	1314	C
25	A	1329	U
25	A	1345	C
25	A	1360	G
25	A	1365	A
25	A	1368	G
25	A	1378	A
25	A	1379	U
25	A	1383	A
25	A	1392	A
25	A	1394	U
25	A	1395	A
25	A	1396	U
25	A	1401	G

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Mol	Chain	Res	Type
25	A	1403	A
25	A	1407	G
25	A	1414	C
25	A	1416	G
25	A	1419	A
25	A	1420	A
25	A	1427	A
25	A	1428	C
25	A	1434	A
25	A	1437	C
25	A	1452	G
25	A	1459	G
25	A	1475	G
25	A	1482	G
25	A	1490	A
25	A	1493	C
25	A	1498	C
25	A	1499	C
25	A	1504	A
25	A	1505	A
25	A	1508	A
25	A	1509	A
25	A	1515	A
25	A	1523	U
25	A	1524	G
25	A	1534	U
25	A	1535	A
25	A	1536	C
25	A	1537	G
25	A	1554	U
25	A	1559	U
25	A	1560	G
25	A	1566	A
25	A	1569	A
25	A	1578	U
25	A	1581	G
25	A	1584	U
25	A	1585	C
25	A	1607	C
25	A	1616	A
25	A	1617	C
25	A	1619	G

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Mol	Chain	Res	Type
25	A	1626	A
25	A	1627	G
25	A	1646	C
25	A	1647	U
25	A	1648	U
25	A	1649	G
25	A	1654	A
25	A	1660	G
25	A	1669	A
25	A	1674	G
25	A	1682	G
25	A	1693	U
25	A	1695	G
25	A	1699	G
25	A	1715	G
25	A	1730	C
25	A	1733	G
25	A	1738	G
25	A	1756	G
25	A	1758	U
25	A	1763	G
25	A	1764	C
25	A	1769	U
25	A	1773	A
25	A	1784	A
25	A	1791	A
25	A	1800	C
25	A	1801	A
25	A	1802	A
25	A	1808	A
25	A	1809	A
25	A	1815	A
25	A	1816	C
25	A	1820	U
25	A	1828	G
25	A	1829	A
25	A	1833	C
25	A	1870	C
25	A	1871	A
25	A	1880	U
25	A	1884	G
25	A	1900	A

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Mol	Chain	Res	Type
25	A	1901	A
25	A	1906	G
25	A	1912	A
25	A	1927	A
25	A	1929	G
25	A	1930	G
25	A	1931	U
25	A	1937	A
25	A	1938	A
25	A	1941	C
25	A	1955	U
25	A	1960	A
25	A	1961	C
25	A	1963	U
25	A	1965	C
25	A	1966	A
25	A	1967	C
25	A	1970	A
25	A	1971	U
25	A	1972	G
25	A	1991	U
25	A	1992	G
25	A	1993	U
25	A	1997	C
25	A	2022	U
25	A	2023	C
25	A	2031	A
25	A	2032	G
25	A	2034	U
25	A	2036	C
25	A	2043	C
25	A	2049	G
25	A	2050	C
25	A	2052	A
25	A	2055	C
25	A	2056	G
25	A	2059	A
25	A	2060	A
25	A	2061	G
25	A	2062	A
25	A	2068	U
25	A	2069	G7M

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Mol	Chain	Res	Type
25	A	2070	A
25	A	2072	C
25	A	2080	A
25	A	2087	G
25	A	2093	G
25	A	2096	C
25	A	2098	U
25	A	2106	U
25	A	2108	A
25	A	2110	G
25	A	2111	U
25	A	2112	G
25	A	2118	U
25	A	2119	A
25	A	2120	G
25	A	2121	G
25	A	2122	U
25	A	2123	G
25	A	2125	G
25	A	2126	A
25	A	2127	G
25	A	2129	C
25	A	2131	U
25	A	2132	U
25	A	2133	G
25	A	2134	A
25	A	2136	G
25	A	2145	C
25	A	2147	A
25	A	2149	U
25	A	2157	G
25	A	2161	C
25	A	2162	G
25	A	2163	A
25	A	2164	C
25	A	2165	C
25	A	2169	A
25	A	2170	A
25	A	2171	A
25	A	2172	U
25	A	2173	A
25	A	2174	C

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Mol	Chain	Res	Type
25	A	2178	C
25	A	2180	U
25	A	2182	U
25	A	2183	A
25	A	2190	G
25	A	2195	U
25	A	2198	A
25	A	2204	G
25	A	2212	A
25	A	2223	G
25	A	2225	A
25	A	2238	G
25	A	2239	G
25	A	2246	G
25	A	2250	G
25	A	2251	OMG
25	A	2268	A
25	A	2279	G
25	A	2283	C
25	A	2287	A
25	A	2296	U
25	A	2297	A
25	A	2305	U
25	A	2309	A
25	A	2310	C
25	A	2312	U
25	A	2321	U
25	A	2325	G
25	A	2326	C
25	A	2327	A
25	A	2331	G
25	A	2333	A
25	A	2334	U
25	A	2335	A
25	A	2345	G
25	A	2347	C
25	A	2350	C
25	A	2354	C
25	A	2357	G
25	A	2373	G
25	A	2383	G
25	A	2385	C

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Mol	Chain	Res	Type
25	A	2388	A
25	A	2392	A
25	A	2402	U
25	A	2403	C
25	A	2406	A
25	A	2422	C
25	A	2427	C
25	A	2428	G
25	A	2430	A
25	A	2435	A
25	A	2441	U
25	A	2445	2MG
25	A	2448	A
25	A	2452	C
25	A	2468	A
25	A	2469	A
25	A	2470	G
25	A	2475	C
25	A	2476	A
25	A	2491	U
25	A	2494	G
25	A	2502	G
25	A	2506	U
25	A	2518	A
25	A	2520	C
25	A	2529	G
25	A	2535	G
25	A	2543	G
25	A	2547	A
25	A	2554	U
25	A	2566	A
25	A	2567	G
25	A	2569	G
25	A	2572	A
25	A	2573	C
25	A	2576	G
25	A	2585	U
25	A	2586	U
25	A	2602	A
25	A	2603	G
25	A	2609	U
25	A	2610	C

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Mol	Chain	Res	Type
25	A	2611	C
25	A	2613	U
25	A	2614	A
25	A	2623	G
25	A	2629	U
25	A	2630	G
25	A	2634	A
25	A	2636	C
25	A	2663	G
25	A	2682	A
25	A	2689	U
25	A	2690	U
25	A	2713	U
25	A	2714	G
25	A	2716	C
25	A	2726	A
25	A	2729	G
25	A	2733	A
25	A	2739	U
25	A	2744	G
25	A	2748	A
25	A	2758	A
25	A	2764	A
25	A	2765	A
25	A	2766	A
25	A	2776	A
25	A	2778	A
25	A	2794	C
25	A	2797	U
25	A	2798	U
25	A	2809	A
25	A	2818	U
25	A	2820	A
25	A	2823	A
25	A	2825	G
25	A	2833	U
25	A	2834	G
25	A	2849	U
25	A	2850	A
25	A	2867	G
25	A	2873	A
25	A	2880	C

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Mol	Chain	Res	Type
25	A	2883	A
25	A	2891	U
25	A	2893	A
25	A	2894	G
26	B	4	C
26	B	25	U
26	B	32	U
26	B	33	G
26	B	35	C
26	B	39	A
26	B	41	G
26	B	88	C
26	B	89	U
26	B	96	G
26	B	109	A

All (26) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
25	A	51	G
25	A	91	A
25	A	158	U
25	A	205	G
25	A	512	G
25	A	545	U
25	A	774	G
25	A	880	G
25	A	1182	G
25	A	1190	G
25	A	1212	G
25	A	1432	G
25	A	1930	G
25	A	1940	U
25	A	2061	G
25	A	2135	A
25	A	2162	G
25	A	2168	G
25	A	2194	U
25	A	2286	G
25	A	2308	G
25	A	2326	C
25	A	2391	G

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Mol	Chain	Res	Type
25	A	2566	A
25	A	2610	C
26	B	88	C

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

43 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	$\#\|Z\| > 2$
25	PSU	A	1917	25	18,21,22	1.53	3 (16%)	22,30,33	1.94	3 (13%)
25	PSU	A	2504	25	18,21,22	1.42	4 (22%)	22,30,33	1.89	4 (18%)
1	G7M	a	527	1	20,26,27	1.59	3 (15%)	17,39,42	1.69	4 (23%)
1	2MG	a	966	1	18,26,27	0.94	1 (5%)	16,38,41	1.23	3 (18%)
24	5MU	y	54	24	19,22,23	1.34	4 (21%)	28,32,35	2.08	7 (25%)
25	PSU	A	2605	25	18,21,22	1.32	2 (11%)	22,30,33	1.90	3 (13%)
25	1MG	A	745	25	18,26,27	0.86	1 (5%)	19,39,42	1.04	2 (10%)
1	PSU	a	516	1	18,21,22	1.38	3 (16%)	22,30,33	1.94	4 (18%)
25	OMU	A	2552	25	19,22,23	1.23	3 (15%)	26,31,34	1.95	8 (30%)
25	PSU	A	2580	25	18,21,22	1.35	2 (11%)	22,30,33	1.88	4 (18%)
25	PSU	A	1911	25	18,21,22	1.40	3 (16%)	22,30,33	2.06	4 (18%)
25	2MG	A	1835	25	18,26,27	0.99	1 (5%)	16,38,41	1.31	2 (12%)
24	6IA	y	37	24	22,29,30	0.79	1 (4%)	22,41,44	1.72	4 (18%)
25	3TD	A	1915	25	18,22,23	4.08	7 (38%)	22,32,35	1.76	3 (13%)
25	6MZ	A	2030	25	18,25,26	0.93	1 (5%)	16,36,39	2.65	4 (25%)
1	MA6	a	1519	1	18,26,27	1.02	2 (11%)	19,38,41	1.81	4 (21%)
1	4OC	a	1402	1	20,23,24	0.78	1 (5%)	26,32,35	1.14	2 (7%)
25	2MA	A	2503	25	17,25,26	1.00	1 (5%)	17,37,40	0.96	2 (11%)
1	5MC	a	1407	1	18,22,23	1.02	2 (11%)	26,32,35	1.32	3 (11%)
24	H2U	y	19	24	18,21,22	0.97	2 (11%)	21,30,33	1.20	2 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
25	5MU	A	747	25	19,22,23	1.35	4 (21%)	28,32,35	1.99	7 (25%)
22	PSU	v	55	22	18,21,22	1.56	3 (16%)	22,30,33	2.08	5 (22%)
25	6MZ	A	1618	25	18,25,26	0.97	1 (5%)	16,36,39	2.11	4 (25%)
25	5MC	A	1962	25	18,22,23	0.92	2 (11%)	26,32,35	1.05	2 (7%)
1	2MG	a	1516	1	18,26,27	0.87	1 (5%)	16,38,41	1.12	2 (12%)
25	PSU	A	955	25	18,21,22	1.41	2 (11%)	22,30,33	2.03	3 (13%)
25	H2U	A	2449	25	18,21,22	1.08	3 (16%)	21,30,33	1.66	3 (14%)
22	H2U	v	20	22	18,21,22	0.95	2 (11%)	21,30,33	1.33	3 (14%)
22	5MU	v	54	22	19,22,23	1.51	3 (15%)	28,32,35	2.10	9 (32%)
1	UR3	a	1498	1	19,22,23	1.06	2 (10%)	26,32,35	1.73	4 (15%)
25	PSU	A	2457	25	18,21,22	1.41	2 (11%)	22,30,33	1.92	4 (18%)
24	PSU	y	55	24	18,21,22	1.49	3 (16%)	22,30,33	1.67	3 (13%)
1	MA6	a	1518	1	18,26,27	0.91	1 (5%)	19,38,41	1.92	6 (31%)
1	5MC	a	967	1	18,22,23	0.93	2 (11%)	26,32,35	1.27	3 (11%)
25	OMG	A	2251	25,24	18,26,27	1.01	1 (5%)	19,38,41	0.98	2 (10%)
25	5MU	A	1939	25	19,22,23	1.38	5 (26%)	28,32,35	2.27	6 (21%)
25	2MG	A	2445	25	18,26,27	0.93	1 (5%)	16,38,41	1.17	3 (18%)
25	G7M	A	2069	25	20,26,27	1.56	3 (15%)	17,39,42	1.56	3 (17%)
1	2MG	a	1207	1	18,26,27	0.92	1 (5%)	16,38,41	1.09	2 (12%)
25	OMC	A	2498	25	19,22,23	0.90	0	26,31,34	1.22	4 (15%)
25	PSU	A	2604	25	18,21,22	1.49	3 (16%)	22,30,33	1.92	3 (13%)
22	4SU	v	8	22	18,21,22	1.71	4 (22%)	26,30,33	2.71	7 (26%)
25	PSU	A	746	25	18,21,22	1.36	2 (11%)	22,30,33	1.84	4 (18%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	PSU	A	1917	25	-	0/7/25/26	0/2/2/2
25	PSU	A	2504	25	-	0/7/25/26	0/2/2/2
1	G7M	a	527	1	2/2/5/5	3/3/25/26	0/3/3/3
1	2MG	a	966	1	-	0/5/27/28	0/3/3/3
24	5MU	y	54	24	-	2/7/25/26	0/2/2/2
25	PSU	A	2605	25	-	0/7/25/26	0/2/2/2
25	1MG	A	745	25	-	0/3/25/26	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	a	516	1	-	0/7/25/26	0/2/2/2
25	OMU	A	2552	25	-	2/9/27/28	0/2/2/2
25	PSU	A	2580	25	-	0/7/25/26	0/2/2/2
25	PSU	A	1911	25	-	0/7/25/26	0/2/2/2
25	2MG	A	1835	25	-	1/5/27/28	0/3/3/3
24	6IA	y	37	24	-	4/9/31/32	0/3/3/3
25	3TD	A	1915	25	-	5/7/25/26	0/2/2/2
25	6MZ	A	2030	25	-	2/5/27/28	0/3/3/3
1	MA6	a	1519	1	-	2/7/29/30	0/3/3/3
1	4OC	a	1402	1	-	2/9/29/30	0/2/2/2
25	2MA	A	2503	25	-	2/3/25/26	0/3/3/3
1	5MC	a	1407	1	-	0/7/25/26	0/2/2/2
24	H2U	y	19	24	-	4/7/38/39	0/2/2/2
25	5MU	A	747	25	-	2/7/25/26	0/2/2/2
22	PSU	v	55	22	-	2/7/25/26	0/2/2/2
25	6MZ	A	1618	25	-	2/5/27/28	0/3/3/3
25	5MC	A	1962	25	-	4/7/25/26	0/2/2/2
1	2MG	a	1516	1	-	0/5/27/28	0/3/3/3
25	PSU	A	955	25	-	0/7/25/26	0/2/2/2
25	H2U	A	2449	25	-	0/7/38/39	0/2/2/2
22	H2U	v	20	22	-	5/7/38/39	0/2/2/2
22	5MU	v	54	22	-	3/7/25/26	0/2/2/2
1	UR3	a	1498	1	-	2/7/25/26	0/2/2/2
25	PSU	A	2457	25	-	0/7/25/26	0/2/2/2
24	PSU	y	55	24	-	1/7/25/26	0/2/2/2
1	MA6	a	1518	1	-	2/7/29/30	0/3/3/3
1	5MC	a	967	1	-	0/7/25/26	0/2/2/2
25	OMG	A	2251	25,24	-	1/5/27/28	0/3/3/3
25	5MU	A	1939	25	-	0/7/25/26	0/2/2/2
25	2MG	A	2445	25	-	2/5/27/28	0/3/3/3
25	G7M	A	2069	25	2/2/5/5	2/3/25/26	0/3/3/3
1	2MG	a	1207	1	-	0/5/27/28	0/3/3/3
25	OMC	A	2498	25	-	0/9/27/28	0/2/2/2
25	PSU	A	2604	25	-	0/7/25/26	0/2/2/2
22	4SU	v	8	22	-	1/7/25/26	0/2/2/2
25	PSU	A	746	25	-	1/7/25/26	0/2/2/2

All (98) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	1915	3TD	C6-C5	11.87	1.49	1.35
25	A	1915	3TD	C2-N1	9.20	1.49	1.37
25	A	1915	3TD	C6-N1	5.79	1.45	1.36
1	a	527	G7M	C5-C4	4.59	1.48	1.39
22	v	8	4SU	C4-S4	-4.57	1.59	1.68
25	A	2069	G7M	C5-C4	4.39	1.47	1.39
24	y	55	PSU	C6-C5	3.70	1.39	1.35
22	v	55	PSU	C6-C5	3.67	1.39	1.35
25	A	2604	PSU	C6-C5	3.56	1.39	1.35
22	v	55	PSU	C4-N3	-3.52	1.32	1.38
25	A	1915	3TD	C2-N3	3.48	1.46	1.38
22	v	8	4SU	C5-C4	-3.44	1.38	1.42
22	v	54	5MU	C2-N1	3.36	1.43	1.38
25	A	2504	PSU	C6-C5	3.21	1.39	1.35
25	A	1917	PSU	C6-C5	3.21	1.39	1.35
25	A	955	PSU	C6-C5	3.19	1.39	1.35
25	A	746	PSU	C6-C5	3.18	1.39	1.35
25	A	2457	PSU	C6-C5	3.18	1.39	1.35
1	a	516	PSU	C6-C5	3.14	1.39	1.35
25	A	2580	PSU	C6-C5	3.08	1.38	1.35
25	A	1911	PSU	C6-C5	3.03	1.38	1.35
24	y	55	PSU	C4-N3	-3.01	1.33	1.38
25	A	1618	6MZ	C5-C4	2.99	1.48	1.40
25	A	2605	PSU	C6-C5	2.97	1.38	1.35
25	A	2030	6MZ	C5-C4	2.95	1.48	1.40
25	A	1911	PSU	C4-N3	-2.94	1.33	1.38
25	A	1939	5MU	C6-C5	2.88	1.39	1.34
22	v	54	5MU	C4-N3	-2.87	1.33	1.38
22	v	55	PSU	C2-N3	-2.86	1.32	1.37
25	A	1915	3TD	O4-C4	-2.86	1.17	1.23
25	A	1835	2MG	C6-N1	-2.84	1.33	1.37
25	A	2504	PSU	C4-N3	-2.79	1.33	1.38
25	A	2449	H2U	C2-N3	-2.79	1.33	1.38
25	A	955	PSU	C4-N3	-2.78	1.33	1.38
25	A	2457	PSU	C4-N3	-2.77	1.33	1.38
1	a	1407	5MC	C6-C5	2.77	1.39	1.34
25	A	2069	G7M	C6-N1	-2.75	1.33	1.37
25	A	2251	OMG	C6-N1	-2.74	1.33	1.37
1	a	1518	MA6	C5-C4	2.73	1.48	1.40
1	a	1519	MA6	C5-C4	2.73	1.48	1.40
25	A	1962	5MC	C6-C5	2.72	1.39	1.34
25	A	747	5MU	C4-N3	-2.71	1.33	1.38
1	a	1498	UR3	C2-N1	2.69	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	2604	PSU	C4-N3	-2.69	1.33	1.38
22	v	20	H2U	C2-N3	-2.67	1.33	1.38
25	A	1917	PSU	C4-N3	-2.67	1.33	1.38
25	A	2605	PSU	C4-N3	-2.66	1.33	1.38
22	v	54	5MU	C6-C5	2.65	1.39	1.34
25	A	1917	PSU	O4'-C1'	-2.61	1.40	1.43
25	A	2580	PSU	C4-N3	-2.58	1.34	1.38
25	A	746	PSU	C4-N3	-2.57	1.34	1.38
24	y	19	H2U	C2-N3	-2.57	1.33	1.38
1	a	516	PSU	C4-N3	-2.56	1.34	1.38
1	a	966	2MG	C6-N1	-2.56	1.34	1.37
25	A	2552	OMU	C4-N3	-2.55	1.34	1.38
24	y	54	5MU	C4-N3	-2.54	1.34	1.38
1	a	527	G7M	C6-N1	-2.53	1.34	1.37
25	A	1915	3TD	C4-N3	2.53	1.45	1.40
25	A	1915	3TD	O2-C2	-2.50	1.18	1.23
25	A	2445	2MG	C6-N1	-2.50	1.34	1.37
1	a	967	5MC	C6-C5	2.50	1.38	1.34
1	a	527	G7M	O2'-C2'	-2.50	1.37	1.43
25	A	1939	5MU	C4-C5	2.49	1.48	1.44
25	A	2449	H2U	C4-N3	-2.47	1.33	1.37
24	y	19	H2U	C4-N3	-2.46	1.33	1.37
25	A	1939	5MU	C4-N3	-2.45	1.34	1.38
24	y	37	6IA	C5-C4	2.45	1.47	1.40
25	A	747	5MU	C6-C5	2.43	1.38	1.34
25	A	2069	G7M	O2'-C2'	-2.41	1.37	1.43
1	a	1207	2MG	C6-N1	-2.36	1.34	1.37
25	A	745	1MG	C5-C4	2.34	1.49	1.43
24	y	55	PSU	C2-N3	-2.33	1.33	1.37
1	a	967	5MC	C6-N1	-2.31	1.34	1.38
25	A	2503	2MA	C2-N3	2.30	1.36	1.31
25	A	1939	5MU	C6-N1	-2.30	1.34	1.38
24	y	54	5MU	C6-C5	2.28	1.38	1.34
25	A	747	5MU	C2-N1	2.26	1.42	1.38
1	a	1516	2MG	C6-N1	-2.25	1.34	1.37
22	v	8	4SU	C4-N3	-2.23	1.35	1.37
25	A	2504	PSU	C2-N3	-2.21	1.33	1.37
24	y	54	5MU	C2-N1	2.18	1.42	1.38
22	v	20	H2U	C4-N3	-2.17	1.33	1.37
1	a	1407	5MC	C6-N1	-2.14	1.34	1.38
25	A	747	5MU	C4-C5	2.14	1.48	1.44
25	A	2552	OMU	C2-N1	2.13	1.41	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	1911	PSU	C2-N3	-2.12	1.33	1.37
22	v	8	4SU	C2-N1	2.12	1.41	1.38
25	A	1962	5MC	C6-N1	-2.11	1.34	1.38
25	A	2552	OMU	C2-N3	-2.11	1.34	1.38
25	A	2449	H2U	C2-N1	-2.08	1.32	1.35
1	a	1498	UR3	C6-C5	2.07	1.39	1.35
25	A	2504	PSU	C4-C5	2.06	1.50	1.44
1	a	1519	MA6	C6-N1	2.05	1.36	1.33
1	a	1402	4OC	C6-C5	2.05	1.39	1.35
25	A	2604	PSU	C4-C5	2.04	1.50	1.44
25	A	1939	5MU	C2-N3	-2.03	1.34	1.38
24	y	54	5MU	C4-C5	2.03	1.48	1.44
1	a	516	PSU	O4'-C1'	-2.02	1.41	1.43

All (164) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	v	8	4SU	C5-C4-S4	-7.22	115.16	124.47
22	v	8	4SU	C4-N3-C2	-6.97	120.57	127.34
25	A	955	PSU	N1-C2-N3	6.62	122.63	115.13
25	A	2030	6MZ	C9-N6-C6	-6.62	117.17	122.87
25	A	2030	6MZ	C2-N1-C6	6.49	122.15	116.59
25	A	1911	PSU	N1-C2-N3	6.43	122.42	115.13
25	A	1618	6MZ	C2-N1-C6	6.38	122.06	116.59
22	v	8	4SU	C5-C4-N3	6.27	120.51	114.69
25	A	2604	PSU	N1-C2-N3	6.21	122.17	115.13
25	A	2457	PSU	N1-C2-N3	6.16	122.11	115.13
25	A	2449	H2U	C4-N3-C2	-6.16	120.68	125.79
1	a	516	PSU	N1-C2-N3	6.15	122.09	115.13
25	A	1917	PSU	N1-C2-N3	6.14	122.09	115.13
25	A	2580	PSU	N1-C2-N3	5.96	121.88	115.13
24	y	37	6IA	C2-N1-C6	5.95	121.70	116.59
25	A	2504	PSU	N1-C2-N3	5.90	121.81	115.13
22	v	55	PSU	N1-C2-N3	5.89	121.80	115.13
25	A	746	PSU	N1-C2-N3	5.84	121.74	115.13
25	A	1939	5MU	C4-N3-C2	-5.72	119.95	127.35
25	A	2605	PSU	N1-C2-N3	5.70	121.59	115.13
24	y	55	PSU	N1-C2-N3	5.53	121.39	115.13
1	a	1498	UR3	C4-N3-C2	-5.50	119.38	124.56
25	A	1915	3TD	N1-C2-N3	5.31	120.33	116.14
24	y	54	5MU	C4-N3-C2	-5.11	120.73	127.35
25	A	1939	5MU	N3-C2-N1	5.10	121.67	114.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	A	747	5MU	N3-C2-N1	5.07	121.62	114.89
24	y	54	5MU	N3-C2-N1	4.95	121.46	114.89
25	A	747	5MU	C4-N3-C2	-4.79	121.15	127.35
25	A	1939	5MU	C5-C4-N3	4.78	119.39	115.31
22	v	54	5MU	N3-C2-N1	4.73	121.17	114.89
24	y	54	5MU	C5-C4-N3	4.72	119.34	115.31
25	A	1939	5MU	C5-C6-N1	-4.66	118.54	123.34
25	A	1911	PSU	C4-N3-C2	-4.59	119.72	126.34
25	A	2552	OMU	C1'-N1-C2	4.52	125.76	117.57
1	a	1519	MA6	C4-C5-N7	-4.51	104.70	109.40
1	a	1518	MA6	C4-C5-N7	-4.51	104.70	109.40
25	A	2552	OMU	N3-C2-N1	4.45	120.80	114.89
25	A	2605	PSU	C4-N3-C2	-4.20	120.29	126.34
22	v	8	4SU	S4-C4-N3	4.18	124.33	120.21
25	A	747	5MU	C5-C4-N3	4.16	118.86	115.31
22	v	54	5MU	C1'-N1-C2	4.15	125.09	117.57
25	A	1939	5MU	O4-C4-C5	-4.14	120.10	124.90
22	v	54	5MU	C4-N3-C2	-4.11	122.03	127.35
24	y	54	5MU	O4-C4-C5	-4.09	120.16	124.90
25	A	1915	3TD	C4-N3-C2	-4.02	120.24	124.61
25	A	747	5MU	O4-C4-C5	-4.02	120.24	124.90
22	v	20	H2U	C4-N3-C2	-4.01	122.46	125.79
25	A	2457	PSU	C4-N3-C2	-4.00	120.57	126.34
1	a	516	PSU	C4-N3-C2	-3.99	120.59	126.34
25	A	955	PSU	C4-N3-C2	-3.99	120.59	126.34
22	v	55	PSU	C6-C5-C4	-3.97	115.42	118.20
1	a	1498	UR3	C1'-N1-C2	3.95	123.67	116.99
25	A	2552	OMU	C4-N3-C2	-3.91	121.43	126.58
25	A	955	PSU	O2-C2-N1	-3.87	118.53	122.79
25	A	2030	6MZ	C4-C5-N7	-3.86	105.38	109.40
25	A	746	PSU	C4-N3-C2	-3.84	120.80	126.34
1	a	1518	MA6	N3-C2-N1	-3.81	122.72	128.68
25	A	1939	5MU	O2-C2-N1	-3.79	117.75	122.79
25	A	2504	PSU	C4-N3-C2	-3.79	120.88	126.34
25	A	2580	PSU	C4-N3-C2	-3.77	120.90	126.34
22	v	8	4SU	N3-C2-N1	3.75	119.86	114.89
1	a	1407	5MC	O2-C2-N3	-3.70	116.31	122.33
25	A	2498	OMC	O2-C2-N3	-3.69	116.33	122.33
1	a	1519	MA6	N3-C2-N1	-3.68	122.92	128.68
22	v	54	5MU	C5-C4-N3	3.68	118.45	115.31
25	A	1917	PSU	O2-C2-N1	-3.64	118.79	122.79
22	v	54	5MU	O2-C2-N3	-3.61	114.78	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	v	55	PSU	C4-N3-C2	-3.59	121.16	126.34
25	A	1917	PSU	C4-N3-C2	-3.55	121.22	126.34
25	A	2604	PSU	O2-C2-N1	-3.54	118.90	122.79
25	A	2604	PSU	C4-N3-C2	-3.54	121.24	126.34
1	a	516	PSU	O2-C2-N1	-3.53	118.91	122.79
1	a	1519	MA6	C10-N6-C6	-3.53	108.84	119.51
25	A	746	PSU	O2-C2-N1	-3.51	118.93	122.79
24	y	19	H2U	C4-N3-C2	-3.50	122.89	125.79
22	v	54	5MU	O4-C4-C5	-3.50	120.85	124.90
25	A	2580	PSU	O2-C2-N1	-3.39	119.06	122.79
22	v	55	PSU	O2-C2-N3	-3.37	115.46	121.82
25	A	2069	G7M	O3'-C3'-C4'	3.36	120.77	111.05
24	y	37	6IA	C12-N6-C6	-3.31	117.32	122.89
25	A	1618	6MZ	C9-N6-C6	-3.26	120.07	122.87
25	A	1835	2MG	C5-C6-N1	3.24	119.68	113.95
25	A	1962	5MC	C5-C6-N1	-3.24	120.00	123.34
25	A	1911	PSU	O2-C2-N1	-3.23	119.23	122.79
25	A	2457	PSU	O2-C2-N1	-3.23	119.24	122.79
25	A	2552	OMU	C5-C4-N3	3.15	119.55	114.84
25	A	1618	6MZ	N3-C2-N1	-3.13	123.78	128.68
1	a	1518	MA6	C9-N6-C6	-3.13	110.04	119.51
24	y	37	6IA	N3-C2-N1	-3.12	123.80	128.68
1	a	527	G7M	O3'-C3'-C2'	3.11	121.89	111.82
1	a	1402	4OC	O2-C2-N3	-3.11	117.27	122.33
25	A	2605	PSU	O2-C2-N1	-3.08	119.40	122.79
1	a	1407	5MC	C5-C6-N1	-3.04	120.21	123.34
24	y	55	PSU	C4-N3-C2	-3.04	121.96	126.34
1	a	1498	UR3	O2-C2-N3	-3.02	117.08	121.34
25	A	2552	OMU	O2-C2-N3	-3.02	115.88	121.50
1	a	1519	MA6	C10-N6-C9	-2.96	106.60	116.12
1	a	527	G7M	O3'-C3'-C4'	2.95	119.56	111.05
25	A	2030	6MZ	N3-C2-N1	-2.93	124.10	128.68
22	v	54	5MU	C1'-N1-C6	-2.92	116.26	121.12
1	a	967	5MC	C5-C6-N1	-2.92	120.33	123.34
22	v	55	PSU	O4-C4-N3	-2.90	114.56	120.12
25	A	2069	G7M	O3'-C3'-C2'	2.86	121.08	111.82
25	A	2504	PSU	O2-C2-N1	-2.86	119.65	122.79
1	a	1518	MA6	C10-N6-C9	-2.82	107.04	116.12
25	A	1915	3TD	O4-C4-N3	-2.81	115.16	120.30
1	a	1518	MA6	N1-C6-N6	-2.79	114.12	117.06
1	a	1498	UR3	C6-N1-C2	-2.77	119.31	121.79
24	y	54	5MU	O2-C2-N1	-2.76	119.12	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	v	20	H2U	C5-C6-N1	-2.71	102.68	111.61
1	a	527	G7M	C3'-C2'-C1'	2.69	105.03	100.98
1	a	967	5MC	C1'-N1-C6	-2.63	116.74	121.12
22	v	54	5MU	C6-N1-C2	-2.62	118.64	121.30
25	A	2552	OMU	O4-C4-C5	-2.58	120.62	125.16
25	A	2503	2MA	C5-C6-N1	2.54	118.41	114.02
25	A	1962	5MC	C5-C4-N3	-2.53	118.94	121.67
24	y	54	5MU	C5-C6-N1	-2.49	120.78	123.34
25	A	747	5MU	C5-C6-N1	-2.48	120.79	123.34
25	A	2069	G7M	C3'-C2'-C1'	2.47	104.69	100.98
1	a	527	G7M	O2'-C2'-C1'	2.46	119.95	110.85
25	A	1911	PSU	C5-C6-N1	-2.44	118.45	122.11
1	a	966	2MG	C5-C6-N1	2.42	118.22	113.95
25	A	2504	PSU	C6-C5-C4	-2.40	116.52	118.20
25	A	2445	2MG	C8-N7-C5	2.39	107.54	102.99
22	v	8	4SU	C1'-N1-C2	2.39	121.89	117.57
24	y	55	PSU	O2-C2-N3	-2.38	117.32	121.82
1	a	1407	5MC	C5-C4-N3	-2.38	119.10	121.67
25	A	2445	2MG	C5-C6-N1	2.37	118.14	113.95
25	A	1618	6MZ	C4-C5-N7	-2.37	106.93	109.40
22	v	20	H2U	C5-C4-N3	2.37	119.31	116.65
1	a	1516	2MG	C8-N7-C5	2.36	107.49	102.99
25	A	2552	OMU	C6-N1-C2	-2.36	117.97	120.99
24	y	54	5MU	C5M-C5-C4	2.33	121.33	118.77
1	a	1402	4OC	C6-C5-C4	2.31	119.78	116.96
25	A	2498	OMC	O2-C2-N1	2.30	123.65	118.89
1	a	966	2MG	C8-N7-C5	2.29	107.36	102.99
25	A	2445	2MG	CM2-N2-C2	-2.29	118.81	123.86
25	A	1835	2MG	C8-N7-C5	2.27	107.32	102.99
22	v	8	4SU	O2-C2-N1	-2.27	119.77	122.79
1	a	1516	2MG	C5-C6-N1	2.27	117.95	113.95
1	a	966	2MG	CM2-N2-C2	-2.26	118.87	123.86
1	a	1207	2MG	C8-N7-C5	2.23	107.23	102.99
25	A	2251	OMG	C8-N7-C5	2.21	107.20	102.99
1	a	1207	2MG	C5-C6-N1	2.20	117.84	113.95
25	A	747	5MU	C5M-C5-C4	2.15	121.13	118.77
25	A	745	1MG	C8-N7-C5	2.14	107.08	102.99
25	A	2457	PSU	C5-C6-N1	-2.13	118.91	122.11
1	a	967	5MC	CM5-C5-C6	-2.12	120.01	122.85
25	A	2498	OMC	C1'-N1-C2	2.12	123.15	118.42
25	A	2580	PSU	O4'-C1'-C2'	2.11	108.13	105.14
22	v	54	5MU	C5-C6-N1	-2.10	121.18	123.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	A	747	5MU	O2-C2-N1	-2.10	119.99	122.79
25	A	2498	OMC	CM2-O2'-C2'	-2.10	109.02	114.52
25	A	2552	OMU	C1'-N1-C6	-2.10	116.27	120.84
1	a	516	PSU	O4'-C1'-C2'	2.10	108.10	105.14
24	y	37	6IA	C4-C5-N7	-2.09	107.22	109.40
25	A	2449	H2U	C5-C6-N1	-2.08	104.77	111.61
25	A	2449	H2U	O2-C2-N1	-2.07	120.51	123.11
25	A	2251	OMG	C5-C6-N1	2.07	117.60	113.95
25	A	746	PSU	C5-C6-N1	-2.07	119.01	122.11
25	A	2503	2MA	C8-N7-C5	2.05	106.89	102.99
25	A	745	1MG	C5-C6-N1	2.05	116.98	113.90
1	a	1518	MA6	C3'-C2'-C1'	2.02	104.02	100.98
24	y	19	H2U	N3-C2-N1	2.02	118.79	116.65

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	a	527	G7M	C4'
1	a	527	G7M	C3'
25	A	2069	G7M	C4'
25	A	2069	G7M	C3'

All (59) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	a	1518	MA6	C5-C6-N6-C9
1	a	1519	MA6	C5-C6-N6-C10
22	v	20	H2U	O4'-C1'-N1-C2
22	v	20	H2U	O4'-C1'-N1-C6
22	v	54	5MU	C3'-C4'-C5'-O5'
22	v	54	5MU	O4'-C4'-C5'-O5'
22	v	55	PSU	O4'-C1'-C5-C4
22	v	55	PSU	O4'-C1'-C5-C6
24	y	19	H2U	O4'-C1'-N1-C6
24	y	19	H2U	C2'-C1'-N1-C2
24	y	19	H2U	C2'-C1'-N1-C6
24	y	54	5MU	C3'-C4'-C5'-O5'
25	A	1618	6MZ	C3'-C4'-C5'-O5'
25	A	1915	3TD	O4'-C1'-C5-C4
25	A	1915	3TD	C2'-C1'-C5-C6
25	A	1915	3TD	O4'-C1'-C5-C6
25	A	2069	G7M	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
25	A	2445	2MG	C3'-C4'-C5'-O5'
25	A	2552	OMU	O4'-C1'-N1-C2
24	y	37	6IA	O4'-C4'-C5'-O5'
24	y	37	6IA	C3'-C4'-C5'-O5'
24	y	54	5MU	O4'-C4'-C5'-O5'
25	A	1618	6MZ	O4'-C4'-C5'-O5'
25	A	2445	2MG	O4'-C4'-C5'-O5'
1	a	527	G7M	O4'-C4'-C5'-O5'
1	a	527	G7M	C3'-C4'-C5'-O5'
25	A	747	5MU	O4'-C4'-C5'-O5'
25	A	1915	3TD	O4'-C4'-C5'-O5'
1	a	1518	MA6	N1-C6-N6-C9
1	a	1519	MA6	N1-C6-N6-C10
25	A	2552	OMU	O4'-C1'-N1-C6
24	y	37	6IA	C12-C13-C14-C16
25	A	2503	2MA	C4'-C5'-O5'-P
25	A	747	5MU	C3'-C4'-C5'-O5'
25	A	1915	3TD	C3'-C4'-C5'-O5'
25	A	2030	6MZ	C3'-C4'-C5'-O5'
1	a	1402	4OC	O4'-C4'-C5'-O5'
1	a	1498	UR3	O4'-C1'-N1-C6
24	y	37	6IA	C4'-C5'-O5'-P
1	a	1498	UR3	O4'-C1'-N1-C2
22	v	20	H2U	C4'-C5'-O5'-P
25	A	2030	6MZ	C4'-C5'-O5'-P
22	v	20	H2U	C3'-C4'-C5'-O5'
22	v	20	H2U	O4'-C4'-C5'-O5'
1	a	527	G7M	C4'-C5'-O5'-P
25	A	2069	G7M	C3'-C4'-C5'-O5'
25	A	1962	5MC	C2'-C1'-N1-C6
25	A	1962	5MC	O4'-C1'-N1-C6
25	A	1835	2MG	C4'-C5'-O5'-P
1	a	1402	4OC	C3'-C4'-C5'-O5'
25	A	2503	2MA	O4'-C4'-C5'-O5'
22	v	54	5MU	C2'-C1'-N1-C2
25	A	746	PSU	O4'-C1'-C5-C6
24	y	55	PSU	C4'-C5'-O5'-P
25	A	2251	OMG	C3'-C4'-C5'-O5'
24	y	19	H2U	O4'-C1'-N1-C2
22	v	8	4SU	O4'-C4'-C5'-O5'
25	A	1962	5MC	O4'-C4'-C5'-O5'
25	A	1962	5MC	C2'-C1'-N1-C2

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

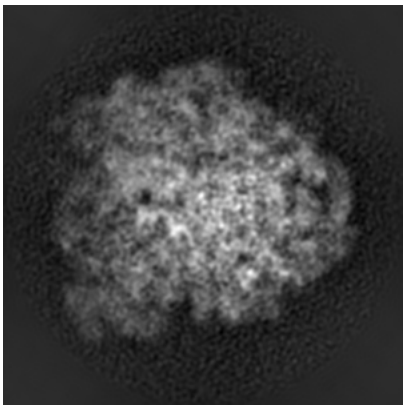
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-4126. 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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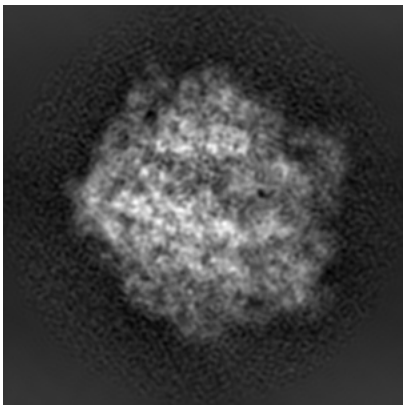
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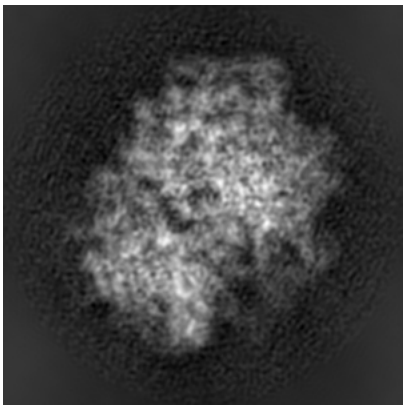
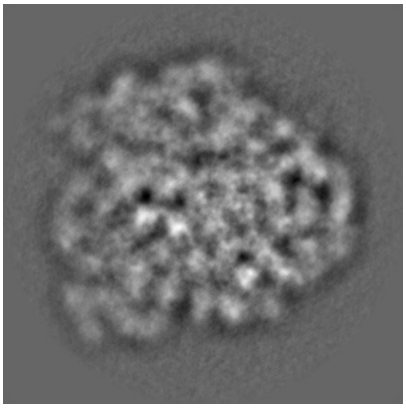
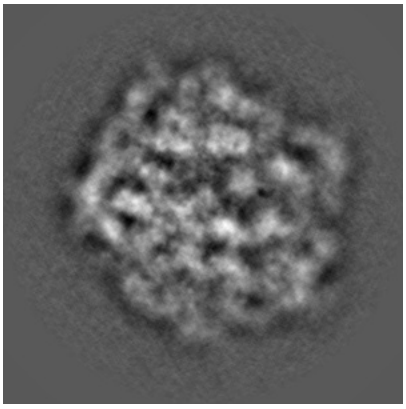
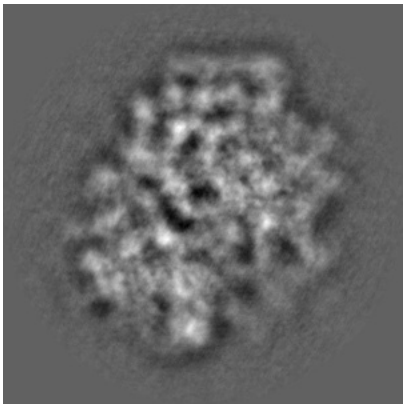

Z

6.1.2 Raw map


X

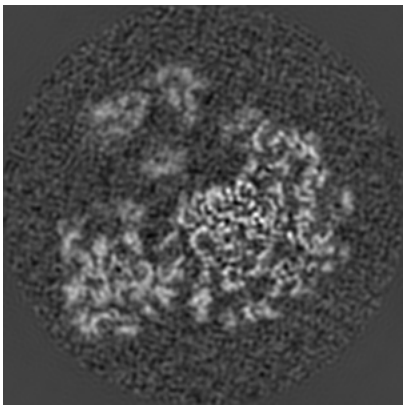

Y

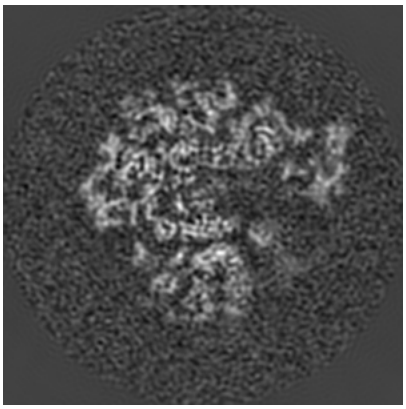

Z

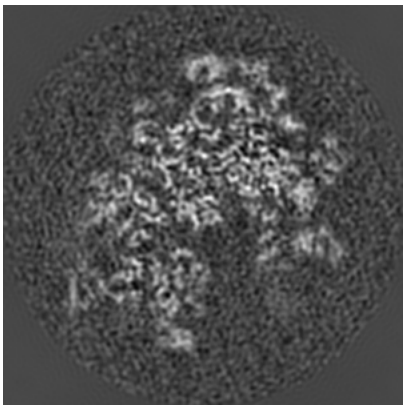
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

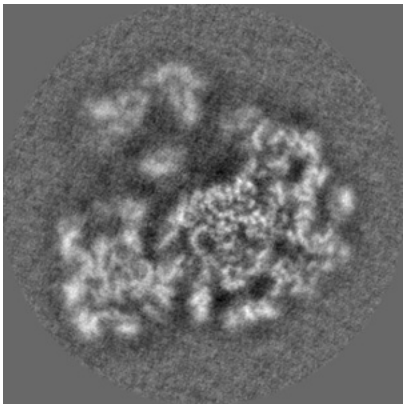
6.2.1 Primary map

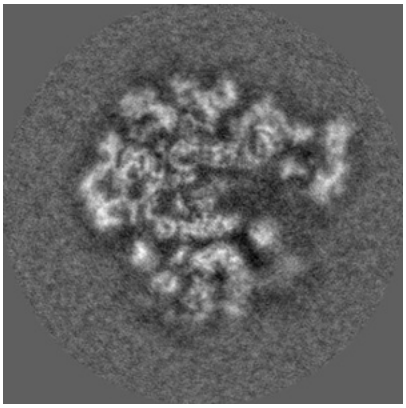

X Index: 136

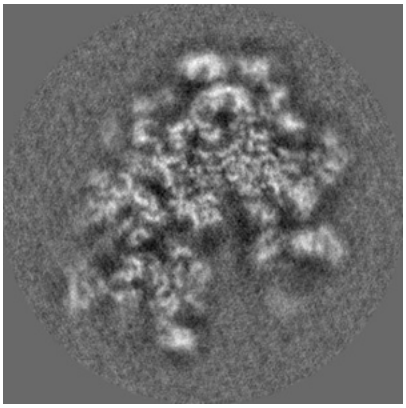

Y Index: 136


Z Index: 136

6.2.2 Raw map


X Index: 136

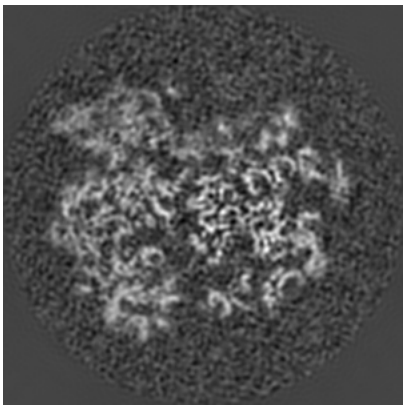

Y Index: 136

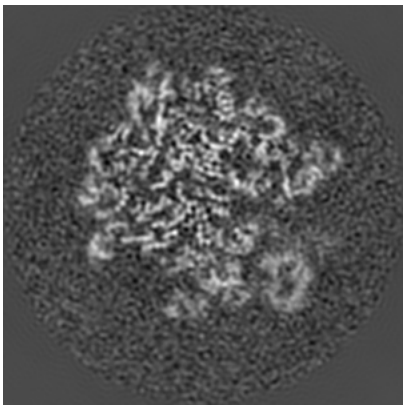

Z Index: 136

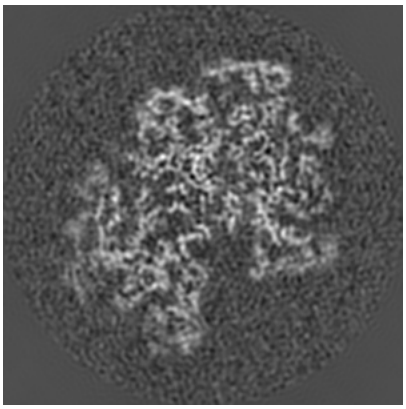
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

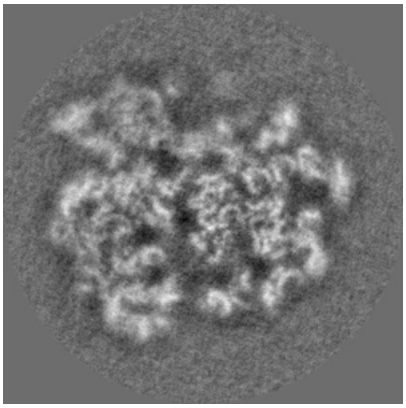
6.3.1 Primary map

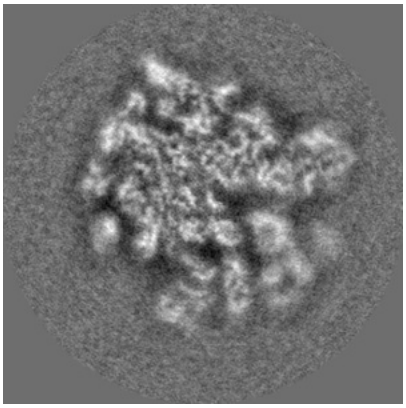

X Index: 119

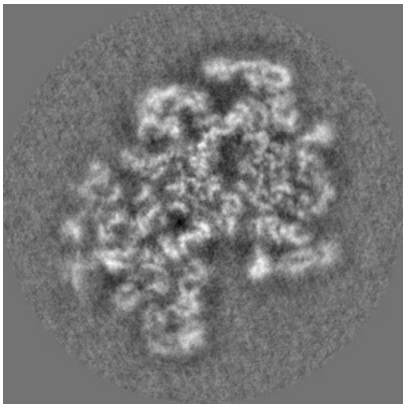

Y Index: 156


Z Index: 127

6.3.2 Raw map


X Index: 119

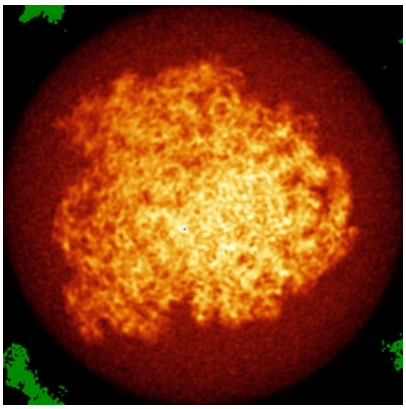

Y Index: 147

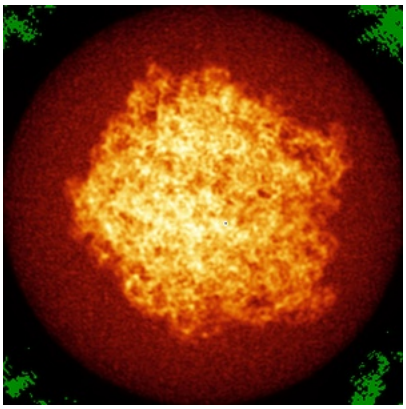

Z Index: 125

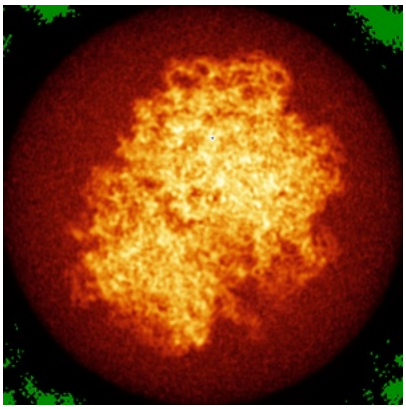
The images above show the largest variance slices of the map in three orthogonal directions.

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

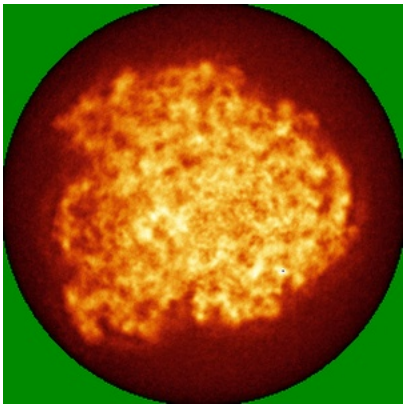
6.4.1 Primary map

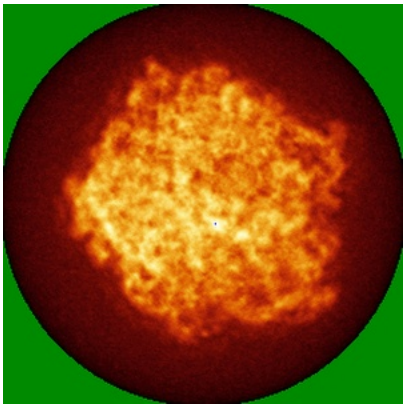

X

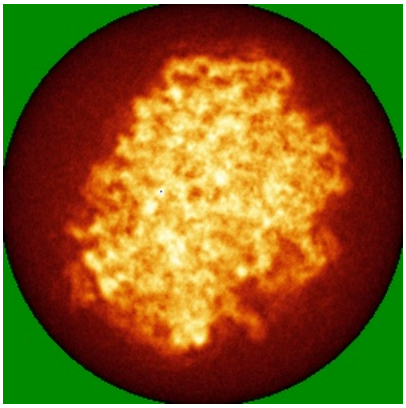

Y


Z

6.4.2 Raw map


X


Y


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.4. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X Y Z

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

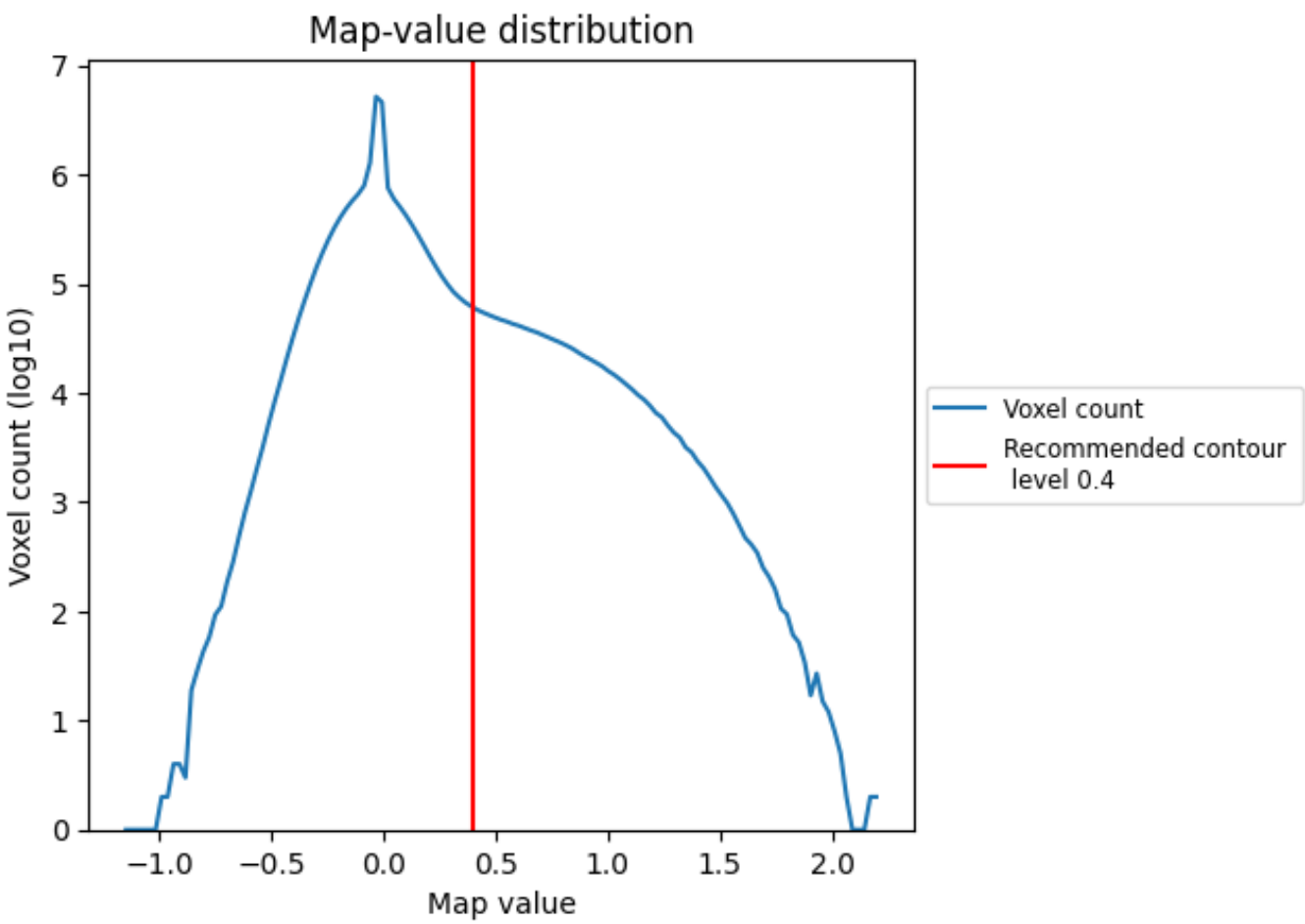
6.6 Mask visualisation (i)

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

7 Map analysis (i)

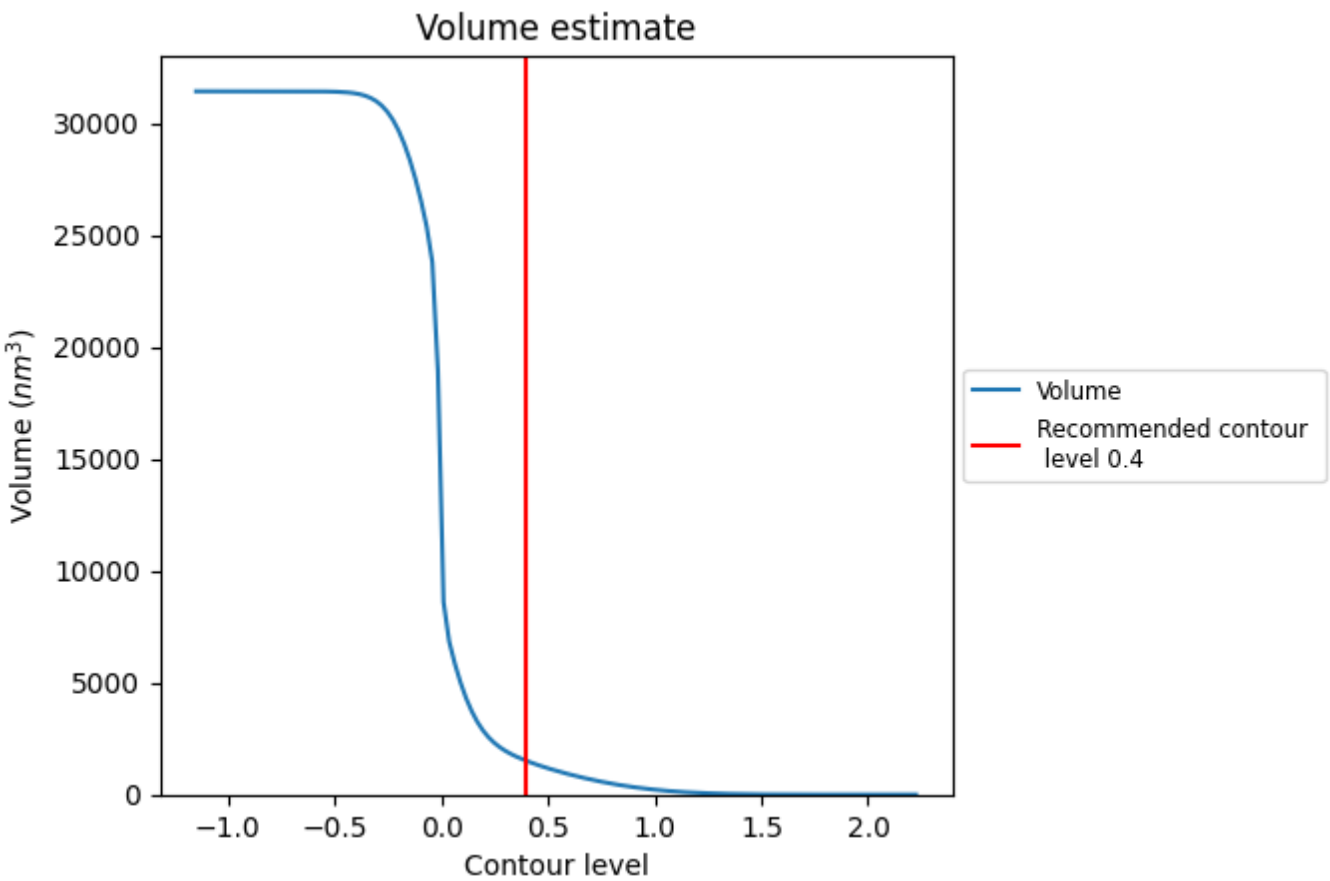
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

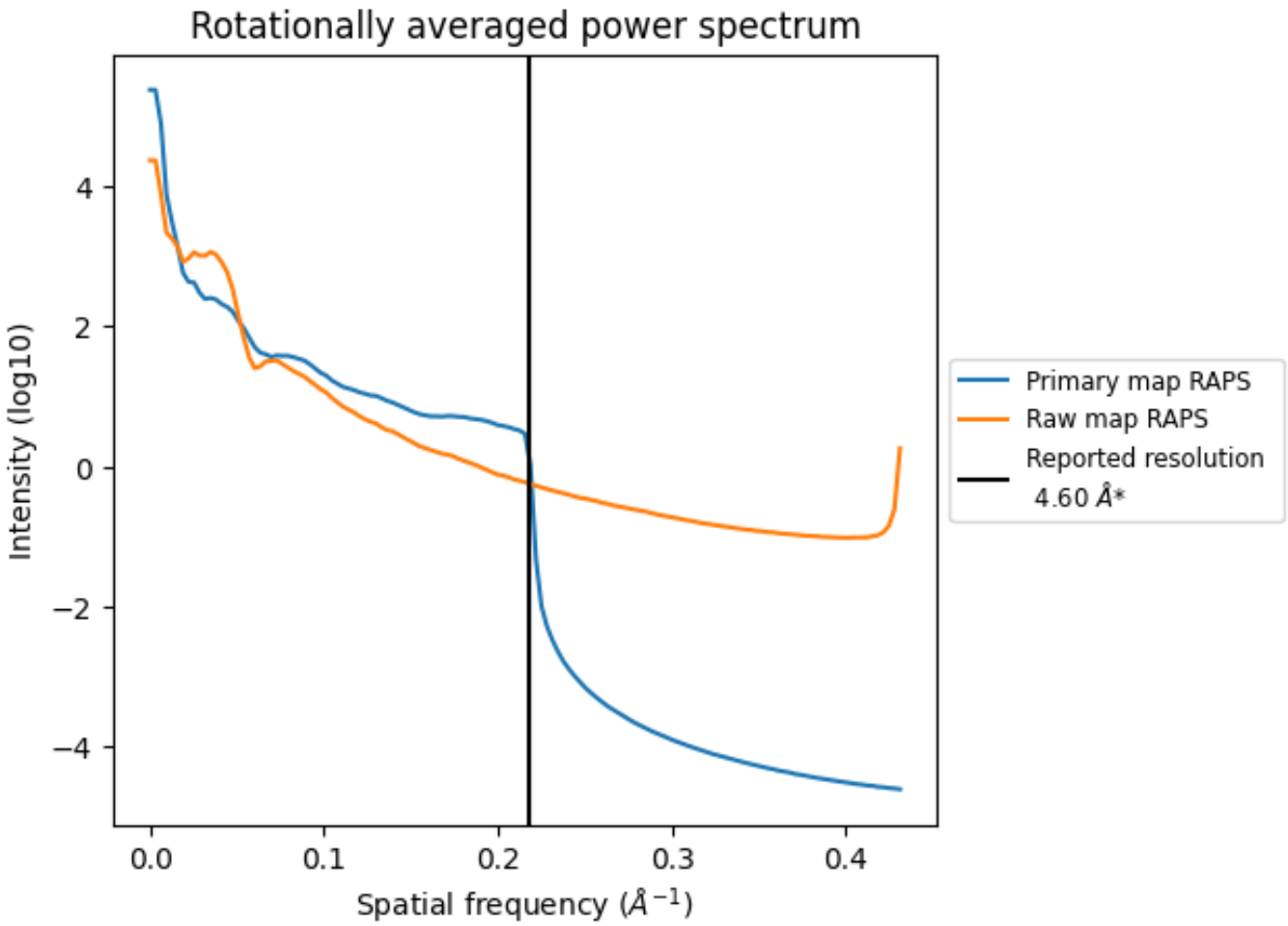
7.2 Volume estimate (i)



The volume at the recommended contour level is 1502 nm^3; this corresponds to an approximate mass of 1357 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)

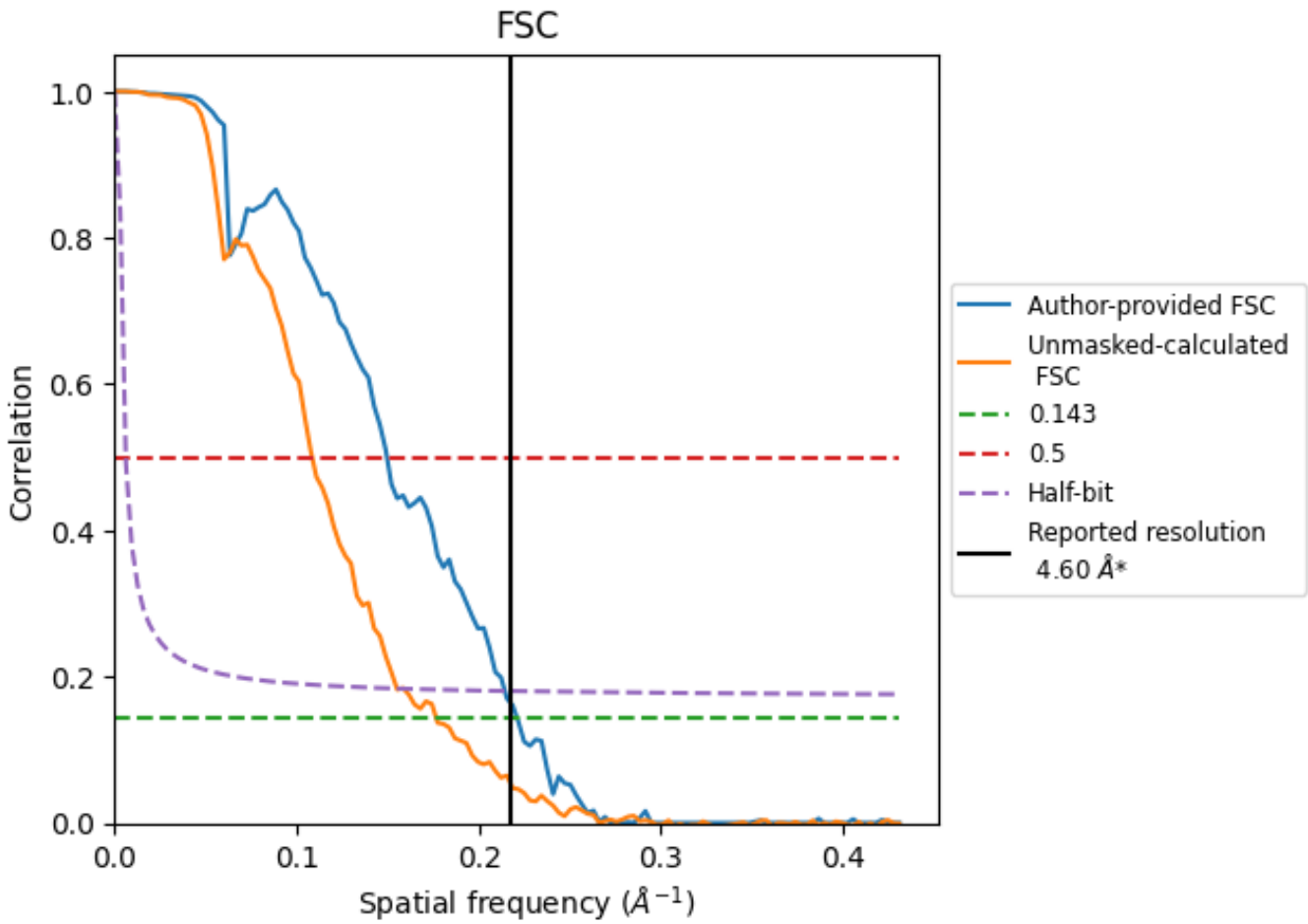


*Reported resolution corresponds to spatial frequency of 0.217 Å^{-1}

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 0.217 Å^{-1}

8.2 Resolution estimates (i)

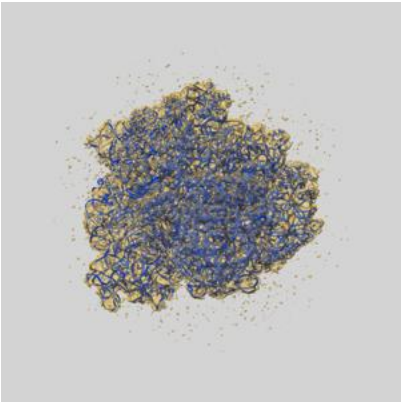
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.60	-	-
Author-provided FSC curve	4.52	6.68	4.66
Unmasked-calculated*	5.66	9.22	6.45

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 5.66 differs from the reported value 4.6 by more than 10 %

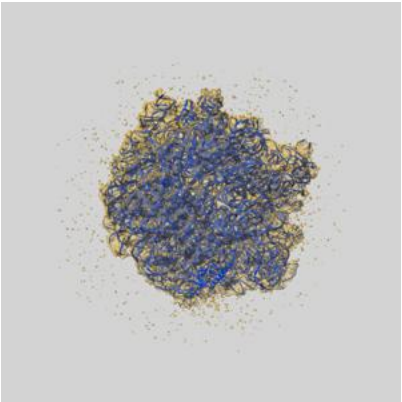
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-4126 and PDB model 5LZF. Per-residue inclusion information can be found in section 3 on page 15.

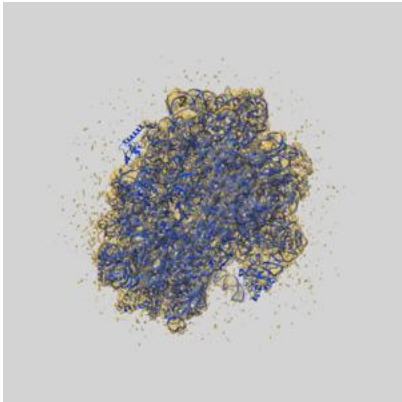
9.1 Map-model overlay (i)



X



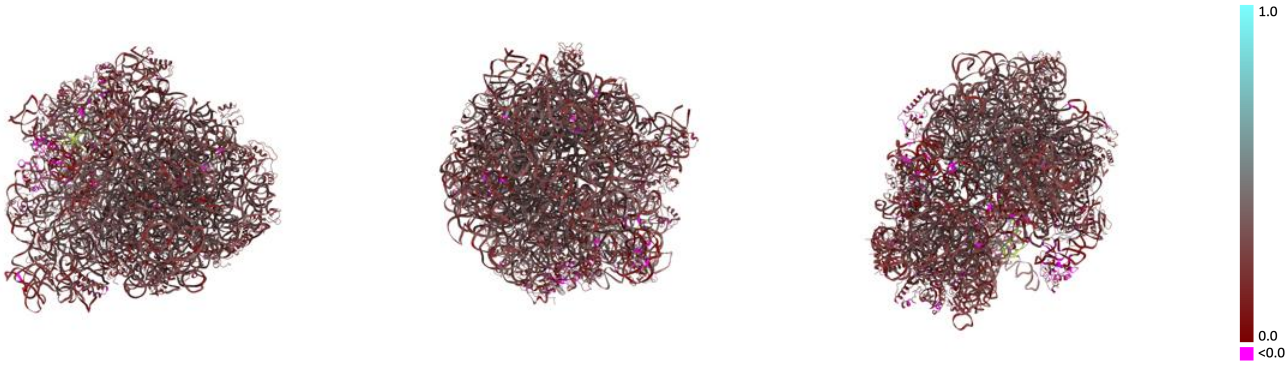
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.4 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

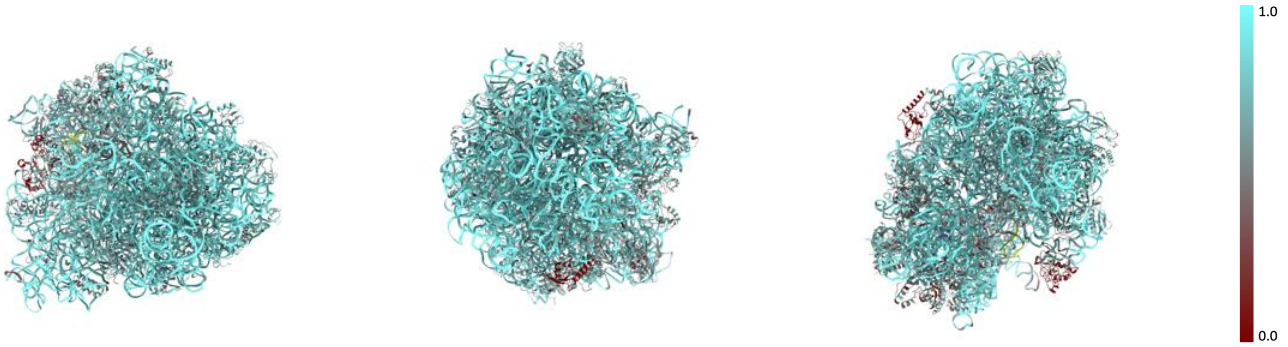
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

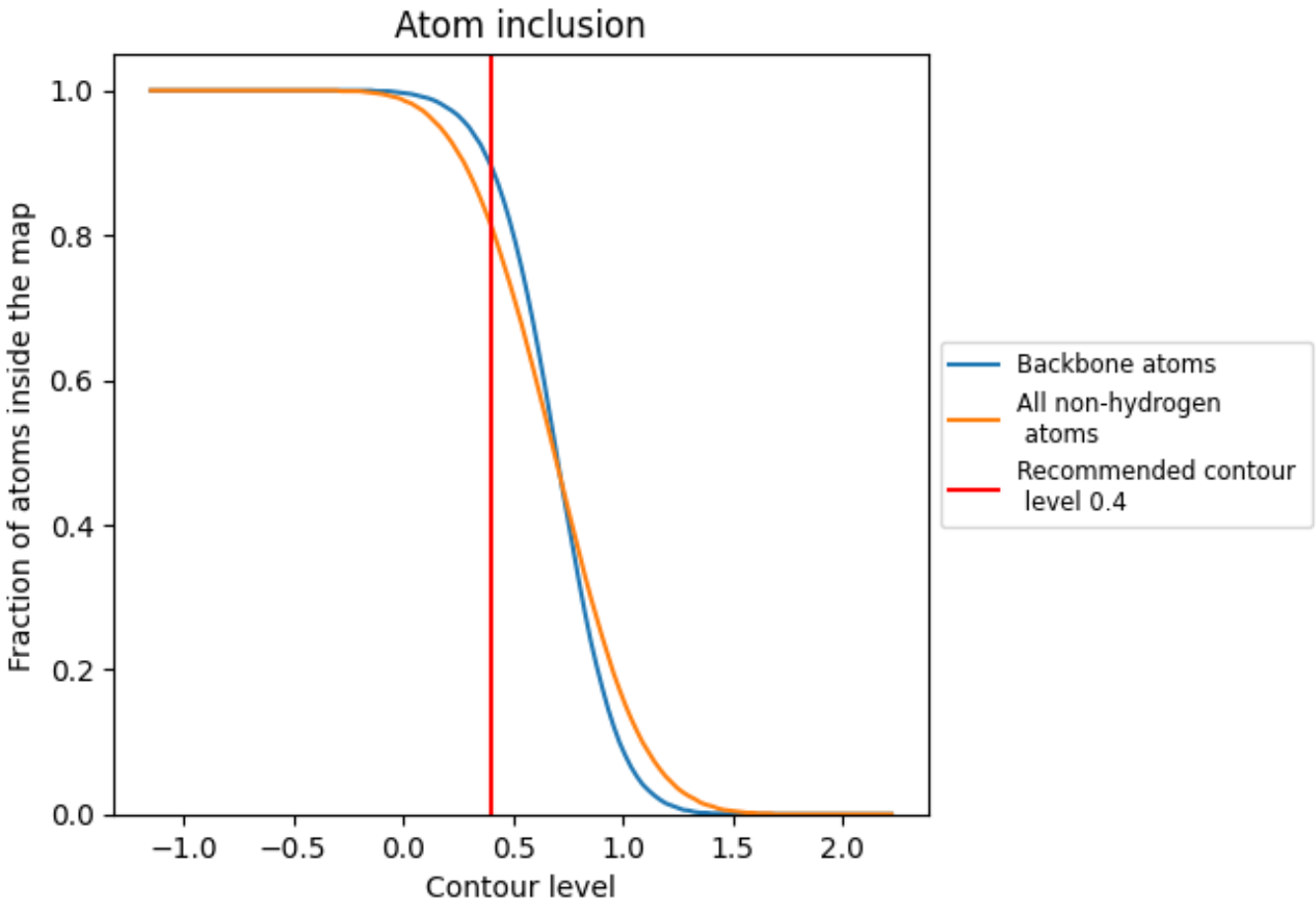
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.4).

9.4 Atom inclusion (i)



At the recommended contour level, 90% of all backbone atoms, 81% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8140	0.2790
0	0.6780	0.2920
1	0.5950	0.2450
2	0.7040	0.2960
3	0.6880	0.3060
4	0.6280	0.2790
6	0.5420	0.1820
A	0.9190	0.3090
B	0.9110	0.2760
C	0.6820	0.2990
D	0.6660	0.2750
E	0.6590	0.2700
F	0.5930	0.1870
G	0.6670	0.2310
H	0.1660	0.1300
I	0.1460	0.0750
J	0.7110	0.2780
K	0.6540	0.2850
L	0.6590	0.2850
M	0.6690	0.2790
N	0.6880	0.2700
O	0.6570	0.2200
P	0.6360	0.2530
Q	0.6980	0.2640
R	0.6930	0.2750
S	0.6720	0.2890
T	0.6470	0.2670
U	0.6680	0.2600
V	0.6540	0.2340
W	0.6400	0.2670
X	0.6870	0.2770
Y	0.6640	0.2000
Z	0.6640	0.2640
a	0.9060	0.2870
b	0.4750	0.2000

Continued on next page...

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Chain	Atom inclusion	Q-score
c	0.6190	0.2400
d	0.5550	0.2030
e	0.6440	0.2550
f	0.6560	0.2440
g	0.5300	0.2020
h	0.6610	0.2500
i	0.5680	0.2120
j	0.5290	0.2150
k	0.6860	0.2640
l	0.6540	0.2750
m	0.5740	0.1910
n	0.6040	0.2220
o	0.6770	0.2330
p	0.6090	0.2380
q	0.6540	0.2510
r	0.6440	0.2290
s	0.5190	0.1910
t	0.6120	0.1890
u	0.5770	0.1960
v	0.8130	0.2110
x	0.4830	0.1870
y	0.5790	0.1740