



## Full wwPDB EM Validation Report ⓘ

Mar 31, 2025 – 06:38 PM JST

PDB ID : 6LSS / pdb\_00006lss  
EMDB ID : EMD-0964  
Title : Cryo-EM structure of a pre-60S ribosomal subunit - state preA  
Authors : Liang, X.; Zuo, M.; Zhang, Y.; Li, N.; Ma, C.; Dong, M.; Gao, N.  
Deposited on : 2020-01-20  
Resolution : 3.23 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

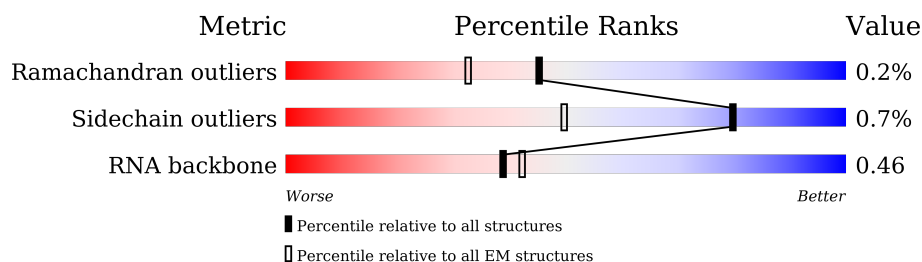
EMDB validation analysis : 0.0.1.dev117  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.42

# 1 Overall quality at a glance

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

The reported resolution of this entry is 3.23 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.



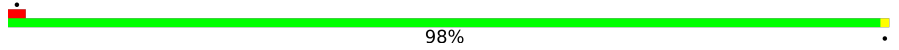



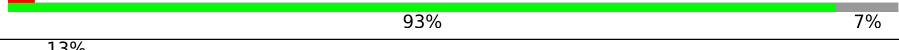
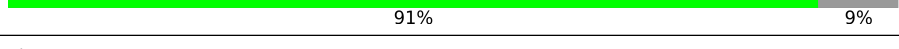
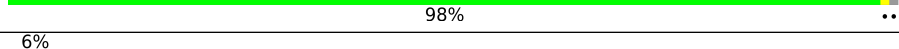
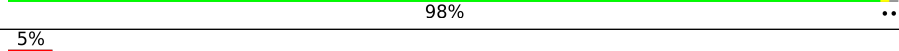
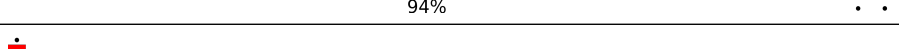
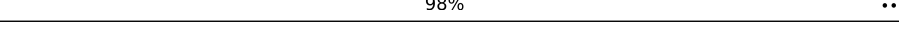
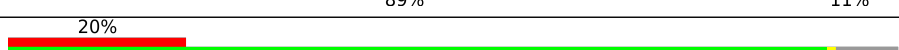
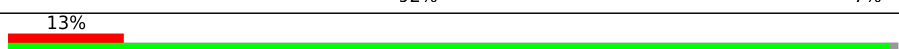
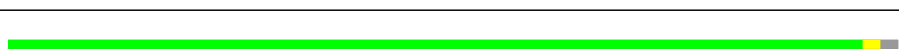
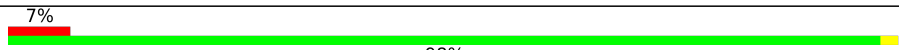
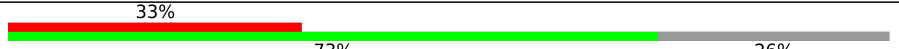

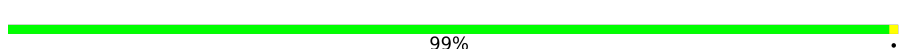
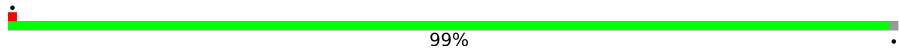
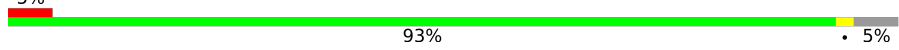
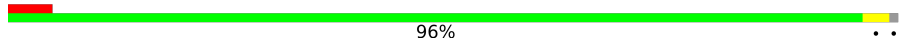
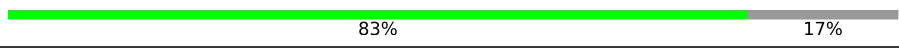
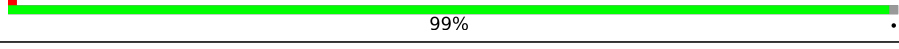

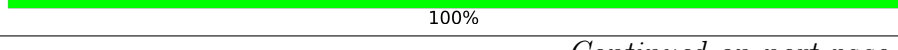

Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	1	731	
2	2	5070	
3	4	634	
4	5	120	
5	6	245	
6	7	163	
7	8	156	
8	9	134	

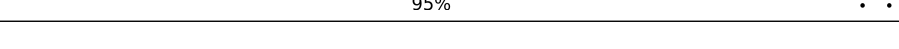

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Mol	Chain	Length	Quality of chain
9	B	403	
10	C	159	
11	D	427	
12	E	115	
13	F	117	
14	G	266	
15	H	123	
16	I	192	
17	K	105	
18	L	148	
19	M	97	
20	N	178	
21	O	70	
22	P	51	
23	Q	211	
24	R	203	
25	S	215	
26	U	204	
27	V	203	
28	W	106	
29	X	92	
30	Y	184	
31	Z	188	
32	a	196	
33	b	176	

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Mol	Chain	Length	Quality of chain
34	c	160	
35	d	128	
36	e	140	
37	g	156	
38	h	145	
39	i	136	
40	j	125	
41	k	135	
42	l	137	
43	m	257	
44	n	110	
45	o	288	
46	p	248	
47	r	297	
48	z	129	

## 2 Entry composition

There are 50 unique types of molecules in this entry. The entry contains 140545 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Nucleolar GTP-binding protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	19	Total	C	N	O	S	0	0
			148	88	23	35	2		

- Molecule 2 is a RNA chain called 28S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	3474	Total	C	N	O	P	0	0
			74611	33280	13653	24205	3473		

- Molecule 3 is a protein called Nucleolar GTP-binding protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	4	620	Total	C	N	O	S	0	0
			5093	3198	935	933	27		

- Molecule 4 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	5	120	Total	C	N	O	P	0	0
			2558	1141	456	842	119		

- Molecule 5 is a protein called Eukaryotic translation initiation factor 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	6	244	Total	C	N	O	S	0	0
			1852	1149	318	372	13		

- Molecule 6 is a protein called Probable ribosome biogenesis protein RLP24.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	7	135	Total	C	N	O	S	0	0
			1159	737	225	187	10		

- Molecule 7 is a RNA chain called 28S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	8	156	Total	C	N	O	P	0	0
			3315	1481	585	1094	155		

- Molecule 8 is a protein called Zinc finger protein 593.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	9	86	Total	C	N	O	S	0	0
			711	433	154	121	3		

- Molecule 9 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	B	402	Total	C	N	O	S	1	0
			3244	2065	609	556	14		

- Molecule 10 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	C	93	Total	C	N	O	S	0	0
			764	476	167	117	4		

- Molecule 11 is a protein called 60S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	D	358	Total	C	N	O	S	0	0
			2853	1797	570	473	13		

- Molecule 12 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	E	98	Total	C	N	O	S	0	0
			764	485	135	138	6		

- Molecule 13 is a protein called 60S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	F	109	Total	C	N	O	S	0	0
			868	544	179	139	6		

- Molecule 14 is a protein called 60S ribosomal protein L7a.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	G	241	Total	C	N	O	S	1	0
			1935	1233	374	324	4		

- Molecule 15 is a protein called 60S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	H	122	Total	C	N	O	S	0	0
			1015	641	205	168	1		

- Molecule 16 is a protein called 60S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	I	190	Total	C	N	O	S	0	0
			1518	956	284	272	6		

- Molecule 17 is a protein called 60S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	K	102	Total	C	N	O	S	0	0
			832	521	177	129	5		

- Molecule 18 is a protein called 60S ribosomal protein L27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	L	147	Total	C	N	O	S	0	0
			1162	736	237	186	3		

- Molecule 19 is a protein called 60S ribosomal protein L37.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	M	86	Total	C	N	O	S	0	0
			705	434	155	111	5		

- Molecule 20 is a protein called 60S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	N	165	Total	C	N	O	S	0	0
			1319	836	245	233	5		

- Molecule 21 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	O	69	Total	C	N	O	S	0	0
			569	366	103	99	1		

- Molecule 22 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	P	50	Total	C	N	O	S	0	0
			444	281	98	64	1		

- Molecule 23 is a protein called 60S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Q	210	Total	C	N	O	S	0	0
			1701	1064	352	281	4		

- Molecule 24 is a protein called Translation machinery-associated protein 16.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	R	150	Total	C	N	O	S	0	0
			1272	793	244	230	5		

- Molecule 25 is a protein called 60S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	S	135	Total	C	N	O	S	0	0
			1111	713	213	178	7		

- Molecule 26 is a protein called 60S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	U	203	Total	C	N	O	S	0	0
			1701	1072	359	266	4		

- Molecule 27 is a protein called 60S ribosomal protein L13a.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	V	201	Total	C	N	O	S	0	0
			1650	1063	321	261	5		

- Molecule 28 is a protein called 60S ribosomal protein L36a.



Mol	Chain	Residues	Atoms					AltConf	Trace
28	W	101	Total	C	N	O	S	0	0
			827	517	170	134	6		

- Molecule 29 is a protein called 60S ribosomal protein L37a.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	X	91	Total	C	N	O	S	0	0
			708	445	136	120	7		

- Molecule 30 is a protein called 60S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Y	153	Total	C	N	O	S	0	0
			1242	776	241	216	9		

- Molecule 31 is a protein called 60S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	Z	187	Total	C	N	O	S	0	0
			1513	944	314	250	5		

- Molecule 32 is a protein called 60S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	a	148	Total	C	N	O	S	0	0
			1239	772	266	192	9		

- Molecule 33 is a protein called 60S ribosomal protein L18a.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	b	176	Total	C	N	O	S	0	0
			1461	930	284	236	11		

- Molecule 34 is a protein called 60S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	c	155	Total	C	N	O	S	0	0
			1264	801	248	210	5		

- Molecule 35 is a protein called 60S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	d	101	Total	C	N	O	S	0	0
			825	529	144	150	2		

- Molecule 36 is a protein called 60S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	e	131	Total	C	N	O	S	0	0
			979	618	184	172	5		

- Molecule 37 is a protein called 60S ribosomal protein L23a.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	g	118	Total	C	N	O	S	0	0
			967	618	181	167	1		

- Molecule 38 is a protein called 60S ribosomal protein L26.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	h	134	Total	C	N	O	S	0	0
			1115	700	226	186	3		

- Molecule 39 is a protein called 60S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	i	135	Total	C	N	O	S	0	0
			1107	714	208	182	3		

- Molecule 40 is a protein called 60S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	j	107	Total	C	N	O	S	0	0
			888	560	171	155	2		

- Molecule 41 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	k	128	Total	C	N	O	S	0	0
			1053	667	216	165	5		

- Molecule 42 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	l	125	Total	C	N	O	S	0	0
			1002	622	207	168	5		

- Molecule 43 is a protein called 60S ribosomal protein L8.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	m	248	Total	C	N	O	S	0	0
			1898	1189	389	314	6		

- Molecule 44 is a protein called 60S ribosomal protein L35a.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	n	109	Total	C	N	O	S	0	0
			876	555	174	144	3		

- Molecule 45 is a protein called 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	o	235	Total	C	N	O	S	0	0
			1897	1217	360	316	4		

- Molecule 46 is a protein called 60S ribosomal protein L7.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	p	225	Total	C	N	O	S	1	0
			1878	1207	361	301	9		

- Molecule 47 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	r	293	Total	C	N	O	S	0	0
			2382	1507	434	427	14		

- Molecule 48 is a protein called Protein LLP homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	z	34	Total	C	N	O	S	0	0
			284	179	61	43	1		

- Molecule 49 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
49	2	229	Total 229	Mg 229	0
49	4	1	Total 1	Mg 1	0
49	5	3	Total 3	Mg 3	0
49	8	5	Total 5	Mg 5	0
49	9	1	Total 1	Mg 1	0
49	B	2	Total 2	Mg 2	0
49	D	1	Total 1	Mg 1	0
49	F	1	Total 1	Mg 1	0
49	L	1	Total 1	Mg 1	0
49	M	1	Total 1	Mg 1	0
49	R	1	Total 1	Mg 1	0
49	k	1	Total 1	Mg 1	0
49	m	1	Total 1	Mg 1	0
49	n	1	Total 1	Mg 1	0
49	p	1	Total 1	Mg 1	0

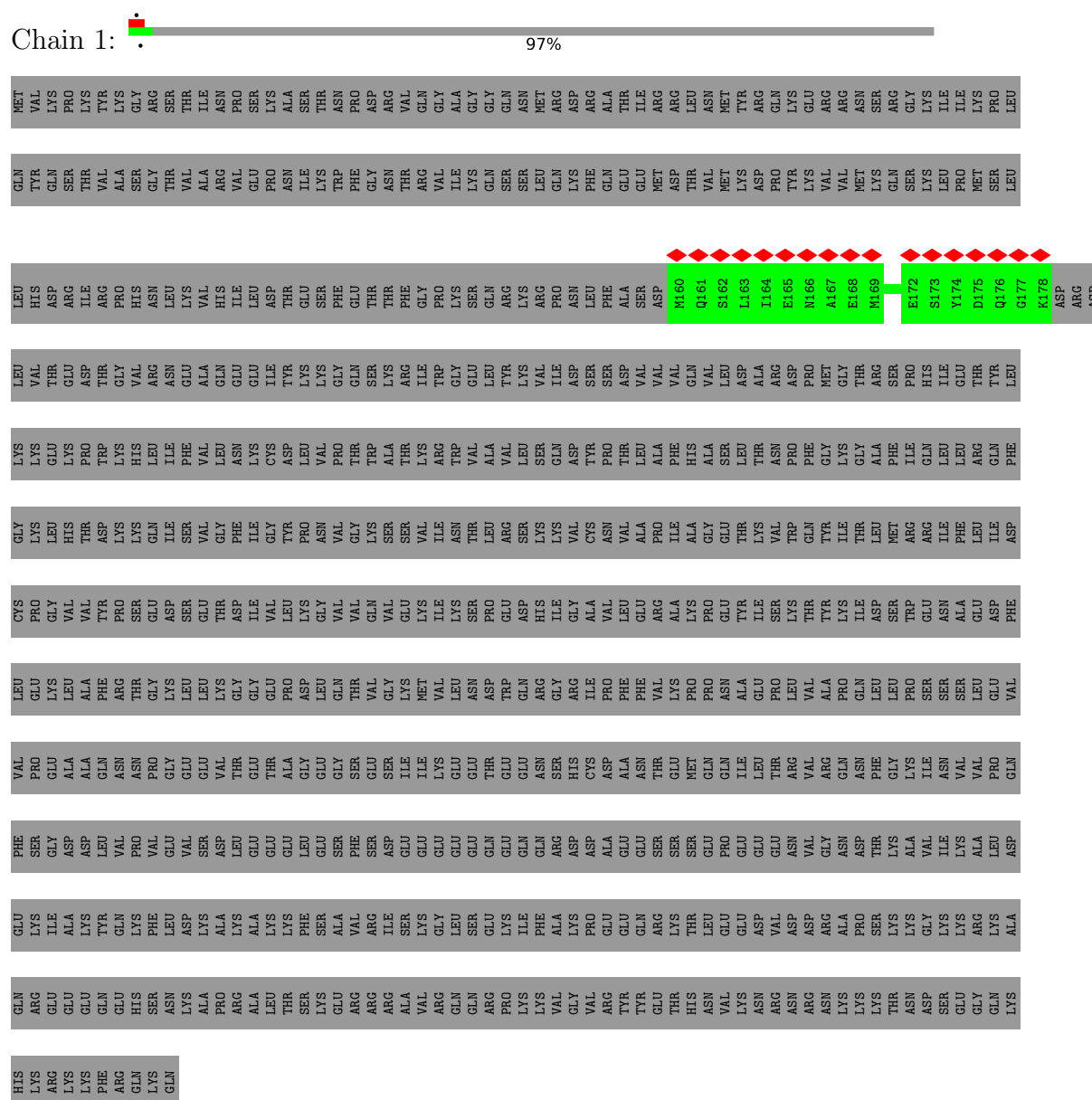
- Molecule 50 is water.

Mol	Chain	Residues	Atoms		AltConf
50	2	13	Total 13	O 13	0
50	k	1	Total 1	O 1	0
50	o	1	Total 1	O 1	0
50	p	1	Total 1	O 1	0

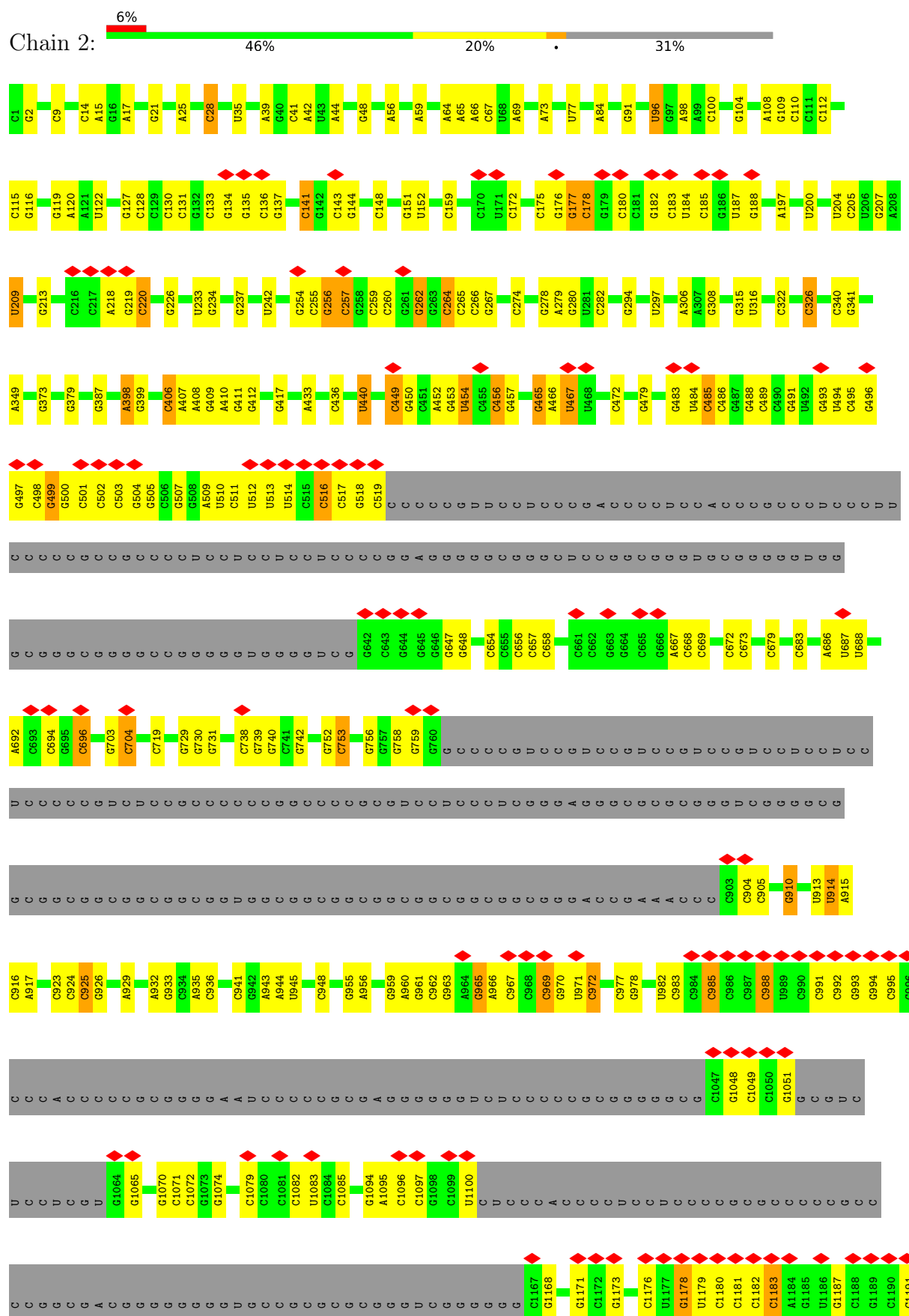
### 3 Residue-property plots

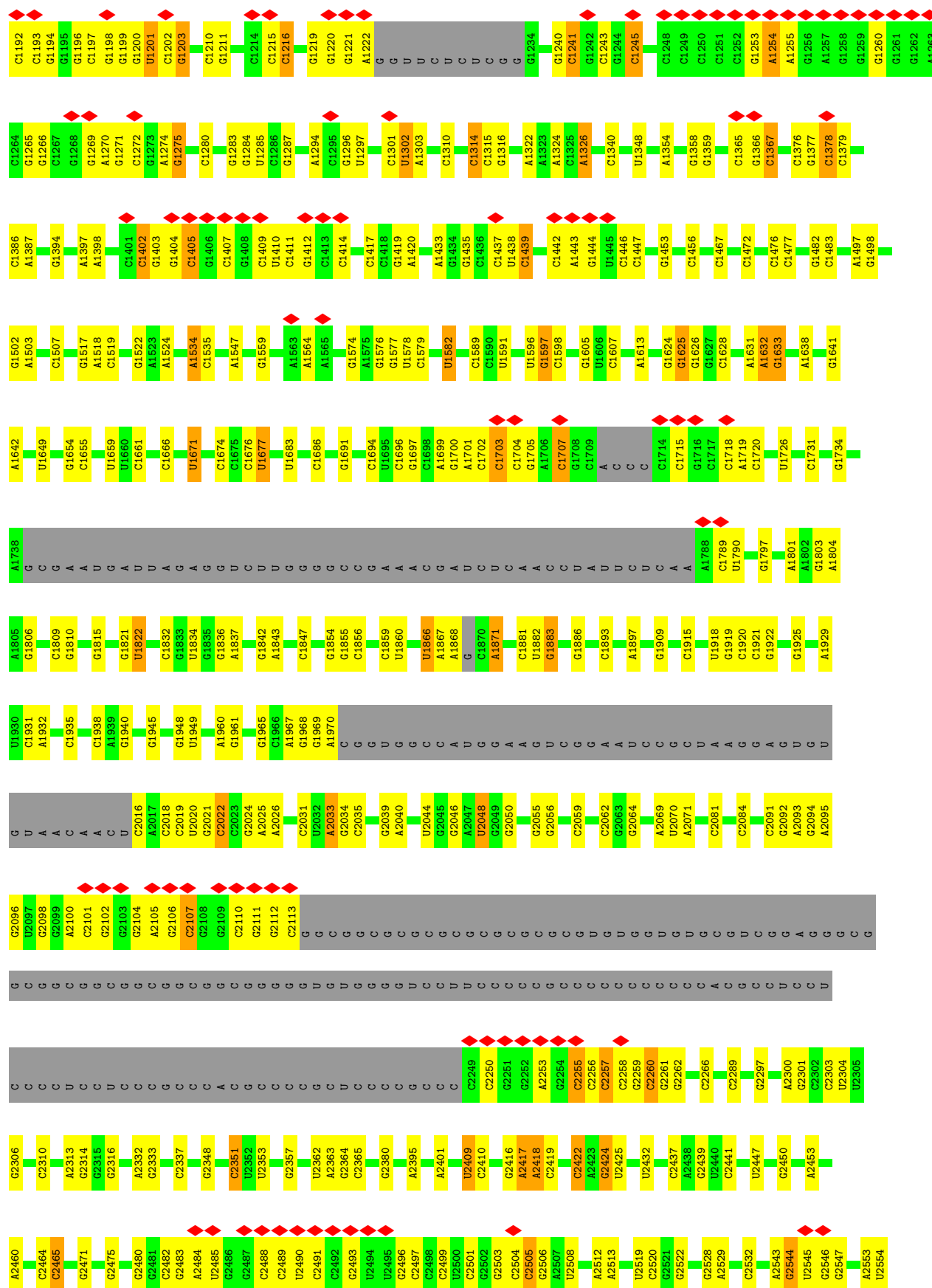
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Nucleolar GTP-binding protein 2



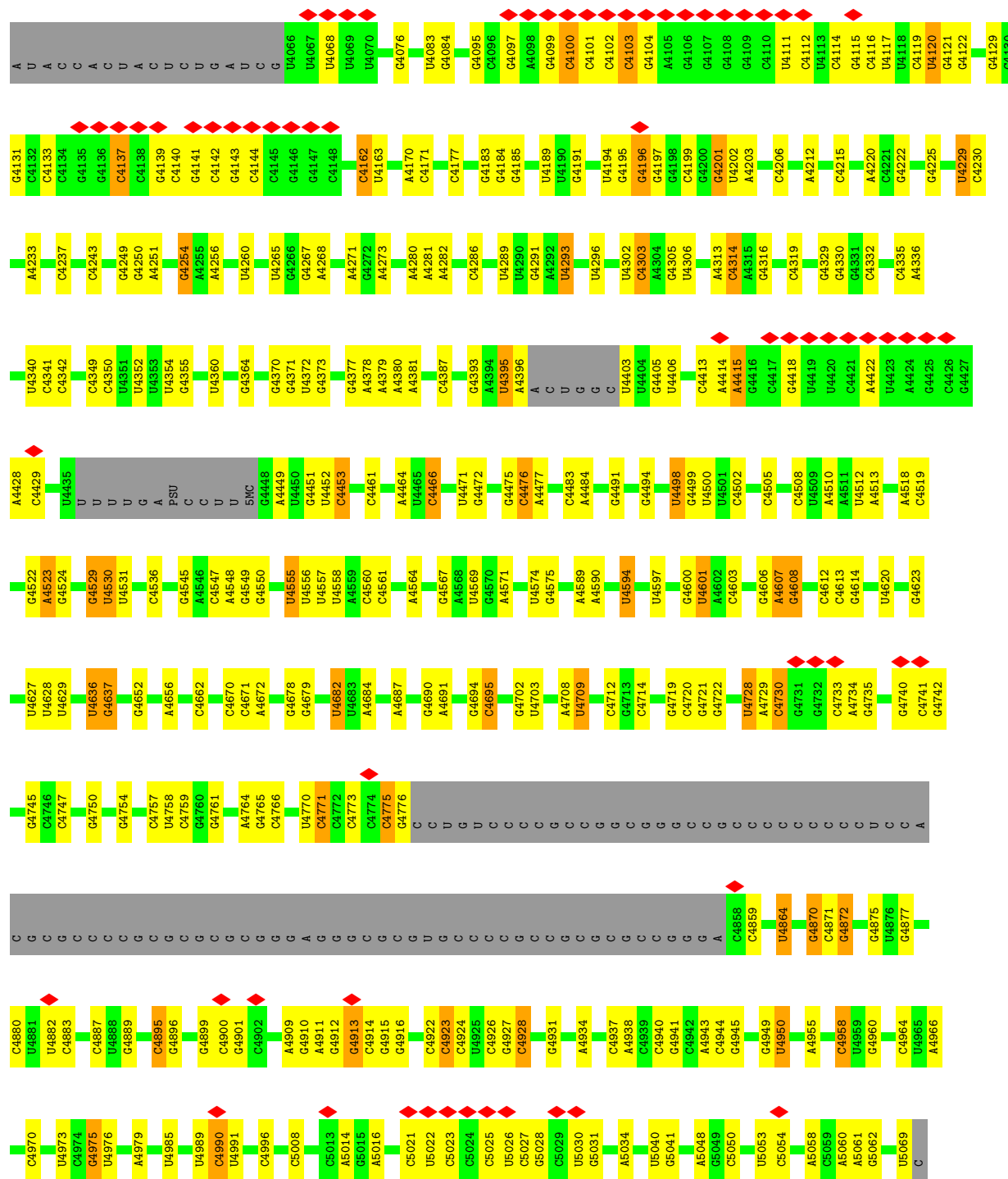
#### • Molecule 2: 28S rRNA

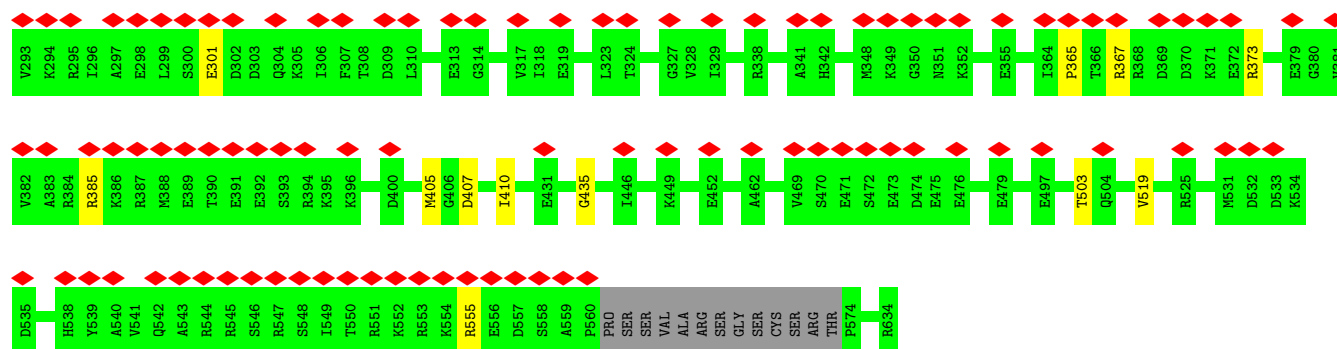




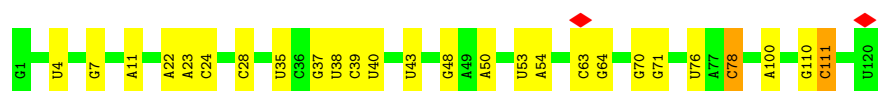
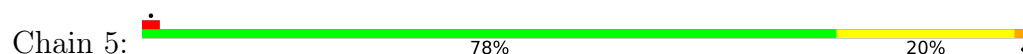




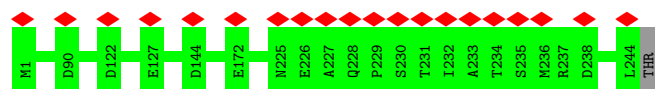




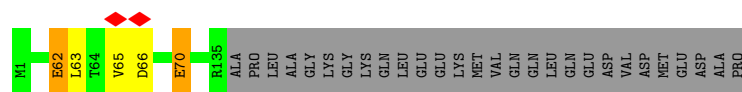
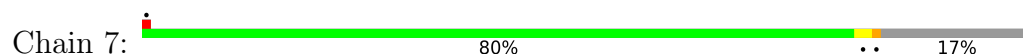
• Molecule 4: 5S rRNA



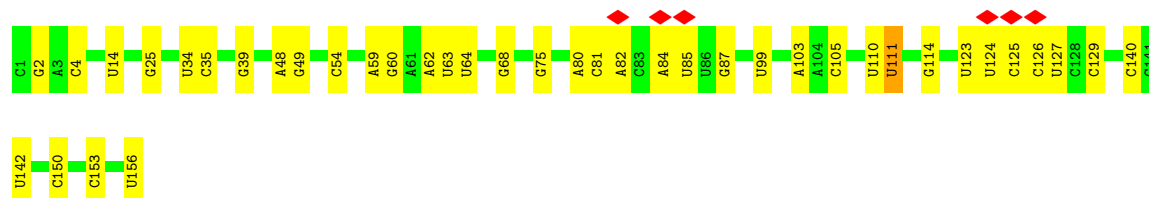
• Molecule 5: Eukaryotic translation initiation factor 6



• Molecule 6: Probable ribosome biogenesis protein RLP24



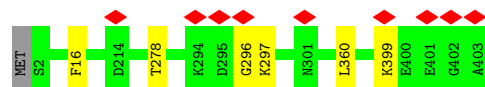
• Molecule 7: 28S rRNA



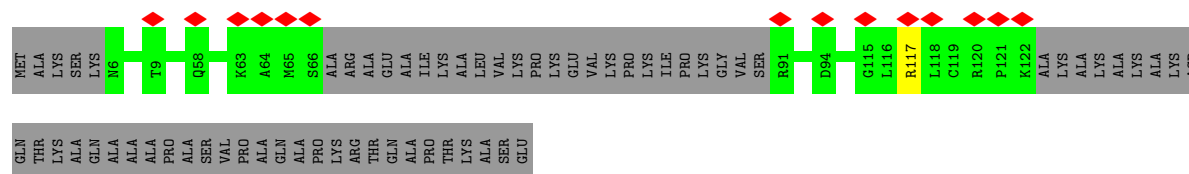
• Molecule 8: Zinc finger protein 593



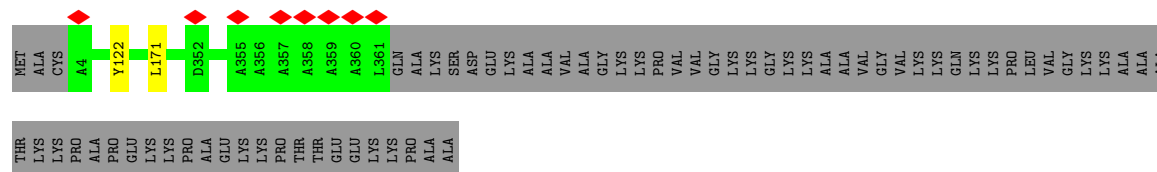
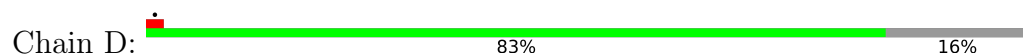
- Molecule 9: 60S ribosomal protein L3



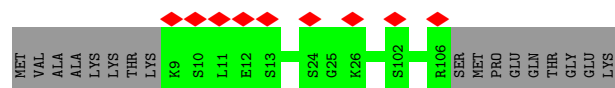
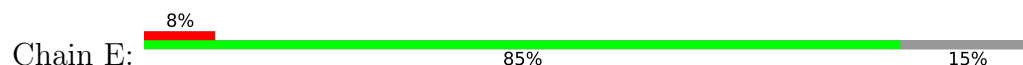
- Molecule 10: 60S ribosomal protein L29



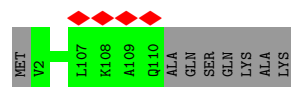
- Molecule 11: 60S ribosomal protein L4



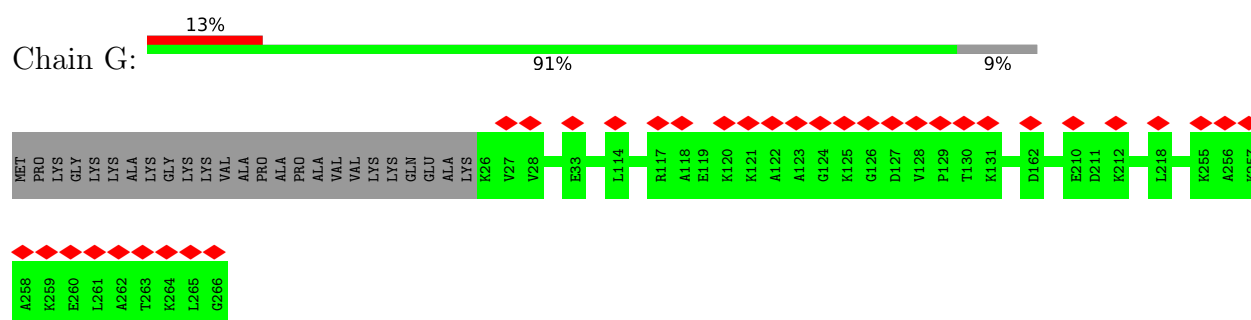
- Molecule 12: 60S ribosomal protein L30



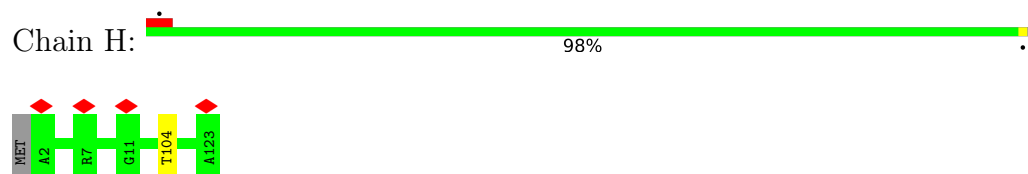
- Molecule 13: 60S ribosomal protein L34



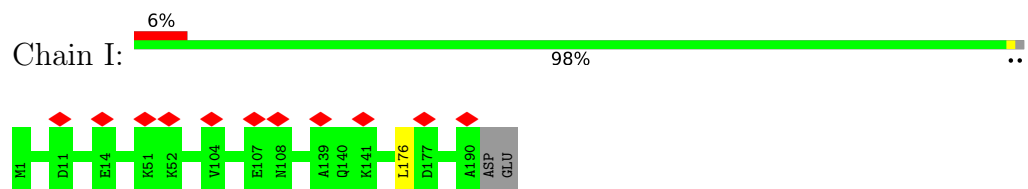
- Molecule 14: 60S ribosomal protein L7a



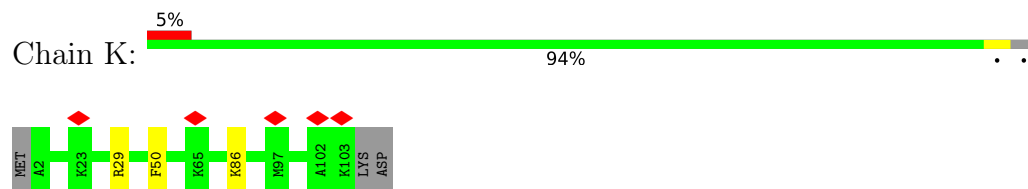
- Molecule 15: 60S ribosomal protein L35



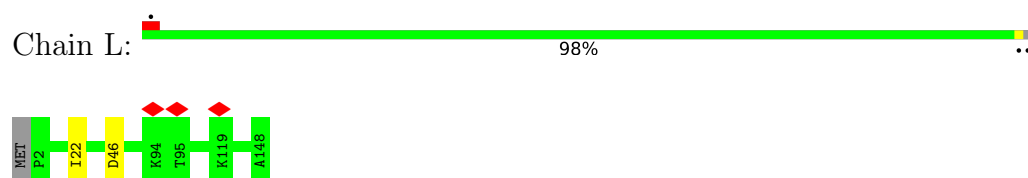
- Molecule 16: 60S ribosomal protein L9



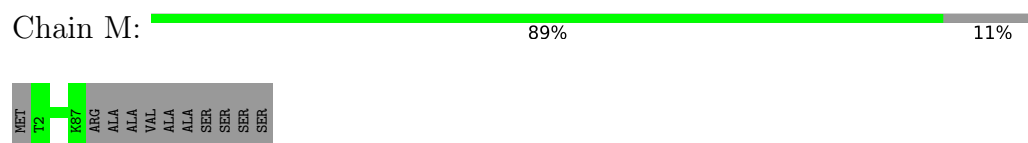
- Molecule 17: 60S ribosomal protein L36



- Molecule 18: 60S ribosomal protein L27a

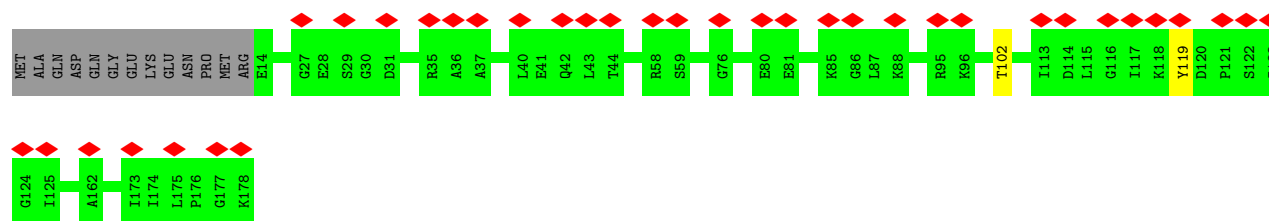


- Molecule 19: 60S ribosomal protein L37

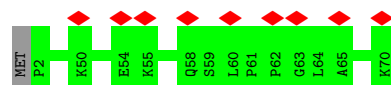


- Molecule 20: 60S ribosomal protein L11





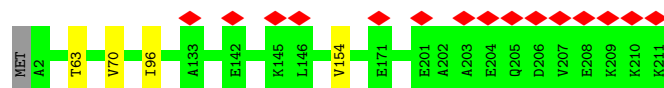
- Molecule 21: 60S ribosomal protein L38



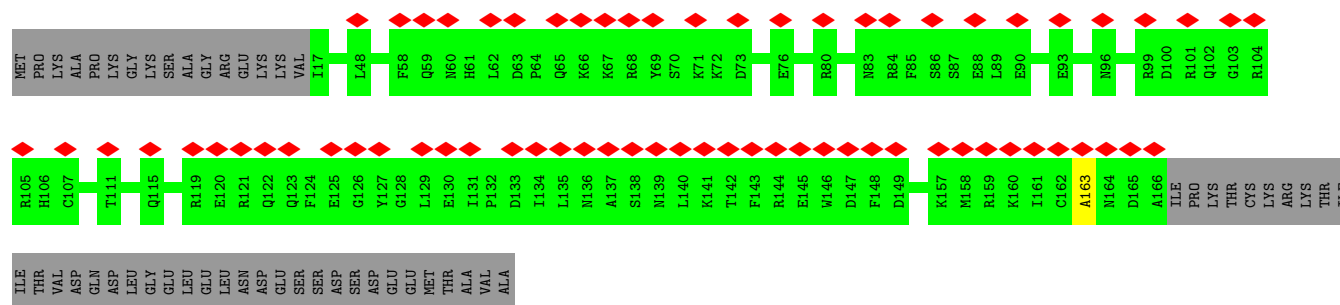
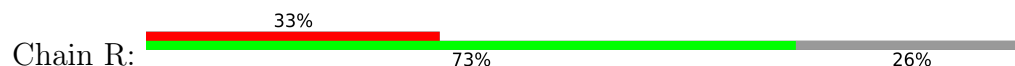
- Molecule 22: 60S ribosomal protein L39



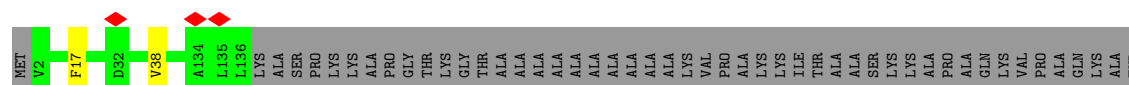
- Molecule 23: 60S ribosomal protein L13



- Molecule 24: Translation machinery-associated protein 16



- Molecule 25: 60S ribosomal protein L14



GLY  
GLN  
LYS  
ALA  
ALA  
PRO  
PRO  
ALA  
PRO  
LYS  
ALA  
GLN  
LYS  
GLY  
GLN  
LYS  
ALA  
ALA  
PRO  
PRO  
GLN  
LYS  
ALA  
ALA  
PRO  
PRO  
LYS  
LYS  
ALA  
SER  
GLY  
LYS  
LYS  
ALA

- Molecule 26: 60S ribosomal protein L15

Chain U:  99%

MET  
G2  
K83  
L134  
R204

- Molecule 27: 60S ribosomal protein L13a

Chain V:  99%

MET  
ALA  
E3  
V4  
K187  
V203

- Molecule 28: 60S ribosomal protein L36a

Chain W:  93% 5% 5%


MET  
V2  
L33  
R81  
D96  
R99  
K100  
G101  
Q102  
VAL  
ILE  
GLN  
PHE

- Molecule 29: 60S ribosomal protein L37a

Chain X:  96% 5% 5%

MET  
A2  
S59  
T63  
R84  
R85  
K90  
D91  
Q92

- Molecule 30: 60S ribosomal protein L17

Chain Y:  83% 17%


MET  
V2  
E154  
GLN  
ILE  
VAL  
PRO  
LYS  
PRO  
GLU  
GLU  
GLU  
VAL  
ALA  
GLN  
LYS  
LYS  
LYS  
ILE  
SER  
GLN  
LYS  
LYS  
LEU  
LYS  
LYS  
GLN  
LYS  
LEU  
MET  
ALA  
ARG  
GLU

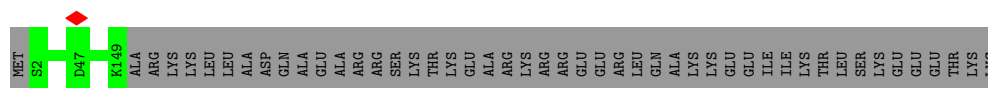
- Molecule 31: 60S ribosomal protein L18

Chain Z:  99%

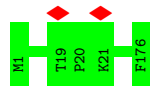
MET  
G2  
V3  
D4  
N188

- Molecule 32: 60S ribosomal protein L19

Chain a:  76% 24%



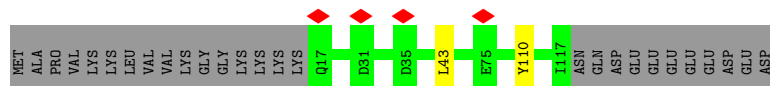
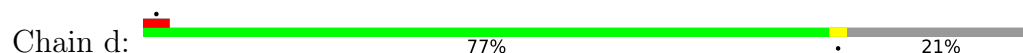
- Molecule 33: 60S ribosomal protein L18a



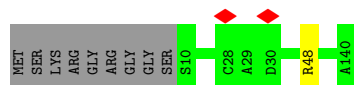
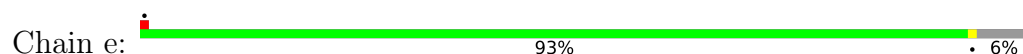
- Molecule 34: 60S ribosomal protein L21



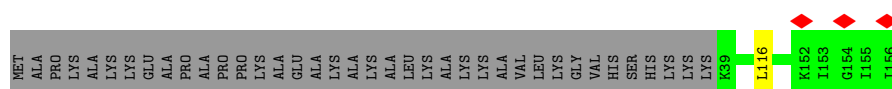
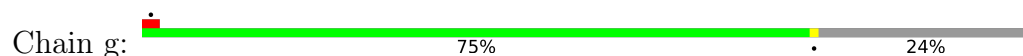
- Molecule 35: 60S ribosomal protein L22



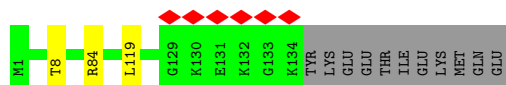
- Molecule 36: 60S ribosomal protein L23



- Molecule 37: 60S ribosomal protein L23a



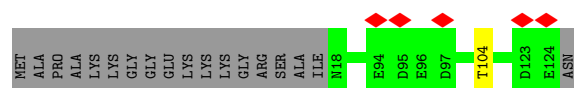
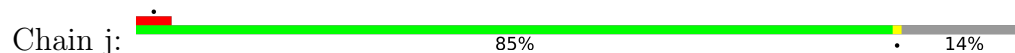
- Molecule 38: 60S ribosomal protein L26



- Molecule 39: 60S ribosomal protein L27



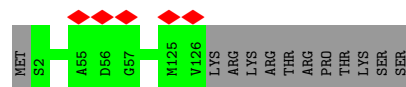
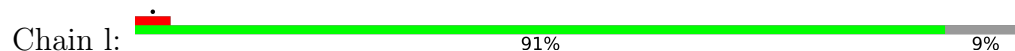
- Molecule 40: 60S ribosomal protein L31



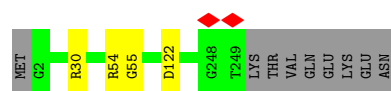
- Molecule 41: 60S ribosomal protein L32



- Molecule 42: 60S ribosomal protein L28



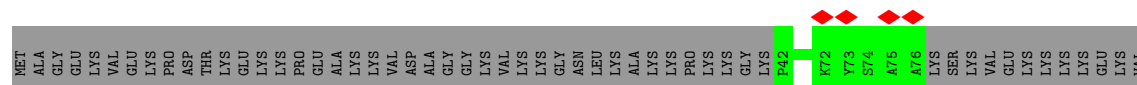
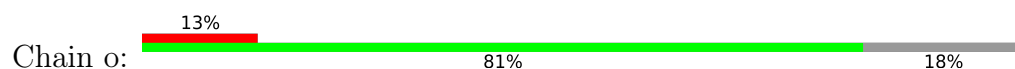
- Molecule 43: 60S ribosomal protein L8



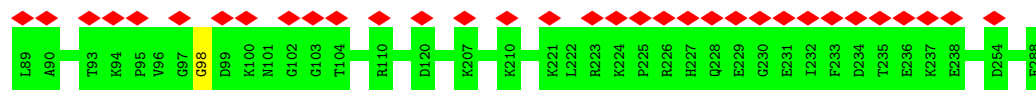
- Molecule 44: 60S ribosomal protein L35a



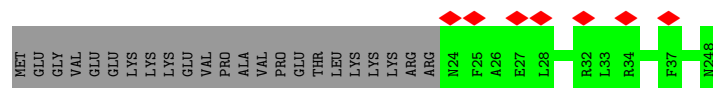
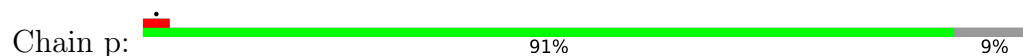
- Molecule 45: 60S ribosomal protein L6



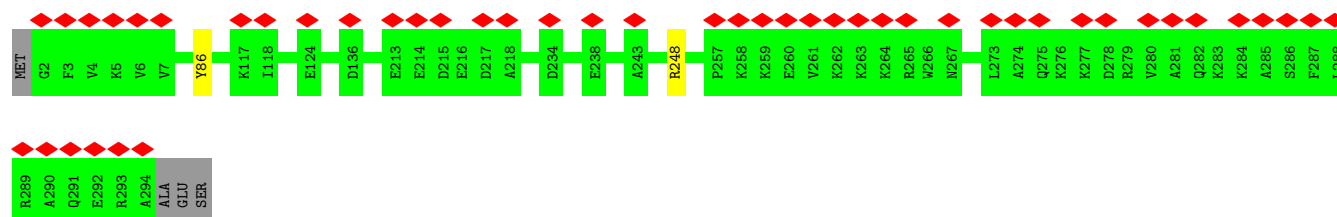




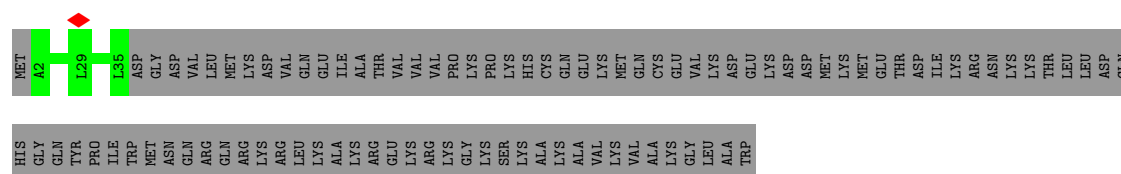
- Molecule 46: 60S ribosomal protein L7



- Molecule 47: 60S ribosomal protein L5



- Molecule 48: Protein LLP homolog



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	10277	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	64	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.377	Depositor
Minimum map value	-0.158	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.012	Depositor
Recommended contour level	0.065	Depositor
Map size ( $\text{\AA}$ )	507.84, 507.84, 507.84	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.058, 1.058, 1.058	Depositor

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, P7G, OMC, 5MU, B9H, E7G, I4U, B8K, UR3, 5MC, 7MG, 2MG, BGH, E6G, MHG, B8T, 1MA, M7A, B8Q, B8H, 6MZ, OMG, P4U, OMU, A2M, B8W, B9B, PSU

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	1	0.28	0/148	0.41	0/196
2	2	0.80	1/81090 (0.0%)	1.19	675/126417 (0.5%)
3	4	0.36	0/5177	0.66	3/6942 (0.0%)
4	5	0.73	0/2858	1.16	16/4455 (0.4%)
5	6	0.40	0/1877	0.62	0/2554
6	7	0.48	0/1181	0.65	1/1563 (0.1%)
7	8	0.85	0/3679	1.08	10/5732 (0.2%)
8	9	0.37	0/723	0.66	0/961
9	B	0.47	0/3315	0.61	1/4435 (0.0%)
10	C	0.33	0/777	0.55	0/1026
11	D	0.45	0/2907	0.61	1/3905 (0.0%)
12	E	0.37	0/774	0.56	0/1038
13	F	0.45	0/878	0.61	0/1170
14	G	0.43	0/1971	0.61	0/2651
15	H	0.39	0/1023	0.53	0/1351
16	I	0.41	0/1537	0.61	0/2066
17	K	0.40	1/843 (0.1%)	0.52	0/1115
18	L	0.47	0/1191	0.55	1/1591 (0.1%)
19	M	0.49	0/720	0.60	0/952
20	N	0.36	0/1341	0.62	1/1793 (0.1%)
21	O	0.39	0/575	0.59	0/761
22	P	0.44	0/454	0.57	0/599
23	Q	0.43	0/1732	0.59	1/2315 (0.0%)
24	R	0.32	0/1293	0.60	0/1725
25	S	0.43	0/1133	0.56	0/1516
26	U	0.48	0/1746	0.55	1/2338 (0.0%)
27	V	0.46	0/1682	0.57	0/2250
28	W	0.41	0/840	0.62	2/1107 (0.2%)
29	X	0.47	0/718	0.55	0/953
30	Y	0.46	0/1268	0.57	0/1701
31	Z	0.43	0/1537	0.59	0/2052

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
32	a	0.43	0/1255	0.54	0/1662
33	b	0.45	0/1501	0.53	0/2013
34	c	0.45	0/1291	0.55	0/1725
35	d	0.41	0/839	0.68	1/1126 (0.1%)
36	e	0.47	0/993	0.60	0/1332
37	g	0.41	0/984	0.56	1/1323 (0.1%)
38	h	0.47	0/1132	0.61	1/1504 (0.1%)
39	i	0.41	0/1130	0.57	1/1507 (0.1%)
40	j	0.46	0/903	0.62	0/1216
41	k	0.49	1/1071 (0.1%)	0.58	0/1429
42	l	0.45	0/1017	0.58	0/1364
43	m	0.47	0/1936	0.65	1/2596 (0.0%)
44	n	0.52	0/895	0.66	2/1198 (0.2%)
45	o	0.38	0/1935	0.61	0/2596
46	p	0.46	0/1916	0.57	0/2553
47	r	0.39	0/2428	0.58	0/3252
48	z	0.39	0/286	0.48	0/372
All	All	0.67	3/148500 (0.0%)	1.01	720/217998 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	4	0	4
9	B	0	2
23	Q	0	1
24	R	0	1
43	m	0	1
44	n	0	1
45	o	0	1
All	All	0	11

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	k	72	SER	CA-CB	-5.74	1.44	1.52
2	2	1577	G	C2-N3	-5.71	1.28	1.32
17	K	50	PHE	C-N	-5.21	1.22	1.34

All (720) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	485	C	C2-N1-C1'	13.46	133.60	118.80
2	2	2257	C	N1-C2-O2	13.20	126.82	118.90
2	2	2255	C	N1-C2-O2	12.76	126.56	118.90
2	2	516	C	N1-C2-O2	12.70	126.52	118.90
2	2	2257	C	C2-N1-C1'	12.40	132.44	118.80
2	2	209	U	C2-N1-C1'	12.24	132.39	117.70
2	2	209	U	N1-C2-O2	12.01	131.21	122.80
2	2	209	U	N3-C2-O2	-11.32	114.28	122.20
2	2	467	U	C2-N1-C1'	11.21	131.16	117.70
2	2	180	C	C5-C6-N1	10.72	126.36	121.00
2	2	3709	U	N3-C2-O2	-10.61	114.77	122.20
2	2	485	C	N1-C2-O2	10.59	125.25	118.90
2	2	2710	C	N1-C2-O2	10.51	125.21	118.90
2	2	2255	C	C2-N1-C1'	10.29	130.12	118.80
2	2	4502	C	N3-C2-O2	-10.23	114.74	121.90
2	2	467	U	N1-C2-O2	10.19	129.93	122.80
2	2	467	U	N3-C2-O2	-10.08	115.15	122.20
2	2	516	C	N3-C2-O2	-10.01	114.89	121.90
2	2	1702	C	N1-C2-O2	9.98	124.89	118.90
2	2	100	C	C2-N1-C1'	9.92	129.72	118.80
2	2	4453	C	N3-C2-O2	-9.89	114.98	121.90
2	2	4453	C	N1-C2-O2	9.88	124.83	118.90
2	2	516	C	C2-N1-C1'	9.86	129.65	118.80
2	2	485	C	C6-N1-C1'	-9.86	108.97	120.80
2	2	4502	C	N1-C2-O2	9.82	124.79	118.90
2	2	1302	U	C2-N1-C1'	9.73	129.38	117.70
2	2	1243	C	C2-N1-C1'	9.69	129.46	118.80
2	2	3587	C	N1-C2-O2	9.65	124.69	118.90
2	2	2257	C	N3-C2-O2	-9.60	115.18	121.90
2	2	472	C	N1-C2-O2	9.40	124.54	118.90
2	2	2022	C	N1-C2-O2	9.37	124.52	118.90
2	2	1702	C	N3-C2-O2	-9.28	115.40	121.90
2	2	2255	C	N3-C2-O2	-9.24	115.43	121.90
2	2	3709	U	N1-C2-O2	9.14	129.20	122.80
2	2	1702	C	C2-N1-C1'	9.14	128.85	118.80
2	2	4950	U	N3-C2-O2	-9.03	115.88	122.20
2	2	4950	U	N1-C2-O2	9.00	129.10	122.80
2	2	2710	C	C2-N1-C1'	8.94	128.63	118.80
2	2	3741	C	N3-C2-O2	-8.91	115.66	121.90
2	2	3741	C	N1-C2-O2	8.81	124.18	118.90
2	2	4895	C	C2-N1-C1'	8.77	128.45	118.80
2	2	2255	C	C6-N1-C2	-8.73	116.81	120.30
2	2	2257	C	C6-N1-C1'	-8.73	110.32	120.80

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*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	115	C	C2-N1-C1'	8.71	128.38	118.80
2	2	4601	U	N1-C2-O2	8.64	128.85	122.80
2	2	4453	C	C2-N1-C1'	8.64	128.30	118.80
2	2	704	C	N1-C2-O2	8.60	124.06	118.90
2	2	2710	C	N3-C2-O2	-8.59	115.89	121.90
2	2	4502	C	C2-N1-C1'	8.59	128.25	118.80
2	2	2255	C	C5-C6-N1	8.58	125.29	121.00
2	2	115	C	N1-C2-O2	8.57	124.04	118.90
2	2	4709	U	N1-C2-O2	8.54	128.78	122.80
2	2	141	C	C2-N1-C1'	8.45	128.09	118.80
2	2	2410	C	C2-N1-C1'	8.35	127.99	118.80
2	2	1241	C	N1-C2-O2	8.35	123.91	118.90
2	2	1079	C	N1-C2-O2	8.32	123.89	118.90
2	2	2410	C	C5-C6-N1	8.21	125.10	121.00
2	2	100	C	N1-C2-O2	8.19	123.81	118.90
2	2	925	C	C6-N1-C2	-8.17	117.03	120.30
2	2	3636	C	C6-N1-C2	-8.06	117.07	120.30
2	2	1216	C	C2-N1-C1'	8.05	127.66	118.80
2	2	1405	C	N1-C2-O2	8.01	123.70	118.90
2	2	77	U	N3-C2-O2	-7.99	116.61	122.20
2	2	100	C	N3-C2-O2	-7.97	116.32	121.90
2	2	2262	G	N3-C4-N9	7.93	130.76	126.00
2	2	1417	C	C2-N1-C1'	7.91	127.50	118.80
2	2	209	U	C6-N1-C1'	-7.85	110.20	121.20
2	2	485	C	N3-C2-O2	-7.82	116.42	121.90
2	2	2022	C	N3-C2-O2	-7.81	116.44	121.90
2	2	456	C	O4'-C1'-N1	7.78	114.42	108.20
2	2	3587	C	C2-N1-C1'	7.78	127.36	118.80
2	2	1097	C	C5-C6-N1	7.77	124.89	121.00
2	2	4950	U	C2-N1-C1'	7.77	127.03	117.70
2	2	4229	U	N3-C2-O2	-7.77	116.76	122.20
2	2	2860	C	C6-N1-C2	-7.74	117.20	120.30
2	2	4773	C	C5-C6-N1	7.74	124.87	121.00
2	2	2262	G	N3-C4-C5	-7.73	124.73	128.60
2	2	4895	C	N1-C2-O2	7.72	123.53	118.90
2	2	516	C	C6-N1-C2	-7.72	117.21	120.30
2	2	220	C	N1-C2-O2	7.72	123.53	118.90
2	2	753	C	C2-N1-C1'	7.72	127.29	118.80
2	2	3587	C	N3-C2-O2	-7.70	116.51	121.90
2	2	2560	C	C6-N1-C2	-7.68	117.23	120.30
2	2	1302	U	N1-C2-O2	7.67	128.17	122.80
2	2	467	U	C6-N1-C1'	-7.66	110.48	121.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	1702	C	C6-N1-C2	-7.65	117.24	120.30
2	2	2257	C	C6-N1-C2	-7.65	117.24	120.30
2	2	4695	C	N1-C2-O2	7.64	123.49	118.90
2	2	4758	U	N3-C2-O2	-7.63	116.86	122.20
4	5	28	C	C6-N1-C2	-7.63	117.25	120.30
2	2	4682	U	N1-C2-O2	7.62	128.13	122.80
2	2	4880	C	N1-C2-O2	7.62	123.47	118.90
2	2	1340	C	C5-C6-N1	7.60	124.80	121.00
2	2	2563	C	N1-C2-O2	7.60	123.46	118.90
2	2	2022	C	C6-N1-C2	-7.59	117.26	120.30
2	2	4926	C	N1-C2-O2	7.58	123.45	118.90
2	2	1191	C	N3-C2-O2	-7.56	116.61	121.90
2	2	2560	C	C5-C6-N1	7.54	124.77	121.00
2	2	4709	U	N3-C2-O2	-7.52	116.93	122.20
2	2	2303	C	C6-N1-C2	-7.51	117.29	120.30
2	2	2410	C	C6-N1-C2	-7.48	117.31	120.30
2	2	454	U	N1-C2-O2	7.44	128.01	122.80
2	2	4502	C	C6-N1-C2	-7.44	117.33	120.30
2	2	753	C	N1-C2-O2	7.42	123.35	118.90
2	2	1241	C	C2-N1-C1'	7.42	126.96	118.80
2	2	971	U	C2-N1-C1'	7.39	126.57	117.70
2	2	485	C	C6-N1-C2	-7.37	117.35	120.30
2	2	4728	U	N1-C2-O2	7.36	127.95	122.80
2	2	2528	G	C4-N9-C1'	7.36	136.06	126.50
2	2	4601	U	N3-C2-O2	-7.34	117.06	122.20
2	2	4926	C	C2-N1-C1'	7.32	126.86	118.80
2	2	1243	C	C6-N1-C2	-7.31	117.38	120.30
2	2	175	C	C6-N1-C2	-7.28	117.39	120.30
2	2	1097	C	C6-N1-C2	-7.28	117.39	120.30
2	2	985	C	C6-N1-C2	-7.27	117.39	120.30
2	2	100	C	C6-N1-C1'	-7.26	112.08	120.80
35	d	43	LEU	CA-CB-CG	7.24	131.96	115.30
2	2	1607	C	C6-N1-C2	-7.22	117.41	120.30
2	2	1726	U	N3-C2-O2	-7.22	117.15	122.20
2	2	2019	C	N3-C2-O2	-7.20	116.86	121.90
2	2	2257	C	C5-C6-N1	7.20	124.60	121.00
2	2	4612	C	N1-C2-O2	7.20	123.22	118.90
2	2	2022	C	C2-N1-C1'	7.20	126.72	118.80
2	2	2262	G	C4-N9-C1'	7.19	135.85	126.50
20	N	119	TYR	C-N-CA	7.19	139.68	121.70
2	2	1437	C	C6-N1-C2	-7.18	117.43	120.30
2	2	925	C	C5-C6-N1	7.18	124.59	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	4728	U	C2-N1-C1'	7.16	126.30	117.70
2	2	965	G	C4-N9-C1'	7.15	135.80	126.50
2	2	1632	A	C2-N3-C4	7.14	114.17	110.60
2	2	1417	C	C6-N1-C2	-7.13	117.45	120.30
2	2	4453	C	C6-N1-C2	-7.12	117.45	120.30
2	2	1720	C	C6-N1-C2	-7.11	117.45	120.30
2	2	2560	C	C2-N1-C1'	7.11	126.62	118.80
2	2	3618	C	C6-N1-C2	-7.11	117.46	120.30
2	2	4229	U	N1-C2-O2	7.10	127.77	122.80
7	8	64	U	N3-C2-O2	-7.10	117.23	122.20
2	2	180	C	C6-N1-C2	-7.09	117.46	120.30
2	2	4709	U	C2-N1-C1'	7.08	126.20	117.70
2	2	985	C	C2-N1-C1'	7.08	126.59	118.80
2	2	2417	A	O4'-C1'-N9	7.08	113.86	108.20
2	2	175	C	N3-C2-O2	-7.07	116.95	121.90
2	2	472	C	N3-C2-O2	-7.03	116.98	121.90
2	2	1302	U	C6-N1-C1'	-7.02	111.37	121.20
9	B	360	LEU	CA-CB-CG	7.00	131.39	115.30
2	2	516	C	C5-C6-N1	6.99	124.49	121.00
2	2	1367	C	N1-C2-O2	6.98	123.09	118.90
2	2	1079	C	C2-N1-C1'	6.98	126.48	118.80
2	2	417	G	O4'-C1'-N9	6.98	113.78	108.20
2	2	2505	C	C6-N1-C2	-6.98	117.51	120.30
2	2	4120	U	C2-N1-C1'	6.97	126.06	117.70
2	2	753	C	N3-C2-O2	-6.96	117.03	121.90
2	2	2351	C	C5-C6-N1	6.94	124.47	121.00
2	2	3587	C	C6-N1-C2	-6.93	117.53	120.30
2	2	4926	C	N3-C2-O2	-6.93	117.05	121.90
2	2	971	U	N1-C2-O2	6.91	127.64	122.80
2	2	1402	C	N1-C2-O2	6.91	123.04	118.90
2	2	4682	U	N3-C2-O2	-6.90	117.37	122.20
2	2	499	G	C4-N9-C1'	6.89	135.46	126.50
2	2	112	C	C2-N1-C1'	6.89	126.38	118.80
2	2	1367	C	C2-N1-C1'	6.88	126.37	118.80
2	2	2814	C	N1-C2-O2	6.88	123.03	118.90
4	5	24	C	C6-N1-C2	-6.88	117.55	120.30
2	2	2094	G	C4-N9-C1'	6.88	135.44	126.50
44	n	105	LEU	C-N-CA	6.87	138.89	121.70
2	2	4662	C	C6-N1-C2	-6.87	117.55	120.30
2	2	1417	C	C5-C6-N1	6.84	124.42	121.00
3	4	257	LEU	CA-CB-CG	6.84	131.03	115.30
4	5	78	C	C5-C6-N1	6.82	124.41	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	449	C	C2-N1-C1'	6.82	126.30	118.80
2	2	4612	C	C6-N1-C2	-6.80	117.58	120.30
2	2	4928	C	C2-N1-C1'	6.80	126.28	118.80
2	2	4728	U	N3-C2-O2	-6.79	117.45	122.20
2	2	4594	U	N3-C2-O2	-6.78	117.45	122.20
2	2	914	U	P-O3'-C3'	6.78	127.84	119.70
2	2	4773	C	N1-C2-O2	6.77	122.96	118.90
2	2	1969	G	N1-C6-O6	-6.76	115.84	119.90
2	2	2351	C	C2-N1-C1'	6.76	126.24	118.80
2	2	4393	G	C5-C6-O6	6.75	132.65	128.60
2	2	2627	C	C6-N1-C2	-6.74	117.60	120.30
2	2	4254	G	C4-N9-C1'	6.74	135.26	126.50
2	2	1096	C	C5-C6-N1	6.72	124.36	121.00
2	2	2853	C	N1-C2-O2	6.71	122.92	118.90
2	2	115	C	C6-N1-C1'	-6.68	112.78	120.80
2	2	1929	A	C2-N3-C4	6.68	113.94	110.60
2	2	914	U	C5-C4-O4	-6.66	121.90	125.90
2	2	1302	U	N3-C2-O2	-6.66	117.54	122.20
2	2	3905	A	P-O3'-C3'	6.66	127.69	119.70
2	2	4887	C	N1-C2-O2	6.65	122.89	118.90
2	2	2410	C	N1-C2-O2	6.64	122.89	118.90
2	2	2528	G	N3-C4-N9	6.64	129.98	126.00
2	2	4887	C	C6-N1-C2	-6.64	117.64	120.30
2	2	1378	C	C2-N1-C1'	6.62	126.09	118.80
2	2	485	C	C5-C6-N1	6.62	124.31	121.00
2	2	4773	C	C2-N1-C1'	6.60	126.06	118.80
2	2	4100	C	C6-N1-C2	-6.59	117.66	120.30
2	2	4608	G	C8-N9-C4	-6.57	103.77	106.40
2	2	2465	C	C5-C6-N1	6.56	124.28	121.00
2	2	4612	C	N3-C2-O2	-6.56	117.31	121.90
2	2	977	C	C2-N1-C1'	6.55	126.01	118.80
2	2	1191	C	N1-C2-O2	6.55	122.83	118.90
2	2	4913	G	P-O3'-C3'	6.55	127.56	119.70
2	2	4758	U	C2-N1-C1'	6.55	125.56	117.70
4	5	78	C	C2-N1-C1'	6.53	125.98	118.80
2	2	2710	C	C6-N1-C1'	-6.52	112.97	120.80
2	2	4601	U	C2-N1-C1'	6.52	125.52	117.70
2	2	1378	C	N1-C2-O2	6.51	122.81	118.90
2	2	1216	C	N1-C2-O2	6.50	122.80	118.90
2	2	1243	C	C6-N1-C1'	-6.49	113.01	120.80
2	2	2760	G	P-O3'-C3'	6.49	127.49	119.70
2	2	4500	U	C2-N1-C1'	6.49	125.49	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	141	C	C5-C6-N1	6.49	124.24	121.00
2	2	2528	G	N3-C4-C5	-6.49	125.36	128.60
2	2	115	C	N3-C2-O2	-6.48	117.36	121.90
2	2	2560	C	N1-C2-O2	6.48	122.79	118.90
2	2	4500	U	C5-C6-N1	6.48	125.94	122.70
2	2	2022	C	C5-C6-N1	6.48	124.24	121.00
2	2	4758	U	N1-C2-O2	6.48	127.33	122.80
2	2	209	U	C5-C6-N1	6.47	125.94	122.70
2	2	495	C	N1-C2-O2	6.47	122.78	118.90
2	2	2255	C	C6-N1-C1'	-6.47	113.04	120.80
2	2	1241	C	N3-C2-O2	-6.46	117.38	121.90
2	2	704	C	C2-N1-C1'	6.46	125.91	118.80
4	5	24	C	C5-C6-N1	6.45	124.23	121.00
2	2	4773	C	C6-N1-C2	-6.44	117.72	120.30
2	2	1666	C	C6-N1-C2	-6.43	117.73	120.30
2	2	454	U	C5-C6-N1	6.42	125.91	122.70
2	2	516	C	C6-N1-C1'	-6.42	113.09	120.80
2	2	2081	C	C6-N1-C2	-6.42	117.73	120.30
2	2	4775	C	C2-N1-C1'	6.42	125.86	118.80
2	2	2860	C	N3-C2-O2	-6.42	117.41	121.90
2	2	965	G	C8-N9-C1'	-6.40	118.67	127.00
2	2	1822	U	C2-N1-C1'	6.40	125.38	117.70
2	2	77	U	N1-C2-O2	6.40	127.28	122.80
7	8	111	U	C2-N1-C1'	6.39	125.36	117.70
2	2	1915	C	N3-C2-O2	-6.39	117.43	121.90
3	4	230	LEU	CA-CB-CG	6.38	129.97	115.30
2	2	719	C	C6-N1-C2	-6.37	117.75	120.30
2	2	2033	A	P-O3'-C3'	6.37	127.35	119.70
2	2	2820	C	N1-C2-O2	6.37	122.72	118.90
2	2	2094	G	N3-C4-C5	-6.37	125.42	128.60
2	2	4133	C	C2-N1-C1'	6.35	125.79	118.80
2	2	963	G	C4-N9-C1'	6.35	134.75	126.50
2	2	2627	C	C2-N1-C1'	6.33	125.77	118.80
2	2	1183	C	N1-C2-O2	6.33	122.70	118.90
11	D	171	LEU	CA-CB-CG	6.33	129.86	115.30
2	2	3739	C	N1-C2-O2	6.33	122.70	118.90
2	2	4940	C	N1-C2-O2	6.32	122.69	118.90
2	2	4895	C	C6-N1-C1'	-6.32	113.22	120.80
2	2	4747	C	C2-N1-C1'	6.32	125.75	118.80
2	2	1809	C	C2-N1-C1'	6.30	125.73	118.80
2	2	4505	C	C5-C6-N1	6.30	124.15	121.00
2	2	1591	U	N1-C2-O2	6.29	127.21	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	449	C	N1-C2-O2	6.29	122.67	118.90
2	2	472	C	C2-N1-C1'	6.29	125.72	118.80
2	2	220	C	C5-C6-N1	6.29	124.14	121.00
2	2	4880	C	N3-C2-O2	-6.27	117.51	121.90
2	2	4360	U	N3-C2-O2	-6.27	117.81	122.20
2	2	141	C	C6-N1-C2	-6.25	117.80	120.30
2	2	4950	U	C5-C6-N1	6.25	125.83	122.70
2	2	4730	C	C6-N1-C2	-6.25	117.80	120.30
4	5	39	C	N1-C2-O2	6.24	122.65	118.90
2	2	2351	C	C6-N1-C2	-6.23	117.81	120.30
2	2	180	C	N1-C2-O2	6.23	122.64	118.90
2	2	4608	G	N7-C8-N9	6.22	116.21	113.10
2	2	2409	U	N1-C2-N3	6.22	118.63	114.90
2	2	4945	G	N3-C4-N9	6.22	129.73	126.00
2	2	988	C	C2-N1-C1'	6.22	125.64	118.80
2	2	2260	C	C2-N1-C1'	6.21	125.64	118.80
2	2	2528	G	C8-N9-C1'	-6.21	118.92	127.00
2	2	2304	U	N3-C2-O2	-6.21	117.85	122.20
2	2	672	C	N1-C2-O2	6.21	122.63	118.90
2	2	2262	G	C8-N9-C1'	-6.21	118.92	127.00
2	2	4923	C	N1-C2-O2	6.21	122.63	118.90
2	2	4471	U	N3-C2-O2	-6.21	117.86	122.20
2	2	1094	G	N3-C4-N9	6.20	129.72	126.00
2	2	148	C	C6-N1-C2	-6.20	117.82	120.30
2	2	4973	U	C2-N1-C1'	6.20	125.14	117.70
2	2	177	G	N3-C4-N9	6.18	129.71	126.00
2	2	100	C	O4'-C1'-N1	6.17	113.14	108.20
2	2	1178	G	N3-C4-C5	-6.17	125.52	128.60
4	5	78	C	C6-N1-C2	-6.16	117.83	120.30
2	2	4887	C	N3-C2-O2	-6.16	117.59	121.90
4	5	28	C	C5-C6-N1	6.16	124.08	121.00
2	2	282	C	N1-C2-O2	6.16	122.59	118.90
2	2	1243	C	N1-C2-O2	6.15	122.59	118.90
2	2	4162	C	C2-N1-C1'	6.15	125.56	118.80
2	2	3924	C	C5-C6-N1	6.14	124.07	121.00
2	2	1607	C	N1-C2-O2	6.14	122.58	118.90
2	2	1216	C	C6-N1-C1'	-6.14	113.44	120.80
2	2	4775	C	C5-C6-N1	6.14	124.07	121.00
2	2	209	U	C6-N1-C2	-6.13	117.32	121.00
2	2	436	C	C6-N1-C2	-6.13	117.85	120.30
2	2	3932	U	N3-C2-O2	-6.13	117.91	122.20
2	2	4505	C	C6-N1-C2	-6.12	117.85	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	4476	C	C2-N1-C1'	6.10	125.51	118.80
2	2	4945	G	C5-C6-O6	-6.10	124.94	128.60
2	2	4500	U	N1-C2-O2	6.09	127.07	122.80
2	2	2563	C	C6-N1-C2	-6.09	117.87	120.30
2	2	4607	A	O4'-C1'-N9	6.09	113.07	108.20
2	2	969	C	C6-N1-C2	-6.08	117.87	120.30
2	2	2563	C	N3-C2-O2	-6.08	117.64	121.90
2	2	4068	U	N1-C2-O2	6.08	127.05	122.80
2	2	220	C	C2-N1-C1'	6.07	125.48	118.80
2	2	2501	C	C5-C6-N1	6.07	124.03	121.00
2	2	4068	U	N3-C2-O2	-6.07	117.95	122.20
2	2	5016	A	O4'-C1'-N9	6.06	113.05	108.20
2	2	96	U	N3-C2-O2	-6.06	117.96	122.20
2	2	2532	C	C5-C6-N1	6.05	124.03	121.00
2	2	2303	C	N3-C2-O2	-6.04	117.67	121.90
2	2	177	G	C4-N9-C1'	6.04	134.35	126.50
2	2	4162	C	N1-C2-O2	6.03	122.52	118.90
2	2	1477	C	C6-N1-C2	-6.03	117.89	120.30
2	2	3734	U	N1-C2-O2	6.02	127.02	122.80
2	2	4990	C	C6-N1-C2	-6.02	117.89	120.30
2	2	965	G	N3-C4-N9	6.01	129.61	126.00
2	2	2505	C	N1-C2-O2	5.99	122.50	118.90
2	2	4199	C	N1-C2-O2	5.99	122.49	118.90
2	2	41	C	C5-C6-N1	5.99	123.99	121.00
2	2	4887	C	C2-N1-C1'	5.98	125.38	118.80
2	2	3870	C	C5-C6-N1	5.98	123.99	121.00
2	2	499	G	C8-N9-C1'	-5.98	119.23	127.00
2	2	2860	C	N1-C2-O2	5.97	122.48	118.90
2	2	1201	U	N1-C2-O2	5.97	126.98	122.80
2	2	3618	C	C5-C6-N1	5.97	123.98	121.00
2	2	2860	C	C2-N1-C1'	5.97	125.36	118.80
2	2	4303	C	N3-C2-O2	-5.97	117.72	121.90
2	2	4612	C	C2-N1-C1'	5.96	125.36	118.80
3	4	271	LEU	CA-CB-CG	5.96	129.00	115.30
2	2	4314	C	N1-C2-O2	5.95	122.47	118.90
2	2	488	G	N7-C8-N9	5.93	116.07	113.10
2	2	3924	C	C6-N1-C2	-5.93	117.93	120.30
2	2	2362	U	N1-C2-O2	5.92	126.94	122.80
2	2	1607	C	N3-C2-O2	-5.91	117.76	121.90
2	2	4206	C	C2-N1-C1'	5.91	125.31	118.80
2	2	2632	U	N1-C2-O2	5.91	126.94	122.80
2	2	2016	C	C6-N1-C2	-5.91	117.94	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	4505	C	N1-C2-O2	5.91	122.45	118.90
2	2	1402	C	N3-C2-O2	-5.91	117.77	121.90
2	2	2094	G	N3-C4-N9	5.90	129.54	126.00
2	2	2255	C	C2-N3-C4	5.90	122.85	119.90
2	2	1297	U	N1-C2-O2	5.90	126.93	122.80
2	2	719	C	C5-C6-N1	5.90	123.95	121.00
2	2	44	A	C2-N3-C4	5.90	113.55	110.60
2	2	2337	C	C6-N1-C2	-5.90	117.94	120.30
2	2	4303	C	C6-N1-C2	-5.90	117.94	120.30
2	2	454	U	C2-N1-C1'	5.89	124.77	117.70
2	2	4923	C	C2-N1-C1'	5.89	125.28	118.80
2	2	4958	C	C6-N1-C2	-5.89	117.94	120.30
2	2	4895	C	N3-C2-O2	-5.89	117.78	121.90
2	2	2506	G	C4-N9-C1'	5.88	134.15	126.50
2	2	4996	C	C6-N1-C2	-5.88	117.95	120.30
2	2	2260	C	N1-C2-O2	5.88	122.43	118.90
2	2	4237	C	C5-C6-N1	5.87	123.94	121.00
2	2	4764	A	N1-C2-N3	-5.87	126.37	129.30
2	2	1405	C	N3-C2-O2	-5.87	117.80	121.90
2	2	4254	G	N3-C4-C5	-5.87	125.67	128.60
6	7	62	GLU	CB-CA-C	5.86	122.12	110.40
2	2	141	C	N1-C2-O2	5.86	122.41	118.90
2	2	1703	C	N1-C2-O2	5.86	122.41	118.90
2	2	2257	C	C2-N3-C4	5.86	122.83	119.90
2	2	2589	C	C6-N1-C2	-5.86	117.96	120.30
2	2	2627	C	C5-C6-N1	5.85	123.92	121.00
37	g	116	LEU	CA-CB-CG	5.85	128.75	115.30
2	2	2499	C	N1-C2-O2	5.84	122.41	118.90
2	2	1597	G	O4'-C1'-N9	5.84	112.87	108.20
2	2	1472	C	N1-C2-O2	5.84	122.40	118.90
2	2	4237	C	C6-N1-C2	-5.83	117.97	120.30
2	2	4771	C	C2-N1-C1'	5.83	125.22	118.80
2	2	1809	C	C6-N1-C2	-5.83	117.97	120.30
2	2	4171	C	N1-C2-O2	5.82	122.39	118.90
2	2	2439	G	N3-C4-N9	5.82	129.49	126.00
2	2	1969	G	C5-C6-O6	5.82	132.09	128.60
2	2	1472	C	C2-N1-C1'	5.81	125.20	118.80
2	2	4950	U	C6-N1-C2	-5.81	117.51	121.00
2	2	991	C	C6-N1-C2	-5.81	117.97	120.30
2	2	1822	U	N1-C2-O2	5.80	126.86	122.80
2	2	2484	A	C2-N3-C4	5.78	113.49	110.60
2	2	1929	A	C4-N9-C1'	5.78	136.70	126.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	914	U	N3-C4-O4	5.78	123.44	119.40
2	2	3657	U	N3-C2-O2	-5.78	118.16	122.20
4	5	76	U	N1-C2-O2	5.78	126.84	122.80
2	2	4229	U	C2-N1-C1'	5.77	124.63	117.70
2	2	4940	C	C6-N1-C2	-5.76	118.00	120.30
2	2	177	G	C8-N9-C1'	-5.76	119.52	127.00
2	2	1579	C	C5-C6-N1	5.76	123.88	121.00
2	2	1577	G	C2-N3-C4	5.75	114.78	111.90
2	2	2727	C	C5-C6-N1	5.75	123.88	121.00
2	2	3709	U	C2-N1-C1'	5.75	124.61	117.70
2	2	4627	U	N1-C2-O2	5.75	126.83	122.80
2	2	1702	C	C6-N1-C1'	-5.75	113.90	120.80
2	2	2048	U	N3-C2-O2	-5.75	118.18	122.20
2	2	4197	G	C8-N9-C4	-5.75	104.10	106.40
2	2	1720	C	C5-C6-N1	5.74	123.87	121.00
2	2	1535	C	C6-N1-C2	-5.74	118.00	120.30
2	2	1467	C	C6-N1-C2	-5.74	118.00	120.30
2	2	654	C	N1-C2-O2	5.73	122.34	118.90
2	2	2593	C	C6-N1-C2	-5.73	118.01	120.30
2	2	2886	U	C2-N1-C1'	5.72	124.57	117.70
2	2	1731	C	C2-N1-C1'	5.71	125.08	118.80
2	2	406	C	P-O3'-C3'	5.71	126.55	119.70
2	2	3590	G	N3-C4-C5	-5.71	125.75	128.60
2	2	5023	C	N1-C2-O2	5.71	122.32	118.90
2	2	4120	U	N1-C2-O2	5.70	126.79	122.80
2	2	972	C	N1-C2-O2	5.70	122.32	118.90
2	2	220	C	C6-N1-C2	-5.70	118.02	120.30
2	2	2031	C	C6-N1-C2	-5.70	118.02	120.30
2	2	4498	U	P-O3'-C3'	5.70	126.54	119.70
2	2	2035	C	C5-C6-N1	5.70	123.85	121.00
2	2	488	G	C8-N9-C4	-5.70	104.12	106.40
2	2	2021	G	C4-N9-C1'	5.69	133.90	126.50
2	2	1315	C	C5-C6-N1	5.69	123.84	121.00
2	2	4940	C	C2-N1-C1'	5.69	125.06	118.80
2	2	4303	C	C2-N1-C1'	5.69	125.05	118.80
2	2	2081	C	C5-C6-N1	5.68	123.84	121.00
2	2	141	C	C6-N1-C1'	-5.68	113.98	120.80
2	2	1847	C	C5-C6-N1	5.68	123.84	121.00
2	2	4137	C	C5-C6-N1	5.68	123.84	121.00
2	2	4340	U	N1-C2-O2	5.68	126.77	122.80
2	2	2791	C	C6-N1-C2	-5.67	118.03	120.30
2	2	3673	C	P-O3'-C3'	5.67	126.50	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	4728	U	C5-C6-N1	5.67	125.53	122.70
2	2	1178	G	N3-C4-N9	5.67	129.40	126.00
28	W	33	LEU	CA-CB-CG	5.67	128.34	115.30
2	2	4522	G	N3-C4-C5	-5.66	125.77	128.60
2	2	4286	C	C5-C6-N1	5.66	123.83	121.00
2	2	965	G	N3-C4-C5	-5.66	125.77	128.60
2	2	1191	C	C6-N1-C2	-5.65	118.04	120.30
2	2	3590	G	N3-C4-N9	5.65	129.39	126.00
2	2	282	C	N3-C2-O2	-5.64	117.95	121.90
2	2	1245	C	C5-C6-N1	5.64	123.82	121.00
7	8	64	U	N1-C2-O2	5.64	126.75	122.80
2	2	1094	G	N3-C4-C5	-5.63	125.78	128.60
2	2	4508	C	C6-N1-C2	-5.63	118.05	120.30
2	2	4695	C	C2-N1-C1'	5.63	124.99	118.80
4	5	76	U	C2-N1-C1'	5.63	124.45	117.70
2	2	1589	C	C6-N1-C2	-5.62	118.05	120.30
2	2	2627	C	N1-C2-O2	5.62	122.27	118.90
2	2	4314	C	N3-C2-O2	-5.62	117.97	121.90
2	2	1577	G	N3-C2-N2	-5.62	115.97	119.90
2	2	4215	C	N1-C2-O2	5.62	122.27	118.90
2	2	1245	C	C6-N1-C2	-5.61	118.05	120.30
2	2	1579	C	C6-N1-C2	-5.61	118.05	120.30
2	2	2632	U	N3-C2-O2	-5.61	118.27	122.20
2	2	2094	G	C8-N9-C1'	-5.61	119.71	127.00
2	2	1192	C	N1-C2-O2	5.61	122.27	118.90
2	2	4137	C	C6-N1-C2	-5.61	118.06	120.30
2	2	985	C	C5-C6-N1	5.60	123.80	121.00
2	2	1598	C	C6-N1-C2	-5.59	118.06	120.30
2	2	3641	U	C5-C6-N1	-5.59	119.90	122.70
2	2	4775	C	C6-N1-C2	-5.59	118.06	120.30
7	8	54	C	N1-C2-O2	5.59	122.26	118.90
2	2	1686	C	N3-C2-O2	-5.59	117.99	121.90
2	2	1386	C	C6-N1-C2	-5.58	118.07	120.30
2	2	1686	C	N1-C2-O2	5.58	122.25	118.90
2	2	4695	C	C5-C6-N1	5.56	123.78	121.00
2	2	1079	C	N3-C2-O2	-5.55	118.01	121.90
2	2	4189	U	N3-C4-O4	5.55	123.29	119.40
2	2	4199	C	N3-C2-O2	-5.55	118.01	121.90
2	2	948	C	C6-N1-C2	-5.55	118.08	120.30
2	2	4340	U	N3-C2-O2	-5.54	118.32	122.20
2	2	4352	U	N3-C2-O2	-5.54	118.32	122.20
2	2	3741	C	C6-N1-C2	-5.53	118.09	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	2337	C	N1-C2-O2	5.53	122.22	118.90
2	2	112	C	C5-C6-N1	5.53	123.77	121.00
2	2	1201	U	C5-C6-N1	5.53	125.47	122.70
2	2	2362	U	N3-C2-O2	-5.52	118.34	122.20
2	2	2850	A	C2-N3-C4	5.52	113.36	110.60
2	2	3587	C	C5-C6-N1	5.51	123.76	121.00
2	2	2048	U	N1-C2-O2	5.51	126.66	122.80
2	2	256	G	C6-C5-N7	-5.51	127.10	130.40
2	2	4709	U	C5-C6-N1	5.50	125.45	122.70
44	n	106	TYR	N-CA-C	5.50	125.83	111.00
2	2	204	U	C5-C6-N1	5.49	125.45	122.70
2	2	205	C	C6-N1-C2	-5.49	118.10	120.30
2	2	971	U	N3-C2-O2	-5.49	118.36	122.20
2	2	963	G	N3-C4-N9	5.49	129.29	126.00
2	2	4864	U	N1-C2-O2	5.49	126.64	122.80
2	2	264	C	C6-N1-C1'	5.48	127.38	120.80
2	2	3598	C	N1-C2-O2	5.48	122.19	118.90
2	2	4289	U	N1-C2-O2	5.48	126.63	122.80
2	2	4395	U	P-O3'-C3'	5.47	126.27	119.70
2	2	4714	C	N1-C2-O2	5.47	122.18	118.90
2	2	499	G	N3-C4-N9	5.47	129.28	126.00
2	2	4453	C	C6-N1-C1'	-5.47	114.24	120.80
2	2	4771	C	N1-C2-O2	5.47	122.18	118.90
2	2	35	U	N3-C2-O2	-5.46	118.38	122.20
2	2	436	C	C2-N1-C1'	5.46	124.81	118.80
2	2	963	G	C8-N9-C1'	-5.46	119.90	127.00
2	2	1696	C	C5-C6-N1	5.46	123.73	121.00
4	5	35	U	N3-C2-O2	-5.46	118.38	122.20
2	2	4928	C	N1-C2-O2	5.45	122.17	118.90
2	2	516	C	C2-N3-C4	5.45	122.63	119.90
2	2	1822	U	N3-C2-O2	-5.45	118.39	122.20
2	2	4973	U	N3-C2-O2	-5.45	118.39	122.20
2	2	4314	C	C6-N1-C2	-5.44	118.12	120.30
2	2	2337	C	C5-C6-N1	5.44	123.72	121.00
2	2	4302	U	N1-C2-O2	5.44	126.61	122.80
43	m	122	ASP	CB-CG-OD1	5.44	123.20	118.30
2	2	2589	C	C5-C6-N1	5.44	123.72	121.00
2	2	4975	G	O4'-C1'-N9	5.44	112.55	108.20
2	2	3631	U	N3-C2-O2	-5.43	118.40	122.20
2	2	454	U	N3-C2-O2	-5.43	118.40	122.20
4	5	39	C	N3-C2-O2	-5.43	118.10	121.90
2	2	679	C	C6-N1-C2	-5.42	118.13	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	1628	C	C6-N1-C2	-5.42	118.13	120.30
2	2	683	C	C6-N1-C2	-5.42	118.13	120.30
2	2	4254	G	C8-N9-C1'	-5.42	119.96	127.00
2	2	2094	G	C2-N3-C4	5.42	114.61	111.90
2	2	753	C	C6-N1-C1'	-5.42	114.30	120.80
2	2	4561	C	C6-N1-C2	-5.42	118.13	120.30
2	2	2353	U	C5-C6-N1	5.41	125.41	122.70
2	2	1655	C	N1-C2-O2	5.41	122.15	118.90
2	2	977	C	C6-N1-C2	-5.41	118.14	120.30
2	2	4555	U	P-O3'-C3'	5.41	126.19	119.70
2	2	4928	C	C6-N1-C2	-5.40	118.14	120.30
2	2	4771	C	C5-C6-N1	5.40	123.70	121.00
18	L	46	ASP	CB-CG-OD1	5.40	123.16	118.30
2	2	1847	C	C6-N1-C2	-5.39	118.14	120.30
2	2	1367	C	N3-C2-O2	-5.39	118.13	121.90
2	2	1633	G	P-O3'-C3'	5.39	126.17	119.70
2	2	2260	C	N3-C2-O2	-5.39	118.13	121.90
2	2	4502	C	C6-N1-C1'	-5.39	114.33	120.80
2	2	294	G	C4-N9-C1'	5.39	133.50	126.50
2	2	262	G	N1-C6-O6	-5.38	116.67	119.90
2	2	3590	G	C4-N9-C1'	5.38	133.50	126.50
2	2	2767	U	N3-C2-O2	-5.38	118.44	122.20
2	2	1535	C	C5-C6-N1	5.37	123.69	121.00
2	2	4682	U	C2-N1-C1'	5.37	124.15	117.70
2	2	4561	C	C2-N1-C1'	5.37	124.71	118.80
2	2	4603	C	C6-N1-C2	-5.37	118.15	120.30
2	2	1096	C	C2-N1-C1'	5.37	124.71	118.80
2	2	1275	G	O4'-C1'-N9	5.37	112.50	108.20
2	2	3680	U	N3-C2-O2	-5.37	118.44	122.20
2	2	96	U	N1-C2-O2	5.37	126.56	122.80
2	2	4406	U	N3-C2-O2	-5.37	118.44	122.20
2	2	4471	U	N1-C2-O2	5.36	126.56	122.80
2	2	180	C	C4-C5-C6	-5.36	114.72	117.40
2	2	2482	C	C6-N1-C2	-5.36	118.16	120.30
2	2	4189	U	C5-C4-O4	-5.36	122.68	125.90
7	8	142	U	C5-C6-N1	5.36	125.38	122.70
2	2	1822	U	C5-C6-N1	5.36	125.38	122.70
2	2	2752	G	N3-C4-N9	5.36	129.22	126.00
2	2	1671	U	N3-C2-O2	-5.36	118.45	122.20
2	2	4352	U	N1-C2-O2	5.35	126.55	122.80
2	2	4476	C	N1-C2-O2	5.35	122.11	118.90
2	2	14	C	N1-C2-O2	5.35	122.11	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	2814	C	N3-C2-O2	-5.35	118.15	121.90
2	2	1915	C	N1-C2-O2	5.35	122.11	118.90
2	2	4766	C	C2-N1-C1'	5.35	124.68	118.80
2	2	1607	C	C5-C6-N1	5.34	123.67	121.00
2	2	1655	C	C6-N1-C2	-5.34	118.16	120.30
2	2	4352	U	C2-N1-C1'	5.34	124.11	117.70
2	2	2021	G	C8-N9-C1'	-5.34	120.06	127.00
2	2	2439	G	C4-N9-C1'	5.34	133.44	126.50
2	2	988	C	N1-C2-O2	5.34	122.10	118.90
2	2	41	C	C6-N1-C2	-5.34	118.17	120.30
4	5	111	C	N1-C2-O2	5.33	122.10	118.90
2	2	2505	C	C5-C6-N1	5.33	123.67	121.00
2	2	1074	G	C4-N9-C1'	5.33	133.43	126.50
2	2	1241	C	C6-N1-C2	-5.33	118.17	120.30
2	2	1439	C	N1-C2-O2	5.33	122.10	118.90
2	2	1703	C	C2-N1-C1'	5.32	124.65	118.80
2	2	4922	C	C6-N1-C2	-5.32	118.17	120.30
2	2	440	U	C2-N1-C1'	5.31	124.08	117.70
2	2	1402	C	C2-N1-C1'	5.31	124.64	118.80
2	2	2031	C	C2-N1-C1'	5.31	124.64	118.80
2	2	1085	C	C6-N1-C2	-5.30	118.18	120.30
2	2	1633	G	OP1-P-O3'	5.30	116.87	105.20
2	2	1447	C	C6-N1-C2	-5.30	118.18	120.30
2	2	112	C	C6-N1-C2	-5.30	118.18	120.30
2	2	1376	C	C2-N1-C1'	5.30	124.63	118.80
2	2	1216	C	O4'-C1'-N1	5.29	112.44	108.20
2	2	4714	C	C5-C6-N1	5.29	123.65	121.00
2	2	669	C	C2-N1-C1'	5.29	124.62	118.80
2	2	3637	U	N3-C2-O2	-5.29	118.50	122.20
2	2	704	C	N3-C2-O2	-5.28	118.21	121.90
2	2	2059	C	C6-N1-C2	-5.28	118.19	120.30
2	2	3711	A	N1-C6-N6	-5.28	115.43	118.60
2	2	322	C	N1-C2-O2	5.27	122.06	118.90
2	2	1591	U	N3-C2-O2	-5.27	118.51	122.20
2	2	2712	G	C4-N9-C1'	5.27	133.35	126.50
2	2	1203	G	C4-N9-C1'	5.27	133.35	126.50
2	2	326	C	C2-N1-C1'	5.27	124.59	118.80
2	2	100	C	C6-N1-C2	-5.26	118.19	120.30
2	2	2820	C	N3-C2-O2	-5.26	118.22	121.90
2	2	9	C	C6-N1-C2	-5.25	118.20	120.30
2	2	180	C	C2-N1-C1'	5.25	124.58	118.80
2	2	2016	C	C5-C6-N1	5.25	123.62	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	2410	C	C2-N3-C4	5.25	122.52	119.90
2	2	4461	C	C6-N1-C2	-5.25	118.20	120.30
2	2	1203	G	C8-N9-C1'	-5.25	120.18	127.00
2	2	2362	U	C2-N1-C1'	5.24	123.99	117.70
2	2	2506	G	C8-N9-C1'	-5.24	120.19	127.00
2	2	4601	U	C5-C6-N1	5.24	125.32	122.70
2	2	242	U	N3-C2-O2	-5.24	118.53	122.20
2	2	2410	C	C6-N1-C1'	-5.24	114.52	120.80
2	2	4342	C	C5-C6-N1	5.24	123.62	121.00
4	5	39	C	C6-N1-C2	-5.24	118.20	120.30
2	2	2653	C	C6-N1-C2	-5.23	118.21	120.30
2	2	977	C	N1-C2-O2	5.23	122.04	118.90
2	2	704	C	C6-N1-C1'	-5.22	114.53	120.80
2	2	2853	C	N3-C2-O2	-5.22	118.25	121.90
2	2	1439	C	C2-N1-C1'	5.22	124.54	118.80
2	2	2760	G	OP2-P-O3'	5.22	116.67	105.20
2	2	1183	C	C6-N1-C2	-5.21	118.21	120.30
26	U	134	LEU	CA-CB-CG	5.21	127.28	115.30
2	2	178	C	N1-C2-O2	5.20	122.02	118.90
2	2	688	U	N1-C2-O2	5.20	126.44	122.80
2	2	2632	U	C2-N1-C1'	5.19	123.93	117.70
2	2	4547	C	C6-N1-C2	-5.19	118.22	120.30
2	2	4712	C	C5-C6-N1	5.19	123.59	121.00
2	2	971	U	C6-N1-C1'	-5.19	113.94	121.20
2	2	1686	C	C6-N1-C2	-5.19	118.22	120.30
2	2	4254	G	N3-C4-N9	5.18	129.11	126.00
2	2	1315	C	C6-N1-C2	-5.18	118.23	120.30
2	2	5023	C	N3-C2-O2	-5.18	118.28	121.90
2	2	1254	A	C2-N3-C4	5.17	113.19	110.60
2	2	2351	C	N1-C2-O2	5.17	122.00	118.90
2	2	2035	C	C6-N1-C2	-5.17	118.23	120.30
2	2	4940	C	N3-C2-O2	-5.17	118.28	121.90
2	2	1314	C	O4'-C1'-N1	5.17	112.33	108.20
2	2	2712	G	N3-C4-N9	5.17	129.10	126.00
2	2	4508	C	C5-C6-N1	5.17	123.58	121.00
2	2	4985	U	N1-C2-O2	5.17	126.42	122.80
2	2	2505	C	N3-C2-O2	-5.17	118.28	121.90
2	2	4201	G	C4-N9-C1'	5.17	133.22	126.50
2	2	4613	C	N1-C2-O2	5.17	122.00	118.90
2	2	3855	C	C5-C6-N1	5.16	123.58	121.00
2	2	1674	C	C5-C6-N1	5.16	123.58	121.00
2	2	308	G	O4'-C1'-N9	5.16	112.33	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	1726	U	N1-C2-O2	5.16	126.41	122.80
2	2	4928	C	N3-C2-O2	-5.16	118.29	121.90
2	2	4341	C	N1-C2-O2	5.16	122.00	118.90
2	2	1079	C	C6-N1-C1'	-5.16	114.61	120.80
2	2	910	G	N3-C4-C5	-5.15	126.02	128.60
2	2	1809	C	C5-C6-N1	5.15	123.58	121.00
2	2	4302	U	N3-C2-O2	-5.15	118.59	122.20
2	2	4964	C	C5-C6-N1	5.15	123.58	121.00
2	2	2544	G	N3-C4-N9	5.15	129.09	126.00
2	2	4926	C	C6-N1-C2	-5.15	118.24	120.30
4	5	78	C	N1-C2-O2	5.15	121.99	118.90
2	2	257	C	N3-C2-O2	-5.14	118.30	121.90
2	2	4627	U	N3-C2-O2	-5.14	118.60	122.20
7	8	111	U	N1-C2-O2	5.14	126.40	122.80
2	2	1183	C	N3-C2-O2	-5.14	118.30	121.90
2	2	2544	G	N3-C4-C5	-5.14	126.03	128.60
7	8	4	C	C5-C6-N1	5.14	123.57	121.00
38	h	119	LEU	CA-CB-CG	5.12	127.08	115.30
2	2	1707	C	C6-N1-C1'	5.12	126.95	120.80
2	2	4764	A	C6-N1-C2	5.12	121.67	118.60
2	2	2501	C	C6-N1-C2	-5.12	118.25	120.30
2	2	67	C	C5-C6-N1	5.12	123.56	121.00
2	2	2501	C	N1-C2-O2	5.11	121.97	118.90
2	2	3636	C	C5-C6-N1	5.11	123.56	121.00
2	2	3840	U	N3-C2-O2	-5.11	118.62	122.20
2	2	4137	C	C2-N1-C1'	5.11	124.42	118.80
2	2	696	C	C6-N1-C2	-5.10	118.26	120.30
2	2	4945	G	C5-C6-N1	5.10	114.05	111.50
2	2	2615	C	N3-C2-O2	-5.09	118.33	121.90
2	2	28	C	C5-C6-N1	5.09	123.55	121.00
2	2	274	C	C6-N1-C2	-5.09	118.26	120.30
2	2	3926	C	N1-C2-O2	5.09	121.95	118.90
2	2	1096	C	C6-N1-C2	-5.09	118.27	120.30
2	2	2497	C	C2-N1-C1'	5.09	124.40	118.80
2	2	4341	C	N3-C2-O2	-5.08	118.34	121.90
2	2	4569	U	N3-C2-O2	-5.08	118.64	122.20
2	2	465	G	C4-N9-C1'	5.08	133.10	126.50
2	2	2304	U	N1-C2-O2	5.08	126.36	122.80
2	2	2670	C	C5-C6-N1	5.08	123.54	121.00
2	2	4612	C	C5-C6-N1	5.08	123.54	121.00
2	2	4766	C	C5-C6-N1	5.08	123.54	121.00
2	2	1340	C	C6-N1-C2	-5.08	118.27	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	2107	C	C2-N1-C1'	5.07	124.38	118.80
2	2	4766	C	C6-N1-C2	-5.07	118.27	120.30
2	2	5008	C	C6-N1-C2	-5.07	118.27	120.30
2	2	4895	C	O4'-C1'-N1	5.07	112.25	108.20
2	2	1696	C	C6-N1-C2	-5.07	118.27	120.30
2	2	4286	C	C6-N1-C2	-5.07	118.27	120.30
2	2	1477	C	C5-C6-N1	5.07	123.53	121.00
2	2	2020	U	N1-C2-O2	5.07	126.34	122.80
2	2	3598	C	C6-N1-C2	-5.07	118.27	120.30
2	2	4695	C	N3-C2-O2	-5.07	118.35	121.90
2	2	1507	C	C6-N1-C2	-5.06	118.28	120.30
2	2	3617	G	C8-N9-C1'	5.06	133.58	127.00
2	2	3680	U	N1-C2-O2	5.06	126.34	122.80
4	5	43	U	N3-C2-O2	-5.06	118.66	122.20
2	2	257	C	N1-C2-O2	5.06	121.94	118.90
2	2	1378	C	C6-N1-C1'	-5.06	114.73	120.80
2	2	4201	G	N3-C4-C5	-5.06	126.07	128.60
2	2	1310	C	C5-C6-N1	5.06	123.53	121.00
2	2	1405	C	C5-C6-N1	5.06	123.53	121.00
2	2	4970	C	C6-N1-C2	-5.06	118.28	120.30
2	2	220	C	N3-C2-O2	-5.05	118.36	121.90
2	2	1707	C	C6-N1-C2	-5.05	118.28	120.30
2	2	2418	A	N7-C8-N9	5.05	116.33	113.80
2	2	2615	C	N1-C2-O2	5.05	121.93	118.90
2	2	28	C	C6-N1-C2	-5.05	118.28	120.30
2	2	4137	C	N1-C2-O2	5.05	121.93	118.90
7	8	81	C	C6-N1-C2	-5.04	118.28	120.30
2	2	3926	C	C5-C6-N1	5.04	123.52	121.00
2	2	4103	C	N1-C2-O2	5.04	121.92	118.90
2	2	467	U	C5-C6-N1	5.04	125.22	122.70
2	2	1386	C	C5-C6-N1	5.03	123.52	121.00
2	2	1476	C	N1-C2-O2	-5.03	115.88	118.90
2	2	4940	C	C5-C6-N1	5.03	123.52	121.00
28	W	81	ARG	NE-CZ-NH1	5.03	122.82	120.30
2	2	2712	G	C8-N9-C1'	-5.03	120.47	127.00
7	8	140	C	C6-N1-C2	-5.03	118.29	120.30
7	8	99	U	N1-C2-O2	5.03	126.32	122.80
39	i	35	ASP	CB-CG-OD1	5.03	122.82	118.30
2	2	4120	U	N3-C2-O2	-5.02	118.68	122.20
2	2	274	C	C5-C6-N1	5.02	123.51	121.00
2	2	2867	C	C2-N1-C1'	5.02	124.32	118.80
2	2	4614	G	C5-C6-O6	5.02	131.61	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	Q	96	ILE	CG1-CB-CG2	-5.02	100.36	111.40
2	2	4466	C	C6-N1-C2	-5.02	118.29	120.30
2	2	4260	U	C2-N1-C1'	5.01	123.72	117.70
2	2	1577	G	N1-C2-N2	5.01	120.71	116.20
2	2	3734	U	N3-C2-O2	-5.01	118.69	122.20

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	4	198	TYR	Peptide
3	4	365	PRO	Peptide
3	4	40	ILE	Peptide
3	4	503	THR	Peptide
9	B	16	PHE	Peptide
9	B	296	GLY	Peptide
23	Q	154	VAL	Peptide
24	R	163	ALA	Peptide
43	m	54	ARG	Peptide
44	n	106	TYR	Peptide
45	o	98	GLY	Peptide

## 5.2 Too-close contacts [i](#)

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

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	17/731 (2%)	17 (100%)	0	0	100	100
3	4	616/634 (97%)	535 (87%)	78 (13%)	3 (0%)	25	58

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	6	242/245 (99%)	224 (93%)	18 (7%)	0	100	100
6	7	133/163 (82%)	124 (93%)	7 (5%)	2 (2%)	8	35
8	9	82/134 (61%)	71 (87%)	10 (12%)	1 (1%)	11	40
9	B	401/403 (100%)	368 (92%)	33 (8%)	0	100	100
10	C	89/159 (56%)	85 (96%)	4 (4%)	0	100	100
11	D	356/427 (83%)	330 (93%)	26 (7%)	0	100	100
12	E	96/115 (84%)	89 (93%)	7 (7%)	0	100	100
13	F	107/117 (92%)	105 (98%)	2 (2%)	0	100	100
14	G	240/266 (90%)	221 (92%)	19 (8%)	0	100	100
15	H	120/123 (98%)	113 (94%)	7 (6%)	0	100	100
16	I	188/192 (98%)	167 (89%)	21 (11%)	0	100	100
17	K	100/105 (95%)	95 (95%)	5 (5%)	0	100	100
18	L	145/148 (98%)	134 (92%)	10 (7%)	1 (1%)	19	51
19	M	84/97 (87%)	80 (95%)	4 (5%)	0	100	100
20	N	163/178 (92%)	144 (88%)	19 (12%)	0	100	100
21	O	67/70 (96%)	64 (96%)	3 (4%)	0	100	100
22	P	48/51 (94%)	46 (96%)	2 (4%)	0	100	100
23	Q	208/211 (99%)	190 (91%)	18 (9%)	0	100	100
24	R	148/203 (73%)	137 (93%)	11 (7%)	0	100	100
25	S	133/215 (62%)	122 (92%)	11 (8%)	0	100	100
26	U	201/204 (98%)	189 (94%)	11 (6%)	1 (0%)	25	58
27	V	199/203 (98%)	193 (97%)	6 (3%)	0	100	100
28	W	99/106 (93%)	89 (90%)	10 (10%)	0	100	100
29	X	89/92 (97%)	83 (93%)	6 (7%)	0	100	100
30	Y	151/184 (82%)	140 (93%)	11 (7%)	0	100	100
31	Z	185/188 (98%)	176 (95%)	9 (5%)	0	100	100
32	a	146/196 (74%)	138 (94%)	8 (6%)	0	100	100
33	b	174/176 (99%)	166 (95%)	8 (5%)	0	100	100
34	c	153/160 (96%)	144 (94%)	9 (6%)	0	100	100
35	d	99/128 (77%)	88 (89%)	11 (11%)	0	100	100
36	e	129/140 (92%)	118 (92%)	11 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
37	g	116/156 (74%)	109 (94%)	7 (6%)	0	100	100
38	h	132/145 (91%)	130 (98%)	2 (2%)	0	100	100
39	i	133/136 (98%)	122 (92%)	11 (8%)	0	100	100
40	j	105/125 (84%)	97 (92%)	8 (8%)	0	100	100
41	k	126/135 (93%)	115 (91%)	11 (9%)	0	100	100
42	l	123/137 (90%)	111 (90%)	12 (10%)	0	100	100
43	m	246/257 (96%)	216 (88%)	29 (12%)	1 (0%)	30	62
44	n	107/110 (97%)	97 (91%)	8 (8%)	2 (2%)	6	31
45	o	231/288 (80%)	210 (91%)	21 (9%)	0	100	100
46	p	224/248 (90%)	210 (94%)	14 (6%)	0	100	100
47	r	291/297 (98%)	269 (92%)	22 (8%)	0	100	100
48	z	32/129 (25%)	30 (94%)	2 (6%)	0	100	100
All	All	7274/8927 (82%)	6701 (92%)	562 (8%)	11 (0%)	45	73

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	7	66	ASP
6	7	70	GLU
44	n	106	TYR
3	4	301	GLU
8	9	99	GLN
3	4	407	ASP
18	L	22	ILE
43	m	55	GLY
3	4	435	GLY
26	U	83	LYS
44	n	107	PRO

### 5.3.2 Protein sidechains ⓘ

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

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



Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	17/654 (3%)	17 (100%)	0	100	100
3	4	562/574 (98%)	554 (99%)	8 (1%)	62	80
5	6	212/213 (100%)	212 (100%)	0	100	100
6	7	126/149 (85%)	122 (97%)	4 (3%)	34	62
8	9	74/114 (65%)	72 (97%)	2 (3%)	40	66
9	B	349/349 (100%)	346 (99%)	3 (1%)	75	87
10	C	78/126 (62%)	77 (99%)	1 (1%)	65	81
11	D	298/348 (86%)	297 (100%)	1 (0%)	91	95
12	E	83/97 (86%)	83 (100%)	0	100	100
13	F	94/100 (94%)	94 (100%)	0	100	100
14	G	204/223 (92%)	204 (100%)	0	100	100
15	H	109/110 (99%)	108 (99%)	1 (1%)	75	87
16	I	169/171 (99%)	168 (99%)	1 (1%)	84	91
17	K	86/89 (97%)	84 (98%)	2 (2%)	45	69
18	L	120/121 (99%)	120 (100%)	0	100	100
19	M	73/80 (91%)	73 (100%)	0	100	100
20	N	138/149 (93%)	137 (99%)	1 (1%)	81	90
21	O	64/65 (98%)	64 (100%)	0	100	100
22	P	47/48 (98%)	46 (98%)	1 (2%)	48	72
23	Q	176/177 (99%)	174 (99%)	2 (1%)	70	84
24	R	138/184 (75%)	138 (100%)	0	100	100
25	S	115/161 (71%)	113 (98%)	2 (2%)	56	76
26	U	171/172 (99%)	171 (100%)	0	100	100
27	V	173/174 (99%)	173 (100%)	0	100	100
28	W	89/94 (95%)	89 (100%)	0	100	100
29	X	74/75 (99%)	71 (96%)	3 (4%)	26	56
30	Y	134/163 (82%)	134 (100%)	0	100	100
31	Z	164/165 (99%)	164 (100%)	0	100	100
32	a	133/175 (76%)	133 (100%)	0	100	100
33	b	157/157 (100%)	157 (100%)	0	100	100
34	c	136/140 (97%)	134 (98%)	2 (2%)	60	78
35	d	91/115 (79%)	90 (99%)	1 (1%)	70	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	e	101/107 (94%)	100 (99%)	1 (1%)	73	85
37	g	106/133 (80%)	106 (100%)	0	100	100
38	h	124/135 (92%)	122 (98%)	2 (2%)	58	77
39	i	117/118 (99%)	115 (98%)	2 (2%)	56	76
40	j	98/110 (89%)	97 (99%)	1 (1%)	73	85
41	k	114/121 (94%)	114 (100%)	0	100	100
42	l	109/121 (90%)	109 (100%)	0	100	100
43	m	190/199 (96%)	189 (100%)	1 (0%)	86	92
44	n	88/89 (99%)	88 (100%)	0	100	100
45	o	208/252 (82%)	208 (100%)	0	100	100
46	p	195/215 (91%)	195 (100%)	0	100	100
47	r	246/250 (98%)	244 (99%)	2 (1%)	79	88
48	z	30/115 (26%)	30 (100%)	0	100	100
All	All	6380/7697 (83%)	6336 (99%)	44 (1%)	80	90

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	4	279	PHE
3	4	367	ARG
3	4	373	ARG
3	4	385	ARG
3	4	405	MET
3	4	410	ILE
3	4	519	VAL
3	4	555	ARG
6	7	62	GLU
6	7	63	LEU
6	7	65	VAL
6	7	70	GLU
8	9	7	THR
8	9	55	LEU
9	B	278	THR
9	B	297	LYS
9	B	399	LYS
10	C	117	ARG
11	D	122	TYR

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Mol	Chain	Res	Type
15	H	104	THR
16	I	176	LEU
17	K	29	ARG
17	K	86	LYS
20	N	102	THR
22	P	21	ARG
23	Q	63	THR
23	Q	70	VAL
25	S	17	PHE
25	S	38	VAL
29	X	59	SER
29	X	63	THR
29	X	84	ARG
34	c	32	ARG
34	c	124	THR
35	d	110	TYR
36	e	48	ARG
38	h	8	THR
38	h	84	ARG
39	i	52	LYS
39	i	108	ARG
40	j	104	THR
43	m	30	ARG
47	r	86	TYR
47	r	248	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (82) such sidechains are listed below:

Mol	Chain	Res	Type
3	4	27	GLN
3	4	98	GLN
3	4	108	ASN
3	4	144	GLN
3	4	157	HIS
3	4	218	GLN
3	4	437	ASN
3	4	601	ASN
5	6	21	ASN
5	6	83	HIS
5	6	162	HIS
5	6	170	GLN
6	7	24	ASN

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Mol	Chain	Res	Type
6	7	87	ASN
6	7	104	GLN
6	7	115	ASN
9	B	109	HIS
9	B	184	GLN
9	B	213	GLN
10	C	58	GLN
10	C	61	ASN
11	D	38	ASN
11	D	50	GLN
11	D	178	ASN
11	D	346	ASN
12	E	19	GLN
12	E	50	ASN
12	E	72	HIS
14	G	43	GLN
14	G	225	ASN
16	I	156	ASN
17	K	92	ASN
18	L	66	ASN
18	L	89	ASN
19	M	30	GLN
19	M	66	HIS
20	N	46	GLN
21	O	28	ASN
23	Q	104	ASN
23	Q	175	ASN
24	R	91	GLN
24	R	102	GLN
26	U	196	ASN
27	V	42	ASN
27	V	167	HIS
27	V	180	GLN
28	W	45	GLN
28	W	51	GLN
30	Y	21	ASN
30	Y	34	GLN
30	Y	56	GLN
30	Y	80	GLN
30	Y	97	ASN
30	Y	118	GLN
30	Y	137	ASN

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Mol	Chain	Res	Type
31	Z	44	ASN
31	Z	188	ASN
32	a	34	ASN
32	a	40	GLN
33	b	66	GLN
33	b	77	ASN
34	c	144	ASN
35	d	17	GLN
35	d	116	GLN
36	e	101	ASN
37	g	108	GLN
37	g	111	GLN
38	h	86	GLN
38	h	96	HIS
40	j	69	ASN
40	j	79	ASN
41	k	52	GLN
41	k	107	ASN
41	k	117	GLN
42	l	4	HIS
42	l	6	GLN
42	l	100	ASN
43	m	216	HIS
44	n	80	ASN
45	o	190	HIS
46	p	39	GLN
47	r	195	HIS

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	2	3428/5070 (67%)	890 (25%)	18 (0%)
4	5	119/120 (99%)	20 (16%)	0
7	8	155/156 (99%)	32 (20%)	0
All	All	3702/5346 (69%)	942 (25%)	18 (0%)

All (942) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	2	2	G
2	2	15	A

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Mol	Chain	Res	Type
2	2	17	A
2	2	21	G
2	2	25	A
2	2	28	C
2	2	39	A
2	2	42	A
2	2	48	G
2	2	56	A
2	2	59	A
2	2	64	A
2	2	65	A
2	2	66	A
2	2	69	A
2	2	73	A
2	2	84	A
2	2	91	G
2	2	96	U
2	2	98	A
2	2	104	G
2	2	108	A
2	2	109	G
2	2	110	C
2	2	116	G
2	2	119	G
2	2	120	A
2	2	122	U
2	2	127	G
2	2	128	C
2	2	130	C
2	2	131	C
2	2	133	C
2	2	134	G
2	2	135	G
2	2	136	C
2	2	137	G
2	2	141	C
2	2	143	C
2	2	144	G
2	2	151	G
2	2	152	U
2	2	159	C
2	2	172	C

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Mol	Chain	Res	Type
2	2	176	G
2	2	177	G
2	2	178	C
2	2	182	G
2	2	183	C
2	2	184	U
2	2	185	C
2	2	187	U
2	2	188	G
2	2	197	A
2	2	200	U
2	2	207	G
2	2	209	U
2	2	213	G
2	2	218	A
2	2	219	G
2	2	220	C
2	2	226	G
2	2	233	U
2	2	234	G
2	2	254	G
2	2	255	C
2	2	256	G
2	2	257	C
2	2	259	C
2	2	260	C
2	2	262	G
2	2	264	C
2	2	265	C
2	2	266	C
2	2	267	G
2	2	278	G
2	2	279	A
2	2	280	G
2	2	297	U
2	2	306	A
2	2	315	G
2	2	316	U
2	2	326	C
2	2	340	C
2	2	341	G
2	2	349	A

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Mol	Chain	Res	Type
2	2	379	G
2	2	387	G
2	2	398	A2M
2	2	399	G
2	2	406	C
2	2	407	A
2	2	408	A
2	2	409	G
2	2	410	A
2	2	411	G
2	2	412	G
2	2	433	A
2	2	440	U
2	2	449	C
2	2	450	G
2	2	452	A
2	2	453	G
2	2	454	U
2	2	456	C
2	2	457	G
2	2	465	G
2	2	466	A
2	2	467	U
2	2	479	G
2	2	483	G
2	2	484	U
2	2	485	C
2	2	486	C
2	2	489	C
2	2	491	G
2	2	493	G
2	2	494	U
2	2	496	G
2	2	497	G
2	2	498	C
2	2	499	G
2	2	500	G
2	2	501	C
2	2	502	C
2	2	503	C
2	2	504	G
2	2	505	G

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Mol	Chain	Res	Type
2	2	507	G
2	2	509	A
2	2	510	U
2	2	511	C
2	2	512	U
2	2	513	U
2	2	514	U
2	2	516	C
2	2	517	C
2	2	518	G
2	2	519	C
2	2	647	G
2	2	648	G
2	2	656	C
2	2	657	C
2	2	658	C
2	2	667	A
2	2	668	C
2	2	673	C
2	2	686	A
2	2	687	U
2	2	692	A
2	2	694	C
2	2	696	C
2	2	703	G
2	2	704	C
2	2	730	G
2	2	731	G
2	2	738	C
2	2	739	G
2	2	740	G
2	2	742	G
2	2	752	G
2	2	753	C
2	2	756	G
2	2	758	G
2	2	759	G
2	2	904	C
2	2	905	C
2	2	910	G
2	2	913	U
2	2	914	U

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Mol	Chain	Res	Type
2	2	915	A
2	2	916	C
2	2	917	A
2	2	923	C
2	2	924	C
2	2	925	C
2	2	926	G
2	2	929	A
2	2	932	A
2	2	933	G
2	2	935	A
2	2	936	C
2	2	941	C
2	2	943	A
2	2	944	A
2	2	945	U
2	2	956	A
2	2	959	G
2	2	960	A
2	2	961	G
2	2	962	C
2	2	965	G
2	2	966	A
2	2	967	C
2	2	969	C
2	2	970	G
2	2	972	C
2	2	982	U
2	2	983	C
2	2	985	C
2	2	988	C
2	2	992	C
2	2	993	G
2	2	994	G
2	2	995	C
2	2	1048	G
2	2	1049	C
2	2	1051	G
2	2	1065	G
2	2	1070	G
2	2	1072	C
2	2	1082	C

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Mol	Chain	Res	Type
2	2	1083	U
2	2	1095	A
2	2	1100	U
2	2	1168	G
2	2	1171	G
2	2	1173	G
2	2	1176	C
2	2	1178	G
2	2	1179	U
2	2	1180	C
2	2	1181	C
2	2	1182	C
2	2	1183	C
2	2	1187	G
2	2	1193	C
2	2	1194	G
2	2	1196	G
2	2	1197	C
2	2	1198	G
2	2	1199	G
2	2	1200	G
2	2	1201	U
2	2	1202	C
2	2	1203	G
2	2	1210	C
2	2	1211	G
2	2	1215	C
2	2	1216	C
2	2	1219	G
2	2	1220	G
2	2	1221	G
2	2	1222	A
2	2	1240	G
2	2	1241	C
2	2	1245	C
2	2	1253	G
2	2	1254	A
2	2	1255	A
2	2	1260	G
2	2	1265	G
2	2	1266	G
2	2	1269	G

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Mol	Chain	Res	Type
2	2	1270	A
2	2	1271	G
2	2	1272	C
2	2	1274	A
2	2	1275	G
2	2	1280	C
2	2	1283	G
2	2	1284	G
2	2	1285	U
2	2	1287	G
2	2	1294	A
2	2	1296	G
2	2	1301	C
2	2	1302	U
2	2	1303	A
2	2	1314	C
2	2	1324	A
2	2	1326	A2M
2	2	1354	A
2	2	1358	G
2	2	1359	G
2	2	1365	C
2	2	1366	G
2	2	1367	C
2	2	1377	G
2	2	1378	C
2	2	1379	C
2	2	1387	A
2	2	1394	G
2	2	1397	A
2	2	1398	A
2	2	1402	C
2	2	1403	G
2	2	1404	G
2	2	1405	C
2	2	1407	C
2	2	1409	C
2	2	1410	U
2	2	1411	C
2	2	1412	G
2	2	1414	C
2	2	1419	G

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Mol	Chain	Res	Type
2	2	1420	A
2	2	1433	A
2	2	1435	G
2	2	1438	U
2	2	1439	C
2	2	1442	C
2	2	1443	A
2	2	1444	G
2	2	1446	C
2	2	1453	G
2	2	1482	G
2	2	1483	C
2	2	1497	A
2	2	1498	G
2	2	1502	G
2	2	1503	A
2	2	1518	A
2	2	1519	C
2	2	1534	A2M
2	2	1547	A
2	2	1559	G
2	2	1564	A
2	2	1576	G
2	2	1578	U
2	2	1582	PSU
2	2	1596	U
2	2	1597	G
2	2	1613	A
2	2	1624	G
2	2	1625	OMG
2	2	1626	G
2	2	1631	A
2	2	1632	A
2	2	1633	G
2	2	1638	A
2	2	1641	G
2	2	1642	A
2	2	1649	U
2	2	1654	G
2	2	1661	C
2	2	1671	U
2	2	1676	C

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Mol	Chain	Res	Type
2	2	1677	PSU
2	2	1691	G
2	2	1694	C
2	2	1697	G
2	2	1699	A
2	2	1700	G
2	2	1701	A
2	2	1703	C
2	2	1704	C
2	2	1705	G
2	2	1707	C
2	2	1715	C
2	2	1718	C
2	2	1719	A
2	2	1734	G
2	2	1789	C
2	2	1790	U
2	2	1801	A
2	2	1803	G
2	2	1804	A
2	2	1806	G
2	2	1810	G
2	2	1815	G
2	2	1821	G
2	2	1822	U
2	2	1832	C
2	2	1834	U
2	2	1836	G
2	2	1837	A
2	2	1842	G
2	2	1843	A
2	2	1854	G
2	2	1855	G
2	2	1856	C
2	2	1859	C
2	2	1866	UR3
2	2	1867	A
2	2	1868	A
2	2	1871	A2M
2	2	1881	C
2	2	1882	U
2	2	1883	OMG

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Mol	Chain	Res	Type
2	2	1886	G
2	2	1893	C
2	2	1897	A
2	2	1918	U
2	2	1919	G
2	2	1920	C
2	2	1921	C
2	2	1922	G
2	2	1925	G
2	2	1931	C
2	2	1932	A
2	2	1935	C
2	2	1938	C
2	2	1940	G
2	2	1945	G
2	2	1948	G
2	2	1949	U
2	2	1960	A
2	2	1961	G
2	2	1965	G
2	2	1967	A
2	2	1968	G
2	2	1970	A
2	2	2018	C
2	2	2022	C
2	2	2024	G
2	2	2025	A
2	2	2026	A
2	2	2033	A
2	2	2034	G
2	2	2039	G
2	2	2040	A
2	2	2044	U
2	2	2046	G
2	2	2048	U
2	2	2055	G
2	2	2056	G
2	2	2062	C
2	2	2064	G
2	2	2069	A
2	2	2070	U
2	2	2071	A

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Mol	Chain	Res	Type
2	2	2084	C
2	2	2091	C
2	2	2092	G
2	2	2093	A
2	2	2095	A
2	2	2096	G
2	2	2098	G
2	2	2100	A
2	2	2101	C
2	2	2102	G
2	2	2104	G
2	2	2105	A
2	2	2106	G
2	2	2107	C
2	2	2110	C
2	2	2111	G
2	2	2112	G
2	2	2113	C
2	2	2250	C
2	2	2253	A
2	2	2255	C
2	2	2256	C
2	2	2257	C
2	2	2258	C
2	2	2259	G
2	2	2260	C
2	2	2261	G
2	2	2266	C
2	2	2289	C
2	2	2300	A
2	2	2301	G
2	2	2306	G
2	2	2310	C
2	2	2313	A
2	2	2314	G
2	2	2316	G
2	2	2332	A
2	2	2333	G
2	2	2348	G
2	2	2351	C
2	2	2357	G
2	2	2395	A

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Mol	Chain	Res	Type
2	2	2409	U
2	2	2416	G
2	2	2417	A
2	2	2418	A
2	2	2419	C
2	2	2422	OMC
2	2	2424	OMG
2	2	2425	U
2	2	2432	U
2	2	2437	C
2	2	2441	C
2	2	2447	U
2	2	2450	G
2	2	2453	A
2	2	2460	A
2	2	2464	C
2	2	2465	C
2	2	2471	G
2	2	2475	G
2	2	2480	G
2	2	2483	G
2	2	2485	U
2	2	2488	C
2	2	2489	C
2	2	2490	U
2	2	2491	C
2	2	2493	G
2	2	2496	G
2	2	2503	G
2	2	2504	C
2	2	2505	C
2	2	2512	A
2	2	2513	A
2	2	2519	U
2	2	2520	C
2	2	2529	A
2	2	2543	A
2	2	2544	G
2	2	2545	U
2	2	2546	G
2	2	2547	G
2	2	2553	A

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Mol	Chain	Res	Type
2	2	2554	U
2	2	2555	G
2	2	2558	C
2	2	2559	G
2	2	2560	C
2	2	2561	C
2	2	2563	C
2	2	2564	G
2	2	2565	A
2	2	2566	G
2	2	2573	A
2	2	2583	C
2	2	2586	G
2	2	2587	A
2	2	2589	C
2	2	2601	A
2	2	2618	G
2	2	2627	C
2	2	2651	C
2	2	2653	C
2	2	2659	A
2	2	2661	U
2	2	2662	G
2	2	2663	G
2	2	2669	C
2	2	2670	C
2	2	2675	G
2	2	2687	U
2	2	2688	G
2	2	2689	C
2	2	2694	G
2	2	2695	A
2	2	2696	A
2	2	2707	U
2	2	2708	U
2	2	2709	C
2	2	2710	C
2	2	2711	G
2	2	2719	C
2	2	2721	G
2	2	2724	G
2	2	2726	G

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Mol	Chain	Res	Type
2	2	2732	G
2	2	2739	C
2	2	2742	G
2	2	2743	A
2	2	2752	G
2	2	2756	G
2	2	2761	U
2	2	2763	U
2	2	2769	U
2	2	2770	C
2	2	2788	U
2	2	2789	A
2	2	2790	U
2	2	2814	C
2	2	2815	A
2	2	2826	U
2	2	2827	G
2	2	2829	U
2	2	2842	G
2	2	2853	C
2	2	2855	G
2	2	2856	C
2	2	2862	G
2	2	2877	G
2	2	2892	C
2	2	2897	G
2	2	2901	G
2	2	2903	G
2	2	2904	U
2	2	2905	C
2	2	2906	G
2	2	2907	G
2	2	2908	U
2	2	2909	C
2	2	3585	G
2	2	3587	C
2	2	3588	C
2	2	3590	G
2	2	3591	C
2	2	3593	C
2	2	3594	C
2	2	3595	U

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Mol	Chain	Res	Type
2	2	3596	A
2	2	3597	G
2	2	3598	C
2	2	3599	A
2	2	3603	G
2	2	3604	A
2	2	3605	C
2	2	3606	U
2	2	3615	G
2	2	3619	G
2	2	3626	G
2	2	3635	A
2	2	3644	U
2	2	3646	A
2	2	3662	A
2	2	3663	A
2	2	3664	G
2	2	3670	C
2	2	3673	C
2	2	3674	G
2	2	3680	U
2	2	3691	G
2	2	3696	C
2	2	3710	G
2	2	3711	A
2	2	3713	U
2	2	3714	G
2	2	3728	A
2	2	3734	U
2	2	3735	G
2	2	3736	A
2	2	3748	A
2	2	3750	G
2	2	3775	A
2	2	3776	G
2	2	3823	G
2	2	3838	U
2	2	3839	G
2	2	3840	U
2	2	3843	C
2	2	3865	A
2	2	3867	A2M

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Mol	Chain	Res	Type
2	2	3877	A
2	2	3878	C
2	2	3879	G
2	2	3881	G
2	2	3898	G
2	2	3903	A
2	2	3904	G
2	2	3905	A
2	2	3906	A
2	2	3915	U
2	2	3916	G
2	2	3923	A
2	2	3938	G
2	2	3939	G
2	2	4076	G
2	2	4084	G
2	2	4095	G
2	2	4097	G
2	2	4099	G
2	2	4100	C
2	2	4101	C
2	2	4102	C
2	2	4103	C
2	2	4104	G
2	2	4111	U
2	2	4112	C
2	2	4114	C
2	2	4115	G
2	2	4116	C
2	2	4117	U
2	2	4119	C
2	2	4120	U
2	2	4121	G
2	2	4122	G
2	2	4131	G
2	2	4137	C
2	2	4139	G
2	2	4140	C
2	2	4141	G
2	2	4142	C
2	2	4143	G
2	2	4144	C

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Mol	Chain	Res	Type
2	2	4162	C
2	2	4163	U
2	2	4170	A
2	2	4177	C
2	2	4183	G
2	2	4184	G
2	2	4191	G
2	2	4195	G
2	2	4196	OMG
2	2	4201	G
2	2	4202	U
2	2	4203	A
2	2	4212	A
2	2	4222	G
2	2	4225	G
2	2	4229	U
2	2	4230	C
2	2	4233	A
2	2	4243	C
2	2	4249	G
2	2	4250	G
2	2	4251	A
2	2	4254	G
2	2	4256	A
2	2	4265	U
2	2	4267	G
2	2	4268	A
2	2	4271	A
2	2	4273	A
2	2	4280	A
2	2	4281	A
2	2	4282	A
2	2	4291	G
2	2	4293	PSU
2	2	4303	C
2	2	4305	G
2	2	4313	A
2	2	4314	C
2	2	4316	G
2	2	4319	C
2	2	4329	G
2	2	4330	G

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Mol	Chain	Res	Type
2	2	4332	C
2	2	4336	A
2	2	4349	C
2	2	4350	C
2	2	4354	U
2	2	4364	G
2	2	4372	U
2	2	4373	G
2	2	4377	G
2	2	4378	A
2	2	4379	A
2	2	4380	A
2	2	4381	A
2	2	4387	C
2	2	4395	U
2	2	4396	A
2	2	4405	G
2	2	4413	C
2	2	4414	A
2	2	4415	1MA
2	2	4418	G
2	2	4422	A
2	2	4428	A
2	2	4429	C
2	2	4449	A
2	2	4451	G
2	2	4452	U
2	2	4453	C
2	2	4464	A
2	2	4466	C
2	2	4475	G
2	2	4476	C
2	2	4477	A
2	2	4484	A
2	2	4491	G
2	2	4498	U
2	2	4499	G
2	2	4510	A
2	2	4512	U
2	2	4513	A
2	2	4518	A
2	2	4519	C

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Mol	Chain	Res	Type
2	2	4523	A2M
2	2	4524	G
2	2	4530	UR3
2	2	4531	U
2	2	4545	G
2	2	4548	A
2	2	4549	G
2	2	4555	U
2	2	4556	U
2	2	4557	U
2	2	4558	U
2	2	4560	C
2	2	4567	G
2	2	4574	U
2	2	4575	G
2	2	4589	A
2	2	4590	A
2	2	4594	U
2	2	4600	G
2	2	4601	U
2	2	4606	G
2	2	4607	A
2	2	4608	G
2	2	4629	U
2	2	4636	PSU
2	2	4637	OMG
2	2	4652	G
2	2	4656	A
2	2	4670	C
2	2	4672	A
2	2	4678	G
2	2	4679	G
2	2	4682	U
2	2	4684	A
2	2	4687	A
2	2	4691	A
2	2	4694	G
2	2	4695	C
2	2	4702	G
2	2	4703	U
2	2	4708	A
2	2	4709	U

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Mol	Chain	Res	Type
2	2	4719	G
2	2	4720	C
2	2	4721	G
2	2	4722	G
2	2	4728	U
2	2	4729	A
2	2	4730	C
2	2	4733	C
2	2	4734	A
2	2	4735	G
2	2	4740	G
2	2	4741	C
2	2	4742	G
2	2	4745	G
2	2	4750	G
2	2	4754	G
2	2	4757	C
2	2	4759	C
2	2	4761	G
2	2	4765	G
2	2	4770	U
2	2	4771	C
2	2	4775	C
2	2	4776	G
2	2	4859	C
2	2	4864	U
2	2	4870	OMG
2	2	4871	C
2	2	4872	2MG
2	2	4875	G
2	2	4877	G
2	2	4882	U
2	2	4883	C
2	2	4889	G
2	2	4895	C
2	2	4896	G
2	2	4899	G
2	2	4900	C
2	2	4901	G
2	2	4909	A
2	2	4910	G
2	2	4911	A

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Mol	Chain	Res	Type
2	2	4912	G
2	2	4914	C
2	2	4915	G
2	2	4916	G
2	2	4923	C
2	2	4924	C
2	2	4927	G
2	2	4928	C
2	2	4931	G
2	2	4934	A
2	2	4937	C
2	2	4938	A
2	2	4941	G
2	2	4943	A
2	2	4944	C
2	2	4949	G
2	2	4950	U
2	2	4955	A
2	2	4958	C
2	2	4960	G
2	2	4966	A
2	2	4975	G
2	2	4976	U
2	2	4979	A
2	2	4989	U
2	2	4990	C
2	2	4991	U
2	2	5014	A
2	2	5021	C
2	2	5022	U
2	2	5025	C
2	2	5026	U
2	2	5027	C
2	2	5028	G
2	2	5030	U
2	2	5031	G
2	2	5034	A
2	2	5040	U
2	2	5041	G
2	2	5048	A
2	2	5050	C
2	2	5053	U

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Mol	Chain	Res	Type
2	2	5054	C
2	2	5058	A
2	2	5060	A
2	2	5061	A
2	2	5062	G
2	2	5069	U
4	5	4	U
4	5	7	G
4	5	11	A
4	5	22	A
4	5	23	A
4	5	37	G
4	5	38	U
4	5	40	U
4	5	48	G
4	5	50	A
4	5	53	U
4	5	54	A
4	5	63	C
4	5	64	G
4	5	70	G
4	5	71	G
4	5	78	C
4	5	100	A
4	5	110	G
4	5	111	C
7	8	2	G
7	8	25	G
7	8	34	U
7	8	35	C
7	8	39	G
7	8	48	A
7	8	49	G
7	8	59	A
7	8	60	G
7	8	62	A
7	8	63	U
7	8	68	G
7	8	75	G
7	8	80	A
7	8	82	A
7	8	84	A

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Mol	Chain	Res	Type
7	8	85	U
7	8	87	G
7	8	103	A
7	8	105	C
7	8	110	U
7	8	111	U
7	8	114	G
7	8	123	U
7	8	124	U
7	8	125	C
7	8	126	C
7	8	127	U
7	8	129	C
7	8	150	C
7	8	153	C
7	8	156	U

All (18) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	2	406	C
2	2	914	U
2	2	955	G
2	2	1071	C
2	2	1613	A
2	2	1625	OMG
2	2	2033	A
2	2	2760	G
2	2	3596	A
2	2	3673	C
2	2	3905	A
2	2	4378	A
2	2	4395	U
2	2	4498	U
2	2	4529	B8W
2	2	4555	U
2	2	4694	G
2	2	4913	G

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

92 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$
2	B8W	2	4529	2	18,26,27	6.22	7 (38%)	21,38,41	2.59	6 (28%)
2	OMC	2	2422	2,49,30	19,22,23	2.89	8 (42%)	26,31,34	1.06	2 (7%)
2	B8H	2	4296	2	19,22,23	6.78	7 (36%)	22,32,35	2.29	5 (22%)
2	B8W	2	4185	2	18,26,27	6.09	7 (38%)	21,38,41	2.43	7 (33%)
2	OMG	2	1316	2,49	18,26,27	2.46	8 (44%)	19,38,41	1.82	5 (26%)
2	OMG	2	1522	2	18,26,27	2.34	8 (44%)	19,38,41	1.51	4 (21%)
2	OMC	2	3909	2	19,22,23	2.91	8 (42%)	26,31,34	1.10	2 (7%)
2	OMG	2	4196	2	18,26,27	2.51	8 (44%)	19,38,41	1.45	4 (21%)
2	OMC	2	2804	2	19,22,23	2.74	7 (36%)	26,31,34	0.99	1 (3%)
2	A2M	2	1524	2	18,25,26	4.14	6 (33%)	18,36,39	3.15	4 (22%)
2	OMG	2	4623	2	18,26,27	2.31	8 (44%)	19,38,41	1.54	4 (21%)
2	PSU	2	1683	2	18,21,22	1.13	2 (11%)	22,30,33	1.80	4 (18%)
2	B9B	2	2754	2	21,28,29	5.59	8 (38%)	23,40,43	2.15	5 (21%)
2	B8W	2	4472	2	18,26,27	6.07	7 (38%)	21,38,41	2.44	6 (28%)
2	7MG	2	2522	2	22,26,27	3.38	10 (45%)	29,39,42	1.98	9 (31%)
2	1MA	2	4415	2	16,25,26	3.96	4 (25%)	18,37,40	1.69	3 (16%)
2	UR3	2	4530	2	19,22,23	2.77	5 (26%)	26,32,35	1.31	2 (7%)
2	A2M	2	3825	2	18,25,26	4.17	7 (38%)	18,36,39	3.01	3 (16%)
2	PSU	2	3729	2	18,21,22	1.07	1 (5%)	22,30,33	1.69	4 (18%)
2	B8W	2	4129	2	18,26,27	6.17	6 (33%)	21,38,41	2.32	9 (42%)
2	BGH	2	3899	2	25,29,30	4.40	17 (68%)	31,43,46	2.56	12 (38%)
7	OMU	8	14	2,7	19,22,23	2.73	7 (36%)	26,31,34	1.75	6 (23%)
2	A2M	2	1534	2,49	18,25,26	4.08	8 (44%)	18,36,39	3.21	4 (22%)
2	PSU	2	3715	2	18,21,22	1.08	1 (5%)	22,30,33	1.67	4 (18%)
2	M7A	2	4564	2	20,25,26	1.96	3 (15%)	28,37,40	3.82	7 (25%)
2	OMG	2	2773	2	18,26,27	2.40	8 (44%)	19,38,41	1.58	4 (21%)
2	OMG	2	373	2	18,26,27	2.34	7 (38%)	19,38,41	1.69	5 (26%)
2	B8K	2	4690	2	24,28,29	4.45	16 (66%)	30,42,45	2.65	11 (36%)
2	P7G	2	1909	2	24,28,29	4.57	11 (45%)	27,41,44	1.68	4 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	OMG	2	4870	2	18,26,27	2.43	8 (44%)	19,38,41	1.46	4 (21%)
2	PSU	2	4403	2	18,21,22	1.02	1 (5%)	22,30,33	1.84	5 (22%)
2	OMG	2	4637	2	18,26,27	2.37	8 (44%)	19,38,41	1.63	4 (21%)
2	OMU	2	4620	2	19,22,23	2.72	7 (36%)	26,31,34	1.72	5 (19%)
2	E7G	2	2297	2	24,27,28	3.65	11 (45%)	30,40,43	2.19	10 (33%)
2	OMG	2	2364	2	18,26,27	2.35	7 (38%)	19,38,41	1.57	4 (21%)
2	B9B	2	237	2	21,28,29	5.68	9 (42%)	23,40,43	2.42	4 (17%)
2	2MG	2	978	2	18,26,27	2.43	7 (38%)	16,38,41	1.46	3 (18%)
2	PSU	2	2508	2	18,21,22	1.00	1 (5%)	22,30,33	1.69	3 (13%)
2	MHG	2	4371	2	29,32,33	3.92	12 (41%)	34,46,49	2.25	11 (32%)
2	OMC	2	2861	2	19,22,23	2.84	7 (36%)	26,31,34	0.95	1 (3%)
2	7MG	2	1605	2	22,26,27	3.38	10 (45%)	29,39,42	1.94	9 (31%)
2	PSU	2	1677	2	18,21,22	1.13	2 (11%)	22,30,33	1.95	5 (22%)
2	B8K	2	3897	2	24,28,29	4.36	15 (62%)	30,42,45	2.49	13 (43%)
2	A2M	2	4571	2	18,25,26	4.25	8 (44%)	18,36,39	2.97	3 (16%)
2	7MG	2	4550	2	22,26,27	3.57	10 (45%)	29,39,42	1.97	9 (31%)
2	OMG	2	1625	2	18,26,27	2.36	8 (44%)	19,38,41	1.52	4 (21%)
2	2MG	2	1517	2	18,26,27	2.31	7 (38%)	16,38,41	1.56	3 (18%)
2	OMC	2	3869	2	19,22,23	2.84	8 (42%)	26,31,34	1.39	3 (11%)
2	UR3	2	4597	2	19,22,23	2.69	7 (36%)	26,32,35	1.87	3 (11%)
2	5MC	2	4335	2	18,22,23	3.40	7 (38%)	26,32,35	1.24	2 (7%)
2	1MA	2	1322	2,49	16,25,26	3.88	4 (25%)	18,37,40	1.67	3 (16%)
2	B9B	2	1574	2	21,28,29	5.64	8 (38%)	23,40,43	2.09	6 (26%)
2	OMU	2	4306	2	19,22,23	2.78	8 (42%)	26,31,34	1.89	5 (19%)
2	OMC	2	4536	2	19,22,23	2.75	7 (36%)	26,31,34	0.92	1 (3%)
2	I4U	2	1659	2,49	21,24,25	4.70	14 (66%)	27,34,37	1.56	6 (22%)
2	OMC	2	2365	2,49	19,22,23	2.75	8 (42%)	26,31,34	0.77	0
2	A2M	2	1871	2	18,25,26	4.25	8 (44%)	18,36,39	2.94	3 (16%)
2	PSU	2	4636	2	18,21,22	1.14	3 (16%)	22,30,33	1.88	4 (18%)
2	OMC	2	3701	2,49	19,22,23	2.82	8 (42%)	26,31,34	0.64	0
2	6MZ	2	4220	2	18,25,26	1.91	3 (16%)	16,36,39	3.55	3 (18%)
2	B8W	2	2380	2	18,26,27	6.12	7 (38%)	21,38,41	2.24	6 (28%)
2	A2M	2	1326	2,49	18,25,26	4.23	7 (38%)	18,36,39	3.19	3 (16%)
2	P7G	2	3880	2	24,28,29	4.73	11 (45%)	27,41,44	1.80	4 (14%)
2	OMC	2	3887	2	19,22,23	2.91	8 (42%)	26,31,34	0.96	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	OMG	2	2424	2	18,26,27	2.47	8 (44%)	19,38,41	1.63	5 (26%)
2	A2M	2	3718	2	18,25,26	4.25	7 (38%)	18,36,39	2.87	3 (16%)
2	B8T	2	4483	2	19,22,23	3.52	8 (42%)	26,31,34	1.26	4 (15%)
2	OMG	2	4370	2	18,26,27	2.39	8 (44%)	19,38,41	1.57	5 (26%)
2	OMG	2	2050	2	18,26,27	2.35	7 (38%)	19,38,41	1.62	4 (21%)
2	PSU	2	4293	2,28	18,21,22	1.01	1 (5%)	22,30,33	1.96	4 (18%)
2	B8T	2	4671	2	19,22,23	3.43	8 (42%)	26,31,34	0.90	1 (3%)
2	A2M	2	398	2	18,25,26	4.18	6 (33%)	18,36,39	2.96	3 (16%)
2	OMG	2	1883	2	18,26,27	2.36	7 (38%)	19,38,41	1.65	4 (21%)
2	E7G	2	1797	2	24,27,28	3.78	11 (45%)	30,40,43	2.18	9 (30%)
2	2MG	2	4872	2	18,26,27	2.25	7 (38%)	16,38,41	1.62	4 (25%)
2	A2M	2	3867	2	18,25,26	4.20	7 (38%)	18,36,39	3.10	4 (22%)
2	A2M	2	2401	2	18,25,26	4.16	7 (38%)	18,36,39	3.19	3 (16%)
2	5MU	2	4083	2	19,22,23	4.69	7 (36%)	28,32,35	3.63	10 (35%)
2	A2M	2	4523	2	18,25,26	4.24	8 (44%)	18,36,39	3.05	4 (22%)
2	B9H	2	2786	2,49	20,25,26	2.73	5 (25%)	22,35,38	2.13	6 (27%)
2	2MG	2	729	2	18,26,27	2.23	7 (38%)	16,38,41	1.47	4 (25%)
2	OMG	2	4494	2	18,26,27	2.40	8 (44%)	19,38,41	1.57	4 (21%)
2	PSU	2	1582	2	18,21,22	1.04	1 (5%)	22,30,33	1.65	3 (13%)
2	PSU	2	4628	2	18,21,22	1.04	1 (5%)	22,30,33	1.75	4 (18%)
2	A2M	2	2363	2,49	18,25,26	4.18	7 (38%)	18,36,39	3.28	3 (16%)
2	E6G	2	4355	2	20,27,28	5.86	9 (45%)	22,39,42	2.74	8 (36%)
2	B8H	2	1860	2	19,22,23	6.76	6 (31%)	22,32,35	2.29	5 (22%)
2	UR3	2	1866	2	19,22,23	2.88	6 (31%)	26,32,35	1.30	2 (7%)
2	P4U	2	1348	2	21,24,25	3.74	8 (38%)	27,33,36	1.17	2 (7%)
2	I4U	2	4194	2,49	21,24,25	4.89	15 (71%)	27,34,37	1.07	1 (3%)
2	B8Q	2	1456	2	17,22,23	2.91	4 (23%)	22,32,35	2.23	6 (27%)
2	A2M	2	3723	2	18,25,26	4.31	7 (38%)	18,36,39	3.07	3 (16%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	B8W	2	4529	2	-	3/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	OMC	2	2422	2,49,30	-	1/9/27/28	0/2/2/2
2	B8H	2	4296	2	-	0/7/25/26	0/2/2/2
2	B8W	2	4185	2	-	2/5/27/28	0/3/3/3
2	OMG	2	1316	2,49	-	0/5/27/28	0/3/3/3
2	OMG	2	1522	2	-	0/5/27/28	0/3/3/3
2	OMC	2	3909	2	-	2/9/27/28	0/2/2/2
2	OMG	2	4196	2	-	0/5/27/28	0/3/3/3
2	OMC	2	2804	2	-	0/9/27/28	0/2/2/2
2	A2M	2	1524	2	-	0/5/27/28	0/3/3/3
2	OMG	2	4623	2	-	0/5/27/28	0/3/3/3
2	PSU	2	1683	2	-	0/7/25/26	0/2/2/2
2	B9B	2	2754	2	-	2/7/29/30	0/3/3/3
2	B8W	2	4472	2	-	2/5/27/28	0/3/3/3
2	7MG	2	2522	2	-	0/7/37/38	0/3/3/3
2	1MA	2	4415	2	-	3/3/25/26	0/3/3/3
2	UR3	2	4530	2	-	0/7/25/26	0/2/2/2
2	A2M	2	3825	2	-	0/5/27/28	0/3/3/3
2	PSU	2	3729	2	-	2/7/25/26	0/2/2/2
2	B8W	2	4129	2	-	2/5/27/28	0/3/3/3
2	BGH	2	3899	2	-	1/13/43/44	0/3/3/3
7	OMU	8	14	2,7	-	1/9/27/28	0/2/2/2
2	A2M	2	1534	2,49	-	3/5/27/28	0/3/3/3
2	PSU	2	3715	2	-	0/7/25/26	0/2/2/2
2	M7A	2	4564	2	-	0/7/37/38	0/3/3/3
2	OMG	2	2773	2	-	2/5/27/28	0/3/3/3
2	OMG	2	373	2	-	1/5/27/28	0/3/3/3
2	B8K	2	4690	2	-	0/11/41/42	0/3/3/3
2	P7G	2	1909	2	-	2/10/40/41	0/3/3/3
2	OMG	2	4870	2	-	3/5/27/28	0/3/3/3
2	PSU	2	4403	2	-	2/7/25/26	0/2/2/2
2	OMG	2	4637	2	-	0/5/27/28	0/3/3/3
2	OMU	2	4620	2	-	0/9/27/28	0/2/2/2
2	E7G	2	2297	2	-	2/9/39/40	0/3/3/3
2	OMG	2	2364	2	-	2/5/27/28	0/3/3/3
2	B9B	2	237	2	-	5/7/29/30	0/3/3/3
2	2MG	2	978	2	-	0/5/27/28	0/3/3/3
2	PSU	2	2508	2	-	1/7/25/26	0/2/2/2
2	MHG	2	4371	2	-	9/16/46/47	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	OMC	2	2861	2	-	2/9/27/28	0/2/2/2
2	7MG	2	1605	2	-	0/7/37/38	0/3/3/3
2	PSU	2	1677	2	-	1/7/25/26	0/2/2/2
2	B8K	2	3897	2	-	3/11/41/42	0/3/3/3
2	A2M	2	4571	2	-	0/5/27/28	0/3/3/3
2	7MG	2	4550	2	-	2/7/37/38	0/3/3/3
2	OMG	2	1625	2	-	2/5/27/28	0/3/3/3
2	2MG	2	1517	2	-	0/5/27/28	0/3/3/3
2	OMC	2	3869	2	-	4/9/27/28	0/2/2/2
2	UR3	2	4597	2	-	0/7/25/26	0/2/2/2
2	5MC	2	4335	2	-	0/7/25/26	0/2/2/2
2	1MA	2	1322	2,49	-	0/3/25/26	0/3/3/3
2	B9B	2	1574	2	-	3/7/29/30	0/3/3/3
2	OMU	2	4306	2	-	0/9/27/28	0/2/2/2
2	OMC	2	4536	2	-	0/9/27/28	0/2/2/2
2	I4U	2	1659	2,49	-	2/9/29/30	0/2/2/2
2	OMC	2	2365	2,49	-	0/9/27/28	0/2/2/2
2	A2M	2	1871	2	-	2/5/27/28	0/3/3/3
2	PSU	2	4636	2	-	4/7/25/26	0/2/2/2
2	OMC	2	3701	2,49	-	4/9/27/28	0/2/2/2
2	6MZ	2	4220	2	-	2/5/27/28	0/3/3/3
2	B8W	2	2380	2	-	0/5/27/28	0/3/3/3
2	A2M	2	1326	2,49	-	1/5/27/28	0/3/3/3
2	P7G	2	3880	2	-	4/10/40/41	0/3/3/3
2	OMC	2	3887	2	-	1/9/27/28	0/2/2/2
2	OMG	2	2424	2	-	2/5/27/28	0/3/3/3
2	A2M	2	3718	2	-	0/5/27/28	0/3/3/3
2	B8T	2	4483	2	-	0/7/27/28	0/2/2/2
2	OMG	2	4370	2	-	0/5/27/28	0/3/3/3
2	OMG	2	2050	2	-	0/5/27/28	0/3/3/3
2	PSU	2	4293	2,28	-	2/7/25/26	0/2/2/2
2	B8T	2	4671	2	-	2/7/27/28	0/2/2/2
2	A2M	2	398	2	-	2/5/27/28	0/3/3/3
2	OMG	2	1883	2	-	2/5/27/28	0/3/3/3
2	E7G	2	1797	2	-	4/9/39/40	0/3/3/3
2	2MG	2	4872	2	-	2/5/27/28	0/3/3/3
2	A2M	2	3867	2	-	4/5/27/28	0/3/3/3
2	A2M	2	2401	2	-	0/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	5MU	2	4083	2	-	0/7/25/26	0/2/2/2
2	A2M	2	4523	2	-	2/5/27/28	0/3/3/3
2	B9H	2	2786	2,49	-	1/12/47/48	0/2/2/2
2	2MG	2	729	2	-	1/5/27/28	0/3/3/3
2	OMG	2	4494	2	-	0/5/27/28	0/3/3/3
2	PSU	2	1582	2	-	2/7/25/26	0/2/2/2
2	PSU	2	4628	2	-	0/7/25/26	0/2/2/2
2	A2M	2	2363	2,49	-	0/5/27/28	0/3/3/3
2	E6G	2	4355	2	-	2/6/28/29	0/3/3/3
2	B8H	2	1860	2	-	2/7/25/26	0/2/2/2
2	UR3	2	1866	2	-	1/7/25/26	0/2/2/2
2	P4U	2	1348	2	-	1/10/29/30	0/2/2/2
2	I4U	2	4194	2,49	-	5/9/29/30	0/2/2/2
2	B8Q	2	1456	2	-	1/7/42/43	0/2/2/2
2	A2M	2	3723	2	-	0/5/27/28	0/3/3/3

All (665) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	4529	B8W	O4'-C1'	17.99	1.66	1.41
2	2	4472	B8W	O4'-C1'	17.81	1.65	1.41
2	2	4129	B8W	O4'-C1'	17.66	1.65	1.41
2	2	2380	B8W	O4'-C1'	17.43	1.65	1.41
2	2	4185	B8W	O4'-C1'	17.22	1.65	1.41
2	2	4296	B8H	C6-C5	-16.73	1.11	1.34
2	2	1860	B8H	C6-C5	-16.52	1.11	1.34
2	2	237	B9B	C2'-C1'	-16.46	1.28	1.53
2	2	4355	E6G	C2'-C1'	-16.42	1.28	1.53
2	2	1574	B9B	C2'-C1'	-16.22	1.29	1.53
2	2	2754	B9B	C2'-C1'	-16.06	1.29	1.53
2	2	4296	B8H	C4-N3	-16.04	1.09	1.38
2	2	1860	B8H	C4-N3	-15.68	1.09	1.38
2	2	4355	E6G	O4'-C1'	15.47	1.62	1.41
2	2	3723	A2M	O4'-C1'	15.41	1.62	1.41
2	2	1871	A2M	O4'-C1'	15.33	1.62	1.41
2	2	2380	B8W	C2'-C1'	-15.25	1.30	1.53
2	2	4129	B8W	C2'-C1'	-15.18	1.30	1.53
2	2	237	B9B	O4'-C1'	15.18	1.62	1.41
2	2	4529	B8W	C2'-C1'	-15.16	1.30	1.53
2	2	3718	A2M	O4'-C1'	15.14	1.62	1.41
2	2	1326	A2M	O4'-C1'	15.09	1.62	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	1574	B9B	O4'-C1'	15.09	1.62	1.41
2	2	4185	B8W	C2'-C1'	-15.08	1.30	1.53
2	2	2754	B9B	O4'-C1'	15.04	1.62	1.41
2	2	4523	A2M	O4'-C1'	15.02	1.62	1.41
2	2	4571	A2M	O4'-C1'	14.86	1.61	1.41
2	2	398	A2M	O4'-C1'	14.78	1.61	1.41
2	2	3825	A2M	O4'-C1'	14.68	1.61	1.41
2	2	3867	A2M	O4'-C1'	14.66	1.61	1.41
2	2	2401	A2M	O4'-C1'	14.61	1.61	1.41
2	2	1524	A2M	O4'-C1'	14.55	1.61	1.41
2	2	2363	A2M	O4'-C1'	14.54	1.61	1.41
2	2	3880	P7G	C8-N9	14.43	1.54	1.46
2	2	4472	B8W	C2'-C1'	-14.39	1.31	1.53
2	2	1534	A2M	O4'-C1'	14.37	1.61	1.41
2	2	4415	1MA	C2-N3	14.31	1.46	1.29
2	2	1909	P7G	C8-N9	14.12	1.53	1.46
2	2	1322	1MA	C2-N3	14.08	1.46	1.29
2	2	1860	B8H	C4-C5	13.13	1.81	1.44
2	2	4296	B8H	C4-C5	12.71	1.80	1.44
2	2	1860	B8H	C6-N1	12.16	1.66	1.36
2	2	4296	B8H	C6-N1	11.87	1.65	1.36
2	2	4194	I4U	C3'-C2'	-10.86	1.23	1.53
2	2	4083	5MU	C6-N1	10.67	1.56	1.38
2	2	1348	P4U	C4-N3	10.66	1.45	1.31
2	2	1659	I4U	C3'-C2'	-10.58	1.24	1.53
2	2	4083	5MU	C2-N1	10.52	1.55	1.38
2	2	3897	B8K	O4'-C4'	10.38	1.68	1.45
2	2	4194	I4U	C4-N3	10.30	1.44	1.31
2	2	4690	B8K	C3'-C4'	-10.21	1.26	1.53
2	2	4690	B8K	O4'-C4'	10.10	1.67	1.45
2	2	1797	E7G	C8-N9	9.95	1.51	1.46
2	2	3899	BGH	C3'-C4'	-9.95	1.27	1.53
2	2	3880	P7G	C5-N7	9.94	1.46	1.35
2	2	3897	B8K	C3'-C4'	-9.89	1.27	1.53
2	2	1659	I4U	C4-N3	9.64	1.43	1.31
2	2	1909	P7G	C5-N7	9.60	1.46	1.35
2	2	3899	BGH	O4'-C4'	9.52	1.66	1.45
2	2	4371	MHG	C8-N9	9.35	1.51	1.46
2	2	2297	E7G	C5-N7	8.85	1.45	1.35
2	2	4083	5MU	C4-C5	8.82	1.59	1.44
2	2	2297	E7G	C8-N9	8.77	1.50	1.46
2	2	4371	MHG	C5-N7	8.76	1.45	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	4335	5MC	C6-C5	8.68	1.48	1.34
2	2	4550	7MG	C8-N9	8.63	1.50	1.46
2	2	1797	E7G	C5-N7	8.46	1.45	1.35
2	2	4129	B8W	C2-N2	8.43	1.50	1.33
2	2	1456	B8Q	C6-C5	8.38	1.52	1.33
2	2	4529	B8W	C2-N2	8.26	1.50	1.33
2	2	2786	B9H	C2-N3	8.20	1.47	1.37
2	2	4472	B8W	C2-N2	8.17	1.50	1.33
2	2	237	B9B	O4'-C4'	-8.16	1.26	1.45
2	2	4185	B8W	C2-N2	8.04	1.50	1.33
2	2	2522	7MG	C5-N7	8.02	1.44	1.35
2	2	4355	E6G	O4'-C4'	-8.01	1.27	1.45
2	2	4083	5MU	C4-N3	-7.93	1.24	1.38
2	2	1605	7MG	C5-N7	7.78	1.44	1.35
2	2	1574	B9B	O4'-C4'	-7.77	1.27	1.45
2	2	2754	B9B	O4'-C4'	-7.73	1.27	1.45
2	2	4371	MHG	C2-N3	7.68	1.46	1.31
2	2	3899	BGH	C8-N9	7.66	1.50	1.46
2	2	2380	B8W	C2-N2	7.62	1.49	1.33
2	2	4550	7MG	C5-N7	7.54	1.44	1.35
2	2	1659	I4U	O4'-C4'	-7.50	1.28	1.45
2	2	1605	7MG	C8-N9	7.48	1.50	1.46
2	2	4194	I4U	O4'-C4'	-7.28	1.28	1.45
2	2	1866	UR3	C2-N1	7.19	1.48	1.38
2	2	4483	B8T	C2-N3	7.11	1.50	1.36
2	2	2522	7MG	C8-N9	7.08	1.49	1.46
2	2	2363	A2M	O4'-C4'	-7.04	1.29	1.45
2	2	1348	P4U	C2-N3	6.97	1.50	1.36
2	2	3867	A2M	O4'-C4'	-6.95	1.29	1.45
2	2	1456	B8Q	C2-N3	6.94	1.47	1.35
2	2	4571	A2M	O4'-C4'	-6.91	1.29	1.45
2	2	4671	B8T	C2-N3	6.90	1.50	1.36
2	2	1524	A2M	O4'-C4'	-6.73	1.30	1.45
2	2	3825	A2M	O4'-C4'	-6.68	1.30	1.45
2	2	4371	MHG	C8-N7	6.67	1.52	1.45
2	2	1866	UR3	C6-C5	6.67	1.50	1.35
2	2	4671	B8T	C4-N3	6.67	1.44	1.32
2	2	4483	B8T	C4-N3	6.66	1.44	1.32
2	2	4530	UR3	C2-N1	6.65	1.48	1.38
2	2	2401	A2M	O4'-C4'	-6.61	1.30	1.45
2	2	4483	B8T	C6-C5	6.61	1.50	1.35
2	2	3880	P7G	C4-N3	6.59	1.49	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	4597	UR3	C6-C5	6.56	1.50	1.35
2	2	398	A2M	O4'-C4'	-6.53	1.30	1.45
2	2	4690	B8K	C8-N9	6.50	1.49	1.46
2	2	1909	P7G	C4-N3	6.50	1.49	1.37
2	2	4671	B8T	C6-C5	6.48	1.50	1.35
2	2	4220	6MZ	C6-N6	6.47	1.45	1.35
2	2	1574	B9B	O6-C6	6.44	1.40	1.35
2	2	3723	A2M	O4'-C4'	-6.43	1.30	1.45
2	2	4530	UR3	C6-C5	6.42	1.50	1.35
2	2	4523	A2M	O4'-C4'	-6.42	1.30	1.45
2	2	4194	I4U	C6-C5	6.42	1.50	1.35
2	2	1326	A2M	O4'-C4'	-6.41	1.30	1.45
2	2	3718	A2M	O4'-C4'	-6.37	1.30	1.45
2	2	1534	A2M	O4'-C4'	-6.35	1.30	1.45
2	2	3887	OMC	C2-N3	6.35	1.49	1.36
2	2	3909	OMC	C6-C5	6.33	1.49	1.35
2	2	4371	MHG	C2-N2	6.32	1.47	1.33
2	2	4355	E6G	O6-C6	6.30	1.40	1.35
2	2	4306	OMU	C2-N3	6.30	1.49	1.38
2	2	1659	I4U	C6-C5	6.29	1.49	1.35
2	2	1871	A2M	O4'-C4'	-6.27	1.31	1.45
2	2	4483	B8T	C4-N4	6.26	1.48	1.35
2	2	4671	B8T	C4-N4	6.23	1.48	1.35
2	2	2786	B9H	C6-C5	6.19	1.47	1.33
2	2	1348	P4U	C6-C5	6.18	1.49	1.35
2	2	1659	I4U	C2-N3	6.18	1.48	1.36
2	2	4335	5MC	C4-N3	6.17	1.44	1.34
2	2	4620	OMU	C2-N3	6.16	1.48	1.38
7	8	14	OMU	C2-N1	6.16	1.48	1.38
2	2	3701	OMC	C2-N3	6.10	1.48	1.36
2	2	2422	OMC	C2-N3	6.04	1.48	1.36
2	2	2861	OMC	C6-C5	6.03	1.49	1.35
2	2	237	B9B	O6-C6	6.02	1.40	1.35
2	2	4371	MHG	C2-N1	6.01	1.46	1.36
2	2	4194	I4U	C2-N3	6.01	1.48	1.36
2	2	2754	B9B	O6-C6	6.01	1.40	1.35
2	2	3897	B8K	O4'-C1'	-6.01	1.27	1.42
2	2	2804	OMC	C2-N3	5.95	1.48	1.36
2	2	2861	OMC	C2-N3	5.93	1.48	1.36
2	2	4690	B8K	C2-N3	5.93	1.47	1.33
7	8	14	OMU	C2-N3	5.88	1.48	1.38
2	2	3701	OMC	C6-C5	5.87	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	4597	UR3	C2-N3	5.87	1.50	1.39
2	2	4536	OMC	C2-N3	5.86	1.48	1.36
2	2	2422	OMC	C6-C5	5.84	1.48	1.35
2	2	4335	5MC	C2-N3	5.83	1.48	1.36
2	2	3897	B8K	C2-N3	5.82	1.47	1.33
2	2	3880	P7G	C2-N2	5.79	1.48	1.34
2	2	2365	OMC	C2-N3	5.74	1.48	1.36
2	2	3869	OMC	C2-N3	5.71	1.47	1.36
2	2	1909	P7G	C2-N2	5.69	1.47	1.34
2	2	4536	OMC	C6-C5	5.68	1.48	1.35
2	2	4185	B8W	O4'-C4'	-5.67	1.32	1.45
2	2	4550	7MG	C2-N3	5.66	1.46	1.33
2	2	4083	5MU	C6-C5	5.64	1.43	1.34
2	2	2365	OMC	C6-C5	5.64	1.48	1.35
2	2	4620	OMU	C2-N1	5.63	1.47	1.38
2	2	3869	OMC	C6-C5	5.61	1.48	1.35
2	2	1866	UR3	C2-N3	5.60	1.49	1.39
2	2	4196	OMG	C2-N3	5.60	1.46	1.33
2	2	4371	MHG	C4-N3	5.58	1.47	1.34
2	2	3909	OMC	C4-N4	5.58	1.47	1.33
2	2	4597	UR3	C2-N1	5.57	1.46	1.38
2	2	4306	OMU	C2-N1	5.55	1.47	1.38
2	2	4530	UR3	C2-N3	5.55	1.49	1.39
2	2	4529	B8W	O4'-C4'	-5.54	1.32	1.45
2	2	3887	OMC	C6-C5	5.54	1.47	1.35
2	2	2380	B8W	O4'-C4'	-5.52	1.32	1.45
2	2	4620	OMU	C6-C5	5.50	1.47	1.35
2	2	4129	B8W	O4'-C4'	-5.50	1.32	1.45
2	2	237	B9B	C2-N2	5.49	1.44	1.33
2	2	4306	OMU	C6-C5	5.49	1.47	1.35
2	2	2804	OMC	C6-C5	5.47	1.47	1.35
2	2	4550	7MG	C4-N3	5.46	1.47	1.34
2	2	2754	B9B	C2-N2	5.46	1.44	1.33
2	2	4371	MHG	C4-N9	5.44	1.44	1.37
2	2	1574	B9B	C2-N2	5.43	1.44	1.33
2	2	4355	E6G	C2-N2	5.42	1.44	1.33
2	2	3880	P7G	C2-N1	5.41	1.46	1.33
2	2	4690	B8K	O4'-C1'	-5.39	1.29	1.42
2	2	2424	OMG	C2-N3	5.38	1.46	1.33
2	2	2297	E7G	C2-N3	5.38	1.46	1.33
2	2	2297	E7G	C4-N3	5.36	1.47	1.34
2	2	3880	P7G	C4-N9	5.36	1.43	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	1797	E7G	C2-N3	5.34	1.46	1.33
2	2	4494	OMG	C2-N3	5.32	1.46	1.33
2	2	3899	BGH	C2-N3	5.32	1.46	1.33
2	2	978	2MG	C2-N2	5.32	1.45	1.33
2	2	3899	BGH	C4-N3	5.31	1.46	1.34
2	2	1797	E7G	C4-N3	5.31	1.46	1.34
2	2	2522	7MG	C2-N3	5.30	1.46	1.33
2	2	4870	OMG	C2-N3	5.30	1.46	1.33
2	2	2522	7MG	C4-N3	5.28	1.46	1.34
2	2	2050	OMG	C2-N3	5.27	1.46	1.33
2	2	3909	OMC	C2-N3	5.27	1.47	1.36
2	2	1316	OMG	C2-N3	5.26	1.46	1.33
2	2	1348	P4U	C5-C4	5.25	1.50	1.43
2	2	4472	B8W	O4'-C4'	-5.24	1.33	1.45
2	2	4637	OMG	C2-N3	5.24	1.45	1.33
2	2	1517	2MG	C2-N2	5.21	1.45	1.33
2	2	1625	OMG	C2-N3	5.21	1.45	1.33
2	2	4550	7MG	C4-N9	5.19	1.43	1.37
2	2	1605	7MG	C2-N3	5.17	1.45	1.33
2	2	1797	E7G	C8-N7	5.12	1.50	1.45
2	2	1605	7MG	C4-N3	5.12	1.46	1.34
2	2	1909	P7G	C2-N1	5.11	1.45	1.33
2	2	3887	OMC	C4-N3	5.09	1.44	1.34
2	2	2364	OMG	C2-N3	5.09	1.45	1.33
2	2	3897	B8K	C8-N9	5.07	1.48	1.46
2	2	3880	P7G	C8-N7	5.02	1.50	1.45
2	2	1348	P4U	O4-C4	5.02	1.40	1.35
2	2	4370	OMG	C2-N3	5.02	1.45	1.33
2	2	3897	B8K	C4-N9	5.01	1.43	1.37
2	2	4564	M7A	C6-N6	5.00	1.46	1.34
2	2	2786	B9H	C2-N1	5.00	1.45	1.38
2	2	4194	I4U	C1'-N1	-4.99	1.33	1.47
2	2	1883	OMG	C2-N3	4.97	1.45	1.33
2	2	4690	B8K	C4-N3	4.95	1.46	1.34
2	2	3897	B8K	C4-N3	4.93	1.46	1.34
2	2	2773	OMG	C2-N3	4.92	1.45	1.33
2	2	4623	OMG	C2-N3	4.89	1.45	1.33
2	2	4564	M7A	C4-N9	4.89	1.47	1.38
7	8	14	OMU	C6-C5	4.88	1.46	1.35
2	2	3899	BGH	O4'-C1'	-4.87	1.30	1.42
2	2	1909	P7G	C4-N9	4.87	1.42	1.35
2	2	4194	I4U	C3'-C4'	4.85	1.65	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	4185	B8W	O3'-C3'	-4.85	1.31	1.43
2	2	3869	OMC	C4-N4	4.85	1.45	1.33
2	2	1522	OMG	C2-N3	4.85	1.45	1.33
2	2	978	2MG	C4-N3	4.83	1.49	1.37
2	2	3887	OMC	C4-N4	4.82	1.45	1.33
2	2	4872	2MG	C2-N2	4.81	1.44	1.33
2	2	1797	E7G	C2-N2	4.81	1.45	1.34
2	2	3899	BGH	C71-N7	4.80	1.50	1.39
2	2	4196	OMG	C4-N3	4.80	1.49	1.37
2	2	1909	P7G	C8-N7	4.77	1.50	1.45
2	2	4415	1MA	C2-N1	4.75	1.44	1.35
2	2	3909	OMC	C4-N3	4.74	1.44	1.34
2	2	2297	E7G	C8-N7	4.73	1.50	1.45
2	2	4483	B8T	C2-N1	4.71	1.50	1.40
2	2	729	2MG	C2-N2	4.70	1.43	1.33
2	2	1517	2MG	C4-N3	4.68	1.48	1.37
2	2	2422	OMC	C4-N4	4.67	1.44	1.33
2	2	2297	E7G	C2-N2	4.67	1.45	1.34
2	2	3869	OMC	C2-N1	4.65	1.50	1.40
2	2	4870	OMG	C4-N3	4.65	1.48	1.37
2	2	4690	B8K	O2'-C2'	-4.64	1.32	1.43
2	2	2422	OMC	C2-N1	4.63	1.50	1.40
2	2	1605	7MG	C2-N2	4.62	1.45	1.34
2	2	1522	OMG	C4-N3	4.61	1.48	1.37
2	2	373	OMG	C2-N3	4.60	1.44	1.33
2	2	3701	OMC	C4-N4	4.60	1.44	1.33
2	2	3880	P7G	C6-N1	4.60	1.46	1.38
2	2	2804	OMC	C4-N4	4.60	1.44	1.33
2	2	2422	OMC	C4-N3	4.60	1.43	1.34
2	2	2380	B8W	O3'-C3'	-4.59	1.32	1.43
2	2	4872	2MG	C4-N3	4.59	1.48	1.37
2	2	1883	OMG	C4-N3	4.58	1.48	1.37
2	2	4550	7MG	C2-N2	4.58	1.45	1.34
2	2	4472	B8W	O3'-C3'	-4.58	1.32	1.43
2	2	4529	B8W	O3'-C3'	-4.58	1.32	1.43
2	2	4494	OMG	C4-N3	4.58	1.48	1.37
2	2	4637	OMG	C4-N3	4.58	1.48	1.37
2	2	4536	OMC	C4-N4	4.58	1.44	1.33
2	2	2804	OMC	C4-N3	4.57	1.43	1.34
2	2	2364	OMG	C4-N3	4.57	1.48	1.37
2	2	3701	OMC	C4-N3	4.56	1.43	1.34
2	2	2365	OMC	C4-N4	4.56	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	729	2MG	C4-N3	4.56	1.48	1.37
2	2	4370	OMG	C4-N3	4.56	1.48	1.37
2	2	2424	OMG	C4-N3	4.54	1.48	1.37
2	2	2522	7MG	C2-N2	4.53	1.45	1.34
2	2	2773	OMG	C4-N3	4.53	1.48	1.37
2	2	2861	OMC	C4-N4	4.51	1.44	1.33
2	2	1322	1MA	C2-N1	4.50	1.44	1.35
2	2	3899	BGH	C2-N2	4.50	1.44	1.34
2	2	2365	OMC	C4-N3	4.49	1.43	1.34
2	2	2522	7MG	C4-N9	4.49	1.42	1.37
2	2	1625	OMG	C4-N3	4.48	1.48	1.37
2	2	1797	E7G	C4-N9	4.48	1.42	1.37
2	2	2050	OMG	C4-N3	4.48	1.48	1.37
2	2	4690	B8K	C4-N9	4.47	1.42	1.37
2	2	1316	OMG	C4-N3	4.46	1.48	1.37
2	2	1659	I4U	C1'-N1	-4.45	1.34	1.47
2	2	373	OMG	C4-N3	4.45	1.48	1.37
2	2	3897	B8K	O2'-C2'	-4.40	1.32	1.43
2	2	2861	OMC	C4-N3	4.40	1.43	1.34
2	2	2861	OMC	C2-N1	4.39	1.49	1.40
2	2	4129	B8W	O3'-C3'	-4.39	1.32	1.43
2	2	4623	OMG	C4-N3	4.38	1.48	1.37
2	2	1909	P7G	C6-N1	4.35	1.45	1.38
2	2	4671	B8T	C2-N1	4.33	1.49	1.40
2	2	4536	OMC	C4-N3	4.33	1.43	1.34
2	2	3869	OMC	C4-N3	4.32	1.43	1.34
2	2	3899	BGH	O2'-C2'	-4.30	1.31	1.42
2	2	1605	7MG	C4-N9	4.27	1.42	1.37
2	2	978	2MG	C2-N1	4.25	1.43	1.36
2	2	4335	5MC	C4-N4	4.25	1.45	1.34
2	2	4536	OMC	C2-N1	4.23	1.49	1.40
2	2	3887	OMC	C2-N1	4.23	1.49	1.40
2	2	2804	OMC	C2-N1	4.22	1.49	1.40
2	2	4872	2MG	C2-N1	4.19	1.43	1.36
2	2	1659	I4U	O4'-C1'	4.18	1.51	1.42
2	2	1659	I4U	C2-N1	4.16	1.49	1.40
2	2	1860	B8H	C2-N3	4.15	1.45	1.38
2	2	1348	P4U	C2-N1	4.12	1.48	1.40
2	2	4196	OMG	C2-N2	4.10	1.43	1.34
2	2	4194	I4U	C5-C4	4.10	1.48	1.43
2	2	2297	E7G	C4-N9	4.06	1.42	1.37
2	2	4194	I4U	C2-N1	4.03	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	3899	BGH	C5-N7	4.01	1.46	1.39
2	2	3701	OMC	C2-N1	4.00	1.48	1.40
2	2	1348	P4U	C6-N1	3.99	1.47	1.38
2	2	4194	I4U	O4'-C1'	3.99	1.51	1.42
2	2	2424	OMG	C2-N2	3.99	1.43	1.34
2	2	4690	B8K	C5-N7	3.98	1.46	1.39
2	2	3880	P7G	C2-N3	3.94	1.47	1.37
7	8	14	OMU	C4-N3	3.94	1.45	1.38
2	2	4296	B8H	C2-N3	3.93	1.45	1.38
2	2	1517	2MG	C2-N1	3.93	1.43	1.36
2	2	4415	1MA	C4-N3	3.91	1.49	1.37
2	2	729	2MG	C2-N1	3.90	1.43	1.36
2	2	2773	OMG	C2-N2	3.90	1.43	1.34
2	2	4335	5MC	C6-N1	3.89	1.44	1.38
2	2	4494	OMG	C2-N2	3.87	1.43	1.34
2	2	4370	OMG	C2-N2	3.87	1.43	1.34
2	2	3899	BGH	C4-N9	3.86	1.42	1.37
2	2	3897	B8K	C2-N2	3.85	1.43	1.34
2	2	4335	5MC	C2-N1	3.85	1.48	1.40
2	2	3880	P7G	C5-C4	3.83	1.45	1.37
2	2	1316	OMG	C2-N2	3.83	1.43	1.34
2	2	4637	OMG	C2-N2	3.79	1.43	1.34
2	2	373	OMG	C2-N2	3.79	1.43	1.34
2	2	1797	E7G	C2-N1	3.78	1.47	1.37
2	2	4564	M7A	C5-N7	3.77	1.48	1.39
2	2	3880	P7G	O6-C6	-3.74	1.17	1.23
2	2	1322	1MA	C4-N3	3.74	1.49	1.37
2	2	1625	OMG	C2-N2	3.74	1.43	1.34
2	2	2050	OMG	C2-N2	3.73	1.43	1.34
2	2	4623	OMG	C2-N2	3.73	1.43	1.34
2	2	1883	OMG	C2-N2	3.73	1.43	1.34
2	2	4196	OMG	C6-N1	3.72	1.43	1.37
2	2	1659	I4U	C3'-C4'	3.72	1.62	1.53
2	2	2365	OMC	C2-N1	3.72	1.48	1.40
2	2	1909	P7G	O6-C6	-3.72	1.17	1.23
2	2	4870	OMG	C2-N2	3.71	1.43	1.34
2	2	4306	OMU	C4-N3	3.68	1.45	1.38
2	2	2297	E7G	C2-N1	3.68	1.46	1.37
2	2	1909	P7G	C5-C4	3.67	1.44	1.37
2	2	4690	B8K	C2-N2	3.67	1.42	1.34
2	2	2424	OMG	C6-N1	3.66	1.43	1.37
2	2	4671	B8T	C5-C4	3.66	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	1522	OMG	C2-N2	3.64	1.42	1.34
2	2	4690	B8K	C5-C6	3.63	1.52	1.43
2	2	2364	OMG	C2-N2	3.60	1.42	1.34
2	2	3897	B8K	C5-N7	3.58	1.45	1.39
2	2	2773	OMG	C6-N1	3.58	1.43	1.37
2	2	4870	OMG	C6-N1	3.55	1.43	1.37
2	2	3897	B8K	C5-C6	3.55	1.52	1.43
2	2	2754	B9B	O2'-C2'	3.53	1.51	1.43
2	2	1456	B8Q	C2-N1	3.51	1.43	1.38
2	2	1316	OMG	C6-N1	3.50	1.43	1.37
2	2	4483	B8T	C5-C4	3.46	1.48	1.40
2	2	373	OMG	C5-C4	-3.45	1.34	1.43
2	2	4690	B8K	O6-C6	-3.44	1.17	1.23
2	2	3909	OMC	C2-N1	3.44	1.47	1.40
2	2	4483	B8T	C6-N1	3.44	1.46	1.38
2	2	3909	OMC	C6-N1	3.43	1.46	1.38
2	2	4571	A2M	O3'-C3'	-3.43	1.34	1.43
2	2	3715	PSU	C6-C5	3.43	1.39	1.35
2	2	4371	MHG	C5-C6	3.42	1.52	1.43
2	2	4494	OMG	C6-N1	3.40	1.42	1.37
2	2	4620	OMU	C4-N3	3.39	1.44	1.38
2	2	237	B9B	O3'-C3'	-3.39	1.35	1.43
2	2	1909	P7G	C2-N3	3.39	1.46	1.37
2	2	3899	BGH	C5-C6	3.38	1.52	1.43
2	2	1866	UR3	C6-N1	3.38	1.46	1.38
2	2	1605	7MG	C2-N1	3.38	1.46	1.37
2	2	1574	B9B	O2'-C2'	3.37	1.50	1.43
2	2	4355	E6G	O2'-C2'	3.37	1.50	1.43
2	2	3897	B8K	O6-C6	-3.37	1.17	1.23
2	2	1625	OMG	C6-N1	3.36	1.42	1.37
2	2	4370	OMG	C6-N1	3.35	1.42	1.37
2	2	2522	7MG	C2-N1	3.32	1.45	1.37
2	2	3899	BGH	C2-N1	3.32	1.45	1.37
2	2	4194	I4U	O2-C2	-3.31	1.17	1.23
2	2	3899	BGH	O6-C6	-3.30	1.17	1.23
2	2	978	2MG	C6-N1	3.30	1.42	1.37
2	2	3869	OMC	O2-C2	-3.28	1.17	1.23
2	2	3729	PSU	C6-C5	3.28	1.39	1.35
2	2	1659	I4U	C5-C4	3.27	1.47	1.43
2	2	1605	7MG	C5-C6	3.27	1.52	1.43
2	2	4530	UR3	C6-N1	3.26	1.45	1.38
2	2	4620	OMU	O4-C4	-3.26	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	3718	A2M	O3'-C3'	-3.26	1.35	1.43
2	2	3723	A2M	O3'-C3'	-3.25	1.35	1.43
2	2	3899	BGH	C6-N1	3.25	1.44	1.38
2	2	2401	A2M	C5-C4	-3.24	1.32	1.40
2	2	1659	I4U	O2-C2	-3.22	1.17	1.23
2	2	373	OMG	C6-N1	3.21	1.42	1.37
2	2	4403	PSU	C6-C5	3.21	1.39	1.35
2	2	4355	E6G	O3'-C3'	-3.21	1.35	1.43
2	2	237	B9B	O2'-C2'	3.21	1.50	1.43
2	2	4083	5MU	O4-C4	-3.20	1.17	1.23
2	2	4550	7MG	C5-C6	3.20	1.51	1.43
2	2	3825	A2M	O3'-C3'	-3.19	1.35	1.43
2	2	3867	A2M	O3'-C3'	-3.19	1.35	1.43
2	2	1522	OMG	C6-N1	3.19	1.42	1.37
2	2	1326	A2M	C6-N6	3.18	1.45	1.34
2	2	4194	I4U	O2'-C2'	3.17	1.50	1.43
2	2	398	A2M	O3'-C3'	-3.17	1.35	1.43
2	2	3723	A2M	O2'-C2'	3.17	1.50	1.42
2	2	1316	OMG	C5-C4	-3.17	1.35	1.43
2	2	4335	5MC	O2-C2	-3.16	1.17	1.23
2	2	1524	A2M	O3'-C3'	-3.16	1.35	1.43
2	2	3897	B8K	C2-N1	3.15	1.45	1.37
2	2	2424	OMG	C5-C4	-3.15	1.35	1.43
2	2	4550	7MG	C2-N1	3.15	1.45	1.37
2	2	2363	A2M	C5-C4	-3.14	1.32	1.40
2	2	4636	PSU	C6-C5	3.14	1.39	1.35
2	2	3825	A2M	C6-N6	3.13	1.45	1.34
2	2	4623	OMG	C5-C4	-3.13	1.35	1.43
2	2	4623	OMG	C6-N1	3.12	1.42	1.37
2	2	1797	E7G	C5-C6	3.12	1.51	1.43
2	2	2364	OMG	C6-N1	3.12	1.42	1.37
2	2	4371	MHG	C6-N1	3.12	1.44	1.38
2	2	2401	A2M	O3'-C3'	-3.11	1.35	1.43
2	2	1574	B9B	C5-C4	-3.10	1.32	1.40
7	8	14	OMU	O4-C4	-3.10	1.18	1.24
2	2	4690	B8K	C2-N1	3.08	1.45	1.37
2	2	1574	B9B	O3'-C3'	-3.08	1.35	1.43
2	2	4306	OMU	O4-C4	-3.08	1.18	1.24
2	2	2861	OMC	C6-N1	3.08	1.45	1.38
2	2	2297	E7G	C6-N1	3.08	1.44	1.38
2	2	2050	OMG	C5-C4	-3.07	1.35	1.43
2	2	2363	A2M	O3'-C3'	-3.06	1.35	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	4494	OMG	C5-C4	-3.06	1.35	1.43
2	2	4637	OMG	C5-C4	-3.06	1.35	1.43
2	2	1883	OMG	C5-C4	-3.05	1.35	1.43
2	2	4637	OMG	C6-N1	3.05	1.42	1.37
2	2	4523	A2M	O3'-C3'	-3.04	1.35	1.43
2	2	1883	OMG	C6-N1	3.04	1.42	1.37
2	2	4370	OMG	C5-C4	-3.04	1.35	1.43
2	2	4523	A2M	C6-N6	3.04	1.45	1.34
2	2	2754	B9B	O3'-C3'	-3.03	1.35	1.43
2	2	2364	OMG	C5-C4	-3.03	1.35	1.43
2	2	1524	A2M	C6-N6	3.02	1.45	1.34
2	2	4523	A2M	C5-C4	-3.02	1.32	1.40
2	2	1659	I4U	O4-C4	3.02	1.41	1.35
2	2	1534	A2M	C5-C4	-3.02	1.32	1.40
2	2	3723	A2M	C6-N6	3.02	1.45	1.34
2	2	2522	7MG	C5-C6	3.01	1.51	1.43
2	2	1522	OMG	C5-C4	-3.01	1.35	1.43
2	2	3701	OMC	C6-N1	2.99	1.45	1.38
2	2	1871	A2M	C6-N6	2.99	1.45	1.34
2	2	1582	PSU	C6-C5	2.99	1.38	1.35
2	2	1326	A2M	C5-C4	-2.99	1.33	1.40
2	2	1871	A2M	O3'-C3'	-2.98	1.36	1.43
2	2	3718	A2M	C5-C4	-2.97	1.33	1.40
2	2	4597	UR3	C6-N1	2.97	1.45	1.38
2	2	3867	A2M	C6-N6	2.97	1.44	1.34
2	2	2297	E7G	C5-C6	2.97	1.51	1.43
2	2	2050	OMG	O6-C6	-2.96	1.17	1.23
2	2	1683	PSU	C6-C5	2.96	1.38	1.35
2	2	4571	A2M	C5-C4	-2.96	1.33	1.40
2	2	1534	A2M	C6-N6	2.96	1.44	1.34
2	2	1316	OMG	O6-C6	-2.95	1.17	1.23
2	2	1517	2MG	C5-C4	-2.95	1.35	1.43
2	2	4872	2MG	C6-N1	2.95	1.42	1.37
2	2	2365	OMC	O2-C2	-2.94	1.18	1.23
2	2	398	A2M	C6-N6	2.94	1.44	1.34
2	2	3825	A2M	C5-C4	-2.94	1.33	1.40
2	2	4220	6MZ	C5-C4	-2.94	1.33	1.40
2	2	1677	PSU	C6-C5	2.94	1.38	1.35
2	2	4571	A2M	C6-N6	2.93	1.44	1.34
2	2	1883	OMG	O6-C6	-2.93	1.17	1.23
2	2	1797	E7G	C6-N1	2.93	1.44	1.38
2	2	237	B9B	C5-C4	-2.93	1.33	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	2050	OMG	C6-N1	2.93	1.42	1.37
2	2	2364	OMG	O6-C6	-2.93	1.17	1.23
2	2	1326	A2M	O3'-C3'	-2.92	1.36	1.43
2	2	1524	A2M	C5-C4	-2.92	1.33	1.40
2	2	2754	B9B	C5-C4	-2.92	1.33	1.40
2	2	3887	OMC	C6-N1	2.92	1.45	1.38
2	2	2401	A2M	C6-N6	2.91	1.44	1.34
2	2	4483	B8T	O2-C2	-2.91	1.18	1.23
2	2	2365	OMC	C6-N1	2.91	1.45	1.38
2	2	3909	OMC	O2-C2	-2.91	1.18	1.23
2	2	978	2MG	C5-C4	-2.90	1.35	1.43
2	2	4306	OMU	O2-C2	-2.90	1.17	1.23
2	2	4194	I4U	C6-N1	2.89	1.45	1.38
2	2	4671	B8T	O2-C2	-2.89	1.18	1.23
2	2	4870	OMG	C5-C6	2.89	1.53	1.47
2	2	1326	A2M	O2'-C2'	2.89	1.50	1.42
2	2	3718	A2M	C6-N6	2.88	1.44	1.34
2	2	4355	E6G	C5-C4	-2.88	1.33	1.40
2	2	4637	OMG	O6-C6	-2.88	1.17	1.23
2	2	2363	A2M	C6-N6	2.88	1.44	1.34
2	2	4690	B8K	C6-N1	2.87	1.44	1.38
2	2	1517	2MG	C6-N1	2.87	1.42	1.37
2	2	1605	7MG	C6-N1	2.87	1.44	1.38
2	2	4671	B8T	C6-N1	2.86	1.44	1.38
2	2	2422	OMC	O2-C2	-2.86	1.18	1.23
2	2	2297	E7G	O6-C6	-2.85	1.18	1.23
2	2	2422	OMC	C6-N1	2.85	1.44	1.38
2	2	4550	7MG	O6-C6	-2.85	1.18	1.23
2	2	1522	OMG	O6-C6	-2.85	1.17	1.23
2	2	4523	A2M	O2'-C2'	2.85	1.49	1.42
2	2	398	A2M	C5-C4	-2.84	1.33	1.40
2	2	3867	A2M	C5-C4	-2.84	1.33	1.40
2	2	2522	7MG	O6-C6	-2.83	1.18	1.23
2	2	1625	OMG	C5-C4	-2.83	1.35	1.43
2	2	2522	7MG	C6-N1	2.82	1.44	1.38
2	2	1871	A2M	C5-C4	-2.82	1.33	1.40
2	2	729	2MG	C5-C4	-2.82	1.35	1.43
2	2	2773	OMG	C5-C4	-2.82	1.35	1.43
2	2	2380	B8W	C5-C4	-2.82	1.33	1.40
2	2	4196	OMG	C5-C6	2.82	1.53	1.47
2	2	1316	OMG	C5-C6	2.82	1.53	1.47
2	2	3867	A2M	O2'-C2'	2.81	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	4083	5MU	O2-C2	-2.81	1.17	1.23
2	2	1534	A2M	O3'-C3'	-2.79	1.36	1.43
2	2	2773	OMG	C5-C6	2.79	1.53	1.47
2	2	3723	A2M	C5-C4	-2.79	1.33	1.40
2	2	2508	PSU	C6-C5	2.79	1.38	1.35
2	2	4870	OMG	C5-C4	-2.78	1.36	1.43
2	2	4571	A2M	O2'-C2'	2.78	1.49	1.42
2	2	729	2MG	C6-N1	2.77	1.42	1.37
7	8	14	OMU	O2-C2	-2.77	1.18	1.23
2	2	4623	OMG	O6-C6	-2.77	1.17	1.23
2	2	4370	OMG	O6-C6	-2.76	1.17	1.23
2	2	978	2MG	C5-C6	2.75	1.53	1.47
2	2	4129	B8W	O2'-C2'	2.74	1.49	1.43
2	2	4690	B8K	O3'-C3'	2.74	1.49	1.43
2	2	4628	PSU	C6-C5	2.73	1.38	1.35
2	2	3869	OMC	C6-N1	2.73	1.44	1.38
2	2	1659	I4U	C6-N1	2.72	1.44	1.38
2	2	4620	OMU	O2-C2	-2.72	1.18	1.23
2	2	2861	OMC	O2-C2	-2.71	1.18	1.23
2	2	1797	E7G	O6-C6	-2.71	1.18	1.23
2	2	1605	7MG	O6-C6	-2.70	1.18	1.23
2	2	4185	B8W	O2'-C2'	2.68	1.49	1.43
2	2	4536	OMC	O2-C2	-2.68	1.18	1.23
2	2	4194	I4U	O4-C4	2.68	1.40	1.35
2	2	398	A2M	O2'-C2'	2.67	1.49	1.42
2	2	4293	PSU	C6-C5	2.66	1.38	1.35
2	2	4494	OMG	O6-C6	-2.65	1.17	1.23
2	2	1517	2MG	O6-C6	-2.65	1.17	1.23
2	2	3897	B8K	O3'-C3'	2.65	1.49	1.43
2	2	3887	OMC	O2-C2	-2.65	1.18	1.23
2	2	1456	B8Q	C6-N1	2.63	1.44	1.38
2	2	2804	OMC	O2-C2	-2.63	1.18	1.23
2	2	1524	A2M	O2'-C2'	2.62	1.49	1.42
2	2	373	OMG	O6-C6	-2.62	1.18	1.23
2	2	4185	B8W	C5-C4	-2.62	1.34	1.40
2	2	3897	B8K	C6-N1	2.62	1.43	1.38
2	2	2363	A2M	O2'-C2'	2.62	1.49	1.42
2	2	2804	OMC	C6-N1	2.62	1.44	1.38
2	2	4371	MHG	C72-C71	2.62	1.58	1.52
2	2	4529	B8W	O2'-C2'	2.60	1.49	1.43
2	2	2424	OMG	O6-C6	-2.60	1.18	1.23
2	2	4371	MHG	O6-C6	-2.60	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	4536	OMC	C6-N1	2.59	1.44	1.38
2	2	2773	OMG	O6-C6	-2.58	1.18	1.23
2	2	3825	A2M	O2'-C2'	2.57	1.49	1.42
2	2	2380	B8W	O2'-C2'	2.57	1.49	1.43
2	2	1659	I4U	O2'-C2'	2.57	1.49	1.43
2	2	4872	2MG	C5-C4	-2.56	1.36	1.43
2	2	1871	A2M	O2'-C2'	2.56	1.49	1.42
2	2	4196	OMG	C2-N1	2.56	1.44	1.37
2	2	3701	OMC	O2-C2	-2.56	1.19	1.23
2	2	4690	B8K	C71-N7	2.55	1.45	1.39
2	2	373	OMG	C5-C6	2.54	1.52	1.47
2	2	1625	OMG	O6-C6	-2.54	1.18	1.23
2	2	4550	7MG	C6-N1	2.53	1.43	1.38
2	2	3718	A2M	O2'-C2'	2.52	1.49	1.42
2	2	4870	OMG	O6-C6	-2.52	1.18	1.23
2	2	1883	OMG	C5-C6	2.52	1.52	1.47
2	2	4370	OMG	C5-C6	2.51	1.52	1.47
2	2	4472	B8W	O2'-C2'	2.50	1.48	1.43
2	2	729	2MG	C5-C6	2.49	1.52	1.47
2	2	4306	OMU	C6-N1	2.45	1.43	1.38
2	2	4196	OMG	O6-C6	-2.45	1.18	1.23
2	2	2401	A2M	O2'-C2'	2.44	1.48	1.42
2	2	4370	OMG	C2-N1	2.44	1.43	1.37
2	2	2786	B9H	C6-N1	2.43	1.43	1.38
2	2	1522	OMG	C5-C6	2.42	1.52	1.47
2	2	2364	OMG	C5-C6	2.42	1.52	1.47
2	2	4415	1MA	C5-C4	-2.42	1.36	1.43
2	2	4296	B8H	O4-C4	-2.41	1.19	1.23
2	2	4472	B8W	C5-C4	-2.41	1.34	1.40
2	2	1322	1MA	C5-C4	-2.40	1.36	1.43
2	2	1625	OMG	C5-C6	2.40	1.52	1.47
2	2	978	2MG	O6-C6	-2.39	1.18	1.23
2	2	4872	2MG	C5-C6	2.38	1.52	1.47
2	2	2424	OMG	C2-N1	2.37	1.43	1.37
2	2	3899	BGH	O5'-C5'	-2.37	1.39	1.44
7	8	14	OMU	C6-N1	2.36	1.43	1.38
2	2	1316	OMG	C2-N1	2.34	1.43	1.37
2	2	4870	OMG	C2-N1	2.34	1.43	1.37
2	2	4597	UR3	O2-C2	-2.34	1.18	1.22
2	2	4196	OMG	C5-C4	-2.33	1.37	1.43
2	2	1517	2MG	C5-C6	2.33	1.52	1.47
2	2	4872	2MG	O6-C6	-2.32	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	729	2MG	O6-C6	-2.31	1.18	1.23
2	2	3909	OMC	C5-C4	2.31	1.48	1.42
2	2	4529	B8W	C5-C4	-2.31	1.34	1.40
2	2	1534	A2M	O2'-C2'	2.30	1.48	1.42
2	2	2424	OMG	C5-C6	2.29	1.52	1.47
2	2	3867	A2M	C2-N3	2.29	1.35	1.32
2	2	1677	PSU	O4'-C1'	-2.29	1.40	1.43
2	2	2050	OMG	C5-C6	2.28	1.52	1.47
2	2	2786	B9H	O2-C2	-2.27	1.18	1.22
2	2	237	B9B	O5'-C5'	-2.26	1.39	1.44
2	2	4494	OMG	C5-C6	2.25	1.52	1.47
2	2	4571	A2M	C2-N3	2.25	1.35	1.32
2	2	4306	OMU	C5-C4	2.25	1.48	1.43
2	2	2773	OMG	C2-N1	2.25	1.43	1.37
2	2	1871	A2M	C2-N3	2.24	1.35	1.32
2	2	2401	A2M	O5'-C5'	-2.24	1.39	1.44
2	2	4571	A2M	O5'-C5'	-2.22	1.39	1.44
2	2	1683	PSU	C4-C5	-2.22	1.37	1.44
2	2	1625	OMG	C2-N1	2.21	1.43	1.37
2	2	4523	A2M	O5'-C5'	-2.21	1.39	1.44
2	2	4296	B8H	C2-N1	-2.21	1.34	1.38
2	2	4623	OMG	C2-N1	2.20	1.43	1.37
2	2	1866	UR3	C5-C4	2.20	1.49	1.43
2	2	4637	OMG	C5-C6	2.19	1.51	1.47
2	2	2422	OMC	C5-C4	2.17	1.47	1.42
2	2	4597	UR3	C5-C4	2.16	1.49	1.43
2	2	4620	OMU	C6-N1	2.16	1.43	1.38
2	2	4636	PSU	C4-C5	-2.16	1.38	1.44
2	2	1871	A2M	O5'-C5'	-2.15	1.39	1.44
2	2	2363	A2M	O5'-C5'	-2.15	1.39	1.44
2	2	4636	PSU	O4'-C1'	-2.14	1.40	1.43
2	2	1866	UR3	C4-N3	2.14	1.45	1.40
2	2	4220	6MZ	C2-N3	2.12	1.35	1.32
2	2	4355	E6G	O5'-C5'	-2.12	1.39	1.44
2	2	3701	OMC	C5-C4	2.10	1.47	1.42
2	2	3869	OMC	C5-C4	2.10	1.47	1.42
2	2	1860	B8H	O4-C4	-2.09	1.19	1.23
2	2	4494	OMG	C2-N1	2.09	1.42	1.37
2	2	1522	OMG	C2-N1	2.07	1.42	1.37
2	2	4597	UR3	C4-N3	2.07	1.45	1.40
2	2	4530	UR3	O2-C2	-2.06	1.18	1.22
2	2	1348	P4U	O2-C2	-2.06	1.19	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	3825	A2M	O5'-C5'	-2.05	1.39	1.44
2	2	3899	BGH	O3'-C3'	2.05	1.47	1.43
2	2	4637	OMG	C2-N1	2.04	1.42	1.37
2	2	3723	A2M	C2-N3	2.04	1.35	1.32
2	2	4623	OMG	C5-C6	2.04	1.51	1.47
2	2	4523	A2M	C2-N3	2.03	1.35	1.32
2	2	1326	A2M	C2-N3	2.03	1.35	1.32
2	2	4194	I4U	O5'-C5'	-2.03	1.39	1.44
2	2	3718	A2M	C5-N7	-2.03	1.32	1.39
2	2	3887	OMC	C5-C4	2.02	1.47	1.42
2	2	2365	OMC	C5-C4	2.01	1.47	1.42
2	2	1534	A2M	C2-N3	2.01	1.35	1.32
2	2	1534	A2M	C5-N7	-2.00	1.32	1.39

All (416) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	4564	M7A	C5-C6-N6	13.64	147.03	123.74
2	2	4220	6MZ	C1'-N9-C4	-12.78	104.18	126.64
2	2	4083	5MU	C5-C4-N3	11.90	125.47	115.31
2	2	4564	M7A	N6-C6-N1	-11.41	93.35	118.35
2	2	2363	A2M	C5-C6-N6	10.14	135.76	120.35
2	2	1326	A2M	C5-C6-N6	9.81	135.25	120.35
2	2	2401	A2M	C5-C6-N6	9.41	134.66	120.35
2	2	1524	A2M	C5-C6-N6	9.39	134.62	120.35
2	2	4083	5MU	C5-C6-N1	-9.34	113.73	123.34
2	2	3723	A2M	C5-C6-N6	9.30	134.48	120.35
2	2	3825	A2M	C5-C6-N6	9.27	134.44	120.35
2	2	3867	A2M	C5-C6-N6	9.15	134.25	120.35
2	2	1534	A2M	C5-C6-N6	9.12	134.21	120.35
2	2	4523	A2M	C5-C6-N6	9.08	134.15	120.35
2	2	398	A2M	C5-C6-N6	9.01	134.05	120.35
2	2	3718	A2M	C5-C6-N6	8.79	133.71	120.35
2	2	4571	A2M	C5-C6-N6	8.67	133.53	120.35
2	2	1871	A2M	C5-C6-N6	8.64	133.48	120.35
2	2	4597	UR3	C4-N3-C2	-7.78	117.24	124.56
2	2	3880	P7G	C4-C5-N7	7.60	110.68	106.67
2	2	2363	A2M	N6-C6-N1	-7.15	103.72	118.57
2	2	1524	A2M	N6-C6-N1	-6.69	104.68	118.57
2	2	3867	A2M	N6-C6-N1	-6.68	104.71	118.57
2	2	237	B9B	O6-C6-N1	-6.65	114.39	120.12
2	2	2786	B9H	C31-N3-C2	6.64	125.51	117.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	2401	A2M	N6-C6-N1	-6.63	104.82	118.57
2	2	1860	B8H	C4-N3-C2	-6.59	118.81	127.35
2	2	1534	A2M	N6-C6-N1	-6.53	105.02	118.57
2	2	1326	A2M	N6-C6-N1	-6.51	105.07	118.57
2	2	4296	B8H	C4-N3-C2	-6.49	118.95	127.35
2	2	2401	A2M	N3-C2-N1	-6.46	118.58	128.68
2	2	3723	A2M	N6-C6-N1	-6.43	105.22	118.57
2	2	4523	A2M	N6-C6-N1	-6.40	105.28	118.57
2	2	3825	A2M	N6-C6-N1	-6.37	105.36	118.57
2	2	1909	P7G	C4-C5-N7	6.32	110.00	106.67
2	2	4571	A2M	N6-C6-N1	-6.29	105.51	118.57
2	2	4371	MHG	C2-N3-C4	6.28	119.83	112.04
2	2	398	A2M	N6-C6-N1	-6.25	105.61	118.57
2	2	4690	B8K	C72-C71-N7	6.21	128.21	118.86
2	2	1871	A2M	N6-C6-N1	-6.18	105.74	118.57
2	2	3718	A2M	N6-C6-N1	-6.13	105.84	118.57
2	2	4355	E6G	N2-C2-N3	6.11	127.75	117.79
2	2	4690	B8K	C5-C6-N1	6.05	121.64	110.99
2	2	4564	M7A	N3-C2-N1	-6.04	119.16	128.60
2	2	3723	A2M	N3-C2-N1	-5.97	119.34	128.68
2	2	3899	BGH	C72-C71-N7	5.94	127.80	118.86
2	2	1326	A2M	N3-C2-N1	-5.93	119.41	128.68
2	2	1456	B8Q	C31-N3-C4	5.93	123.18	114.25
2	2	4690	B8K	C4-C5-N7	5.92	110.17	104.91
2	2	1871	A2M	N3-C2-N1	-5.89	119.47	128.68
2	2	4523	A2M	N3-C2-N1	-5.88	119.49	128.68
2	2	4355	E6G	O6-C6-N1	5.85	125.17	120.12
2	2	3899	BGH	C5-C6-N1	5.79	121.19	110.99
2	2	1524	A2M	N3-C2-N1	-5.78	119.65	128.68
2	2	2363	A2M	N3-C2-N1	-5.77	119.65	128.68
2	2	4571	A2M	N3-C2-N1	-5.75	119.70	128.68
2	2	4185	B8W	N3-C2-N1	-5.73	119.58	127.22
2	2	3897	B8K	C72-C71-N7	5.69	127.42	118.86
2	2	3897	B8K	C5-C6-N1	5.68	121.00	110.99
2	2	2297	E7G	C4-C5-N7	5.67	109.95	104.91
2	2	398	A2M	N3-C2-N1	-5.66	119.84	128.68
2	2	1534	A2M	N3-C2-N1	-5.65	119.85	128.68
2	2	4306	OMU	C4-N3-C2	-5.64	119.14	126.58
2	2	4472	B8W	N3-C2-N1	-5.64	119.70	127.22
2	2	4296	B8H	N3-C2-N1	5.49	121.07	115.14
2	2	1456	B8Q	N3-C2-N1	5.47	123.56	117.13
2	2	3867	A2M	N3-C2-N1	-5.46	120.15	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	1797	E7G	C4-C5-N7	5.45	109.76	104.91
2	2	237	B9B	N3-C2-N1	-5.45	119.95	127.22
2	2	2297	E7G	C5-C6-N1	5.45	120.59	110.99
2	2	4355	E6G	N3-C2-N1	-5.43	119.98	127.22
2	2	3825	A2M	N3-C2-N1	-5.42	120.21	128.68
2	2	4371	MHG	C4-C5-N7	5.41	109.73	104.91
2	2	4129	B8W	N3-C2-N1	-5.41	120.00	127.22
2	2	4083	5MU	O4-C4-C5	-5.35	118.70	124.90
2	2	4220	6MZ	N3-C2-N1	-5.34	120.33	128.68
2	2	4293	PSU	N1-C2-N3	5.32	121.16	115.13
2	2	4529	B8W	N3-C2-N1	-5.27	120.19	127.22
2	2	1860	B8H	N3-C2-N1	5.24	120.80	115.14
2	2	3718	A2M	N3-C2-N1	-5.23	120.50	128.68
2	2	3899	BGH	C4-C5-N7	5.21	109.54	104.91
2	2	4472	B8W	C2-N3-C4	5.20	121.29	115.36
2	2	1677	PSU	C4-N3-C2	-5.18	118.88	126.34
2	2	4415	1MA	N1-C2-N3	-5.17	119.99	126.02
2	2	2754	B9B	N3-C2-N1	-5.17	120.33	127.22
2	2	1797	E7G	C5-C6-N1	5.15	120.07	110.99
2	2	237	B9B	C2-N3-C4	5.12	121.20	115.36
2	2	2754	B9B	O6-C6-N1	-5.11	115.71	120.12
2	2	4529	B8W	O6-C6-N1	5.10	126.10	119.03
2	2	2522	7MG	C5-C6-N1	5.10	119.97	110.99
2	2	2380	B8W	O6-C6-N1	5.09	126.08	119.03
2	2	4371	MHG	C5-C6-N1	5.00	119.81	110.99
2	2	4185	B8W	C2-N3-C4	5.00	121.07	115.36
2	2	1574	B9B	N3-C2-N1	-4.99	120.57	127.22
2	2	1677	PSU	N1-C2-N3	4.95	120.74	115.13
2	2	4550	7MG	C5-C6-N1	4.95	119.71	110.99
2	2	4636	PSU	C4-N3-C2	-4.95	119.21	126.34
7	8	14	OMU	C4-N3-C2	-4.93	120.08	126.58
2	2	4620	OMU	C4-N3-C2	-4.91	120.10	126.58
2	2	4403	PSU	N1-C2-N3	4.87	120.64	115.13
2	2	1605	7MG	C5-C6-N1	4.86	119.55	110.99
2	2	4083	5MU	N3-C2-N1	4.83	121.30	114.89
2	2	4529	B8W	N2-C2-N3	4.79	125.60	117.79
2	2	4293	PSU	C4-N3-C2	-4.77	119.46	126.34
2	2	4083	5MU	C4-N3-C2	-4.77	121.18	127.35
2	2	1322	1MA	N1-C2-N3	-4.75	120.48	126.02
2	2	1866	UR3	C4-N3-C2	-4.75	120.09	124.56
2	2	4129	B8W	N2-C2-N3	4.68	125.42	117.79
2	2	4628	PSU	N1-C2-N3	4.67	120.43	115.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	1574	B9B	O6-C6-N1	-4.67	116.09	120.12
2	2	3899	BGH	C2-N3-C4	4.64	120.57	112.30
2	2	4636	PSU	N1-C2-N3	4.63	120.38	115.13
2	2	4306	OMU	N3-C2-N1	4.62	121.03	114.89
2	2	4403	PSU	C4-N3-C2	-4.56	119.77	126.34
2	2	2508	PSU	C4-N3-C2	-4.53	119.81	126.34
2	2	4530	UR3	C4-N3-C2	-4.51	120.32	124.56
2	2	1683	PSU	C4-N3-C2	-4.49	119.87	126.34
2	2	1683	PSU	N1-C2-N3	4.48	120.20	115.13
2	2	3715	PSU	N1-C2-N3	4.43	120.15	115.13
2	2	4690	B8K	C2-N3-C4	4.43	120.19	112.30
2	2	4564	M7A	N3-C4-N9	4.43	132.46	126.87
2	2	4355	E6G	C2-N3-C4	4.41	120.39	115.36
2	2	3897	B8K	C4-C5-N7	4.40	108.83	104.91
2	2	4529	B8W	C2-N3-C4	4.40	120.38	115.36
2	2	4083	5MU	C5M-C5-C6	-4.36	117.02	122.85
2	2	4472	B8W	N2-C2-N3	4.35	124.88	117.79
2	2	1456	B8Q	O2-C2-N3	-4.35	116.56	122.95
2	2	2297	E7G	C2-N3-C4	4.35	120.05	112.30
2	2	2380	B8W	N3-C2-N1	-4.33	121.44	127.22
2	2	1574	B9B	C2-N3-C4	4.33	120.30	115.36
2	2	1659	I4U	C5-C4-N3	-4.32	118.33	124.91
2	2	3715	PSU	C4-N3-C2	-4.31	120.13	126.34
2	2	1534	A2M	O4'-C1'-C2'	-4.30	99.12	106.59
2	2	1797	E7G	C2-N3-C4	4.29	119.94	112.30
2	2	1582	PSU	C4-N3-C2	-4.23	120.25	126.34
2	2	2508	PSU	N1-C2-N3	4.23	119.92	115.13
2	2	1605	7MG	C2-N3-C4	4.22	119.81	112.30
2	2	4083	5MU	C5M-C5-C4	4.20	123.39	118.77
2	2	4335	5MC	C5-C6-N1	-4.20	119.02	123.34
2	2	3729	PSU	N1-C2-N3	4.19	119.88	115.13
2	2	3897	B8K	C2-N3-C4	4.19	119.76	112.30
2	2	4129	B8W	C2-N3-C4	4.18	120.13	115.36
2	2	1322	1MA	C5-C6-N1	4.18	120.12	113.90
2	2	4690	B8K	N9-C8-N7	4.17	108.92	103.33
2	2	2522	7MG	C2-N3-C4	4.17	119.72	112.30
2	2	4472	B8W	O6-C6-N1	4.16	124.79	119.03
2	2	2754	B9B	C2-N3-C4	4.09	120.02	115.36
2	2	4620	OMU	N3-C2-N1	4.08	120.31	114.89
2	2	1517	2MG	C5-C6-N1	4.06	121.11	113.95
2	2	1883	OMG	C5-C6-N1	4.01	121.04	113.95
2	2	4185	B8W	N2-C2-N3	4.01	124.32	117.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	4550	7MG	C2-N3-C4	4.00	119.43	112.30
2	2	4628	PSU	C4-N3-C2	-3.97	120.62	126.34
2	2	2050	OMG	C5-C6-N1	3.96	120.94	113.95
2	2	4872	2MG	CM2-N2-C2	-3.94	115.16	123.86
2	2	1582	PSU	N1-C2-N3	3.93	119.59	115.13
2	2	1316	OMG	C5-C6-N1	3.93	120.89	113.95
2	2	4415	1MA	C5-C6-N1	3.90	119.72	113.90
2	2	4529	B8W	O4'-C4'-C3'	-3.89	97.41	105.11
2	2	3869	OMC	O2-C2-N3	-3.87	116.04	122.33
2	2	4637	OMG	C5-C6-N1	3.87	120.78	113.95
2	2	4550	7MG	C5-C4-N3	-3.84	120.81	128.13
7	8	14	OMU	C5-C4-N3	3.82	120.55	114.84
2	2	2424	OMG	C5-C6-N1	3.81	120.68	113.95
2	2	1348	P4U	C5-C4-N3	-3.77	119.17	124.91
2	2	4185	B8W	O6-C6-N1	3.76	124.25	119.03
2	2	4494	OMG	C5-C6-N1	3.75	120.58	113.95
2	2	2786	B9H	C6-N1-C2	-3.75	118.43	121.79
2	2	2380	B8W	N2-C2-N3	3.70	123.83	117.79
2	2	3899	BGH	N9-C8-N7	3.70	108.30	103.33
2	2	373	OMG	C5-C6-N1	3.68	120.45	113.95
2	2	1860	B8H	C5-C4-N3	3.65	124.83	116.58
2	2	2364	OMG	C5-C6-N1	3.64	120.39	113.95
2	2	3729	PSU	C4-N3-C2	-3.63	121.11	126.34
2	2	237	B9B	C3'-C2'-C1'	3.63	106.44	100.98
2	2	1797	E7G	C5-C4-N3	-3.61	121.25	128.13
2	2	3899	BGH	C5-C4-N9	3.60	111.02	106.35
2	2	4306	OMU	O2-C2-N1	-3.60	118.00	122.79
2	2	978	2MG	C5-C6-N1	3.59	120.30	113.95
2	2	4296	B8H	C5-C4-N3	3.59	124.69	116.58
2	2	1316	OMG	C2-N1-C6	-3.52	118.61	125.10
2	2	1522	OMG	C5-C6-N1	3.52	120.17	113.95
2	2	1797	E7G	C5-C4-N9	3.48	110.87	106.35
2	2	2786	B9H	O3'-C3'-C2'	3.47	121.03	111.17
2	2	2297	E7G	C5-C4-N3	-3.47	121.51	128.13
2	2	4371	MHG	C5-C4-N3	-3.47	121.52	128.13
2	2	2522	7MG	C5-C4-N3	-3.47	121.53	128.13
2	2	2380	B8W	C2-N3-C4	3.47	119.31	115.36
2	2	4370	OMG	C5-C6-N1	3.46	120.06	113.95
2	2	4623	OMG	C5-C6-N1	3.46	120.06	113.95
2	2	3729	PSU	C6-N1-C2	-3.40	119.21	122.68
2	2	1605	7MG	C5-C4-N3	-3.39	121.68	128.13
2	2	4872	2MG	C5-C6-N1	3.38	119.92	113.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	1605	7MG	C5-C4-N9	3.36	110.71	106.35
2	2	2773	OMG	C5-C6-N1	3.35	119.87	113.95
2	2	2364	OMG	C2-N1-C6	-3.34	118.94	125.10
2	2	729	2MG	C5-C6-N1	3.34	119.85	113.95
7	8	14	OMU	O4-C4-C5	-3.33	119.30	125.16
2	2	2050	OMG	C2-N1-C6	-3.32	118.99	125.10
2	2	4564	M7A	C2-N3-C4	3.30	119.56	111.75
2	2	1574	B9B	C1'-N9-C4	-3.30	120.84	126.64
2	2	4196	OMG	C5-C6-N1	3.28	119.74	113.95
2	2	3897	B8K	C5-C4-N9	3.27	110.60	106.35
2	2	2754	B9B	C3'-C2'-C1'	3.27	105.91	100.98
2	2	4637	OMG	C2-N1-C6	-3.25	119.11	125.10
2	2	4690	B8K	C5-C4-N9	3.25	110.57	106.35
2	2	4371	MHG	C2-N1-C6	-3.25	120.75	124.48
2	2	4355	E6G	O4'-C4'-C3'	-3.23	98.73	105.11
2	2	4355	E6G	N2-C2-N1	-3.21	112.26	117.25
2	2	1860	B8H	O2-C2-N1	-3.20	119.26	122.87
2	2	1883	OMG	C2-N1-C6	-3.18	119.24	125.10
2	2	1625	OMG	C5-C6-N1	3.18	119.56	113.95
2	2	4550	7MG	C5-C4-N9	3.17	110.46	106.35
2	2	4628	PSU	C6-N1-C2	-3.14	119.47	122.68
2	2	4690	B8K	C6-C5-C4	-3.14	116.15	122.62
2	2	3729	PSU	O2-C2-N1	-3.14	119.33	122.79
2	2	4870	OMG	C5-C6-N1	3.13	119.47	113.95
2	2	1909	P7G	N9-C8-N7	3.11	107.83	103.38
7	8	14	OMU	C1'-N1-C2	3.11	123.20	117.57
2	2	2522	7MG	C5-C4-N9	3.11	110.38	106.35
2	2	4194	I4U	C5-C4-N3	-3.10	120.19	124.91
2	2	2424	OMG	C2-N1-C6	-3.10	119.39	125.10
2	2	4494	OMG	C2-N1-C6	-3.09	119.40	125.10
2	2	1625	OMG	C2-N1-C6	-3.06	119.46	125.10
2	2	3899	BGH	C6-C5-C4	-3.06	116.31	122.62
2	2	3899	BGH	C5-C4-N3	-3.06	122.31	128.13
2	2	4306	OMU	C5-C4-N3	3.06	119.41	114.84
2	2	3869	OMC	C1'-N1-C2	3.05	125.22	118.42
2	2	1683	PSU	O2-C2-N1	-3.04	119.44	122.79
2	2	3897	B8K	N9-C8-N7	3.01	107.37	103.33
2	2	4550	7MG	C4-C5-N7	3.00	109.70	105.53
2	2	4371	MHG	C5-C4-N9	3.00	110.25	106.35
2	2	4690	B8K	C5-C4-N3	-3.00	122.42	128.13
2	2	4335	5MC	CM5-C5-C6	-2.99	118.85	122.85
2	2	1316	OMG	C8-N7-C5	2.99	108.69	102.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	4296	B8H	O2-C2-N1	-2.99	119.51	122.87
2	2	4628	PSU	O2-C2-N1	-2.99	119.50	122.79
2	2	4129	B8W	C2-N1-C6	2.98	120.86	116.08
2	2	4870	OMG	C2-N1-C6	-2.97	119.62	125.10
2	2	4620	OMU	C5-C4-N3	2.97	119.29	114.84
2	2	2380	B8W	C1'-N9-C4	-2.96	121.45	126.64
2	2	3897	B8K	C5-C4-N3	-2.95	122.52	128.13
2	2	2424	OMG	O6-C6-C5	-2.94	118.62	124.37
2	2	1522	OMG	C2-N1-C6	-2.94	119.68	125.10
2	2	1456	B8Q	C6-N1-C2	-2.93	119.16	121.79
2	2	2380	B8W	C3'-C2'-C1'	2.93	105.38	100.98
2	2	1574	B9B	C3'-C2'-C1'	2.92	105.37	100.98
2	2	1517	2MG	O6-C6-C5	-2.91	118.68	124.37
2	2	3897	B8K	C6-C5-C4	-2.91	116.62	122.62
2	2	2522	7MG	C4-C5-N7	2.90	109.56	105.53
2	2	4196	OMG	C2-N1-C6	-2.89	119.77	125.10
2	2	2754	B9B	C1'-N9-C4	-2.89	121.56	126.64
2	2	2422	OMC	O2-C2-N3	-2.89	117.64	122.33
2	2	373	OMG	C2-N1-C6	-2.88	119.79	125.10
2	2	4620	OMU	O2-C2-N1	-2.88	118.95	122.79
2	2	2773	OMG	C8-N7-C5	2.87	108.46	102.99
2	2	1605	7MG	C4-C5-N7	2.86	109.49	105.53
2	2	373	OMG	C8-N7-C5	2.85	108.42	102.99
2	2	2297	E7G	O6-C6-C5	-2.85	120.55	127.54
2	2	4564	M7A	C4-N9-C1'	-2.85	119.84	126.60
2	2	2773	OMG	C2-N1-C6	-2.84	119.88	125.10
2	2	4293	PSU	C6-N1-C2	-2.83	119.79	122.68
2	2	4597	UR3	C3U-N3-C2	2.83	122.27	117.31
2	2	4550	7MG	N9-C8-N7	2.83	107.42	103.38
2	2	4403	PSU	O2-C2-N1	-2.82	119.68	122.79
2	2	2786	B9H	O2-C2-N1	-2.81	116.13	122.72
2	2	4355	E6G	C2-N1-C6	2.80	120.58	116.08
2	2	4370	OMG	C2-N1-C6	-2.80	119.95	125.10
2	2	4371	MHG	N1-C2-N3	-2.78	119.65	123.95
2	2	4083	5MU	O2-C2-N1	-2.77	119.10	122.79
2	2	2297	E7G	C2-N1-C6	-2.76	120.06	125.10
2	2	4623	OMG	C2-N1-C6	-2.75	120.04	125.10
2	2	1797	E7G	N9-C8-N7	2.74	107.30	103.38
2	2	1625	OMG	C8-N7-C5	2.74	108.21	102.99
2	2	2297	E7G	C5-C4-N9	2.74	109.90	106.35
7	8	14	OMU	N3-C2-N1	2.74	118.53	114.89
2	2	4636	PSU	O2-C2-N1	-2.73	119.78	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	4872	2MG	O6-C6-C5	-2.73	119.04	124.37
2	2	4370	OMG	C8-N7-C5	2.72	108.17	102.99
2	2	978	2MG	C8-N7-C5	2.71	108.16	102.99
2	2	4530	UR3	C6-N1-C2	-2.71	119.36	121.79
2	2	4637	OMG	O6-C6-C5	-2.71	119.08	124.37
2	2	1683	PSU	C6-N1-C2	-2.70	119.92	122.68
2	2	1797	E7G	C2-N1-C6	-2.70	120.18	125.10
2	2	1677	PSU	O2-C2-N1	-2.70	119.82	122.79
2	2	4637	OMG	C8-N7-C5	2.69	108.12	102.99
2	2	4690	B8K	C2-N1-C6	-2.68	120.21	125.10
2	2	4220	6MZ	C2-N1-C6	2.66	118.87	116.59
2	2	4293	PSU	O2-C2-N1	-2.66	119.86	122.79
2	2	4870	OMG	C8-N7-C5	2.65	108.03	102.99
2	2	4185	B8W	C2-N1-C6	2.64	120.33	116.08
2	2	2364	OMG	C8-N7-C5	2.64	108.02	102.99
2	2	1316	OMG	O6-C6-C5	-2.62	119.25	124.37
2	2	3897	B8K	O3'-C3'-C2'	-2.62	103.34	111.82
2	2	4129	B8W	C4-C5-N7	-2.61	106.68	109.40
2	2	4371	MHG	C71-C72-C73	-2.60	106.91	114.20
2	2	4494	OMG	O6-C6-C5	-2.58	119.33	124.37
2	2	4623	OMG	C8-N7-C5	2.58	107.90	102.99
2	2	4483	B8T	O3'-C3'-C2'	2.58	120.16	111.82
2	2	2861	OMC	O2-C2-N3	-2.57	118.14	122.33
2	2	4690	B8K	O6-C6-C5	-2.55	121.29	127.54
2	2	1860	B8H	O4-C4-N3	-2.54	115.24	120.12
2	2	4494	OMG	C8-N7-C5	2.54	107.83	102.99
2	2	2050	OMG	O6-C6-C5	-2.54	119.42	124.37
2	2	4083	5MU	C6-N1-C2	-2.53	118.74	121.30
2	2	1522	OMG	C8-N7-C5	2.52	107.80	102.99
2	2	2050	OMG	C8-N7-C5	2.52	107.78	102.99
2	2	1605	7MG	N9-C8-N7	2.51	106.97	103.38
2	2	2424	OMG	C8-N7-C5	2.51	107.77	102.99
2	2	1582	PSU	O2-C2-N1	-2.51	120.03	122.79
2	2	4671	B8T	C6-C5-C4	2.50	120.02	116.96
2	2	3869	OMC	C6-C5-C4	2.50	121.54	117.50
2	2	1316	OMG	N2-C2-N1	2.50	122.03	116.71
2	2	4296	B8H	O4-C4-N3	-2.50	115.33	120.12
2	2	1883	OMG	C8-N7-C5	2.49	107.74	102.99
2	2	1797	E7G	O6-C6-C5	-2.49	121.44	127.54
2	2	1456	B8Q	C31-N3-C2	2.49	121.40	117.79
2	2	3897	B8K	O4'-C1'-C2'	-2.48	101.23	106.64
2	2	2522	7MG	C2-N1-C6	-2.48	120.58	125.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	1883	OMG	O6-C6-C5	-2.48	119.53	124.37
2	2	2522	7MG	O6-C6-C5	-2.48	121.47	127.54
2	2	1322	1MA	C8-N7-C5	2.48	107.71	102.99
2	2	4483	B8T	O3'-C3'-C4'	2.47	118.20	111.05
2	2	3897	B8K	C2-N1-C6	-2.46	120.61	125.10
2	2	4196	OMG	C8-N7-C5	2.46	107.67	102.99
2	2	729	2MG	C8-N7-C5	2.44	107.64	102.99
2	2	4306	OMU	O4-C4-C5	-2.44	120.87	125.16
2	2	3899	BGH	C2-N1-C6	-2.43	120.67	125.10
2	2	4550	7MG	C2-N1-C6	-2.42	120.68	125.10
2	2	1659	I4U	O4'-C1'-C2'	-2.41	101.38	106.64
2	2	3909	OMC	C5-C4-N4	2.41	124.36	120.57
2	2	2522	7MG	N9-C8-N7	2.41	106.82	103.38
2	2	4536	OMC	O2-C2-N3	-2.40	118.42	122.33
2	2	1605	7MG	O6-C6-C5	-2.40	121.65	127.54
2	2	4623	OMG	O6-C6-C5	-2.40	119.69	124.37
2	2	4472	B8W	O4'-C1'-C2'	-2.39	103.43	106.93
2	2	2786	B9H	O3'-C3'-C4'	2.38	117.94	111.05
2	2	729	2MG	CM2-N2-C2	-2.38	118.62	123.86
2	2	4415	1MA	C8-N7-C5	2.37	107.51	102.99
2	2	3715	PSU	O2-C2-N1	-2.36	120.19	122.79
2	2	3880	P7G	N9-C8-N7	2.36	106.76	103.38
2	2	4620	OMU	O4-C4-C5	-2.36	121.00	125.16
2	2	2508	PSU	O2-C2-N1	-2.36	120.19	122.79
2	2	1605	7MG	C2-N1-C6	-2.36	120.80	125.10
2	2	1909	P7G	C71-N7-C5	2.36	130.10	124.52
2	2	3715	PSU	C6-N1-C2	-2.36	120.27	122.68
2	2	4483	B8T	C6-C5-C4	2.35	119.84	116.96
2	2	4403	PSU	C6-N1-C2	-2.35	120.28	122.68
2	2	3899	BGH	N1-C2-N3	-2.35	118.94	123.32
2	2	4483	B8T	O2-C2-N3	-2.32	118.56	122.33
2	2	1524	A2M	O4'-C4'-C3'	-2.30	100.55	105.11
2	2	4129	B8W	C3'-C2'-C1'	2.30	104.44	100.98
2	2	4371	MHG	O6-C6-C5	-2.29	121.93	127.54
2	2	1517	2MG	C8-N7-C5	2.28	107.34	102.99
2	2	3867	A2M	O4'-C4'-C3'	-2.28	100.60	105.11
2	2	1909	P7G	N3-C2-N1	-2.28	119.07	123.32
2	2	2364	OMG	O6-C6-C5	-2.28	119.92	124.37
7	8	14	OMU	C1'-N1-C6	-2.27	115.90	120.84
2	2	1348	P4U	O2-C2-N3	-2.27	118.65	122.33
2	2	373	OMG	O6-C6-C5	-2.26	119.95	124.37
2	2	4129	B8W	C5-C6-N1	-2.26	118.96	123.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	729	2MG	O6-C6-C5	-2.25	119.97	124.37
2	2	4196	OMG	O6-C6-C5	-2.25	119.97	124.37
2	2	1625	OMG	O6-C6-C5	-2.24	119.99	124.37
2	2	4083	5MU	O4-C4-N3	-2.24	115.82	120.12
2	2	2786	B9H	C32-C31-N3	2.23	117.14	112.47
2	2	2422	OMC	C1'-N1-C2	2.23	123.40	118.42
2	2	978	2MG	O6-C6-C5	-2.23	120.02	124.37
2	2	4370	OMG	O6-C6-C5	-2.23	120.03	124.37
2	2	3880	P7G	N2-C2-N3	2.22	121.44	116.71
2	2	4597	UR3	O2-C2-N1	-2.22	117.53	122.72
2	2	4564	M7A	C5-C4-N3	-2.22	121.42	126.62
2	2	4636	PSU	C6-N1-C2	-2.21	120.42	122.68
2	2	2773	OMG	N2-C2-N1	2.21	121.42	116.71
2	2	373	OMG	N1-C2-N3	-2.21	119.19	123.32
2	2	4529	B8W	C2-N1-C6	2.21	119.63	116.08
2	2	1659	I4U	O4'-C4'-C3'	-2.20	100.76	105.11
2	2	2804	OMC	O2-C2-N3	-2.20	118.75	122.33
2	2	1522	OMG	O6-C6-C5	-2.19	120.10	124.37
2	2	4550	7MG	N9-C4-N3	2.18	128.73	125.47
2	2	2297	E7G	N9-C8-N7	2.18	106.50	103.38
2	2	1659	I4U	O2-C2-N3	-2.16	118.81	122.33
2	2	2297	E7G	C6-C5-C4	-2.16	118.16	122.62
2	2	4550	7MG	O6-C6-C5	-2.16	122.24	127.54
2	2	4403	PSU	O4'-C1'-C2'	2.16	108.19	105.14
2	2	3909	OMC	C4-N3-C2	2.15	123.73	120.25
2	2	4129	B8W	O6-C6-N1	2.15	122.00	119.03
2	2	4371	MHG	C72-C71-N7	2.11	114.49	112.41
2	2	4690	B8K	N1-C2-N3	-2.11	119.39	123.32
2	2	1677	PSU	C6-N1-C2	-2.10	120.53	122.68
2	2	4370	OMG	N2-C2-N1	2.10	121.18	116.71
2	2	4185	B8W	C1'-N9-C4	-2.10	122.96	126.64
2	2	3880	P7G	N3-C2-N1	-2.09	119.42	123.32
2	2	3899	BGH	O6-C6-N1	-2.09	116.12	120.12
2	2	1456	B8Q	C1'-N1-C2	2.08	120.51	116.99
2	2	1866	UR3	C1'-N1-C2	2.08	120.50	116.99
2	2	2297	E7G	N9-C4-N3	2.08	128.57	125.47
2	2	3899	BGH	C2'-C1'-N9	-2.08	109.92	114.14
2	2	4472	B8W	C2-N1-C6	2.08	119.41	116.08
2	2	1797	E7G	C8-N7-C71	2.07	125.43	120.50
2	2	1605	7MG	C6-C5-C4	-2.06	118.36	122.62
2	2	2424	OMG	N1-C2-N3	-2.06	119.47	123.32
2	2	1659	I4U	C6-N1-C2	-2.06	116.92	120.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	1677	PSU	O4'-C1'-C2'	2.06	108.04	105.14
2	2	2522	7MG	C6-C5-C4	-2.05	118.39	122.62
2	2	3897	B8K	N1-C2-N3	-2.05	119.49	123.32
2	2	4185	B8W	O4'-C4'-C3'	-2.05	101.06	105.11
2	2	4872	2MG	C8-N7-C5	2.05	106.89	102.99
2	2	1574	B9B	N2-C2-N1	2.04	120.43	117.25
2	2	4129	B8W	O6-C6-C5	2.04	118.92	116.01
2	2	4355	E6G	C5-C6-N1	-2.03	119.39	123.26
2	2	4870	OMG	O6-C6-C5	-2.03	120.41	124.37
2	2	4371	MHG	C6-C5-C4	-2.02	118.45	122.62
2	2	3897	B8K	O6-C6-N1	-2.01	116.26	120.12
2	2	1659	I4U	O4-C41-C42	2.01	112.47	107.14
2	2	4523	A2M	C3'-C2'-C1'	2.00	106.66	102.89

There are no chirality outliers.

All (128) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	8	14	OMU	C1'-C2'-O2'-CM2
2	2	237	B9B	C5-C6-O6-C61
2	2	237	B9B	N1-C6-O6-C61
2	2	237	B9B	C3'-C4'-C5'-O5'
2	2	237	B9B	O4'-C4'-C5'-O5'
2	2	398	A2M	O4'-C4'-C5'-O5'
2	2	1348	P4U	N3-C4-O4-C41
2	2	1574	B9B	C5-C6-O6-C61
2	2	1574	B9B	N1-C6-O6-C61
2	2	1582	PSU	C3'-C4'-C5'-O5'
2	2	1582	PSU	O4'-C4'-C5'-O5'
2	2	1625	OMG	C3'-C4'-C5'-O5'
2	2	1797	E7G	C72-C71-N7-C5
2	2	1871	A2M	O4'-C4'-C5'-O5'
2	2	1871	A2M	C3'-C4'-C5'-O5'
2	2	1883	OMG	O4'-C4'-C5'-O5'
2	2	1883	OMG	C3'-C4'-C5'-O5'
2	2	2297	E7G	C72-C71-N7-C5
2	2	2424	OMG	O4'-C4'-C5'-O5'
2	2	2424	OMG	C3'-C4'-C5'-O5'
2	2	2754	B9B	C5-C6-O6-C61
2	2	2754	B9B	N1-C6-O6-C61
2	2	2861	OMC	C1'-C2'-O2'-CM2
2	2	3701	OMC	C2'-C1'-N1-C2

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Mol	Chain	Res	Type	Atoms
2	2	3701	OMC	C2'-C1'-N1-C6
2	2	3867	A2M	C3'-C4'-C5'-O5'
2	2	3867	A2M	C1'-C2'-O2'-CM'
2	2	3869	OMC	O4'-C1'-N1-C2
2	2	4129	B8W	C5-C6-O6-C61
2	2	4129	B8W	N1-C6-O6-C61
2	2	4185	B8W	C5-C6-O6-C61
2	2	4185	B8W	N1-C6-O6-C61
2	2	4194	I4U	C3'-C4'-C5'-O5'
2	2	4194	I4U	O4'-C4'-C5'-O5'
2	2	4355	E6G	C5-C6-O6-C61
2	2	4355	E6G	N1-C6-O6-C61
2	2	4403	PSU	O4'-C1'-C5-C4
2	2	4403	PSU	O4'-C1'-C5-C6
2	2	4415	1MA	O4'-C4'-C5'-O5'
2	2	4472	B8W	C5-C6-O6-C61
2	2	4472	B8W	N1-C6-O6-C61
2	2	4523	A2M	O4'-C4'-C5'-O5'
2	2	4529	B8W	C5-C6-O6-C61
2	2	4529	B8W	N1-C6-O6-C61
2	2	4636	PSU	C2'-C1'-C5-C6
2	2	4636	PSU	C3'-C4'-C5'-O5'
2	2	4636	PSU	O4'-C4'-C5'-O5'
2	2	4870	OMG	O4'-C4'-C5'-O5'
2	2	4870	OMG	C3'-C4'-C5'-O5'
2	2	1659	I4U	O4'-C4'-C5'-O5'
2	2	1797	E7G	O4'-C4'-C5'-O5'
2	2	2364	OMG	O4'-C4'-C5'-O5'
2	2	3897	B8K	C3'-C4'-C5'-O5'
2	2	3897	B8K	O4'-C4'-C5'-O5'
2	2	4220	6MZ	C3'-C4'-C5'-O5'
2	2	4293	PSU	O4'-C4'-C5'-O5'
2	2	4371	MHG	O4'-C4'-C5'-O5'
2	2	4415	1MA	C3'-C4'-C5'-O5'
2	2	4872	2MG	O4'-C4'-C5'-O5'
2	2	1574	B9B	O6-C61-C62-C63
2	2	398	A2M	C3'-C4'-C5'-O5'
2	2	1797	E7G	C3'-C4'-C5'-O5'
2	2	3867	A2M	O4'-C4'-C5'-O5'
2	2	3880	P7G	O4'-C4'-C5'-O5'
2	2	4220	6MZ	O4'-C4'-C5'-O5'
2	2	4293	PSU	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
2	2	4523	A2M	C3'-C4'-C5'-O5'
2	2	4529	B8W	O4'-C4'-C5'-O5'
2	2	4872	2MG	C3'-C4'-C5'-O5'
2	2	3909	OMC	O4'-C4'-C5'-O5'
2	2	237	B9B	O6-C61-C62-C63
2	2	3869	OMC	O4'-C1'-N1-C6
2	2	1625	OMG	O4'-C4'-C5'-O5'
2	2	2364	OMG	C3'-C4'-C5'-O5'
2	2	3880	P7G	N7-C71-C72-C73
2	2	1797	E7G	C72-C71-N7-C8
2	2	2773	OMG	O4'-C4'-C5'-O5'
2	2	3729	PSU	O4'-C4'-C5'-O5'
2	2	3899	BGH	O4'-C4'-C5'-O5'
2	2	4371	MHG	C3'-C4'-C5'-O5'
2	2	4371	MHG	C2'-C1'-N9-C8
2	2	4371	MHG	C75-C73-C74-C76
2	2	1534	A2M	C3'-C2'-O2'-CM'
2	2	4371	MHG	C72-C73-C74-C76
2	2	1326	A2M	C4'-C5'-O5'-P
2	2	3867	A2M	C4'-C5'-O5'-P
2	2	4870	OMG	C4'-C5'-O5'-P
2	2	3880	P7G	C3'-C4'-C5'-O5'
2	2	4371	MHG	C72-C71-N7-C5
2	2	2861	OMC	O4'-C4'-C5'-O5'
2	2	1909	P7G	C72-C71-N7-C8
2	2	3887	OMC	C4'-C5'-O5'-P
2	2	3897	B8K	C4'-C5'-O5'-P
2	2	4194	I4U	C4'-C5'-O5'-P
2	2	4550	7MG	O4'-C4'-C5'-O5'
2	2	3869	OMC	C3'-C2'-O2'-CM2
2	2	2786	B9H	C32-C31-N3-C2
2	2	1866	UR3	C4'-C5'-O5'-P
2	2	3701	OMC	O4'-C1'-N1-C6
2	2	2297	E7G	C72-C71-N7-C8
2	2	1534	A2M	C4'-C5'-O5'-P
2	2	4550	7MG	C3'-C4'-C5'-O5'
2	2	4371	MHG	C72-C71-N7-C8
2	2	4194	I4U	C42-C41-O4-C4
2	2	1860	B8H	O4'-C1'-C5-C4
2	2	3869	OMC	C4'-C5'-O5'-P
2	2	4671	B8T	C2'-C1'-N1-C6
2	2	1860	B8H	C4'-C5'-O5'-P

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Mol	Chain	Res	Type	Atoms
2	2	1909	P7G	O4'-C4'-C5'-O5'
2	2	2422	OMC	O4'-C4'-C5'-O5'
2	2	2508	PSU	O4'-C4'-C5'-O5'
2	2	4371	MHG	O4'-C1'-N9-C8
2	2	373	OMG	C4'-C5'-O5'-P
2	2	4415	1MA	C4'-C5'-O5'-P
2	2	1659	I4U	C3'-C4'-C5'-O5'
2	2	2773	OMG	C3'-C4'-C5'-O5'
2	2	3729	PSU	C3'-C4'-C5'-O5'
2	2	3909	OMC	C3'-C4'-C5'-O5'
2	2	4671	B8T	O4'-C1'-N1-C6
2	2	3701	OMC	O4'-C1'-N1-C2
2	2	729	2MG	O4'-C4'-C5'-O5'
2	2	1456	B8Q	C3'-C4'-C5'-O5'
2	2	1677	PSU	O4'-C1'-C5-C6
2	2	4636	PSU	O4'-C1'-C5-C6
2	2	1534	A2M	O4'-C4'-C5'-O5'
2	2	3880	P7G	C72-C71-N7-C8
2	2	4194	I4U	C43-C41-O4-C4
2	2	4371	MHG	C4'-C5'-O5'-P

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 250 ligands modelled in this entry, 250 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.



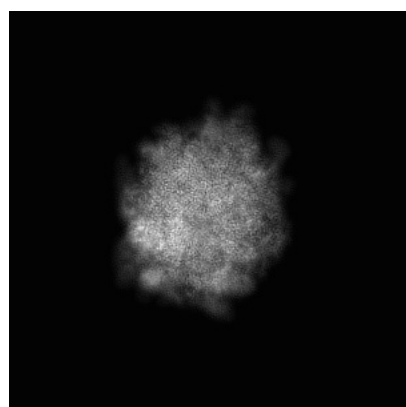
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0964. These allow visual inspection of the internal detail of the map and identification of artifacts.

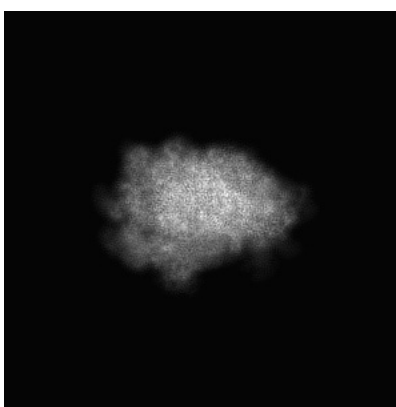
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

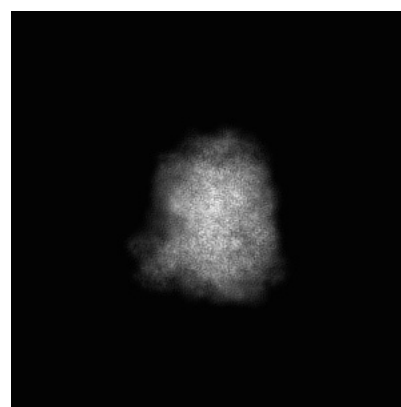
#### 6.1.1 Primary map



X



Y

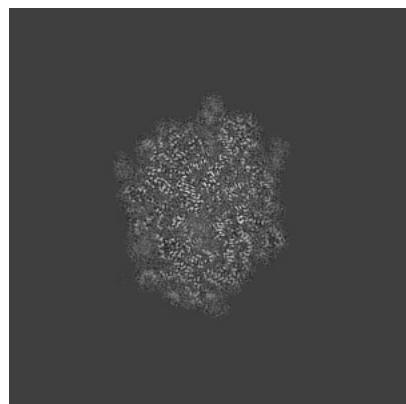


Z

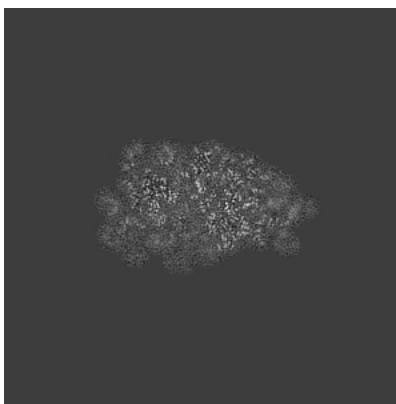
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

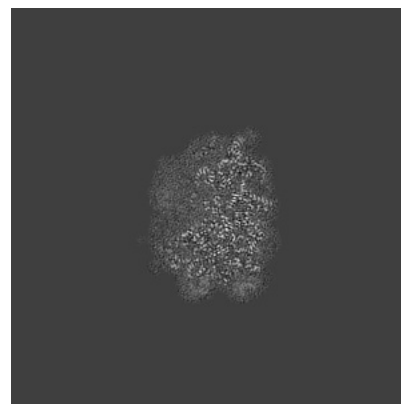
#### 6.2.1 Primary map



X Index: 240



Y Index: 240

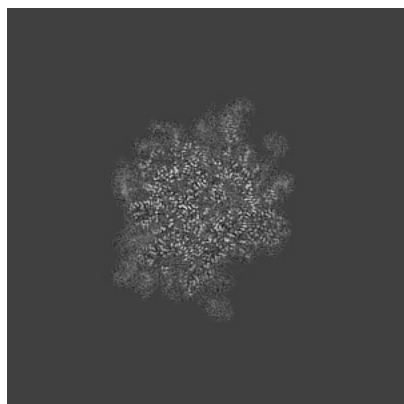


Z Index: 240

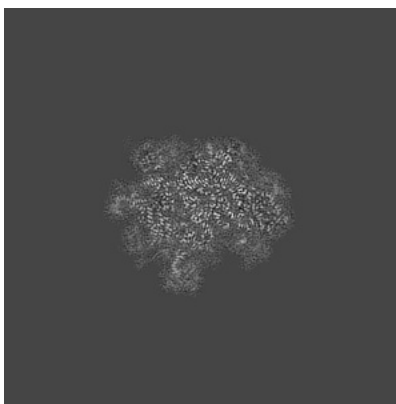
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

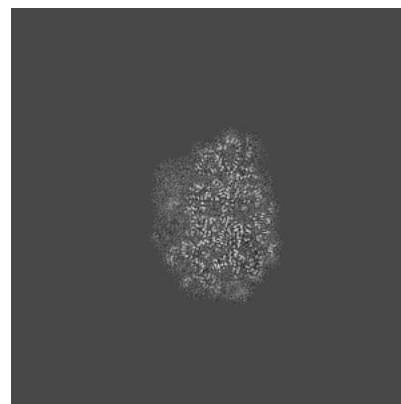
### 6.3.1 Primary map



X Index: 258



Y Index: 201

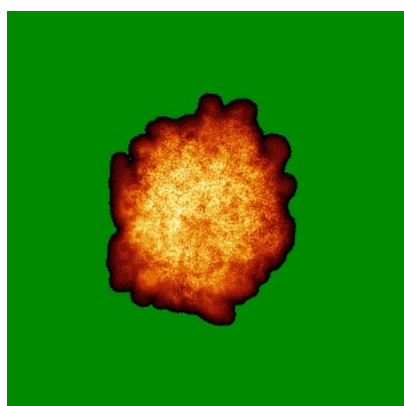


Z Index: 252

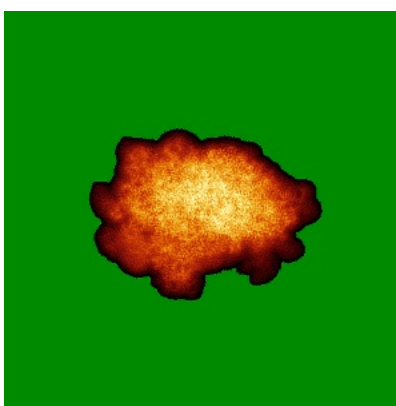
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

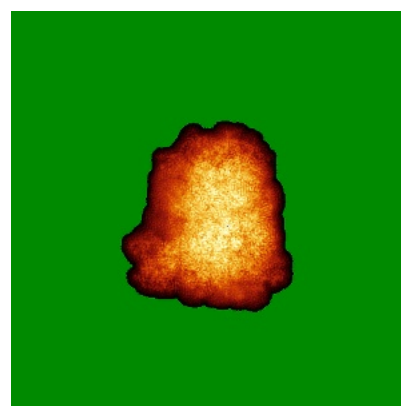
### 6.4.1 Primary map



X



Y

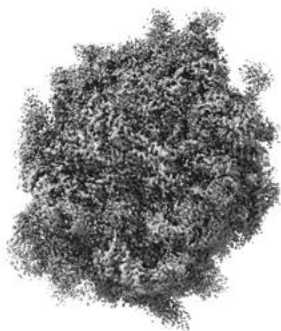


Z

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](#)

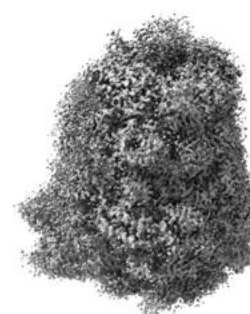
### 6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.065. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

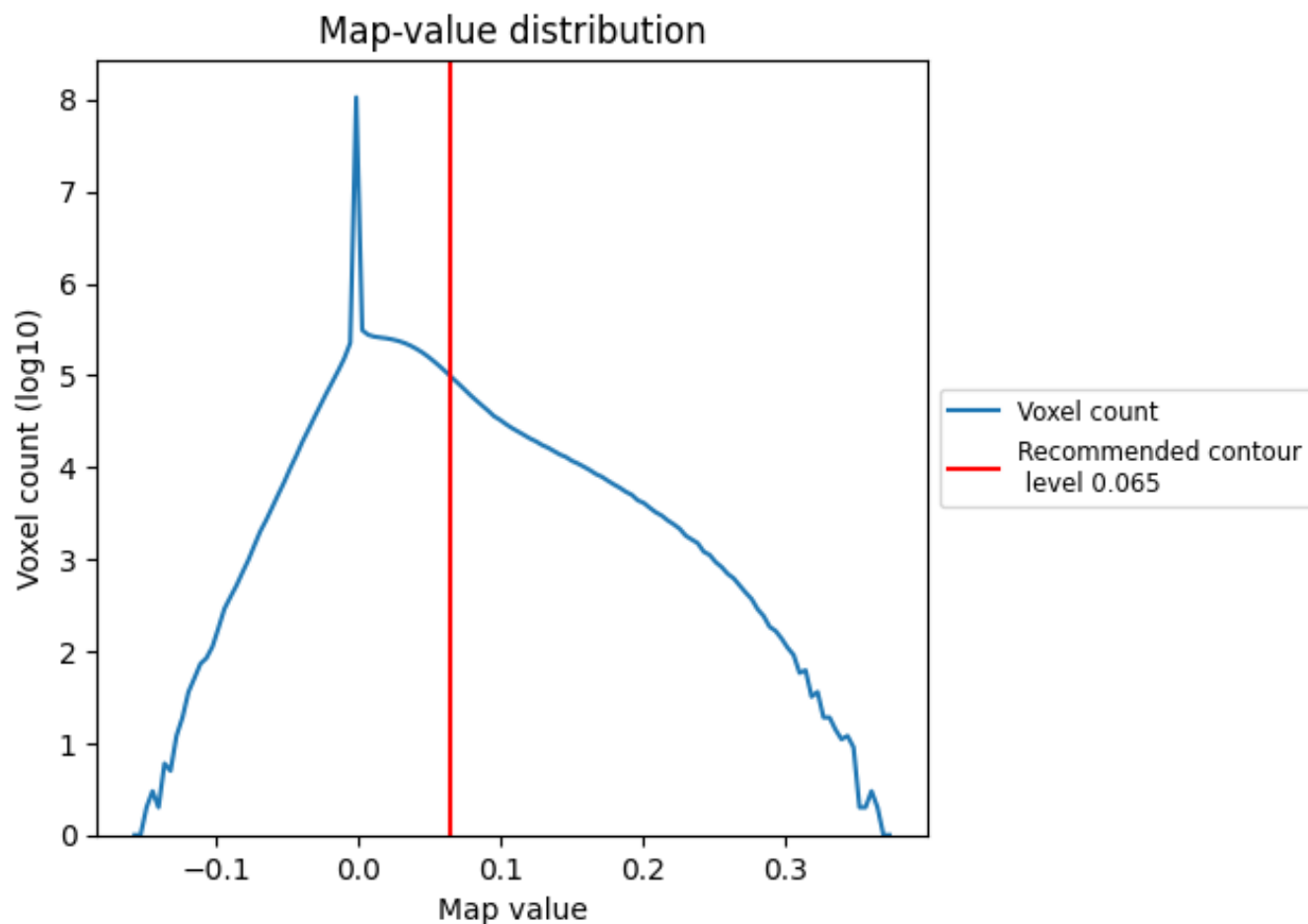
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

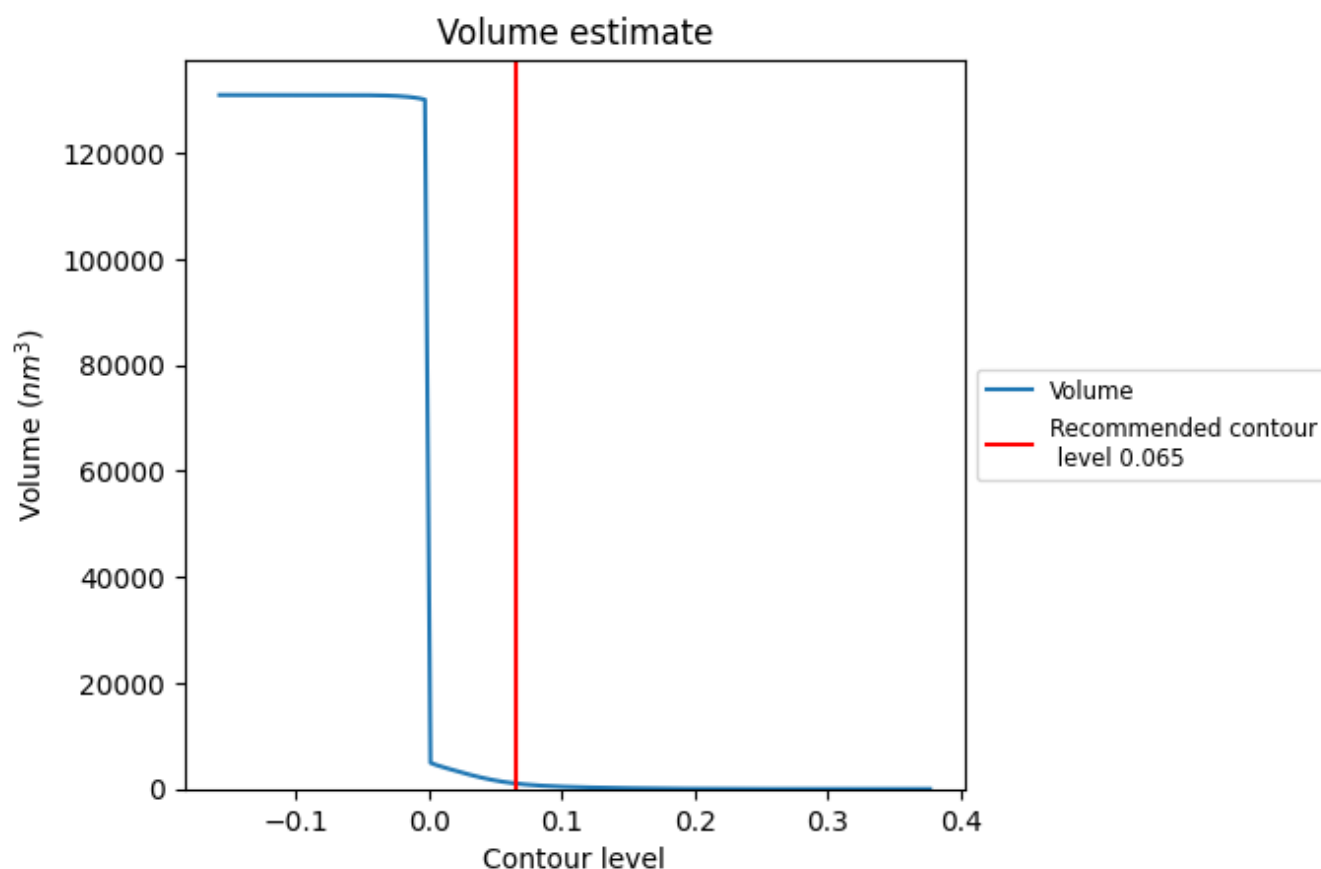
This section contains the results of statistical analysis of the map.

### 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.

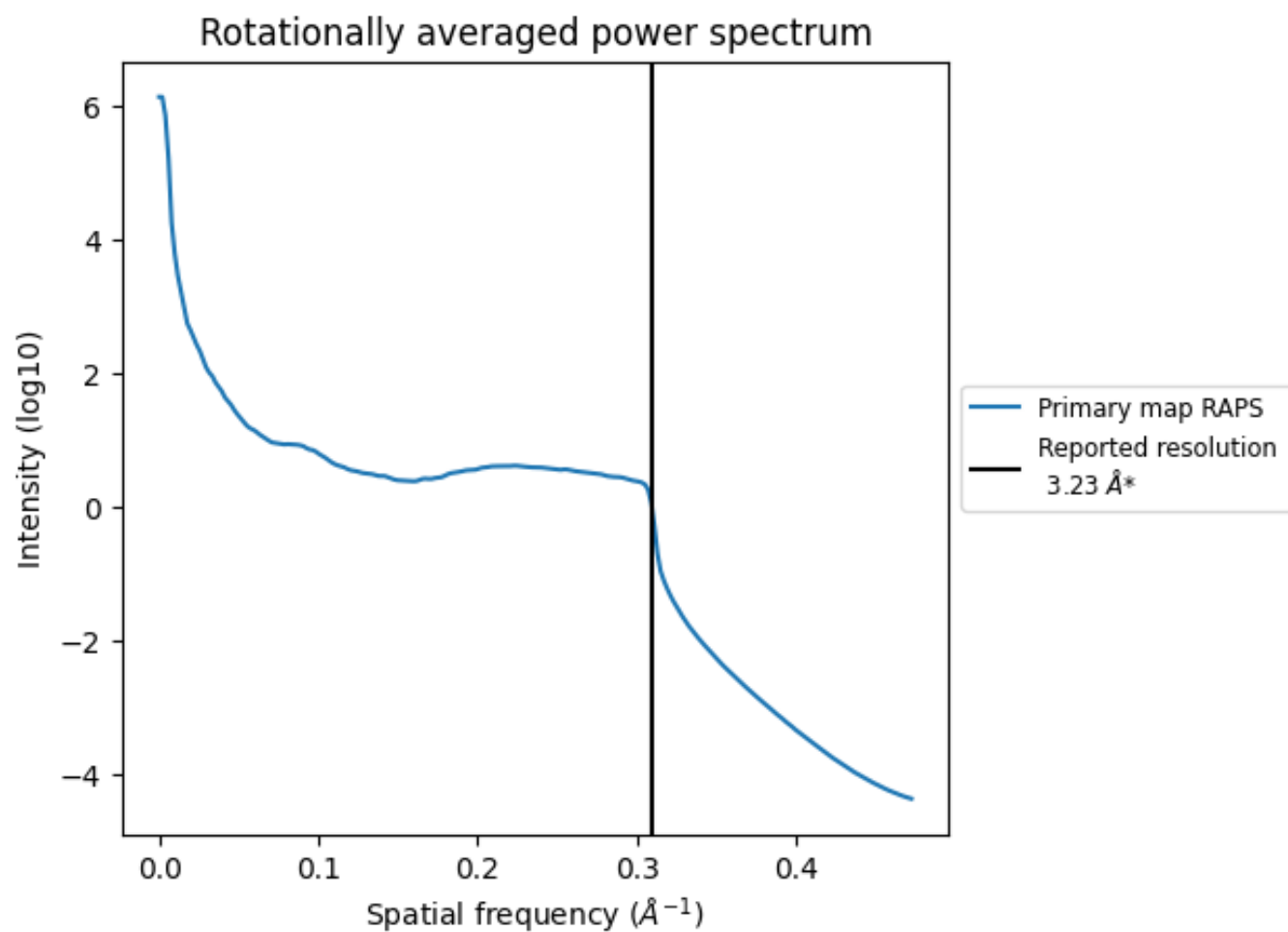
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1045 nm<sup>3</sup>; this corresponds to an approximate mass of 944 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 ⓘ



\*Reported resolution corresponds to spatial frequency of 0.310 Å<sup>-1</sup>

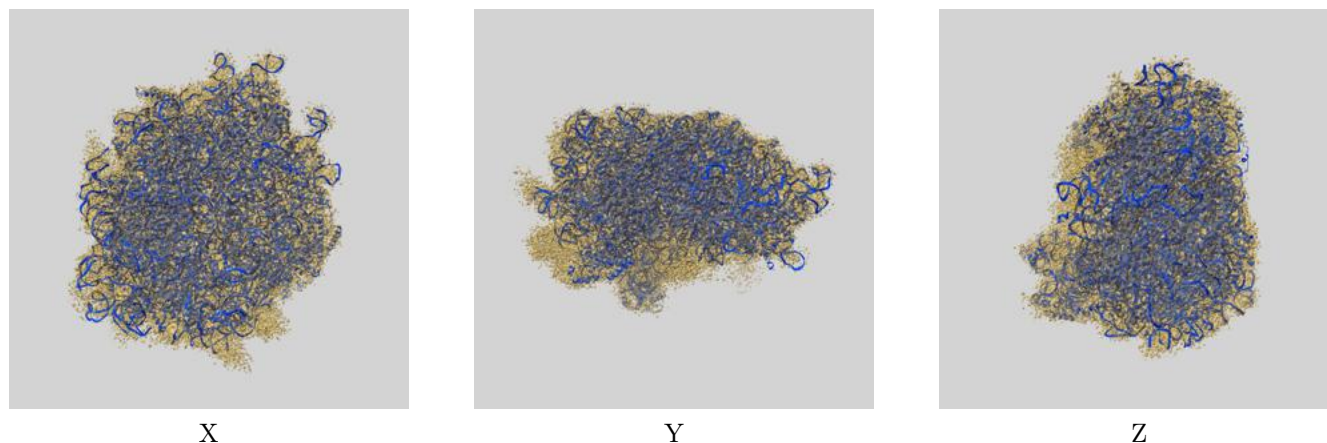
## 8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-0964 and PDB model 6LSS. Per-residue inclusion information can be found in [section 3](#) on [page 13](#).

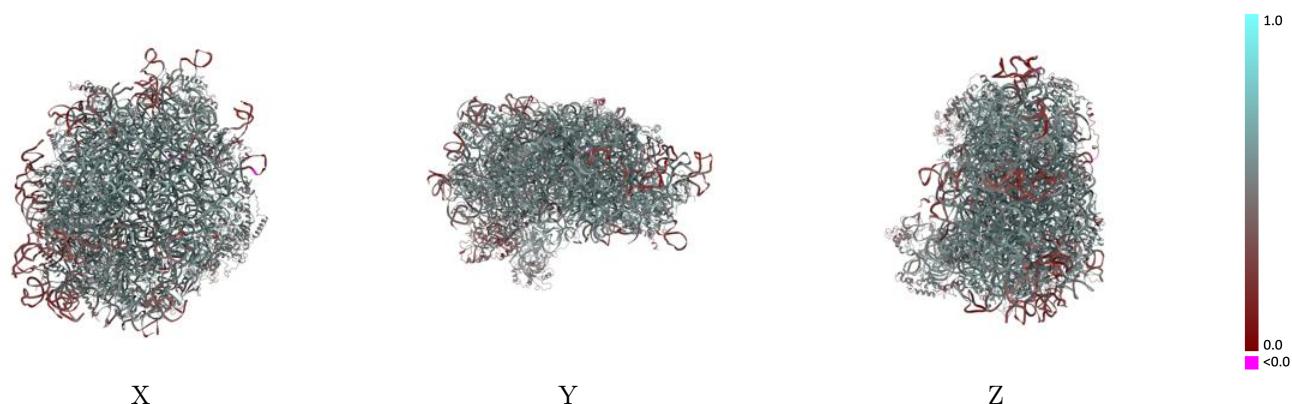
### 9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.065 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

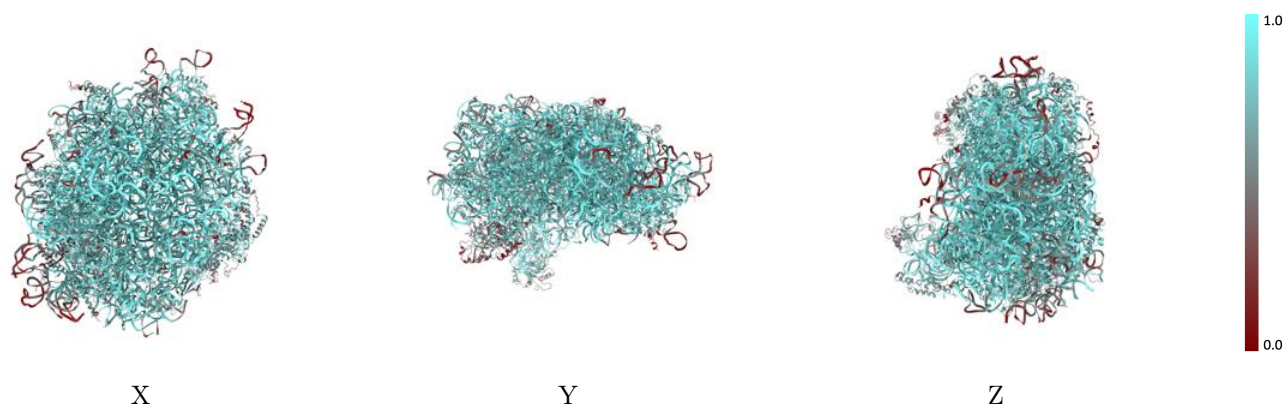


## 9.2 Q-score mapped to coordinate model [i](#)



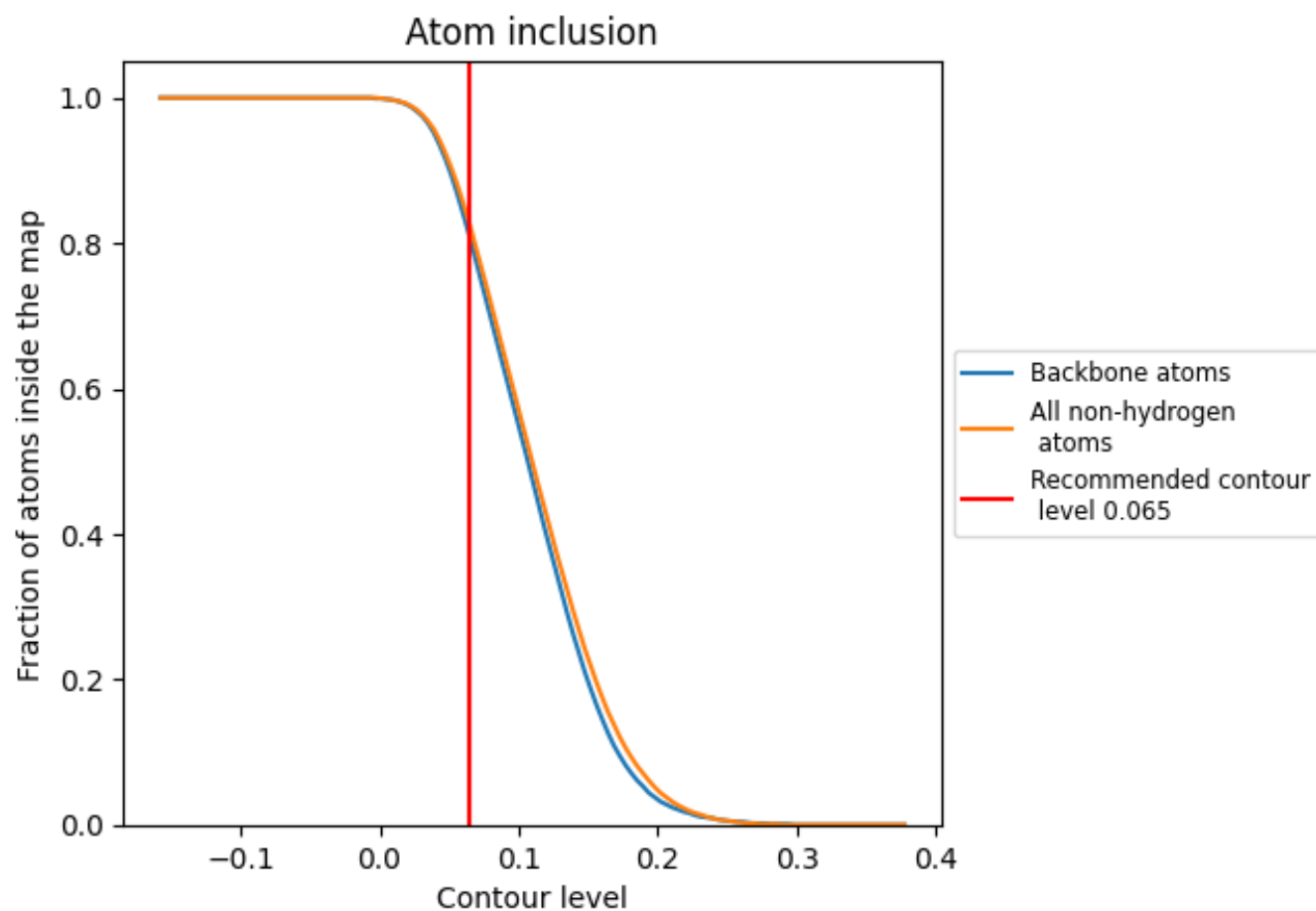
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.065).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 81% of all backbone atoms, 82% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary ⓘ





























The table lists the average atom inclusion at the recommended contour level (0.065) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8240	 0.5150
1	 0.2250	 0.3490
2	 0.8480	 0.5010
4	 0.6350	 0.4600
5	 0.9100	 0.5160
6	 0.7040	 0.5070
7	 0.7970	 0.5370
8	 0.9110	 0.5400
9	 0.7750	 0.5180
B	 0.8620	 0.5620
C	 0.7330	 0.4790
D	 0.8830	 0.5660
E	 0.7150	 0.5260
F	 0.8560	 0.5530
G	 0.7140	 0.5090
H	 0.8140	 0.5490
I	 0.7600	 0.5200
K	 0.7830	 0.5200
L	 0.8970	 0.5790
M	 0.9440	 0.5800
N	 0.5780	 0.4230
O	 0.6800	 0.5060
P	 0.9170	 0.5750
Q	 0.7950	 0.5280
R	 0.4480	 0.3980
S	 0.8330	 0.5430
U	 0.9310	 0.5890
V	 0.8710	 0.5640
W	 0.8190	 0.5370
X	 0.8240	 0.5460
Y	 0.8960	 0.5710
Z	 0.8960	 0.5800
a	 0.8370	 0.5550
b	 0.8760	 0.5710
c	 0.8610	 0.5510



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Chain	Atom inclusion	Q-score
d	 0.7340	 0.5120
e	 0.8380	 0.5350
g	 0.8310	 0.5480
h	 0.8250	 0.5530
i	 0.7730	 0.5370
j	 0.8160	 0.5480
k	 0.8930	 0.5780
l	 0.8540	 0.5610
m	 0.8810	 0.5670
n	 0.9040	 0.5820
o	 0.7010	 0.4950
p	 0.8580	 0.5540
r	 0.6740	 0.4820
z	 0.7400	 0.5190