



Full wwPDB EM Validation Report ⓘ

Oct 15, 2021 – 01:50 am BST

PDB ID : 7PJZ
EMDB ID : EMD-13465
Title : Structure of the 70S-EF-G-GDP ribosome complex with tRNAs in chimeric state 2 (CHI2-EF-G-GDP)
Authors : Petrychenko, V.; Peng, B.Z.; Schwarzer, A.C.; Peske, F.; Rodnina, M.V.; Fischer, N.
Deposited on : 2021-08-24
Resolution : 6.00 Å (reported)
Based on initial models : 4AQY, 5J9Z, 5LZD, 6YSS

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

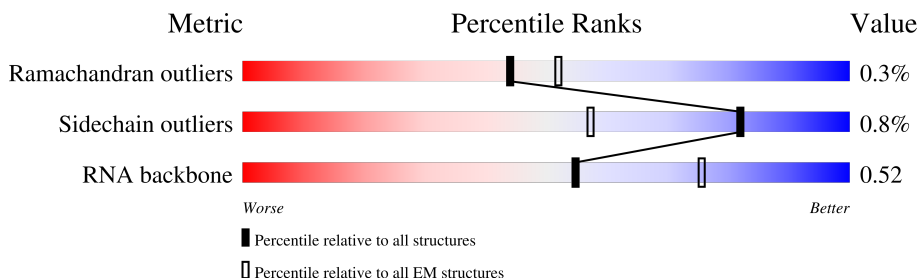
EMDB validation analysis : 0.0.0.dev97
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.23.2

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 6.00 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	0	57	
2	1	55	
3	2	46	
4	3	65	
5	4	38	
6	5	165	
7	6	70	
8	A	2903	

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Mol	Chain	Length	Quality of chain
9	B	120	32% 59% 9%
10	C	273	5% 96%
11	D	209	100%
12	E	201	100%
13	F	179	98%
14	G	177	97%
15	H	149	47% 99%
16	I	142	43% 99%
17	J	142	6% 99%
18	K	123	10% 96%
19	L	144	6% 97%
20	M	136	97%
21	N	127	93% 6%
22	O	117	97%
23	P	115	5% 98%
24	Q	118	98%
25	R	103	98%
26	S	110	96%
27	T	100	90% 7%
28	U	104	94%
29	V	94	99%
30	W	85	87% 12%
31	X	78	94% 5%
32	Y	63	98%
33	Z	59	98%


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Mol	Chain	Length	Quality of chain
34	a	1542	39% 49% 11%
35	b	240	21% 88% 9%
36	c	233	88% 12%
37	d	206	5% 97%
38	e	167	92% 6%
39	f	135	74% 26%
40	g	179	16% 83% 16%
41	h	130	6% 99%
42	i	130	5% 97%
43	j	103	5% 94% 5%
44	k	129	89% 10%
45	l	124	5% 96%
46	m	118	5% 97%
47	n	102	5% 98%
48	o	89	98%
49	p	82	6% 99%
50	q	84	94% 5%
51	r	75	84% 13%
52	s	92	86% 11%
53	t	87	98%
54	u	71	8% 90% 8%
55	v	77	43% 47% 10%
56	w	76	11% 46% 42% 12%
57	x	704	21% 92% 5%
58	y	2	50% 50%

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Mol	Chain	Length	Quality of chain
59	z	33	 21% 9% 70%

2 Entry composition

There are 62 unique types of molecules in this entry. The entry contains 152440 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 50S ribosomal protein L32.

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

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

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

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

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

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

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

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

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

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

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

- Molecule 7 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	6	66	522	323	99	94	6	0	0

- Molecule 8 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
8	A	2903	62338	27816	11471	20148	2903	0	0

- Molecule 9 is a RNA chain called 5S ribosomal RNA.

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

- Molecule 10 is a protein called 50S ribosomal protein L2.

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

- Molecule 11 is a protein called 50S ribosomal protein L3.

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

- Molecule 12 is a protein called 50S ribosomal protein L4.

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

- Molecule 13 is a protein called 50S ribosomal protein L5.

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

- Molecule 14 is a protein called 50S ribosomal protein L6.

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

- Molecule 15 is a protein called 50S ribosomal protein L9.

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

- Molecule 16 is a protein called 50S ribosomal protein L11.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 25 is a protein called 50S ribosomal protein L21.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 34 is a RNA chain called 16S ribosomal RNA.

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

- Molecule 35 is a protein called 30S ribosomal protein S2.

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

- Molecule 36 is a protein called 30S ribosomal protein S3.

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

- Molecule 37 is a protein called 30S ribosomal protein S4.

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

- Molecule 38 is a protein called 30S ribosomal protein S5.

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

- Molecule 39 is a protein called 30S ribosomal protein S6.

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

- Molecule 40 is a protein called 30S ribosomal protein S7.

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

- Molecule 41 is a protein called 30S ribosomal protein S8.

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

- Molecule 42 is a protein called 30S ribosomal protein S9.

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

- Molecule 43 is a protein called 30S ribosomal protein S10.

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

- Molecule 44 is a protein called 30S ribosomal protein S11.

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

- Molecule 45 is a protein called 30S ribosomal protein S12.

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

- Molecule 46 is a protein called 30S ribosomal protein S13.

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

- Molecule 47 is a protein called 30S ribosomal protein S14.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 48 is a protein called 30S ribosomal protein S15.

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

- Molecule 49 is a protein called 30S ribosomal protein S16.

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

- Molecule 50 is a protein called 30S ribosomal protein S17.

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

- Molecule 51 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	r	65	Total	C	N	O	S	0	0
			535	339	100	95	1		

- Molecule 52 is a protein called 30S ribosomal protein S19.

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

- Molecule 53 is a protein called 30S ribosomal protein S20.

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

- Molecule 54 is a protein called 30S ribosomal protein S21.

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

- Molecule 55 is a RNA chain called P-site tRNA(fMet).

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	N	O	P			S
55	v	77	1642	733	297	534	77	1	0	0

- Molecule 56 is a RNA chain called P-site fMet-Phe-tRNA(Phe).

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

- Molecule 57 is a protein called Elongation factor G.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
57	x	669	5192	3275	900	994	23	1	0

- Molecule 58 is a protein called Dipeptide (FME-PHE).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
58	y	2	21	15	2	3	1	0	0

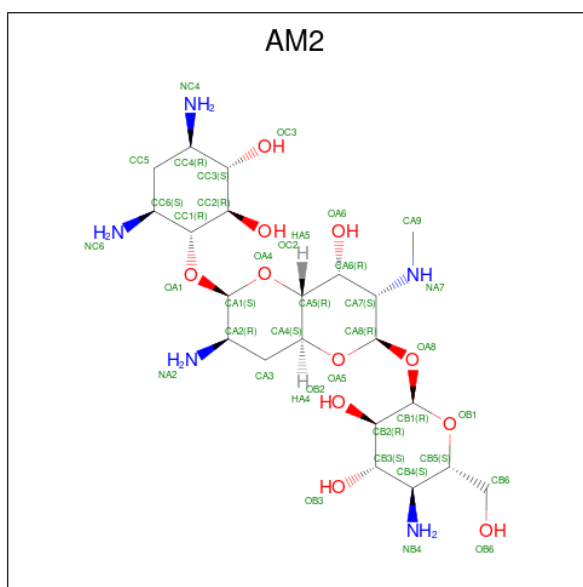
- Molecule 59 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
59	z	10	208	93	29	76	10	0	0

- Molecule 60 is ZINC ION (three-letter code: ZN) (formula: Zn).

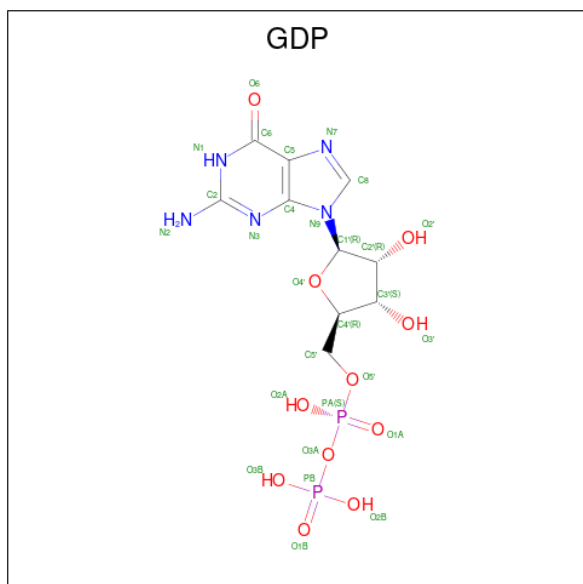
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
60	6	1	1	1	0

- Molecule 61 is APRAMYCIN (three-letter code: AM2) (formula: C₂₁H₄₁N₅O₁₁).



Mol	Chain	Residues	Atoms				AltConf
61	a	1	Total	C	N	O	0
			37	21	5	11	

- Molecule 62 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).

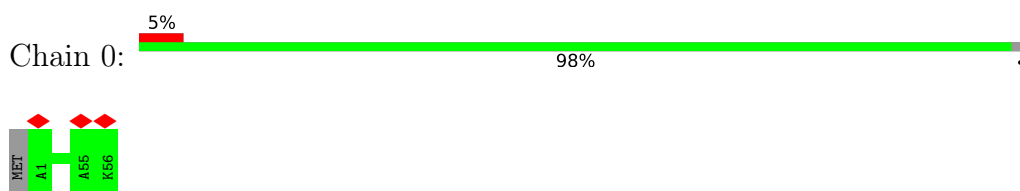


Mol	Chain	Residues	Atoms					AltConf
62	x	1	Total	C	N	O	P	0
			28	10	5	11	2	

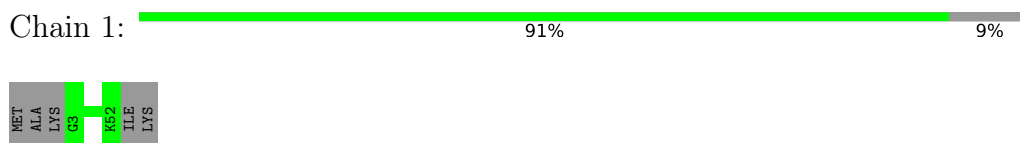
3 Residue-property plots [i](#)

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

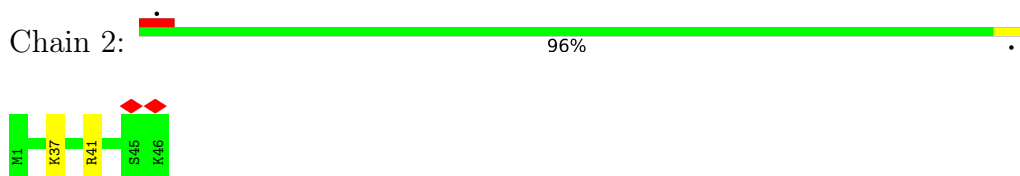
- Molecule 1: 50S ribosomal protein L32



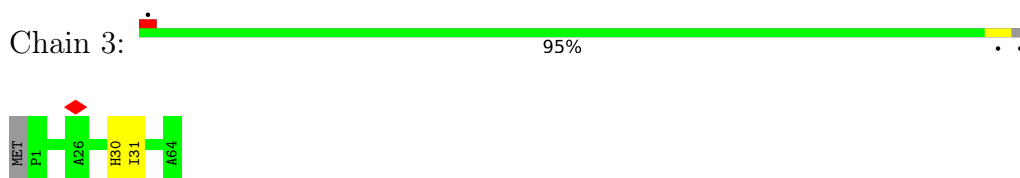
- Molecule 2: 50S ribosomal protein L33



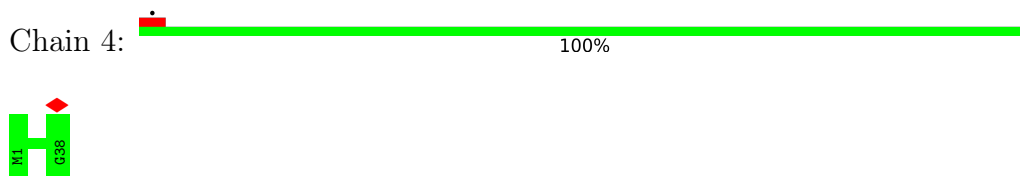
- Molecule 3: 50S ribosomal protein L34



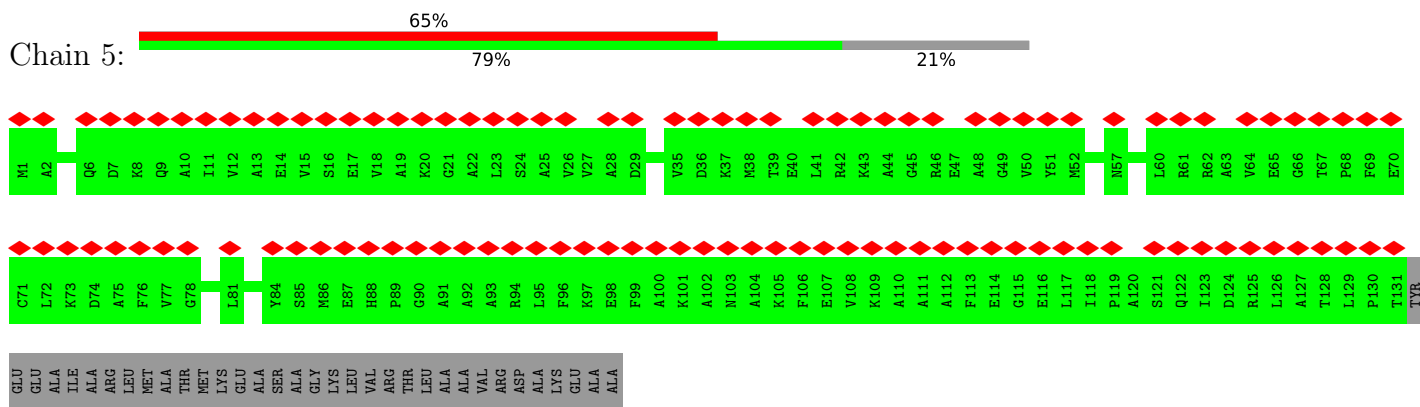
- Molecule 4: 50S ribosomal protein L35



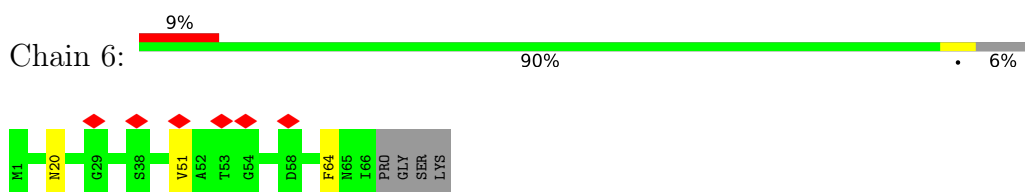
- Molecule 5: 50S ribosomal protein L36



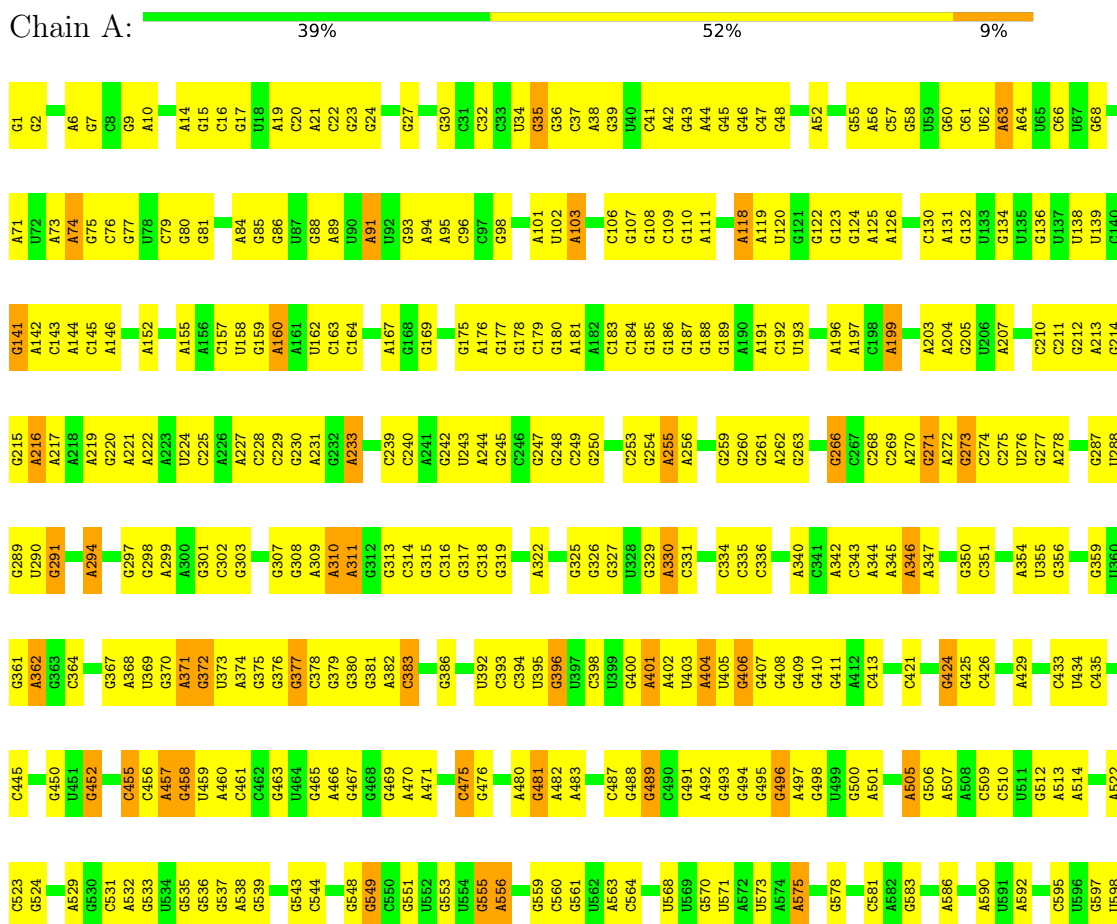
• Molecule 6: 50S ribosomal protein L10



• Molecule 7: 50S ribosomal protein L31

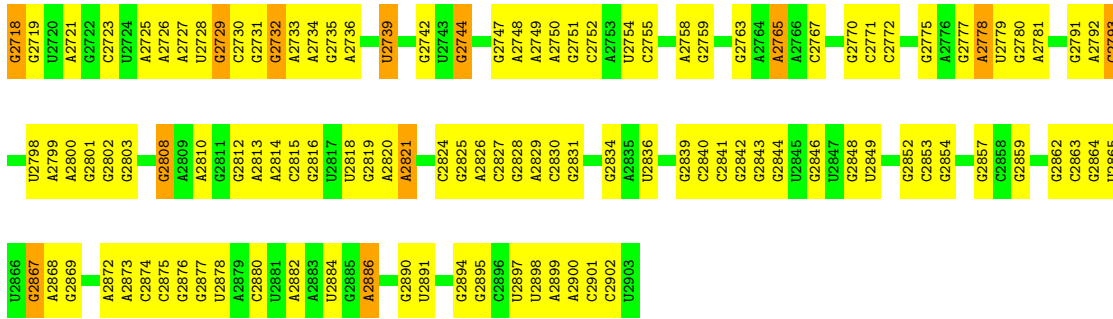


• Molecule 8: 23S ribosomal RNA

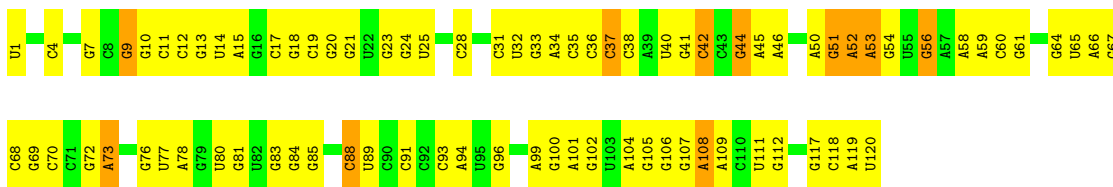


G1628	G1631	A1634	C1638	C1639	C1550	A1551	A1552	A1553	C1556	C1557	C1558	C1561	C1566	C1567	A1569	A1570	A1571	A1572	A1573	C1577	A1578	A1580	A1583	A1584	C1585	A1586	C1587	C1588	A1589	A1590	A1591	C1592	A1593	A1596	C1600	C1603	C1604	C1606	C1607	U1608	A1609	A1610	C1615	C1616	A1617	C1618	C1619	A1626	G1627																																																																												
G1472	G1473	U1474	G1475	C1476	U1477	U1478	G1479	G1482	A1490	C1491	G1492	C1493	U1497	C1498	G1501	A1502	A1503	G1511	G1512	U1513	G1514	A1515	G1516	G1517	C1518	G1519	U1520	G1521	A1522	U1523	G1524	A1525	C1526	G1527	A1528	G1529	G1530	C1531	A1532	C1533	C1534	A1535	C1536	G1537	G1538	U1539	G1540	C1541	C1542	C1543	A1544	A1548	A1549																																																																								
A1395	C1398	C1399	U1400	U1401	U1402	A1403	C1404	G1407	G1408	U1409	G1410	U1415	G1416	C1417	G1418	A1419	A1420	G1421	G1422	G1423	G1424	G1425	G1426	A1427	C1428	G1429	G1430	A1433	A1434	G1435	G1436	G1445	G1448	G1449	G1450	C1451	G1452	A1453	C1454	G1455	G1456	U1457	U1458	G1459	U1460	C1461	U1462	C1463	A1465	A1469	A1471																																																																										
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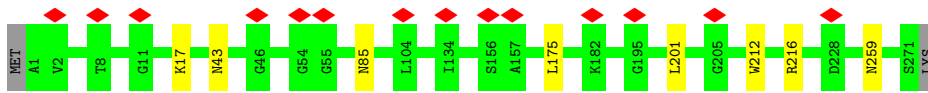
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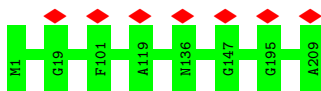
• Molecule 9: 5S ribosomal RNA



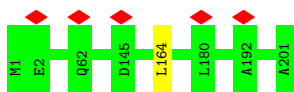
• Molecule 10: 50S ribosomal protein L2



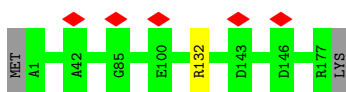
• Molecule 11: 50S ribosomal protein L3



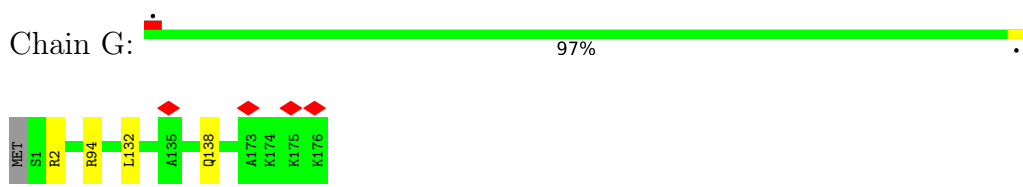
• Molecule 12: 50S ribosomal protein L4



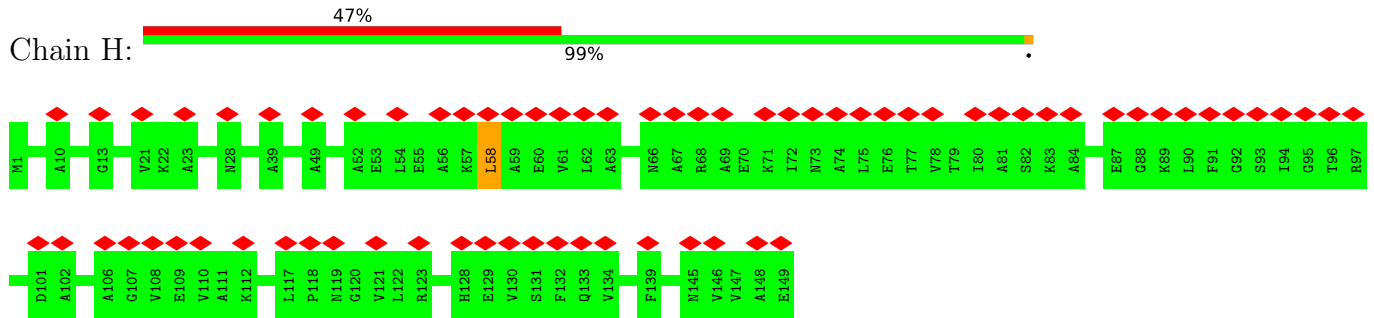
• Molecule 13: 50S ribosomal protein L5



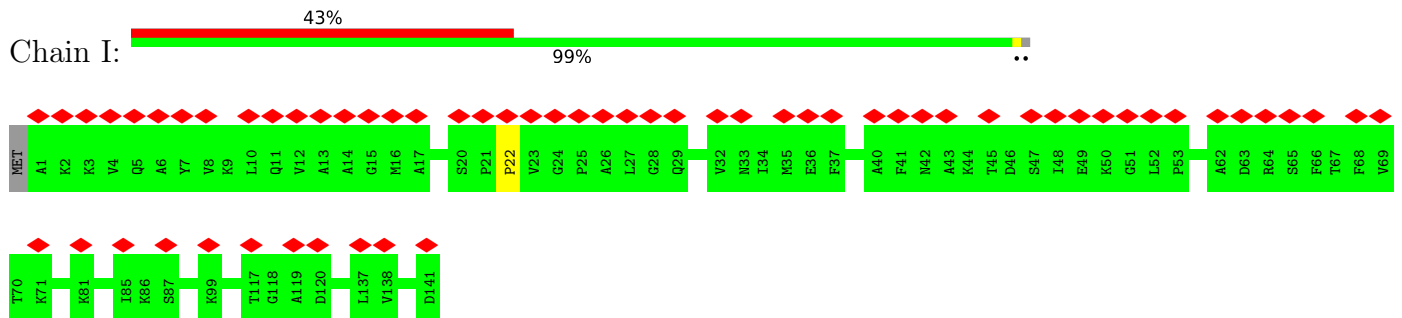
- Molecule 14: 50S ribosomal protein L6



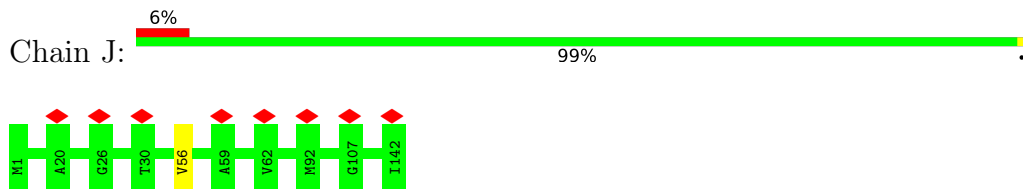
- Molecule 15: 50S ribosomal protein L9



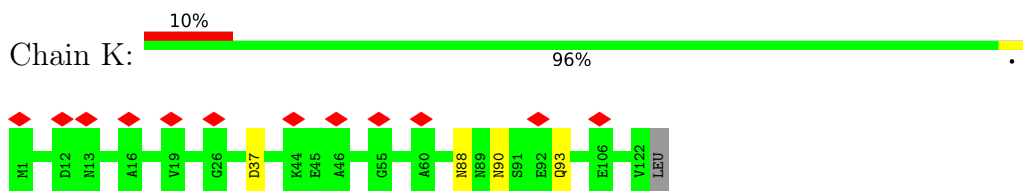
- Molecule 16: 50S ribosomal protein L11



- Molecule 17: 50S ribosomal protein L13

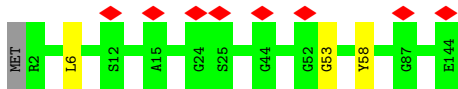


- Molecule 18: 50S ribosomal protein L14

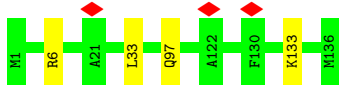


- Molecule 19: 50S ribosomal protein L15

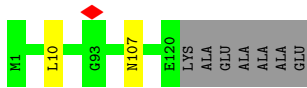




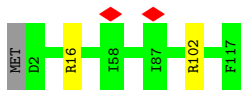
- Molecule 20: 50S ribosomal protein L16



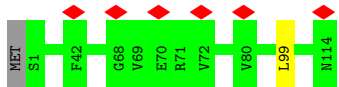
- Molecule 21: 50S ribosomal protein L17



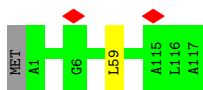
- Molecule 22: 50S ribosomal protein L18



- Molecule 23: 50S ribosomal protein L19



- Molecule 24: 50S ribosomal protein L20



- Molecule 25: 50S ribosomal protein L21




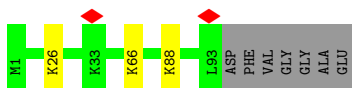
- Molecule 26: 50S ribosomal protein L22

Chain S:  96%



- Molecule 27: 50S ribosomal protein L23

Chain T:  90% 7%



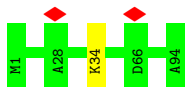
- Molecule 28: 50S ribosomal protein L24

Chain U:  94%



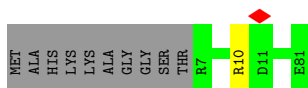
- Molecule 29: 50S ribosomal protein L25

Chain V:  99%



- Molecule 30: 50S ribosomal protein L27

Chain W:  87% 12%



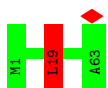
- Molecule 31: 50S ribosomal protein L28

Chain X:  94% 5%



- Molecule 32: 50S ribosomal protein L29

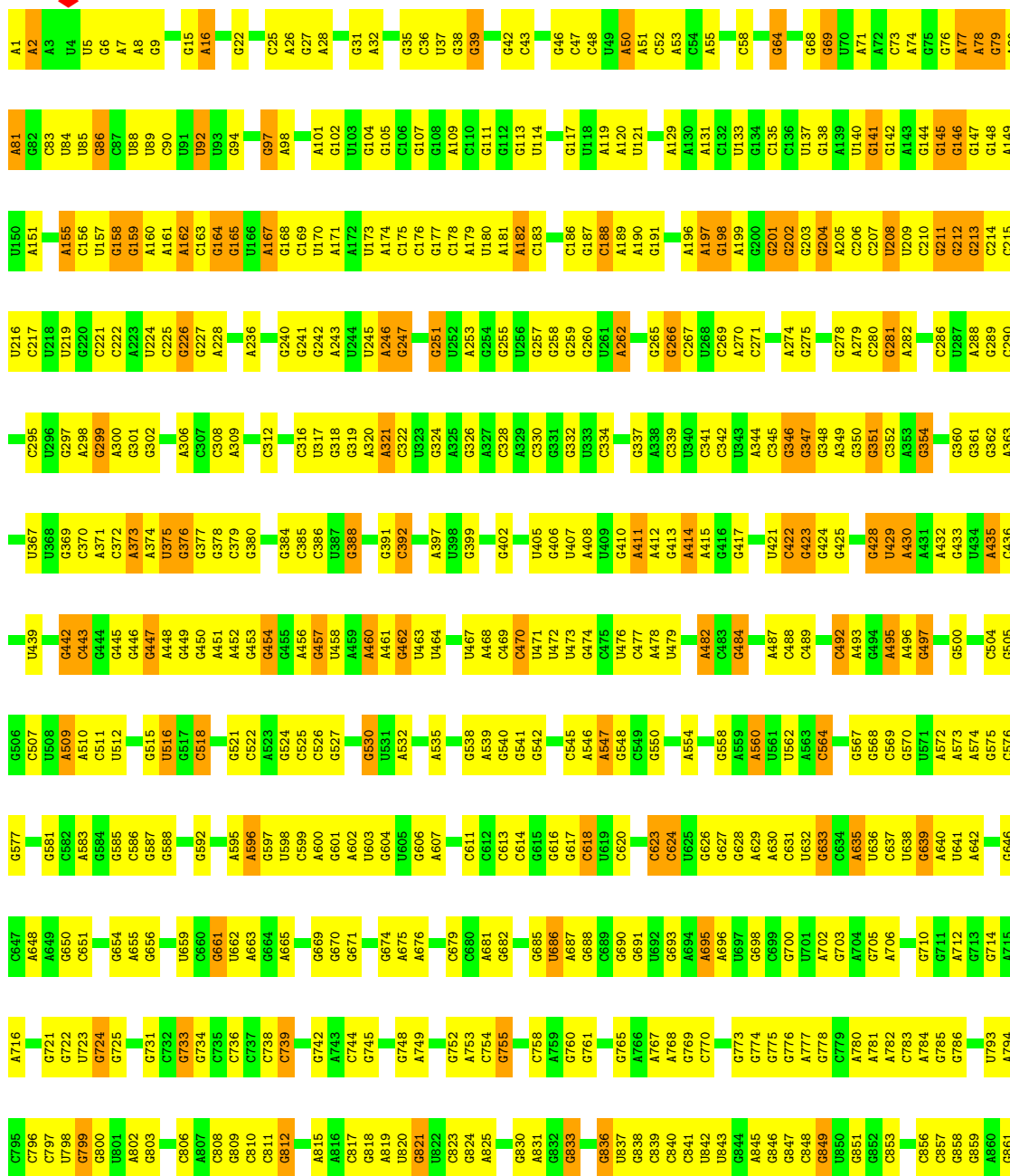
Chain Y:  98%

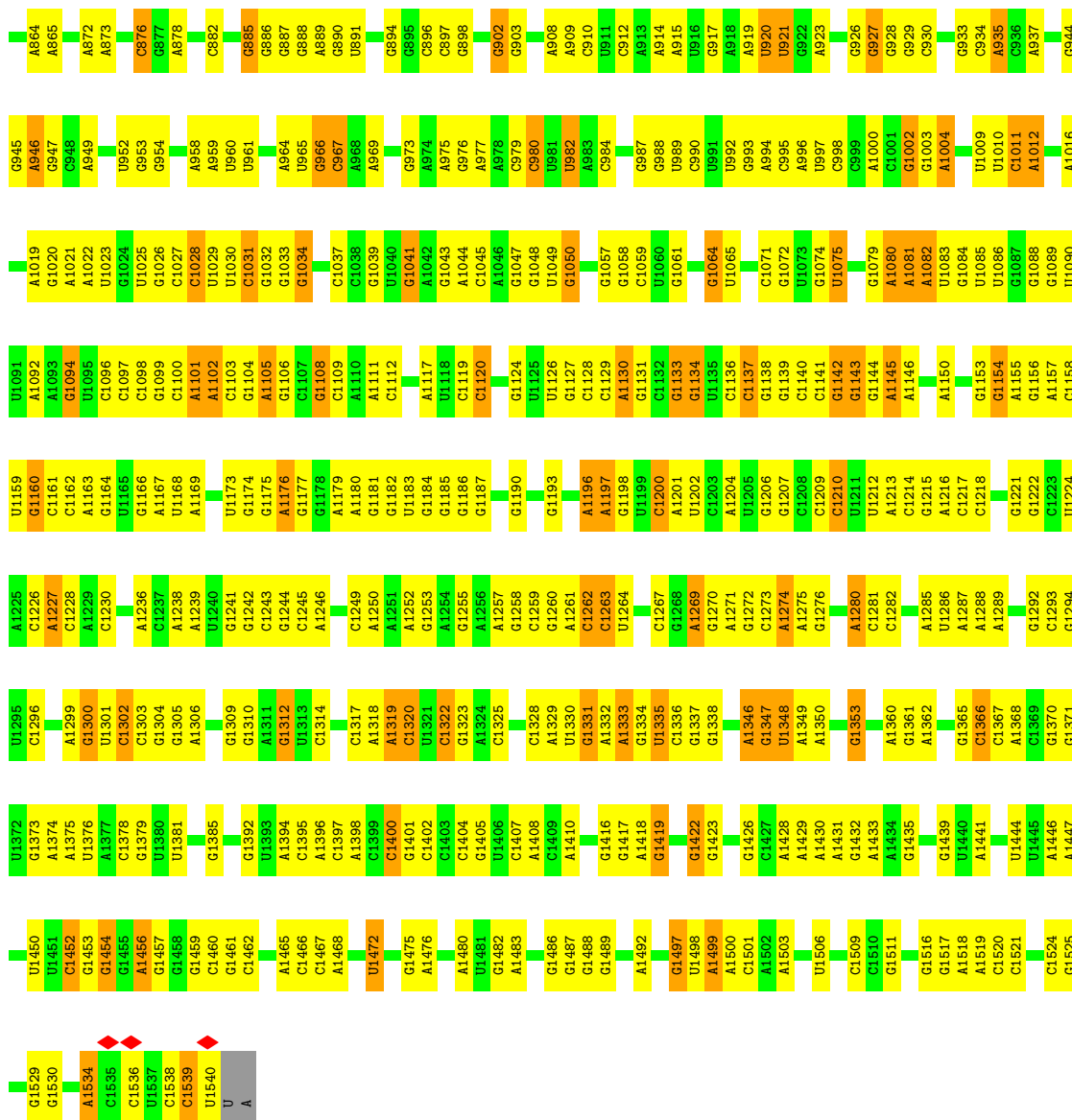


• Molecule 33: 50S ribosomal protein L30

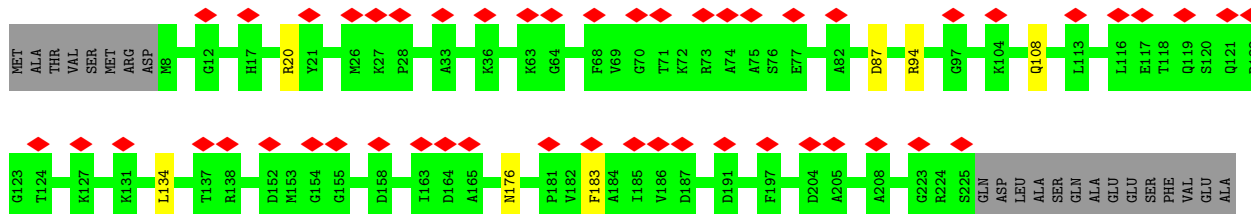
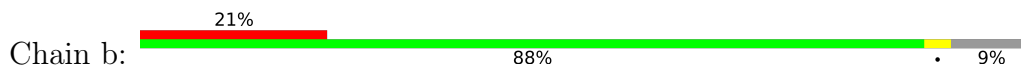


• Molecule 34: 16S ribosomal RNA

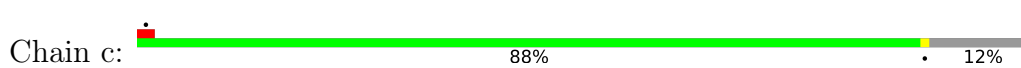


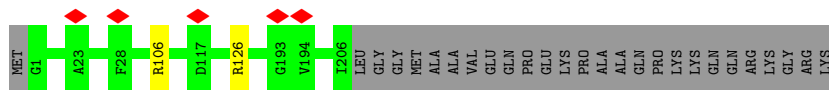


• Molecule 35: 30S ribosomal protein S2

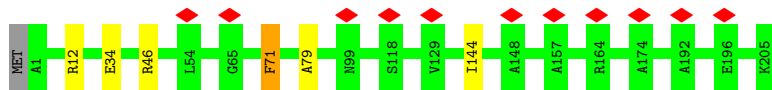


• Molecule 36: 30S ribosomal protein S3

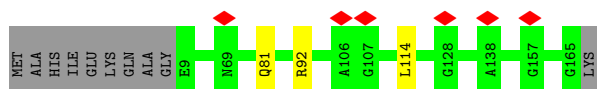
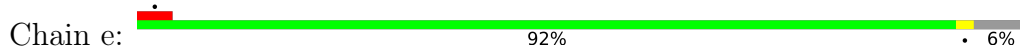




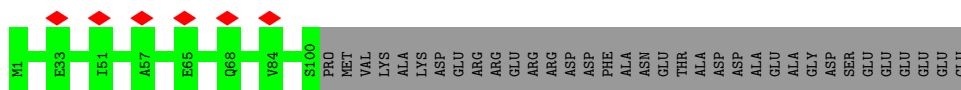
- Molecule 37: 30S ribosomal protein S4



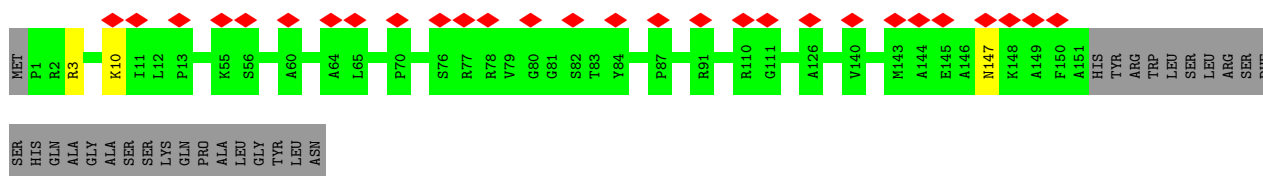
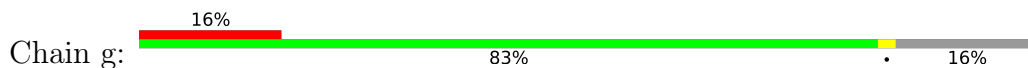
- Molecule 38: 30S ribosomal protein S5



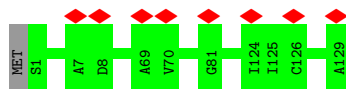
- Molecule 39: 30S ribosomal protein S6



- Molecule 40: 30S ribosomal protein S7



- Molecule 41: 30S ribosomal protein S8

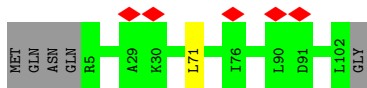
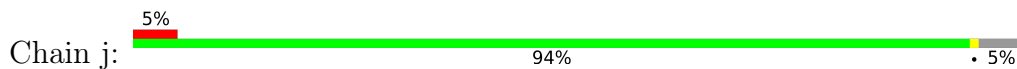


- Molecule 42: 30S ribosomal protein S9

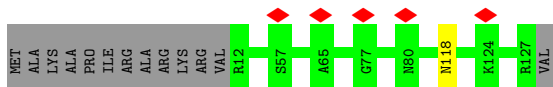
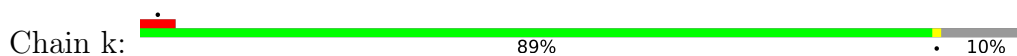




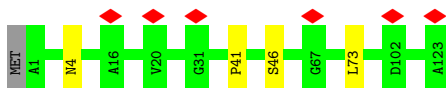
- Molecule 43: 30S ribosomal protein S10



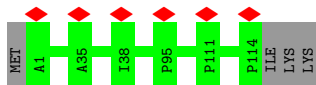
- Molecule 44: 30S ribosomal protein S11



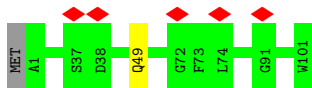
- Molecule 45: 30S ribosomal protein S12



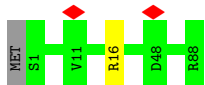
- Molecule 46: 30S ribosomal protein S13



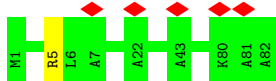
- Molecule 47: 30S ribosomal protein S14



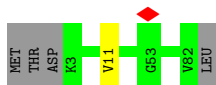
- Molecule 48: 30S ribosomal protein S15



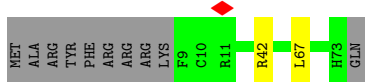
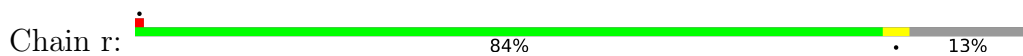
- Molecule 49: 30S ribosomal protein S16



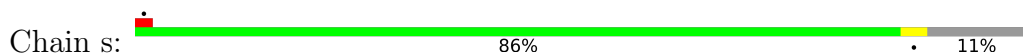
- Molecule 50: 30S ribosomal protein S17



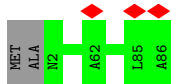
- Molecule 51: 30S ribosomal protein S18



- Molecule 52: 30S ribosomal protein S19



- Molecule 53: 30S ribosomal protein S20



- Molecule 54: 30S ribosomal protein S21

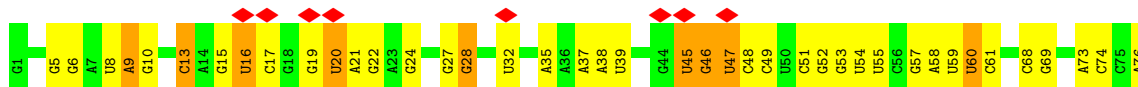


- Molecule 55: P-site tRNA(fMet)

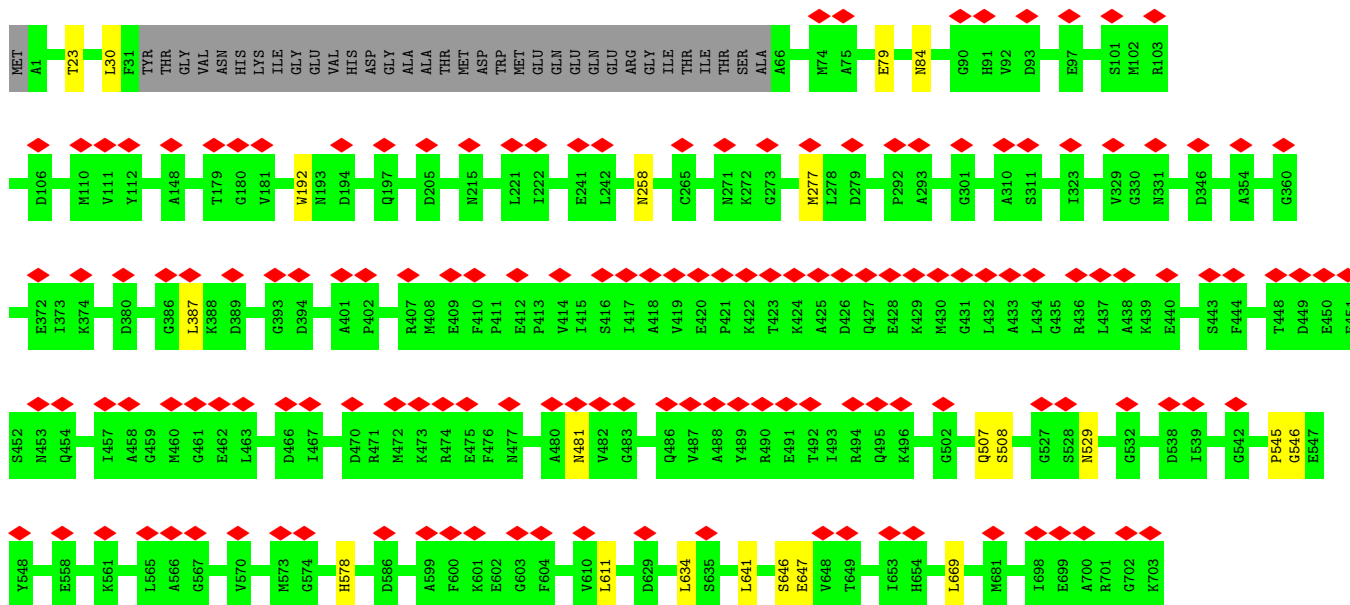
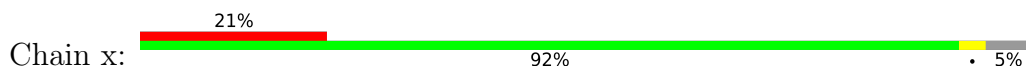




• Molecule 56: P-site fMet-Phe-tRNA(Phe)



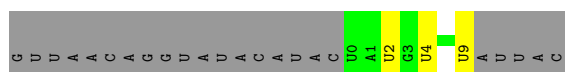
• Molecule 57: Elongation factor G



• Molecule 58: Dipeptide (FME-PHE)



• Molecule 59: mRNA



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	6168	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 ($e^-/\text{\AA}^2$)	30	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1200	Depositor
Magnification	59000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	10.963	Depositor
Minimum map value	-5.358	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	1.5	Depositor
Map size (\AA)	334.08, 334.08, 334.08	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.16, 1.16, 1.16	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: AM2, OMC, 3TD, ZN, 4SU, 6MZ, PSU, 5MU, 4OC, 2MG, MA6, GDP, FME, OMG, OMU, 1MG, G7M, 2MA, 5MC, MIA, H2U, UR3

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	0	0.81	0/450	1.06	0/599
2	1	0.71	0/416	1.15	0/554
3	2	0.82	0/380	1.08	1/498 (0.2%)
4	3	0.81	0/513	1.07	0/676
5	4	0.77	0/303	1.17	0/397
6	5	0.31	0/646	0.62	0/898
7	6	0.76	0/531	1.04	0/709
8	A	1.65	635/69266 (0.9%)	1.90	2790/108055 (2.6%)
9	B	1.68	28/2873 (1.0%)	2.02	154/4478 (3.4%)
10	C	0.78	1/2121 (0.0%)	1.05	4/2852 (0.1%)
11	D	0.76	0/1586	0.99	0/2134
12	E	0.74	0/1571	0.99	1/2113 (0.0%)
13	F	0.79	0/1434	0.99	1/1926 (0.1%)
14	G	0.76	0/1343	0.98	2/1816 (0.1%)
15	H	0.62	0/1122	0.87	1/1515 (0.1%)
16	I	0.37	0/692	0.66	0/960
17	J	0.82	0/1152	1.03	1/1551 (0.1%)
18	K	0.73	0/947	1.01	0/1268
19	L	0.72	0/1054	1.17	2/1403 (0.1%)
20	M	0.83	0/1093	1.08	3/1460 (0.2%)
21	N	0.77	1/973 (0.1%)	1.14	1/1301 (0.1%)
22	O	0.73	0/902	0.94	2/1209 (0.2%)
23	P	0.81	0/929	1.02	1/1242 (0.1%)
24	Q	0.82	0/960	1.04	1/1278 (0.1%)
25	R	0.81	0/829	1.04	0/1107
26	S	0.79	0/864	1.10	4/1156 (0.3%)
27	T	0.82	0/744	1.10	1/994 (0.1%)
28	U	0.93	1/787 (0.1%)	1.12	1/1051 (0.1%)
29	V	0.93	0/766	0.99	0/1025
30	W	0.76	0/582	1.02	0/769
31	X	0.87	2/635 (0.3%)	1.17	2/848 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	Y	0.77	0/510	1.08	1/677 (0.1%)
33	Z	0.78	0/453	1.12	0/605
34	a	1.52	254/36725 (0.7%)	1.85	1350/57285 (2.4%)
35	b	0.62	0/1735	0.86	2/2338 (0.1%)
36	c	0.73	0/1651	0.93	1/2225 (0.0%)
37	d	0.70	0/1665	0.96	1/2227 (0.0%)
38	e	0.73	0/1154	1.00	1/1554 (0.1%)
39	f	0.71	0/835	0.89	0/1128
40	g	0.63	0/1195	0.86	1/1602 (0.1%)
41	h	0.66	0/989	0.86	0/1326
42	i	0.65	0/1034	0.93	1/1375 (0.1%)
43	j	0.66	0/796	0.94	1/1077 (0.1%)
44	k	0.65	0/885	0.94	0/1195
45	l	0.75	0/969	1.09	1/1300 (0.1%)
46	m	0.65	0/892	0.95	0/1193
47	n	0.68	0/811	0.97	0/1081
48	o	0.66	0/722	0.97	0/964
49	p	0.70	0/659	0.96	1/884 (0.1%)
50	q	0.81	0/657	1.00	1/881 (0.1%)
51	r	0.73	1/544 (0.2%)	0.98	1/731 (0.1%)
52	s	0.66	0/675	1.02	2/908 (0.2%)
53	t	0.79	0/671	0.90	0/888
54	u	0.59	0/512	0.91	0/683
55	v	1.45	16/1745 (0.9%)	1.88	65/2716 (2.4%)
56	w	1.09	2/1650 (0.1%)	1.48	27/2569 (1.1%)
57	x	0.72	1/5288 (0.0%)	0.95	6/7152 (0.1%)
58	y	0.29	0/11	0.79	0/13
59	z	0.89	0/230	1.17	0/355
All	All	1.39	942/164127 (0.6%)	1.68	4436/244774 (1.8%)

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
4	3	0	1
25	R	0	1
28	U	0	1
32	Y	0	1
35	b	0	1
37	d	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
54	u	0	1
57	x	0	1
All	All	0	10

All (942) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	1	G	OP3-P	-10.75	1.48	1.61
9	B	1	U	OP3-P	-10.72	1.48	1.61
55	v	1	C	OP3-P	-10.66	1.48	1.61
8	A	1055	G	N9-C4	-10.60	1.29	1.38
34	a	640	A	N9-C4	-9.66	1.32	1.37
8	A	1139	G	N9-C4	-9.09	1.30	1.38
34	a	101	A	N9-C4	-9.00	1.32	1.37
34	a	1155	A	N9-C4	-8.98	1.32	1.37
8	A	482	A	N9-C4	-8.90	1.32	1.37
8	A	843	G	N9-C4	-8.69	1.30	1.38
34	a	604	G	N9-C4	-8.66	1.31	1.38
34	a	201	G	N9-C4	-8.46	1.31	1.38
34	a	1081	A	O3'-P	8.44	1.71	1.61
8	A	1548	A	N9-C4	-8.43	1.32	1.37
8	A	2763	G	N9-C4	-8.37	1.31	1.38
34	a	858	G	N9-C4	-8.32	1.31	1.38
8	A	1025	G	N9-C4	-8.31	1.31	1.38
8	A	2235	G	N9-C4	-8.26	1.31	1.38
8	A	2814	A	N9-C4	-8.23	1.32	1.37
8	A	1687	G	N9-C4	-8.21	1.31	1.38
8	A	1425	G	N9-C4	-8.19	1.31	1.38
8	A	217	A	N9-C4	-8.18	1.32	1.37
8	A	2576	G	N3-C4	-8.11	1.29	1.35
8	A	1277	G	N9-C4	-8.10	1.31	1.38
8	A	126	A	N9-C4	-8.05	1.33	1.37
34	a	542	G	N9-C4	-7.97	1.31	1.38
34	a	1431	A	N9-C4	-7.94	1.33	1.37
8	A	920	A	N9-C4	-7.92	1.33	1.37
8	A	344	A	N9-C4	-7.88	1.33	1.37
8	A	780	G	N9-C4	-7.80	1.31	1.38
8	A	2657	A	N9-C4	-7.78	1.33	1.37
8	A	1165	A	N9-C4	-7.76	1.33	1.37
9	B	119	A	N9-C4	-7.68	1.33	1.37
34	a	461	A	N9-C4	-7.67	1.33	1.37
8	A	522	A	N9-C4	-7.62	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	a	321	A	N9-C4	-7.60	1.33	1.37
34	a	954	G	N9-C4	-7.56	1.31	1.38
34	a	628	G	N9-C4	-7.54	1.31	1.38
8	A	1022	G	N9-C4	-7.53	1.31	1.38
8	A	1492	G	N9-C4	-7.53	1.31	1.38
8	A	2228	G	N9-C4	-7.51	1.31	1.38
8	A	505	A	N9-C4	-7.50	1.33	1.37
8	A	2097	A	N9-C4	-7.50	1.33	1.37
8	A	2461	A	N9-C4	-7.50	1.33	1.37
8	A	1674	G	N9-C4	-7.49	1.31	1.38
8	A	1650	A	N9-C4	-7.48	1.33	1.37
34	a	888	G	N9-C4	-7.47	1.31	1.38
55	v	12	G	N9-C4	-7.47	1.31	1.38
8	A	1385	A	N9-C4	-7.47	1.33	1.37
34	a	460	A	N9-C4	-7.47	1.33	1.37
8	A	1450	G	N9-C4	-7.46	1.31	1.38
8	A	2770	G	N9-C4	-7.45	1.31	1.38
8	A	180	G	N9-C4	-7.45	1.31	1.38
8	A	2418	A	N9-C4	-7.44	1.33	1.37
34	a	1289	A	N9-C4	-7.41	1.33	1.37
8	A	1433	A	N9-C4	-7.40	1.33	1.37
8	A	1642	G	N9-C4	-7.40	1.32	1.38
8	A	457	A	N9-C4	-7.38	1.33	1.37
34	a	768	A	N9-C4	-7.37	1.33	1.37
8	A	2225	A	N9-C4	-7.36	1.33	1.37
8	A	1522	A	N9-C4	-7.35	1.33	1.37
34	a	909	A	N9-C4	-7.32	1.33	1.37
8	A	1684	G	N9-C4	-7.32	1.32	1.38
8	A	2199	A	N9-C4	-7.32	1.33	1.37
8	A	2525	G	N9-C4	-7.31	1.32	1.38
8	A	2389	G	N9-C4	-7.31	1.32	1.38
34	a	617	G	N9-C4	-7.30	1.32	1.38
8	A	2727	A	N9-C4	-7.30	1.33	1.37
8	A	347	A	N9-C4	-7.29	1.33	1.37
8	A	1503	A	N9-C4	-7.29	1.33	1.37
55	v	72	A	N9-C4	-7.28	1.33	1.37
34	a	592	G	N9-C4	-7.28	1.32	1.38
8	A	2663	G	N9-C4	-7.27	1.32	1.38
34	a	42	G	N9-C4	-7.24	1.32	1.38
34	a	413	G	N9-C4	-7.24	1.32	1.38
8	A	1371	G	N9-C4	-7.23	1.32	1.38
8	A	2706	A	N9-C4	-7.22	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	a	274	A	N9-C4	-7.21	1.33	1.37
8	A	207	A	N9-C4	-7.18	1.33	1.37
8	A	1843	C	N1-C6	-7.17	1.32	1.37
8	A	2010	G	N9-C4	-7.17	1.32	1.38
34	a	831	A	N9-C4	-7.17	1.33	1.37
8	A	1055	G	C2-N3	-7.16	1.27	1.32
8	A	1374	G	N9-C4	-7.16	1.32	1.38
8	A	2813	A	N9-C4	-7.15	1.33	1.37
34	a	1012	A	N9-C4	-7.11	1.33	1.37
8	A	761	A	N9-C4	-7.11	1.33	1.37
8	A	833	A	N9-C4	-7.10	1.33	1.37
8	A	1525	A	N9-C4	-7.10	1.33	1.37
34	a	1488	G	N9-C4	-7.09	1.32	1.38
34	a	262	A	N9-C4	-7.09	1.33	1.37
8	A	315	G	N9-C4	-7.07	1.32	1.38
8	A	45	G	N9-C4	-7.06	1.32	1.38
34	a	1417	G	N9-C4	-7.06	1.32	1.38
8	A	1749	A	N9-C4	-7.04	1.33	1.37
34	a	228	A	N9-C4	-7.04	1.33	1.37
34	a	265	G	N9-C4	-7.03	1.32	1.38
8	A	1593	A	N9-C4	-7.01	1.33	1.37
8	A	1970	A	N9-C4	-6.98	1.33	1.37
8	A	340	A	N9-C4	-6.97	1.33	1.37
8	A	2458	G	N9-C4	-6.97	1.32	1.38
34	a	521	G	N9-C4	-6.97	1.32	1.38
8	A	2566	A	N9-C4	-6.96	1.33	1.37
8	A	1745	A	N9-C4	-6.96	1.33	1.37
9	B	20	G	N9-C4	-6.96	1.32	1.38
34	a	1156	G	N9-C4	-6.95	1.32	1.38
8	A	1016	G	N9-C4	-6.95	1.32	1.38
9	B	23	G	N9-C4	-6.94	1.32	1.38
34	a	155	A	N9-C4	-6.94	1.33	1.37
9	B	34	A	N9-C4	-6.93	1.33	1.37
8	A	943	A	N9-C4	-6.93	1.33	1.37
8	A	1596	A	N9-C4	-6.93	1.33	1.37
8	A	1216	G	N9-C4	-6.92	1.32	1.38
8	A	1347	A	N9-C4	-6.91	1.33	1.37
8	A	1292	G	N9-C4	-6.91	1.32	1.38
8	A	1867	G	N9-C4	-6.90	1.32	1.38
8	A	1091	G	N9-C4	-6.90	1.32	1.38
8	A	1021	A	N9-C4	-6.90	1.33	1.37
8	A	800	A	N9-C4	-6.89	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	1570	A	N9-C4	-6.88	1.33	1.37
34	a	889	A	N9-C4	-6.88	1.33	1.37
8	A	2435	A	N9-C4	-6.88	1.33	1.37
8	A	2576	G	C2-N3	-6.87	1.27	1.32
8	A	44	A	N9-C4	-6.86	1.33	1.37
34	a	988	G	N9-C4	-6.85	1.32	1.38
34	a	1432	G	N9-C4	-6.85	1.32	1.38
34	a	648	A	N9-C4	-6.84	1.33	1.37
8	A	354	A	N9-C4	-6.84	1.33	1.37
8	A	2040	G	N9-C4	-6.84	1.32	1.38
34	a	1244	G	N9-C4	-6.83	1.32	1.38
8	A	1336	A	N9-C4	-6.82	1.33	1.37
8	A	310	A	N9-C4	-6.82	1.33	1.37
55	v	46	A	N9-C4	-6.82	1.33	1.37
8	A	1527	G	N9-C4	-6.81	1.32	1.38
34	a	411	A	N9-C4	-6.81	1.33	1.37
34	a	241	G	N9-C4	-6.81	1.32	1.38
8	A	2536	G	N9-C4	-6.79	1.32	1.38
8	A	1220	G	N9-C4	-6.79	1.32	1.38
8	A	188	G	N9-C4	-6.79	1.32	1.38
34	a	201	G	C2-N3	-6.78	1.27	1.32
8	A	111	A	N9-C4	-6.78	1.33	1.37
8	A	1047	G	N9-C4	-6.78	1.32	1.38
34	a	77	A	N9-C4	-6.78	1.33	1.37
8	A	2411	A	N9-C4	-6.77	1.33	1.37
9	B	54	G	N9-C4	-6.77	1.32	1.38
8	A	1266	G	N9-C4	-6.77	1.32	1.38
34	a	246	A	N9-C4	-6.76	1.33	1.37
8	A	708	G	N9-C4	-6.75	1.32	1.38
8	A	696	G	N9-C4	-6.73	1.32	1.38
8	A	2351	G	N9-C4	-6.72	1.32	1.38
8	A	2665	A	N9-C4	-6.71	1.33	1.37
8	A	301	G	N9-C4	-6.71	1.32	1.38
8	A	1952	A	N9-C4	-6.71	1.33	1.37
8	A	1905	C	N1-C6	-6.69	1.33	1.37
34	a	1142	G	N9-C4	-6.68	1.32	1.38
8	A	2353	G	N9-C4	-6.68	1.32	1.38
8	A	146	A	N9-C4	-6.67	1.33	1.37
8	A	1022	G	N3-C4	-6.67	1.30	1.35
8	A	1906	G	N9-C8	-6.67	1.33	1.37
8	A	1228	G	N9-C4	-6.67	1.32	1.38
8	A	203	A	N9-C4	-6.67	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	2576	G	N9-C4	-6.67	1.32	1.38
8	A	2803	G	N9-C4	-6.67	1.32	1.38
8	A	1721	G	N9-C4	-6.66	1.32	1.38
8	A	124	G	N9-C4	-6.66	1.32	1.38
8	A	536	G	N9-C4	-6.65	1.32	1.38
8	A	949	G	N9-C4	-6.65	1.32	1.38
8	A	2432	A	N9-C4	-6.64	1.33	1.37
8	A	2481	G	N9-C4	-6.64	1.32	1.38
8	A	1750	G	N9-C4	-6.63	1.32	1.38
8	A	24	G	N9-C4	-6.63	1.32	1.38
8	A	514	A	N9-C4	-6.63	1.33	1.37
8	A	523	C	N1-C6	-6.61	1.33	1.37
34	a	151	A	C6-N6	-6.59	1.28	1.33
8	A	213	A	N9-C4	-6.59	1.33	1.37
34	a	1329	A	N9-C4	-6.58	1.33	1.37
8	A	260	G	N9-C4	-6.58	1.32	1.38
8	A	2003	A	N9-C4	-6.58	1.33	1.37
8	A	1713	A	N9-C4	-6.57	1.33	1.37
8	A	2485	G	N9-C4	-6.57	1.32	1.38
8	A	666	A	N9-C4	-6.56	1.33	1.37
8	A	1	G	N9-C4	-6.56	1.32	1.38
8	A	1163	G	N9-C4	-6.55	1.32	1.38
8	A	14	A	C6-N6	-6.55	1.28	1.33
34	a	167	A	N9-C4	-6.54	1.33	1.37
8	A	74	A	N9-C4	-6.54	1.33	1.37
8	A	2369	A	N9-C4	-6.54	1.33	1.37
34	a	809	G	N9-C4	-6.53	1.32	1.38
8	A	2632	A	N9-C4	-6.52	1.33	1.37
8	A	1543	G	N9-C4	-6.52	1.32	1.38
34	a	923	A	N9-C4	-6.52	1.33	1.37
8	A	2323	G	N9-C4	-6.51	1.32	1.38
8	A	2557	G	N9-C4	-6.51	1.32	1.38
34	a	212	G	N9-C8	-6.51	1.33	1.37
8	A	1218	G	N9-C4	-6.50	1.32	1.38
55	v	9	G	N9-C4	-6.50	1.32	1.38
8	A	231	A	N9-C4	-6.49	1.33	1.37
8	A	2640	G	N9-C4	-6.49	1.32	1.38
8	A	2876	G	N9-C4	-6.49	1.32	1.38
8	A	1631	G	N9-C4	-6.49	1.32	1.38
34	a	663	A	N9-C4	-6.49	1.33	1.37
8	A	1367	A	N9-C4	-6.48	1.33	1.37
34	a	780	A	N9-C4	-6.48	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	2775	G	N9-C4	-6.47	1.32	1.38
34	a	1497	G	N9-C4	-6.46	1.32	1.38
8	A	1187	G	N9-C4	-6.46	1.32	1.38
8	A	2005	A	N9-C4	-6.46	1.33	1.37
8	A	671	C	N1-C6	-6.46	1.33	1.37
8	A	289	G	N9-C4	-6.45	1.32	1.38
8	A	1202	G	N9-C4	-6.45	1.32	1.38
8	A	1922	G	N9-C4	-6.45	1.32	1.38
34	a	260	G	N9-C4	-6.43	1.32	1.38
8	A	1984	G	N9-C4	-6.43	1.32	1.38
34	a	78	A	N9-C4	-6.43	1.33	1.37
8	A	1337	G	N9-C4	-6.42	1.32	1.38
8	A	818	G	N9-C4	-6.42	1.32	1.38
34	a	1143	G	N9-C4	-6.42	1.32	1.38
8	A	42	A	N9-C4	-6.42	1.33	1.37
8	A	38	A	N9-C4	-6.41	1.34	1.37
8	A	176	A	N9-C4	-6.41	1.34	1.37
34	a	1374	A	C5-C6	-6.41	1.35	1.41
8	A	2414	G	N9-C4	-6.40	1.32	1.38
8	A	2058	A	N9-C4	-6.39	1.34	1.37
34	a	432	A	N9-C4	-6.39	1.34	1.37
8	A	2472	G	N9-C4	-6.39	1.32	1.38
8	A	1423	G	N9-C4	-6.39	1.32	1.38
8	A	1424	G	N9-C4	-6.38	1.32	1.38
34	a	1430	A	N9-C4	-6.38	1.34	1.37
8	A	214	G	N9-C4	-6.38	1.32	1.38
34	a	1476	A	N9-C4	-6.38	1.34	1.37
8	A	793	A	N9-C4	-6.37	1.34	1.37
8	A	1378	A	N9-C4	-6.37	1.34	1.37
9	B	59	A	N9-C4	-6.37	1.34	1.37
34	a	326	G	N9-C4	-6.37	1.32	1.38
34	a	1089	G	N9-C4	-6.36	1.32	1.38
34	a	629	A	N9-C4	-6.36	1.34	1.37
34	a	1306	A	N9-C4	-6.36	1.34	1.37
34	a	921	U	C5'-C4'	6.35	1.58	1.51
8	A	988	A	N9-C4	-6.33	1.34	1.37
55	v	15	G	N9-C4	-6.33	1.32	1.38
34	a	1098	C	N1-C2	-6.33	1.33	1.40
8	A	1904	G	N9-C4	-6.32	1.32	1.38
8	A	144	A	N9-C4	-6.31	1.34	1.37
8	A	85	G	N9-C4	-6.31	1.32	1.38
8	A	1142	A	N9-C4	-6.30	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	1918	A	N9-C4	-6.30	1.34	1.37
8	A	2894	G	N9-C4	-6.30	1.32	1.38
8	A	951	C	N1-C6	-6.30	1.33	1.37
8	A	1735	A	N9-C4	-6.29	1.34	1.37
8	A	73	A	N9-C4	-6.29	1.34	1.37
34	a	1133	G	N9-C4	-6.28	1.32	1.38
8	A	469	G	C5-C6	-6.28	1.36	1.42
34	a	1088	G	C2-N3	-6.28	1.27	1.32
8	A	844	A	N9-C4	-6.28	1.34	1.37
8	A	1106	G	N9-C4	-6.27	1.32	1.38
8	A	1664	A	N9-C4	-6.27	1.34	1.37
8	A	1674	G	N9-C8	-6.26	1.33	1.37
8	A	1735	A	C5-C6	-6.26	1.35	1.41
8	A	2844	G	N9-C4	-6.26	1.32	1.38
8	A	1762	A	N9-C4	-6.26	1.34	1.37
8	A	814	C	N1-C6	-6.26	1.33	1.37
8	A	1237	A	N9-C4	-6.25	1.34	1.37
8	A	2603	G	N9-C4	-6.25	1.32	1.38
9	B	33	G	N9-C4	-6.25	1.32	1.38
8	A	830	G	N9-C4	-6.25	1.32	1.38
8	A	297	G	N9-C4	-6.24	1.32	1.38
8	A	2765	A	N9-C4	-6.24	1.34	1.37
34	a	1111	A	N9-C4	-6.23	1.34	1.37
8	A	410	G	N9-C4	-6.23	1.32	1.38
34	a	919	A	N9-C4	-6.23	1.34	1.37
8	A	1723	G	N9-C4	-6.23	1.32	1.38
34	a	98	A	N9-C4	-6.22	1.34	1.37
34	a	1050	G	N9-C4	-6.22	1.32	1.38
8	A	2719	G	N9-C4	-6.22	1.32	1.38
8	A	1377	G	N9-C4	-6.22	1.32	1.38
8	A	1890	A	N9-C4	-6.22	1.34	1.37
8	A	2624	G	N9-C4	-6.21	1.32	1.38
8	A	303	G	N9-C4	-6.21	1.32	1.38
8	A	704	G	N9-C4	-6.21	1.32	1.38
8	A	1652	A	N9-C4	-6.21	1.34	1.37
34	a	1179	A	N9-C4	-6.21	1.34	1.37
8	A	1251	C	N1-C6	-6.21	1.33	1.37
34	a	987	G	N9-C4	-6.20	1.32	1.38
34	a	456	A	N3-C4	-6.20	1.31	1.34
8	A	2416	C	N1-C6	-6.19	1.33	1.37
8	A	655	A	N9-C4	-6.19	1.34	1.37
8	A	1230	A	N9-C4	-6.19	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	255	A	N9-C4	-6.18	1.34	1.37
8	A	1449	G	N9-C4	-6.18	1.33	1.38
34	a	478	A	N9-C4	-6.18	1.34	1.37
34	a	1405	G	N9-C4	-6.18	1.33	1.38
8	A	682	G	N9-C4	-6.18	1.33	1.38
8	A	2009	A	N9-C4	-6.17	1.34	1.37
8	A	2857	G	N9-C4	-6.16	1.33	1.38
8	A	1009	A	N9-C4	-6.15	1.34	1.37
8	A	1029	A	N9-C4	-6.15	1.34	1.37
8	A	1112	G	N9-C4	-6.15	1.33	1.38
8	A	1465	G	N9-C4	-6.15	1.33	1.38
34	a	1108	G	N9-C4	-6.14	1.33	1.38
8	A	751	A	N9-C4	-6.14	1.34	1.37
8	A	2513	A	C6-N1	-6.14	1.31	1.35
8	A	270	A	N9-C4	-6.13	1.34	1.37
8	A	722	A	N9-C4	-6.13	1.34	1.37
8	A	1381	G	N9-C4	-6.13	1.33	1.38
8	A	2284	A	N9-C4	-6.13	1.34	1.37
8	A	1317	G	N9-C4	-6.13	1.33	1.38
34	a	775	G	N9-C4	-6.13	1.33	1.38
34	a	1312	G	N9-C4	-6.12	1.33	1.38
34	a	1088	G	N9-C4	-6.11	1.33	1.38
34	a	1480	A	N9-C4	-6.11	1.34	1.37
34	a	920	U	O3'-P	6.11	1.68	1.61
34	a	778	G	N9-C4	-6.11	1.33	1.38
8	A	123	G	N9-C4	-6.10	1.33	1.38
34	a	1221	G	N9-C4	-6.10	1.33	1.38
8	A	178	G	N9-C4	-6.10	1.33	1.38
8	A	1383	A	N9-C4	-6.10	1.34	1.37
8	A	1655	A	N9-C4	-6.10	1.34	1.37
8	A	1960	A	N9-C4	-6.10	1.34	1.37
9	B	101	A	N9-C4	-6.10	1.34	1.37
8	A	2448	A	N9-C4	-6.09	1.34	1.37
8	A	940	G	N9-C4	-6.09	1.33	1.38
8	A	1193	G	N9-C4	-6.09	1.33	1.38
8	A	2524	G	N9-C4	-6.09	1.33	1.38
9	B	21	G	N9-C4	-6.09	1.33	1.38
8	A	1767	G	N9-C4	-6.08	1.33	1.38
8	A	2316	G	N9-C4	-6.08	1.33	1.38
34	a	1375	A	N9-C4	-6.08	1.34	1.37
8	A	771	G	N9-C4	-6.08	1.33	1.38
34	a	1435	G	N9-C4	-6.08	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	a	1323	G	N9-C8	-6.07	1.33	1.37
34	a	259	G	N9-C4	-6.06	1.33	1.38
8	A	636	G	N9-C4	-6.06	1.33	1.38
8	A	1358	G	N9-C4	-6.06	1.33	1.38
8	A	888	C	N1-C6	-6.05	1.33	1.37
8	A	1139	G	N3-C4	-6.05	1.31	1.35
8	A	1626	A	N9-C4	-6.04	1.34	1.37
34	a	1333	A	N9-C4	-6.04	1.34	1.37
34	a	462	G	N7-C5	-6.03	1.35	1.39
8	A	673	C	N1-C6	-6.03	1.33	1.37
8	A	1540	G	N9-C4	-6.03	1.33	1.38
8	A	39	G	N9-C4	-6.03	1.33	1.38
8	A	1311	G	N9-C4	-6.03	1.33	1.38
8	A	2631	G	N9-C4	-6.03	1.33	1.38
34	a	833	G	N9-C4	-6.03	1.33	1.38
34	a	1323	G	N9-C4	-6.02	1.33	1.38
8	A	1186	G	N9-C4	-6.02	1.33	1.38
8	A	1974	C	N1-C6	-6.02	1.33	1.37
8	A	2694	G	N9-C4	-6.02	1.33	1.38
8	A	271	G	N9-C4	-6.01	1.33	1.38
8	A	2846	G	N9-C4	-6.01	1.33	1.38
8	A	401	A	N9-C4	-6.00	1.34	1.37
8	A	1169	A	N9-C4	-6.00	1.34	1.37
34	a	509	A	N9-C4	-6.00	1.34	1.37
8	A	317	G	N9-C4	-5.99	1.33	1.38
34	a	849	G	N9-C4	-5.99	1.33	1.38
34	a	1428	A	N9-C4	-5.99	1.34	1.37
8	A	254	G	N9-C8	-5.99	1.33	1.37
8	A	1425	G	N3-C4	-5.98	1.31	1.35
8	A	679	C	N1-C6	-5.98	1.33	1.37
8	A	259	G	N9-C4	-5.97	1.33	1.38
8	A	926	G	N9-C4	-5.97	1.33	1.38
8	A	1139	G	C5-C4	-5.97	1.34	1.38
8	A	1666	G	N9-C4	-5.97	1.33	1.38
8	A	2223	G	N9-C4	-5.97	1.33	1.38
9	B	102	G	N9-C4	-5.97	1.33	1.38
8	A	1805	A	N9-C4	-5.97	1.34	1.37
8	A	551	G	N9-C4	-5.97	1.33	1.38
8	A	1034	G	N9-C4	-5.97	1.33	1.38
8	A	1697	G	N9-C4	-5.97	1.33	1.38
8	A	2444	G	N9-C4	-5.97	1.33	1.38
34	a	627	G	N9-C4	-5.96	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	a	446	G	N9-C4	-5.95	1.33	1.38
8	A	1530	G	N9-C4	-5.95	1.33	1.38
34	a	802	A	N9-C4	-5.95	1.34	1.37
8	A	1588	G	N9-C4	-5.94	1.33	1.38
8	A	368	A	N9-C4	-5.94	1.34	1.37
34	a	917	G	N9-C4	-5.94	1.33	1.38
34	a	921	U	P-O5'	5.94	1.65	1.59
8	A	21	A	N9-C4	-5.93	1.34	1.37
8	A	381	G	N9-C4	-5.93	1.33	1.38
8	A	404	A	N9-C4	-5.93	1.34	1.37
8	A	630	G	N9-C4	-5.93	1.33	1.38
8	A	1746	A	N9-C4	-5.93	1.34	1.37
8	A	1047	G	C2-N3	-5.93	1.28	1.32
8	A	1667	G	N9-C4	-5.93	1.33	1.38
34	a	410	G	N9-C4	-5.93	1.33	1.38
8	A	382	A	N9-C4	-5.92	1.34	1.37
8	A	778	G	N9-C4	-5.92	1.33	1.38
34	a	1276	G	N9-C4	-5.92	1.33	1.38
8	A	592	A	N9-C4	-5.91	1.34	1.37
34	a	1019	A	N9-C4	-5.91	1.34	1.37
55	v	6	G	N9-C4	-5.91	1.33	1.38
55	v	73	A	N9-C4	-5.91	1.34	1.37
8	A	638	G	N9-C4	-5.91	1.33	1.38
34	a	1061	G	N9-C4	-5.91	1.33	1.38
8	A	706	A	N9-C4	-5.90	1.34	1.37
8	A	2686	G	N9-C4	-5.90	1.33	1.38
34	a	949	A	N9-C4	-5.90	1.34	1.37
34	a	332	G	N9-C4	-5.89	1.33	1.38
9	B	24	G	N9-C4	-5.89	1.33	1.38
8	A	1977	A	N9-C4	-5.89	1.34	1.37
34	a	402	G	N9-C4	-5.88	1.33	1.38
34	a	319	G	N9-C4	-5.88	1.33	1.38
9	B	44	G	N9-C4	-5.88	1.33	1.38
28	U	59	GLU	CA-CB	-5.88	1.41	1.53
8	A	58	G	N9-C4	-5.87	1.33	1.38
8	A	629	G	N9-C4	-5.87	1.33	1.38
8	A	94	A	N9-C4	-5.87	1.34	1.37
34	a	181	A	C5-C6	-5.87	1.35	1.41
8	A	2077	A	N9-C4	-5.86	1.34	1.37
34	a	1362	A	N9-C4	-5.86	1.34	1.37
8	A	675	A	N9-C4	-5.86	1.34	1.37
8	A	1281	G	N9-C4	-5.86	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	a	320	A	N9-C4	-5.86	1.34	1.37
34	a	786	G	N9-C4	-5.86	1.33	1.38
8	A	1678	A	N9-C4	-5.86	1.34	1.37
34	a	915	A	N9-C4	-5.86	1.34	1.37
8	A	1154	G	N9-C4	-5.85	1.33	1.38
8	A	1826	G	N9-C4	-5.85	1.33	1.38
8	A	1973	G	N9-C4	-5.85	1.33	1.38
34	a	722	G	N9-C4	-5.85	1.33	1.38
8	A	122	G	N9-C4	-5.84	1.33	1.38
8	A	1178	C	N1-C6	-5.84	1.33	1.37
8	A	1308	A	N9-C4	-5.83	1.34	1.37
34	a	50	A	N9-C4	-5.83	1.34	1.37
8	A	2373	G	N9-C4	-5.82	1.33	1.38
8	A	2816	G	N9-C4	-5.82	1.33	1.38
8	A	2191	A	N9-C4	-5.82	1.34	1.37
8	A	1501	G	N9-C4	-5.82	1.33	1.38
8	A	2671	G	N9-C4	-5.82	1.33	1.38
8	A	977	G	N9-C4	-5.82	1.33	1.38
8	A	1420	A	N9-C4	-5.82	1.34	1.37
8	A	1538	G	N9-C4	-5.82	1.33	1.38
8	A	2899	A	C5-C6	-5.82	1.35	1.41
8	A	1873	G	N9-C4	-5.81	1.33	1.38
34	a	68	G	N9-C4	-5.81	1.33	1.38
8	A	2071	A	N9-C4	-5.81	1.34	1.37
8	A	2730	C	N1-C6	-5.81	1.33	1.37
8	A	1106	G	C2-N3	-5.80	1.28	1.32
55	v	21	A	N9-C4	-5.80	1.34	1.37
34	a	1487	G	N9-C4	-5.79	1.33	1.38
8	A	1194	A	N9-C4	-5.79	1.34	1.37
34	a	408	A	N9-C4	-5.79	1.34	1.37
8	A	1875	G	N9-C4	-5.78	1.33	1.38
9	B	104	A	N9-C4	-5.78	1.34	1.37
8	A	219	A	N9-C4	-5.78	1.34	1.37
8	A	152	A	N9-C4	-5.78	1.34	1.37
8	A	1025	G	C2-N3	-5.78	1.28	1.32
8	A	936	A	N9-C4	-5.77	1.34	1.37
34	a	452	A	C6-N1	-5.77	1.31	1.35
8	A	359	G	N9-C4	-5.77	1.33	1.38
34	a	1418	A	N9-C4	-5.77	1.34	1.37
8	A	95	A	N9-C4	-5.76	1.34	1.37
8	A	1025	G	N3-C4	-5.76	1.31	1.35
8	A	952	G	N9-C4	-5.76	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	2569	G	N9-C4	-5.76	1.33	1.38
8	A	2471	A	N9-C4	-5.76	1.34	1.37
8	A	2437	G	N9-C4	-5.75	1.33	1.38
8	A	1011	G	N9-C4	-5.75	1.33	1.38
8	A	481	G	N9-C4	-5.75	1.33	1.38
8	A	2436	G	N9-C4	-5.75	1.33	1.38
34	a	752	G	N9-C4	-5.75	1.33	1.38
34	a	1108	G	N3-C4	-5.75	1.31	1.35
9	B	78	A	N9-C4	-5.74	1.34	1.37
9	B	73	A	N9-C4	-5.74	1.34	1.37
8	A	2669	G	N9-C4	-5.74	1.33	1.38
8	A	497	A	N9-C4	-5.73	1.34	1.37
8	A	861	A	N9-C4	-5.73	1.34	1.37
8	A	1417	C	N1-C6	-5.73	1.33	1.37
34	a	300	A	N9-C4	-5.73	1.34	1.37
8	A	1192	G	N9-C4	-5.72	1.33	1.38
34	a	1374	A	C6-N6	-5.72	1.29	1.33
8	A	1189	A	N9-C4	-5.72	1.34	1.37
8	A	2577	A	N9-C4	-5.72	1.34	1.37
8	A	1933	G	N9-C4	-5.71	1.33	1.38
34	a	830	G	N9-C4	-5.71	1.33	1.38
8	A	997	G	N9-C4	-5.71	1.33	1.38
8	A	2415	G	N9-C4	-5.71	1.33	1.38
8	A	2526	G	N9-C4	-5.71	1.33	1.38
34	a	606	G	N9-C4	-5.71	1.33	1.38
8	A	1482	G	N9-C4	-5.70	1.33	1.38
55	v	26	G	N9-C4	-5.70	1.33	1.38
8	A	843	G	C2-N3	-5.70	1.28	1.32
8	A	590	A	N9-C4	-5.69	1.34	1.37
34	a	380	G	N9-C4	-5.69	1.33	1.38
8	A	2501	C	N1-C6	-5.69	1.33	1.37
8	A	2355	G	N9-C4	-5.69	1.33	1.38
8	A	924	G	N9-C4	-5.69	1.33	1.38
8	A	1225	G	N9-C4	-5.69	1.33	1.38
55	v	52	G	N9-C4	-5.69	1.33	1.38
34	a	1104	G	N9-C4	-5.68	1.33	1.38
8	A	618	G	N9-C4	-5.68	1.33	1.38
8	A	633	A	N9-C4	-5.68	1.34	1.37
8	A	1771	C	N3-C4	-5.67	1.29	1.33
8	A	1863	G	N9-C4	-5.67	1.33	1.38
8	A	1661	G	N9-C4	-5.67	1.33	1.38
34	a	749	A	N9-C4	-5.67	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	802	A	N9-C4	-5.67	1.34	1.37
34	a	146	G	N9-C4	-5.67	1.33	1.38
34	a	1074	G	N3-C4	-5.67	1.31	1.35
8	A	91	A	N9-C4	-5.67	1.34	1.37
34	a	1461	G	N9-C4	-5.67	1.33	1.38
8	A	2670	A	N9-C4	-5.66	1.34	1.37
8	A	55	G	N9-C4	-5.66	1.33	1.38
8	A	2328	A	N9-C4	-5.66	1.34	1.37
9	B	105	G	N9-C4	-5.66	1.33	1.38
34	a	706	A	N9-C4	-5.66	1.34	1.37
8	A	261	G	N9-C4	-5.65	1.33	1.38
8	A	1182	G	N9-C4	-5.65	1.33	1.38
8	A	35	G	N9-C4	-5.65	1.33	1.38
8	A	2435	A	C6-N6	-5.65	1.29	1.33
34	a	373	A	N9-C4	-5.65	1.34	1.37
8	A	836	G	N9-C4	-5.64	1.33	1.38
34	a	947	G	N9-C4	-5.64	1.33	1.38
34	a	824	G	N9-C4	-5.64	1.33	1.38
8	A	713	G	N9-C4	-5.64	1.33	1.38
34	a	361	G	N9-C4	-5.64	1.33	1.38
8	A	575	A	N9-C4	-5.64	1.34	1.37
34	a	682	G	N9-C4	-5.64	1.33	1.38
8	A	1566	A	N9-C4	-5.63	1.34	1.37
8	A	693	A	N9-C4	-5.63	1.34	1.37
8	A	1115	G	N9-C4	-5.63	1.33	1.38
8	A	2840	C	N1-C6	-5.63	1.33	1.37
34	a	243	A	N9-C4	-5.63	1.34	1.37
8	A	469	G	N9-C4	-5.62	1.33	1.38
8	A	342	A	N9-C4	-5.62	1.34	1.37
8	A	2839	G	N9-C4	-5.62	1.33	1.38
34	a	630	A	N9-C4	-5.61	1.34	1.37
34	a	1190	G	N9-C4	-5.61	1.33	1.38
8	A	256	A	N9-C4	-5.61	1.34	1.37
55	v	43	A	N9-C4	-5.60	1.34	1.37
8	A	1492	G	C2-N3	-5.59	1.28	1.32
8	A	1569	A	N9-C4	-5.59	1.34	1.37
55	v	63	G	N9-C4	-5.58	1.33	1.38
8	A	2088	A	N9-C4	-5.58	1.34	1.37
8	A	2170	A	N9-C4	-5.57	1.34	1.37
34	a	451	A	N9-C4	-5.57	1.34	1.37
34	a	1134	G	C2-N3	-5.57	1.28	1.32
34	a	1092	A	N9-C4	-5.57	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	a	117	G	N9-C4	-5.56	1.33	1.38
8	A	2853	C	N1-C6	-5.56	1.33	1.37
34	a	255	G	N9-C4	-5.56	1.33	1.38
34	a	691	G	N9-C4	-5.56	1.33	1.38
34	a	104	G	N9-C4	-5.55	1.33	1.38
8	A	309	A	N9-C4	-5.55	1.34	1.37
8	A	2744	G	N9-C4	-5.55	1.33	1.38
8	A	362	A	O3'-P	-5.54	1.54	1.61
34	a	825	A	N9-C4	-5.54	1.34	1.37
9	B	100	G	N9-C4	-5.53	1.33	1.38
8	A	899	A	N9-C4	-5.53	1.34	1.37
34	a	655	A	N9-C4	-5.53	1.34	1.37
8	A	1401	G	N9-C4	-5.53	1.33	1.38
8	A	1681	G	N9-C4	-5.53	1.33	1.38
34	a	1253	G	N9-C4	-5.53	1.33	1.38
34	a	1459	G	N9-C4	-5.53	1.33	1.38
9	B	60	C	N1-C2	-5.52	1.34	1.40
8	A	553	G	N9-C4	-5.52	1.33	1.38
8	A	2644	G	N9-C4	-5.52	1.33	1.38
34	a	742	G	N9-C4	-5.52	1.33	1.38
8	A	6	A	N9-C4	-5.51	1.34	1.37
8	A	2509	G	N9-C4	-5.51	1.33	1.38
8	A	1378	A	C5-C6	-5.51	1.36	1.41
8	A	1274	A	N9-C4	-5.51	1.34	1.37
8	A	1456	G	N9-C4	-5.51	1.33	1.38
34	a	1074	G	N9-C4	-5.51	1.33	1.38
8	A	2553	G	N9-C4	-5.51	1.33	1.38
8	A	134	G	N9-C4	-5.50	1.33	1.38
8	A	2664	G	N9-C4	-5.50	1.33	1.38
8	A	233	A	N9-C4	-5.50	1.34	1.37
34	a	1252	A	N9-C4	-5.49	1.34	1.37
34	a	1098	C	C2-N3	-5.49	1.31	1.35
8	A	1719	G	N9-C4	-5.49	1.33	1.38
8	A	307	G	N9-C4	-5.49	1.33	1.38
8	A	2590	A	N9-C4	-5.48	1.34	1.37
8	A	1419	A	N9-C4	-5.48	1.34	1.37
8	A	1551	A	N9-C4	-5.48	1.34	1.37
8	A	2227	A	N9-C4	-5.48	1.34	1.37
8	A	971	G	N9-C4	-5.48	1.33	1.38
8	A	2218	G	N9-C4	-5.47	1.33	1.38
8	A	212	G	N9-C4	-5.47	1.33	1.38
8	A	1945	G	N9-C4	-5.47	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	a	1048	G	N9-C4	-5.46	1.33	1.38
8	A	1040	A	N9-C4	-5.46	1.34	1.37
8	A	1966	A	N9-C4	-5.46	1.34	1.37
8	A	2574	G	N9-C4	-5.46	1.33	1.38
8	A	1278	C	N1-C6	-5.46	1.33	1.37
8	A	1686	C	C2-N3	-5.45	1.31	1.35
8	A	319	G	N9-C4	-5.45	1.33	1.38
8	A	595	C	N1-C6	-5.45	1.33	1.37
8	A	925	A	N9-C4	-5.45	1.34	1.37
8	A	2426	A	N9-C4	-5.45	1.34	1.37
34	a	1299	A	N9-C4	-5.45	1.34	1.37
8	A	2530	A	N9-C4	-5.44	1.34	1.37
8	A	668	A	N9-C4	-5.44	1.34	1.37
8	A	1171	G	N3-C4	-5.44	1.31	1.35
8	A	2430	A	C5-C6	-5.44	1.36	1.41
8	A	1010	A	N9-C4	-5.43	1.34	1.37
34	a	859	G	N9-C4	-5.43	1.33	1.38
8	A	2070	A	N9-C4	-5.43	1.34	1.37
8	A	1388	G	N9-C4	-5.43	1.33	1.38
8	A	93	G	N9-C4	-5.43	1.33	1.38
8	A	792	A	N9-C4	-5.42	1.34	1.37
8	A	1958	C	N1-C6	-5.42	1.33	1.37
8	A	1987	A	N9-C4	-5.42	1.34	1.37
8	A	1519	G	N9-C4	-5.42	1.33	1.38
8	A	266	G	C6-N1	-5.42	1.35	1.39
8	A	1861	G	N9-C4	-5.42	1.33	1.38
8	A	1800	C	N1-C6	-5.41	1.33	1.37
8	A	2407	A	C5-C6	-5.41	1.36	1.41
51	r	42	ARG	CA-C	-5.41	1.38	1.52
8	A	2253	G	N9-C4	-5.41	1.33	1.38
8	A	506	G	N9-C4	-5.41	1.33	1.38
8	A	1807	G	N9-C4	-5.41	1.33	1.38
34	a	493	A	N9-C4	-5.41	1.34	1.37
8	A	2270	A	N9-C4	-5.41	1.34	1.37
9	B	107	G	N9-C4	-5.40	1.33	1.38
34	a	27	G	N9-C4	-5.40	1.33	1.38
8	A	9	G	N9-C4	-5.40	1.33	1.38
8	A	470	A	N9-C4	-5.40	1.34	1.37
34	a	959	A	N9-C4	-5.40	1.34	1.37
8	A	1121	C	N1-C6	-5.40	1.33	1.37
34	a	935	A	N9-C4	-5.40	1.34	1.37
8	A	555	G	N9-C4	-5.39	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	636	G	N9-C8	-5.39	1.34	1.37
8	A	1177	G	N9-C4	-5.39	1.33	1.38
8	A	311	A	N9-C4	-5.39	1.34	1.37
8	A	2094	A	N9-C4	-5.39	1.34	1.37
34	a	1117	A	N9-C4	-5.39	1.34	1.37
57	x	192	TRP	CB-CG	-5.39	1.40	1.50
8	A	1171	G	C2-N3	-5.39	1.28	1.32
34	a	1329	A	C5-C4	-5.39	1.34	1.38
8	A	2705	A	N9-C4	-5.38	1.34	1.37
34	a	1088	G	N3-C4	-5.38	1.31	1.35
8	A	340	A	C5-C6	-5.38	1.36	1.41
8	A	1797	G	N9-C4	-5.38	1.33	1.38
8	A	2821	A	N9-C4	-5.38	1.34	1.37
34	a	487	A	N9-C4	-5.38	1.34	1.37
34	a	878	A	N9-C4	-5.38	1.34	1.37
34	a	492	C	N1-C2	-5.38	1.34	1.40
34	a	541	G	N9-C4	-5.38	1.33	1.38
8	A	425	G	N9-C4	-5.38	1.33	1.38
8	A	262	A	N9-C4	-5.37	1.34	1.37
8	A	2781	A	N9-C4	-5.37	1.34	1.37
31	X	16	ASN	CA-CB	-5.37	1.39	1.53
8	A	1214	A	N9-C4	-5.37	1.34	1.37
8	A	2679	A	N9-C4	-5.37	1.34	1.37
34	a	1204	A	N9-C4	-5.37	1.34	1.37
8	A	2898	U	C2-N3	-5.37	1.33	1.37
8	A	48	G	N9-C4	-5.37	1.33	1.38
8	A	1889	A	N9-C4	-5.37	1.34	1.37
8	A	2082	A	C6-N6	-5.36	1.29	1.33
8	A	1093	G	N9-C4	-5.36	1.33	1.38
8	A	1479	G	N9-C4	-5.36	1.33	1.38
55	v	12	G	C2-N3	-5.36	1.28	1.32
8	A	820	A	N9-C4	-5.36	1.34	1.37
8	A	1998	A	C6-N1	-5.36	1.31	1.35
8	A	2778	A	N9-C4	-5.36	1.34	1.37
8	A	1587	G	N9-C4	-5.35	1.33	1.38
8	A	1095	A	N9-C4	-5.35	1.34	1.37
8	A	1568	G	C6-N1	-5.35	1.35	1.39
34	a	257	G	N9-C4	-5.35	1.33	1.38
34	a	585	G	N9-C4	-5.35	1.33	1.38
34	a	1145	A	N9-C4	-5.35	1.34	1.37
8	A	2465	C	N1-C6	-5.34	1.33	1.37
8	A	2840	C	C5-C6	-5.34	1.30	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	a	288	A	N9-C4	-5.34	1.34	1.37
34	a	432	A	C5-C6	-5.34	1.36	1.41
8	A	823	C	N1-C6	-5.34	1.33	1.37
8	A	1178	C	C4-N4	-5.34	1.29	1.33
8	A	1549	A	N9-C4	-5.34	1.34	1.37
8	A	2235	G	C2-N3	-5.34	1.28	1.32
8	A	192	C	N1-C6	-5.34	1.33	1.37
8	A	197	A	N9-C4	-5.33	1.34	1.37
8	A	1426	G	N9-C4	-5.33	1.33	1.38
8	A	2412	A	N9-C4	-5.33	1.34	1.37
8	A	424	G	N9-C4	-5.33	1.33	1.38
8	A	2407	A	N9-C4	-5.33	1.34	1.37
9	B	64	G	N9-C4	-5.33	1.33	1.38
8	A	460	A	N9-C4	-5.32	1.34	1.37
8	A	2051	A	N9-C4	-5.32	1.34	1.37
34	a	1368	A	N9-C4	-5.32	1.34	1.37
9	B	42	C	N1-C6	-5.32	1.33	1.37
55	v	29	G	N9-C4	-5.32	1.33	1.38
8	A	2900	A	N9-C4	-5.32	1.34	1.37
8	A	1369	G	N9-C4	-5.31	1.33	1.38
8	A	1682	G	N9-C4	-5.31	1.33	1.38
34	a	838	G	N9-C4	-5.31	1.33	1.38
8	A	1435	G	N9-C4	-5.30	1.33	1.38
8	A	2641	G	N9-C4	-5.30	1.33	1.38
8	A	953	G	N9-C4	-5.30	1.33	1.38
8	A	1384	A	N9-C4	-5.30	1.34	1.37
8	A	2230	G	N9-C4	-5.30	1.33	1.38
8	A	1653	G	N9-C4	-5.29	1.33	1.38
8	A	1803	A	N9-C4	-5.29	1.34	1.37
8	A	2708	G	N9-C4	-5.29	1.33	1.38
34	a	1433	A	N9-C4	-5.29	1.34	1.37
8	A	549	G	N9-C4	-5.29	1.33	1.38
8	A	697	G	N9-C4	-5.29	1.33	1.38
8	A	1643	G	N9-C4	-5.29	1.33	1.38
34	a	129	A	N9-C4	-5.29	1.34	1.37
34	a	1500	A	N9-C4	-5.29	1.34	1.37
8	A	1008	A	N9-C4	-5.28	1.34	1.37
8	A	2571	U	C2-N3	-5.28	1.34	1.37
8	A	2516	A	N9-C4	-5.28	1.34	1.37
8	A	2890	G	N9-C4	-5.28	1.33	1.38
34	a	1081	A	C3'-O3'	5.28	1.49	1.42
8	A	966	G	N9-C4	-5.28	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	1075	C	C2-N3	-5.27	1.31	1.35
8	A	2082	A	C5-C4	-5.27	1.35	1.38
8	A	1557	C	N1-C6	-5.26	1.33	1.37
8	A	463	G	N9-C4	-5.26	1.33	1.38
8	A	1846	G	N9-C4	-5.26	1.33	1.38
8	A	672	C	N1-C6	-5.26	1.33	1.37
8	A	862	G	N9-C4	-5.26	1.33	1.38
8	A	2792	A	N9-C4	-5.26	1.34	1.37
8	A	216	A	N9-C4	-5.26	1.34	1.37
8	A	1362	C	N1-C6	-5.25	1.33	1.37
34	a	800	G	N9-C4	-5.25	1.33	1.38
34	a	1176	A	N9-C4	-5.25	1.34	1.37
8	A	1139	G	C2-N3	-5.25	1.28	1.32
8	A	2095	A	N9-C4	-5.25	1.34	1.37
34	a	535	A	N9-C4	-5.25	1.34	1.37
34	a	638	U	C2-N3	-5.25	1.34	1.37
8	A	888	C	N3-C4	-5.25	1.30	1.33
8	A	1703	G	N9-C4	-5.25	1.33	1.38
8	A	1858	A	N9-C4	-5.25	1.34	1.37
34	a	1163	A	N9-C4	-5.25	1.34	1.37
8	A	88	G	C6-N1	-5.25	1.35	1.39
8	A	1017	G	N9-C4	-5.25	1.33	1.38
8	A	1013	C	N1-C6	-5.24	1.34	1.37
8	A	1117	C	N1-C6	-5.24	1.34	1.37
8	A	1448	G	N9-C4	-5.24	1.33	1.38
8	A	2281	A	C6-N6	-5.24	1.29	1.33
34	a	1319	A	N9-C4	-5.24	1.34	1.37
34	a	908	A	N9-C4	-5.24	1.34	1.37
8	A	2829	A	N9-C4	-5.24	1.34	1.37
9	B	50	A	N9-C4	-5.24	1.34	1.37
34	a	716	A	N9-C4	-5.24	1.34	1.37
8	A	2547	A	C6-N1	-5.24	1.31	1.35
34	a	903	G	N9-C4	-5.24	1.33	1.38
56	w	38	A	N9-C4	-5.24	1.34	1.37
8	A	621	A	N9-C4	-5.23	1.34	1.37
8	A	1477	A	N9-C4	-5.23	1.34	1.37
8	A	1517	G	N9-C4	-5.23	1.33	1.38
8	A	1169	A	C5-C6	-5.23	1.36	1.41
8	A	728	G	N9-C4	-5.23	1.33	1.38
34	a	1057	G	N9-C4	-5.23	1.33	1.38
8	A	2012	G	N9-C4	-5.23	1.33	1.38
34	a	1182	G	N9-C4	-5.23	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	a	1154	G	N9-C4	-5.22	1.33	1.38
8	A	721	A	N9-C4	-5.22	1.34	1.37
8	A	2567	G	N9-C4	-5.22	1.33	1.38
8	A	81	G	N9-C4	-5.22	1.33	1.38
8	A	732	C	N1-C6	-5.22	1.34	1.37
8	A	2659	G	N9-C4	-5.22	1.33	1.38
8	A	2826	A	N9-C4	-5.22	1.34	1.37
8	A	2848	G	N9-C4	-5.22	1.33	1.38
9	B	10	G	N9-C4	-5.22	1.33	1.38
34	a	53	A	N9-C4	-5.22	1.34	1.37
8	A	2080	A	N9-C4	-5.21	1.34	1.37
8	A	2484	G	N9-C4	-5.21	1.33	1.38
34	a	378	G	N9-C4	-5.21	1.33	1.38
34	a	1322	C	N1-C6	-5.21	1.34	1.37
8	A	1057	A	N9-C4	-5.21	1.34	1.37
8	A	1628	G	N9-C4	-5.21	1.33	1.38
8	A	1260	A	N9-C4	-5.21	1.34	1.37
8	A	2281	A	N9-C4	-5.21	1.34	1.37
8	A	2464	G	N9-C4	-5.21	1.33	1.38
34	a	654	G	C6-N1	-5.21	1.35	1.39
34	a	898	G	N9-C4	-5.21	1.33	1.38
8	A	495	G	N9-C4	-5.21	1.33	1.38
8	A	1072	C	N1-C6	-5.21	1.34	1.37
8	A	1342	A	N9-C4	-5.21	1.34	1.37
8	A	2654	A	N9-C4	-5.21	1.34	1.37
8	A	340	A	C6-N6	-5.20	1.29	1.33
34	a	947	G	N9-C8	-5.20	1.34	1.37
8	A	1811	G	N9-C4	-5.20	1.33	1.38
34	a	1274	A	N9-C4	-5.20	1.34	1.37
34	a	1456	A	N9-C4	-5.20	1.34	1.37
8	A	1120	G	N9-C4	-5.20	1.33	1.38
34	a	2	A	N9-C4	-5.20	1.34	1.37
8	A	1975	G	N9-C4	-5.20	1.33	1.38
34	a	767	A	N9-C4	-5.19	1.34	1.37
34	a	500	G	N9-C4	-5.19	1.33	1.38
34	a	1310	G	N9-C4	-5.19	1.33	1.38
8	A	1638	C	N1-C6	-5.19	1.34	1.37
34	a	428	G	N9-C4	-5.19	1.33	1.38
34	a	581	G	N9-C4	-5.19	1.33	1.38
8	A	726	G	N9-C4	-5.19	1.33	1.38
34	a	1044	A	N9-C4	-5.19	1.34	1.37
9	B	28	C	N1-C6	-5.18	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	C	212	TRP	CB-CG	-5.18	1.41	1.50
8	A	2271	G	N9-C4	-5.18	1.33	1.38
8	A	2663	G	N3-C4	-5.18	1.31	1.35
34	a	1465	A	N9-C4	-5.18	1.34	1.37
8	A	220	G	C6-N1	-5.18	1.35	1.39
34	a	1120	C	N1-C6	-5.18	1.34	1.37
8	A	2097	A	C5-C6	-5.18	1.36	1.41
8	A	2217	G	N9-C4	-5.18	1.33	1.38
8	A	2678	C	N1-C6	-5.17	1.34	1.37
8	A	834	G	N9-C4	-5.17	1.33	1.38
8	A	2515	C	N1-C6	-5.17	1.34	1.37
34	a	760	G	N9-C4	-5.17	1.33	1.38
8	A	14	A	C5-C6	-5.17	1.36	1.41
34	a	928	G	N9-C4	-5.17	1.33	1.38
8	A	1711	A	C6-N1	-5.17	1.31	1.35
8	A	856	G	N9-C4	-5.16	1.33	1.38
8	A	979	A	N9-C4	-5.16	1.34	1.37
8	A	1194	A	C6-N1	-5.16	1.31	1.35
34	a	242	G	N9-C4	-5.16	1.33	1.38
34	a	592	G	C2-N3	-5.16	1.28	1.32
8	A	950	G	N9-C4	-5.16	1.33	1.38
34	a	1454	G	N9-C4	-5.16	1.33	1.38
8	A	1989	G	N9-C4	-5.15	1.33	1.38
8	A	2864	G	N9-C4	-5.15	1.33	1.38
34	a	1222	G	N9-C4	-5.15	1.33	1.38
8	A	2383	G	N9-C4	-5.15	1.33	1.38
8	A	1022	G	C2-N3	-5.15	1.28	1.32
8	A	2268	A	N9-C4	-5.15	1.34	1.37
34	a	119	A	N9-C4	-5.15	1.34	1.37
8	A	2758	A	N9-C4	-5.15	1.34	1.37
8	A	1039	A	N9-C4	-5.14	1.34	1.37
34	a	765	G	N9-C4	-5.14	1.33	1.38
34	a	1157	A	N9-C4	-5.14	1.34	1.37
8	A	1410	G	N9-C4	-5.14	1.33	1.38
8	A	327	G	N9-C4	-5.14	1.33	1.38
8	A	939	G	N9-C4	-5.14	1.33	1.38
8	A	2661	G	N9-C4	-5.14	1.33	1.38
8	A	247	G	N9-C4	-5.13	1.33	1.38
34	a	16	A	N9-C4	-5.13	1.34	1.37
34	a	602	A	C5-C6	-5.13	1.36	1.41
34	a	1047	G	N9-C4	-5.13	1.33	1.38
34	a	654	G	C5-C6	-5.12	1.37	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	1005	C	N3-C4	-5.12	1.30	1.33
8	A	1502	A	N9-C4	-5.12	1.34	1.37
34	a	38	G	N9-C4	-5.12	1.33	1.38
8	A	556	A	N9-C4	-5.12	1.34	1.37
8	A	80	G	N9-C4	-5.12	1.33	1.38
8	A	1725	U	C2-N3	-5.12	1.34	1.37
8	A	2575	C	N1-C6	-5.12	1.34	1.37
8	A	1055	G	N3-C4	-5.12	1.31	1.35
8	A	15	G	C6-N1	-5.11	1.35	1.39
56	w	53	G	N9-C4	-5.11	1.33	1.38
8	A	1425	G	C2-N3	-5.11	1.28	1.32
34	a	286	C	N1-C6	-5.11	1.34	1.37
8	A	136	G	N9-C4	-5.11	1.33	1.38
8	A	1370	C	N1-C6	-5.11	1.34	1.37
8	A	2335	A	N9-C4	-5.11	1.34	1.37
8	A	1104	C	N1-C2	-5.11	1.35	1.40
8	A	2777	G	N9-C4	-5.11	1.33	1.38
34	a	1039	G	N9-C4	-5.11	1.33	1.38
8	A	230	G	N9-C4	-5.10	1.33	1.38
34	a	861	G	N9-C4	-5.10	1.33	1.38
34	a	1404	C	N1-C2	-5.10	1.35	1.40
34	a	81	A	C5-C6	-5.10	1.36	1.41
8	A	132	G	N9-C4	-5.10	1.33	1.38
8	A	429	A	N9-C4	-5.10	1.34	1.37
8	A	877	A	N9-C4	-5.09	1.34	1.37
34	a	318	G	N9-C4	-5.09	1.33	1.38
8	A	2843	G	N9-C4	-5.09	1.33	1.38
34	a	227	G	N9-C4	-5.09	1.33	1.38
34	a	109	A	N9-C4	-5.08	1.34	1.37
34	a	1186	G	N9-C4	-5.08	1.33	1.38
34	a	52	C	N1-C6	-5.08	1.34	1.37
8	A	1335	C	N1-C6	-5.08	1.34	1.37
8	A	2663	G	C2-N3	-5.08	1.28	1.32
8	A	118	A	N9-C4	-5.08	1.34	1.37
9	B	84	G	N9-C4	-5.08	1.33	1.38
8	A	2544	G	N9-C4	-5.08	1.33	1.38
34	a	602	A	N9-C4	-5.08	1.34	1.37
8	A	1656	C	N1-C6	-5.07	1.34	1.37
34	a	362	G	N9-C4	-5.07	1.33	1.38
9	B	96	G	N9-C4	-5.07	1.33	1.38
34	a	1103	C	N1-C6	-5.07	1.34	1.37
8	A	1238	G	N9-C4	-5.07	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	1685	C	N1-C6	-5.07	1.34	1.37
8	A	1824	G	N9-C4	-5.07	1.33	1.38
34	a	247	G	N9-C4	-5.07	1.33	1.38
34	a	1331	G	N9-C4	-5.07	1.33	1.38
8	A	998	C	N1-C6	-5.07	1.34	1.37
8	A	1672	A	N9-C4	-5.07	1.34	1.37
8	A	2190	G	N9-C4	-5.07	1.33	1.38
34	a	138	G	N9-C4	-5.07	1.33	1.38
34	a	278	G	N9-C4	-5.07	1.33	1.38
8	A	2435	A	C5-C6	-5.06	1.36	1.41
34	a	595	A	N9-C4	-5.06	1.34	1.37
8	A	180	G	C2-N3	-5.06	1.28	1.32
8	A	2547	A	N9-C4	-5.06	1.34	1.37
34	a	980	C	N1-C6	-5.06	1.34	1.37
34	a	35	G	N9-C4	-5.06	1.33	1.38
8	A	1686	C	N1-C2	-5.06	1.35	1.40
8	A	1403	A	C6-N1	-5.06	1.32	1.35
8	A	43	G	N9-C4	-5.05	1.33	1.38
8	A	2780	G	N9-C4	-5.05	1.33	1.38
8	A	812	C	N1-C6	-5.05	1.34	1.37
8	A	1930	G	N9-C4	-5.05	1.33	1.38
34	a	812	G	N9-C4	-5.05	1.33	1.38
8	A	1634	A	N9-C4	-5.05	1.34	1.37
8	A	2516	A	C5-C6	-5.05	1.36	1.41
8	A	1999	C	N3-C4	-5.04	1.30	1.33
8	A	2279	G	N9-C4	-5.04	1.33	1.38
34	a	1058	G	N9-C4	-5.04	1.33	1.38
8	A	2897	U	N1-C2	-5.04	1.34	1.38
8	A	1147	A	N9-C4	-5.04	1.34	1.37
34	a	79	G	N9-C4	-5.04	1.33	1.38
8	A	1743	G	N9-C4	-5.04	1.33	1.38
8	A	1932	A	N9-C4	-5.04	1.34	1.37
8	A	2349	G	N9-C4	-5.04	1.33	1.38
34	a	151	A	N9-C4	-5.03	1.34	1.37
21	N	107	ASN	C-N	-5.03	1.22	1.34
34	a	430	A	N9-C4	-5.03	1.34	1.37
8	A	583	G	N9-C4	-5.03	1.33	1.38
8	A	900	A	N9-C8	-5.03	1.33	1.37
34	a	953	G	N9-C4	-5.03	1.33	1.38
8	A	1553	A	N9-C4	-5.03	1.34	1.37
8	A	1749	A	C5-C6	-5.03	1.36	1.41
8	A	2082	A	N9-C4	-5.03	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	46	A	N9-C4	-5.03	1.34	1.37
34	a	1102	A	C6-N1	-5.03	1.32	1.35
8	A	1696	G	N9-C4	-5.02	1.33	1.38
8	A	2377	A	N9-C4	-5.02	1.34	1.37
8	A	1477	A	C6-N6	-5.02	1.29	1.33
55	v	4	G	N9-C4	-5.02	1.33	1.38
8	A	1421	G	N9-C4	-5.02	1.33	1.38
8	A	1869	G	N9-C4	-5.02	1.33	1.38
8	A	2077	A	C5-C6	-5.02	1.36	1.41
8	A	488	G	N9-C4	-5.01	1.33	1.38
8	A	2877	G	N9-C4	-5.01	1.33	1.38
8	A	2199	A	C5-C6	-5.01	1.36	1.41
8	A	2854	G	N9-C4	-5.01	1.33	1.38
8	A	2470	G	N9-C4	-5.01	1.33	1.38
31	X	28	PHE	C-N	-5.01	1.22	1.34
8	A	1333	G	N9-C4	-5.00	1.33	1.38
8	A	2014	A	N9-C4	-5.00	1.34	1.37
8	A	189	G	N9-C4	-5.00	1.33	1.38
8	A	1037	G	N9-C4	-5.00	1.33	1.38
8	A	2834	G	N9-C4	-5.00	1.33	1.38
34	a	656	G	N9-C4	-5.00	1.33	1.38
8	A	1216	G	C2-N3	-5.00	1.28	1.32
8	A	1740	G	N9-C4	-5.00	1.33	1.38
8	A	2721	A	N9-C4	-5.00	1.34	1.37
8	A	2802	G	N9-C4	-5.00	1.33	1.38

All (4436) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	1055	G	N3-C4-C5	16.27	136.74	128.60
34	a	921	U	C6-N1-C2	-14.36	112.39	121.00
8	A	1055	G	N3-C4-N9	-14.11	117.53	126.00
34	a	201	G	N3-C4-C5	12.85	135.03	128.60
34	a	604	G	N3-C4-C5	12.82	135.01	128.60
8	A	469	G	C4-C5-N7	12.69	115.87	110.80
34	a	920	U	OP1-P-O3'	12.60	132.93	105.20
34	a	201	G	N3-C4-N9	-12.60	118.44	126.00
8	A	469	G	N9-C4-C5	-12.48	100.41	105.40
34	a	797	C	C6-N1-C2	12.38	125.25	120.30
8	A	843	G	N3-C4-C5	12.33	134.76	128.60
34	a	456	A	N1-C2-N3	12.17	135.38	129.30
34	a	921	U	O4'-C1'-N1	12.16	117.93	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	1604	C	C6-N1-C2	11.96	125.08	120.30
34	a	921	U	C5-C6-N1	11.84	128.62	122.70
8	A	2235	G	N3-C4-C5	11.79	134.49	128.60
55	v	12	G	N3-C4-C5	11.78	134.49	128.60
34	a	1088	G	N3-C4-N9	-11.77	118.94	126.00
8	A	2767	C	C6-N1-C2	11.69	124.98	120.30
34	a	1143	G	N3-C4-C5	11.42	134.31	128.60
8	A	1687	G	N3-C4-N9	-11.40	119.16	126.00
34	a	858	G	N3-C4-N9	-11.40	119.16	126.00
34	a	921	U	OP1-P-OP2	-11.30	102.65	119.60
8	A	180	G	N3-C4-C5	11.24	134.22	128.60
8	A	1492	G	N3-C4-C5	11.20	134.20	128.60
34	a	542	G	N3-C4-C5	11.19	134.19	128.60
34	a	1129	C	C6-N1-C2	11.12	124.75	120.30
8	A	1277	G	N3-C4-C5	11.10	134.15	128.60
34	a	920	U	P-O3'-C3'	11.04	132.95	119.70
8	A	2576	G	N3-C2-N2	-11.02	112.19	119.90
9	B	31	C	C6-N1-C2	10.98	124.69	120.30
8	A	2198	A	N1-C6-N6	-10.96	112.02	118.60
8	A	814	C	C6-N1-C2	10.96	124.68	120.30
8	A	780	G	N3-C4-N9	-10.92	119.45	126.00
8	A	1022	G	N3-C4-N9	-10.86	119.48	126.00
8	A	1492	G	N3-C4-N9	-10.83	119.50	126.00
8	A	1450	G	N3-C4-C5	10.74	133.97	128.60
8	A	1810	A	N1-C6-N6	10.74	125.04	118.60
34	a	592	G	N3-C4-C5	10.73	133.97	128.60
55	v	17	C	O4'-C1'-N1	-10.73	99.62	108.20
34	a	241	G	N3-C4-C5	10.71	133.95	128.60
8	A	1425	G	N3-C4-C5	10.69	133.94	128.60
34	a	1134	G	N3-C4-N9	-10.65	119.61	126.00
34	a	1081	A	P-O3'-C3'	10.62	132.44	119.70
8	A	2663	G	N3-C4-N9	-10.59	119.65	126.00
8	A	2763	G	N3-C4-C5	10.57	133.89	128.60
34	a	858	G	N3-C4-C5	10.51	133.86	128.60
34	a	42	G	N3-C4-C5	10.50	133.85	128.60
8	A	2146	C	C6-N1-C2	10.49	124.50	120.30
8	A	1684	G	N3-C4-C5	10.45	133.82	128.60
8	A	1117	C	C6-N1-C2	10.45	124.48	120.30
34	a	954	G	N3-C4-C5	10.41	133.81	128.60
34	a	201	G	C2-N3-C4	-10.40	106.70	111.90
8	A	2663	G	N3-C4-C5	10.38	133.79	128.60
34	a	158	G	O4'-C1'-N9	-10.37	99.90	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	a	1244	G	N3-C4-C5	10.37	133.78	128.60
8	A	1022	G	N3-C2-N2	-10.35	112.66	119.90
8	A	2010	G	N3-C4-C5	10.35	133.77	128.60
8	A	1091	G	N3-C4-C5	10.34	133.77	128.60
8	A	1025	G	N3-C4-C5	10.32	133.76	128.60
8	A	1686	C	C6-N1-C2	10.32	124.43	120.30
8	A	1013	C	C6-N1-C2	10.29	124.42	120.30
34	a	181	A	C5-C6-N6	-10.29	115.47	123.70
8	A	1378	A	N1-C6-N6	10.28	124.77	118.60
8	A	536	G	N3-C4-N9	-10.27	119.84	126.00
34	a	190	A	N1-C6-N6	10.26	124.75	118.60
34	a	1082	A	OP1-P-OP2	-10.25	104.23	119.60
8	A	2839	G	C2-N3-C4	-10.24	106.78	111.90
8	A	1016	G	N3-C4-C5	10.23	133.72	128.60
8	A	1047	G	N3-C4-N9	-10.21	119.87	126.00
8	A	1527	G	N3-C4-C5	10.20	133.70	128.60
8	A	318	C	C6-N1-C2	10.19	124.38	120.30
55	v	12	G	N3-C4-N9	-10.17	119.90	126.00
34	a	988	G	N3-C4-C5	10.14	133.67	128.60
8	A	314	C	C6-N1-C2	10.14	124.36	120.30
9	B	76	G	O5'-P-OP1	-10.13	96.58	105.70
8	A	2803	G	N3-C4-C5	10.08	133.64	128.60
8	A	1908	C	C6-N1-C2	10.07	124.33	120.30
8	A	1025	G	N3-C4-N9	-10.05	119.97	126.00
8	A	696	G	N3-C4-C5	10.03	133.62	128.60
8	A	1371	G	N3-C4-C5	10.02	133.61	128.60
34	a	521	G	N3-C4-C5	10.00	133.60	128.60
8	A	1216	G	N3-C4-C5	9.99	133.59	128.60
9	B	20	G	N3-C4-C5	9.98	133.59	128.60
8	A	1721	G	N3-C4-C5	9.97	133.59	128.60
34	a	1050	G	N3-C4-N9	-9.97	120.02	126.00
8	A	1652	A	N1-C6-N6	9.96	124.58	118.60
34	a	1143	G	C8-N9-C4	9.94	110.37	106.40
34	a	888	G	N3-C4-C5	9.93	133.56	128.60
34	a	920	U	OP2-P-O3'	-9.91	83.39	105.20
8	A	1674	G	N3-C4-C5	9.91	133.56	128.60
8	A	752	A	O4'-C1'-N9	9.89	116.11	108.20
8	A	1642	G	N3-C4-C5	9.89	133.54	128.60
34	a	1418	A	C8-N9-C4	9.89	109.75	105.80
8	A	2338	C	C6-N1-C2	9.88	124.25	120.30
34	a	1050	G	N3-C4-C5	9.88	133.54	128.60
34	a	175	C	C6-N1-C2	9.87	124.25	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	a	888	G	N3-C4-N9	-9.84	120.10	126.00
34	a	617	G	N3-C4-C5	9.84	133.52	128.60
8	A	1789	A	C2'-C3'-O3'	9.83	131.13	109.50
8	A	2576	G	N1-C2-N2	9.83	125.05	116.20
34	a	181	A	N1-C6-N6	9.80	124.48	118.60
8	A	2414	G	N3-C4-N9	-9.79	120.13	126.00
8	A	2525	G	C8-N9-C4	9.78	110.31	106.40
8	A	1604	C	N3-C4-C5	9.76	125.80	121.90
9	B	54	G	N3-C4-C5	9.73	133.46	128.60
8	A	1064	C	N1-C2-O2	-9.70	113.08	118.90
8	A	2576	G	N3-C4-N9	-9.67	120.20	126.00
34	a	1108	G	N3-C2-N2	-9.66	113.14	119.90
55	v	9	G	N3-C4-C5	9.66	133.43	128.60
8	A	2389	G	N3-C4-N9	-9.63	120.22	126.00
8	A	1139	G	N3-C4-C5	9.62	133.41	128.60
8	A	2525	G	N3-C4-C5	9.62	133.41	128.60
8	A	52	A	N1-C6-N6	9.60	124.36	118.60
8	A	2496	C	N1-C2-O2	9.60	124.66	118.90
8	A	301	G	N3-C4-C5	9.59	133.39	128.60
8	A	180	G	N3-C4-N9	-9.59	120.25	126.00
8	A	1178	C	N3-C4-C5	9.57	125.73	121.90
8	A	2430	A	N1-C6-N6	9.56	124.34	118.60
34	a	640	A	C8-N9-C4	9.56	109.62	105.80
8	A	1025	G	C2-N3-C4	-9.55	107.13	111.90
8	A	1425	G	N3-C4-N9	-9.55	120.27	126.00
8	A	1745	A	C8-N9-C4	9.53	109.61	105.80
34	a	651	C	C6-N1-C2	9.54	124.11	120.30
8	A	1465	G	N3-C4-C5	9.53	133.37	128.60
8	A	1054	A	N9-C4-C5	-9.52	101.99	105.80
34	a	1088	G	C5-C6-O6	9.50	134.30	128.60
8	A	2665	A	C8-N9-C4	9.49	109.60	105.80
34	a	628	G	N3-C4-C5	9.48	133.34	128.60
34	a	1156	G	N3-C4-C5	9.48	133.34	128.60
55	v	17	C	N1-C1'-C2'	9.47	126.32	114.00
8	A	1904	G	N3-C4-C5	9.46	133.33	128.60
8	A	289	G	N3-C4-C5	9.43	133.32	128.60
8	A	1941	C	C6-N1-C2	9.43	124.07	120.30
8	A	1642	G	N3-C4-N9	-9.42	120.34	126.00
8	A	2254	C	C6-N1-C2	9.42	124.07	120.30
8	A	2381	A	C4'-C3'-O3'	9.41	131.81	113.00
8	A	45	G	N3-C4-C5	9.39	133.29	128.60
8	A	780	G	N3-C4-C5	9.38	133.29	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	2526	G	C2-N3-C4	-9.38	107.21	111.90
34	a	1289	A	N1-C6-N6	9.37	124.22	118.60
8	A	2235	G	N3-C4-N9	-9.37	120.38	126.00
8	A	260	G	N3-C4-C5	9.37	133.28	128.60
8	A	178	G	N3-C4-C5	9.36	133.28	128.60
9	B	54	G	C2-N3-C4	-9.34	107.23	111.90
8	A	2154	A	N1-C6-N6	9.34	124.20	118.60
8	A	1277	G	N3-C4-N9	-9.32	120.41	126.00
8	A	2763	G	N3-C4-N9	-9.31	120.41	126.00
8	A	2338	C	N3-C4-C5	9.30	125.62	121.90
8	A	1266	G	N3-C4-N9	-9.30	120.42	126.00
8	A	1543	G	N3-C4-C5	9.30	133.25	128.60
8	A	2153	C	C6-N1-C2	9.29	124.02	120.30
8	A	1163	G	N3-C4-C5	9.29	133.25	128.60
8	A	1317	G	N3-C4-C5	9.29	133.24	128.60
8	A	359	G	N3-C4-N9	-9.28	120.43	126.00
8	A	1631	G	N3-C4-N9	-9.27	120.44	126.00
8	A	536	G	N3-C4-C5	9.27	133.23	128.60
8	A	1425	G	C2-N3-C4	-9.26	107.27	111.90
8	A	2770	G	N3-C4-C5	9.23	133.22	128.60
8	A	843	G	N3-C4-N9	-9.23	120.46	126.00
34	a	1227	A	N1-C6-N6	-9.23	113.06	118.60
56	w	15	G	N1-C2-N2	-9.21	107.91	116.20
8	A	469	G	C8-N9-C4	9.21	110.08	106.40
34	a	1253	G	N3-C4-N9	-9.19	120.48	126.00
8	A	2803	G	C8-N9-C4	9.19	110.08	106.40
34	a	987	G	N3-C4-C5	9.19	133.19	128.60
8	A	124	G	N3-C4-C5	9.19	133.19	128.60
8	A	1424	G	N3-C4-C5	9.19	133.19	128.60
34	a	1432	G	N3-C4-C5	9.19	133.19	128.60
8	A	708	G	N3-C4-C5	9.18	133.19	128.60
8	A	2631	G	N3-C4-C5	9.18	133.19	128.60
8	A	2770	G	N3-C4-N9	-9.17	120.50	126.00
8	A	949	G	N3-C4-C5	9.17	133.18	128.60
8	A	1922	G	N3-C4-C5	9.17	133.18	128.60
34	a	1088	G	N3-C4-C5	9.16	133.18	128.60
34	a	1222	G	C2-N3-C4	-9.12	107.34	111.90
8	A	1687	G	N3-C4-C5	9.12	133.16	128.60
8	A	1449	G	N3-C4-N9	-9.11	120.54	126.00
8	A	1022	G	O4'-C1'-N9	9.09	115.47	108.20
8	A	1171	G	N3-C2-N2	-9.09	113.54	119.90
8	A	1867	G	N3-C4-C5	9.09	133.14	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	a	1488	G	N3-C4-C5	9.09	133.14	128.60
56	w	68	C	C6-N1-C2	9.09	123.93	120.30
8	A	2551	C	N3-C4-N4	-9.08	111.64	118.00
8	A	1374	G	N3-C4-C5	9.06	133.13	128.60
8	A	2458	G	N3-C4-C5	9.06	133.13	128.60
8	A	865	C	N3-C4-N4	-9.04	111.67	118.00
34	a	1088	G	C2-N3-C4	-9.04	107.38	111.90
8	A	297	G	N3-C4-C5	9.03	133.11	128.60
8	A	1530	G	N3-C4-C5	9.02	133.11	128.60
34	a	617	G	N3-C4-N9	-9.02	120.59	126.00
34	a	809	G	N3-C4-C5	9.01	133.10	128.60
8	A	1482	G	N3-C4-C5	9.00	133.10	128.60
8	A	482	A	C8-N9-C4	9.00	109.40	105.80
34	a	1432	G	N3-C4-N9	-8.99	120.61	126.00
8	A	1909	C	C6-N1-C2	8.99	123.89	120.30
8	A	1656	C	C6-N1-C2	8.97	123.89	120.30
8	A	1072	C	C6-N1-C2	8.97	123.89	120.30
34	a	42	G	C2-N3-C4	-8.96	107.42	111.90
34	a	682	G	N3-C4-C5	8.97	133.08	128.60
8	A	315	G	N3-C4-C5	8.96	133.08	128.60
8	A	307	G	N3-C4-C5	8.96	133.08	128.60
34	a	1142	G	N3-C4-C5	8.96	133.08	128.60
34	a	637	C	C6-N1-C2	8.95	123.88	120.30
34	a	592	G	C2-N3-C4	-8.94	107.43	111.90
8	A	2485	G	N3-C4-C5	8.94	133.07	128.60
8	A	2496	C	N3-C2-O2	-8.94	115.64	121.90
8	A	361	G	C4-C5-N7	8.94	114.37	110.80
34	a	413	G	N3-C4-C5	8.93	133.06	128.60
34	a	1276	G	N3-C4-C5	8.93	133.06	128.60
8	A	1450	G	C2-N3-C4	-8.93	107.44	111.90
8	A	1666	G	N3-C4-N9	-8.93	120.64	126.00
8	A	1220	G	N3-C4-C5	8.92	133.06	128.60
34	a	1289	A	C5-C6-N6	-8.92	116.56	123.70
8	A	1894	C	C6-N1-C2	8.91	123.87	120.30
8	A	1721	G	C2-N3-C4	-8.90	107.45	111.90
8	A	2223	G	N3-C4-N9	-8.90	120.66	126.00
8	A	672	C	C6-N1-C2	8.88	123.85	120.30
8	A	24	G	N3-C4-C5	8.87	133.03	128.60
8	A	673	C	C6-N1-C2	8.86	123.84	120.30
9	B	23	G	N3-C4-C5	8.86	133.03	128.60
34	a	320	A	C8-N9-C4	8.85	109.34	105.80
8	A	2154	A	C5-C6-N6	-8.85	116.62	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	2223	G	N3-C4-C5	8.85	133.02	128.60
8	A	1311	G	N3-C4-C5	8.85	133.02	128.60
8	A	1449	G	N3-C4-C5	8.84	133.02	128.60
34	a	917	G	N3-C4-C5	8.84	133.02	128.60
8	A	675	A	N1-C6-N6	8.84	123.90	118.60
8	A	217	A	C8-N9-C4	8.84	109.33	105.80
34	a	1133	G	N3-C4-C5	8.83	133.02	128.60
55	v	9	G	N3-C4-N9	-8.83	120.70	126.00
34	a	1089	G	N3-C4-C5	8.81	133.01	128.60
34	a	1241	G	N3-C4-C5	8.80	133.00	128.60
34	a	1405	G	N3-C4-C5	8.80	133.00	128.60
8	A	2526	G	N3-C4-C5	8.79	133.00	128.60
34	a	953	G	C8-N9-C4	8.79	109.92	106.40
8	A	303	G	N3-C4-C5	8.79	133.00	128.60
8	A	781	A	N1-C6-N6	-8.79	113.33	118.60
8	A	1606	C	C6-N1-C2	8.79	123.81	120.30
34	a	1025	U	C5-C6-N1	8.78	127.09	122.70
8	A	2040	G	N3-C4-C5	8.78	132.99	128.60
8	A	675	A	C5-C6-N6	-8.78	116.68	123.70
34	a	1417	G	N3-C4-C5	8.78	132.99	128.60
34	a	1418	A	N9-C4-C5	-8.76	102.30	105.80
8	A	578	G	N1-C2-N2	-8.76	108.32	116.20
8	A	2894	G	N3-C4-C5	8.76	132.98	128.60
34	a	1081	A	C4-N9-C1'	8.76	142.06	126.30
8	A	1423	G	N3-C4-C5	8.75	132.97	128.60
8	A	2857	G	N3-C4-C5	8.74	132.97	128.60
9	B	102	G	N3-C4-C5	8.74	132.97	128.60
8	A	214	G	N3-C4-C5	8.73	132.97	128.60
34	a	823	C	C6-N1-C2	8.73	123.79	120.30
8	A	1450	G	N3-C4-N9	-8.73	120.76	126.00
8	A	2536	G	N3-C4-C5	8.73	132.96	128.60
8	A	2557	G	N3-C4-C5	8.72	132.96	128.60
9	B	119	A	C8-N9-C4	8.72	109.29	105.80
55	v	9	G	C4-N9-C1'	-8.72	115.17	126.50
8	A	2848	G	N3-C4-N9	-8.71	120.77	126.00
8	A	1984	G	N3-C4-C5	8.70	132.95	128.60
34	a	592	G	N3-C4-N9	-8.70	120.78	126.00
8	A	1216	G	C2-N3-C4	-8.70	107.55	111.90
8	A	818	G	N3-C4-C5	8.69	132.95	128.60
8	A	1718	G	C2-N3-C4	-8.69	107.56	111.90
8	A	381	G	N3-C4-C5	8.68	132.94	128.60
8	A	271	G	N3-C4-C5	8.68	132.94	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	1631	G	N3-C4-C5	8.68	132.94	128.60
8	A	2857	G	N3-C4-N9	-8.66	120.80	126.00
8	A	2472	G	N3-C4-C5	8.66	132.93	128.60
8	A	2894	G	N3-C4-N9	-8.66	120.80	126.00
8	A	469	G	C5-C6-O6	-8.66	123.40	128.60
34	a	847	G	C2-N3-C4	-8.66	107.57	111.90
8	A	2362	C	C6-N1-C2	8.65	123.76	120.30
34	a	461	A	C2-N3-C4	-8.65	106.27	110.60
8	A	1106	G	N3-C4-C5	8.64	132.92	128.60
8	A	188	G	N3-C4-C5	8.64	132.92	128.60
8	A	1767	G	N3-C4-C5	8.63	132.92	128.60
8	A	1735	A	N9-C4-C5	-8.63	102.35	105.80
8	A	818	G	C2-N3-C4	-8.63	107.59	111.90
8	A	1202	G	N3-C4-C5	8.63	132.91	128.60
8	A	2665	A	N9-C4-C5	-8.62	102.35	105.80
8	A	1022	G	N3-C4-C5	8.61	132.91	128.60
34	a	833	G	N3-C4-C5	8.61	132.90	128.60
34	a	1081	A	C8-N9-C1'	-8.60	112.21	127.70
9	B	11	C	C5-C4-N4	-8.58	114.19	120.20
8	A	2353	G	N3-C4-N9	-8.58	120.86	126.00
34	a	1209	C	C6-N1-C2	8.57	123.73	120.30
8	A	1112	G	N3-C4-C5	8.57	132.89	128.60
8	A	1292	G	N3-C4-C5	8.57	132.89	128.60
8	A	696	G	C8-N9-C4	8.56	109.82	106.40
34	a	117	G	C8-N9-C4	8.54	109.82	106.40
8	A	1652	A	C5-C6-N6	-8.53	116.88	123.70
55	v	15	G	N3-C4-C5	8.52	132.86	128.60
8	A	32	C	C6-N1-C2	8.52	123.71	120.30
8	A	1218	G	N3-C4-C5	8.52	132.86	128.60
8	A	1650	A	C8-N9-C4	8.52	109.21	105.80
8	A	315	G	N3-C4-N9	-8.51	120.89	126.00
8	A	778	G	N3-C4-C5	8.51	132.85	128.60
8	A	1218	G	C2-N3-C4	-8.51	107.65	111.90
34	a	1374	A	N9-C4-C5	-8.50	102.40	105.80
8	A	2716	C	C6-N1-C2	8.50	123.70	120.30
34	a	631	C	C6-N1-C2	8.50	123.70	120.30
8	A	726	G	C2-N3-C4	-8.50	107.65	111.90
8	A	425	G	N3-C4-C5	8.49	132.85	128.60
9	B	33	G	N3-C4-C5	8.49	132.85	128.60
8	A	2846	G	N3-C4-N9	-8.48	120.91	126.00
8	A	2010	G	N3-C4-N9	-8.48	120.91	126.00
8	A	361	G	N9-C4-C5	-8.48	102.01	105.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	1232	G	C2-N3-C4	-8.48	107.66	111.90
8	A	220	G	C2-N3-C4	-8.47	107.66	111.90
8	A	1106	G	N3-C4-N9	-8.47	120.92	126.00
8	A	1	G	N3-C4-C5	8.46	132.83	128.60
8	A	551	G	N3-C4-C5	8.46	132.83	128.60
8	A	2501	C	C6-N1-C2	8.46	123.68	120.30
9	B	56	G	C8-N9-C4	8.45	109.78	106.40
8	A	1750	G	N3-C4-C5	8.45	132.82	128.60
34	a	380	G	N3-C4-N9	-8.45	120.93	126.00
8	A	1674	G	C2-N3-C4	-8.45	107.67	111.90
8	A	2378	A	N1-C6-N6	8.44	123.67	118.60
8	A	2876	G	N3-C4-C5	8.45	132.82	128.60
34	a	908	A	C8-N9-C4	8.44	109.18	105.80
34	a	1312	G	N3-C4-C5	8.44	132.82	128.60
8	A	2524	G	N3-C4-C5	8.43	132.82	128.60
8	A	144	A	N9-C4-C5	-8.42	102.43	105.80
34	a	1226	C	C6-N1-C2	8.41	123.66	120.30
8	A	1028	A	C5-C6-N6	-8.41	116.97	123.70
8	A	1009	A	C8-N9-C4	8.40	109.16	105.80
34	a	79	G	N3-C4-C5	8.40	132.80	128.60
8	A	2316	G	N3-C4-C5	8.40	132.80	128.60
8	A	638	G	N3-C4-C5	8.39	132.79	128.60
8	A	1617	C	O4'-C1'-N1	8.39	114.91	108.20
8	A	2420	C	C6-N1-C2	8.39	123.66	120.30
34	a	158	G	C5-C6-O6	-8.38	123.57	128.60
34	a	859	G	N3-C4-C5	8.38	132.79	128.60
8	A	1540	G	N3-C4-C5	8.38	132.79	128.60
8	A	2414	G	N3-C4-C5	8.38	132.79	128.60
8	A	2353	G	N3-C4-C5	8.38	132.79	128.60
34	a	265	G	N3-C4-C5	8.38	132.79	128.60
8	A	1465	G	C2-N3-C4	-8.37	107.71	111.90
8	A	706	A	C8-N9-C4	8.37	109.15	105.80
8	A	940	G	N3-C4-C5	8.37	132.78	128.60
34	a	786	G	N3-C4-C5	8.36	132.78	128.60
34	a	1098	C	C6-N1-C1'	8.36	130.83	120.80
34	a	1104	G	N3-C4-C5	8.35	132.78	128.60
8	A	618	G	N3-C4-C5	8.35	132.77	128.60
9	B	54	G	N3-C4-N9	-8.33	121.00	126.00
34	a	1190	G	N3-C4-C5	8.33	132.77	128.60
34	a	1454	G	N3-C4-C5	8.33	132.77	128.60
8	A	1588	G	N3-C4-C5	8.33	132.76	128.60
8	A	1538	G	N3-C4-C5	8.33	132.76	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	1861	G	N3-C4-N9	-8.33	121.00	126.00
8	A	704	G	N3-C4-N9	-8.32	121.00	126.00
8	A	2640	G	N3-C4-C5	8.32	132.76	128.60
8	A	1527	G	N3-C4-N9	-8.32	121.01	126.00
55	v	6	G	N3-C4-C5	8.31	132.76	128.60
34	a	1190	G	N3-C4-N9	-8.31	121.01	126.00
8	A	1369	G	C2-N3-C4	-8.31	107.75	111.90
8	A	2228	G	N3-C4-N9	-8.31	121.02	126.00
8	A	1960	A	N9-C4-C5	-8.31	102.48	105.80
8	A	1667	G	N3-C4-N9	-8.29	121.02	126.00
8	A	359	G	N3-C4-C5	8.29	132.75	128.60
8	A	2624	G	N3-C4-N9	-8.29	121.03	126.00
8	A	1158	C	C6-N1-C2	8.29	123.61	120.30
34	a	752	G	N3-C4-C5	8.29	132.74	128.60
8	A	330	A	N1-C6-N6	-8.29	113.63	118.60
8	A	1054	A	C8-N9-C4	8.29	109.11	105.80
8	A	1337	G	N3-C4-C5	8.29	132.74	128.60
34	a	920	U	C6-N1-C2	-8.28	116.03	121.00
8	A	812	C	C6-N1-C2	8.28	123.61	120.30
56	w	15	G	N3-C2-N2	8.28	125.69	119.90
34	a	797	C	N3-C4-C5	8.27	125.21	121.90
8	A	997	G	N3-C4-C5	8.26	132.73	128.60
34	a	1405	G	N3-C4-N9	-8.26	121.04	126.00
8	A	887	A	O5'-P-OP2	-8.26	98.27	105.70
8	A	2228	G	N3-C4-C5	8.26	132.73	128.60
34	a	980	C	C6-N1-C2	8.26	123.60	120.30
8	A	704	G	C4-N9-C1'	-8.25	115.78	126.50
8	A	2512	C	N3-C4-N4	-8.25	112.23	118.00
34	a	290	C	C6-N1-C2	8.25	123.60	120.30
8	A	85	G	N3-C4-C5	8.24	132.72	128.60
8	A	2694	G	N3-C4-C5	8.24	132.72	128.60
55	v	4	G	N3-C4-N9	-8.24	121.05	126.00
34	a	270	A	N9-C4-C5	-8.24	102.50	105.80
8	A	469	G	N3-C2-N2	8.24	125.67	119.90
34	a	446	G	N3-C4-C5	8.23	132.71	128.60
8	A	1041	G	N3-C4-C5	8.22	132.71	128.60
8	A	1169	A	N9-C4-C5	-8.22	102.51	105.80
8	A	977	G	N3-C4-C5	8.21	132.71	128.60
34	a	1156	G	N3-C4-N9	-8.21	121.08	126.00
8	A	45	G	N3-C4-N9	-8.20	121.08	126.00
8	A	1524	G	C2-N3-C4	-8.21	107.80	111.90
8	A	1745	A	N9-C4-C5	-8.20	102.52	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	1139	G	C8-N9-C4	8.20	109.68	106.40
8	A	2323	G	N3-C4-C5	8.19	132.70	128.60
34	a	260	G	N3-C4-C5	8.19	132.69	128.60
34	a	1375	A	O4'-C1'-N9	-8.19	101.65	108.20
8	A	1228	G	N3-C4-C5	8.19	132.69	128.60
34	a	1098	C	C2-N1-C1'	-8.19	109.80	118.80
8	A	673	C	N3-C4-C5	8.18	125.17	121.90
8	A	559	G	C2-N3-C4	-8.18	107.81	111.90
8	A	1186	G	N3-C4-C5	8.18	132.69	128.60
34	a	1048	G	N3-C4-C5	8.18	132.69	128.60
34	a	1418	A	C5-C6-N6	-8.18	117.16	123.70
8	A	42	A	C8-N9-C4	8.16	109.07	105.80
9	B	21	G	N3-C4-C5	8.16	132.68	128.60
34	a	1221	G	N3-C4-C5	8.16	132.68	128.60
34	a	388	G	O5'-P-OP1	-8.16	98.36	105.70
8	A	1541	C	C6-N1-C2	8.15	123.56	120.30
8	A	297	G	N3-C4-N9	-8.15	121.11	126.00
8	A	2767	C	N3-C4-C5	8.15	125.16	121.90
9	B	31	C	N3-C4-C5	8.15	125.16	121.90
34	a	1244	G	C8-N9-C4	8.15	109.66	106.40
8	A	1012	U	C5-C4-O4	-8.15	121.01	125.90
8	A	951	C	C6-N1-C2	8.14	123.56	120.30
8	A	1501	G	N3-C4-C5	8.13	132.66	128.60
8	A	303	G	C8-N9-C4	8.12	109.65	106.40
55	v	46	A	N1-C6-N6	8.12	123.47	118.60
8	A	1320	C	N3-C4-C5	8.12	125.15	121.90
9	B	20	G	N3-C4-N9	-8.12	121.13	126.00
8	A	14	A	C5-C6-N6	-8.12	117.21	123.70
8	A	2639	A	N1-C6-N6	8.12	123.47	118.60
8	A	1367	A	C8-N9-C4	8.11	109.05	105.80
8	A	819	A	C5-C6-N6	-8.11	117.21	123.70
8	A	2624	G	N3-C4-C5	8.11	132.66	128.60
8	A	1723	G	N3-C4-C5	8.11	132.65	128.60
34	a	120	A	O4'-C1'-N9	8.11	114.69	108.20
8	A	2082	A	C5-C6-N6	-8.10	117.22	123.70
10	C	175	LEU	CA-CB-CG	8.10	133.92	115.30
34	a	849	G	N3-C4-C5	8.09	132.65	128.60
8	A	2481	G	N3-C4-C5	8.09	132.64	128.60
8	A	2521	C	C6-N1-C2	8.09	123.53	120.30
8	A	39	G	N3-C4-C5	8.07	132.63	128.60
34	a	1418	A	N1-C6-N6	8.07	123.44	118.60
8	A	134	G	N3-C4-C5	8.06	132.63	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	a	1142	G	C2-N3-C4	-8.06	107.87	111.90
34	a	604	G	N3-C4-N9	-8.06	121.16	126.00
8	A	816	C	N3-C4-C5	8.06	125.12	121.90
34	a	432	A	C8-N9-C4	8.06	109.02	105.80
8	A	361	G	N1-C6-O6	8.06	124.73	119.90
8	A	2472	G	C8-N9-C4	8.06	109.62	106.40
8	A	989	G	O4'-C1'-N9	8.05	114.64	108.20
8	A	1378	A	C5-C6-N6	-8.05	117.26	123.70
8	A	1401	G	N3-C4-C5	8.05	132.62	128.60
8	A	1028	A	N1-C6-N6	8.04	123.43	118.60
8	A	2430	A	C5-C6-N6	-8.04	117.26	123.70
8	A	481	G	N3-C4-C5	8.04	132.62	128.60
8	A	1055	G	C4-N9-C1'	-8.04	116.05	126.50
34	a	560	A	O4'-C1'-N9	-8.03	101.77	108.20
8	A	1666	G	N3-C4-C5	8.03	132.62	128.60
34	a	742	G	N3-C4-N9	-8.03	121.18	126.00
8	A	126	A	N1-C6-N6	8.03	123.42	118.60
8	A	2143	C	C5-C4-N4	-8.03	114.58	120.20
34	a	259	G	N3-C4-C5	8.02	132.61	128.60
34	a	1050	G	C4-N9-C1'	-8.02	116.08	126.50
8	A	469	G	N9-C1'-C2'	-8.02	103.18	112.00
8	A	2603	G	N3-C4-C5	8.02	132.61	128.60
34	a	775	G	N3-C4-C5	8.01	132.60	128.60
8	A	317	G	N3-C4-C5	8.01	132.60	128.60
8	A	180	G	C4-N9-C1'	-8.00	116.10	126.50
34	a	1417	G	N3-C4-N9	-8.00	121.20	126.00
34	a	954	G	C2-N3-C4	-8.00	107.90	111.90
8	A	268	C	C6-N1-C2	8.00	123.50	120.30
34	a	1253	G	N3-C4-C5	8.00	132.60	128.60
8	A	1047	G	N3-C4-C5	7.99	132.60	128.60
34	a	346	G	C4-C5-N7	7.99	114.00	110.80
34	a	1098	C	N3-C4-N4	-7.99	112.40	118.00
8	A	2199	A	C8-N9-C4	7.99	109.00	105.80
34	a	921	U	O5'-P-OP2	7.99	120.29	110.70
8	A	664	G	C2-N3-C4	-7.99	107.91	111.90
8	A	301	G	N3-C4-N9	-7.99	121.21	126.00
34	a	1108	G	N3-C4-N9	-7.99	121.21	126.00
55	v	64	G	N3-C4-C5	7.99	132.59	128.60
8	A	940	G	C8-N9-C4	7.98	109.59	106.40
8	A	830	G	N3-C4-C5	7.98	132.59	128.60
9	B	38	C	C6-N1-C2	7.98	123.49	120.30
8	A	1381	G	N3-C4-C5	7.98	132.59	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	2093	G	C8-N9-C4	7.98	109.59	106.40
34	a	27	G	N3-C4-C5	7.98	132.59	128.60
34	a	410	G	N3-C4-C5	7.98	132.59	128.60
34	a	606	G	N3-C4-C5	7.97	132.58	128.60
34	a	1435	G	C2-N3-C4	-7.97	107.92	111.90
8	A	2225	A	C8-N9-C4	7.96	108.99	105.80
8	A	2671	G	N3-C4-C5	7.96	132.58	128.60
8	A	2	G	N9-C4-C5	-7.96	102.22	105.40
8	A	974	G	O4'-C1'-N9	7.96	114.56	108.20
8	A	1170	C	C5-C6-N1	7.96	124.98	121.00
34	a	838	G	N3-C4-C5	7.96	132.58	128.60
34	a	1461	G	C2-N3-C4	-7.96	107.92	111.90
34	a	308	C	C6-N1-C2	7.95	123.48	120.30
34	a	151	A	C5-C6-N1	7.94	121.67	117.70
8	A	289	G	C2-N3-C4	-7.94	107.93	111.90
34	a	361	G	N3-C4-C5	7.93	132.57	128.60
55	v	63	G	N3-C4-C5	7.93	132.57	128.60
8	A	583	G	N3-C4-N9	-7.93	121.24	126.00
8	A	1492	G	C4-N9-C1'	-7.93	116.19	126.50
34	a	312	C	C6-N1-C2	7.93	123.47	120.30
8	A	2659	G	N3-C4-C5	7.92	132.56	128.60
8	A	1374	G	N3-C4-N9	-7.92	121.25	126.00
8	A	1192	G	C8-N9-C4	7.92	109.57	106.40
34	a	1047	G	N3-C4-C5	7.91	132.55	128.60
8	A	303	G	C2-N3-C4	-7.90	107.95	111.90
34	a	1019	A	C8-N9-C4	7.90	108.96	105.80
8	A	2389	G	N3-C4-C5	7.89	132.55	128.60
8	A	1055	G	C2-N3-C4	-7.89	107.95	111.90
8	A	2667	C	N3-C4-N4	-7.89	112.48	118.00
34	a	1497	G	N3-C4-C5	7.89	132.54	128.60
34	a	830	G	N3-C4-C5	7.89	132.54	128.60
9	B	23	G	C2-N3-C4	-7.88	107.96	111.90
8	A	1193	G	C8-N9-C4	7.88	109.55	106.40
8	A	2631	G	N3-C4-N9	-7.88	121.27	126.00
8	A	410	G	N3-C4-C5	7.88	132.54	128.60
8	A	1091	G	N3-C4-N9	-7.88	121.27	126.00
8	A	1824	G	C2-N3-C4	-7.87	107.96	111.90
8	A	1519	G	N3-C4-C5	7.87	132.53	128.60
8	A	1804	C	C6-N1-C2	7.86	123.44	120.30
8	A	1381	G	N3-C4-N9	-7.86	121.28	126.00
34	a	770	C	C6-N1-C2	7.86	123.44	120.30
34	a	1273	C	C6-N1-C2	7.86	123.44	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	2899	A	C4-C5-N7	7.86	114.63	110.70
8	A	1404	C	N3-C4-C5	7.85	125.04	121.90
34	a	954	G	C8-N9-C4	7.85	109.54	106.40
8	A	188	G	N3-C4-N9	-7.85	121.29	126.00
9	B	108	A	C5-C6-N6	-7.84	117.43	123.70
8	A	1863	G	N3-C4-C5	7.84	132.52	128.60
8	A	1455	G	C2-N3-C4	-7.83	107.98	111.90
8	A	2154	A	C4-C5-N7	7.83	114.61	110.70
8	A	1774	C	C6-N1-C2	7.83	123.43	120.30
34	a	1323	G	C8-N9-C4	7.83	109.53	106.40
8	A	998	C	C6-N1-C2	7.83	123.43	120.30
8	A	816	C	C6-N1-C2	7.82	123.43	120.30
8	A	2686	G	N3-C4-C5	7.82	132.51	128.60
8	A	1867	G	N3-C4-N9	-7.82	121.31	126.00
8	A	136	G	N3-C4-C5	7.82	132.51	128.60
8	A	1861	G	N3-C4-C5	7.82	132.51	128.60
8	A	570	G	N1-C2-N2	-7.81	109.17	116.20
8	A	1186	G	N3-C4-N9	-7.81	121.31	126.00
34	a	1423	G	C2-N3-C4	-7.80	108.00	111.90
8	A	2569	G	N3-C4-C5	7.80	132.50	128.60
8	A	1	G	N3-C4-N9	-7.79	121.32	126.00
8	A	1112	G	C2-N3-C4	-7.79	108.00	111.90
8	A	1091	G	C2-N3-C4	-7.79	108.00	111.90
8	A	2669	G	N3-C4-C5	7.79	132.49	128.60
34	a	627	G	N3-C4-C5	7.79	132.49	128.60
34	a	1098	C	C5-C4-N4	7.78	125.65	120.20
8	A	837	C	C6-N1-C2	7.78	123.41	120.30
8	A	1591	A	N9-C4-C5	-7.78	102.69	105.80
34	a	851	G	O4'-C1'-N9	-7.78	101.98	108.20
8	A	926	G	N3-C4-C5	7.77	132.49	128.60
8	A	578	G	N3-C2-N2	7.76	125.33	119.90
8	A	1538	G	N3-C4-N9	-7.76	121.34	126.00
8	A	2339	C	C6-N1-C2	7.76	123.41	120.30
8	A	1374	G	C2-N3-C4	-7.76	108.02	111.90
8	A	1960	A	C8-N9-C4	7.76	108.90	105.80
8	A	2699	C	C6-N1-C2	7.76	123.40	120.30
55	v	26	G	N3-C4-N9	-7.76	121.34	126.00
8	A	1423	G	N3-C4-N9	-7.76	121.35	126.00
34	a	1134	G	N3-C4-C5	7.76	132.48	128.60
8	A	123	G	C2-N3-C4	-7.75	108.02	111.90
8	A	704	G	N3-C4-C5	7.75	132.48	128.60
8	A	1905	C	C6-N1-C2	7.75	123.40	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	1941	C	N3-C4-C5	7.75	125.00	121.90
34	a	456	A	C2-N3-C4	-7.75	106.72	110.60
8	A	1735	A	C4-C5-N7	7.75	114.57	110.70
9	B	24	G	O4'-C1'-N9	-7.75	102.00	108.20
8	A	506	G	N3-C4-C5	7.75	132.47	128.60
8	A	2470	G	C8-N9-C4	7.75	109.50	106.40
8	A	2440	C	C6-N1-C2	7.75	123.40	120.30
8	A	124	G	N3-C4-N9	-7.74	121.35	126.00
8	A	671	C	C6-N1-C2	7.74	123.40	120.30
8	A	2050	C	N1-C2-O2	7.74	123.54	118.90
8	A	848	C	C6-N1-C2	7.74	123.39	120.30
8	A	2545	G	C2-N3-C4	-7.73	108.03	111.90
34	a	858	G	N3-C2-N2	-7.73	114.49	119.90
8	A	1011	G	C2-N3-C4	-7.73	108.04	111.90
8	A	1903	G	C8-N9-C4	7.73	109.49	106.40
8	A	37	C	C6-N1-C2	7.72	123.39	120.30
8	A	819	A	N1-C6-N6	7.72	123.23	118.60
8	A	122	G	N3-C4-C5	7.71	132.46	128.60
8	A	1719	G	N3-C4-C5	7.71	132.46	128.60
8	A	2510	C	C6-N1-C2	7.70	123.38	120.30
34	a	474	G	N3-C4-C5	7.70	132.45	128.60
8	A	630	G	N3-C4-C5	7.70	132.45	128.60
34	a	1459	G	N3-C4-C5	7.70	132.45	128.60
34	a	1374	A	C5-C6-N6	-7.70	117.54	123.70
8	A	1721	G	C8-N9-C4	7.70	109.48	106.40
8	A	1193	G	N3-C4-C5	7.69	132.44	128.60
8	A	629	G	N3-C4-C5	7.69	132.44	128.60
8	A	273	G	N3-C4-C5	7.68	132.44	128.60
8	A	2481	G	C2-N3-C4	-7.68	108.06	111.90
8	A	1435	G	N3-C4-C5	7.68	132.44	128.60
8	A	2632	A	C8-N9-C4	7.68	108.87	105.80
8	A	696	G	C2-N3-C4	-7.68	108.06	111.90
9	B	21	G	C2-N3-C4	-7.68	108.06	111.90
8	A	1543	G	N3-C4-N9	-7.67	121.40	126.00
8	A	2606	C	N3-C2-O2	-7.67	116.53	121.90
34	a	1061	G	N3-C4-C5	7.67	132.44	128.60
8	A	1904	G	C8-N9-C4	7.67	109.47	106.40
34	a	492	C	C2-N1-C1'	-7.67	110.36	118.80
8	A	2576	G	N9-C4-C5	7.67	108.47	105.40
8	A	189	G	C8-N9-C4	7.67	109.47	106.40
8	A	1986	C	C6-N1-C2	7.67	123.37	120.30
8	A	2661	G	C2-N3-C4	-7.67	108.07	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	2667	C	C5-C4-N4	7.67	125.57	120.20
8	A	47	C	C6-N1-C2	7.66	123.36	120.30
8	A	2606	C	N1-C2-O2	7.66	123.50	118.90
8	A	2864	G	C8-N9-C4	7.66	109.46	106.40
34	a	1222	G	N1-C2-N3	7.66	128.49	123.90
8	A	299	A	C8-N9-C4	7.65	108.86	105.80
8	A	630	G	N3-C4-N9	-7.65	121.41	126.00
34	a	542	G	N3-C4-N9	-7.65	121.41	126.00
8	A	843	G	C8-N9-C4	7.65	109.46	106.40
8	A	991	C	C6-N1-C2	7.65	123.36	120.30
8	A	713	G	N3-C4-N9	-7.64	121.41	126.00
34	a	1487	G	N3-C4-C5	7.64	132.42	128.60
8	A	1404	C	C6-N1-C2	7.64	123.36	120.30
34	a	265	G	C2-N3-C4	-7.64	108.08	111.90
9	B	105	G	C8-N9-C4	7.64	109.45	106.40
8	A	126	A	C8-N9-C4	7.63	108.85	105.80
8	A	424	G	N3-C4-C5	7.63	132.41	128.60
8	A	1038	G	N3-C4-C5	7.63	132.41	128.60
8	A	2073	C	C6-N1-C2	7.63	123.35	120.30
56	w	9	A	C4'-C3'-O3'	7.63	128.25	113.00
8	A	103	A	N1-C6-N6	7.62	123.17	118.60
34	a	203	G	C4-N9-C1'	-7.62	116.59	126.50
8	A	336	C	C6-N1-C2	7.62	123.35	120.30
34	a	1293	C	C6-N1-C2	7.62	123.35	120.30
8	A	1281	G	N3-C4-C5	7.61	132.41	128.60
8	A	1661	G	N3-C4-C5	7.61	132.41	128.60
8	A	2657	A	C8-N9-C4	7.61	108.84	105.80
8	A	1875	G	N3-C4-C5	7.61	132.40	128.60
34	a	1108	G	N3-C4-C5	7.61	132.40	128.60
8	A	1482	G	C2-N3-C4	-7.60	108.10	111.90
8	A	1588	G	C2-N3-C4	-7.60	108.10	111.90
34	a	247	G	N3-C4-C5	7.59	132.40	128.60
34	a	628	G	C8-N9-C4	7.59	109.44	106.40
8	A	1823	G	C2-N3-C4	-7.59	108.10	111.90
8	A	307	G	C8-N9-C4	7.58	109.43	106.40
8	A	1653	G	C2-N3-C4	-7.58	108.11	111.90
34	a	228	A	C8-N9-C4	7.58	108.83	105.80
34	a	803	G	N1-C2-N2	-7.58	109.37	116.20
8	A	2077	A	N9-C4-C5	-7.58	102.77	105.80
8	A	1279	G	N9-C4-C5	-7.58	102.37	105.40
34	a	241	G	C2-N3-C4	-7.58	108.11	111.90
9	B	105	G	N3-C4-C5	7.58	132.39	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	1076	C	N1-C2-O2	7.57	123.44	118.90
8	A	2775	G	N3-C4-C5	7.57	132.38	128.60
9	B	51	G	C8-N9-C4	7.57	109.43	106.40
8	A	2714	G	C2-N3-C4	-7.57	108.12	111.90
55	v	15	G	C2-N3-C4	-7.57	108.12	111.90
34	a	889	A	C8-N9-C4	7.57	108.83	105.80
8	A	1587	G	N3-C4-C5	7.56	132.38	128.60
9	B	64	G	N3-C4-C5	7.56	132.38	128.60
34	a	599	C	C6-N1-C2	7.56	123.32	120.30
8	A	1086	A	C8-N9-C4	-7.56	102.78	105.80
8	A	1975	G	C8-N9-C4	7.56	109.42	106.40
8	A	2641	G	N3-C4-C5	7.56	132.38	128.60
8	A	2744	G	N3-C4-C5	7.56	132.38	128.60
8	A	482	A	C4-C5-C6	-7.56	113.22	117.00
9	B	56	G	N9-C4-C5	-7.55	102.38	105.40
8	A	103	A	C5-C6-N6	-7.55	117.66	123.70
8	A	939	G	C2-N3-C4	-7.55	108.13	111.90
34	a	1071	C	N3-C4-C5	7.55	124.92	121.90
8	A	974	G	C2-N3-C4	-7.55	108.13	111.90
34	a	646	G	C2-N3-C4	-7.55	108.13	111.90
8	A	256	A	C8-N9-C4	7.54	108.82	105.80
8	A	1946	U	C6-N1-C2	7.54	125.53	121.00
9	B	7	G	C2-N3-C4	-7.54	108.13	111.90
34	a	380	G	N3-C4-C5	7.54	132.37	128.60
8	A	55	G	N3-C4-C5	7.54	132.37	128.60
8	A	2890	G	N3-C4-C5	7.54	132.37	128.60
8	A	1875	G	N3-C4-N9	-7.53	121.48	126.00
8	A	1945	G	C2-N3-C4	-7.53	108.14	111.90
8	A	2234	G	C2-N3-C4	-7.53	108.14	111.90
34	a	269	C	C6-N1-C2	7.53	123.31	120.30
8	A	2844	G	C2-N3-C4	-7.52	108.14	111.90
34	a	797	C	N3-C4-N4	-7.52	112.73	118.00
8	A	1169	A	C4-C5-N7	7.52	114.46	110.70
8	A	2045	C	N3-C4-C5	7.52	124.91	121.90
8	A	2228	G	C2-N3-C4	-7.52	108.14	111.90
34	a	319	G	N3-C4-C5	7.52	132.36	128.60
8	A	461	C	C6-N1-C2	7.51	123.31	120.30
8	A	638	G	C2-N3-C4	-7.51	108.14	111.90
8	A	1200	C	C6-N1-C2	7.51	123.31	120.30
8	A	1652	A	N9-C4-C5	-7.51	102.80	105.80
34	a	146	G	N3-C4-C5	7.51	132.36	128.60
8	A	1216	G	N3-C4-N9	-7.51	121.49	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	1482	G	N3-C4-N9	-7.51	121.49	126.00
34	a	1404	C	C6-N1-C2	7.51	123.30	120.30
8	A	2641	G	N3-C4-N9	-7.51	121.50	126.00
8	A	1643	G	N3-C4-N9	-7.51	121.50	126.00
55	v	9	G	C8-N9-C1'	7.51	136.76	127.00
8	A	76	C	C6-N1-C2	7.50	123.30	120.30
34	a	1227	A	C5-C6-N6	7.50	129.70	123.70
34	a	181	A	N9-C4-C5	-7.50	102.80	105.80
8	A	318	C	N3-C4-C5	7.49	124.90	121.90
8	A	1430	G	C2-N3-C4	-7.49	108.15	111.90
34	a	1294	G	C8-N9-C4	7.49	109.40	106.40
34	a	1016	A	N1-C6-N6	7.49	123.09	118.60
8	A	814	C	N3-C4-C5	7.49	124.90	121.90
8	A	1770	G	C2-N3-C4	-7.49	108.16	111.90
34	a	1405	G	C4-N9-C1'	-7.49	116.76	126.50
8	A	1425	G	N3-C2-N2	-7.48	114.66	119.90
8	A	2470	G	N3-C4-C5	7.48	132.34	128.60
8	A	2846	G	N3-C4-C5	7.48	132.34	128.60
34	a	1500	A	N1-C6-N6	-7.48	114.11	118.60
8	A	1933	G	C2-N3-C4	-7.48	108.16	111.90
34	a	278	G	N3-C4-C5	7.48	132.34	128.60
8	A	707	G	C2-N3-C4	-7.48	108.16	111.90
8	A	549	G	N3-C4-C5	7.47	132.34	128.60
8	A	2444	G	N3-C4-N9	-7.47	121.52	126.00
8	A	1459	G	N3-C4-N9	-7.47	121.52	126.00
8	A	510	C	C6-N1-C2	-7.47	117.31	120.30
34	a	159	G	N1-C6-O6	-7.47	115.42	119.90
34	a	617	G	C2-N3-C4	-7.47	108.16	111.90
8	A	2190	G	N3-C4-C5	7.47	132.34	128.60
8	A	1987	A	C8-N9-C4	7.47	108.79	105.80
8	A	1705	A	N9-C4-C5	-7.47	102.81	105.80
34	a	748	G	N3-C4-C5	7.47	132.33	128.60
14	G	132	LEU	CA-CB-CG	7.46	132.47	115.30
8	A	2844	G	N3-C4-C5	7.46	132.33	128.60
8	A	1922	G	C2-N3-C4	-7.45	108.17	111.90
8	A	1968	G	C8-N9-C4	7.45	109.38	106.40
8	A	728	G	C2-N3-C4	-7.45	108.17	111.90
34	a	1182	G	N3-C4-C5	7.45	132.32	128.60
8	A	2541	A	N1-C6-N6	-7.45	114.13	118.60
8	A	793	A	N1-C6-N6	7.45	123.07	118.60
8	A	1022	G	C2-N3-C4	-7.45	108.18	111.90
8	A	1192	G	N3-C4-C5	7.45	132.32	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	289	G	N3-C4-N9	-7.44	121.53	126.00
8	A	84	A	C8-N9-C4	7.44	108.78	105.80
34	a	696	A	N1-C6-N6	7.44	123.06	118.60
8	A	445	C	C6-N1-C2	7.43	123.27	120.30
8	A	1807	G	N3-C4-C5	7.43	132.32	128.60
34	a	990	C	C6-N1-C2	7.43	123.27	120.30
8	A	2688	G	C8-N9-C4	7.43	109.37	106.40
34	a	432	A	N9-C4-C5	-7.43	102.83	105.80
8	A	660	C	C6-N1-C2	7.43	123.27	120.30
34	a	824	G	C8-N9-C4	7.42	109.37	106.40
8	A	455	C	N3-C4-N4	-7.42	112.81	118.00
8	A	1139	G	N3-C4-N9	-7.41	121.55	126.00
8	A	344	A	C8-N9-C4	7.41	108.77	105.80
8	A	1639	C	C6-N1-C2	7.41	123.27	120.30
34	a	487	A	C5-C6-N6	-7.41	117.77	123.70
8	A	2816	G	N3-C4-C5	7.41	132.30	128.60
34	a	361	G	N3-C4-N9	-7.41	121.56	126.00
8	A	952	G	N3-C4-C5	7.40	132.30	128.60
8	A	2008	C	C6-N1-C2	7.40	123.26	120.30
8	A	261	G	N3-C4-C5	7.40	132.30	128.60
8	A	1399	C	C6-N1-C2	7.40	123.26	120.30
34	a	518	C	O4'-C1'-N1	-7.39	102.29	108.20
8	A	1358	G	N3-C4-C5	7.39	132.29	128.60
34	a	332	G	N3-C4-C5	7.39	132.29	128.60
8	A	1037	G	N3-C4-C5	7.39	132.29	128.60
8	A	2509	G	N3-C4-C5	7.39	132.29	128.60
9	B	51	G	N9-C4-C5	-7.38	102.45	105.40
34	a	1154	G	N3-C4-C5	7.38	132.29	128.60
34	a	651	C	N3-C4-C5	7.38	124.85	121.90
8	A	1034	G	N3-C4-C5	7.38	132.29	128.60
34	a	851	G	C2-N3-C4	-7.38	108.21	111.90
34	a	181	A	C4-C5-N7	7.38	114.39	110.70
8	A	178	G	C2-N3-C4	-7.37	108.21	111.90
8	A	1225	G	N3-C4-C5	7.37	132.29	128.60
8	A	1631	G	C4-N9-C1'	-7.37	116.92	126.50
34	a	408	A	C8-N9-C4	7.37	108.75	105.80
34	a	1255	G	N3-C4-C5	7.37	132.29	128.60
34	a	604	G	C2-N3-C4	-7.37	108.22	111.90
8	A	2277	G	N3-C4-C5	7.37	132.28	128.60
34	a	257	G	N3-C4-C5	7.37	132.28	128.60
8	A	212	G	N3-C4-C5	7.37	132.28	128.60
34	a	1429	A	C8-N9-C4	7.36	108.75	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	1177	G	N3-C4-C5	7.36	132.28	128.60
8	A	2557	G	N3-C4-N9	-7.36	121.58	126.00
34	a	806	C	C6-N1-C2	7.36	123.24	120.30
8	A	123	G	N3-C4-C5	7.36	132.28	128.60
8	A	2281	A	C8-N9-C4	7.36	108.74	105.80
9	B	33	G	N3-C4-N9	-7.36	121.58	126.00
8	A	2481	G	N3-C4-N9	-7.35	121.59	126.00
34	a	278	G	N3-C4-N9	-7.35	121.59	126.00
8	A	1182	G	N3-C4-C5	7.35	132.28	128.60
8	A	393	C	C6-N1-C2	7.34	123.24	120.30
8	A	1154	G	C8-N9-C4	7.34	109.34	106.40
21	N	10	LEU	CA-CB-CG	7.34	132.19	115.30
56	w	6	G	N3-C4-C5	7.34	132.27	128.60
34	a	255	G	N3-C4-C5	7.34	132.27	128.60
34	a	332	G	C2-N3-C4	-7.34	108.23	111.90
34	a	1323	G	N3-C4-C5	7.34	132.27	128.60
34	a	682	G	N3-C4-N9	-7.34	121.60	126.00
8	A	609	A	N1-C6-N6	7.34	123.00	118.60
8	A	205	G	O4'-C1'-N9	7.34	114.07	108.20
8	A	771	G	N3-C4-C5	7.34	132.27	128.60
8	A	1553	A	N1-C6-N6	7.34	123.00	118.60
34	a	360	G	N3-C4-C5	7.33	132.27	128.60
34	a	654	G	C4-C5-N7	7.33	113.73	110.80
8	A	79	C	C6-N1-C2	7.33	123.23	120.30
8	A	1894	C	N3-C4-N4	-7.33	112.87	118.00
34	a	119	A	N1-C6-N6	7.33	123.00	118.60
8	A	2395	C	C6-N1-C2	7.32	123.23	120.30
34	a	630	A	C8-N9-C4	7.32	108.73	105.80
8	A	2316	G	C2-N3-C4	-7.32	108.24	111.90
8	A	81	G	N3-C4-C5	7.32	132.26	128.60
34	a	320	A	N9-C4-C5	-7.32	102.87	105.80
34	a	987	G	N3-C4-N9	-7.32	121.61	126.00
8	A	146	A	N9-C4-C5	-7.32	102.87	105.80
34	a	953	G	N9-C4-C5	-7.31	102.47	105.40
8	A	319	G	N3-C4-C5	7.31	132.26	128.60
8	A	343	C	C6-N1-C2	7.31	123.22	120.30
8	A	2153	C	N3-C2-O2	7.31	127.02	121.90
34	a	141	G	N3-C4-C5	7.31	132.25	128.60
34	a	742	G	N3-C4-C5	7.31	132.25	128.60
34	a	775	G	N3-C4-N9	-7.31	121.61	126.00
34	a	346	G	N9-C4-C5	-7.30	102.48	105.40
34	a	838	G	C8-N9-C4	7.30	109.32	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	a	1524	C	C6-N1-C2	7.30	123.22	120.30
34	a	1488	G	C2-N3-C4	-7.29	108.25	111.90
8	A	1062	G	N3-C2-N2	7.29	125.01	119.90
8	A	2780	G	N3-C4-C5	7.29	132.25	128.60
8	A	950	G	C2-N3-C4	-7.29	108.25	111.90
55	v	6	G	N3-C4-N9	-7.29	121.62	126.00
8	A	259	G	N3-C4-C5	7.29	132.25	128.60
8	A	735	A	C8-N9-C4	7.29	108.72	105.80
34	a	541	G	N3-C4-C5	7.29	132.24	128.60
34	a	518	C	N3-C4-N4	7.29	123.10	118.00
34	a	1048	G	C8-N9-C4	7.29	109.31	106.40
8	A	1332	G	O4'-C1'-N9	7.28	114.02	108.20
8	A	2248	C	C2-N1-C1'	7.28	126.81	118.80
34	a	521	G	C2-N3-C4	-7.28	108.26	111.90
55	v	12	G	C2-N3-C4	-7.28	108.26	111.90
55	v	76	A	O4'-C1'-N9	7.28	114.02	108.20
8	A	780	G	C2-N3-C4	-7.28	108.26	111.90
8	A	249	C	C6-N1-C2	7.28	123.21	120.30
8	A	1169	A	C5-N7-C8	-7.28	100.26	103.90
8	A	2199	A	N9-C4-C5	-7.27	102.89	105.80
8	A	80	G	N3-C4-C5	7.27	132.24	128.60
8	A	1182	G	C2-N3-C4	-7.27	108.26	111.90
8	A	770	G	N3-C4-C5	7.27	132.24	128.60
8	A	2464	G	N3-C4-N9	-7.27	121.64	126.00
34	a	809	G	N3-C4-N9	-7.27	121.64	126.00
34	a	655	A	C8-N9-C4	7.27	108.71	105.80
8	A	1930	G	C8-N9-C4	7.27	109.31	106.40
8	A	927	A	N1-C6-N6	7.26	122.96	118.60
8	A	2549	G	C8-N9-C4	7.26	109.30	106.40
9	B	100	G	C2-N3-C4	-7.26	108.27	111.90
34	a	318	G	N3-C4-N9	-7.26	121.65	126.00
8	A	636	G	N3-C4-C5	7.25	132.23	128.60
8	A	2363	G	N3-C4-C5	7.25	132.23	128.60
8	A	93	G	C2-N3-C4	-7.25	108.28	111.90
8	A	496	G	C8-N9-C4	7.25	109.30	106.40
34	a	453	G	C8-N9-C1'	-7.25	117.58	127.00
8	A	2444	G	C2-N3-C4	-7.25	108.28	111.90
8	A	728	G	N3-C4-C5	7.25	132.22	128.60
8	A	2663	G	N3-C2-N2	-7.24	114.83	119.90
8	A	2715	C	N3-C4-C5	7.24	124.80	121.90
34	a	1011	C	N3-C4-N4	-7.24	112.93	118.00
8	A	407	G	N3-C4-C5	7.24	132.22	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	326	G	N3-C4-C5	7.24	132.22	128.60
34	a	604	G	C8-N9-C4	7.24	109.30	106.40
8	A	1221	C	C6-N1-C2	7.24	123.19	120.30
34	a	1312	G	C2-N3-C4	-7.24	108.28	111.90
34	a	824	G	N3-C4-C5	7.24	132.22	128.60
8	A	371	A	N1-C6-N6	7.23	122.94	118.60
8	A	2603	G	N3-C4-N9	-7.23	121.66	126.00
8	A	2708	G	C8-N9-C4	7.23	109.29	106.40
34	a	1294	G	N3-C4-C5	7.23	132.22	128.60
34	a	1487	G	C2-N3-C4	-7.23	108.28	111.90
34	a	158	G	N1-C6-O6	7.23	124.24	119.90
8	A	2877	G	C8-N9-C4	7.23	109.29	106.40
8	A	1775	U	C6-N1-C2	7.22	125.33	121.00
8	A	960	A	N1-C6-N6	7.22	122.93	118.60
34	a	670	G	N3-C4-C5	7.22	132.21	128.60
34	a	1488	G	C8-N9-C4	7.22	109.29	106.40
8	A	1187	G	N3-C4-N9	-7.22	121.67	126.00
34	a	487	A	N1-C6-N6	7.22	122.93	118.60
34	a	857	C	C6-N1-C2	7.22	123.19	120.30
8	A	481	G	C4-N9-C1'	-7.22	117.12	126.50
34	a	953	G	C4-C5-N7	7.22	113.69	110.80
34	a	1476	A	C8-N9-C4	7.22	108.69	105.80
8	A	191	A	N1-C6-N6	7.21	122.93	118.60
8	A	506	G	C4-N9-C1'	-7.21	117.12	126.50
8	A	1377	G	N3-C4-C5	7.21	132.21	128.60
8	A	2110	G	C4-N9-C1'	7.21	135.88	126.50
9	B	81	G	C2-N3-C4	-7.21	108.30	111.90
34	a	1312	G	O4'-C1'-N9	-7.21	102.43	108.20
34	a	1244	G	C4-N9-C1'	-7.21	117.13	126.50
34	a	104	G	N3-C4-N9	-7.20	121.68	126.00
34	a	1312	G	C8-N9-C4	7.20	109.28	106.40
8	A	1202	G	C8-N9-C4	7.20	109.28	106.40
8	A	58	G	N3-C4-N9	-7.19	121.68	126.00
34	a	800	G	N3-C4-C5	7.19	132.20	128.60
8	A	888	C	O4'-C1'-N1	7.19	113.95	108.20
34	a	859	G	N3-C4-N9	-7.19	121.69	126.00
8	A	1081	U	O4'-C1'-N1	7.19	113.95	108.20
9	B	80	U	C6-N1-C2	7.19	125.31	121.00
8	A	1317	G	C2-N3-C4	-7.18	108.31	111.90
8	A	2253	G	C2-N3-C4	-7.18	108.31	111.90
8	A	1371	G	N3-C4-N9	-7.18	121.69	126.00
8	A	2190	G	C2-N3-C4	-7.18	108.31	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	a	1433	A	N1-C6-N6	7.18	122.91	118.60
8	A	2391	G	C4-N9-C1'	-7.18	117.17	126.50
34	a	1227	A	N9-C4-C5	7.18	108.67	105.80
34	a	402	G	N3-C4-C5	7.17	132.19	128.60
8	A	1047	G	N3-C2-N2	-7.17	114.88	119.90
8	A	2383	G	N3-C4-C5	7.17	132.19	128.60
8	A	2715	C	C6-N1-C2	7.17	123.17	120.30
34	a	1323	G	C2-N3-C4	-7.17	108.31	111.90
8	A	1968	G	N9-C4-C5	-7.17	102.53	105.40
34	a	1374	A	C4-C5-N7	7.17	114.28	110.70
8	A	14	A	C5-C6-N1	7.17	121.28	117.70
8	A	2854	G	N3-C4-C5	7.17	132.18	128.60
8	A	1178	C	N3-C4-N4	-7.17	112.98	118.00
8	A	875	G	N3-C4-C5	7.16	132.18	128.60
8	A	1388	G	N3-C4-C5	7.16	132.18	128.60
8	A	2415	G	N3-C4-N9	-7.16	121.70	126.00
8	A	240	C	C6-N1-C2	7.16	123.16	120.30
34	a	671	G	N3-C4-C5	7.16	132.18	128.60
8	A	469	G	C5-N7-C8	-7.16	100.72	104.30
8	A	2719	G	N3-C4-C5	7.16	132.18	128.60
9	B	96	G	N3-C4-C5	7.16	132.18	128.60
34	a	1050	G	C8-N9-C1'	7.16	136.30	127.00
8	A	2456	C	C6-N1-C2	7.15	123.16	120.30
8	A	570	G	N3-C4-N9	7.15	130.29	126.00
8	A	1697	G	N3-C4-C5	7.15	132.18	128.60
34	a	661	G	C8-N9-C4	7.15	109.26	106.40
8	A	371	A	C5-C6-N6	-7.15	117.98	123.70
8	A	721	A	N9-C4-C5	-7.15	102.94	105.80
34	a	445	G	N3-C4-C5	7.15	132.17	128.60
8	A	381	G	C8-N9-C4	7.15	109.26	106.40
8	A	247	G	N3-C4-C5	7.14	132.17	128.60
34	a	928	G	N3-C4-C5	7.14	132.17	128.60
8	A	899	A	N1-C6-N6	7.14	122.88	118.60
34	a	1486	G	C2-N3-C4	-7.14	108.33	111.90
34	a	1105	A	N9-C4-C5	-7.14	102.95	105.80
8	A	713	G	N3-C4-C5	7.13	132.17	128.60
8	A	2686	G	C2-N3-C4	-7.13	108.33	111.90
8	A	2839	G	N3-C4-C5	7.13	132.17	128.60
8	A	1810	A	C5-C6-N6	-7.13	117.99	123.70
8	A	1178	C	C2-N3-C4	-7.13	116.33	119.90
8	A	1456	G	N3-C4-C5	7.13	132.16	128.60
8	A	361	G	C5-N7-C8	-7.13	100.74	104.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	2508	G	C8-N9-C4	7.13	109.25	106.40
8	A	510	C	N3-C2-O2	-7.12	116.91	121.90
8	A	707	G	N3-C4-C5	7.12	132.16	128.60
34	a	929	G	N3-C4-C5	7.12	132.16	128.60
8	A	1873	G	N3-C4-C5	7.12	132.16	128.60
8	A	2206	C	C6-N1-C2	7.12	123.15	120.30
8	A	2734	A	C8-N9-C4	7.12	108.65	105.80
8	A	327	G	N3-C4-C5	7.12	132.16	128.60
8	A	1028	A	N9-C4-C5	-7.11	102.96	105.80
34	a	1472	U	C2-N1-C1'	7.11	126.23	117.70
8	A	1156	A	C8-N9-C4	7.11	108.64	105.80
8	A	2844	G	N3-C4-N9	-7.11	121.74	126.00
34	a	851	G	N9-C4-C5	-7.11	102.56	105.40
34	a	518	C	C6-N1-C1'	-7.10	112.28	120.80
34	a	1375	A	C8-N9-C4	7.10	108.64	105.80
8	A	1408	G	C2-N3-C4	-7.10	108.35	111.90
8	A	1745	A	C5-C6-N6	-7.10	118.02	123.70
8	A	2349	G	N3-C4-C5	7.10	132.15	128.60
34	a	243	A	N1-C2-N3	7.10	132.85	129.30
34	a	246	A	N1-C6-N6	7.10	122.86	118.60
34	a	698	G	N3-C4-N9	-7.10	121.74	126.00
8	A	2218	G	C2-N3-C4	-7.10	108.35	111.90
8	A	1220	G	N3-C4-N9	-7.10	121.74	126.00
34	a	460	A	O4'-C1'-N9	-7.10	102.52	108.20
8	A	2437	G	N3-C4-C5	7.10	132.15	128.60
8	A	2208	C	C2'-C3'-O3'	7.10	125.11	109.50
8	A	24	G	C2-N3-C4	-7.09	108.35	111.90
34	a	542	G	C8-N9-C4	7.09	109.24	106.40
8	A	2843	G	N3-C4-C5	7.09	132.15	128.60
34	a	691	G	C4-N9-C1'	-7.09	117.28	126.50
8	A	2248	C	C6-N1-C1'	-7.09	112.29	120.80
8	A	52	A	C5-C6-N6	-7.09	118.03	123.70
9	B	40	U	O4'-C1'-N1	-7.09	102.53	108.20
8	A	1378	A	C4-C5-N7	7.09	114.24	110.70
8	A	2524	G	C8-N9-C4	7.09	109.23	106.40
34	a	104	G	N3-C4-C5	7.09	132.14	128.60
8	A	260	G	C2-N3-C4	-7.08	108.36	111.90
8	A	2899	A	N9-C4-C5	-7.08	102.97	105.80
34	a	1112	C	C6-N1-C2	7.08	123.13	120.30
8	A	122	G	N3-C4-N9	-7.08	121.75	126.00
8	A	2168	G	P-O3'-C3'	-7.08	111.20	119.70
8	A	1178	C	N3-C2-O2	-7.08	116.94	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	102	G	C8-N9-C4	7.08	109.23	106.40
9	B	84	G	N3-C4-C5	7.08	132.14	128.60
26	S	42	LYS	CA-CB-CG	7.08	128.97	113.40
8	A	48	G	N3-C4-C5	7.07	132.14	128.60
34	a	518	C	C5-C4-N4	-7.07	115.25	120.20
34	a	545	C	C6-N1-C2	7.07	123.13	120.30
34	a	1143	G	N9-C4-C5	-7.07	102.57	105.40
34	a	585	G	N3-C4-C5	7.07	132.13	128.60
8	A	2840	C	C6-N1-C2	7.07	123.13	120.30
34	a	639	G	C8-N9-C4	7.07	109.23	106.40
34	a	550	G	N3-C4-C5	7.06	132.13	128.60
8	A	27	G	O4'-C1'-N9	7.06	113.85	108.20
8	A	1016	G	N3-C4-N9	-7.06	121.76	126.00
8	A	629	G	C8-N9-C4	7.06	109.22	106.40
8	A	1333	G	C8-N9-C4	7.06	109.22	106.40
8	A	1642	G	C2-N3-C4	-7.06	108.37	111.90
8	A	1900	A	O4'-C1'-N9	7.06	113.85	108.20
8	A	956	G	N3-C4-C5	7.06	132.13	128.60
34	a	241	G	N3-C4-N9	-7.06	121.77	126.00
34	a	953	G	N3-C4-C5	7.06	132.13	128.60
34	a	1487	G	N3-C4-N9	-7.06	121.77	126.00
8	A	815	C	N3-C4-C5	7.05	124.72	121.90
8	A	1337	G	N3-C4-N9	-7.05	121.77	126.00
8	A	2235	G	C2-N3-C4	-7.05	108.37	111.90
34	a	362	G	N3-C4-C5	7.05	132.13	128.60
34	a	898	G	N3-C4-C5	7.05	132.13	128.60
8	A	1721	G	N3-C4-N9	-7.05	121.77	126.00
34	a	348	G	C8-N9-C4	7.05	109.22	106.40
34	a	799	G	C8-N9-C4	7.05	109.22	106.40
8	A	1115	G	N3-C4-C5	7.04	132.12	128.60
8	A	2373	G	N3-C4-C5	7.04	132.12	128.60
34	a	833	G	N3-C4-N9	-7.04	121.78	126.00
8	A	350	G	C2-N3-C4	-7.04	108.38	111.90
8	A	1766	G	C8-N9-C4	7.04	109.22	106.40
8	A	1843	C	N1-C2-O2	7.04	123.12	118.90
8	A	1973	G	N3-C4-C5	7.04	132.12	128.60
8	A	2355	G	N3-C4-C5	7.04	132.12	128.60
8	A	996	A	C8-N9-C4	7.03	108.61	105.80
8	A	2618	G	N1-C6-O6	-7.03	115.68	119.90
34	a	800	G	C2-N3-C4	-7.03	108.38	111.90
8	A	939	G	N3-C4-C5	7.03	132.12	128.60
8	A	1190	G	C8-N9-C4	7.03	109.21	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	2040	G	C8-N9-C4	7.03	109.21	106.40
34	a	226	G	N3-C2-N2	7.03	124.82	119.90
8	A	488	G	N3-C4-C5	7.03	132.12	128.60
8	A	2282	G	N1-C6-O6	-7.03	115.68	119.90
8	A	1154	G	N3-C4-C5	7.02	132.11	128.60
9	B	19	C	C6-N1-C2	7.02	123.11	120.30
8	A	1893	C	C6-N1-C2	7.02	123.11	120.30
34	a	1174	G	N3-C4-C5	7.02	132.11	128.60
8	A	188	G	C2-N3-C4	-7.02	108.39	111.90
8	A	954	G	C2-N3-C4	-7.01	108.39	111.90
8	A	2557	G	C8-N9-C4	7.01	109.21	106.40
34	a	1	A	N7-C8-N9	7.01	117.31	113.80
34	a	81	A	C4-C5-N7	7.01	114.21	110.70
34	a	848	C	C6-N1-C2	7.01	123.10	120.30
8	A	2719	G	N3-C4-N9	-7.00	121.80	126.00
8	A	705	A	N1-C6-N6	7.00	122.80	118.60
8	A	2407	A	N9-C4-C5	-7.00	103.00	105.80
8	A	1055	G	C4-C5-C6	-7.00	114.60	118.80
8	A	2869	G	N3-C4-N9	-7.00	121.80	126.00
34	a	1020	G	C8-N9-C4	7.00	109.20	106.40
34	a	326	G	C2-N3-C4	-6.99	108.40	111.90
8	A	672	C	N3-C4-C5	6.99	124.70	121.90
34	a	1019	A	N9-C4-C5	-6.99	103.00	105.80
34	a	1104	G	C8-N9-C4	6.99	109.20	106.40
8	A	1377	G	N3-C4-N9	-6.99	121.81	126.00
8	A	2198	A	C5-C6-N6	6.99	129.29	123.70
34	a	742	G	N3-C2-N2	-6.99	115.01	119.90
34	a	1435	G	N3-C4-C5	6.99	132.09	128.60
34	a	887	G	N3-C4-C5	6.99	132.09	128.60
8	A	682	G	N3-C4-C5	6.99	132.09	128.60
8	A	1279	G	C4-C5-N7	6.99	113.59	110.80
34	a	521	G	C8-N9-C4	6.99	109.19	106.40
8	A	1060	U	C5-C4-O4	-6.98	121.71	125.90
8	A	35	G	N3-C4-C5	6.98	132.09	128.60
8	A	1684	G	C4-N9-C1'	-6.98	117.42	126.50
34	a	696	A	N9-C4-C5	-6.98	103.01	105.80
34	a	1025	U	C2-N1-C1'	6.98	126.08	117.70
8	A	500	G	N3-C4-C5	6.98	132.09	128.60
8	A	917	A	N1-C6-N6	6.97	122.78	118.60
8	A	1681	G	N3-C4-C5	6.97	132.09	128.60
8	A	2198	A	C6-C5-N7	6.97	137.18	132.30
8	A	2708	G	N3-C4-C5	6.97	132.09	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	2864	G	N3-C4-C5	6.97	132.09	128.60
8	A	1479	G	N3-C4-C5	6.97	132.08	128.60
34	a	242	G	N3-C4-C5	6.96	132.08	128.60
34	a	1011	C	C2-N1-C1'	-6.96	111.14	118.80
8	A	2	G	C4-C5-N7	6.96	113.58	110.80
34	a	626	G	C2-N3-C4	-6.96	108.42	111.90
8	A	1093	G	N3-C4-C5	6.96	132.08	128.60
8	A	2549	G	N9-C4-C5	-6.96	102.62	105.40
55	v	26	G	N3-C4-C5	6.96	132.08	128.60
8	A	1163	G	C8-N9-C4	6.96	109.18	106.40
8	A	93	G	N3-C4-C5	6.96	132.08	128.60
34	a	886	G	N3-C4-C5	6.96	132.08	128.60
34	a	1439	G	N3-C4-C5	6.96	132.08	128.60
8	A	1574	C	C6-N1-C2	6.96	123.08	120.30
8	A	1227	G	C2-N3-C4	-6.95	108.42	111.90
8	A	334	C	C6-N1-C2	6.95	123.08	120.30
8	A	413	C	C6-N1-C2	6.95	123.08	120.30
8	A	1897	G	N3-C4-C5	6.95	132.07	128.60
34	a	1175	G	C2-N3-C4	-6.95	108.43	111.90
34	a	53	A	C8-N9-C4	6.94	108.58	105.80
8	A	830	G	N3-C4-N9	-6.94	121.83	126.00
34	a	518	C	C2-N1-C1'	6.94	126.44	118.80
8	A	1048	A	N1-C6-N6	6.94	122.76	118.60
8	A	144	A	C4-C5-N7	6.94	114.17	110.70
8	A	2567	G	N3-C4-C5	6.94	132.07	128.60
8	A	340	A	C8-N9-C4	6.93	108.57	105.80
8	A	2551	C	C6-N1-C2	6.93	123.07	120.30
8	A	1989	G	N3-C4-C5	6.93	132.06	128.60
8	A	2507	C	C6-N1-C2	6.93	123.07	120.30
8	A	1807	G	N3-C4-N9	-6.92	121.84	126.00
8	A	2868	A	N1-C6-N6	6.92	122.75	118.60
34	a	1043	G	N3-C4-C5	6.92	132.06	128.60
34	a	274	A	C8-N9-C4	6.92	108.57	105.80
8	A	1548	A	C8-N9-C4	6.92	108.57	105.80
8	A	335	C	C6-N1-C2	6.92	123.07	120.30
8	A	463	G	N3-C4-C5	6.92	132.06	128.60
34	a	151	A	C5-C6-N6	-6.92	118.16	123.70
34	a	760	G	N3-C4-C5	6.92	132.06	128.60
8	A	795	C	N3-C4-C5	6.92	124.67	121.90
8	A	1233	C	N3-C4-N4	-6.92	113.16	118.00
8	A	1723	G	C2-N3-C4	-6.91	108.44	111.90
8	A	523	C	C6-N1-C2	6.91	123.06	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	1797	G	N3-C4-C5	6.91	132.06	128.60
8	A	2567	G	N3-C4-N9	-6.91	121.85	126.00
55	v	26	G	N3-C2-N2	-6.91	115.06	119.90
8	A	708	G	C2-N3-C4	-6.91	108.45	111.90
8	A	1171	G	C8-N9-C4	-6.91	103.64	106.40
8	A	1628	G	C8-N9-C4	6.91	109.16	106.40
8	A	2735	G	C2-N3-C4	-6.91	108.44	111.90
34	a	117	G	N3-C4-C5	6.91	132.05	128.60
8	A	1708	C	C6-N1-C2	6.91	123.06	120.30
8	A	1631	G	C6-C5-N7	6.91	134.54	130.40
8	A	1697	G	N3-C4-N9	-6.90	121.86	126.00
8	A	461	C	N3-C4-N4	-6.90	113.17	118.00
8	A	553	G	N3-C4-C5	6.90	132.05	128.60
8	A	560	C	C6-N1-C2	6.90	123.06	120.30
34	a	413	G	C2-N3-C4	-6.90	108.45	111.90
34	a	628	G	N3-C4-N9	-6.90	121.86	126.00
34	a	211	G	C2-N3-C4	6.90	115.35	111.90
34	a	295	C	C6-N1-C2	6.90	123.06	120.30
8	A	950	G	N3-C4-C5	6.90	132.05	128.60
8	A	1054	A	C4-C5-N7	6.90	114.15	110.70
8	A	506	G	N3-C4-N9	-6.89	121.86	126.00
8	A	2878	U	C6-N1-C2	6.89	125.14	121.00
34	a	921	U	C6-N1-C1'	6.89	130.85	121.20
8	A	2391	G	C8-N9-C4	6.89	109.16	106.40
34	a	1079	G	N3-C4-C5	6.89	132.05	128.60
55	v	4	G	N3-C4-C5	6.89	132.05	128.60
8	A	1062	G	N1-C2-N2	-6.89	110.00	116.20
8	A	1686	C	N3-C4-C5	6.89	124.66	121.90
8	A	1717	A	N1-C6-N6	6.89	122.73	118.60
8	A	1277	G	C8-N9-C4	6.88	109.15	106.40
34	a	1143	G	C2-N3-C4	-6.88	108.46	111.90
8	A	2867	G	C4-N9-C1'	-6.88	117.56	126.50
8	A	322	A	N1-C6-N6	-6.88	114.47	118.60
8	A	359	G	C4-N9-C1'	-6.88	117.56	126.50
8	A	2399	G	N3-C4-C5	6.88	132.04	128.60
8	A	1424	G	N3-C4-N9	-6.88	121.88	126.00
34	a	39	G	N3-C4-C5	6.88	132.04	128.60
8	A	1304	A	C8-N9-C4	6.87	108.55	105.80
8	A	1933	G	N3-C4-C5	6.87	132.04	128.60
8	A	1013	C	N3-C4-C5	6.87	124.65	121.90
8	A	1652	A	C4-C5-N7	6.87	114.14	110.70
8	A	1719	G	N3-C4-N9	-6.87	121.88	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	2458	G	C2-N3-C4	-6.87	108.47	111.90
8	A	2536	G	N3-C4-N9	-6.87	121.88	126.00
34	a	201	G	C4-N9-C1'	-6.87	117.57	126.50
8	A	2218	G	N3-C4-C5	6.87	132.03	128.60
8	A	2631	G	C4-N9-C1'	-6.87	117.57	126.50
9	B	17	C	C6-N1-C2	6.87	123.05	120.30
34	a	1157	A	C8-N9-C4	6.87	108.55	105.80
8	A	877	A	C8-N9-C4	6.86	108.55	105.80
8	A	2164	C	O4'-C1'-N1	-6.86	102.71	108.20
8	A	675	A	C4-C5-N7	6.86	114.13	110.70
8	A	2576	G	C6-C5-N7	6.86	134.52	130.40
34	a	903	G	N3-C4-C5	6.86	132.03	128.60
34	a	119	A	C5-C6-N6	-6.86	118.22	123.70
55	v	5	G	N3-C4-C5	6.86	132.03	128.60
8	A	862	G	N3-C4-C5	6.85	132.03	128.60
55	v	43	A	N9-C4-C5	-6.85	103.06	105.80
8	A	317	G	C8-N9-C4	6.85	109.14	106.40
8	A	2669	G	C8-N9-C4	6.85	109.14	106.40
8	A	618	G	N3-C4-N9	-6.85	121.89	126.00
8	A	949	G	C2-N3-C4	-6.85	108.48	111.90
8	A	1975	G	N3-C4-C5	6.85	132.02	128.60
8	A	41	C	C6-N1-C2	6.84	123.04	120.30
8	A	1713	A	C8-N9-C4	6.84	108.54	105.80
8	A	843	G	C2-N3-C4	-6.84	108.48	111.90
8	A	1333	G	N3-C4-C5	6.84	132.02	128.60
8	A	2496	C	C2-N1-C1'	6.84	126.32	118.80
34	a	410	G	N3-C4-N9	-6.84	121.90	126.00
8	A	2484	G	N3-C4-C5	6.84	132.02	128.60
8	A	2525	G	N3-C4-N9	-6.84	121.90	126.00
8	A	2815	C	C6-N1-C2	6.84	123.03	120.30
34	a	270	A	C4-C5-N7	6.84	114.12	110.70
8	A	1426	G	C2-N3-C4	-6.83	108.48	111.90
8	A	2659	G	N3-C4-N9	-6.83	121.90	126.00
8	A	1501	G	C2-N3-C4	-6.83	108.48	111.90
8	A	2045	C	C6-N1-C2	6.83	123.03	120.30
34	a	151	A	N9-C4-C5	-6.83	103.07	105.80
8	A	45	G	C2-N3-C4	-6.83	108.48	111.90
8	A	126	A	N9-C4-C5	-6.83	103.07	105.80
8	A	1244	A	N9-C4-C5	-6.83	103.07	105.80
34	a	954	G	N3-C4-N9	-6.83	121.90	126.00
8	A	259	G	N3-C4-N9	-6.83	121.91	126.00
34	a	225	C	C6-N1-C2	6.83	123.03	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	936	A	N9-C4-C5	-6.82	103.07	105.80
8	A	1165	A	C8-N9-C4	6.82	108.53	105.80
8	A	1218	G	N3-C4-N9	-6.82	121.91	126.00
55	v	52	G	N3-C4-C5	6.82	132.01	128.60
8	A	2671	G	N3-C4-N9	-6.82	121.91	126.00
8	A	2848	G	N3-C4-C5	6.82	132.01	128.60
34	a	445	G	N3-C4-N9	-6.81	121.91	126.00
8	A	2414	G	C4-N9-C1'	-6.81	117.64	126.50
9	B	60	C	C6-N1-C2	6.81	123.03	120.30
34	a	266	G	O4'-C1'-N9	6.81	113.65	108.20
34	a	691	G	N3-C4-C5	6.81	132.01	128.60
9	B	24	G	N3-C4-C5	6.81	132.01	128.60
8	A	771	G	N3-C4-N9	-6.81	121.92	126.00
8	A	2277	G	N3-C4-N9	-6.81	121.91	126.00
8	A	2157	G	O5'-P-OP1	-6.81	99.57	105.70
8	A	2525	G	C4-N9-C1'	-6.81	117.65	126.50
34	a	894	G	N3-C4-N9	-6.81	121.92	126.00
8	A	2628	C	N3-C4-C5	6.80	124.62	121.90
9	B	64	G	C8-N9-C4	6.80	109.12	106.40
9	B	78	A	C8-N9-C4	6.80	108.52	105.80
34	a	226	G	N1-C2-N2	-6.80	110.08	116.20
8	A	2230	G	C2-N3-C4	-6.80	108.50	111.90
34	a	142	G	N3-C4-N9	-6.80	121.92	126.00
34	a	68	G	N3-C4-C5	6.79	132.00	128.60
8	A	2803	G	C4-N9-C1'	-6.79	117.67	126.50
34	a	1374	A	C5-C6-N1	6.79	121.10	117.70
8	A	220	G	O4'-C1'-N9	-6.79	102.77	108.20
34	a	1081	A	O3'-P-O5'	6.79	116.90	104.00
8	A	247	G	N3-C4-N9	-6.79	121.93	126.00
8	A	1705	A	C4-C5-N7	6.79	114.09	110.70
9	B	107	G	N3-C4-N9	-6.79	121.93	126.00
8	A	718	A	N9-C4-C5	-6.78	103.09	105.80
8	A	1266	G	N3-C4-C5	6.78	131.99	128.60
34	a	1432	G	C2-N3-C4	-6.78	108.51	111.90
8	A	1403	A	N9-C4-C5	-6.78	103.09	105.80
9	B	64	G	C2-N3-C4	-6.78	108.51	111.90
34	a	640	A	N3-C4-C5	6.78	131.55	126.80
34	a	688	G	N3-C4-C5	6.78	131.99	128.60
8	A	1115	G	C2-N3-C4	-6.78	108.51	111.90
34	a	453	G	C4-N9-C1'	6.78	135.31	126.50
8	A	1178	C	N1-C2-O2	6.78	122.97	118.90
8	A	313	G	N3-C4-C5	6.77	131.99	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	1743	G	N3-C4-C5	6.77	131.99	128.60
34	a	164	G	N3-C4-C5	6.77	131.99	128.60
8	A	398	C	C6-N1-C2	6.77	123.01	120.30
8	A	1387	A	N9-C4-C5	-6.77	103.09	105.80
34	a	1102	A	N9-C4-C5	-6.77	103.09	105.80
8	A	1346	G	N3-C4-C5	6.77	131.98	128.60
9	B	51	G	C8-N9-C1'	-6.77	118.20	127.00
8	A	1767	G	N3-C4-N9	-6.76	121.94	126.00
9	B	83	G	C8-N9-C4	6.76	109.10	106.40
8	A	888	C	N3-C2-O2	-6.76	117.17	121.90
8	A	924	G	N3-C4-C5	6.76	131.98	128.60
8	A	953	G	C8-N9-C4	6.76	109.10	106.40
8	A	1517	G	C2-N3-C4	-6.76	108.52	111.90
8	A	2351	G	N3-C4-C5	6.76	131.98	128.60
34	a	38	G	N3-C4-C5	6.76	131.98	128.60
34	a	696	A	C5-C6-N6	-6.76	118.29	123.70
34	a	988	G	N3-C4-N9	-6.76	121.95	126.00
8	A	813	U	C6-N1-C2	6.75	125.05	121.00
8	A	1382	G	N3-C4-C5	6.75	131.98	128.60
8	A	1477	A	C4-C5-N7	6.75	114.08	110.70
34	a	109	A	N1-C6-N6	6.75	122.65	118.60
8	A	271	G	C2-N3-C4	-6.75	108.52	111.90
8	A	1017	G	N3-C4-C5	6.75	131.97	128.60
8	A	2235	G	C4-N9-C1'	-6.75	117.72	126.50
8	A	2142	A	O4'-C1'-N9	-6.75	102.80	108.20
34	a	1462	C	C6-N1-C2	6.75	123.00	120.30
8	A	1034	G	C2-N3-C4	-6.75	108.53	111.90
8	A	1517	G	N3-C4-C5	6.75	131.97	128.60
10	C	201	LEU	CA-CB-CG	-6.75	99.79	115.30
8	A	1846	G	N3-C4-C5	6.74	131.97	128.60
34	a	199	A	N9-C4-C5	-6.74	103.10	105.80
8	A	1336	A	C8-N9-C4	6.74	108.50	105.80
34	a	778	G	N3-C4-C5	6.74	131.97	128.60
34	a	1483	A	N1-C6-N6	6.74	122.64	118.60
9	B	111	U	C6-N1-C2	6.74	125.04	121.00
8	A	2876	G	N3-C4-N9	-6.74	121.96	126.00
55	v	15	G	N3-C4-N9	-6.74	121.96	126.00
9	B	37	C	N3-C4-N4	-6.73	113.29	118.00
8	A	2678	C	N3-C4-C5	6.73	124.59	121.90
34	a	1417	G	C2-N3-C4	-6.73	108.53	111.90
8	A	1092	C	C6-N1-C2	6.73	122.99	120.30
8	A	1904	G	C2-N3-C4	-6.73	108.53	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	a	1061	G	C2-N3-C4	-6.73	108.53	111.90
8	A	2235	G	C8-N9-C4	6.73	109.09	106.40
8	A	2444	G	N3-C4-C5	6.73	131.96	128.60
34	a	297	G	N3-C4-C5	6.73	131.96	128.60
56	w	53	G	N3-C4-C5	6.73	131.96	128.60
8	A	1093	G	N3-C4-N9	-6.73	121.97	126.00
8	A	335	C	N3-C4-C5	6.72	124.59	121.90
8	A	425	G	C8-N9-C4	6.72	109.09	106.40
8	A	340	A	C5-C6-N6	-6.72	118.32	123.70
8	A	916	G	C4-C5-N7	6.72	113.49	110.80
8	A	1826	G	N3-C4-C5	6.72	131.96	128.60
8	A	570	G	C4-N9-C1'	6.72	135.23	126.50
8	A	1338	G	C2-N3-C4	-6.72	108.54	111.90
8	A	2458	G	N3-C4-N9	-6.71	121.97	126.00
8	A	1123	C	N3-C4-N4	-6.71	113.30	118.00
8	A	1220	G	C4-N9-C1'	-6.71	117.77	126.50
8	A	2803	G	N3-C4-N9	-6.71	121.97	126.00
34	a	602	A	N9-C4-C5	-6.71	103.11	105.80
34	a	1196	A	N1-C6-N6	6.71	122.63	118.60
34	a	1020	G	N3-C4-C5	6.71	131.95	128.60
8	A	2542	A	N1-C6-N6	-6.71	114.58	118.60
34	a	432	A	C5-C6-N6	-6.71	118.34	123.70
8	A	1090	A	P-O3'-C3'	6.70	127.75	119.70
8	A	2279	G	N3-C4-C5	6.70	131.95	128.60
8	A	729	G	O4'-C1'-N9	6.70	113.56	108.20
8	A	2093	G	N3-C4-C5	6.70	131.95	128.60
8	A	1239	G	N3-C4-C5	6.70	131.95	128.60
34	a	691	G	N3-C4-N9	-6.70	121.98	126.00
34	a	1043	G	N3-C4-N9	-6.70	121.98	126.00
34	a	1310	G	N3-C4-C5	6.70	131.95	128.60
8	A	2138	G	N3-C4-C5	6.70	131.95	128.60
9	B	102	G	C2-N3-C4	-6.70	108.55	111.90
8	A	1426	G	N3-C4-C5	6.70	131.95	128.60
8	A	1682	G	N3-C4-C5	6.70	131.95	128.60
34	a	425	G	N3-C4-N9	-6.70	121.98	126.00
9	B	83	G	N3-C4-C5	6.69	131.95	128.60
34	a	1190	G	N3-C2-N2	-6.69	115.22	119.90
34	a	1419	G	C4-N9-C1'	6.69	135.20	126.50
34	a	25	C	C6-N1-C2	6.69	122.98	120.30
9	B	112	G	N3-C4-C5	6.69	131.94	128.60
34	a	626	G	N3-C4-C5	6.69	131.94	128.60
34	a	888	G	N3-C2-N2	-6.69	115.22	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	988	A	C8-N9-C4	6.69	108.47	105.80
8	A	1590	A	N9-C4-C5	-6.69	103.13	105.80
8	A	1844	C	N3-C4-C5	6.68	124.57	121.90
8	A	2121	G	O4'-C1'-N9	6.68	113.55	108.20
8	A	37	C	N3-C4-C5	6.68	124.57	121.90
8	A	466	A	N1-C6-N6	-6.68	114.59	118.60
8	A	1477	A	N9-C4-C5	-6.68	103.13	105.80
8	A	1062	G	N9-C4-C5	-6.67	102.73	105.40
34	a	1423	G	N3-C4-C5	6.67	131.94	128.60
8	A	1684	G	N3-C4-N9	-6.67	122.00	126.00
34	a	1300	G	C2-N3-C4	-6.67	108.56	111.90
8	A	524	G	N3-C4-C5	6.67	131.94	128.60
8	A	537	G	C8-N9-C4	6.67	109.07	106.40
34	a	1003	G	N3-C4-C5	6.67	131.94	128.60
8	A	303	G	N9-C4-C5	-6.67	102.73	105.40
34	a	402	G	C2-N3-C4	-6.67	108.57	111.90
56	w	13	C	C2'-C3'-O3'	6.66	124.36	113.70
8	A	1492	G	C8-N9-C1'	6.66	135.66	127.00
34	a	410	G	C4-N9-C1'	-6.66	117.84	126.50
34	a	886	G	C2-N3-C4	-6.66	108.57	111.90
8	A	669	G	N3-C2-N2	-6.66	115.24	119.90
8	A	2663	G	C2-N3-C4	-6.66	108.57	111.90
34	a	1461	G	N3-C4-C5	6.66	131.93	128.60
34	a	141	G	N3-C4-N9	-6.65	122.01	126.00
34	a	1258	G	N3-C4-C5	6.65	131.93	128.60
34	a	765	G	N3-C4-C5	6.65	131.93	128.60
8	A	712	G	N3-C4-C5	6.65	131.93	128.60
8	A	1186	G	C2-N3-C4	-6.65	108.57	111.90
34	a	917	G	C2-N3-C4	-6.65	108.58	111.90
8	A	2575	C	N3-C4-C5	6.65	124.56	121.90
8	A	2323	G	N3-C4-N9	-6.65	122.01	126.00
8	A	2867	G	N3-C4-N9	-6.65	122.01	126.00
34	a	1025	U	C6-N1-C2	-6.65	117.01	121.00
55	v	53	G	N3-C4-C5	6.65	131.92	128.60
8	A	843	G	C4-N9-C1'	-6.64	117.86	126.50
8	A	1158	C	N3-C4-N4	-6.64	113.35	118.00
8	A	1628	G	N3-C4-C5	6.64	131.92	128.60
8	A	401	A	O4'-C1'-N9	-6.64	102.89	108.20
34	a	227	G	N3-C4-C5	6.64	131.92	128.60
8	A	1540	G	C2-N3-C4	-6.64	108.58	111.90
34	a	616	G	C8-N9-C4	6.63	109.05	106.40
34	a	705	G	C2-N3-C4	-6.63	108.58	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	a	1117	A	N1-C6-N6	6.63	122.58	118.60
34	a	1322	C	O4'-C1'-N1	6.63	113.50	108.20
8	A	469	G	N1-C6-O6	6.63	123.88	119.90
34	a	778	G	N3-C4-N9	-6.63	122.02	126.00
34	a	830	G	C2-N3-C4	-6.63	108.59	111.90
55	v	46	A	C5-C6-N6	-6.63	118.40	123.70
8	A	1401	G	C2-N3-C4	-6.63	108.59	111.90
8	A	1717	A	C5-C6-N6	-6.62	118.40	123.70
8	A	2207	C	C6-N1-C2	6.62	122.95	120.30
8	A	2378	A	C6-C5-N7	-6.62	127.66	132.30
8	A	1016	G	C8-N9-C4	6.62	109.05	106.40
34	a	187	G	N3-C4-C5	6.62	131.91	128.60
8	A	1849	G	N3-C4-C5	6.62	131.91	128.60
34	a	1094	G	N1-C2-N2	-6.62	110.24	116.20
34	a	1362	A	C8-N9-C4	6.62	108.45	105.80
8	A	617	G	C8-N9-C4	6.62	109.05	106.40
8	A	1120	G	N3-C4-C5	6.62	131.91	128.60
8	A	2174	C	C6-N1-C1'	6.62	128.74	120.80
34	a	920	U	C5-C6-N1	6.62	126.01	122.70
8	A	494	G	N3-C4-N9	-6.61	122.03	126.00
8	A	2217	G	N3-C4-C5	6.61	131.91	128.60
8	A	2502	G	N3-C4-C5	6.61	131.91	128.60
34	a	435	A	N9-C4-C5	-6.61	103.16	105.80
34	a	319	G	N3-C4-N9	-6.61	122.03	126.00
34	a	838	G	N9-C4-C5	-6.61	102.76	105.40
8	A	1266	G	C2-N3-C4	-6.61	108.60	111.90
8	A	2877	G	N3-C4-C5	6.61	131.90	128.60
34	a	1245	C	C6-N1-C2	6.61	122.94	120.30
8	A	2677	G	N3-C4-C5	6.60	131.90	128.60
34	a	1106	G	N3-C4-N9	-6.60	122.04	126.00
8	A	2527	C	N3-C4-N4	-6.60	113.38	118.00
8	A	493	G	C2-N3-C4	-6.60	108.60	111.90
8	A	132	G	C2-N3-C4	-6.60	108.60	111.90
8	A	953	G	N3-C4-C5	6.60	131.90	128.60
8	A	2640	G	N3-C4-N9	-6.60	122.04	126.00
8	A	2834	G	N3-C4-C5	6.59	131.90	128.60
34	a	488	C	C6-N1-C1'	-6.59	112.89	120.80
8	A	1238	G	N3-C4-C5	6.59	131.90	128.60
8	A	2461	A	C8-N9-C4	6.59	108.44	105.80
34	a	1185	G	C8-N9-C4	6.59	109.04	106.40
8	A	178	G	N3-C4-N9	-6.58	122.05	126.00
8	A	346	A	N1-C6-N6	6.58	122.55	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	1399	C	N3-C4-C5	6.58	124.53	121.90
8	A	408	G	C2-N3-C4	-6.58	108.61	111.90
8	A	2010	G	C2-N3-C4	-6.58	108.61	111.90
8	A	2436	G	N3-C4-C5	6.58	131.89	128.60
34	a	1241	G	C8-N9-C4	6.58	109.03	106.40
8	A	359	G	C8-N9-C1'	6.58	135.56	127.00
8	A	856	G	N3-C4-C5	6.58	131.89	128.60
8	A	1703	G	N3-C4-C5	6.58	131.89	128.60
8	A	1398	C	N3-C4-C5	6.58	124.53	121.90
8	A	494	G	N3-C4-C5	6.57	131.89	128.60
8	A	1171	G	N3-C4-N9	-6.57	122.06	126.00
35	b	134	LEU	CA-CB-CG	6.57	130.42	115.30
8	A	1295	C	C6-N1-C2	6.57	122.93	120.30
8	A	1469	A	N9-C1'-C2'	-6.57	104.77	112.00
34	a	639	G	N3-C4-C5	6.57	131.88	128.60
8	A	966	G	N3-C4-C5	6.57	131.88	128.60
52	s	28	LYS	CB-CG-CD	-6.57	94.52	111.60
8	A	2665	A	N1-C6-N6	6.56	122.54	118.60
34	a	851	G	C4-C5-N7	6.56	113.43	110.80
34	a	1361	G	C2-N3-C4	-6.56	108.62	111.90
34	a	1521	C	C6-N1-C2	6.56	122.93	120.30
8	A	1120	G	C2-N3-C4	-6.56	108.62	111.90
8	A	1456	G	N3-C4-N9	-6.56	122.06	126.00
8	A	2363	G	N3-C4-N9	-6.56	122.06	126.00
34	a	1089	G	N3-C4-N9	-6.56	122.06	126.00
8	A	681	G	C2-N3-C4	-6.56	108.62	111.90
8	A	1123	C	C6-N1-C2	6.56	122.92	120.30
8	A	1888	G	N3-C4-C5	6.56	131.88	128.60
8	A	1984	G	N3-C4-N9	-6.56	122.07	126.00
34	a	348	G	N3-C4-C5	6.56	131.88	128.60
34	a	752	G	N3-C4-N9	-6.56	122.07	126.00
8	A	1149	G	C8-N9-C4	6.56	109.02	106.40
8	A	848	C	N3-C4-C5	6.55	124.52	121.90
8	A	974	G	C6-C5-N7	-6.55	126.47	130.40
34	a	1108	G	N1-C2-N2	6.55	122.10	116.20
34	a	1314	C	C6-N1-C2	6.55	122.92	120.30
8	A	107	G	N3-C4-C5	6.55	131.88	128.60
8	A	1149	G	N3-C4-C5	6.55	131.88	128.60
8	A	424	G	C8-N9-C4	6.54	109.02	106.40
8	A	475	C	O4'-C1'-N1	6.54	113.43	108.20
8	A	498	G	N3-C4-N9	-6.54	122.07	126.00
8	A	2436	G	C8-N9-C4	6.54	109.02	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	a	768	A	C8-N9-C4	6.54	108.42	105.80
34	a	1081	A	OP2-P-O3'	6.54	119.59	105.20
34	a	682	G	C4-N9-C1'	-6.54	118.00	126.50
8	A	319	G	C2-N3-C4	-6.54	108.63	111.90
8	A	1075	C	C6-N1-C2	6.54	122.92	120.30
8	A	1663	G	N3-C4-C5	6.54	131.87	128.60
8	A	549	G	C2-N3-C4	-6.54	108.63	111.90
8	A	118	A	C8-N9-C4	6.54	108.42	105.80
8	A	189	G	N3-C4-C5	6.54	131.87	128.60
8	A	2812	G	N3-C4-C5	6.54	131.87	128.60
8	A	1367	A	N9-C4-C5	-6.53	103.19	105.80
34	a	1057	G	C2-N3-C4	-6.53	108.63	111.90
34	a	204	G	N9-C1'-C2'	-6.53	104.81	112.00
8	A	899	A	N9-C4-C5	-6.53	103.19	105.80
8	A	1810	A	C6-C5-N7	-6.53	127.73	132.30
8	A	2411	A	C5-C6-N6	-6.53	118.47	123.70
55	v	12	G	C4-N9-C1'	-6.53	118.01	126.50
8	A	1139	G	C4-C5-C6	-6.53	114.88	118.80
8	A	2652	C	N3-C4-C5	6.53	124.51	121.90
8	A	1	G	C2-N3-C4	-6.53	108.64	111.90
8	A	268	C	N3-C4-C5	6.53	124.51	121.90
8	A	340	A	N9-C4-C5	-6.53	103.19	105.80
34	a	882	C	C6-N1-C2	6.53	122.91	120.30
8	A	917	A	C5-C6-N6	-6.52	118.48	123.70
8	A	1858	A	C8-N9-C4	6.52	108.41	105.80
8	A	2073	C	N3-C4-C5	6.52	124.51	121.90
8	A	409	G	C2-N3-C4	-6.52	108.64	111.90
34	a	445	G	C4-N9-C1'	-6.52	118.02	126.50
8	A	2665	A	C5-C6-N6	-6.52	118.48	123.70
8	A	549	G	C8-N9-C4	6.52	109.01	106.40
8	A	2153	C	N1-C2-O2	-6.52	114.99	118.90
34	a	798	U	C6-N1-C2	6.52	124.91	121.00
34	a	1111	A	C8-N9-C4	6.52	108.41	105.80
8	A	370	G	O4'-C1'-N9	-6.51	102.99	108.20
34	a	1244	G	C2-N3-C4	-6.51	108.64	111.90
8	A	695	G	C2-N3-C4	-6.51	108.64	111.90
9	B	13	G	N3-C4-C5	6.51	131.86	128.60
8	A	997	G	C2-N3-C4	-6.51	108.64	111.90
8	A	1960	A	C4-C5-N7	6.51	113.95	110.70
8	A	2253	G	N3-C4-C5	6.51	131.85	128.60
34	a	1134	G	C8-N9-C1'	6.51	135.46	127.00
8	A	85	G	C2-N3-C4	-6.51	108.65	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	721	A	C8-N9-C4	6.51	108.40	105.80
8	A	1465	G	N3-C4-N9	-6.51	122.10	126.00
8	A	2802	G	C2-N3-C4	-6.51	108.65	111.90
34	a	606	G	N3-C4-N9	-6.51	122.10	126.00
34	a	1075	U	O4'-C1'-N1	-6.51	102.99	108.20
34	a	784	A	N9-C4-C5	-6.50	103.20	105.80
8	A	86	G	C8-N9-C4	6.50	109.00	106.40
8	A	1919	A	O4'-C1'-N9	-6.50	103.00	108.20
8	A	2659	G	C4-N9-C1'	-6.50	118.05	126.50
34	a	449	G	C2-N3-C4	-6.50	108.65	111.90
8	A	1165	A	C4-C5-C6	-6.50	113.75	117.00
8	A	1436	G	C2-N3-C4	-6.50	108.65	111.90
8	A	1867	G	C2-N3-C4	-6.50	108.65	111.90
8	A	551	G	N3-C4-N9	-6.50	122.10	126.00
34	a	767	A	C8-N9-C4	6.50	108.40	105.80
34	a	758	C	C6-N1-C2	6.50	122.90	120.30
8	A	1873	G	N3-C4-N9	-6.49	122.10	126.00
9	B	107	G	N3-C4-C5	6.49	131.85	128.60
34	a	190	A	C5-C6-N6	-6.49	118.51	123.70
34	a	1501	C	N3-C4-C5	6.49	124.50	121.90
8	A	1306	C	C6-N1-C2	6.49	122.90	120.30
8	A	1424	G	C2-N3-C4	-6.49	108.66	111.90
8	A	1686	C	N3-C4-N4	-6.49	113.46	118.00
8	A	1334	G	C2-N3-C4	-6.49	108.66	111.90
8	A	2882	A	C8-N9-C4	6.49	108.40	105.80
8	A	833	A	C8-N9-C4	6.49	108.39	105.80
8	A	1844	C	C6-N1-C2	6.49	122.89	120.30
8	A	1511	G	N3-C4-C5	6.48	131.84	128.60
8	A	261	G	N3-C4-N9	-6.48	122.11	126.00
8	A	2230	G	N3-C4-C5	6.48	131.84	128.60
8	A	2661	G	N3-C4-C5	6.48	131.84	128.60
34	a	391	G	N3-C4-C5	6.48	131.84	128.60
8	A	52	A	N9-C4-C5	-6.48	103.21	105.80
8	A	1311	G	N3-C4-N9	-6.48	122.11	126.00
34	a	1141	C	C6-N1-C2	-6.48	117.71	120.30
8	A	1557	C	C6-N1-C2	6.48	122.89	120.30
34	a	846	G	N9-C4-C5	-6.48	102.81	105.40
8	A	9	G	N3-C4-N9	-6.48	122.11	126.00
8	A	1011	G	N3-C4-C5	6.48	131.84	128.60
8	A	1479	G	N3-C4-N9	-6.48	122.11	126.00
8	A	1448	G	N3-C4-C5	6.47	131.84	128.60
8	A	2126	A	O4'-C1'-N9	-6.47	103.02	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	522	A	O4'-C1'-N9	-6.47	103.02	108.20
8	A	1544	A	C5-C6-N6	-6.47	118.53	123.70
8	A	2008	C	N3-C4-C5	6.47	124.49	121.90
8	A	697	G	N3-C4-C5	6.47	131.83	128.60
8	A	2716	C	N3-C4-C5	6.47	124.49	121.90
8	A	14	A	N9-C4-C5	-6.47	103.21	105.80
8	A	179	C	C6-N1-C2	6.47	122.89	120.30
8	A	260	G	N3-C4-N9	-6.47	122.12	126.00
8	A	1279	G	C8-N9-C4	6.47	108.99	106.40
8	A	2083	G	N3-C2-N2	6.47	124.43	119.90
8	A	450	G	N3-C4-C5	6.46	131.83	128.60
8	A	1973	G	C2-N3-C4	-6.46	108.67	111.90
8	A	2281	A	N9-C4-C5	-6.46	103.21	105.80
9	B	52	A	C5-C6-N6	-6.46	118.53	123.70
34	a	1419	G	C8-N9-C1'	-6.46	118.60	127.00
8	A	319	G	N3-C4-N9	-6.46	122.12	126.00
8	A	871	U	C6-N1-C2	6.46	124.88	121.00
8	A	2414	G	C6-C5-N7	6.46	134.28	130.40
8	A	2842	G	N3-C4-C5	6.46	131.83	128.60
34	a	337	G	N3-C4-C5	6.46	131.83	128.60
34	a	1198	G	N3-C4-C5	6.46	131.83	128.60
8	A	1448	G	N3-C4-N9	-6.46	122.12	126.00
34	a	227	G	C2-N3-C4	-6.46	108.67	111.90
34	a	191	G	C2-N3-C4	-6.46	108.67	111.90
8	A	1930	G	N3-C4-C5	6.46	131.83	128.60
8	A	2643	G	C2-N3-C4	-6.46	108.67	111.90
8	A	2867	G	C8-N9-C1'	6.46	135.39	127.00
34	a	774	G	N3-C4-N9	-6.46	122.13	126.00
34	a	1134	G	C5-C6-O6	6.46	132.47	128.60
8	A	1348	C	O4'-C1'-N1	-6.45	103.04	108.20
34	a	602	A	C4-C5-N7	6.45	113.93	110.70
8	A	294	A	O4'-C1'-N9	-6.45	103.04	108.20
8	A	507	A	C8-N9-C4	6.45	108.38	105.80
8	A	1740	G	C2-N3-C4	-6.45	108.67	111.90
9	B	52	A	N1-C6-N6	6.45	122.47	118.60
8	A	570	G	N3-C2-N2	6.45	124.41	119.90
10	C	17	LYS	CA-CB-CG	6.45	127.59	113.40
8	A	1933	G	N3-C4-N9	-6.45	122.13	126.00
8	A	1969	A	C5-C6-N6	-6.45	118.54	123.70
8	A	2619	C	N3-C4-N4	-6.45	113.49	118.00
8	A	2688	G	N3-C4-C5	6.45	131.82	128.60
34	a	722	G	N3-C4-C5	6.45	131.82	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	a	259	G	N3-C4-N9	-6.44	122.13	126.00
34	a	912	C	N1-C2-O2	6.44	122.77	118.90
8	A	2234	G	N3-C4-C5	6.44	131.82	128.60
8	A	44	A	C8-N9-C4	6.44	108.38	105.80
9	B	93	C	C6-N1-C1'	-6.44	113.07	120.80
8	A	406	G	C2-N3-C4	-6.44	108.68	111.90
8	A	543	G	N3-C4-C5	6.44	131.82	128.60
8	A	452	G	C2-N3-C4	-6.44	108.68	111.90
34	a	442	G	C4-C5-N7	6.43	113.37	110.80
34	a	1289	A	C4-C5-N7	6.43	113.92	110.70
8	A	1041	G	C8-N9-C4	6.43	108.97	106.40
8	A	2168	G	O4'-C1'-N9	-6.43	103.06	108.20
34	a	55	A	N1-C6-N6	6.43	122.46	118.60
34	a	1039	G	N3-C4-C5	6.42	131.81	128.60
8	A	2217	G	C2-N3-C4	-6.42	108.69	111.90
36	c	126	ARG	NE-CZ-NH2	-6.42	117.09	120.30
8	A	2082	A	N1-C6-N6	6.42	122.45	118.60
8	A	2863	C	N1-C2-O2	6.42	122.75	118.90
9	B	108	A	N9-C4-C5	-6.42	103.23	105.80
34	a	371	A	N9-C4-C5	-6.42	103.23	105.80
34	a	1133	G	C8-N9-C4	6.42	108.97	106.40
8	A	2430	A	O4'-C1'-N9	6.42	113.33	108.20
34	a	774	G	N3-C4-C5	6.42	131.81	128.60
8	A	819	A	N9-C4-C5	-6.41	103.23	105.80
34	a	654	G	C2-N3-C4	-6.41	108.69	111.90
8	A	77	G	C2-N3-C4	-6.41	108.69	111.90
34	a	378	G	N3-C4-C5	6.41	131.81	128.60
8	A	38	A	C4-C5-C6	-6.41	113.80	117.00
9	B	119	A	N3-C4-C5	6.41	131.29	126.80
8	A	708	G	C8-N9-C4	6.41	108.96	106.40
8	A	1274	A	C8-N9-C4	6.41	108.36	105.80
8	A	2002	G	N3-C4-C5	6.41	131.81	128.60
8	A	2174	C	C2-N1-C1'	-6.41	111.75	118.80
34	a	841	C	C6-N1-C2	6.41	122.86	120.30
9	B	70	C	C6-N1-C2	6.41	122.86	120.30
8	A	1783	A	C5-C6-N6	-6.41	118.58	123.70
23	P	99	LEU	CA-CB-CG	-6.41	100.56	115.30
34	a	282	A	N1-C6-N6	6.41	122.44	118.60
34	a	808	C	C6-N1-C2	6.41	122.86	120.30
34	a	1500	A	C5-C6-N6	6.41	128.82	123.70
34	a	831	A	C8-N9-C4	6.40	108.36	105.80
8	A	2127	G	O4'-C1'-N9	-6.40	103.08	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	a	346	G	C5-C6-O6	-6.40	124.76	128.60
34	a	921	U	P-O5'-C5'	6.40	131.14	120.90
8	A	476	G	N3-C4-C5	6.40	131.80	128.60
8	A	2612	C	C6-N1-C2	6.40	122.86	120.30
8	A	2411	A	C8-N9-C4	6.40	108.36	105.80
8	A	457	A	C8-N9-C4	6.40	108.36	105.80
34	a	656	G	N3-C4-C5	6.40	131.80	128.60
8	A	748	G	N3-C4-C5	6.39	131.80	128.60
8	A	1277	G	C2-N3-C4	-6.39	108.70	111.90
8	A	1726	C	C6-N1-C2	6.39	122.86	120.30
34	a	987	G	C4-N9-C1'	-6.39	118.19	126.50
8	A	1158	C	N3-C4-C5	6.39	124.46	121.90
8	A	2652	C	C6-N1-C2	6.39	122.86	120.30
34	a	604	G	C4-N9-C1'	-6.39	118.19	126.50
8	A	2134	A	C5'-C4'-C3'	-6.39	105.78	116.00
9	B	10	G	N3-C4-C5	6.39	131.79	128.60
8	A	132	G	N3-C4-C5	6.39	131.79	128.60
8	A	496	G	N3-C4-C5	6.39	131.79	128.60
8	A	1674	G	N3-C4-N9	-6.39	122.17	126.00
8	A	2467	C	C6-N1-C2	6.39	122.86	120.30
8	A	875	G	C2-N3-C4	-6.38	108.71	111.90
34	a	522	C	N3-C4-C5	6.38	124.45	121.90
34	a	1134	G	C4-N9-C1'	-6.38	118.20	126.50
34	a	346	G	C6-C5-N7	-6.38	126.57	130.40
8	A	141	G	N3-C4-C5	6.38	131.79	128.60
8	A	1667	G	N3-C4-C5	6.38	131.79	128.60
8	A	1369	G	N3-C4-C5	6.38	131.79	128.60
9	B	10	G	C2-N3-C4	-6.38	108.71	111.90
34	a	1162	C	C6-N1-C2	6.38	122.85	120.30
8	A	469	G	N1-C2-N2	-6.38	110.46	116.20
8	A	1029	A	N1-C6-N6	6.38	122.43	118.60
8	A	2864	G	N9-C4-C5	-6.38	102.85	105.40
34	a	830	G	N3-C4-N9	-6.38	122.17	126.00
8	A	1542	U	C6-N1-C2	6.37	124.82	121.00
8	A	2862	G	N3-C4-C5	6.37	131.79	128.60
8	A	618	G	C2-N3-C4	-6.37	108.72	111.90
34	a	1329	A	C4-C5-C6	-6.37	113.81	117.00
8	A	1295	C	N3-C4-C5	6.37	124.45	121.90
8	A	2	G	C8-N9-C4	6.37	108.95	106.40
8	A	748	G	C4-N9-C1'	-6.37	118.22	126.50
8	A	1099	G	N3-C4-N9	-6.37	122.18	126.00
34	a	339	C	N3-C4-N4	-6.37	113.54	118.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	1041	G	C4-N9-C1'	-6.37	118.22	126.50
8	A	1389	G	N3-C4-C5	6.37	131.78	128.60
9	B	85	G	C8-N9-C4	6.37	108.95	106.40
8	A	245	G	N3-C4-C5	6.37	131.78	128.60
8	A	1643	G	N3-C4-C5	6.37	131.78	128.60
8	A	2133	G	N3-C4-N9	-6.37	122.18	126.00
8	A	786	C	C6-N1-C2	6.36	122.85	120.30
8	A	2140	G	N3-C4-N9	-6.36	122.18	126.00
34	a	540	G	N3-C4-N9	-6.36	122.18	126.00
8	A	794	A	C5-C6-N1	6.36	120.88	117.70
8	A	962	G	C2-N3-C4	-6.36	108.72	111.90
8	A	1684	G	C8-N9-C4	6.36	108.94	106.40
8	A	1735	A	C5-N7-C8	-6.36	100.72	103.90
8	A	2005	A	C8-N9-C4	6.36	108.34	105.80
8	A	2536	G	C2-N3-C4	-6.36	108.72	111.90
9	B	59	A	C8-N9-C4	6.36	108.34	105.80
34	a	371	A	C8-N9-C4	6.36	108.34	105.80
8	A	1028	A	C4-C5-N7	6.36	113.88	110.70
8	A	2295	C	N1-C2-O2	6.36	122.72	118.90
8	A	682	G	C2-N3-C4	-6.36	108.72	111.90
8	A	1371	G	C2-N3-C4	-6.36	108.72	111.90
8	A	88	G	C8-N9-C4	6.35	108.94	106.40
8	A	1116	G	N3-C4-C5	6.35	131.78	128.60
34	a	243	A	C2-N3-C4	-6.35	107.42	110.60
34	a	446	G	N3-C4-N9	-6.35	122.19	126.00
34	a	1104	G	C2-N3-C4	-6.35	108.72	111.90
8	A	2512	C	C5-C4-N4	6.35	124.65	120.20
34	a	215	C	C6-N1-C2	6.35	122.84	120.30
8	A	1530	G	N3-C4-N9	-6.35	122.19	126.00
34	a	812	G	N3-C4-N9	-6.35	122.19	126.00
8	A	693	A	N9-C4-C5	-6.35	103.26	105.80
34	a	722	G	N3-C4-N9	-6.35	122.19	126.00
8	A	1281	G	N3-C4-N9	-6.35	122.19	126.00
8	A	881	G	N1-C6-O6	6.34	123.71	119.90
34	a	151	A	C4-C5-N7	6.34	113.87	110.70
8	A	180	G	C8-N9-C1'	6.34	135.24	127.00
8	A	598	U	C6-N1-C2	6.34	124.80	121.00
8	A	2406	A	O4'-C1'-N9	-6.34	103.13	108.20
34	a	1071	C	C6-N1-C2	6.34	122.84	120.30
8	A	1863	G	C2-N3-C4	-6.34	108.73	111.90
8	A	2657	A	N9-C4-C5	-6.33	103.27	105.80
8	A	2474	U	C2-N1-C1'	6.33	125.30	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	a	98	A	C8-N9-C4	6.33	108.33	105.80
34	a	165	G	C2-N3-C4	-6.33	108.73	111.90
8	A	1112	G	N3-C4-N9	-6.33	122.20	126.00
8	A	2154	A	N9-C4-C5	-6.33	103.27	105.80
34	a	1164	G	N3-C4-C5	6.33	131.76	128.60
34	a	1221	G	N3-C4-N9	-6.33	122.20	126.00
8	A	2543	G	C2-N3-C4	-6.33	108.74	111.90
34	a	42	G	N3-C4-N9	-6.33	122.20	126.00
34	a	146	G	C2-N3-C4	-6.33	108.74	111.90
8	A	20	C	N3-C4-N4	-6.32	113.57	118.00
8	A	122	G	C2-N3-C4	-6.32	108.74	111.90
8	A	655	A	C8-N9-C4	6.32	108.33	105.80
8	A	1858	A	N9-C4-C5	-6.32	103.27	105.80
8	A	2485	G	N3-C4-N9	-6.32	122.20	126.00
8	A	2644	G	N3-C4-C5	6.32	131.76	128.60
56	w	45	U	C4'-C3'-O3'	6.32	125.64	113.00
8	A	1631	G	C8-N9-C4	6.32	108.93	106.40
9	B	108	A	N1-C6-N6	6.32	122.39	118.60
8	A	2	G	C2-N3-C4	-6.32	108.74	111.90
8	A	1311	G	O4'-C1'-N9	-6.32	103.14	108.20
8	A	1358	G	C2-N3-C4	-6.32	108.74	111.90
34	a	521	G	N3-C4-N9	-6.32	122.21	126.00
34	a	748	G	N3-C4-N9	-6.32	122.21	126.00
8	A	1895	C	C6-N1-C2	6.32	122.83	120.30
8	A	406	G	N3-C4-N9	-6.32	122.21	126.00
8	A	1036	G	N3-C4-C5	6.32	131.76	128.60
34	a	369	G	N3-C4-C5	6.32	131.76	128.60
34	a	1259	C	C6-N1-C2	6.32	122.83	120.30
34	a	1457	G	N3-C4-C5	6.32	131.76	128.60
8	A	869	G	C2-N3-C4	-6.32	108.74	111.90
8	A	1313	U	C2-N1-C1'	6.32	125.28	117.70
8	A	378	C	N3-C4-N4	-6.31	113.58	118.00
8	A	2190	G	C4-C5-N7	6.31	113.33	110.80
8	A	2629	U	O4'-C1'-N1	6.31	113.25	108.20
8	A	1519	G	C2-N3-C4	-6.31	108.74	111.90
8	A	1805	A	C8-N9-C4	6.31	108.33	105.80
8	A	2221	G	C2-N3-C4	-6.31	108.74	111.90
34	a	247	G	C2-N3-C4	-6.31	108.74	111.90
34	a	1230	C	N1-C2-O2	6.31	122.69	118.90
34	a	255	G	N3-C4-N9	-6.31	122.21	126.00
8	A	1389	G	C8-N9-C4	6.31	108.92	106.40
8	A	1810	A	N9-C4-C5	-6.31	103.28	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	2714	G	N1-C2-N2	-6.31	110.52	116.20
34	a	839	C	N3-C4-C5	6.31	124.42	121.90
34	a	821	G	C8-N9-C4	6.31	108.92	106.40
8	A	2501	C	N3-C4-C5	6.30	124.42	121.90
9	B	15	A	N1-C6-N6	-6.30	114.82	118.60
34	a	202	G	C8-N9-C4	6.30	108.92	106.40
34	a	1155	A	N3-C4-C5	6.30	131.21	126.80
8	A	882	G	C2-N3-C4	-6.29	108.75	111.90
8	A	1170	C	C2-N1-C1'	6.29	125.72	118.80
55	v	43	A	C8-N9-C4	6.29	108.32	105.80
8	A	2810	A	N1-C6-N6	6.29	122.38	118.60
34	a	187	G	N3-C4-N9	-6.29	122.22	126.00
34	a	1312	G	N9-C4-C5	-6.29	102.88	105.40
8	A	763	G	N3-C4-N9	-6.29	122.23	126.00
8	A	1846	G	C2-N3-C4	-6.29	108.75	111.90
8	A	2077	A	C4-C5-N7	6.29	113.84	110.70
8	A	2839	G	C8-N9-C4	6.29	108.92	106.40
8	A	2004	G	C2-N3-C4	-6.29	108.76	111.90
34	a	326	G	N3-C4-N9	-6.29	122.23	126.00
8	A	1740	G	N3-C4-C5	6.29	131.74	128.60
8	A	1765	U	C6-N1-C2	6.29	124.77	121.00
9	B	100	G	N3-C4-C5	6.29	131.74	128.60
34	a	1134	G	N9-C4-C5	6.29	107.91	105.40
9	B	119	A	N9-C4-C5	-6.28	103.29	105.80
8	A	361	G	C5-C6-O6	-6.28	124.83	128.60
34	a	886	G	C8-N9-C4	6.28	108.91	106.40
8	A	1572	A	C5-C6-N6	-6.28	118.68	123.70
34	a	1043	G	C4-N9-C1'	-6.28	118.34	126.50
8	A	1600	C	C6-N1-C2	6.28	122.81	120.30
34	a	97	G	N3-C4-N9	-6.28	122.23	126.00
34	a	675	A	C5-N7-C8	-6.28	100.76	103.90
8	A	1863	G	C8-N9-C4	6.28	108.91	106.40
8	A	262	A	C8-N9-C4	6.27	108.31	105.80
8	A	1885	A	C8-N9-C4	6.27	108.31	105.80
8	A	2489	U	O4'-C1'-N1	-6.27	103.19	108.20
34	a	451	A	C8-N9-C4	6.27	108.31	105.80
8	A	22	C	C6-N1-C2	6.27	122.81	120.30
8	A	253	C	C6-N1-C2	6.27	122.81	120.30
8	A	570	G	C8-N9-C1'	-6.27	118.85	127.00
8	A	2505	G	C8-N9-C1'	-6.27	118.85	127.00
34	a	442	G	N1-C2-N2	-6.27	110.56	116.20
34	a	1294	G	N9-C4-C5	-6.27	102.89	105.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	w	53	G	C2-N3-C4	-6.27	108.77	111.90
8	A	764	A	N1-C6-N6	-6.26	114.84	118.60
8	A	936	A	C4-C5-N7	6.26	113.83	110.70
8	A	96	C	C6-N1-C2	6.26	122.81	120.30
8	A	2840	C	N3-C4-C5	6.26	124.41	121.90
34	a	847	G	N3-C4-C5	6.26	131.73	128.60
8	A	204	A	N1-C6-N6	6.26	122.36	118.60
34	a	167	A	N9-C4-C5	-6.26	103.30	105.80
34	a	260	G	N3-C4-N9	-6.26	122.24	126.00
8	A	1473	G	N3-C4-C5	6.26	131.73	128.60
34	a	623	C	N3-C4-C5	6.26	124.40	121.90
8	A	2091	C	N3-C4-N4	-6.26	113.62	118.00
8	A	98	G	N3-C4-N9	-6.26	122.25	126.00
8	A	1092	C	N3-C4-C5	6.26	124.40	121.90
8	A	2857	G	C4-N9-C1'	-6.26	118.37	126.50
9	B	44	G	N3-C4-C5	6.26	131.73	128.60
9	B	42	C	C6-N1-C2	6.25	122.80	120.30
8	A	923	G	C8-N9-C4	6.25	108.90	106.40
8	A	1036	G	C2-N3-C4	-6.25	108.77	111.90
8	A	1459	G	N3-C4-C5	6.25	131.73	128.60
8	A	2430	A	C4-C5-N7	6.25	113.83	110.70
34	a	450	G	N3-C4-N9	-6.25	122.25	126.00
34	a	685	G	N3-C4-C5	6.25	131.73	128.60
8	A	1323	C	N3-C4-C5	6.25	124.40	121.90
8	A	1867	G	C8-N9-C4	6.25	108.90	106.40
8	A	570	G	C6-C5-N7	-6.25	126.65	130.40
34	a	500	G	N3-C4-C5	6.25	131.72	128.60
8	A	2516	A	C5-N7-C8	-6.25	100.78	103.90
8	A	302	C	C6-N1-C2	6.24	122.80	120.30
8	A	1086	A	N7-C8-N9	6.24	116.92	113.80
8	A	1410	G	N3-C4-C5	6.24	131.72	128.60
8	A	2082	A	C8-N9-C4	6.24	108.30	105.80
34	a	695	A	N9-C1'-C2'	-6.24	105.14	112.00
34	a	1329	A	C8-N9-C4	6.24	108.30	105.80
9	B	99	A	N1-C6-N6	6.24	122.34	118.60
34	a	1134	G	C6-C5-N7	6.24	134.14	130.40
34	a	1371	G	C2-N3-C4	-6.24	108.78	111.90
8	A	696	G	N3-C4-N9	-6.24	122.26	126.00
8	A	2308	G	N3-C4-C5	6.24	131.72	128.60
34	a	474	G	N3-C4-N9	-6.24	122.26	126.00
8	A	704	G	C8-N9-C1'	6.23	135.10	127.00
8	A	1479	G	C2-N3-C4	-6.23	108.78	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	a	492	C	N1-C2-O2	-6.23	115.16	118.90
8	A	690	G	N3-C4-N9	-6.23	122.26	126.00
8	A	726	G	N3-C4-C5	6.23	131.72	128.60
34	a	1041	G	N3-C4-C5	6.23	131.72	128.60
8	A	2180	U	O4'-C1'-N1	-6.23	103.22	108.20
8	A	634	C	C6-N1-C2	6.23	122.79	120.30
34	a	1348	U	C5-C4-O4	-6.23	122.16	125.90
34	a	947	G	C2-N3-C4	-6.23	108.79	111.90
34	a	1422	G	N9-C4-C5	-6.23	102.91	105.40
8	A	43	G	N3-C4-C5	6.22	131.71	128.60
8	A	1922	G	N3-C4-N9	-6.22	122.27	126.00
34	a	1497	G	N3-C4-N9	-6.22	122.27	126.00
8	A	1891	G	C8-N9-C4	6.22	108.89	106.40
34	a	1057	G	N3-C4-C5	6.22	131.71	128.60
8	A	144	A	C8-N9-C4	6.22	108.29	105.80
34	a	1197	A	N9-C4-C5	-6.22	103.31	105.80
8	A	778	G	N3-C4-N9	-6.22	122.27	126.00
8	A	1388	G	C2-N3-C4	-6.22	108.79	111.90
8	A	471	A	N1-C6-N6	6.22	122.33	118.60
8	A	1684	G	C2-N3-C4	-6.22	108.79	111.90
8	A	1036	G	C8-N9-C4	6.22	108.89	106.40
8	A	1823	G	N3-C4-C5	6.22	131.71	128.60
34	a	982	U	C5-C4-O4	-6.22	122.17	125.90
8	A	146	A	C4-C5-N7	6.21	113.81	110.70
8	A	1029	A	C5-N7-C8	-6.21	100.79	103.90
8	A	1055	G	C8-N9-C1'	6.21	135.08	127.00
8	A	1906	G	C2-N3-C4	-6.21	108.79	111.90
8	A	2083	G	N1-C2-N2	-6.21	110.61	116.20
8	A	1077	A	N1-C6-N6	6.21	122.33	118.60
8	A	2685	G	C2-N3-C4	-6.21	108.80	111.90
8	A	371	A	N9-C4-C5	-6.21	103.32	105.80
8	A	2553	G	N3-C4-C5	6.21	131.70	128.60
34	a	540	G	N3-C4-C5	6.21	131.70	128.60
34	a	318	G	N3-C4-C5	6.20	131.70	128.60
34	a	1286	U	N1-C1'-C2'	-6.20	105.18	112.00
55	v	29	G	N3-C4-C5	6.20	131.70	128.60
34	a	509	A	N1-C6-N6	6.20	122.32	118.60
8	A	629	G	C4-N9-C1'	-6.20	118.44	126.50
34	a	495	A	N9-C4-C5	-6.20	103.32	105.80
34	a	1016	A	C5-C6-N6	-6.20	118.74	123.70
8	A	2846	G	C2-N3-C4	-6.20	108.80	111.90
8	A	726	G	N3-C4-N9	-6.20	122.28	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	1567	G	N3-C4-C5	6.20	131.70	128.60
8	A	2679	A	C8-N9-C4	6.20	108.28	105.80
34	a	1088	G	N9-C4-C5	6.20	107.88	105.40
8	A	402	A	C5-C6-N6	-6.19	118.75	123.70
8	A	749	A	N1-C6-N6	-6.19	114.88	118.60
55	v	28	C	C6-N1-C2	6.19	122.78	120.30
8	A	14	A	C4-C5-N7	6.19	113.80	110.70
8	A	1107	G	N3-C4-C5	6.19	131.70	128.60
8	A	1588	G	N3-C4-N9	-6.19	122.28	126.00
34	a	176	C	C6-N1-C2	6.19	122.78	120.30
34	a	661	G	N9-C4-C5	-6.19	102.92	105.40
8	A	409	G	N3-C4-C5	6.19	131.70	128.60
8	A	537	G	N3-C4-C5	6.19	131.69	128.60
8	A	1920	C	N3-C4-C5	6.19	124.38	121.90
8	A	2763	G	C2-N3-C4	-6.19	108.81	111.90
34	a	145	G	N3-C2-N2	-6.19	115.57	119.90
8	A	461	C	N3-C4-C5	6.19	124.38	121.90
34	a	1154	G	C2-N3-C4	-6.19	108.81	111.90
8	A	1435	G	C2-N3-C4	-6.19	108.81	111.90
8	A	2003	A	C8-N9-C4	6.19	108.28	105.80
8	A	2400	G	N3-C4-C5	6.18	131.69	128.60
34	a	488	C	O4'-C1'-N1	-6.18	103.25	108.20
34	a	947	G	N3-C4-C5	6.18	131.69	128.60
8	A	56	A	N9-C4-C5	-6.18	103.33	105.80
8	A	298	G	C8-N9-C4	6.18	108.87	106.40
8	A	992	C	C6-N1-C2	6.18	122.77	120.30
8	A	1977	A	C8-N9-C4	6.18	108.27	105.80
8	A	2640	G	C2-N3-C4	-6.18	108.81	111.90
34	a	1112	C	N3-C4-C5	6.18	124.37	121.90
8	A	1735	A	C8-N9-C4	6.18	108.27	105.80
8	A	2015	A	O4'-C1'-N9	-6.18	103.25	108.20
34	a	454	G	C2-N3-C4	-6.18	108.81	111.90
34	a	851	G	N3-C4-C5	6.18	131.69	128.60
8	A	675	A	C5-N7-C8	-6.18	100.81	103.90
8	A	891	G	N3-C4-C5	6.18	131.69	128.60
8	A	1503	A	C8-N9-C4	6.18	108.27	105.80
8	A	2694	G	C2-N3-C4	-6.18	108.81	111.90
34	a	724	G	C8-N9-C4	6.18	108.87	106.40
8	A	1731	G	N3-C4-C5	6.18	131.69	128.60
9	B	28	C	C6-N1-C2	6.18	122.77	120.30
34	a	1221	G	C2-N3-C4	-6.18	108.81	111.90
8	A	1292	G	C2-N3-C4	-6.17	108.81	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	119	A	C4-C5-C6	-6.17	113.91	117.00
34	a	1099	G	N3-C4-C5	6.17	131.69	128.60
8	A	183	C	C6-N1-C2	6.17	122.77	120.30
34	a	748	G	C2-N3-C4	-6.17	108.81	111.90
34	a	760	G	C2-N3-C4	-6.17	108.81	111.90
34	a	1429	A	N9-C4-C5	-6.17	103.33	105.80
8	A	2154	A	C5-N7-C8	-6.17	100.82	103.90
9	B	99	A	C5-C6-N6	-6.17	118.77	123.70
55	v	12	G	C8-N9-C4	6.17	108.87	106.40
8	A	1653	G	N3-C4-C5	6.17	131.68	128.60
34	a	627	G	C8-N9-C4	6.17	108.87	106.40
34	a	800	G	N3-C4-N9	-6.17	122.30	126.00
8	A	2148	G	C2-N3-C4	-6.17	108.82	111.90
34	a	98	A	C2-N3-C4	-6.17	107.52	110.60
8	A	1124	G	N3-C4-C5	6.16	131.68	128.60
8	A	1807	G	N3-C2-N2	-6.16	115.58	119.90
55	v	42	G	N3-C4-C5	6.16	131.68	128.60
8	A	1016	G	C2-N3-C4	-6.16	108.82	111.90
8	A	1639	C	N3-C4-C5	6.16	124.36	121.90
8	A	2610	C	N3-C4-C5	6.16	124.36	121.90
34	a	302	G	N3-C4-N9	-6.16	122.30	126.00
34	a	1150	A	C8-N9-C4	-6.16	103.34	105.80
34	a	1439	G	C2-N3-C4	-6.16	108.82	111.90
8	A	1842	G	C2-N3-C4	-6.16	108.82	111.90
8	A	732	C	C6-N1-C2	6.16	122.76	120.30
8	A	1674	G	C8-N9-C4	6.16	108.86	106.40
8	A	1826	G	N3-C4-N9	-6.16	122.31	126.00
34	a	1186	G	N3-C4-C5	6.16	131.68	128.60
8	A	301	G	C2-N3-C4	-6.15	108.82	111.90
34	a	1289	A	N9-C4-C5	-6.15	103.34	105.80
8	A	24	G	N3-C4-N9	-6.15	122.31	126.00
8	A	325	G	C8-N9-C4	6.15	108.86	106.40
8	A	2332	C	N3-C4-N4	-6.15	113.69	118.00
34	a	1253	G	C6-C5-N7	6.15	134.09	130.40
34	a	1328	C	C6-N1-C2	6.15	122.76	120.30
34	a	1426	G	C2-N3-C4	-6.15	108.83	111.90
8	A	488	G	N3-C4-N9	-6.15	122.31	126.00
8	A	2304	G	N3-C4-C5	6.15	131.67	128.60
34	a	1379	G	N3-C4-C5	6.15	131.67	128.60
34	a	259	G	C2-N3-C4	-6.15	108.83	111.90
34	a	540	G	C2-N3-C4	-6.15	108.83	111.90
9	B	88	C	O4'-C1'-N1	-6.15	103.28	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	a	487	A	N9-C4-C5	-6.15	103.34	105.80
8	A	20	C	N3-C4-C5	6.14	124.36	121.90
8	A	42	A	C4-C5-C6	-6.14	113.93	117.00
8	A	956	G	C8-N9-C4	6.14	108.86	106.40
8	A	2160	C	O4'-C1'-N1	-6.14	103.29	108.20
8	A	2628	C	C6-N1-C2	6.14	122.76	120.30
9	B	37	C	C5-C4-N4	6.14	124.50	120.20
34	a	101	A	N3-C4-C5	6.14	131.10	126.80
34	a	217	C	N3-C2-O2	-6.14	117.60	121.90
8	A	867	C	N3-C4-N4	-6.14	113.70	118.00
34	a	190	A	N9-C4-C5	-6.14	103.34	105.80
8	A	856	G	C2-N3-C4	-6.14	108.83	111.90
8	A	2544	G	C2-N3-C4	-6.14	108.83	111.90
8	A	977	G	N3-C4-N9	-6.13	122.32	126.00
8	A	482	A	N3-C4-C5	6.13	131.09	126.80
8	A	659	G	N1-C2-N2	-6.13	110.68	116.20
8	A	2238	G	O4'-C1'-N9	6.13	113.11	108.20
34	a	903	G	C2-N3-C4	-6.13	108.83	111.90
8	A	1565	C	C6-N1-C2	6.13	122.75	120.30
8	A	2678	C	C6-N1-C2	6.13	122.75	120.30
34	a	541	G	N3-C4-N9	-6.13	122.32	126.00
8	A	2485	G	C2-N3-C4	-6.13	108.83	111.90
8	A	2895	G	C2-N3-C4	-6.13	108.83	111.90
34	a	626	G	C8-N9-C4	6.13	108.85	106.40
8	A	66	C	C6-N1-C2	6.13	122.75	120.30
8	A	106	C	C6-N1-C2	6.13	122.75	120.30
34	a	769	G	N3-C4-C5	6.13	131.66	128.60
34	a	1314	C	N3-C4-C5	6.13	124.35	121.90
56	w	51	C	C6-N1-C2	6.13	122.75	120.30
8	A	2814	A	C8-N9-C4	6.13	108.25	105.80
9	B	54	G	C5-C6-O6	6.13	132.28	128.60
8	A	907	G	C2-N3-C4	-6.12	108.84	111.90
8	A	1403	A	C8-N9-C4	6.12	108.25	105.80
8	A	1048	A	C5-C6-N6	-6.12	118.80	123.70
8	A	1092	C	N3-C4-N4	-6.12	113.71	118.00
8	A	1681	G	N3-C4-N9	-6.12	122.33	126.00
34	a	635	A	C4-C5-N7	6.12	113.76	110.70
34	a	849	G	C2-N3-C4	-6.12	108.84	111.90
8	A	217	A	N3-C4-C5	6.12	131.08	126.80
8	A	1154	G	N9-C4-C5	-6.12	102.95	105.40
34	a	1374	A	C8-N9-C4	6.12	108.25	105.80
34	a	1072	G	C2-N3-C4	-6.11	108.84	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	a	1106	G	N3-C4-C5	6.11	131.66	128.60
34	a	1293	C	N3-C4-C5	6.11	124.34	121.90
8	A	2525	G	C4-C5-C6	-6.11	115.13	118.80
8	A	2828	G	N1-C2-N2	-6.11	110.70	116.20
34	a	1155	A	C8-N9-C4	6.11	108.24	105.80
8	A	239	C	C6-N1-C2	6.11	122.74	120.30
8	A	289	G	C8-N9-C1'	6.11	134.94	127.00
34	a	236	A	C4-C5-N7	6.11	113.75	110.70
55	v	64	G	C2-N3-C4	-6.11	108.85	111.90
8	A	80	G	C8-N9-C4	6.11	108.84	106.40
34	a	1431	A	N1-C6-N6	6.11	122.26	118.60
8	A	960	A	C5-C6-N6	-6.10	118.82	123.70
8	A	455	C	C6-N1-C2	6.10	122.74	120.30
8	A	359	G	N3-C2-N2	-6.10	115.63	119.90
8	A	2775	G	C8-N9-C4	6.10	108.84	106.40
34	a	632	U	O4'-C1'-N1	-6.10	103.32	108.20
34	a	885	G	C8-N9-C4	6.10	108.84	106.40
8	A	510	C	N1-C2-O2	6.10	122.56	118.90
8	A	1811	G	C8-N9-C4	6.10	108.84	106.40
8	A	1905	C	C2-N3-C4	-6.10	116.85	119.90
8	A	2418	A	C8-N9-C4	6.10	108.24	105.80
52	s	46	LEU	CA-CB-CG	-6.10	101.28	115.30
8	A	778	G	C2-N3-C4	-6.10	108.85	111.90
8	A	2022	U	O4'-C1'-N1	-6.10	103.32	108.20
9	B	9	G	N9-C4-C5	-6.10	102.96	105.40
8	A	230	G	C2-N3-C4	-6.09	108.85	111.90
8	A	1945	G	N3-C4-C5	6.09	131.65	128.60
34	a	424	G	C2-N3-C4	-6.09	108.85	111.90
34	a	432	A	N1-C6-N6	6.09	122.26	118.60
8	A	925	A	N9-C4-C5	-6.09	103.36	105.80
8	A	1868	C	C6-N1-C2	6.09	122.74	120.30
34	a	203	G	C8-N9-C1'	6.09	134.92	127.00
8	A	2137	U	C4-C5-C6	-6.09	116.05	119.70
8	A	1042	G	C2-N3-C4	-6.09	108.86	111.90
8	A	1606	C	N3-C4-C5	6.09	124.33	121.90
34	a	1198	G	N3-C4-N9	-6.09	122.35	126.00
9	B	37	C	C2-N1-C1'	-6.08	112.11	118.80
9	B	61	G	N1-C2-N2	-6.08	110.72	116.20
34	a	50	A	C8-N9-C4	6.08	108.23	105.80
34	a	733	G	C2-N3-C4	-6.08	108.86	111.90
8	A	1961	C	C6-N1-C2	6.08	122.73	120.30
34	a	1143	G	C4-C5-N7	6.08	113.23	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	a	755	G	N3-C4-C5	6.08	131.64	128.60
34	a	930	C	C6-N1-C2	6.08	122.73	120.30
8	A	954	G	N3-C4-C5	6.08	131.64	128.60
8	A	2744	G	C2-N3-C4	-6.08	108.86	111.90
8	A	191	A	C5-C6-N6	-6.08	118.84	123.70
8	A	465	G	N3-C4-C5	6.08	131.64	128.60
8	A	1347	A	C8-N9-C4	6.08	108.23	105.80
8	A	2040	G	C2-N3-C4	-6.08	108.86	111.90
34	a	581	G	N3-C4-C5	6.08	131.64	128.60
8	A	897	C	N1-C2-O2	6.07	122.54	118.90
9	B	20	G	C2-N3-C4	-6.07	108.86	111.90
34	a	1347	G	C8-N9-C4	6.07	108.83	106.40
8	A	495	G	N3-C4-C5	6.07	131.64	128.60
8	A	1528	A	C5-C6-N6	-6.07	118.84	123.70
8	A	1225	G	N3-C4-N9	-6.07	122.36	126.00
8	A	1356	G	C2-N3-C4	-6.07	108.87	111.90
8	A	1781	U	C6-N1-C2	6.07	124.64	121.00
34	a	568	G	N3-C4-C5	6.07	131.63	128.60
8	A	1357	C	C6-N1-C2	6.07	122.73	120.30
8	A	1767	G	C8-N9-C4	6.07	108.83	106.40
8	A	2014	A	O5'-P-OP1	-6.07	100.24	105.70
8	A	2239	G	C2-N3-C4	-6.07	108.87	111.90
34	a	341	C	C6-N1-C2	6.07	122.73	120.30
34	a	679	C	C6-N1-C2	6.07	122.73	120.30
8	A	9	G	N3-C4-C5	6.06	131.63	128.60
34	a	495	A	C8-N9-C4	6.06	108.23	105.80
8	A	1026	G	C8-N9-C1'	-6.06	119.12	127.00
34	a	1305	G	C2-N3-C4	-6.06	108.87	111.90
8	A	996	A	N9-C4-C5	-6.06	103.38	105.80
8	A	347	A	C8-N9-C4	6.06	108.22	105.80
34	a	1405	G	C8-N9-C1'	6.06	134.87	127.00
9	B	23	G	O4'-C1'-N9	-6.06	103.36	108.20
8	A	455	C	C5-C4-N4	6.05	124.44	120.20
8	A	1334	G	N3-C4-C5	6.05	131.63	128.60
34	a	92	U	O4'-C1'-N1	-6.05	103.36	108.20
8	A	1521	G	N3-C4-C5	6.05	131.63	128.60
8	A	555	G	N3-C4-N9	-6.05	122.37	126.00
8	A	808	G	C8-N9-C4	6.05	108.82	106.40
8	A	1734	G	C2-N3-C4	-6.05	108.88	111.90
8	A	88	G	N9-C4-C5	-6.05	102.98	105.40
8	A	1477	A	C5-C6-N6	-6.04	118.86	123.70
8	A	2414	G	C8-N9-C1'	6.04	134.86	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	a	386	C	N1-C2-O2	6.04	122.53	118.90
34	a	602	A	C5-N7-C8	-6.04	100.88	103.90
8	A	536	G	N3-C2-N2	-6.04	115.67	119.90
34	a	600	A	N9-C4-C5	-6.04	103.38	105.80
55	v	52	G	N3-C4-N9	-6.04	122.38	126.00
8	A	270	A	O4'-C1'-N9	6.04	113.03	108.20
8	A	1194	A	C8-N9-C4	6.04	108.22	105.80
8	A	180	G	C2-N3-C4	-6.04	108.88	111.90
8	A	1422	G	N3-C4-C5	6.04	131.62	128.60
8	A	1512	C	N3-C4-N4	-6.04	113.77	118.00
8	A	1591	A	C4-C5-N7	6.04	113.72	110.70
8	A	2100	G	C2-N3-C4	-6.04	108.88	111.90
8	A	2381	A	C2'-C3'-O3'	6.04	123.36	113.70
34	a	413	G	C8-N9-C4	6.04	108.81	106.40
34	a	449	G	N3-C4-C5	6.04	131.62	128.60
8	A	843	G	C4-C5-C6	-6.04	115.18	118.80
8	A	751	A	C8-N9-C4	6.04	108.21	105.80
34	a	786	G	N3-C4-N9	-6.04	122.38	126.00
8	A	469	G	C6-C5-N7	-6.03	126.78	130.40
8	A	671	C	N3-C4-C5	6.03	124.31	121.90
8	A	1840	G	C2-N3-C4	-6.03	108.88	111.90
8	A	2395	C	N3-C4-C5	6.03	124.31	121.90
34	a	442	G	C2-N3-C4	-6.03	108.88	111.90
34	a	1350	A	C8-N9-C4	6.03	108.21	105.80
8	A	1797	G	C2-N3-C4	-6.03	108.88	111.90
8	A	2154	A	C6-C5-N7	-6.03	128.08	132.30
8	A	2840	C	C4-C5-C6	-6.03	114.38	117.40
34	a	691	G	C8-N9-C1'	6.03	134.84	127.00
8	A	1133	A	O4'-C1'-N9	6.03	113.02	108.20
34	a	433	G	C2-N3-C4	-6.03	108.89	111.90
34	a	803	G	C2-N3-C4	-6.03	108.89	111.90
8	A	2050	C	N3-C2-O2	-6.03	117.68	121.90
34	a	1331	G	N3-C4-N9	-6.03	122.38	126.00
34	a	1459	G	N3-C4-N9	-6.03	122.38	126.00
8	A	469	G	C2-N3-C4	-6.03	108.89	111.90
8	A	538	A	C8-N9-C4	6.03	108.21	105.80
8	A	1382	G	C2-N3-C4	-6.03	108.89	111.90
34	a	101	A	N3-C4-N9	-6.03	122.58	127.40
8	A	997	G	N3-C4-N9	-6.02	122.39	126.00
34	a	178	C	C6-N1-C2	-6.02	117.89	120.30
34	a	443	C	O4'-C1'-N1	-6.02	103.38	108.20
34	a	1465	A	C8-N9-C4	6.02	108.21	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	1532	A	N9-C4-C5	-6.02	103.39	105.80
34	a	350	G	C2-N3-C4	-6.02	108.89	111.90
8	A	1689	A	C8-N9-C4	6.02	108.21	105.80
9	B	84	G	C8-N9-C4	6.02	108.81	106.40
8	A	1972	G	C5'-C4'-O4'	6.02	116.32	109.10
8	A	2097	A	C4-C5-N7	6.02	113.71	110.70
8	A	2729	G	C2-N3-C4	-6.02	108.89	111.90
31	X	70	LEU	CA-CB-CG	-6.02	101.46	115.30
34	a	988	G	C8-N9-C4	6.02	108.81	106.40
34	a	1102	A	C8-N9-C4	6.02	108.21	105.80
8	A	214	G	N3-C4-N9	-6.01	122.39	126.00
8	A	361	G	C6-C5-N7	-6.01	126.79	130.40
8	A	1047	G	C6-C5-N7	6.01	134.01	130.40
34	a	841	C	N1-C1'-C2'	-6.01	105.38	112.00
8	A	2464	G	N3-C4-C5	6.01	131.61	128.60
34	a	538	G	N3-C4-C5	6.01	131.61	128.60
34	a	1182	G	N3-C4-N9	-6.01	122.39	126.00
8	A	245	G	C8-N9-C4	6.01	108.80	106.40
8	A	1836	C	N3-C4-N4	-6.01	113.79	118.00
8	A	2729	G	C4-C5-N7	6.01	113.20	110.80
8	A	2816	G	C8-N9-C4	6.01	108.81	106.40
9	B	73	A	N1-C6-N6	6.01	122.21	118.60
55	v	41	C	N3-C4-C5	6.01	124.31	121.90
8	A	820	A	C8-N9-C4	6.01	108.20	105.80
8	A	2876	G	C2-N3-C4	-6.01	108.90	111.90
8	A	63	A	C2-N3-C4	-6.01	107.60	110.60
8	A	2574	G	C2-N3-C4	-6.01	108.90	111.90
8	A	1590	A	C8-N9-C4	6.00	108.20	105.80
8	A	1904	G	N3-C4-N9	-6.00	122.40	126.00
34	a	1334	G	C4-N9-C1'	-6.00	118.70	126.50
34	a	8	A	C8-N9-C4	6.00	108.20	105.80
34	a	586	C	N3-C4-N4	-6.00	113.80	118.00
34	a	639	G	N9-C4-C5	-6.00	103.00	105.40
8	A	2830	C	C6-N1-C1'	-6.00	113.60	120.80
8	A	39	G	C2-N3-C4	-6.00	108.90	111.90
34	a	623	C	C6-N1-C1'	-6.00	113.60	120.80
34	a	1263	C	C6-N1-C2	6.00	122.70	120.30
8	A	77	G	N3-C4-C5	6.00	131.60	128.60
8	A	377	G	C2-N3-C4	-6.00	108.90	111.90
34	a	190	A	C6-C5-N7	-6.00	128.10	132.30
8	A	660	C	N3-C4-C5	6.00	124.30	121.90
8	A	126	A	C5-C6-N6	-5.99	118.91	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	426	C	C6-N1-C2	5.99	122.70	120.30
8	A	2834	G	N3-C4-N9	-5.99	122.41	126.00
34	a	42	G	C5-N7-C8	-5.99	101.30	104.30
34	a	1	A	C5-N7-C8	-5.99	100.91	103.90
34	a	79	G	N3-C4-N9	-5.99	122.41	126.00
34	a	921	U	N3-C2-O2	-5.99	118.01	122.20
34	a	1048	G	N9-C4-C5	-5.99	103.00	105.40
8	A	2394	C	O5'-P-OP1	-5.99	100.31	105.70
8	A	2735	G	N3-C4-C5	5.99	131.59	128.60
34	a	656	G	C4-N9-C1'	-5.99	118.72	126.50
34	a	933	G	N3-C4-C5	5.99	131.59	128.60
34	a	1509	C	N3-C4-N4	-5.99	113.81	118.00
8	A	1166	G	N1-C2-N2	-5.99	110.81	116.20
8	A	2516	A	C4-C5-N7	5.99	113.69	110.70
34	a	783	C	C6-N1-C2	5.99	122.69	120.30
34	a	1119	C	C6-N1-C2	5.99	122.69	120.30
34	a	1483	A	N9-C4-C5	-5.99	103.41	105.80
8	A	1401	G	N3-C4-N9	-5.98	122.41	126.00
8	A	1492	G	C2-N3-C4	-5.98	108.91	111.90
8	A	58	G	N3-C4-C5	5.98	131.59	128.60
8	A	1228	G	C2-N3-C4	-5.98	108.91	111.90
8	A	1368	G	N3-C4-C5	5.98	131.59	128.60
9	B	73	A	C5-C6-N6	-5.98	118.92	123.70
13	F	132	ARG	CA-CB-CG	-5.98	100.24	113.40
34	a	246	A	C2-N3-C4	-5.98	107.61	110.60
34	a	637	C	N3-C4-C5	5.98	124.29	121.90
8	A	330	A	C5-C6-N1	5.98	120.69	117.70
8	A	1567	G	C8-N9-C4	5.98	108.79	106.40
8	A	2316	G	N3-C4-N9	-5.98	122.41	126.00
34	a	917	G	N3-C4-N9	-5.98	122.41	126.00
8	A	1760	C	C6-N1-C2	5.98	122.69	120.30
8	A	2729	G	C5-N7-C8	-5.98	101.31	104.30
8	A	2812	G	C2-N3-C4	-5.98	108.91	111.90
8	A	2642	G	N3-C4-C5	5.98	131.59	128.60
34	a	1081	A	C8-N9-C4	-5.98	103.41	105.80
8	A	2901	C	N3-C4-C5	5.97	124.29	121.90
9	B	102	G	N3-C4-N9	-5.97	122.42	126.00
8	A	1378	A	C5-N7-C8	-5.97	100.91	103.90
8	A	1210	G	N3-C4-C5	5.97	131.59	128.60
8	A	2551	C	N3-C4-C5	5.97	124.29	121.90
8	A	425	G	N3-C4-N9	-5.97	122.42	126.00
8	A	1047	G	C4-N9-C1'	-5.97	118.74	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	a	754	C	C2-N3-C4	5.97	122.89	119.90
34	a	902	G	N3-C4-C5	5.97	131.59	128.60
34	a	947	G	C5-N7-C8	-5.97	101.31	104.30
34	a	1217	C	C6-N1-C2	5.97	122.69	120.30
8	A	1028	A	C8-N9-C4	5.97	108.19	105.80
8	A	1358	G	C4-C5-N7	5.97	113.19	110.80
8	A	1750	G	C2-N3-C4	-5.97	108.92	111.90
8	A	2683	C	C5-C4-N4	5.97	124.38	120.20
8	A	375	G	C8-N9-C4	5.96	108.78	106.40
8	A	1548	A	N9-C4-C5	-5.96	103.41	105.80
8	A	1661	G	C2-N3-C4	-5.96	108.92	111.90
8	A	2050	C	N3-C4-N4	-5.96	113.83	118.00
28	U	46	LYS	CD-CE-NZ	-5.96	97.98	111.70
34	a	297	G	N3-C4-N9	-5.96	122.42	126.00
8	A	1048	A	N9-C4-C5	-5.96	103.42	105.80
9	B	56	G	C4-C5-N7	5.96	113.19	110.80
34	a	497	G	N3-C4-C5	5.96	131.58	128.60
8	A	1906	G	C5-C6-O6	5.96	132.18	128.60
34	a	1238	A	C5-C6-N6	-5.96	118.93	123.70
8	A	21	A	C8-N9-C4	5.96	108.18	105.80
8	A	57	C	C6-N1-C2	5.96	122.68	120.30
8	A	1168	G	N3-C4-C5	5.96	131.58	128.60
8	A	2294	G	C8-N9-C4	5.96	108.78	106.40
34	a	585	G	C2-N3-C4	-5.96	108.92	111.90
8	A	1384	A	N1-C6-N6	5.96	122.17	118.60
34	a	79	G	C8-N9-C4	5.96	108.78	106.40
8	A	1515	A	C5-C6-N6	-5.96	118.94	123.70
8	A	1862	G	N1-C2-N2	-5.96	110.84	116.20
9	B	23	G	N3-C4-N9	-5.96	122.43	126.00
8	A	134	G	C2-N3-C4	-5.95	108.92	111.90
9	B	85	G	N3-C4-C5	5.95	131.58	128.60
34	a	1329	A	C4-N9-C1'	-5.95	115.58	126.30
8	A	2040	G	N3-C4-N9	-5.95	122.43	126.00
8	A	900	A	C5-N7-C8	-5.95	100.92	103.90
8	A	1593	A	C4-C5-N7	5.95	113.67	110.70
8	A	2496	C	C6-N1-C1'	-5.95	113.66	120.80
27	T	66	LYS	CD-CE-NZ	5.95	125.39	111.70
34	a	1034	G	N3-C2-N2	-5.95	115.73	119.90
8	A	1382	G	N3-C4-N9	-5.95	122.43	126.00
9	B	112	G	N3-C4-N9	-5.95	122.43	126.00
34	a	509	A	O4'-C1'-N9	5.95	112.96	108.20
34	a	1088	G	N1-C6-O6	-5.95	116.33	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	a	1098	C	N1-C2-N3	5.95	123.36	119.20
8	A	1422	G	C2-N3-C4	-5.95	108.93	111.90
8	A	2339	C	N3-C4-C5	5.95	124.28	121.90
34	a	988	G	C2-N3-C4	-5.95	108.93	111.90
34	a	1028	C	O4'-C1'-N1	-5.95	103.44	108.20
8	A	175	G	C2-N3-C4	-5.94	108.93	111.90
8	A	1726	C	N3-C4-C5	5.94	124.28	121.90
8	A	2092	U	C5-C4-O4	-5.94	122.33	125.90
8	A	2808	G	N3-C4-C5	5.94	131.57	128.60
34	a	724	G	N3-C4-C5	5.94	131.57	128.60
34	a	809	G	C4-N9-C1'	-5.94	118.77	126.50
8	A	425	G	C2-N3-C4	-5.94	108.93	111.90
8	A	704	G	C8-N9-C4	5.94	108.78	106.40
8	A	2557	G	N1-C6-O6	-5.94	116.33	119.90
34	a	542	G	C2-N3-C4	-5.94	108.93	111.90
34	a	1328	C	N3-C4-C5	5.94	124.28	121.90
56	w	6	G	C2-N3-C4	-5.94	108.93	111.90
8	A	2664	G	N3-C4-C5	5.94	131.57	128.60
34	a	274	A	N9-C4-C5	-5.94	103.42	105.80
8	A	61	C	C6-N1-C2	5.93	122.67	120.30
8	A	402	A	N1-C6-N6	5.93	122.16	118.60
8	A	1969	A	N1-C6-N6	5.93	122.16	118.60
8	A	289	G	C4-N9-C1'	-5.93	118.79	126.50
8	A	728	G	N3-C4-N9	-5.93	122.44	126.00
8	A	2256	G	N3-C4-C5	5.93	131.56	128.60
8	A	340	A	C4-C5-N7	5.93	113.66	110.70
34	a	796	C	C6-N1-C2	5.93	122.67	120.30
34	a	838	G	C2-N3-C4	-5.93	108.94	111.90
8	A	364	C	N1-C2-O2	5.93	122.46	118.90
34	a	654	G	N9-C4-C5	-5.93	103.03	105.40
34	a	725	G	N3-C4-C5	5.93	131.56	128.60
8	A	2508	G	N3-C4-C5	5.92	131.56	128.60
8	A	2524	G	N3-C4-N9	-5.92	122.45	126.00
34	a	928	G	N3-C4-N9	-5.92	122.44	126.00
55	v	30	G	N3-C4-C5	5.92	131.56	128.60
8	A	2616	C	C6-N1-C2	5.92	122.67	120.30
34	a	257	G	C2-N3-C4	-5.92	108.94	111.90
34	a	1309	G	N9-C4-C5	-5.92	103.03	105.40
9	B	52	A	N9-C4-C5	-5.92	103.43	105.80
34	a	360	G	N3-C4-N9	-5.92	122.45	126.00
8	A	506	G	C8-N9-C1'	5.92	134.69	127.00
8	A	899	A	C8-N9-C4	5.92	108.17	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	2739	U	C2-N1-C1'	-5.92	110.60	117.70
8	A	2775	G	N3-C4-N9	-5.92	122.45	126.00
56	w	16	U	C5'-C4'-O4'	5.92	116.20	109.10
8	A	103	A	N9-C4-C5	-5.92	103.43	105.80
8	A	1544	A	N9-C4-C5	-5.92	103.43	105.80
8	A	1907	G	C8-N9-C4	5.92	108.77	106.40
8	A	2369	A	C2-N3-C4	-5.92	107.64	110.60
8	A	945	A	N1-C6-N6	5.92	122.15	118.60
8	A	1387	A	C4-C5-N7	5.92	113.66	110.70
8	A	307	G	C4-N9-C1'	-5.91	118.81	126.50
8	A	831	G	C4-N9-C1'	-5.91	118.81	126.50
8	A	1374	G	C8-N9-C4	5.91	108.77	106.40
8	A	2196	C	C6-N1-C2	5.91	122.67	120.30
8	A	2864	G	C4-C5-N7	5.91	113.17	110.80
34	a	1002	G	N3-C4-C5	5.91	131.56	128.60
8	A	2190	G	O4'-C1'-N9	-5.91	103.47	108.20
34	a	760	G	C8-N9-C4	5.91	108.77	106.40
8	A	647	G	C8-N9-C4	5.91	108.76	106.40
8	A	900	A	N7-C8-N9	5.91	116.75	113.80
34	a	973	G	N1-C6-O6	-5.91	116.35	119.90
8	A	2659	G	C8-N9-C4	5.91	108.76	106.40
9	B	23	G	C5-N7-C8	-5.91	101.35	104.30
8	A	998	C	N3-C4-N4	-5.91	113.87	118.00
8	A	2736	A	N9-C4-C5	-5.91	103.44	105.80
34	a	334	C	C6-N1-C1'	-5.91	113.71	120.80
34	a	1422	G	C8-N9-C4	5.91	108.76	106.40
34	a	1466	C	N3-C2-O2	-5.91	117.77	121.90
8	A	146	A	C8-N9-C4	5.90	108.16	105.80
34	a	1472	U	C6-N1-C1'	-5.90	112.94	121.20
8	A	2505	G	C4-N9-C1'	5.90	134.17	126.50
8	A	2624	G	C2-N3-C4	-5.90	108.95	111.90
34	a	265	G	N3-C4-N9	-5.90	122.46	126.00
34	a	933	G	C2-N3-C4	-5.90	108.95	111.90
8	A	1238	G	C2-N3-C4	-5.90	108.95	111.90
8	A	2179	C	O4'-C1'-N1	-5.90	103.48	108.20
8	A	2407	A	C5-C6-N6	-5.90	118.98	123.70
8	A	2825	G	N3-C2-N2	-5.90	115.77	119.90
34	a	775	G	C8-N9-C4	5.90	108.76	106.40
8	A	1093	G	N3-C2-N2	-5.90	115.77	119.90
8	A	1162	G	N3-C4-C5	5.90	131.55	128.60
8	A	1718	G	N3-C4-C5	5.90	131.55	128.60
34	a	1079	G	N3-C4-N9	-5.90	122.46	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	a	1418	A	C4-C5-N7	5.90	113.65	110.70
8	A	1746	A	C8-N9-C4	5.90	108.16	105.80
8	A	2442	C	N3-C4-N4	-5.90	113.87	118.00
34	a	158	G	C5-N7-C8	-5.90	101.35	104.30
8	A	845	A	N9-C4-C5	-5.89	103.44	105.80
34	a	146	G	N3-C4-N9	-5.89	122.46	126.00
34	a	1144	G	N3-C4-N9	-5.89	122.46	126.00
8	A	664	G	N3-C4-C5	5.89	131.55	128.60
34	a	1004	A	O5'-P-OP1	-5.89	100.40	105.70
8	A	191	A	N9-C4-C5	-5.89	103.44	105.80
8	A	536	G	C6-C5-N7	5.89	133.93	130.40
8	A	1596	A	C4-C5-C6	-5.89	114.06	117.00
8	A	1715	G	N3-C4-C5	5.89	131.54	128.60
8	A	2557	G	C5-C6-O6	5.89	132.13	128.60
8	A	2665	A	C4-C5-N7	5.89	113.64	110.70
34	a	629	A	C8-N9-C4	5.89	108.16	105.80
8	A	273	G	C2-N3-C4	-5.89	108.96	111.90
8	A	1163	G	N3-C4-N9	-5.89	122.47	126.00
8	A	1750	G	N3-C4-N9	-5.88	122.47	126.00
34	a	77	A	C8-N9-C4	5.88	108.15	105.80
34	a	78	A	C2-N3-C4	-5.88	107.66	110.60
8	A	854	C	N3-C4-C5	5.88	124.25	121.90
34	a	640	A	C2-N3-C4	-5.88	107.66	110.60
34	a	1243	C	C6-N1-C2	5.88	122.65	120.30
8	A	1308	A	C8-N9-C4	5.88	108.15	105.80
8	A	2114	A	P-O3'-C3'	-5.88	112.65	119.70
8	A	2780	G	N3-C4-N9	-5.88	122.47	126.00
34	a	167	A	C4-C5-N7	5.88	113.64	110.70
8	A	1530	G	C2-N3-C4	-5.88	108.96	111.90
34	a	778	G	C2-N3-C4	-5.88	108.96	111.90
8	A	1317	G	N3-C4-N9	-5.88	122.47	126.00
8	A	2437	G	N3-C4-N9	-5.88	122.47	126.00
34	a	460	A	C2-N3-C4	-5.88	107.66	110.60
34	a	487	A	C4-C5-N7	5.88	113.64	110.70
34	a	604	G	C4-C5-N7	5.88	113.15	110.80
34	a	1047	G	N3-C4-N9	-5.88	122.47	126.00
8	A	865	C	C5-C4-N4	5.87	124.31	120.20
8	A	1244	A	C4-C5-N7	5.87	113.64	110.70
8	A	630	G	C4-N9-C1'	-5.87	118.87	126.50
8	A	780	G	C4-N9-C1'	-5.87	118.87	126.50
8	A	2270	A	C8-N9-C4	5.87	108.15	105.80
34	a	920	U	C2-N1-C1'	5.87	124.75	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	493	G	N3-C4-C5	5.87	131.53	128.60
8	A	1216	G	C8-N9-C4	5.87	108.75	106.40
8	A	1292	G	N3-C4-N9	-5.87	122.48	126.00
34	a	858	G	C2-N3-C4	-5.87	108.97	111.90
34	a	1241	G	C2-N3-C4	-5.87	108.97	111.90
8	A	48	G	C8-N9-C4	5.87	108.75	106.40
8	A	897	C	C2-N1-C1'	5.87	125.25	118.80
8	A	949	G	N3-C4-N9	-5.87	122.48	126.00
8	A	1239	G	N3-C4-N9	-5.87	122.48	126.00
34	a	35	G	N3-C4-C5	5.87	131.53	128.60
34	a	260	G	C2-N3-C4	-5.87	108.97	111.90
34	a	550	G	C4-N9-C1'	-5.87	118.87	126.50
34	a	1153	G	N3-C4-C5	5.87	131.53	128.60
34	a	1422	G	C2-N3-C4	-5.87	108.97	111.90
34	a	833	G	C2-N3-C4	-5.87	108.97	111.90
34	a	1111	A	N9-C4-C5	-5.87	103.45	105.80
34	a	1206	G	C2-N3-C4	-5.86	108.97	111.90
8	A	498	G	N3-C4-C5	5.86	131.53	128.60
9	B	11	C	N3-C4-N4	5.86	122.10	118.00
8	A	175	G	N3-C4-C5	5.86	131.53	128.60
8	A	1095	A	O4'-C1'-N9	-5.86	103.51	108.20
8	A	1435	G	N3-C4-N9	-5.86	122.48	126.00
34	a	1058	G	C2-N3-C4	-5.86	108.97	111.90
8	A	731	C	C6-N1-C2	5.86	122.64	120.30
8	A	2597	G	N3-C4-C5	5.86	131.53	128.60
34	a	428	G	N3-C4-C5	5.86	131.53	128.60
8	A	1793	C	N3-C4-N4	-5.86	113.90	118.00
8	A	2792	A	N9-C4-C5	-5.86	103.46	105.80
8	A	2869	G	C2-N3-C4	-5.86	108.97	111.90
34	a	81	A	N9-C4-C5	-5.86	103.46	105.80
8	A	1165	A	N3-C4-C5	5.86	130.90	126.80
8	A	2083	G	N9-C4-C5	-5.86	103.06	105.40
8	A	2355	G	N3-C4-N9	-5.86	122.49	126.00
9	B	11	C	C6-N1-C1'	-5.86	113.77	120.80
34	a	755	G	C8-N9-C4	5.86	108.74	106.40
34	a	894	G	N3-C4-C5	5.86	131.53	128.60
34	a	1048	G	C4-C5-N7	5.86	113.14	110.80
34	a	1187	G	N3-C4-C5	5.86	131.53	128.60
8	A	677	A	N1-C6-N6	-5.85	115.09	118.60
8	A	1755	A	N1-C6-N6	-5.85	115.09	118.60
34	a	745	G	N3-C4-C5	5.85	131.53	128.60
8	A	39	G	N3-C4-N9	-5.85	122.49	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	623	C	C6-N1-C2	5.85	122.64	120.30
8	A	758	C	C6-N1-C2	5.85	122.64	120.30
8	A	1169	A	N1-C6-N6	5.85	122.11	118.60
8	A	1378	A	N9-C4-C5	-5.85	103.46	105.80
8	A	2460	U	C6-N1-C2	5.85	124.51	121.00
8	A	2472	G	N3-C4-N9	-5.85	122.49	126.00
8	A	2827	C	C6-N1-C2	5.85	122.64	120.30
9	B	117	G	N3-C4-C5	5.85	131.53	128.60
34	a	504	C	C6-N1-C2	5.85	122.64	120.30
34	a	624	C	N3-C4-N4	-5.85	113.90	118.00
8	A	553	G	C2-N3-C4	-5.85	108.97	111.90
8	A	1055	G	C8-N9-C4	5.85	108.74	106.40
34	a	616	G	N3-C4-C5	5.85	131.53	128.60
8	A	350	G	N9-C4-C5	-5.85	103.06	105.40
8	A	1117	C	N3-C4-C5	5.85	124.24	121.90
8	A	1652	A	C5-N7-C8	-5.85	100.98	103.90
8	A	2671	G	C2-N3-C4	-5.85	108.97	111.90
34	a	69	G	N3-C4-C5	5.85	131.53	128.60
8	A	2759	G	N3-C4-C5	5.85	131.52	128.60
9	B	60	C	N3-C2-O2	5.85	125.99	121.90
34	a	838	G	C4-C5-N7	5.85	113.14	110.80
34	a	1094	G	N3-C2-N2	5.85	123.99	119.90
8	A	227	A	N1-C6-N6	-5.85	115.09	118.60
8	A	1830	C	C6-N1-C2	5.84	122.64	120.30
34	a	878	A	O5'-P-OP1	-5.84	100.44	105.70
34	a	888	G	N1-C2-N2	5.84	121.46	116.20
34	a	944	G	N3-C4-N9	-5.84	122.49	126.00
8	A	1553	A	C5-C6-N6	-5.84	119.03	123.70
8	A	2859	G	N3-C4-C5	5.84	131.52	128.60
34	a	442	G	N3-C2-N2	5.84	123.99	119.90
34	a	597	G	N3-C4-C5	5.84	131.52	128.60
8	A	670	A	N1-C6-N6	5.84	122.10	118.60
8	A	2482	A	C8-N9-C4	5.84	108.14	105.80
34	a	1325	C	N1-C2-O2	5.84	122.40	118.90
8	A	1345	C	C6-N1-C2	5.84	122.64	120.30
8	A	1418	G	N3-C4-C5	5.84	131.52	128.60
8	A	1512	C	C6-N1-C2	5.84	122.63	120.30
8	A	2391	G	N3-C4-C5	5.84	131.52	128.60
34	a	347	G	N3-C4-C5	5.84	131.52	128.60
34	a	493	A	O4'-C1'-N9	-5.84	103.53	108.20
8	A	144	A	C5-N7-C8	-5.83	100.98	103.90
8	A	989	G	N3-C4-N9	-5.83	122.50	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	1650	A	C4-C5-C6	-5.83	114.08	117.00
8	A	2294	G	N3-C4-C5	5.83	131.52	128.60
8	A	2718	G	C8-N9-C4	5.83	108.73	106.40
8	A	570	G	N3-C4-C5	-5.83	125.68	128.60
8	A	2419	U	C6-N1-C2	5.83	124.50	121.00
34	a	28	A	C4-C5-N7	5.83	113.62	110.70
34	a	785	G	N3-C4-C5	5.83	131.52	128.60
8	A	1038	G	C8-N9-C4	5.83	108.73	106.40
8	A	303	G	C4-C5-N7	5.83	113.13	110.80
34	a	211	G	P-O5'-C5'	-5.83	111.57	120.90
8	A	549	G	N9-C4-C5	-5.83	103.07	105.40
8	A	831	G	N3-C4-C5	5.83	131.51	128.60
8	A	2165	C	C6-N1-C2	5.83	122.63	120.30
8	A	2351	G	N3-C4-N9	-5.83	122.50	126.00
55	v	76	A	C8-N9-C4	5.83	108.13	105.80
31	X	21	LEU	CA-CB-CG	-5.83	101.90	115.30
34	a	203	G	C6-C5-N7	5.83	133.90	130.40
8	A	1616	A	C8-N9-C4	5.83	108.13	105.80
34	a	1047	G	C2-N3-C4	-5.83	108.99	111.90
8	A	555	G	N3-C4-C5	5.82	131.51	128.60
8	A	2351	G	C8-N9-C4	5.82	108.73	106.40
34	a	1185	G	N3-C4-C5	5.82	131.51	128.60
34	a	1459	G	C2-N3-C4	-5.82	108.99	111.90
8	A	350	G	N3-C4-C5	5.82	131.51	128.60
8	A	564	C	C6-N1-C2	5.82	122.63	120.30
8	A	1408	G	N3-C4-C5	5.82	131.51	128.60
8	A	2137	U	N3-C4-O4	-5.82	115.33	119.40
34	a	1304	G	N3-C4-C5	5.82	131.51	128.60
8	A	185	G	C4-N9-C1'	-5.82	118.94	126.50
8	A	212	G	C2-N3-C4	-5.82	108.99	111.90
8	A	244	A	C8-N9-C4	5.82	108.13	105.80
8	A	271	G	C8-N9-C4	5.82	108.73	106.40
8	A	383	C	N3-C4-C5	5.82	124.23	121.90
8	A	1173	U	C2-N1-C1'	5.82	124.68	117.70
8	A	1492	G	N3-C2-N2	-5.82	115.83	119.90
8	A	2355	G	C2-N3-C4	-5.82	108.99	111.90
8	A	2655	G	N3-C4-C5	5.82	131.51	128.60
8	A	2901	C	N1-C2-O2	5.81	122.39	118.90
8	A	63	A	N1-C2-N3	5.81	132.21	129.30
8	A	291	G	C2-N3-C4	-5.81	108.99	111.90
34	a	117	G	N9-C4-C5	-5.81	103.08	105.40
34	a	1090	U	C6-N1-C2	5.81	124.49	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	2150	C	N3-C4-C5	5.81	124.22	121.90
34	a	236	A	N9-C4-C5	-5.81	103.48	105.80
8	A	1237	A	C2-N3-C4	-5.81	107.69	110.60
34	a	803	G	N3-C2-N2	5.81	123.97	119.90
34	a	1373	G	C8-N9-C4	5.81	108.72	106.40
8	A	1511	G	C2-N3-C4	-5.81	109.00	111.90
8	A	2407	A	C4-C5-N7	5.81	113.60	110.70
8	A	2544	G	N3-C4-N9	-5.81	122.52	126.00
34	a	998	C	N3-C4-N4	-5.81	113.94	118.00
34	a	1371	G	N3-C4-C5	5.81	131.50	128.60
34	a	76	G	N3-C4-C5	5.80	131.50	128.60
8	A	73	A	C8-N9-C4	5.80	108.12	105.80
8	A	314	C	N3-C4-C5	5.80	124.22	121.90
8	A	380	G	C8-N9-C4	5.80	108.72	106.40
8	A	2465	C	C6-N1-C2	5.80	122.62	120.30
34	a	681	A	N9-C4-C5	-5.80	103.48	105.80
34	a	784	A	C8-N9-C4	5.80	108.12	105.80
34	a	1133	G	C4-N9-C1'	-5.80	118.96	126.50
34	a	1331	G	N3-C4-C5	5.80	131.50	128.60
8	A	1449	G	C4-N9-C1'	-5.80	118.96	126.50
8	A	1529	G	C8-N9-C1'	-5.80	119.46	127.00
34	a	654	G	N1-C6-O6	5.80	123.38	119.90
8	A	96	C	N3-C4-C5	5.80	124.22	121.90
8	A	367	G	C2-N3-C4	-5.80	109.00	111.90
8	A	155	A	N9-C4-C5	-5.79	103.48	105.80
8	A	375	G	N1-C2-N2	-5.79	110.99	116.20
8	A	2461	A	N9-C4-C5	-5.79	103.48	105.80
34	a	312	C	N3-C4-C5	5.79	124.22	121.90
34	a	1059	C	N3-C4-N4	-5.79	113.95	118.00
8	A	1966	A	N1-C6-N6	5.79	122.07	118.60
34	a	321	A	C8-N9-C4	5.79	108.11	105.80
34	a	1143	G	N1-C6-O6	5.79	123.37	119.90
8	A	270	A	C4-C5-C6	-5.79	114.11	117.00
8	A	1528	A	N1-C6-N6	5.79	122.07	118.60
34	a	255	G	C2-N3-C4	-5.79	109.01	111.90
34	a	1043	G	C8-N9-C1'	5.79	134.52	127.00
55	v	72	A	C8-N9-C4	5.79	108.11	105.80
8	A	1465	G	C5-N7-C8	-5.78	101.41	104.30
34	a	1244	G	N3-C4-N9	-5.78	122.53	126.00
8	A	2378	A	N7-C8-N9	5.78	116.69	113.80
8	A	535	G	C2-N3-C4	-5.78	109.01	111.90
8	A	856	G	C8-N9-C4	5.78	108.71	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	1099	G	C2-N3-C4	-5.78	109.01	111.90
8	A	1228	G	C8-N9-C4	5.78	108.71	106.40
8	A	2483	C	C6-N1-C2	5.78	122.61	120.30
20	M	33	LEU	CA-CB-CG	-5.78	102.01	115.30
34	a	324	G	C4-N9-C1'	-5.78	118.99	126.50
34	a	442	G	C6-C5-N7	-5.78	126.93	130.40
34	a	27	G	C8-N9-C4	5.78	108.71	106.40
8	A	1193	G	N9-C4-C5	-5.78	103.09	105.40
8	A	2343	U	P-O3'-C3'	5.78	126.63	119.70
34	a	203	G	O4'-C1'-N9	5.77	112.82	108.20
34	a	1272	G	N3-C4-C5	5.77	131.49	128.60
8	A	1471	G	C8-N9-C1'	-5.77	119.50	127.00
34	a	611	C	N3-C4-N4	-5.77	113.96	118.00
34	a	1482	G	C2-N3-C4	-5.77	109.01	111.90
8	A	310	A	C8-N9-C4	5.77	108.11	105.80
8	A	1115	G	N3-C4-N9	-5.77	122.54	126.00
8	A	1271	G	C8-N9-C4	5.77	108.71	106.40
12	E	164	LEU	CA-CB-CG	-5.77	102.03	115.30
34	a	809	G	C8-N9-C4	5.77	108.71	106.40
34	a	927	G	N3-C4-C5	5.77	131.49	128.60
8	A	793	A	C5-C6-N6	-5.77	119.08	123.70
8	A	2516	A	N9-C4-C5	-5.77	103.49	105.80
34	a	241	G	C8-N9-C4	5.77	108.71	106.40
8	A	376	G	N3-C4-N9	-5.77	122.54	126.00
8	A	1385	A	C8-N9-C4	5.77	108.11	105.80
8	A	1655	A	C8-N9-C4	5.77	108.11	105.80
8	A	1893	C	N3-C4-N4	-5.77	113.96	118.00
8	A	2694	G	C8-N9-C4	5.77	108.71	106.40
8	A	2777	G	N3-C4-C5	5.77	131.48	128.60
34	a	1511	G	C4-C5-N7	5.77	113.11	110.80
8	A	68	G	C8-N9-C4	5.77	108.71	106.40
8	A	2018	G	C2-N3-C4	-5.77	109.02	111.90
34	a	628	G	C2-N3-C4	-5.77	109.02	111.90
56	w	68	C	N3-C4-C5	5.77	124.21	121.90
8	A	401	A	N9-C4-C5	-5.76	103.49	105.80
8	A	531	C	O4'-C1'-N1	-5.76	103.59	108.20
8	A	536	G	C4-N9-C1'	-5.76	119.01	126.50
8	A	1894	C	N3-C4-C5	5.76	124.21	121.90
8	A	2618	G	C5-C6-O6	5.76	132.06	128.60
34	a	274	A	N3-C4-C5	5.76	130.84	126.80
34	a	429	U	O4'-C1'-N1	-5.76	103.59	108.20
8	A	2198	A	C4-C5-C6	-5.76	114.12	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	58	A	O5'-P-OP2	-5.76	100.51	105.70
34	a	362	G	N3-C4-N9	-5.76	122.54	126.00
34	a	435	A	C4-C5-N7	5.76	113.58	110.70
34	a	1224	U	O4'-C1'-N1	-5.76	103.59	108.20
8	A	1094	U	O4'-C1'-N1	5.76	112.81	108.20
8	A	1152	C	C6-N1-C2	5.76	122.60	120.30
8	A	1649	G	C8-N9-C4	5.76	108.70	106.40
8	A	2547	A	N9-C4-C5	-5.76	103.50	105.80
34	a	201	G	C8-N9-C1'	5.76	134.49	127.00
8	A	998	C	N3-C4-C5	5.76	124.20	121.90
8	A	2143	C	N3-C4-N4	5.76	122.03	118.00
8	A	2400	G	C2-N3-C4	-5.76	109.02	111.90
8	A	2874	C	C6-N1-C2	5.76	122.60	120.30
34	a	656	G	N3-C4-N9	-5.76	122.54	126.00
57	x	669	LEU	CA-CB-CG	5.76	128.55	115.30
9	B	34	A	C2-N3-C4	-5.76	107.72	110.60
8	A	853	C	N3-C4-C5	5.76	124.20	121.90
8	A	1532	A	C4-C5-N7	5.76	113.58	110.70
34	a	1280	A	N1-C6-N6	-5.76	115.15	118.60
8	A	145	C	N3-C4-C5	5.75	124.20	121.90
8	A	1233	C	C6-N1-C2	5.75	122.60	120.30
8	A	1008	A	C8-N9-C4	5.75	108.10	105.80
8	A	1703	G	C8-N9-C4	5.75	108.70	106.40
8	A	2839	G	N9-C4-C5	-5.75	103.10	105.40
9	B	61	G	N3-C2-N2	5.75	123.93	119.90
34	a	821	G	N3-C4-C5	5.75	131.48	128.60
8	A	271	G	N1-C6-O6	5.75	123.35	119.90
8	A	697	G	C2-N3-C4	-5.75	109.02	111.90
8	A	2012	G	C4-C5-N7	5.75	113.10	110.80
8	A	2792	A	C8-N9-C4	5.75	108.10	105.80
34	a	242	G	N3-C4-N9	-5.75	122.55	126.00
34	a	586	C	C6-N1-C2	5.75	122.60	120.30
34	a	929	G	C2-N3-C4	-5.75	109.03	111.90
8	A	1303	G	N3-C4-C5	5.75	131.47	128.60
34	a	526	C	N3-C4-C5	5.75	124.20	121.90
8	A	551	G	C2-N3-C4	-5.75	109.03	111.90
8	A	581	C	C2-N1-C1'	5.75	125.12	118.80
8	A	469	G	N3-C4-C5	5.75	131.47	128.60
8	A	512	G	N3-C4-C5	5.75	131.47	128.60
34	a	81	A	C5-C6-N6	-5.75	119.10	123.70
8	A	177	G	C2-N3-C4	-5.74	109.03	111.90
8	A	467	G	N3-C4-C5	5.74	131.47	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	2801	G	C8-N9-C4	5.74	108.70	106.40
34	a	1081	A	N7-C8-N9	5.74	116.67	113.80
8	A	1527	G	C2-N3-C4	-5.74	109.03	111.90
55	v	46	A	C8-N9-C4	5.74	108.10	105.80
8	A	382	A	C8-N9-C4	5.74	108.10	105.80
8	A	2323	G	C2-N3-C4	-5.74	109.03	111.90
55	v	21	A	C4-C5-C6	-5.74	114.13	117.00
8	A	2080	A	C8-N9-C4	5.74	108.10	105.80
8	A	2510	C	N3-C4-N4	-5.74	113.98	118.00
34	a	347	G	C2-N3-C4	-5.74	109.03	111.90
34	a	423	G	O4'-C1'-N9	5.74	112.79	108.20
56	w	47	U	C5'-C4'-O4'	5.74	115.98	109.10
8	A	1952	A	C8-N9-C4	5.73	108.09	105.80
8	A	2735	G	C8-N9-C4	5.73	108.69	106.40
34	a	1128	C	C6-N1-C2	5.73	122.59	120.30
8	A	316	C	C6-N1-C2	5.73	122.59	120.30
8	A	2109	U	O5'-P-OP1	5.73	117.58	110.70
8	A	2828	G	C2-N3-C4	-5.73	109.03	111.90
8	A	381	G	N3-C4-N9	-5.73	122.56	126.00
8	A	631	A	C8-N9-C4	5.73	108.09	105.80
8	A	1492	G	C6-C5-N7	5.73	133.84	130.40
8	A	2574	G	N3-C4-C5	5.73	131.46	128.60
8	A	481	G	C8-N9-C1'	5.73	134.45	127.00
8	A	1356	G	N3-C4-C5	5.73	131.46	128.60
8	A	2641	G	C4-N9-C1'	-5.73	119.05	126.50
34	a	910	C	C6-N1-C2	5.73	122.59	120.30
8	A	270	A	N1-C6-N6	-5.73	115.17	118.60
8	A	1153	C	C2-N1-C1'	5.73	125.10	118.80
8	A	1166	G	C2-N3-C4	-5.73	109.04	111.90
8	A	705	A	C8-N9-C4	5.72	108.09	105.80
8	A	1905	C	C5-C6-N1	-5.72	118.14	121.00
8	A	2411	A	N9-C4-C5	-5.72	103.51	105.80
8	A	2592	G	C2-N3-C4	-5.72	109.04	111.90
34	a	102	G	N3-C4-C5	5.72	131.46	128.60
34	a	1276	G	C4-C5-N7	5.72	113.09	110.80
8	A	655	A	N9-C4-C5	-5.72	103.51	105.80
8	A	1062	G	C4-C5-N7	5.72	113.09	110.80
8	A	2092	U	C6-N1-C1'	-5.72	113.19	121.20
8	A	2275	C	C6-N1-C2	-5.72	118.01	120.30
34	a	177	G	C8-N9-C1'	-5.72	119.56	127.00
34	a	550	G	N3-C4-N9	-5.72	122.57	126.00
34	a	674	G	C4-N9-C1'	5.72	133.94	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	539	G	C2-N3-C4	-5.72	109.04	111.90
8	A	1192	G	C2-N3-C4	-5.72	109.04	111.90
8	A	2204	G	C2-N3-C4	-5.72	109.04	111.90
8	A	2305	U	C6-N1-C2	5.72	124.43	121.00
8	A	20	C	C6-N1-C2	5.72	122.59	120.30
8	A	2383	G	N3-C4-N9	-5.72	122.57	126.00
34	a	35	G	C2-N3-C4	-5.72	109.04	111.90
34	a	42	G	C4-C5-N7	5.72	113.09	110.80
34	a	1312	G	C4-C5-N7	5.72	113.09	110.80
8	A	834	G	N3-C4-C5	5.72	131.46	128.60
8	A	1378	A	O4'-C1'-N9	-5.72	103.63	108.20
8	A	1661	G	N3-C4-N9	-5.72	122.57	126.00
34	a	28	A	N9-C4-C5	-5.72	103.51	105.80
34	a	428	G	C4-N9-C1'	-5.72	119.07	126.50
8	A	1568	G	C2-N3-C4	-5.71	109.04	111.90
34	a	399	G	N3-C4-C5	5.71	131.46	128.60
34	a	604	G	C4-C5-C6	-5.71	115.37	118.80
8	A	2894	G	C4-N9-C1'	-5.71	119.07	126.50
34	a	164	G	C2-N3-C4	-5.71	109.04	111.90
8	A	664	G	N1-C2-N2	-5.71	111.06	116.20
8	A	1745	A	N1-C6-N6	5.71	122.03	118.60
8	A	2366	A	N1-C6-N6	5.71	122.03	118.60
34	a	457	G	N3-C4-C5	5.71	131.46	128.60
8	A	1857	G	C2-N3-C4	-5.71	109.05	111.90
8	A	2116	G	C8-N9-C4	5.71	108.68	106.40
8	A	2433	A	N1-C6-N6	-5.71	115.17	118.60
8	A	2199	A	C4-C5-N7	5.71	113.56	110.70
9	B	42	C	N1-C1'-C2'	-5.71	105.72	112.00
9	B	112	G	C2-N3-C4	-5.71	109.05	111.90
34	a	198	G	C2-N3-C4	-5.71	109.05	111.90
34	a	349	A	N9-C4-C5	-5.71	103.52	105.80
8	A	674	G	N9-C1'-C2'	-5.71	105.72	112.00
8	A	1037	G	N3-C4-N9	-5.71	122.58	126.00
8	A	2044	C	O4'-C1'-N1	-5.71	103.64	108.20
9	B	44	G	C2-N3-C4	-5.71	109.05	111.90
34	a	319	G	C4-N9-C1'	-5.71	119.08	126.50
34	a	1262	C	C6-N1-C1'	-5.71	113.95	120.80
8	A	2414	G	C2-N3-C4	-5.71	109.05	111.90
8	A	2899	A	C5-N7-C8	-5.71	101.05	103.90
9	B	54	G	C5-C6-N1	-5.71	108.65	111.50
34	a	1196	A	C5-C6-N6	-5.71	119.14	123.70
8	A	155	A	C4-C5-N7	5.70	113.55	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	951	C	N3-C4-C5	5.70	124.18	121.90
8	A	2367	G	C8-N9-C4	5.70	108.68	106.40
9	B	76	G	C2-N3-C4	-5.70	109.05	111.90
34	a	429	U	C2-N1-C1'	-5.70	110.86	117.70
34	a	927	G	C2-N3-C4	-5.70	109.05	111.90
34	a	1396	A	C5-C6-N1	5.70	120.55	117.70
34	a	1430	A	C8-N9-C4	5.70	108.08	105.80
34	a	836	G	C8-N9-C4	5.70	108.68	106.40
8	A	269	C	N3-C4-C5	5.70	124.18	121.90
8	A	372	G	C2-N3-C4	-5.70	109.05	111.90
8	A	785	G	C2-N3-C4	-5.70	109.05	111.90
8	A	854	C	C6-N1-C2	5.70	122.58	120.30
8	A	1099	G	N3-C4-C5	5.70	131.45	128.60
8	A	1277	G	C4-C5-C6	-5.70	115.38	118.80
8	A	1889	A	C8-N9-C4	5.70	108.08	105.80
8	A	1966	A	C8-N9-C4	5.70	108.08	105.80
8	A	2508	G	C2-N3-C4	-5.70	109.05	111.90
34	a	101	A	C4-C5-C6	-5.70	114.15	117.00
8	A	1604	C	N3-C4-N4	-5.70	114.01	118.00
8	A	30	G	C2-N3-C4	-5.70	109.05	111.90
8	A	86	G	N3-C4-C5	5.70	131.45	128.60
8	A	697	G	O4'-C1'-N9	-5.70	103.64	108.20
8	A	815	C	C6-N1-C2	5.70	122.58	120.30
34	a	1081	A	N3-C4-C5	-5.70	122.81	126.80
8	A	2713	U	O4'-C1'-N1	-5.69	103.64	108.20
9	B	9	G	C8-N9-C1'	-5.69	119.60	127.00
34	a	585	G	N3-C4-N9	-5.69	122.58	126.00
8	A	354	A	C8-N9-C4	5.69	108.08	105.80
8	A	693	A	C8-N9-C4	5.69	108.08	105.80
34	a	674	G	N1-C2-N3	5.69	127.31	123.90
8	A	27	G	C2-N3-C4	-5.69	109.06	111.90
8	A	271	G	C4-C5-N7	5.69	113.08	110.80
8	A	313	G	C2-N3-C4	-5.69	109.05	111.90
8	A	1685	C	C6-N1-C2	5.69	122.58	120.30
8	A	2297	A	C2-N3-C4	-5.69	107.75	110.60
8	A	2643	G	N3-C4-C5	5.69	131.45	128.60
55	v	41	C	N3-C4-N4	-5.69	114.02	118.00
8	A	497	A	N1-C6-N6	-5.69	115.19	118.60
8	A	636	G	N3-C4-N9	-5.69	122.59	126.00
8	A	1048	A	C8-N9-C4	5.69	108.08	105.80
8	A	837	C	N3-C4-N4	-5.69	114.02	118.00
34	a	413	G	N1-C6-O6	5.69	123.31	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	2097	A	N9-C4-C5	-5.69	103.53	105.80
34	a	674	G	C2-N3-C4	-5.69	109.06	111.90
34	a	846	G	C4-C5-N7	5.69	113.07	110.80
34	a	1230	C	N3-C4-C5	5.69	124.17	121.90
8	A	481	G	N3-C4-N9	-5.68	122.59	126.00
8	A	1984	G	C2-N3-C4	-5.68	109.06	111.90
8	A	2280	G	N3-C4-C5	5.68	131.44	128.60
8	A	1001	A	N1-C6-N6	5.68	122.01	118.60
8	A	2054	A	C8-N9-C4	5.68	108.07	105.80
8	A	2430	A	C5-N7-C8	-5.68	101.06	103.90
8	A	398	C	N3-C4-N4	-5.68	114.02	118.00
22	O	16	ARG	CG-CD-NE	-5.68	99.87	111.80
8	A	410	G	N3-C4-N9	-5.68	122.59	126.00
8	A	956	G	N3-C4-N9	-5.68	122.59	126.00
8	A	1074	G	N3-C4-N9	-5.68	122.59	126.00
8	A	1916	A	N9-C1'-C2'	-5.68	105.75	112.00
34	a	1096	C	C6-N1-C2	5.68	122.57	120.30
8	A	770	G	C8-N9-C4	5.68	108.67	106.40
8	A	1587	G	C8-N9-C4	5.68	108.67	106.40
8	A	2846	G	N3-C2-N2	-5.68	115.92	119.90
34	a	213	G	N3-C4-N9	-5.68	122.59	126.00
8	A	57	C	N3-C4-C5	5.68	124.17	121.90
8	A	1361	G	C2-N3-C4	-5.67	109.06	111.90
8	A	108	G	C2-N3-C4	-5.67	109.06	111.90
8	A	952	G	N3-C4-N9	-5.67	122.60	126.00
8	A	1543	G	C4-N9-C1'	-5.67	119.12	126.50
34	a	1185	G	C2-N3-C4	-5.67	109.06	111.90
34	a	1309	G	C4-C5-N7	5.67	113.07	110.80
8	A	488	G	C4-N9-C1'	-5.67	119.13	126.50
8	A	1696	G	C2-N3-C4	-5.67	109.06	111.90
8	A	2718	G	N3-C4-C5	5.67	131.44	128.60
34	a	326	G	N3-C4-C5	5.67	131.44	128.60
8	A	1346	G	C8-N9-C4	5.67	108.67	106.40
8	A	2137	U	N1-C2-N3	-5.67	111.50	114.90
9	B	88	C	C2-N1-C1'	5.67	125.04	118.80
8	A	326	G	N3-C4-N9	-5.67	122.60	126.00
8	A	2110	G	C8-N9-C1'	-5.67	119.63	127.00
34	a	885	G	N3-C4-C5	5.67	131.43	128.60
8	A	1421	G	N3-C4-C5	5.67	131.43	128.60
8	A	1719	G	C2-N3-C4	-5.67	109.07	111.90
8	A	2415	G	N3-C4-C5	5.67	131.43	128.60
8	A	2839	G	N1-C2-N2	-5.67	111.10	116.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	396	G	C4-C5-N7	5.67	113.07	110.80
9	B	14	U	C6-N1-C2	5.66	124.40	121.00
34	a	450	G	N3-C4-C5	5.66	131.43	128.60
55	v	72	A	N3-C4-C5	5.66	130.76	126.80
8	A	2674	G	C8-N9-C4	5.66	108.67	106.40
8	A	923	G	N3-C4-C5	5.66	131.43	128.60
8	A	938	G	N3-C4-C5	5.66	131.43	128.60
8	A	2142	A	C4-N9-C1'	5.66	136.49	126.30
8	A	2407	A	N1-C6-N6	5.66	122.00	118.60
34	a	167	A	C8-N9-C4	5.66	108.06	105.80
8	A	91	A	C8-N9-C4	5.66	108.06	105.80
8	A	919	U	C6-N1-C2	5.66	124.39	121.00
8	A	2326	C	N3-C4-N4	-5.66	114.04	118.00
8	A	497	A	C8-N9-C4	5.66	108.06	105.80
8	A	693	A	C4-C5-N7	5.66	113.53	110.70
8	A	1106	G	C4-N9-C1'	-5.66	119.15	126.50
8	A	1189	A	N1-C6-N6	5.66	121.99	118.60
8	A	1230	A	N9-C4-C5	-5.66	103.54	105.80
8	A	2736	A	C8-N9-C4	5.66	108.06	105.80
55	v	5	G	N3-C4-N9	-5.65	122.61	126.00
34	a	1331	G	C6-C5-N7	5.65	133.79	130.40
8	A	675	A	N9-C4-C5	-5.65	103.54	105.80
8	A	2440	C	N3-C4-C5	5.65	124.16	121.90
34	a	181	A	C5-N7-C8	-5.65	101.07	103.90
8	A	425	G	C4-N9-C1'	-5.65	119.16	126.50
8	A	1933	G	C5-C6-O6	5.65	131.99	128.60
8	A	2549	G	C4-C5-N7	5.65	113.06	110.80
8	A	684	G	C2-N3-C4	-5.65	109.08	111.90
9	B	11	C	O4'-C1'-N1	-5.65	103.68	108.20
8	A	2544	G	N3-C4-C5	5.64	131.42	128.60
34	a	1190	G	N1-C2-N2	5.64	121.28	116.20
8	A	126	A	N3-C4-C5	5.64	130.75	126.80
8	A	971	G	N3-C4-C5	5.64	131.42	128.60
8	A	1142	A	C2-N3-C4	-5.64	107.78	110.60
34	a	1002	G	N3-C4-N9	-5.64	122.61	126.00
8	A	1615	C	C6-N1-C2	5.64	122.56	120.30
8	A	1974	C	N3-C4-C5	5.64	124.16	121.90
8	A	2077	A	C8-N9-C4	5.64	108.06	105.80
34	a	542	G	N9-C4-C5	-5.64	103.14	105.40
8	A	1558	C	C6-N1-C2	5.64	122.56	120.30
8	A	2121	G	C6-C5-N7	-5.64	127.02	130.40
9	B	118	C	C6-N1-C2	5.64	122.56	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	1	G	O4'-C1'-N9	-5.63	103.69	108.20
8	A	375	G	C2-N3-C4	-5.63	109.08	111.90
8	A	1278	C	C6-N1-C2	5.63	122.55	120.30
8	A	2742	G	N3-C4-C5	5.63	131.42	128.60
34	a	433	G	N3-C4-C5	5.63	131.42	128.60
8	A	134	G	C4-C5-N7	5.63	113.05	110.80
8	A	763	G	N3-C4-C5	5.63	131.42	128.60
8	A	1743	G	C2-N3-C4	-5.63	109.08	111.90
8	A	2550	G	N3-C4-C5	5.63	131.42	128.60
34	a	227	G	C8-N9-C4	5.63	108.65	106.40
8	A	695	G	N3-C4-C5	5.63	131.42	128.60
8	A	1007	C	C6-N1-C2	5.63	122.55	120.30
8	A	2123	G	C8-N9-C4	5.63	108.65	106.40
8	A	2426	A	C8-N9-C4	5.63	108.05	105.80
9	B	4	C	C6-N1-C2	5.63	122.55	120.30
34	a	1371	G	N3-C4-N9	-5.63	122.62	126.00
8	A	781	A	C5-C6-N6	5.63	128.20	123.70
8	A	1238	G	C8-N9-C4	5.63	108.65	106.40
8	A	2721	A	N1-C6-N6	5.63	121.98	118.60
8	A	308	G	N3-C4-C5	5.63	131.41	128.60
8	A	1095	A	N1-C2-N3	5.63	132.12	129.30
8	A	1702	G	C2-N3-C4	-5.63	109.09	111.90
8	A	1857	G	N3-C4-C5	5.63	131.41	128.60
8	A	2719	G	C2-N3-C4	-5.63	109.09	111.90
34	a	379	C	N3-C4-N4	-5.63	114.06	118.00
8	A	376	G	N3-C4-C5	5.63	131.41	128.60
8	A	2151	U	N1-C1'-C2'	-5.63	105.81	112.00
34	a	495	A	C5-C6-N6	-5.63	119.20	123.70
8	A	52	A	C6-C5-N7	-5.62	128.36	132.30
8	A	2623	G	C8-N9-C4	5.62	108.65	106.40
9	B	68	C	C6-N1-C2	5.62	122.55	120.30
55	v	29	G	C2-N3-C4	-5.62	109.09	111.90
8	A	424	G	C2-N3-C4	-5.62	109.09	111.90
8	A	882	G	N3-C4-C5	5.62	131.41	128.60
8	A	1369	G	N3-C4-N9	-5.62	122.63	126.00
34	a	859	G	C8-N9-C4	5.62	108.65	106.40
8	A	1038	G	C2-N3-C4	-5.62	109.09	111.90
34	a	861	G	N3-C4-C5	5.62	131.41	128.60
8	A	460	A	C8-N9-C4	5.62	108.05	105.80
8	A	524	G	C2-N3-C4	-5.62	109.09	111.90
8	A	2490	G	C4-C5-N7	5.62	113.05	110.80
8	A	351	C	O4'-C1'-N1	-5.62	103.71	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	2470	G	C2-N3-C4	-5.62	109.09	111.90
34	a	944	G	N3-C4-C5	5.62	131.41	128.60
34	a	1262	C	C2-N1-C1'	5.62	124.98	118.80
8	A	400	G	C4-C5-N7	5.62	113.05	110.80
8	A	536	G	C2-N3-C4	-5.62	109.09	111.90
8	A	1007	C	N3-C4-C5	5.62	124.15	121.90
8	A	263	G	O4'-C1'-N9	-5.61	103.71	108.20
8	A	488	G	C8-N9-C4	5.61	108.65	106.40
8	A	2273	A	C8-N9-C4	5.61	108.05	105.80
34	a	858	G	C6-C5-N7	5.61	133.77	130.40
55	v	23	C	C6-N1-C2	-5.61	118.06	120.30
8	A	908	C	C6-N1-C2	5.61	122.55	120.30
8	A	2886	A	N1-C6-N6	5.61	121.97	118.60
8	A	406	G	N3-C4-C5	5.61	131.41	128.60
8	A	495	G	C8-N9-C4	5.61	108.64	106.40
8	A	1543	G	C8-N9-C4	5.61	108.64	106.40
8	A	2742	G	N3-C4-N9	-5.61	122.63	126.00
34	a	27	G	C2-N3-C4	-5.61	109.09	111.90
34	a	417	G	C2-N3-C4	-5.61	109.09	111.90
8	A	254	G	N3-C4-C5	5.61	131.40	128.60
8	A	1451	C	N3-C4-N4	-5.61	114.07	118.00
8	A	1972	G	C5'-C4'-C3'	5.61	124.97	116.00
8	A	2793	C	C6-N1-C2	5.61	122.54	120.30
8	A	1745	A	C4-C5-N7	5.61	113.50	110.70
34	a	162	A	O4'-C1'-N9	5.61	112.69	108.20
34	a	1105	A	C8-N9-C4	5.61	108.04	105.80
8	A	346	A	N9-C4-C5	-5.61	103.56	105.80
8	A	581	C	C6-N1-C1'	-5.61	114.07	120.80
8	A	1182	G	N3-C4-N9	-5.61	122.64	126.00
34	a	639	G	C2-N3-C4	-5.61	109.10	111.90
8	A	109	C	N3-C4-N4	-5.60	114.08	118.00
8	A	940	G	C2-N3-C4	-5.60	109.10	111.90
8	A	1968	G	C4-C5-N7	5.60	113.04	110.80
8	A	1974	C	C6-N1-C2	5.60	122.54	120.30
34	a	482	A	C5-C6-N6	-5.60	119.22	123.70
8	A	1152	C	N3-C4-C5	5.60	124.14	121.90
8	A	1367	A	N1-C6-N6	5.60	121.96	118.60
8	A	2389	G	C6-C5-N7	5.60	133.76	130.40
8	A	2397	G	N1-C2-N2	-5.60	111.16	116.20
34	a	775	G	C2-N3-C4	-5.60	109.10	111.90
34	a	915	A	C8-N9-C4	5.60	108.04	105.80
8	A	704	G	C6-C5-N7	5.60	133.76	130.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	1030	C	C6-N1-C2	5.60	122.54	120.30
8	A	1689	A	C5-C6-N6	-5.60	119.22	123.70
34	a	623	C	C6-N1-C2	5.60	122.54	120.30
34	a	1475	G	C2-N3-C4	-5.60	109.10	111.90
8	A	761	A	C8-N9-C4	5.60	108.04	105.80
8	A	1193	G	C2-N3-C4	-5.60	109.10	111.90
34	a	784	A	C4-C5-N7	5.60	113.50	110.70
8	A	1544	A	N1-C6-N6	5.60	121.96	118.60
8	A	1934	C	N3-C4-N4	-5.60	114.08	118.00
8	A	1230	A	C8-N9-C4	5.59	108.04	105.80
8	A	1451	C	C5-C4-N4	5.59	124.12	120.20
8	A	2320	U	C6-N1-C2	5.59	124.36	121.00
8	A	2854	G	C8-N9-C4	5.59	108.64	106.40
9	B	72	G	N3-C4-C5	5.59	131.40	128.60
34	a	151	A	C5-N7-C8	-5.59	101.10	103.90
34	a	461	A	N3-C4-C5	5.59	130.72	126.80
8	A	23	G	N3-C4-C5	5.59	131.40	128.60
8	A	193	U	C6-N1-C2	5.59	124.36	121.00
8	A	1429	G	C8-N9-C4	5.59	108.64	106.40
8	A	2024	G	N1-C2-N2	-5.59	111.17	116.20
34	a	1375	A	N9-C4-C5	-5.59	103.56	105.80
55	v	46	A	N9-C4-C5	-5.59	103.56	105.80
8	A	211	C	C2-N1-C1'	5.59	124.95	118.80
8	A	522	A	C4-C5-N7	5.59	113.50	110.70
34	a	674	G	N7-C8-N9	5.59	115.89	113.10
37	d	12	ARG	NE-CZ-NH2	-5.59	117.50	120.30
8	A	1345	C	N3-C4-C5	5.59	124.14	121.90
8	A	2217	G	C5-N7-C8	-5.59	101.51	104.30
34	a	535	A	C8-N9-C4	5.59	108.03	105.80
8	A	1532	A	O4'-C1'-N9	-5.58	103.73	108.20
8	A	2191	A	C2-N3-C4	-5.58	107.81	110.60
34	a	898	G	C8-N9-C4	5.58	108.63	106.40
8	A	726	G	N1-C2-N3	5.58	127.25	123.90
8	A	2670	A	C8-N9-C4	5.58	108.03	105.80
8	A	2839	G	C5-C6-N1	-5.58	108.71	111.50
8	A	2340	A	N9-C4-C5	-5.58	103.57	105.80
10	C	216	ARG	CG-CD-NE	5.58	123.52	111.80
8	A	463	G	N3-C4-N9	-5.58	122.65	126.00
8	A	1421	G	C8-N9-C4	5.58	108.63	106.40
8	A	2271	G	O4'-C1'-N9	-5.58	103.74	108.20
8	A	1538	G	C2-N3-C4	-5.57	109.11	111.90
8	A	1696	G	N3-C4-C5	5.57	131.39	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	93	C	C2-N1-C1'	5.57	124.93	118.80
34	a	597	G	N3-C4-N9	-5.57	122.66	126.00
34	a	851	G	C8-N9-C4	5.57	108.63	106.40
8	A	882	G	N3-C4-N9	-5.57	122.66	126.00
8	A	2744	G	N3-C4-N9	-5.57	122.66	126.00
8	A	230	G	N3-C4-C5	5.57	131.38	128.60
8	A	561	G	N3-C4-C5	5.57	131.38	128.60
8	A	628	G	N3-C4-C5	5.57	131.38	128.60
8	A	727	A	O4'-C1'-N9	-5.57	103.74	108.20
8	A	904	G	N3-C4-C5	5.57	131.38	128.60
8	A	922	C	C6-N1-C2	5.57	122.53	120.30
8	A	1708	C	N3-C4-C5	5.57	124.13	121.90
8	A	2150	C	O4'-C1'-N1	5.57	112.66	108.20
34	a	36	C	C6-N1-C2	5.57	122.53	120.30
8	A	855	G	N3-C4-C5	5.57	131.38	128.60
34	a	799	G	N3-C4-C5	5.57	131.38	128.60
8	A	465	G	N3-C4-N9	-5.57	122.66	126.00
8	A	799	G	N3-C4-N9	-5.57	122.66	126.00
8	A	1503	A	N3-C4-C5	5.57	130.70	126.80
8	A	1811	G	N3-C4-C5	5.57	131.38	128.60
8	A	2901	C	N3-C2-O2	-5.57	118.00	121.90
8	A	721	A	C4-C5-N7	5.57	113.48	110.70
34	a	712	A	N9-C4-C5	-5.57	103.57	105.80
34	a	201	G	C6-C5-N7	5.56	133.74	130.40
34	a	337	G	C8-N9-C4	5.56	108.62	106.40
8	A	899	A	C5-C6-N6	-5.56	119.25	123.70
8	A	1137	G	N3-C4-C5	5.56	131.38	128.60
8	A	1767	G	C4-N9-C1'	-5.56	119.27	126.50
8	A	2378	A	C5-N7-C8	-5.56	101.12	103.90
8	A	2481	G	C8-N9-C4	5.56	108.62	106.40
8	A	2890	G	C4-C5-N7	5.56	113.03	110.80
34	a	1353	G	N3-C4-N9	-5.56	122.66	126.00
8	A	1596	A	C8-N9-C4	5.56	108.03	105.80
34	a	15	G	C2-N3-C4	-5.56	109.12	111.90
9	B	101	A	C8-N9-C4	5.56	108.02	105.80
8	A	424	G	N3-C4-N9	-5.56	122.67	126.00
8	A	609	A	C5-C6-N6	-5.56	119.25	123.70
8	A	819	A	C4-C5-N7	5.56	113.48	110.70
8	A	1221	C	N3-C4-C5	5.56	124.12	121.90
8	A	2472	G	C4-N9-C1'	-5.56	119.28	126.50
34	a	43	C	C6-N1-C2	5.56	122.52	120.30
34	a	847	G	N3-C4-N9	-5.56	122.67	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
42	i	86	LEU	CB-CG-CD2	-5.56	101.55	111.00
8	A	470	A	N1-C6-N6	5.56	121.93	118.60
8	A	1333	G	N9-C4-C5	-5.56	103.18	105.40
8	A	1347	A	C4-C5-C6	-5.56	114.22	117.00
34	a	1011	C	C5-C4-N4	5.56	124.09	120.20
8	A	329	G	C8-N9-C4	5.55	108.62	106.40
8	A	1202	G	N3-C4-N9	-5.55	122.67	126.00
8	A	1529	G	N9-C4-C5	-5.55	103.18	105.40
8	A	1715	G	N3-C4-N9	-5.55	122.67	126.00
34	a	402	G	N3-C4-N9	-5.55	122.67	126.00
34	a	623	C	N1-C2-O2	5.55	122.23	118.90
8	A	381	G	C4-N9-C1'	-5.55	119.28	126.50
8	A	997	G	C8-N9-C4	5.55	108.62	106.40
8	A	1215	G	N1-C2-N2	-5.55	111.21	116.20
8	A	1407	G	C2-N3-C4	-5.55	109.13	111.90
34	a	456	A	N7-C8-N9	5.55	116.57	113.80
8	A	1685	C	N3-C4-N4	-5.55	114.12	118.00
8	A	1824	G	N3-C4-C5	5.55	131.37	128.60
8	A	2502	G	C4-N9-C1'	-5.55	119.29	126.50
32	Y	19	LEU	CA-CB-CG	5.55	128.06	115.30
34	a	685	G	N3-C4-N9	-5.55	122.67	126.00
34	a	1329	A	C4-C5-N7	5.55	113.47	110.70
8	A	522	A	N9-C4-C5	-5.54	103.58	105.80
8	A	1384	A	C5-C6-N6	-5.54	119.27	123.70
34	a	1255	G	C8-N9-C4	5.54	108.62	106.40
8	A	1643	G	C5-C6-O6	5.54	131.93	128.60
34	a	1133	G	C2-N3-C4	-5.54	109.13	111.90
8	A	346	A	C5-C6-N6	-5.54	119.27	123.70
8	A	361	G	C8-N9-C1'	-5.54	119.80	127.00
8	A	402	A	N9-C4-C5	-5.54	103.58	105.80
8	A	799	G	N3-C4-C5	5.54	131.37	128.60
8	A	81	G	C8-N9-C4	5.54	108.61	106.40
8	A	124	G	C2-N3-C4	-5.54	109.13	111.90
8	A	881	G	C2-N3-C4	-5.54	109.13	111.90
8	A	1846	G	N3-C4-N9	-5.54	122.68	126.00
8	A	2524	G	C2-N3-C4	-5.54	109.13	111.90
8	A	2852	G	C2-N3-C4	-5.54	109.13	111.90
9	B	106	G	N3-C4-C5	5.54	131.37	128.60
8	A	73	A	N1-C6-N6	-5.54	115.28	118.60
8	A	254	G	C2-N3-C4	-5.54	109.13	111.90
8	A	707	G	C8-N9-C4	5.54	108.61	106.40
8	A	1587	G	C2-N3-C4	-5.54	109.13	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	2899	A	C5-C6-N6	-5.54	119.27	123.70
34	a	682	G	C8-N9-C4	5.54	108.61	106.40
34	a	1293	C	N3-C4-N4	-5.54	114.12	118.00
26	S	82	MET	N-CA-CB	5.54	120.56	110.60
34	a	569	C	N3-C4-C5	5.54	124.11	121.90
8	A	522	A	C5-N7-C8	-5.53	101.13	103.90
8	A	2444	G	C5-C6-O6	5.53	131.92	128.60
9	B	70	C	N3-C4-C5	5.53	124.11	121.90
34	a	225	C	N3-C4-C5	5.53	124.11	121.90
34	a	856	C	C6-N1-C2	5.53	122.51	120.30
34	a	990	C	N3-C4-C5	5.53	124.11	121.90
8	A	134	G	C8-N9-C4	5.53	108.61	106.40
8	A	733	G	N3-C4-C5	5.53	131.37	128.60
8	A	1168	G	C4-C5-N7	5.53	113.01	110.80
8	A	2014	A	O4'-C1'-N9	-5.53	103.78	108.20
8	A	2484	G	N9-C1'-C2'	-5.53	105.92	112.00
34	a	197	A	C4-C5-C6	-5.53	114.24	117.00
55	v	63	G	C2-N3-C4	-5.53	109.14	111.90
8	A	500	G	C2-N3-C4	-5.52	109.14	111.90
8	A	1009	A	N9-C4-C5	-5.52	103.59	105.80
8	A	1055	G	C6-C5-N7	5.52	133.71	130.40
8	A	1358	G	C5-N7-C8	-5.52	101.54	104.30
8	A	361	G	O4'-C1'-N9	-5.52	103.78	108.20
8	A	1473	G	C8-N9-C4	5.52	108.61	106.40
8	A	681	G	N3-C4-C5	5.52	131.36	128.60
34	a	1011	C	C6-N1-C1'	5.52	127.42	120.80
8	A	904	G	C2-N3-C4	-5.52	109.14	111.90
8	A	1349	C	C6-N1-C2	5.52	122.51	120.30
8	A	1593	A	N9-C4-C5	-5.52	103.59	105.80
8	A	2110	G	C8-N9-C4	-5.52	104.19	106.40
34	a	38	G	N3-C4-N9	-5.52	122.69	126.00
34	a	265	G	C8-N9-C4	5.52	108.61	106.40
8	A	1573	G	N3-C4-C5	5.51	131.36	128.60
8	A	2186	G	N7-C8-N9	5.51	115.86	113.10
34	a	474	G	C4-N9-C1'	-5.51	119.33	126.50
34	a	627	G	N3-C4-N9	-5.51	122.69	126.00
34	a	1454	G	N3-C4-N9	-5.51	122.69	126.00
8	A	787	C	C6-N1-C2	5.51	122.50	120.30
8	A	2812	G	N3-C4-N9	-5.51	122.69	126.00
34	a	1302	C	C6-N1-C2	5.51	122.50	120.30
8	A	1749	A	C4-C5-N7	5.51	113.46	110.70
8	A	2127	G	N3-C4-C5	5.51	131.36	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	a	302	G	N3-C4-C5	5.51	131.35	128.60
34	a	588	G	N9-C4-C5	-5.51	103.20	105.40
34	a	1334	G	N3-C4-C5	5.51	131.36	128.60
8	A	160	A	C5'-C4'-O4'	5.51	115.71	109.10
8	A	471	A	C8-N9-C1'	-5.51	117.78	127.70
8	A	775	G	C2-N3-C4	-5.51	109.14	111.90
8	A	1077	A	C5-C6-N6	-5.51	119.29	123.70
8	A	2379	G	C2-N3-C4	-5.51	109.14	111.90
9	B	96	G	N3-C4-N9	-5.51	122.69	126.00
8	A	2767	C	C5-C6-N1	-5.51	118.25	121.00
8	A	1191	G	C8-N9-C4	5.51	108.60	106.40
8	A	2557	G	C2-N3-C4	-5.51	109.15	111.90
9	B	117	G	C2-N3-C4	-5.51	109.15	111.90
34	a	776	G	C8-N9-C4	5.51	108.60	106.40
34	a	1044	A	N9-C4-C5	-5.51	103.60	105.80
34	a	1175	G	N3-C4-C5	5.51	131.35	128.60
34	a	1296	C	C6-N1-C2	5.51	122.50	120.30
8	A	2575	C	C2-N3-C4	-5.50	117.15	119.90
8	A	2875	C	N1-C2-O2	5.50	122.20	118.90
8	A	936	A	C5-N7-C8	-5.50	101.15	103.90
8	A	1220	G	C8-N9-C1'	5.50	134.16	127.00
8	A	1845	G	C2-N3-C4	-5.50	109.15	111.90
8	A	2730	C	N3-C4-C5	5.50	124.10	121.90
34	a	1155	A	C2-N3-C4	-5.50	107.85	110.60
34	a	278	G	C4-N9-C1'	-5.50	119.35	126.50
34	a	424	G	N3-C4-C5	5.50	131.35	128.60
34	a	1252	A	C8-N9-C4	5.50	108.00	105.80
34	a	1323	G	N9-C4-C5	-5.50	103.20	105.40
8	A	1888	G	N3-C4-N9	-5.50	122.70	126.00
8	A	939	G	N3-C4-N9	-5.50	122.70	126.00
34	a	635	A	N9-C4-C5	-5.50	103.60	105.80
8	A	177	G	O4'-C1'-N9	5.50	112.60	108.20
8	A	2802	G	N3-C4-C5	5.50	131.35	128.60
34	a	613	C	C2-N1-C1'	5.50	124.85	118.80
8	A	899	A	N9-C1'-C2'	-5.50	105.95	112.00
8	A	1039	A	N1-C6-N6	5.50	121.90	118.60
8	A	2416	C	C6-N1-C2	5.50	122.50	120.30
8	A	733	G	N3-C4-N9	-5.49	122.70	126.00
8	A	815	C	C6-N1-C1'	-5.49	114.21	120.80
8	A	1226	A	C4-C5-C6	-5.49	114.25	117.00
8	A	1514	G	C5-C6-O6	-5.49	125.30	128.60
8	A	2284	A	C8-N9-C4	5.49	108.00	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	493	G	N3-C4-N9	-5.49	122.70	126.00
8	A	708	G	N3-C4-N9	-5.49	122.70	126.00
34	a	1347	G	C4-N9-C1'	-5.49	119.36	126.50
8	A	695	G	C8-N9-C4	5.49	108.60	106.40
8	A	857	G	O4'-C1'-N9	-5.49	103.81	108.20
8	A	1619	G	C2-N3-C4	-5.49	109.15	111.90
8	A	1945	G	N9-C4-C5	-5.49	103.20	105.40
8	A	2253	G	N3-C4-N9	-5.49	122.71	126.00
34	a	77	A	N3-C4-C5	5.49	130.64	126.80
34	a	456	A	C6-N1-C2	-5.49	115.31	118.60
8	A	1291	C	C6-N1-C2	5.49	122.50	120.30
8	A	2293	G	N3-C4-C5	5.49	131.34	128.60
8	A	2338	C	N3-C4-N4	-5.49	114.16	118.00
34	a	1335	U	O4'-C1'-N1	-5.49	103.81	108.20
8	A	56	A	C4-C5-N7	5.49	113.44	110.70
8	A	489	G	C8-N9-C4	5.49	108.59	106.40
8	A	1910	G	C8-N9-C4	5.49	108.59	106.40
8	A	875	G	N3-C4-N9	-5.49	122.71	126.00
8	A	1445	G	C2-N3-C4	-5.49	109.16	111.90
34	a	203	G	N3-C4-N9	-5.49	122.71	126.00
8	A	1151	A	N9-C4-C5	-5.48	103.61	105.80
34	a	1454	G	C8-N9-C4	5.48	108.59	106.40
34	a	158	G	C4-C5-N7	5.48	112.99	110.80
34	a	177	G	C5-N7-C8	-5.48	101.56	104.30
34	a	177	G	N7-C8-N9	5.48	115.84	113.10
34	a	300	A	N1-C6-N6	5.48	121.89	118.60
34	a	385	C	N3-C4-N4	-5.48	114.16	118.00
34	a	624	C	N3-C2-O2	-5.48	118.06	121.90
8	A	895	U	O4'-C1'-N1	5.48	112.58	108.20
8	A	930	G	C4-N9-C1'	-5.48	119.38	126.50
8	A	1567	G	C2-N3-C4	-5.48	109.16	111.90
8	A	793	A	N9-C4-C5	-5.48	103.61	105.80
8	A	1723	G	N3-C4-N9	-5.48	122.71	126.00
8	A	1965	C	C6-N1-C2	5.48	122.49	120.30
8	A	2618	G	N3-C4-N9	-5.48	122.71	126.00
34	a	1288	A	N9-C4-C5	-5.48	103.61	105.80
8	A	1180	U	C6-N1-C2	5.48	124.29	121.00
8	A	1587	G	N3-C4-N9	-5.48	122.71	126.00
8	A	2574	G	N1-C6-O6	-5.48	116.61	119.90
34	a	1058	G	N3-C4-C5	5.48	131.34	128.60
8	A	2525	G	N7-C8-N9	-5.48	110.36	113.10
8	A	376	G	C2-N3-C4	-5.47	109.16	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	50	A	C4-C5-N7	5.47	113.44	110.70
34	a	188	C	N1-C1'-C2'	-5.47	105.98	112.00
34	a	897	C	C6-N1-C2	5.47	122.49	120.30
8	A	16	C	N3-C4-N4	-5.47	114.17	118.00
8	A	718	A	C8-N9-C4	5.47	107.99	105.80
56	w	68	C	N3-C4-N4	-5.47	114.17	118.00
8	A	828	U	O4'-C1'-N1	-5.47	103.82	108.20
8	A	1861	G	C2-N3-C4	-5.47	109.17	111.90
8	A	2169	A	O4'-C1'-N9	5.47	112.58	108.20
8	A	2857	G	C8-N9-C1'	5.47	134.11	127.00
9	B	21	G	C4-C5-N7	5.47	112.99	110.80
9	B	77	U	C6-N1-C2	5.47	124.28	121.00
34	a	539	A	N9-C4-C5	-5.47	103.61	105.80
34	a	1337	G	N3-C4-C5	5.47	131.34	128.60
8	A	2505	G	N3-C2-N2	5.47	123.73	119.90
8	A	841	G	N3-C4-C5	5.47	131.33	128.60
8	A	989	G	C2-N3-C4	-5.47	109.17	111.90
8	A	1226	A	C5-C6-N1	5.47	120.43	117.70
8	A	2051	A	C5-C6-N6	-5.47	119.33	123.70
34	a	681	A	C4-C5-N7	5.47	113.43	110.70
34	a	1209	C	N3-C4-C5	5.47	124.09	121.90
8	A	1017	G	C8-N9-C4	5.46	108.58	106.40
8	A	1222	U	C6-N1-C2	5.46	124.28	121.00
8	A	1416	G	N3-C4-N9	-5.46	122.72	126.00
8	A	2121	G	N3-C4-N9	5.46	129.28	126.00
8	A	217	A	C4-C5-C6	-5.46	114.27	117.00
34	a	765	G	C2-N3-C4	-5.46	109.17	111.90
8	A	189	G	N9-C4-C5	-5.46	103.22	105.40
8	A	586	A	N9-C4-C5	-5.46	103.62	105.80
8	A	759	G	N3-C4-C5	5.46	131.33	128.60
8	A	1261	C	N3-C4-C5	5.46	124.08	121.90
8	A	1600	C	N3-C4-N4	-5.46	114.18	118.00
8	A	2579	C	N1-C2-O2	5.46	122.18	118.90
34	a	141	G	C2-N3-C4	-5.46	109.17	111.90
34	a	587	G	N3-C4-C5	5.46	131.33	128.60
8	A	2190	G	C5-C6-N1	-5.46	108.77	111.50
34	a	484	G	N3-C4-C5	5.46	131.33	128.60
8	A	400	G	N9-C4-C5	-5.46	103.22	105.40
8	A	869	G	N3-C4-C5	5.46	131.33	128.60
8	A	1368	G	C8-N9-C4	5.46	108.58	106.40
8	A	2217	G	C4-C5-N7	5.46	112.98	110.80
8	A	2767	C	N3-C4-N4	-5.46	114.18	118.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	a	547	A	C8-N9-C4	5.46	107.98	105.80
34	a	744	C	N3-C4-N4	-5.46	114.18	118.00
8	A	220	G	N7-C8-N9	5.46	115.83	113.10
8	A	471	A	C6-C5-N7	-5.46	128.48	132.30
8	A	640	C	C2-N1-C1'	5.46	124.80	118.80
8	A	1540	G	N3-C4-N9	-5.46	122.73	126.00
8	A	2373	G	N3-C4-N9	-5.46	122.73	126.00
34	a	525	C	C6-N1-C2	5.46	122.48	120.30
34	a	627	G	C4-N9-C1'	-5.46	119.41	126.50
34	a	675	A	N7-C8-N9	5.46	116.53	113.80
34	a	688	G	C2-N3-C4	-5.46	109.17	111.90
34	a	453	G	N1-C2-N2	-5.46	111.29	116.20
8	A	7	G	C2-N3-C4	-5.45	109.17	111.90
8	A	951	C	N3-C4-N4	-5.45	114.18	118.00
8	A	1862	G	C2-N3-C4	-5.45	109.17	111.90
8	A	1865	U	O4'-C1'-N1	5.45	112.56	108.20
34	a	1109	C	C6-N1-C2	5.45	122.48	120.30
56	w	5	G	N3-C4-C5	5.45	131.33	128.60
8	A	45	G	C8-N9-C4	5.45	108.58	106.40
8	A	514	A	C8-N9-C4	5.45	107.98	105.80
8	A	60	G	N3-C4-N9	-5.45	122.73	126.00
8	A	2413	G	C5-C6-O6	5.45	131.87	128.60
34	a	309	A	C8-N9-C4	5.45	107.98	105.80
34	a	1289	A	C8-N9-C4	5.45	107.98	105.80
8	A	212	G	N3-C4-N9	-5.45	122.73	126.00
8	A	1540	G	C5-N7-C8	-5.45	101.58	104.30
8	A	1908	C	N3-C4-C5	5.45	124.08	121.90
34	a	1288	A	C4-C5-N7	5.45	113.42	110.70
34	a	1310	G	C2-N3-C4	-5.45	109.18	111.90
8	A	73	A	C4-C5-C6	-5.45	114.28	117.00
8	A	1346	G	C2-N3-C4	-5.45	109.18	111.90
8	A	1713	A	N3-C4-C5	5.45	130.61	126.80
8	A	2862	G	C2-N3-C4	-5.45	109.18	111.90
34	a	168	G	N1-C6-O6	-5.45	116.63	119.90
34	a	601	G	N3-C4-C5	5.45	131.32	128.60
8	A	261	G	C2-N3-C4	-5.44	109.18	111.90
8	A	301	G	O4'-C1'-N9	5.44	112.56	108.20
8	A	1398	C	C6-N1-C2	5.44	122.48	120.30
8	A	1768	C	C6-N1-C2	5.44	122.48	120.30
8	A	2600	A	C8-N9-C4	5.44	107.98	105.80
8	A	487	C	N3-C2-O2	-5.44	118.09	121.90
8	A	793	A	C8-N9-C4	5.44	107.98	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	1728	C	C2-N1-C1'	-5.44	112.81	118.80
8	A	2164	C	C5-C4-N4	-5.44	116.39	120.20
9	B	69	G	N3-C4-C5	5.44	131.32	128.60
34	a	1210	C	N3-C4-C5	5.44	124.08	121.90
34	a	1255	G	N3-C4-N9	-5.44	122.73	126.00
8	A	1755	A	C5-C6-N6	5.44	128.05	123.70
8	A	2732	G	O4'-C1'-N9	-5.44	103.85	108.20
34	a	849	G	N3-C4-N9	-5.44	122.73	126.00
34	a	1034	G	N3-C4-N9	-5.44	122.73	126.00
56	w	27	G	N3-C4-C5	5.44	131.32	128.60
8	A	1863	G	N3-C4-N9	-5.44	122.74	126.00
8	A	1448	G	C2-N3-C4	-5.44	109.18	111.90
8	A	2603	G	C2-N3-C4	-5.44	109.18	111.90
34	a	407	U	C6-N1-C2	5.44	124.26	121.00
34	a	1011	C	P-O3'-C3'	-5.44	113.18	119.70
8	A	214	G	C2-N3-C4	-5.44	109.18	111.90
8	A	891	G	C2-N3-C4	-5.44	109.18	111.90
8	A	1171	G	N7-C8-N9	5.44	115.82	113.10
8	A	1556	C	N3-C4-N4	-5.43	114.20	118.00
34	a	1226	C	N3-C4-C5	5.43	124.07	121.90
8	A	1126	A	C5-C6-N6	-5.43	119.35	123.70
8	A	2869	G	N3-C4-C5	5.43	131.32	128.60
34	a	786	G	C2-N3-C4	-5.43	109.18	111.90
34	a	1476	A	N9-C4-C5	-5.43	103.63	105.80
8	A	1124	G	N3-C4-N9	-5.43	122.74	126.00
8	A	1518	C	N3-C4-C5	5.43	124.07	121.90
34	a	107	G	C8-N9-C4	5.43	108.57	106.40
34	a	698	G	N3-C4-C5	5.43	131.31	128.60
34	a	778	G	N3-C2-N2	-5.43	116.10	119.90
34	a	1467	C	C6-N1-C2	5.43	122.47	120.30
8	A	56	A	C8-N9-C4	5.43	107.97	105.80
8	A	186	G	N3-C4-C5	5.43	131.31	128.60
8	A	1492	G	C4-C5-C6	-5.43	115.54	118.80
8	A	2576	G	N3-C4-C5	5.43	131.31	128.60
34	a	1431	A	C8-N9-C4	5.43	107.97	105.80
8	A	103	A	C4-C5-N7	5.43	113.41	110.70
8	A	1519	G	N3-C4-N9	-5.43	122.74	126.00
8	A	1577	C	N1-C2-O2	5.43	122.16	118.90
34	a	1362	A	C5-C6-N1	5.43	120.41	117.70
34	a	1482	G	N3-C4-C5	5.43	131.31	128.60
8	A	597	G	C2-N3-C4	-5.42	109.19	111.90
8	A	2170	A	C4-N9-C1'	-5.42	116.54	126.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	2894	G	C2-N3-C4	-5.42	109.19	111.90
34	a	600	A	C8-N9-C4	5.42	107.97	105.80
8	A	203	A	C5-N7-C8	-5.42	101.19	103.90
8	A	1553	A	C4-C5-N7	5.42	113.41	110.70
8	A	211	C	C6-N1-C1'	-5.42	114.29	120.80
8	A	1429	G	N3-C4-C5	5.42	131.31	128.60
8	A	1521	G	N3-C4-N9	-5.42	122.75	126.00
8	A	2865	U	C6-N1-C2	5.42	124.25	121.00
34	a	1050	G	C6-C5-N7	5.42	133.65	130.40
8	A	551	G	C8-N9-C4	5.42	108.57	106.40
8	A	2435	A	C4-C5-N7	5.42	113.41	110.70
34	a	432	A	C4-C5-N7	5.42	113.41	110.70
34	a	1179	A	C8-N9-C4	5.42	107.97	105.80
34	a	1272	G	C2-N3-C4	-5.42	109.19	111.90
34	a	1416	G	N3-C4-C5	5.42	131.31	128.60
8	A	916	G	C5-N7-C8	-5.42	101.59	104.30
34	a	587	G	C8-N9-C4	5.42	108.57	106.40
34	a	1039	G	N3-C4-N9	-5.42	122.75	126.00
34	a	1454	G	C2-N3-C4	-5.42	109.19	111.90
8	A	2190	G	C6-N1-C2	5.42	128.35	125.10
34	a	39	G	C2-N3-C4	-5.42	109.19	111.90
34	a	497	G	N3-C4-N9	-5.42	122.75	126.00
34	a	1044	A	C5-N7-C8	-5.42	101.19	103.90
34	a	1161	C	C6-N1-C2	5.42	122.47	120.30
34	a	1289	A	C5-N7-C8	-5.42	101.19	103.90
8	A	739	A	O4'-C1'-N9	-5.42	103.87	108.20
8	A	836	G	N3-C4-C5	5.42	131.31	128.60
8	A	2315	G	C2-N3-C4	-5.42	109.19	111.90
8	A	2414	G	C5-C6-O6	5.41	131.85	128.60
8	A	2663	G	C4-N9-C1'	-5.41	119.46	126.50
9	B	108	A	C4-C5-N7	5.41	113.41	110.70
34	a	258	G	C2-N3-C4	-5.41	109.19	111.90
8	A	66	C	N3-C4-N4	-5.41	114.21	118.00
8	A	460	A	N9-C4-C5	-5.41	103.64	105.80
8	A	1804	C	N3-C4-C5	5.41	124.06	121.90
8	A	2644	G	C2-N3-C4	-5.41	109.19	111.90
34	a	138	G	N3-C4-C5	5.41	131.31	128.60
34	a	497	G	C2-N3-C4	-5.41	109.19	111.90
34	a	923	A	C5-N7-C8	-5.41	101.19	103.90
8	A	43	G	C8-N9-C4	5.41	108.56	106.40
8	A	327	G	C2-N3-C4	-5.41	109.19	111.90
8	A	559	G	C8-N9-C4	5.41	108.56	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	757	G	N3-C4-N9	-5.41	122.75	126.00
8	A	1354	A	N1-C6-N6	5.41	121.85	118.60
8	A	2844	G	O4'-C1'-N9	-5.41	103.87	108.20
34	a	1047	G	C8-N9-C4	5.41	108.56	106.40
8	A	15	G	N1-C2-N2	-5.41	111.33	116.20
8	A	1450	G	C5-C6-N1	-5.41	108.80	111.50
34	a	1186	G	C8-N9-C4	5.41	108.56	106.40
34	a	1489	G	C2-N3-C4	-5.41	109.19	111.90
8	A	1277	G	C4-N9-C1'	-5.41	119.47	126.50
34	a	488	C	C2-N1-C1'	5.41	124.75	118.80
8	A	230	G	N3-C4-N9	-5.41	122.76	126.00
8	A	1075	C	N3-C4-N4	-5.41	114.22	118.00
8	A	1161	C	C6-N1-C2	5.41	122.46	120.30
8	A	1459	G	C2-N3-C4	-5.41	109.20	111.90
9	B	100	G	C8-N9-C4	5.41	108.56	106.40
34	a	851	G	C8-N9-C1'	-5.41	119.97	127.00
8	A	925	A	C4-C5-N7	5.40	113.40	110.70
8	A	2315	G	N3-C4-C5	5.40	131.30	128.60
8	A	2819	G	C2-N3-C4	-5.40	109.20	111.90
8	A	617	G	N3-C4-C5	5.40	131.30	128.60
34	a	413	G	N3-C2-N2	-5.40	116.12	119.90
8	A	231	A	C2-N3-C4	-5.40	107.90	110.60
8	A	383	C	C6-N1-C2	5.40	122.46	120.30
34	a	81	A	C5-N7-C8	-5.40	101.20	103.90
34	a	413	G	N3-C4-N9	-5.40	122.76	126.00
34	a	1075	U	C2-N1-C1'	5.40	124.18	117.70
34	a	1154	G	C8-N9-C4	5.40	108.56	106.40
8	A	1278	C	N3-C4-C5	5.40	124.06	121.90
34	a	675	A	C5-C6-N6	-5.40	119.38	123.70
8	A	656	G	C2-N3-C4	-5.40	109.20	111.90
8	A	1160	G	N3-C4-N9	-5.40	122.76	126.00
8	A	2097	A	C5-N7-C8	-5.40	101.20	103.90
8	A	2801	G	N3-C4-C5	5.40	131.30	128.60
9	B	84	G	C2-N3-C4	-5.40	109.20	111.90
34	a	903	G	N3-C4-N9	-5.40	122.76	126.00
34	a	1092	A	N3-C4-N9	-5.40	123.08	127.40
34	a	1215	G	N3-C4-C5	5.40	131.30	128.60
8	A	2	G	N3-C4-C5	5.40	131.30	128.60
8	A	1041	G	N3-C4-N9	-5.39	122.76	126.00
8	A	1336	A	N9-C4-C5	-5.39	103.64	105.80
34	a	1081	A	N3-C4-N9	5.39	131.72	127.40
8	A	24	G	C8-N9-C4	5.39	108.56	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	68	G	N3-C4-C5	5.39	131.30	128.60
8	A	1189	A	C2-N3-C4	-5.39	107.90	110.60
8	A	122	G	O5'-P-OP2	-5.39	100.85	105.70
8	A	1518	C	C6-N1-C2	5.39	122.46	120.30
8	A	1577	C	N3-C4-N4	-5.39	114.23	118.00
8	A	2813	A	C4-C5-C6	-5.39	114.31	117.00
34	a	86	G	C4-C5-N7	5.39	112.96	110.80
34	a	280	C	C6-N1-C2	5.39	122.46	120.30
34	a	742	G	N1-C2-N2	5.39	121.05	116.20
34	a	39	G	N3-C4-N9	-5.39	122.77	126.00
34	a	1294	G	C4-C5-N7	5.39	112.95	110.80
34	a	831	A	N3-C4-C5	5.39	130.57	126.80
8	A	851	C	C6-N1-C2	5.38	122.45	120.30
8	A	1459	G	C5-C6-O6	5.38	131.83	128.60
34	a	299	G	N3-C4-C5	5.38	131.29	128.60
8	A	1107	G	C2-N3-C4	-5.38	109.21	111.90
34	a	1142	G	N3-C4-N9	-5.38	122.77	126.00
8	A	30	G	C5-C6-O6	5.38	131.83	128.60
8	A	1212	G	N3-C4-N9	-5.38	122.77	126.00
8	A	2610	C	O4'-C1'-N1	5.38	112.50	108.20
34	a	141	G	N9-C1'-C2'	-5.38	106.08	112.00
34	a	548	G	C8-N9-C4	5.38	108.55	106.40
8	A	560	C	N3-C4-C5	5.38	124.05	121.90
8	A	1202	G	C4-N9-C1'	-5.38	119.51	126.50
8	A	1099	G	C5-C6-O6	5.38	131.83	128.60
8	A	2193	G	N3-C4-C5	5.38	131.29	128.60
8	A	2315	G	C8-N9-C1'	5.38	133.99	127.00
34	a	288	A	C8-N9-C4	5.38	107.95	105.80
34	a	350	G	N3-C4-C5	5.38	131.29	128.60
34	a	1175	G	N3-C4-N9	-5.38	122.77	126.00
8	A	666	A	C8-N9-C4	5.38	107.95	105.80
8	A	1561	C	N3-C4-C5	5.38	124.05	121.90
8	A	1947	C	C6-N1-C2	5.38	122.45	120.30
34	a	1204	A	C8-N9-C4	5.38	107.95	105.80
8	A	180	G	C8-N9-C4	5.38	108.55	106.40
8	A	1100	C	N3-C4-N4	-5.38	114.24	118.00
8	A	1276	A	N9-C4-C5	-5.38	103.65	105.80
8	A	1042	G	N3-C4-C5	5.37	131.29	128.60
8	A	2405	G	C4-N9-C1'	-5.37	119.51	126.50
34	a	887	G	N3-C4-N9	-5.37	122.78	126.00
34	a	1144	G	N3-C4-C5	5.37	131.29	128.60
8	A	621	A	O5'-P-OP2	-5.37	100.87	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	1028	A	N9-C1'-C2'	-5.37	106.09	112.00
8	A	1112	G	N3-C2-N2	-5.37	116.14	119.90
8	A	1177	G	N3-C2-N2	-5.37	116.14	119.90
8	A	1450	G	O4'-C1'-N9	-5.37	103.90	108.20
34	a	876	C	C6-N1-C1'	-5.37	114.35	120.80
8	A	1110	G	C2-N3-C4	-5.37	109.22	111.90
8	A	1389	G	C2-N3-C4	-5.37	109.22	111.90
9	B	65	U	C6-N1-C2	5.37	124.22	121.00
26	S	42	LYS	N-CA-CB	-5.37	100.94	110.60
8	A	394	C	N3-C4-N4	-5.37	114.24	118.00
8	A	1095	A	C2-N3-C4	-5.37	107.92	110.60
15	H	58	LEU	CB-CG-CD2	5.37	120.13	111.00
34	a	640	A	C4-C5-C6	-5.37	114.32	117.00
8	A	1423	G	C8-N9-C4	5.37	108.55	106.40
8	A	1631	G	C8-N9-C1'	5.37	133.97	127.00
8	A	2490	G	N3-C4-C5	5.37	131.28	128.60
8	A	2640	G	C8-N9-C4	5.37	108.55	106.40
8	A	2655	G	N3-C4-N9	-5.37	122.78	126.00
34	a	270	A	C5-N7-C8	-5.37	101.22	103.90
8	A	290	U	N3-C2-O2	5.36	125.95	122.20
8	A	1049	C	N3-C4-C5	5.36	124.05	121.90
8	A	1241	A	N1-C6-N6	5.36	121.82	118.60
8	A	1475	G	C8-N9-C4	5.36	108.55	106.40
34	a	445	G	C8-N9-C1'	5.36	133.97	127.00
34	a	898	G	N3-C4-N9	-5.36	122.78	126.00
34	a	1044	A	C4-C5-N7	5.36	113.38	110.70
8	A	1735	A	C5-C6-N6	-5.36	119.41	123.70
8	A	670	A	C5-C6-N6	-5.36	119.41	123.70
8	A	1054	A	N1-C6-N6	5.36	121.82	118.60
8	A	2383	G	C2-N3-C4	-5.36	109.22	111.90
34	a	492	C	C6-N1-C1'	5.36	127.23	120.80
8	A	220	G	N1-C2-N3	5.36	127.11	123.90
8	A	556	A	N1-C6-N6	5.36	121.81	118.60
8	A	1107	G	N3-C4-N9	-5.36	122.78	126.00
14	G	94	ARG	NE-CZ-NH2	-5.36	117.62	120.30
8	A	410	G	C2-N3-C4	-5.36	109.22	111.90
8	A	1128	G	N3-C4-N9	-5.36	122.79	126.00
8	A	2485	G	O4'-C1'-N9	-5.36	103.92	108.20
8	A	260	G	C8-N9-C4	5.35	108.54	106.40
8	A	2128	G	N3-C4-N9	-5.35	122.79	126.00
8	A	36	G	N3-C4-C5	5.35	131.28	128.60
8	A	1820	U	C6-N1-C2	5.35	124.21	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	2281	A	C4-C5-N7	5.35	113.38	110.70
34	a	339	C	C5-C4-N4	5.35	123.95	120.20
34	a	1097	C	C6-N1-C1'	-5.35	114.38	120.80
8	A	1522	A	C5-C6-N6	-5.35	119.42	123.70
8	A	2505	G	N1-C2-N2	-5.35	111.38	116.20
8	A	152	A	C4-C5-N7	5.35	113.38	110.70
34	a	599	C	N3-C4-C5	5.35	124.04	121.90
8	A	797	G	N3-C4-C5	5.35	131.27	128.60
8	A	1561	C	C6-N1-C2	5.35	122.44	120.30
8	A	1590	A	C4-C5-N7	5.35	113.37	110.70
8	A	2494	G	C8-N9-C4	5.35	108.54	106.40
8	A	2551	C	C5-C4-N4	5.35	123.94	120.20
20	M	133	LYS	CD-CE-NZ	5.35	124.00	111.70
34	a	246	A	N3-C4-C5	5.35	130.54	126.80
34	a	896	C	C6-N1-C2	5.35	122.44	120.30
34	a	1150	A	N7-C8-N9	5.35	116.47	113.80
34	a	1222	G	N3-C2-N2	-5.35	116.16	119.90
34	a	1333	A	N1-C6-N6	5.35	121.81	118.60
34	a	1379	G	N3-C4-N9	-5.35	122.79	126.00
34	a	1525	G	C2-N3-C4	-5.35	109.23	111.90
8	A	1280	G	C8-N9-C4	5.35	108.54	106.40
9	B	64	G	N9-C4-C5	-5.35	103.26	105.40
8	A	326	G	C4-N9-C1'	-5.34	119.55	126.50
8	A	734	A	N1-C6-N6	-5.34	115.39	118.60
8	A	2418	A	N9-C4-C5	-5.34	103.66	105.80
8	A	2502	G	N3-C4-N9	-5.34	122.79	126.00
8	A	2868	A	C5-C6-N6	-5.34	119.42	123.70
9	B	33	G	C2-N3-C4	-5.34	109.23	111.90
34	a	1276	G	C2-N3-C4	-5.34	109.23	111.90
8	A	307	G	N3-C4-N9	-5.34	122.80	126.00
8	A	1426	G	N3-C4-N9	-5.34	122.80	126.00
8	A	2545	G	N1-C2-N3	5.34	127.11	123.90
34	a	1367	C	N3-C4-C5	5.34	124.04	121.90
8	A	273	G	C4-C5-N7	5.34	112.94	110.80
8	A	1022	G	N1-C2-N2	5.34	121.00	116.20
8	A	2150	C	C6-N1-C2	5.34	122.44	120.30
8	A	2525	G	C6-C5-N7	5.34	133.60	130.40
9	B	32	U	C6-N1-C2	5.34	124.20	121.00
34	a	1157	A	C4-C5-C6	-5.34	114.33	117.00
34	a	1499	A	N1-C6-N6	5.34	121.80	118.60
55	v	64	G	N3-C4-N9	-5.34	122.80	126.00
8	A	1928	A	C5-C6-N6	-5.34	119.43	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	a	1294	G	C2-N3-C4	-5.34	109.23	111.90
8	A	407	G	C2-N3-C4	-5.34	109.23	111.90
8	A	718	A	C4-C5-N7	5.34	113.37	110.70
8	A	2353	G	C2-N3-C4	-5.34	109.23	111.90
8	A	2373	G	C2-N3-C4	-5.34	109.23	111.90
34	a	554	A	N1-C6-N6	-5.34	115.40	118.60
34	a	1392	G	N3-C4-C5	5.34	131.27	128.60
8	A	1140	C	N3-C4-C5	5.33	124.03	121.90
34	a	324	G	N3-C4-C5	5.33	131.27	128.60
34	a	1230	C	N3-C2-O2	-5.33	118.17	121.90
34	a	1417	G	C8-N9-C4	5.33	108.53	106.40
56	w	20	U	C2'-C3'-O3'	5.33	122.24	113.70
8	A	679	C	N3-C4-C5	5.33	124.03	121.90
8	A	765	C	C6-N1-C2	5.33	122.43	120.30
8	A	2094	A	C8-N9-C4	5.33	107.93	105.80
8	A	2237	G	N3-C4-N9	-5.33	122.80	126.00
34	a	351	G	O4'-C1'-N9	-5.33	103.93	108.20
34	a	530	G	N3-C4-C5	5.33	131.27	128.60
34	a	1226	C	N3-C4-N4	-5.33	114.27	118.00
34	a	1365	G	N3-C4-C5	5.33	131.27	128.60
34	a	1366	C	C6-N1-C2	5.33	122.43	120.30
8	A	374	A	C5-C6-N6	-5.33	119.44	123.70
8	A	727	A	C8-N9-C1'	-5.33	118.10	127.70
8	A	2526	G	N3-C4-N9	-5.33	122.80	126.00
34	a	567	G	N3-C4-C5	5.33	131.26	128.60
8	A	2863	C	C6-N1-C1'	-5.33	114.40	120.80
34	a	102	G	C4-N9-C1'	-5.33	119.57	126.50
34	a	1099	G	N3-C4-N9	-5.33	122.80	126.00
34	a	1158	C	O4'-C1'-N1	5.33	112.46	108.20
8	A	364	C	C6-N1-C2	5.33	122.43	120.30
8	A	1685	C	N3-C4-C5	5.33	124.03	121.90
9	B	105	G	C2-N3-C4	-5.33	109.24	111.90
34	a	52	C	C6-N1-C2	5.33	122.43	120.30
34	a	696	A	C4-C5-N7	5.33	113.36	110.70
34	a	1405	G	C6-C5-N7	5.33	133.60	130.40
45	l	73	LEU	CA-CB-CG	-5.33	103.04	115.30
8	A	146	A	C5-N7-C8	-5.33	101.24	103.90
8	A	2349	G	C8-N9-C4	5.33	108.53	106.40
34	a	853	C	C6-N1-C2	5.33	122.43	120.30
34	a	859	G	C4-N9-C1'	-5.33	119.57	126.50
8	A	904	G	C5-N7-C8	-5.33	101.64	104.30
8	A	1449	G	C2-N3-C4	-5.33	109.24	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	1454	C	C6-N1-C2	5.33	122.43	120.30
8	A	2303	G	N3-C4-C5	5.33	131.26	128.60
20	M	97	GLN	CA-CB-CG	-5.33	101.68	113.40
34	a	1088	G	N1-C2-N3	5.33	127.10	123.90
8	A	7	G	N3-C4-C5	5.32	131.26	128.60
8	A	1358	G	O4'-C1'-N9	-5.32	103.94	108.20
34	a	53	A	C4-C5-C6	-5.32	114.34	117.00
51	r	67	LEU	CA-CB-CG	-5.32	103.06	115.30
8	A	1202	G	C4-C5-C6	-5.32	115.61	118.80
8	A	1423	G	C4-N9-C1'	-5.32	119.58	126.50
8	A	1522	A	C4-C5-C6	-5.32	114.34	117.00
34	a	101	A	C4-N9-C1'	-5.32	116.72	126.30
8	A	429	A	C5-N7-C8	-5.32	101.24	103.90
34	a	175	C	C5-C6-N1	-5.32	118.34	121.00
34	a	386	C	N3-C4-N4	-5.32	114.28	118.00
8	A	359	G	C2-N3-C4	-5.32	109.24	111.90
8	A	1607	C	C6-N1-C2	5.32	122.43	120.30
8	A	2186	G	C5-N7-C8	-5.32	101.64	104.30
34	a	633	G	C2-N3-C4	-5.32	109.24	111.90
34	a	733	G	N3-C4-C5	5.32	131.26	128.60
8	A	651	G	N3-C4-C5	5.32	131.26	128.60
8	A	1124	G	C2-N3-C4	-5.32	109.24	111.90
8	A	1138	G	N1-C6-O6	-5.32	116.71	119.90
9	B	105	G	N3-C4-N9	-5.32	122.81	126.00
34	a	257	G	N3-C4-N9	-5.32	122.81	126.00
34	a	811	C	C6-N1-C1'	-5.32	114.42	120.80
34	a	592	G	C4-N9-C1'	-5.31	119.59	126.50
34	a	1034	G	N3-C4-C5	5.31	131.26	128.60
8	A	1280	G	N3-C4-C5	5.31	131.26	128.60
8	A	1281	G	C2-N3-C4	-5.31	109.24	111.90
9	B	88	C	C6-N1-C1'	-5.31	114.42	120.80
34	a	1082	A	O4'-C1'-N9	5.31	112.45	108.20
55	v	6	G	C2-N3-C4	-5.31	109.24	111.90
8	A	1074	G	C8-N9-C1'	5.31	133.91	127.00
57	x	30	LEU	CA-CB-CG	5.31	127.52	115.30
8	A	463	G	C2-N3-C4	-5.31	109.25	111.90
8	A	1738	G	C2-N3-C4	-5.31	109.25	111.90
8	A	2647	U	C6-N1-C2	5.31	124.19	121.00
8	A	2848	G	C4-N9-C1'	-5.31	119.60	126.50
8	A	1156	A	N9-C4-C5	-5.31	103.68	105.80
34	a	306	A	N9-C1'-C2'	-5.31	106.16	112.00
34	a	635	A	C5-N7-C8	-5.31	101.25	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	a	768	A	N3-C4-C5	5.31	130.51	126.80
34	a	833	G	C4-N9-C1'	-5.31	119.60	126.50
8	A	1743	G	N3-C4-N9	-5.31	122.82	126.00
8	A	2235	G	C4-C5-C6	-5.31	115.62	118.80
34	a	98	A	N3-C4-C5	5.31	130.51	126.80
8	A	297	G	C2-N3-C4	-5.30	109.25	111.90
8	A	330	A	O4'-C1'-N9	5.30	112.44	108.20
8	A	2843	G	C8-N9-C4	5.30	108.52	106.40
34	a	26	A	C8-N9-C4	5.30	107.92	105.80
8	A	136	G	N3-C4-N9	-5.30	122.82	126.00
34	a	377	G	N3-C4-C5	5.30	131.25	128.60
34	a	1180	A	C5-C6-N6	-5.30	119.46	123.70
34	a	1435	G	C5-C6-O6	5.30	131.78	128.60
8	A	705	A	N9-C4-C5	-5.30	103.68	105.80
8	A	1171	G	N9-C4-C5	5.30	107.52	105.40
8	A	1244	A	C8-N9-C4	5.30	107.92	105.80
8	A	2524	G	C4-N9-C1'	-5.30	119.61	126.50
9	B	60	C	N1-C2-O2	-5.30	115.72	118.90
34	a	548	G	N3-C4-C5	5.30	131.25	128.60
8	A	1436	G	N3-C4-C5	5.30	131.25	128.60
8	A	2461	A	C2-N3-C4	-5.30	107.95	110.60
8	A	2723	C	C6-N1-C2	5.30	122.42	120.30
34	a	111	G	O4'-C1'-N9	-5.30	103.96	108.20
34	a	1074	G	N3-C4-C5	5.30	131.25	128.60
8	A	253	C	N3-C4-N4	-5.29	114.29	118.00
8	A	311	A	C8-N9-C4	5.29	107.92	105.80
9	B	93	C	N1-C2-O2	5.29	122.08	118.90
34	a	391	G	N3-C4-N9	-5.29	122.82	126.00
34	a	1282	C	O4'-C1'-N1	-5.29	103.97	108.20
34	a	1346	A	C8-N9-C1'	-5.29	118.17	127.70
8	A	35	G	N3-C4-N9	-5.29	122.83	126.00
34	a	1238	A	N1-C6-N6	5.29	121.77	118.60
8	A	2415	G	N3-C2-N2	-5.29	116.20	119.90
8	A	2633	G	N1-C6-O6	-5.29	116.73	119.90
34	a	849	G	C8-N9-C4	5.29	108.52	106.40
34	a	1181	G	C2-N3-C4	-5.29	109.25	111.90
55	v	66	C	C6-N1-C2	5.29	122.42	120.30
8	A	1471	G	N1-C2-N2	-5.29	111.44	116.20
34	a	858	G	N1-C2-N2	5.29	120.96	116.20
34	a	946	A	C4-C5-N7	5.29	113.34	110.70
8	A	659	G	N3-C2-N2	5.29	123.60	119.90
8	A	17	G	N3-C4-C5	5.29	131.24	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	814	C	C4-C5-C6	-5.29	114.76	117.40
8	A	964	C	C6-N1-C2	5.29	122.41	120.30
8	A	1052	C	N3-C4-N4	-5.29	114.30	118.00
8	A	1449	G	N3-C2-N2	-5.29	116.20	119.90
8	A	2116	G	N3-C4-C5	5.29	131.24	128.60
8	A	2248	C	N1-C2-O2	5.29	122.07	118.90
34	a	474	G	C2-N3-C4	-5.29	109.26	111.90
34	a	642	A	C8-N9-C4	5.29	107.92	105.80
34	a	1347	G	C6-C5-N7	5.29	133.57	130.40
8	A	245	G	C2-N3-C4	-5.28	109.26	111.90
8	A	647	G	N3-C4-C5	5.28	131.24	128.60
8	A	661	A	N9-C4-C5	-5.28	103.69	105.80
8	A	2201	G	C5-C6-O6	5.28	131.77	128.60
8	A	2201	G	N3-C4-N9	-5.28	122.83	126.00
9	B	10	G	C8-N9-C4	5.28	108.51	106.40
34	a	370	C	O4'-C1'-N1	-5.28	103.97	108.20
8	A	186	G	C8-N9-C4	5.28	108.51	106.40
34	a	714	G	O4'-C1'-N9	-5.28	103.97	108.20
8	A	326	G	C2-N3-C4	-5.28	109.26	111.90
8	A	1313	U	C6-N1-C1'	-5.28	113.81	121.20
8	A	1593	A	N3-C4-C5	5.28	130.50	126.80
8	A	1961	C	N3-C4-C5	5.28	124.01	121.90
8	A	659	G	C2-N3-C4	-5.28	109.26	111.90
8	A	344	A	N3-C4-C5	5.28	130.49	126.80
8	A	1034	G	N3-C4-N9	-5.28	122.83	126.00
8	A	1072	C	C5-C6-N1	-5.28	118.36	121.00
8	A	1197	G	C4-N9-C1'	-5.28	119.64	126.50
8	A	1514	G	N1-C6-O6	5.28	123.07	119.90
8	A	2416	C	C6-N1-C1'	-5.28	114.47	120.80
8	A	2505	G	N3-C4-N9	5.28	129.17	126.00
8	A	2669	G	C2-N3-C4	-5.28	109.26	111.90
34	a	1218	C	C6-N1-C2	5.28	122.41	120.30
8	A	1128	G	N3-C4-C5	5.28	131.24	128.60
8	A	1689	A	N1-C6-N6	5.28	121.77	118.60
8	A	1849	G	C2-N3-C4	-5.28	109.26	111.90
34	a	1246	A	C8-N9-C4	5.28	107.91	105.80
34	a	1293	C	C4-C5-C6	-5.28	114.76	117.40
8	A	207	A	C5-N7-C8	-5.27	101.26	103.90
8	A	1470	A	C5-C6-N6	-5.27	119.48	123.70
8	A	2476	A	N9-C4-C5	-5.27	103.69	105.80
8	A	263	G	C8-N9-C1'	-5.27	120.14	127.00
8	A	1337	G	C4-N9-C1'	-5.27	119.64	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	2269	G	C2-N3-C4	-5.27	109.26	111.90
34	a	546	A	C8-N9-C4	5.27	107.91	105.80
8	A	1389	G	N9-C4-C5	-5.27	103.29	105.40
8	A	2338	C	C5-C6-N1	-5.27	118.36	121.00
8	A	2461	A	O4'-C1'-N9	-5.27	103.98	108.20
8	A	720	U	C6-N1-C2	5.27	124.16	121.00
8	A	940	G	N3-C4-N9	-5.27	122.84	126.00
8	A	1277	G	C6-C5-N7	5.27	133.56	130.40
8	A	2014	A	N1-C6-N6	5.27	121.76	118.60
8	A	2717	C	N3-C4-C5	5.27	124.01	121.90
34	a	1426	G	N3-C4-C5	5.27	131.24	128.60
34	a	1452	C	C2-N1-C1'	-5.27	113.00	118.80
8	A	865	C	N3-C4-C5	5.27	124.01	121.90
8	A	882	G	N3-C2-N2	-5.27	116.21	119.90
8	A	2258	C	O4'-C1'-N1	-5.27	103.99	108.20
8	A	2271	G	C2-N3-C4	-5.27	109.27	111.90
8	A	2369	A	N3-C4-C5	5.27	130.49	126.80
8	A	2882	A	N9-C4-C5	-5.27	103.69	105.80
34	a	686	U	C5-C4-O4	-5.27	122.74	125.90
3	2	37	LYS	CD-CE-NZ	5.27	123.81	111.70
26	S	16	LYS	CD-CE-NZ	5.27	123.81	111.70
8	A	55	G	C2-N3-C4	-5.26	109.27	111.90
8	A	85	G	C8-N9-C4	5.26	108.50	106.40
8	A	152	A	C5-N7-C8	-5.26	101.27	103.90
8	A	739	A	C5-C6-N6	-5.26	119.49	123.70
8	A	926	G	C2-N3-C4	-5.26	109.27	111.90
8	A	929	U	C6-N1-C2	5.26	124.16	121.00
8	A	1178	C	C6-N1-C2	5.26	122.41	120.30
34	a	522	C	C6-N1-C2	5.26	122.41	120.30
34	a	588	G	C8-N9-C4	5.26	108.51	106.40
34	a	1075	U	C6-N1-C1'	-5.26	113.83	121.20
34	a	1177	G	C2-N3-C4	-5.26	109.27	111.90
34	a	1489	G	N3-C4-C5	5.26	131.23	128.60
55	v	74	C	C6-N1-C2	5.26	122.41	120.30
34	a	155	A	N3-C4-C5	5.26	130.48	126.80
34	a	348	G	N9-C4-C5	-5.26	103.30	105.40
57	x	611	LEU	CA-CB-CG	-5.26	103.19	115.30
8	A	1296	G	N3-C4-C5	5.26	131.23	128.60
8	A	2508	G	C4-N9-C1'	-5.26	119.66	126.50
34	a	247	G	N3-C4-N9	-5.26	122.84	126.00
55	v	70	G	C5-N7-C8	-5.26	101.67	104.30
8	A	48	G	N3-C4-N9	-5.26	122.84	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	656	G	N3-C4-C5	5.26	131.23	128.60
8	A	2886	A	C8-N9-C4	5.26	107.90	105.80
34	a	1117	A	C4-C5-N7	5.26	113.33	110.70
8	A	2686	G	N3-C4-N9	-5.26	122.84	126.00
8	A	2133	G	N3-C4-C5	5.26	131.23	128.60
8	A	2520	C	N3-C4-C5	5.26	124.00	121.90
8	A	2831	G	N3-C4-C5	5.26	131.23	128.60
34	a	542	G	C4-C5-N7	5.26	112.90	110.80
8	A	187	G	C2-N3-C4	-5.25	109.27	111.90
8	A	921	C	N3-C4-C5	5.25	124.00	121.90
8	A	1689	A	N9-C4-C5	-5.25	103.70	105.80
8	A	2435	A	N9-C4-C5	-5.25	103.70	105.80
34	a	912	C	C2-N1-C1'	5.25	124.58	118.80
34	a	1534	A	O4'-C1'-N9	5.25	112.40	108.20
55	v	46	A	C4-C5-N7	5.25	113.33	110.70
8	A	32	C	N3-C4-C5	5.25	124.00	121.90
8	A	1401	G	C5-C6-O6	5.25	131.75	128.60
8	A	2677	G	C2-N3-C4	-5.25	109.27	111.90
8	A	401	A	C4-C5-N7	5.25	113.33	110.70
8	A	1910	G	N9-C1'-C2'	-5.25	106.22	112.00
34	a	659	U	C6-N1-C2	5.25	124.15	121.00
8	A	1573	G	N3-C4-N9	-5.25	122.85	126.00
8	A	2824	C	N3-C4-C5	5.25	124.00	121.90
34	a	392	C	O4'-C1'-N1	-5.25	104.00	108.20
34	a	648	A	C4-C5-N7	5.25	113.32	110.70
34	a	1457	G	C8-N9-C4	5.25	108.50	106.40
8	A	701	G	C8-N9-C4	5.25	108.50	106.40
8	A	926	G	N3-C4-N9	-5.25	122.85	126.00
8	A	1925	C	C6-N1-C2	5.25	122.40	120.30
34	a	669	G	C8-N9-C4	5.25	108.50	106.40
34	a	1139	G	C6-C5-N7	-5.25	127.25	130.40
34	a	1400	C	C6-N1-C2	5.25	122.40	120.30
55	v	76	A	C5-C6-N6	-5.25	119.50	123.70
8	A	299	A	N9-C4-C5	-5.25	103.70	105.80
8	A	2886	A	C5-C6-N6	-5.25	119.50	123.70
34	a	102	G	N3-C4-N9	-5.25	122.85	126.00
8	A	680	C	C6-N1-C1'	-5.24	114.51	120.80
8	A	1369	G	N1-C2-N3	5.24	127.05	123.90
8	A	1524	G	N1-C2-N2	-5.24	111.48	116.20
9	B	53	A	N9-C4-C5	-5.24	103.70	105.80
34	a	198	G	N3-C4-C5	5.24	131.22	128.60
8	A	2900	A	C5-N7-C8	-5.24	101.28	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	a	1143	G	C4-N9-C1'	-5.24	119.69	126.50
34	a	1227	A	C4-C5-N7	-5.24	108.08	110.70
8	A	210	C	N1-C2-O2	5.24	122.05	118.90
8	A	1093	G	O4'-C1'-N9	-5.24	104.01	108.20
8	A	1892	C	C6-N1-C2	5.24	122.40	120.30
8	A	1945	G	C8-N9-C4	5.24	108.50	106.40
8	A	2004	G	N3-C4-C5	5.24	131.22	128.60
8	A	2509	G	N3-C4-N9	-5.24	122.86	126.00
34	a	222	C	N1-C2-O2	-5.24	115.76	118.90
34	a	749	A	C8-N9-C4	5.24	107.90	105.80
34	a	1061	G	C4-C5-N7	5.24	112.90	110.80
8	A	66	C	C5-C6-N1	-5.24	118.38	121.00
8	A	1157	G	N1-C2-N2	-5.24	111.49	116.20
8	A	1241	A	N9-C4-C5	-5.24	103.70	105.80
8	A	1580	A	N9-C4-C5	-5.24	103.70	105.80
34	a	425	G	C2-N3-C4	-5.24	109.28	111.90
34	a	460	A	N3-C4-N9	-5.24	123.21	127.40
34	a	639	G	C4-C5-N7	5.24	112.89	110.80
8	A	549	G	C4-C5-N7	5.24	112.89	110.80
8	A	1110	G	N3-C4-C5	5.24	131.22	128.60
8	A	2222	C	N3-C4-N4	-5.24	114.33	118.00
8	A	315	G	C4-N9-C1'	-5.24	119.69	126.50
8	A	982	C	C6-N1-C2	5.24	122.39	120.30
8	A	2271	G	N3-C4-C5	5.24	131.22	128.60
8	A	2453	A	C5-C6-N1	5.24	120.32	117.70
24	Q	59	LEU	CA-CB-CG	-5.24	103.26	115.30
34	a	722	G	N3-C2-N2	-5.24	116.23	119.90
34	a	1058	G	C8-N9-C4	5.24	108.50	106.40
8	A	183	C	N3-C4-N4	-5.23	114.34	118.00
8	A	1733	G	N3-C4-C5	5.23	131.22	128.60
8	A	2218	G	C4-C5-N7	5.23	112.89	110.80
34	a	408	A	C4-C5-C6	-5.23	114.38	117.00
8	A	350	G	C4-C5-N7	5.23	112.89	110.80
8	A	1669	A	N9-C4-C5	-5.23	103.71	105.80
8	A	2591	C	C2-N1-C1'	5.23	124.56	118.80
34	a	64	G	C4-C5-N7	5.23	112.89	110.80
34	a	873	A	N9-C4-C5	-5.23	103.71	105.80
34	a	937	A	C8-N9-C4	5.23	107.89	105.80
8	A	89	A	C8-N9-C4	5.23	107.89	105.80
8	A	2002	G	C8-N9-C4	5.23	108.49	106.40
9	B	46	A	C8-N9-C4	5.23	107.89	105.80
9	B	54	G	C6-N1-C2	5.23	128.24	125.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	a	58	C	C6-N1-C2	5.23	122.39	120.30
34	a	81	A	N1-C6-N6	5.23	121.74	118.60
34	a	282	A	C5-C6-N6	-5.23	119.52	123.70
34	a	354	G	C8-N9-C4	5.23	108.49	106.40
34	a	1196	A	N9-C4-C5	-5.23	103.71	105.80
8	A	870	U	C6-N1-C2	5.23	124.14	121.00
9	B	12	C	N3-C2-O2	-5.23	118.24	121.90
34	a	761	G	N3-C4-C5	5.23	131.21	128.60
8	A	37	C	C5-C6-N1	-5.23	118.39	121.00
8	A	270	A	C6-C5-N7	5.23	135.96	132.30
8	A	1092	C	C2-N3-C4	-5.23	117.29	119.90
8	A	1240	U	C2-N1-C1'	-5.23	111.43	117.70
8	A	1684	G	C4-C5-C6	-5.23	115.66	118.80
8	A	2611	C	N1-C2-O2	5.23	122.04	118.90
8	A	2665	A	O4'-C1'-N9	-5.23	104.02	108.20
8	A	217	A	N7-C8-N9	-5.23	111.19	113.80
8	A	1060	U	N3-C4-O4	5.23	123.06	119.40
8	A	2049	G	C2-N3-C4	-5.23	109.29	111.90
34	a	1021	A	N9-C4-C5	-5.23	103.71	105.80
34	a	1281	C	N3-C4-C5	5.23	123.99	121.90
8	A	118	A	C5-C6-N6	-5.22	119.52	123.70
8	A	402	A	C6-C5-N7	-5.22	128.64	132.30
8	A	888	C	C5-C4-N4	5.22	123.86	120.20
8	A	1771	C	N1-C2-O2	5.22	122.03	118.90
8	A	2407	A	C8-N9-C4	5.22	107.89	105.80
8	A	227	A	C5-C6-N6	5.22	127.88	123.70
8	A	661	A	C4-C5-N7	5.22	113.31	110.70
8	A	2523	G	C8-N9-C4	5.22	108.49	106.40
8	A	38	A	C8-N9-C4	5.22	107.89	105.80
8	A	977	G	C8-N9-C4	5.22	108.49	106.40
8	A	1143	A	C5-C6-N6	-5.22	119.52	123.70
8	A	1227	G	C8-N9-C4	5.22	108.49	106.40
8	A	2012	G	N9-C4-C5	-5.22	103.31	105.40
34	a	241	G	C4-N9-C1'	-5.22	119.72	126.50
55	v	21	A	C8-N9-C4	5.22	107.89	105.80
8	A	138	U	C6-N1-C2	5.22	124.13	121.00
8	A	544	C	N1-C2-O2	5.22	122.03	118.90
8	A	1474	U	C6-N1-C2	5.22	124.13	121.00
34	a	435	A	C8-N9-C4	5.22	107.89	105.80
38	e	114	LEU	CA-CB-CG	-5.22	103.30	115.30
8	A	974	G	N1-C2-N3	5.22	127.03	123.90
8	A	1707	G	C2-N3-C4	-5.22	109.29	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	w	28	G	N3-C4-C5	5.22	131.21	128.60
34	a	226	G	C8-N9-C4	5.21	108.49	106.40
8	A	1593	A	C8-N9-C4	5.21	107.89	105.80
8	A	2430	A	C6-C5-N7	-5.21	128.65	132.30
34	a	246	A	C8-N9-C4	5.21	107.89	105.80
8	A	270	A	C4-N9-C1'	-5.21	116.92	126.30
8	A	1119	U	O4'-C1'-N1	-5.21	104.03	108.20
34	a	1511	G	N3-C4-C5	5.21	131.21	128.60
8	A	76	C	N3-C4-C5	5.21	123.98	121.90
8	A	2844	G	N3-C2-N2	-5.21	116.25	119.90
34	a	542	G	C4-N9-C1'	-5.21	119.73	126.50
57	x	641	LEU	CA-CB-CG	5.21	127.28	115.30
8	A	1424	G	C8-N9-C4	5.21	108.48	106.40
8	A	1501	G	N3-C4-N9	-5.21	122.88	126.00
8	A	2082	A	C5-C6-N1	5.21	120.30	117.70
8	A	2384	U	C6-N1-C2	5.21	124.12	121.00
8	A	2566	A	N3-C4-C5	5.21	130.44	126.80
34	a	236	A	C5-N7-C8	-5.21	101.30	103.90
8	A	60	G	C2-N3-C4	-5.21	109.30	111.90
8	A	912	C	N3-C4-C5	5.21	123.98	121.90
34	a	196	A	N1-C6-N6	-5.21	115.48	118.60
8	A	2339	C	N3-C4-N4	-5.21	114.36	118.00
8	A	2631	G	C8-N9-C4	5.21	108.48	106.40
8	A	2894	G	N3-C2-N2	-5.21	116.26	119.90
17	J	56	VAL	CG1-CB-CG2	5.21	119.23	110.90
34	a	799	G	N9-C4-C5	-5.21	103.32	105.40
8	A	844	A	C5-N7-C8	-5.20	101.30	103.90
8	A	2579	C	C6-N1-C1'	-5.20	114.56	120.80
34	a	661	G	O4'-C1'-N9	-5.20	104.04	108.20
43	j	71	LEU	CA-CB-CG	-5.20	103.33	115.30
8	A	203	A	C2-N3-C4	-5.20	108.00	110.60
8	A	1850	G	C2-N3-C4	-5.20	109.30	111.90
34	a	175	C	N3-C4-C5	5.20	123.98	121.90
34	a	423	G	C6-C5-N7	-5.20	127.28	130.40
34	a	581	G	C2-N3-C4	-5.20	109.30	111.90
34	a	1539	C	O4'-C1'-N1	5.20	112.36	108.20
8	A	136	G	C8-N9-C4	5.20	108.48	106.40
8	A	818	G	O4'-C1'-N9	-5.20	104.04	108.20
8	A	1220	G	C4-C5-C6	-5.20	115.68	118.80
8	A	2349	G	C2-N3-C4	-5.20	109.30	111.90
8	A	2655	G	C4-N9-C1'	-5.20	119.74	126.50
8	A	1335	C	C6-N1-C2	5.20	122.38	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	2051	A	C4-C5-N7	5.20	113.30	110.70
34	a	564	C	O4'-C1'-N1	5.20	112.36	108.20
34	a	332	G	C8-N9-C4	5.20	108.48	106.40
34	a	596	A	N9-C4-C5	-5.20	103.72	105.80
34	a	946	A	N9-C4-C5	-5.20	103.72	105.80
8	A	289	G	C5-N7-C8	-5.20	101.70	104.30
8	A	1774	C	N3-C4-N4	-5.20	114.36	118.00
34	a	1156	G	C8-N9-C4	5.20	108.48	106.40
34	a	1182	G	C2-N3-C4	-5.20	109.30	111.90
8	A	2569	G	C8-N9-C4	5.19	108.48	106.40
8	A	2854	G	C4-C5-N7	5.19	112.88	110.80
34	a	567	G	C2-N3-C4	-5.19	109.30	111.90
56	w	60	U	C5'-C4'-O4'	5.19	115.33	109.10
8	A	2125	G	O4'-C1'-N9	5.19	112.35	108.20
8	A	2432	A	C8-N9-C4	5.19	107.88	105.80
34	a	251	G	C2-N3-C4	-5.19	109.30	111.90
34	a	385	C	C6-N1-C2	5.19	122.38	120.30
34	a	1320	C	C6-N1-C2	5.19	122.38	120.30
8	A	126	A	C4-C5-N7	5.19	113.30	110.70
8	A	492	A	N1-C6-N6	5.19	121.71	118.60
8	A	1168	G	C2-N3-C4	-5.19	109.31	111.90
8	A	1449	G	C8-N9-C1'	5.19	133.75	127.00
8	A	2051	A	N9-C4-C5	-5.19	103.72	105.80
8	A	2771	C	C6-N1-C2	5.19	122.38	120.30
8	A	2836	U	C6-N1-C2	5.19	124.11	121.00
34	a	334	C	C2-N1-C1'	5.19	124.51	118.80
34	a	1137	C	C6-N1-C2	5.19	122.38	120.30
8	A	125	A	N1-C6-N6	5.19	121.71	118.60
8	A	1055	G	N3-C2-N2	-5.19	116.27	119.90
8	A	2352	A	N1-C6-N6	5.19	121.71	118.60
34	a	755	G	C2-N3-C4	-5.19	109.31	111.90
8	A	213	A	C8-N9-C4	5.19	107.88	105.80
8	A	836	G	O4'-C1'-N9	-5.19	104.05	108.20
8	A	2763	G	C4-N9-C1'	-5.19	119.76	126.50
8	A	35	G	C2-N3-C4	-5.19	109.31	111.90
8	A	2338	C	C2-N3-C4	-5.19	117.31	119.90
8	A	2413	G	C2-N3-C4	-5.19	109.31	111.90
9	B	21	G	C5-N7-C8	-5.19	101.71	104.30
56	w	74	C	N3-C2-O2	-5.19	118.27	121.90
8	A	704	G	C2-N3-C4	-5.18	109.31	111.90
8	A	1120	G	C8-N9-C4	5.18	108.47	106.40
8	A	1163	G	C2-N3-C4	-5.18	109.31	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	a	1164	G	C2-N3-C4	-5.18	109.31	111.90
8	A	1025	G	C5-C6-N1	-5.18	108.91	111.50
8	A	1774	C	C5-C6-N1	-5.18	118.41	121.00
8	A	2318	G	N3-C4-C5	5.18	131.19	128.60
34	a	105	G	N3-C4-C5	5.18	131.19	128.60
34	a	378	G	C2-N3-C4	-5.18	109.31	111.90
34	a	1019	A	C4-C5-N7	5.18	113.29	110.70
8	A	79	C	N3-C4-C5	5.18	123.97	121.90
8	A	456	C	N3-C4-N4	-5.18	114.37	118.00
8	A	781	A	N1-C2-N3	5.18	131.89	129.30
8	A	1461	C	N1-C2-O2	-5.18	115.79	118.90
8	A	1885	A	N1-C6-N6	5.18	121.71	118.60
8	A	1906	G	N3-C4-N9	-5.18	122.89	126.00
8	A	2502	G	C8-N9-C4	5.18	108.47	106.40
34	a	1405	G	C4-C5-C6	-5.18	115.69	118.80
8	A	864	G	C2-N3-C4	-5.18	109.31	111.90
8	A	1043	C	N3-C2-O2	5.18	125.53	121.90
8	A	1119	U	C6-N1-C2	5.18	124.11	121.00
8	A	1739	A	N1-C6-N6	5.18	121.71	118.60
8	A	2110	G	C6-C5-N7	-5.18	127.29	130.40
34	a	526	C	N1-C2-O2	5.18	122.01	118.90
8	A	886	A	O4'-C1'-N9	5.18	112.34	108.20
34	a	603	U	C2-N1-C1'	5.18	123.91	117.70
8	A	350	G	N1-C6-O6	5.18	123.01	119.90
8	A	421	C	N3-C4-N4	-5.18	114.38	118.00
8	A	2190	G	N1-C6-O6	5.18	123.01	119.90
8	A	2810	A	C5-C6-N6	-5.18	119.56	123.70
9	B	31	C	C5-C6-N1	-5.18	118.41	121.00
9	B	33	G	C8-N9-C4	5.18	108.47	106.40
34	a	447	G	N3-C4-C5	5.18	131.19	128.60
34	a	489	C	N3-C4-N4	-5.18	114.38	118.00
34	a	1064	G	N3-C4-C5	5.18	131.19	128.60
8	A	1927	A	C5-C6-N6	-5.17	119.56	123.70
8	A	2021	C	C6-N1-C1'	-5.17	114.59	120.80
8	A	2810	A	N9-C4-C5	-5.17	103.73	105.80
9	B	24	G	C2-N3-C4	-5.17	109.31	111.90
34	a	554	A	C8-N9-C4	5.17	107.87	105.80
8	A	350	G	C8-N9-C4	5.17	108.47	106.40
8	A	712	G	C2-N3-C4	-5.17	109.31	111.90
8	A	1858	A	C5-C6-N6	-5.17	119.56	123.70
8	A	1862	G	N3-C2-N2	5.17	123.52	119.90
34	a	1020	G	C2-N3-C4	-5.17	109.31	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	a	669	G	N3-C4-C5	5.17	131.19	128.60
56	w	47	U	C5'-C4'-C3'	5.17	124.27	116.00
8	A	317	G	C2-N3-C4	-5.17	109.32	111.90
8	A	2279	G	C8-N9-C4	5.17	108.47	106.40
8	A	2557	G	C6-C5-N7	5.17	133.50	130.40
34	a	600	A	C4-C5-N7	5.17	113.28	110.70
34	a	1080	A	C5-N7-C8	-5.17	101.31	103.90
34	a	77	A	N9-C4-C5	-5.17	103.73	105.80
34	a	987	G	C8-N9-C1'	5.17	133.72	127.00
8	A	489	G	N3-C4-C5	5.17	131.18	128.60
8	A	1025	G	O4'-C1'-N9	-5.17	104.07	108.20
8	A	1908	C	N3-C4-N4	-5.17	114.38	118.00
8	A	2484	G	N3-C4-N9	-5.17	122.90	126.00
8	A	2655	G	C2-N3-C4	-5.17	109.32	111.90
8	A	207	A	C4-C5-N7	5.16	113.28	110.70
8	A	922	C	N3-C4-C5	5.16	123.97	121.90
8	A	1706	C	N1-C2-O2	5.16	122.00	118.90
8	A	1992	G	N1-C2-N2	-5.16	111.55	116.20
34	a	178	C	C2-N3-C4	-5.16	117.32	119.90
34	a	349	A	C8-N9-C4	5.16	107.87	105.80
34	a	696	A	C8-N9-C4	5.16	107.86	105.80
34	a	953	G	N9-C1'-C2'	-5.16	106.32	112.00
34	a	1258	G	N3-C4-N9	-5.16	122.90	126.00
8	A	533	G	C2-N3-C4	-5.16	109.32	111.90
8	A	1311	G	C2-N3-C4	-5.16	109.32	111.90
8	A	2490	G	C2-N3-C4	-5.16	109.32	111.90
34	a	773	G	C8-N9-C4	5.16	108.47	106.40
34	a	1198	G	N1-C6-O6	-5.16	116.80	119.90
8	A	220	G	C5-C6-N1	-5.16	108.92	111.50
8	A	1549	A	C5-N7-C8	-5.16	101.32	103.90
34	a	695	A	N1-C6-N6	5.16	121.70	118.60
34	a	912	C	C6-N1-C1'	-5.16	114.61	120.80
8	A	1336	A	C4-C5-C6	-5.16	114.42	117.00
8	A	344	A	N9-C4-C5	-5.16	103.74	105.80
8	A	2507	C	N3-C4-C5	5.16	123.96	121.90
8	A	2523	G	N3-C4-C5	5.16	131.18	128.60
34	a	15	G	C8-N9-C1'	-5.16	120.30	127.00
34	a	670	G	N3-C4-N9	-5.16	122.91	126.00
8	A	1733	G	C8-N9-C4	5.16	108.46	106.40
8	A	2223	G	N3-C2-N2	-5.16	116.29	119.90
8	A	2295	C	C6-N1-C1'	-5.16	114.61	120.80
34	a	1497	G	C4-C5-C6	-5.16	115.71	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	x	277	MET	CA-CB-CG	5.16	122.06	113.30
8	A	2830	C	C2-N1-C1'	5.15	124.47	118.80
8	A	1125	G	N3-C4-N9	-5.15	122.91	126.00
8	A	1553	A	N9-C4-C5	-5.15	103.74	105.80
8	A	2352	A	C8-N9-C4	5.15	107.86	105.80
9	B	94	A	N9-C4-C5	-5.15	103.74	105.80
34	a	97	G	C4-N9-C1'	-5.15	119.80	126.50
34	a	376	G	C2-N3-C4	-5.15	109.32	111.90
34	a	654	G	C6-C5-N7	-5.15	127.31	130.40
34	a	1130	A	C4-N9-C1'	5.15	135.57	126.30
34	a	1385	G	N3-C4-C5	5.15	131.18	128.60
34	a	1483	A	C5-C6-N6	-5.15	119.58	123.70
35	b	94	ARG	CG-CD-NE	5.15	122.62	111.80
55	v	42	G	N3-C4-N9	-5.15	122.91	126.00
8	A	204	A	C5-C6-N6	-5.15	119.58	123.70
8	A	1378	A	C6-C5-N7	-5.15	128.69	132.30
8	A	2491	U	N1-C1'-C2'	-5.15	106.33	112.00
34	a	603	U	C6-N1-C1'	-5.15	113.99	121.20
55	v	53	G	C2-N3-C4	-5.15	109.33	111.90
8	A	466	A	N9-C4-C5	5.15	107.86	105.80
8	A	1663	G	C8-N9-C4	5.15	108.46	106.40
9	B	52	A	C4-C5-N7	5.15	113.28	110.70
34	a	1362	A	C4-C5-C6	-5.15	114.43	117.00
8	A	1704	C	C6-N1-C1'	-5.15	114.62	120.80
34	a	1241	G	N3-C4-N9	-5.15	122.91	126.00
8	A	1029	A	N7-C8-N9	5.15	116.37	113.80
8	A	1986	C	N3-C4-C5	5.15	123.96	121.90
19	L	6	LEU	CA-CB-CG	-5.15	103.46	115.30
8	A	143	C	N3-C4-N4	-5.14	114.40	118.00
8	A	672	C	N1-C2-O2	5.14	121.99	118.90
8	A	1530	G	C4-N9-C1'	-5.14	119.81	126.50
34	a	1088	G	C6-C5-N7	5.14	133.49	130.40
8	A	1104	C	C5-C6-N1	5.14	123.57	121.00
8	A	2168	G	C2-N3-C4	-5.14	109.33	111.90
9	B	69	G	N3-C4-N9	-5.14	122.92	126.00
8	A	263	G	C2-N3-C4	-5.14	109.33	111.90
34	a	377	G	N3-C4-N9	-5.14	122.92	126.00
8	A	107	G	C2-N3-C4	-5.14	109.33	111.90
8	A	581	C	N1-C2-O2	5.14	121.98	118.90
8	A	2570	G	C2-N3-C4	-5.14	109.33	111.90
34	a	888	G	C4-N9-C1'	-5.14	119.82	126.50
34	a	1525	G	N3-C4-C5	5.14	131.17	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	1055	G	N1-C2-N2	5.14	120.82	116.20
8	A	2727	A	C8-N9-C4	5.14	107.86	105.80
34	a	182	A	C5-C6-N6	-5.14	119.59	123.70
8	A	371	A	C8-N9-C4	5.14	107.86	105.80
8	A	375	G	N3-C2-N2	5.14	123.50	119.90
8	A	1540	G	C4-C5-N7	5.14	112.85	110.80
8	A	2027	G	N3-C4-C5	5.14	131.17	128.60
8	A	2623	G	N9-C4-C5	-5.14	103.34	105.40
8	A	2824	C	C6-N1-C2	5.14	122.36	120.30
8	A	735	A	N9-C4-C5	-5.13	103.75	105.80
8	A	1017	G	C2-N3-C4	-5.13	109.33	111.90
8	A	1226	A	N1-C6-N6	-5.13	115.52	118.60
8	A	1333	G	C2-N3-C4	-5.13	109.33	111.90
34	a	208	U	N1-C1'-C2'	-5.13	106.35	112.00
34	a	810	C	C6-N1-C2	5.13	122.35	120.30
8	A	1090	A	O4'-C1'-N9	-5.13	104.09	108.20
8	A	2308	G	C8-N9-C4	5.13	108.45	106.40
8	A	2648	G	C2-N3-C4	-5.13	109.33	111.90
9	B	50	A	N9-C4-C5	-5.13	103.75	105.80
8	A	1477	A	C5-N7-C8	-5.13	101.33	103.90
34	a	275	G	C8-N9-C4	5.13	108.45	106.40
34	a	457	G	C2-N3-C4	-5.13	109.33	111.90
34	a	542	G	C4-C5-C6	-5.13	115.72	118.80
34	a	1198	G	C5-C6-O6	5.13	131.68	128.60
8	A	2777	G	C8-N9-C4	5.13	108.45	106.40
8	A	1166	G	N3-C2-N2	5.13	123.49	119.90
8	A	1833	C	C6-N1-C2	5.13	122.35	120.30
8	A	2464	G	C4-N9-C1'	-5.13	119.83	126.50
8	A	2731	G	N3-C4-C5	5.13	131.16	128.60
34	a	410	G	C8-N9-C1'	5.13	133.67	127.00
34	a	1180	A	C4-C5-N7	5.13	113.26	110.70
8	A	346	A	C4-C5-N7	5.13	113.26	110.70
8	A	1088	A	C4-C5-C6	5.13	119.56	117.00
8	A	1811	G	C2-N3-C4	-5.13	109.34	111.90
8	A	2038	G	C4-C5-N7	5.13	112.85	110.80
8	A	2841	C	C6-N1-C2	5.13	122.35	120.30
9	B	9	G	C6-C5-N7	-5.13	127.32	130.40
34	a	846	G	C8-N9-C1'	-5.13	120.33	127.00
34	a	1043	G	C2-N3-C4	-5.13	109.34	111.90
34	a	1080	A	N7-C8-N9	5.13	116.36	113.80
34	a	1215	G	N3-C4-N9	-5.13	122.92	126.00
8	A	927	A	C5-C6-N6	-5.12	119.60	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	2674	G	C2-N3-C4	-5.12	109.34	111.90
34	a	1271	A	C8-N9-C4	5.12	107.85	105.80
8	A	130	C	N1-C2-O2	5.12	121.97	118.90
8	A	560	C	N3-C4-N4	-5.12	114.41	118.00
8	A	586	A	C8-N9-C4	5.12	107.85	105.80
8	A	2052	A	N9-C4-C5	-5.12	103.75	105.80
8	A	2190	G	C5-N7-C8	-5.12	101.74	104.30
8	A	2634	A	N9-C4-C5	-5.12	103.75	105.80
8	A	1600	C	N3-C4-C5	5.12	123.95	121.90
8	A	1805	A	C4-C5-C6	-5.12	114.44	117.00
8	A	2868	A	N9-C4-C5	-5.12	103.75	105.80
8	A	630	G	C6-C5-N7	5.12	133.47	130.40
8	A	1074	G	C4-N9-C1'	-5.12	119.84	126.50
50	q	11	VAL	CG1-CB-CG2	-5.12	102.71	110.90
8	A	512	G	N3-C4-N9	-5.12	122.93	126.00
8	A	748	G	C8-N9-C1'	5.12	133.65	127.00
8	A	949	G	C8-N9-C4	5.12	108.45	106.40
8	A	976	G	N3-C4-C5	5.12	131.16	128.60
34	a	489	C	C6-N1-C2	5.12	122.35	120.30
34	a	1392	G	N3-C4-N9	-5.12	122.93	126.00
8	A	771	G	C2-N3-C4	-5.12	109.34	111.90
8	A	890	C	C5-C4-N4	5.12	123.78	120.20
8	A	2020	A	N9-C4-C5	-5.12	103.75	105.80
8	A	2282	G	C5-C6-N1	5.12	114.06	111.50
34	a	739	C	N3-C4-N4	-5.12	114.42	118.00
56	w	16	U	C1'-C2'-O2'	5.12	125.94	110.60
8	A	81	G	N3-C4-N9	-5.11	122.93	126.00
8	A	401	A	N1-C6-N6	5.11	121.67	118.60
8	A	2443	C	N3-C4-N4	-5.11	114.42	118.00
34	a	988	G	C4-N9-C1'	-5.11	119.85	126.50
8	A	394	C	C6-N1-C2	5.11	122.34	120.30
8	A	1011	G	N3-C4-N9	-5.11	122.93	126.00
8	A	85	G	N3-C4-N9	-5.11	122.93	126.00
8	A	164	C	N3-C4-C5	5.11	123.94	121.90
8	A	408	G	N3-C4-C5	5.11	131.16	128.60
8	A	2097	A	N3-C4-C5	5.11	130.38	126.80
8	A	2201	G	C2-N3-C4	-5.11	109.34	111.90
8	A	2830	C	N1-C2-O2	5.11	121.97	118.90
34	a	423	G	C4-N9-C1'	5.11	133.14	126.50
34	a	454	G	N3-C4-C5	5.11	131.16	128.60
34	a	861	G	N3-C4-N9	-5.11	122.93	126.00
8	A	110	G	N3-C4-C5	5.11	131.16	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	52	A	C8-N9-C4	5.11	107.84	105.80
34	a	1160	G	C2-N3-C4	-5.11	109.35	111.90
55	v	43	A	N1-C6-N6	5.11	121.67	118.60
55	v	70	G	C2-N3-C4	-5.11	109.35	111.90
8	A	1429	G	C2-N3-C4	-5.11	109.35	111.90
8	A	1688	U	N1-C2-O2	-5.11	119.22	122.80
8	A	2864	G	C2-N3-C4	-5.11	109.35	111.90
34	a	1430	A	C4-C5-C6	-5.11	114.45	117.00
8	A	433	C	N3-C4-C5	5.11	123.94	121.90
8	A	457	A	N1-C6-N6	5.11	121.66	118.60
8	A	1320	C	C2-N3-C4	-5.11	117.35	119.90
8	A	2391	G	C8-N9-C1'	5.11	133.64	127.00
8	A	2772	C	C6-N1-C1'	-5.11	114.67	120.80
8	A	812	C	C5-C6-N1	-5.10	118.45	121.00
8	A	1671	U	C5'-C4'-C3'	-5.10	107.83	116.00
8	A	2354	C	N3-C4-N4	-5.10	114.43	118.00
34	a	147	G	N3-C4-C5	5.10	131.15	128.60
34	a	155	A	C4-C5-C6	-5.10	114.45	117.00
34	a	1401	G	C5'-C4'-C3'	-5.10	107.83	116.00
8	A	500	G	N3-C4-N9	-5.10	122.94	126.00
8	A	950	G	C8-N9-C4	5.10	108.44	106.40
8	A	998	C	N1-C2-O2	5.10	121.96	118.90
8	A	1472	C	C6-N1-C2	5.10	122.34	120.30
34	a	422	C	C6-N1-C2	5.10	122.34	120.30
34	a	1108	G	C2-N3-C4	-5.10	109.35	111.90
8	A	130	C	N3-C2-O2	-5.10	118.33	121.90
8	A	2632	A	C4-C5-C6	-5.10	114.45	117.00
34	a	681	A	C5-C6-N6	-5.10	119.62	123.70
34	a	1304	G	N3-C4-N9	-5.10	122.94	126.00
34	a	1331	G	N1-C2-N2	5.10	120.79	116.20
8	A	401	A	C5-C6-N6	-5.10	119.62	123.70
8	A	802	A	N1-C6-N6	-5.10	115.54	118.60
8	A	1557	C	N3-C4-C5	5.10	123.94	121.90
8	A	2110	G	N7-C8-N9	5.10	115.65	113.10
34	a	137	U	C6-N1-C2	5.10	124.06	121.00
34	a	785	G	C4-C5-N7	5.10	112.84	110.80
34	a	1431	A	C2-N3-C4	-5.10	108.05	110.60
8	A	975	A	N9-C1'-C2'	-5.10	106.39	112.00
8	A	2303	G	N3-C4-N9	-5.10	122.94	126.00
8	A	2898	U	C6-N1-C2	5.10	124.06	121.00
34	a	442	G	C5-N7-C8	-5.10	101.75	104.30
8	A	924	G	C2-N3-C4	-5.09	109.35	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	1423	G	C6-C5-N7	5.09	133.46	130.40
8	A	1571	A	O4'-C1'-N9	5.09	112.28	108.20
8	A	2097	A	C8-N9-C4	5.09	107.84	105.80
8	A	2241	A	C5-C6-N1	5.09	120.25	117.70
8	A	2435	A	C8-N9-C4	5.09	107.84	105.80
8	A	19	A	N9-C4-C5	-5.09	103.76	105.80
8	A	392	U	C6-N1-C2	5.09	124.06	121.00
8	A	1230	A	C4-C5-N7	5.09	113.25	110.70
8	A	2632	A	N9-C4-C5	-5.09	103.76	105.80
34	a	265	G	O4'-C1'-N9	-5.09	104.12	108.20
8	A	310	A	C4-C5-C6	-5.09	114.45	117.00
8	A	450	G	C8-N9-C4	5.09	108.44	106.40
8	A	2280	G	C2-N3-C4	-5.09	109.35	111.90
8	A	612	G	N3-C4-N9	-5.09	122.95	126.00
8	A	659	G	C8-N9-C1'	-5.09	120.38	127.00
8	A	1548	A	C4-C5-C6	-5.09	114.45	117.00
8	A	1639	C	N1-C2-O2	5.09	121.95	118.90
56	w	35	A	C8-N9-C4	5.09	107.84	105.80
8	A	199	A	N1-C6-N6	-5.09	115.55	118.60
8	A	914	G	C8-N9-C4	5.09	108.44	106.40
8	A	1684	G	C8-N9-C1'	5.09	133.61	127.00
8	A	1903	G	N3-C4-C5	5.09	131.14	128.60
8	A	2013	A	N9-C4-C5	-5.09	103.77	105.80
8	A	1650	A	N9-C4-C5	-5.09	103.77	105.80
8	A	1737	G	C2-N3-C4	-5.09	109.36	111.90
8	A	2303	G	C2-N3-C4	-5.09	109.36	111.90
19	L	53	GLY	N-CA-C	5.09	125.82	113.10
8	A	1606	C	C5-C6-N1	-5.08	118.46	121.00
8	A	2461	A	N3-C4-C5	5.08	130.36	126.80
34	a	1276	G	C5-N7-C8	-5.08	101.76	104.30
8	A	583	G	N3-C4-C5	5.08	131.14	128.60
8	A	1142	A	N3-C4-C5	5.08	130.36	126.80
8	A	2227	A	C8-N9-C4	5.08	107.83	105.80
8	A	2363	G	C4-N9-C1'	-5.08	119.89	126.50
9	B	7	G	N3-C4-C5	5.08	131.14	128.60
34	a	53	A	N9-C4-C5	-5.08	103.77	105.80
34	a	412	A	N1-C6-N6	5.08	121.65	118.60
34	a	998	C	C6-N1-C2	5.08	122.33	120.30
34	a	1166	G	N3-C4-C5	5.08	131.14	128.60
57	x	634	LEU	CA-CB-CG	-5.08	103.61	115.30
8	A	831	G	N3-C4-N9	-5.08	122.95	126.00
8	A	1068	G	N3-C2-N2	-5.08	116.34	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	1114	C	C6-N1-C2	5.08	122.33	120.30
34	a	1081	A	N9-C1'-C2'	5.08	120.61	114.00
34	a	1141	C	C5-C4-N4	5.08	123.76	120.20
34	a	1468	A	C5-C6-N6	-5.08	119.63	123.70
8	A	975	A	O4'-C1'-N9	-5.08	104.14	108.20
8	A	1616	A	N9-C4-C5	-5.08	103.77	105.80
34	a	1309	G	C2-N3-C4	-5.08	109.36	111.90
34	a	1462	C	N3-C4-C5	5.08	123.93	121.90
8	A	1092	C	N1-C1'-C2'	-5.08	106.41	112.00
8	A	1418	G	C8-N9-C4	5.08	108.43	106.40
8	A	1445	G	N3-C4-C5	5.08	131.14	128.60
8	A	2499	C	N3-C4-C5	5.08	123.93	121.90
8	A	2630	G	N3-C4-C5	5.08	131.14	128.60
34	a	457	G	N3-C4-N9	-5.08	122.95	126.00
34	a	1282	C	C6-N1-C2	5.08	122.33	120.30
34	a	1422	G	N3-C4-C5	5.08	131.14	128.60
8	A	301	G	C8-N9-C4	5.08	108.43	106.40
8	A	1762	A	C4-C5-C6	-5.08	114.46	117.00
34	a	410	G	C8-N9-C4	5.08	108.43	106.40
34	a	598	U	O4'-C1'-N1	-5.08	104.14	108.20
34	a	952	U	C6-N1-C2	5.08	124.05	121.00
34	a	1200	C	N3-C4-C5	5.08	123.93	121.90
8	A	325	G	N3-C4-C5	5.07	131.14	128.60
8	A	379	G	C2-N3-C4	-5.07	109.36	111.90
8	A	974	G	C5-N7-C8	-5.07	101.76	104.30
8	A	2135	A	O5'-P-OP2	-5.07	101.13	105.70
34	a	1174	G	C8-N9-C4	5.07	108.43	106.40
34	a	1337	G	O4'-C1'-N9	-5.07	104.14	108.20
56	w	24	G	N3-C4-N9	-5.07	122.96	126.00
8	A	309	A	C8-N9-C4	5.07	107.83	105.80
8	A	1452	G	N3-C2-N2	-5.07	116.35	119.90
8	A	2040	G	C4-N9-C1'	-5.07	119.91	126.50
34	a	953	G	C5-C6-O6	-5.07	125.56	128.60
8	A	1168	G	N9-C4-C5	-5.07	103.37	105.40
8	A	1323	C	N3-C4-N4	-5.07	114.45	118.00
34	a	670	G	C2-N3-C4	-5.07	109.36	111.90
8	A	1936	A	O4'-C1'-N9	5.07	112.25	108.20
8	A	2815	C	N3-C4-C5	5.07	123.93	121.90
34	a	825	A	C8-N9-C4	5.07	107.83	105.80
8	A	1178	C	C5-C6-N1	-5.07	118.47	121.00
8	A	1370	C	C6-N1-C2	5.07	122.33	120.30
34	a	682	G	N9-C1'-C2'	-5.07	106.42	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	808	G	N9-C4-C5	-5.07	103.37	105.40
8	A	1588	G	C4-N9-C1'	-5.07	119.91	126.50
8	A	1994	C	C5-C4-N4	5.07	123.75	120.20
8	A	2201	G	N3-C4-C5	5.07	131.13	128.60
34	a	601	G	C2-N3-C4	-5.07	109.37	111.90
34	a	785	G	C2-N3-C4	-5.07	109.37	111.90
34	a	920	U	N3-C2-O2	-5.07	118.66	122.20
55	v	12	G	C6-C5-N7	5.07	133.44	130.40
8	A	269	C	C6-N1-C2	5.06	122.33	120.30
8	A	457	A	N3-C4-C5	5.06	130.34	126.80
8	A	2484	G	C2-N3-C4	-5.06	109.37	111.90
8	A	2875	C	C6-N1-C1'	-5.06	114.72	120.80
34	a	203	G	C8-N9-C4	5.06	108.43	106.40
34	a	274	A	C4-C5-N7	5.06	113.23	110.70
8	A	2022	U	C2-N1-C1'	5.06	123.78	117.70
8	A	2212	A	C8-N9-C4	5.06	107.83	105.80
34	a	648	A	N3-C4-C5	5.06	130.34	126.80
34	a	923	A	C4-C5-N7	5.06	113.23	110.70
34	a	1376	U	O4'-C1'-N1	-5.06	104.15	108.20
8	A	1016	G	C4-N9-C1'	-5.06	119.92	126.50
34	a	1466	C	N3-C4-N4	-5.06	114.46	118.00
8	A	522	A	C2-N3-C4	-5.06	108.07	110.60
8	A	1074	G	N3-C2-N2	-5.06	116.36	119.90
8	A	1797	G	N3-C4-N9	-5.06	122.96	126.00
8	A	1897	G	C8-N9-C4	5.06	108.42	106.40
8	A	2281	A	C5-C6-N1	5.06	120.23	117.70
8	A	2331	G	N3-C4-C5	5.06	131.13	128.60
8	A	2509	G	C8-N9-C4	5.06	108.42	106.40
8	A	2657	A	C4-C5-N7	5.06	113.23	110.70
34	a	411	A	N3-C4-C5	5.06	130.34	126.80
34	a	1031	C	C2-N1-C1'	5.06	124.37	118.80
34	a	1101	A	O4'-C1'-N9	5.06	112.25	108.20
8	A	266	G	C2-N3-C4	-5.06	109.37	111.90
8	A	2624	G	N3-C2-N2	-5.06	116.36	119.90
8	A	2867	G	N3-C4-C5	5.06	131.13	128.60
8	A	1153	C	C5-C6-N1	5.06	123.53	121.00
8	A	1541	C	N3-C4-C5	5.06	123.92	121.90
8	A	2087	G	N3-C4-C5	5.06	131.13	128.60
8	A	342	A	C8-N9-C4	5.05	107.82	105.80
8	A	867	C	C5-C4-N4	5.05	123.74	120.20
8	A	1127	A	N1-C6-N6	5.05	121.63	118.60
8	A	1361	G	N1-C2-N3	5.05	126.93	123.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	2002	G	C2-N3-C4	-5.05	109.37	111.90
9	B	119	A	C4-C5-N7	5.05	113.23	110.70
49	p	5	ARG	CB-CA-C	5.05	120.51	110.40
55	v	43	A	C4-C5-N7	5.05	113.23	110.70
8	A	458	G	O4'-C1'-N9	5.05	112.24	108.20
8	A	2148	G	O4'-C1'-N9	5.05	112.24	108.20
8	A	1762	A	C8-N9-C4	5.05	107.82	105.80
9	B	23	G	C4-C5-N7	5.05	112.82	110.80
34	a	190	A	C4-C5-N7	5.05	113.23	110.70
34	a	1129	C	N3-C2-O2	5.05	125.44	121.90
34	a	1177	G	N3-C4-C5	5.05	131.13	128.60
34	a	1215	G	C2-N3-C4	-5.05	109.37	111.90
8	A	1088	A	N3-C4-N9	5.05	131.44	127.40
8	A	1116	G	C2-N3-C4	-5.05	109.38	111.90
8	A	1501	G	C8-N9-C4	5.05	108.42	106.40
8	A	2170	A	C4-C5-C6	-5.05	114.47	117.00
8	A	2319	G	N3-C4-C5	5.05	131.12	128.60
34	a	618	C	C6-N1-C2	5.05	122.32	120.30
34	a	1197	A	C4-C5-N7	5.05	113.22	110.70
34	a	113	G	N3-C4-N9	-5.05	122.97	126.00
34	a	149	A	N1-C6-N6	-5.05	115.57	118.60
34	a	738	C	C5'-C4'-C3'	-5.05	107.92	116.00
34	a	1253	G	C5-C6-O6	5.05	131.63	128.60
8	A	136	G	C2-N3-C4	-5.05	109.38	111.90
8	A	316	C	N3-C2-O2	5.05	125.43	121.90
8	A	471	A	N9-C4-C5	-5.05	103.78	105.80
8	A	1548	A	C4-C5-N7	5.05	113.22	110.70
8	A	2023	C	C6-N1-C2	5.05	122.32	120.30
34	a	507	C	C6-N1-C2	5.05	122.32	120.30
34	a	1269	A	O4'-C1'-N9	5.05	112.24	108.20
56	w	45	U	C2'-C3'-O3'	5.05	121.77	113.70
34	a	799	G	C2-N3-C4	-5.04	109.38	111.90
34	a	1089	G	C8-N9-C4	5.04	108.42	106.40
34	a	1117	A	N9-C4-C5	-5.04	103.78	105.80
8	A	834	G	C2-N3-C4	-5.04	109.38	111.90
8	A	1940	U	O4'-C1'-N1	5.04	112.23	108.20
8	A	1975	G	C2-N3-C4	-5.04	109.38	111.90
8	A	2050	C	C5-C4-N4	5.04	123.73	120.20
8	A	2282	G	O4'-C1'-N9	5.04	112.23	108.20
9	B	91	C	C6-N1-C2	5.04	122.32	120.30
34	a	1216	A	N9-C4-C5	-5.04	103.78	105.80
8	A	141	G	O4'-C1'-N9	5.04	112.23	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	676	A	C5-C6-N6	-5.04	119.67	123.70
8	A	2411	A	C4-C5-N7	5.04	113.22	110.70
8	A	2895	G	N1-C2-N3	5.04	126.92	123.90
34	a	281	G	C8-N9-C4	5.04	108.42	106.40
34	a	462	G	C8-N9-C4	-5.04	104.38	106.40
34	a	637	C	C4-C5-C6	-5.04	114.88	117.40
8	A	315	G	C8-N9-C4	5.04	108.42	106.40
8	A	2803	G	N7-C8-N9	-5.04	110.58	113.10
34	a	135	C	C5-C4-N4	-5.04	116.67	120.20
34	a	712	A	C8-N9-C4	5.04	107.82	105.80
34	a	1452	C	C6-N1-C2	5.04	122.32	120.30
8	A	881	G	C4-C5-N7	5.04	112.82	110.80
8	A	1189	A	O4'-C1'-N9	-5.04	104.17	108.20
8	A	2803	G	C4-C5-C6	-5.04	115.78	118.80
8	A	2814	A	C4-C5-C6	-5.04	114.48	117.00
34	a	1089	G	C4-N9-C1'	-5.04	119.95	126.50
34	a	1373	G	N3-C4-C5	5.04	131.12	128.60
8	A	1337	G	C2-N3-C4	-5.04	109.38	111.90
8	A	2375	G	N3-C4-C5	5.04	131.12	128.60
34	a	164	G	N3-C4-N9	-5.04	122.98	126.00
34	a	541	G	C4-N9-C1'	-5.04	119.95	126.50
8	A	1044	C	O4'-C1'-N1	-5.04	104.17	108.20
8	A	1207	C	N3-C4-N4	-5.04	114.48	118.00
8	A	1278	C	N3-C4-N4	-5.04	114.48	118.00
8	A	1847	G	O4'-C1'-N9	-5.04	104.17	108.20
34	a	375	U	C6-N1-C2	5.04	124.02	121.00
34	a	414	A	N9-C4-C5	-5.04	103.79	105.80
8	A	2813	A	C4-N9-C1'	-5.03	117.24	126.30
8	A	2553	G	N3-C4-N9	-5.03	122.98	126.00
8	A	849	A	C4-C5-N7	5.03	113.22	110.70
8	A	856	G	N9-C4-C5	-5.03	103.39	105.40
8	A	1151	A	C8-N9-C4	5.03	107.81	105.80
34	a	1003	G	N3-C4-N9	-5.03	122.98	126.00
56	w	52	G	N3-C4-C5	5.03	131.11	128.60
8	A	175	G	C4-C5-N7	5.03	112.81	110.80
8	A	184	C	N1-C1'-C2'	-5.03	106.47	112.00
8	A	1371	G	N1-C6-O6	5.03	122.92	119.90
8	A	2009	A	C4-C5-C6	-5.03	114.49	117.00
34	a	408	A	N9-C4-C5	-5.03	103.79	105.80
8	A	748	G	N3-C4-N9	-5.03	122.98	126.00
8	A	2140	G	N3-C4-C5	5.03	131.11	128.60
8	A	2294	G	C2-N3-C4	-5.03	109.39	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	g	3	ARG	CG-CD-NE	5.03	122.35	111.80
55	v	9	G	C2-N3-C4	-5.03	109.39	111.90
8	A	483	A	N1-C6-N6	5.02	121.61	118.60
8	A	1372	U	N1-C2-O2	-5.02	119.28	122.80
9	B	19	C	N3-C4-C5	5.02	123.91	121.90
34	a	489	C	N3-C4-C5	5.02	123.91	121.90
34	a	423	G	C8-N9-C1'	-5.02	120.47	127.00
34	a	530	G	N3-C4-N9	-5.02	122.99	126.00
34	a	558	G	N3-C4-C5	5.02	131.11	128.60
8	A	1631	G	N7-C8-N9	-5.02	110.59	113.10
8	A	640	C	C6-N1-C1'	-5.02	114.78	120.80
8	A	1552	A	C8-N9-C4	5.02	107.81	105.80
8	A	1652	A	C8-N9-C4	5.02	107.81	105.80
8	A	2848	G	C6-C5-N7	5.02	133.41	130.40
34	a	695	A	C5-C6-N6	-5.02	119.69	123.70
8	A	1544	A	C4-C5-N7	5.02	113.21	110.70
8	A	2279	G	N3-C4-N9	-5.02	122.99	126.00
34	a	613	C	C6-N1-C1'	-5.02	114.78	120.80
34	a	102	G	C8-N9-C4	5.02	108.41	106.40
8	A	673	C	C2-N3-C4	-5.01	117.39	119.90
8	A	974	G	N7-C8-N9	5.01	115.61	113.10
8	A	1755	A	N9-C4-C5	5.01	107.81	105.80
8	A	2116	G	N9-C4-C5	-5.01	103.39	105.40
22	O	102	ARG	NE-CZ-NH2	5.01	122.81	120.30
34	a	1012	A	C2-N3-C4	-5.01	108.09	110.60
8	A	1471	G	C4-N9-C1'	5.01	133.02	126.50
9	B	11	C	C2-N1-C1'	5.01	124.31	118.80
8	A	1279	G	N3-C4-C5	5.01	131.11	128.60
8	A	2137	U	C6-N1-C2	5.01	124.01	121.00
8	A	2412	A	N1-C6-N6	5.01	121.61	118.60
34	a	671	G	C2-N3-C4	-5.01	109.39	111.90
8	A	301	G	C4-N9-C1'	-5.01	119.99	126.50
8	A	1012	U	N3-C4-O4	5.01	122.91	119.40
8	A	1208	C	C6-N1-C2	5.01	122.30	120.30
34	a	482	A	N1-C6-N6	5.01	121.61	118.60
8	A	570	G	C4-C5-C6	5.01	121.81	118.80
8	A	1831	G	C8-N9-C4	5.01	108.40	106.40
34	a	648	A	N9-C4-C5	-5.01	103.80	105.80
34	a	1366	C	N3-C4-C5	5.01	123.90	121.90
8	A	770	G	N3-C4-N9	-5.01	123.00	126.00
8	A	2013	A	C4-C5-N7	5.01	113.20	110.70
8	A	2224	G	N3-C4-C5	5.01	131.10	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	44	G	N3-C4-N9	-5.01	123.00	126.00
8	A	1666	G	C4-N9-C1'	-5.00	119.99	126.50
34	a	470	C	N1-C1'-C2'	-5.00	106.49	112.00
8	A	1194	A	N9-C4-C5	-5.00	103.80	105.80
8	A	1515	A	N1-C6-N6	5.00	121.60	118.60
8	A	1987	A	N9-C4-C5	-5.00	103.80	105.80
34	a	1460	C	C6-N1-C2	5.00	122.30	120.30
55	v	5	G	C4-N9-C1'	-5.00	119.99	126.50
8	A	1177	G	N3-C4-N9	-5.00	123.00	126.00
8	A	1989	G	C2-N3-C4	-5.00	109.40	111.90
8	A	2093	G	C2-N3-C4	-5.00	109.40	111.90
34	a	831	A	N9-C4-C5	-5.00	103.80	105.80
34	a	1292	G	N3-C4-C5	5.00	131.10	128.60

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	3	30	HIS	Peptide
25	R	51	VAL	Peptide
28	U	97	SER	Peptide
32	Y	19	LEU	Peptide
35	b	87	ASP	Peptide
37	d	34	GLU	Peptide
37	d	71	PHE	Peptide
37	d	79	ALA	Peptide
54	u	12	ASP	Peptide
57	x	646	SER	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	0	54/57 (95%)	53 (98%)	1 (2%)	0	100	100
2	1	48/55 (87%)	46 (96%)	2 (4%)	0	100	100
3	2	44/46 (96%)	41 (93%)	3 (7%)	0	100	100
4	3	62/65 (95%)	56 (90%)	5 (8%)	1 (2%)	9	44
5	4	36/38 (95%)	31 (86%)	5 (14%)	0	100	100
6	5	129/165 (78%)	107 (83%)	22 (17%)	0	100	100
7	6	64/70 (91%)	57 (89%)	5 (8%)	2 (3%)	4	27
10	C	269/273 (98%)	245 (91%)	24 (9%)	0	100	100
11	D	207/209 (99%)	190 (92%)	17 (8%)	0	100	100
12	E	199/201 (99%)	191 (96%)	8 (4%)	0	100	100
13	F	175/179 (98%)	157 (90%)	18 (10%)	0	100	100
14	G	174/177 (98%)	163 (94%)	11 (6%)	0	100	100
15	H	147/149 (99%)	126 (86%)	21 (14%)	0	100	100
16	I	139/142 (98%)	124 (89%)	14 (10%)	1 (1%)	22	62
17	J	140/142 (99%)	134 (96%)	6 (4%)	0	100	100
18	K	120/123 (98%)	109 (91%)	11 (9%)	0	100	100
19	L	141/144 (98%)	124 (88%)	17 (12%)	0	100	100
20	M	134/136 (98%)	122 (91%)	12 (9%)	0	100	100
21	N	118/127 (93%)	109 (92%)	9 (8%)	0	100	100
22	O	114/117 (97%)	107 (94%)	7 (6%)	0	100	100
23	P	112/115 (97%)	101 (90%)	11 (10%)	0	100	100
24	Q	115/118 (98%)	113 (98%)	2 (2%)	0	100	100
25	R	101/103 (98%)	91 (90%)	9 (9%)	1 (1%)	15	54
26	S	108/110 (98%)	99 (92%)	9 (8%)	0	100	100
27	T	91/100 (91%)	81 (89%)	9 (10%)	1 (1%)	14	52
28	U	100/104 (96%)	89 (89%)	10 (10%)	1 (1%)	15	54
29	V	92/94 (98%)	92 (100%)	0	0	100	100
30	W	73/85 (86%)	68 (93%)	5 (7%)	0	100	100
31	X	75/78 (96%)	70 (93%)	5 (7%)	0	100	100
32	Y	61/63 (97%)	57 (93%)	3 (5%)	1 (2%)	9	44

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
33	Z	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
35	b	216/240 (90%)	180 (83%)	35 (16%)	1 (0%)	29	69
36	c	204/233 (88%)	193 (95%)	11 (5%)	0	100	100
37	d	203/206 (98%)	172 (85%)	30 (15%)	1 (0%)	29	69
38	e	155/167 (93%)	140 (90%)	15 (10%)	0	100	100
39	f	98/135 (73%)	89 (91%)	9 (9%)	0	100	100
40	g	149/179 (83%)	134 (90%)	15 (10%)	0	100	100
41	h	127/130 (98%)	118 (93%)	9 (7%)	0	100	100
42	i	125/130 (96%)	106 (85%)	19 (15%)	0	100	100
43	j	96/103 (93%)	78 (81%)	18 (19%)	0	100	100
44	k	114/129 (88%)	103 (90%)	11 (10%)	0	100	100
45	l	121/124 (98%)	104 (86%)	16 (13%)	1 (1%)	19	60
46	m	112/118 (95%)	100 (89%)	12 (11%)	0	100	100
47	n	99/102 (97%)	90 (91%)	9 (9%)	0	100	100
48	o	86/89 (97%)	82 (95%)	4 (5%)	0	100	100
49	p	80/82 (98%)	68 (85%)	12 (15%)	0	100	100
50	q	78/84 (93%)	65 (83%)	13 (17%)	0	100	100
51	r	63/75 (84%)	54 (86%)	9 (14%)	0	100	100
52	s	80/92 (87%)	72 (90%)	8 (10%)	0	100	100
53	t	83/87 (95%)	82 (99%)	1 (1%)	0	100	100
54	u	63/71 (89%)	51 (81%)	12 (19%)	0	100	100
57	x	666/704 (95%)	588 (88%)	71 (11%)	7 (1%)	14	52
All	All	6516/6924 (94%)	5877 (90%)	621 (10%)	18 (0%)	44	76

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	6	64	PHE
57	x	387	LEU
57	x	545	PRO
57	x	546	GLY
4	3	31	ILE
57	x	647	GLU
28	U	98	ASN

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Mol	Chain	Res	Type
57	x	507	GLN
57	x	508	SER
32	Y	19	LEU
35	b	20	ARG
57	x	79	GLU
25	R	52	PRO
27	T	88	LYS
45	l	41	PRO
7	6	51	VAL
16	I	22	PRO
37	d	144	ILE

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	47/48 (98%)	47 (100%)	0	100	100
2	1	45/49 (92%)	45 (100%)	0	100	100
3	2	38/38 (100%)	37 (97%)	1 (3%)	46	67
4	3	51/52 (98%)	51 (100%)	0	100	100
5	4	34/34 (100%)	34 (100%)	0	100	100
7	6	59/62 (95%)	58 (98%)	1 (2%)	60	78
10	C	216/218 (99%)	213 (99%)	3 (1%)	67	80
11	D	164/164 (100%)	164 (100%)	0	100	100
12	E	165/165 (100%)	165 (100%)	0	100	100
13	F	148/150 (99%)	148 (100%)	0	100	100
14	G	137/138 (99%)	135 (98%)	2 (2%)	65	80
15	H	114/114 (100%)	113 (99%)	1 (1%)	78	88
17	J	116/116 (100%)	116 (100%)	0	100	100
18	K	103/104 (99%)	99 (96%)	4 (4%)	32	56
19	L	102/103 (99%)	101 (99%)	1 (1%)	76	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	M	109/109 (100%)	108 (99%)	1 (1%)	78	88
21	N	100/103 (97%)	100 (100%)	0	100	100
22	O	86/87 (99%)	86 (100%)	0	100	100
23	P	99/100 (99%)	99 (100%)	0	100	100
24	Q	89/90 (99%)	89 (100%)	0	100	100
25	R	84/84 (100%)	84 (100%)	0	100	100
26	S	93/93 (100%)	92 (99%)	1 (1%)	73	84
27	T	80/84 (95%)	79 (99%)	1 (1%)	69	82
28	U	83/85 (98%)	83 (100%)	0	100	100
29	V	78/78 (100%)	77 (99%)	1 (1%)	69	82
30	W	57/63 (90%)	56 (98%)	1 (2%)	59	77
31	X	67/68 (98%)	67 (100%)	0	100	100
32	Y	55/55 (100%)	55 (100%)	0	100	100
33	Z	48/49 (98%)	48 (100%)	0	100	100
35	b	180/198 (91%)	177 (98%)	3 (2%)	60	78
36	c	170/190 (90%)	169 (99%)	1 (1%)	86	92
37	d	172/173 (99%)	170 (99%)	2 (1%)	71	84
38	e	114/126 (90%)	112 (98%)	2 (2%)	59	77
39	f	87/116 (75%)	87 (100%)	0	100	100
40	g	124/147 (84%)	122 (98%)	2 (2%)	62	79
41	h	104/105 (99%)	104 (100%)	0	100	100
42	i	105/107 (98%)	105 (100%)	0	100	100
43	j	86/90 (96%)	86 (100%)	0	100	100
44	k	89/99 (90%)	88 (99%)	1 (1%)	73	84
45	l	103/104 (99%)	101 (98%)	2 (2%)	57	75
46	m	92/96 (96%)	92 (100%)	0	100	100
47	n	79/84 (94%)	78 (99%)	1 (1%)	69	82
48	o	76/77 (99%)	75 (99%)	1 (1%)	69	82
49	p	65/65 (100%)	65 (100%)	0	100	100
50	q	74/78 (95%)	74 (100%)	0	100	100
51	r	56/65 (86%)	56 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
52	s	72/79 (91%)	71 (99%)	1 (1%)	67	80
53	t	65/66 (98%)	65 (100%)	0	100	100
54	u	46/61 (75%)	46 (100%)	0	100	100
57	x	551/578 (95%)	545 (99%)	6 (1%)	73	84
58	y	1/1 (100%)	1 (100%)	0	100	100
All	All	5178/5408 (96%)	5138 (99%)	40 (1%)	82	89

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	2	41	ARG
7	6	20	ASN
10	C	43	ASN
10	C	85	ASN
10	C	259	ASN
14	G	2	ARG
14	G	138	GLN
15	H	58	LEU
18	K	37	ASP
18	K	88	ASN
18	K	90	ASN
18	K	93	GLN
19	L	58	TYR
20	M	6	ARG
26	S	46	LEU
27	T	26	LYS
29	V	34	LYS
30	W	10	ARG
35	b	108	GLN
35	b	176	ASN
35	b	183	PHE
36	c	106	ARG
37	d	46	ARG
37	d	71	PHE
38	e	81	GLN
38	e	92	ARG
40	g	10	LYS
40	g	147	ASN
44	k	118	ASN
45	l	4	ASN

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Mol	Chain	Res	Type
45	l	46	SER
47	n	49	GLN
48	o	16	ARG
52	s	80	ARG
57	x	23	THR
57	x	84	ASN
57	x	258	ASN
57	x	481	ASN
57	x	529	ASN
57	x	578	HIS

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

Mol	Chain	Res	Type
2	l	44	GLN
38	e	81	GLN
44	k	21	HIS

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
34	a	1536/1542 (99%)	447 (29%)	0
55	v	76/77 (98%)	20 (26%)	0
56	w	74/76 (97%)	23 (31%)	0
59	z	9/33 (27%)	3 (33%)	0
8	A	2898/2903 (99%)	593 (20%)	39 (1%)
9	B	119/120 (99%)	21 (17%)	3 (2%)
All	All	4712/4751 (99%)	1107 (23%)	42 (0%)

All (1107) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
8	A	10	A
8	A	34	U
8	A	35	G
8	A	46	G
8	A	62	U
8	A	63	A
8	A	64	A
8	A	71	A

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Mol	Chain	Res	Type
8	A	74	A
8	A	75	G
8	A	91	A
8	A	101	A
8	A	102	U
8	A	103	A
8	A	118	A
8	A	119	A
8	A	120	U
8	A	131	A
8	A	139	U
8	A	141	G
8	A	142	A
8	A	157	C
8	A	158	U
8	A	159	G
8	A	160	A
8	A	162	U
8	A	163	C
8	A	167	A
8	A	169	G
8	A	181	A
8	A	196	A
8	A	199	A
8	A	215	G
8	A	216	A
8	A	221	A
8	A	222	A
8	A	224	U
8	A	225	C
8	A	228	C
8	A	229	C
8	A	233	A
8	A	242	G
8	A	243	U
8	A	248	G
8	A	250	G
8	A	255	A
8	A	266	G
8	A	271	G
8	A	272	A
8	A	273	G

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Mol	Chain	Res	Type
8	A	274	C
8	A	275	C
8	A	276	U
8	A	277	G
8	A	278	A
8	A	287	G
8	A	288	U
8	A	291	G
8	A	294	A
8	A	311	A
8	A	330	A
8	A	331	C
8	A	345	A
8	A	346	A
8	A	355	U
8	A	356	G
8	A	362	A
8	A	369	U
8	A	371	A
8	A	372	G
8	A	373	U
8	A	377	G
8	A	383	C
8	A	386	G
8	A	395	U
8	A	396	G
8	A	401	A
8	A	403	U
8	A	404	A
8	A	405	U
8	A	406	G
8	A	411	G
8	A	424	G
8	A	434	U
8	A	435	C
8	A	452	G
8	A	455	C
8	A	457	A
8	A	458	G
8	A	459	U
8	A	475	C
8	A	480	A

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Mol	Chain	Res	Type
8	A	481	G
8	A	489	G
8	A	491	G
8	A	496	G
8	A	501	A
8	A	505	A
8	A	509	C
8	A	513	A
8	A	529	A
8	A	532	A
8	A	548	G
8	A	549	G
8	A	556	A
8	A	563	A
8	A	568	U
8	A	571	U
8	A	573	U
8	A	575	A
8	A	603	A
8	A	613	A
8	A	614	A
8	A	615	U
8	A	622	G
8	A	627	A
8	A	637	A
8	A	645	C
8	A	646	U
8	A	647	G
8	A	653	U
8	A	654	A
8	A	655	A
8	A	669	G
8	A	670	A
8	A	677	A
8	A	682	G
8	A	685	A
8	A	686	U
8	A	730	A
8	A	740	C
8	A	747	5MC
8	A	762	U
8	A	764	A

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Mol	Chain	Res	Type
8	A	765	C
8	A	774	G
8	A	775	G
8	A	776	G
8	A	782	A
8	A	784	G
8	A	785	G
8	A	791	C
8	A	792	A
8	A	805	G
8	A	812	C
8	A	819	A
8	A	827	U
8	A	828	U
8	A	831	G
8	A	845	A
8	A	846	U
8	A	847	U
8	A	856	G
8	A	859	G
8	A	866	A
8	A	869	G
8	A	874	G
8	A	875	G
8	A	876	C
8	A	877	A
8	A	882	G
8	A	883	G
8	A	884	U
8	A	885	C
8	A	886	A
8	A	887	A
8	A	888	C
8	A	890	C
8	A	891	G
8	A	892	A
8	A	893	C
8	A	894	U
8	A	895	U
8	A	896	A
8	A	899	A
8	A	903	C

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Mol	Chain	Res	Type
8	A	907	G
8	A	910	A
8	A	914	G
8	A	927	A
8	A	931	U
8	A	938	G
8	A	941	A
8	A	945	A
8	A	946	C
8	A	959	A
8	A	961	C
8	A	973	A
8	A	974	G
8	A	983	A
8	A	984	A
8	A	990	A
8	A	995	C
8	A	996	A
8	A	999	U
8	A	1005	C
8	A	1012	U
8	A	1013	C
8	A	1025	G
8	A	1026	G
8	A	1033	U
8	A	1040	A
8	A	1044	C
8	A	1045	C
8	A	1046	A
8	A	1047	G
8	A	1048	A
8	A	1057	A
8	A	1058	U
8	A	1059	G
8	A	1060	U
8	A	1061	U
8	A	1062	G
8	A	1063	G
8	A	1064	C
8	A	1065	U
8	A	1066	U
8	A	1067	A

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Mol	Chain	Res	Type
8	A	1068	G
8	A	1069	A
8	A	1070	A
8	A	1072	C
8	A	1073	A
8	A	1074	G
8	A	1075	C
8	A	1076	C
8	A	1079	C
8	A	1080	A
8	A	1081	U
8	A	1082	U
8	A	1083	U
8	A	1084	A
8	A	1085	A
8	A	1086	A
8	A	1087	G
8	A	1088	A
8	A	1089	A
8	A	1091	G
8	A	1092	C
8	A	1093	G
8	A	1094	U
8	A	1095	A
8	A	1097	U
8	A	1099	G
8	A	1100	C
8	A	1101	U
8	A	1102	C
8	A	1103	A
8	A	1105	U
8	A	1106	G
8	A	1107	G
8	A	1111	A
8	A	1112	G
8	A	1115	G
8	A	1117	C
8	A	1120	G
8	A	1130	U
8	A	1132	U
8	A	1133	A
8	A	1135	C

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Mol	Chain	Res	Type
8	A	1139	G
8	A	1172	C
8	A	1174	U
8	A	1175	A
8	A	1176	U
8	A	1177	G
8	A	1178	C
8	A	1179	G
8	A	1180	U
8	A	1204	A
8	A	1227	G
8	A	1247	A
8	A	1253	A
8	A	1255	U
8	A	1256	G
8	A	1271	G
8	A	1272	A
8	A	1294	U
8	A	1300	G
8	A	1301	A
8	A	1332	G
8	A	1341	G
8	A	1345	C
8	A	1359	A
8	A	1365	A
8	A	1368	G
8	A	1378	A
8	A	1379	U
8	A	1380	G
8	A	1383	A
8	A	1395	A
8	A	1408	G
8	A	1415	U
8	A	1416	G
8	A	1419	A
8	A	1420	A
8	A	1427	A
8	A	1428	C
8	A	1433	A
8	A	1452	G
8	A	1454	C
8	A	1455	G

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Mol	Chain	Res	Type
8	A	1458	U
8	A	1460	U
8	A	1461	C
8	A	1482	G
8	A	1490	A
8	A	1491	G
8	A	1493	C
8	A	1497	U
8	A	1498	C
8	A	1515	A
8	A	1523	U
8	A	1529	G
8	A	1534	U
8	A	1535	A
8	A	1536	C
8	A	1558	C
8	A	1566	A
8	A	1569	A
8	A	1578	U
8	A	1583	A
8	A	1584	U
8	A	1585	C
8	A	1603	A
8	A	1608	A
8	A	1610	A
8	A	1634	A
8	A	1647	U
8	A	1648	U
8	A	1649	G
8	A	1654	A
8	A	1674	G
8	A	1675	C
8	A	1698	A
8	A	1715	G
8	A	1729	U
8	A	1730	C
8	A	1731	G
8	A	1732	C
8	A	1738	G
8	A	1744	A
8	A	1757	A
8	A	1764	C

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Mol	Chain	Res	Type
8	A	1773	A
8	A	1784	A
8	A	1786	A
8	A	1787	A
8	A	1789	A
8	A	1790	C
8	A	1800	C
8	A	1801	A
8	A	1807	G
8	A	1808	A
8	A	1809	A
8	A	1811	G
8	A	1816	C
8	A	1827	U
8	A	1829	A
8	A	1835	2MG
8	A	1848	A
8	A	1857	G
8	A	1869	G
8	A	1884	G
8	A	1896	G
8	A	1900	A
8	A	1901	A
8	A	1906	G
8	A	1912	A
8	A	1913	A
8	A	1914	C
8	A	1927	A
8	A	1929	G
8	A	1930	G
8	A	1931	U
8	A	1937	A
8	A	1938	A
8	A	1939	5MU
8	A	1955	U
8	A	1960	A
8	A	1967	C
8	A	1970	A
8	A	1971	U
8	A	1972	G
8	A	1982	U
8	A	1991	U

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Mol	Chain	Res	Type
8	A	1997	C
8	A	2020	A
8	A	2022	U
8	A	2023	C
8	A	2031	A
8	A	2032	G
8	A	2033	A
8	A	2036	C
8	A	2043	C
8	A	2049	G
8	A	2055	C
8	A	2056	G
8	A	2060	A
8	A	2061	G
8	A	2062	A
8	A	2069	G7M
8	A	2072	C
8	A	2100	G
8	A	2104	C
8	A	2105	U
8	A	2107	G
8	A	2108	A
8	A	2109	U
8	A	2110	G
8	A	2111	U
8	A	2112	G
8	A	2113	U
8	A	2114	A
8	A	2115	G
8	A	2116	G
8	A	2118	U
8	A	2120	G
8	A	2121	G
8	A	2123	G
8	A	2125	G
8	A	2126	A
8	A	2129	C
8	A	2131	U
8	A	2132	U
8	A	2133	G
8	A	2134	A
8	A	2136	G

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Mol	Chain	Res	Type
8	A	2140	G
8	A	2141	G
8	A	2143	C
8	A	2144	G
8	A	2145	C
8	A	2146	C
8	A	2147	A
8	A	2149	U
8	A	2151	U
8	A	2153	C
8	A	2155	U
8	A	2156	G
8	A	2157	G
8	A	2158	A
8	A	2159	G
8	A	2164	C
8	A	2165	C
8	A	2170	A
8	A	2171	A
8	A	2172	U
8	A	2173	A
8	A	2174	C
8	A	2176	A
8	A	2177	C
8	A	2179	C
8	A	2181	U
8	A	2185	U
8	A	2186	G
8	A	2187	U
8	A	2188	U
8	A	2189	U
8	A	2193	G
8	A	2198	A
8	A	2203	U
8	A	2204	G
8	A	2208	C
8	A	2210	U
8	A	2211	A
8	A	2225	A
8	A	2238	G
8	A	2239	G
8	A	2266	A

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Mol	Chain	Res	Type
8	A	2273	A
8	A	2278	A
8	A	2279	G
8	A	2283	C
8	A	2287	A
8	A	2288	A
8	A	2289	G
8	A	2297	A
8	A	2305	U
8	A	2309	A
8	A	2310	C
8	A	2312	U
8	A	2319	G
8	A	2320	U
8	A	2322	A
8	A	2325	G
8	A	2333	A
8	A	2334	U
8	A	2336	A
8	A	2344	U
8	A	2345	G
8	A	2346	A
8	A	2347	C
8	A	2350	C
8	A	2357	G
8	A	2361	G
8	A	2371	G
8	A	2381	A
8	A	2382	G
8	A	2383	G
8	A	2385	C
8	A	2402	U
8	A	2406	A
8	A	2407	A
8	A	2408	U
8	A	2410	G
8	A	2423	U
8	A	2425	A
8	A	2426	A
8	A	2428	G
8	A	2429	G
8	A	2430	A

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Mol	Chain	Res	Type
8	A	2432	A
8	A	2435	A
8	A	2441	U
8	A	2445	2MG
8	A	2447	G
8	A	2448	A
8	A	2475	C
8	A	2476	A
8	A	2478	A
8	A	2487	G
8	A	2494	G
8	A	2502	G
8	A	2504	PSU
8	A	2505	G
8	A	2518	A
8	A	2520	C
8	A	2529	G
8	A	2535	G
8	A	2547	A
8	A	2554	U
8	A	2556	C
8	A	2566	A
8	A	2567	G
8	A	2573	C
8	A	2576	G
8	A	2584	U
8	A	2585	U
8	A	2602	A
8	A	2609	U
8	A	2613	U
8	A	2615	U
8	A	2619	C
8	A	2621	G
8	A	2629	U
8	A	2630	G
8	A	2638	G
8	A	2646	C
8	A	2654	A
8	A	2656	U
8	A	2663	G
8	A	2689	U
8	A	2690	U

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Mol	Chain	Res	Type
8	A	2702	G
8	A	2714	G
8	A	2718	G
8	A	2725	A
8	A	2726	A
8	A	2729	G
8	A	2732	G
8	A	2733	A
8	A	2739	U
8	A	2744	G
8	A	2747	G
8	A	2748	A
8	A	2749	A
8	A	2750	A
8	A	2751	G
8	A	2752	C
8	A	2754	U
8	A	2755	C
8	A	2765	A
8	A	2778	A
8	A	2779	U
8	A	2791	G
8	A	2793	C
8	A	2798	U
8	A	2799	A
8	A	2800	A
8	A	2808	G
8	A	2818	U
8	A	2820	A
8	A	2821	A
8	A	2849	U
8	A	2867	G
8	A	2872	A
8	A	2873	A
8	A	2880	C
8	A	2884	U
8	A	2886	A
8	A	2891	U
8	A	2902	C
9	B	9	G
9	B	18	G
9	B	25	U

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Mol	Chain	Res	Type
9	B	35	C
9	B	36	C
9	B	37	C
9	B	41	G
9	B	42	C
9	B	44	G
9	B	45	A
9	B	51	G
9	B	52	A
9	B	53	A
9	B	56	G
9	B	67	G
9	B	73	A
9	B	88	C
9	B	89	U
9	B	108	A
9	B	109	A
9	B	120	U
34	a	2	A
34	a	5	U
34	a	6	G
34	a	7	A
34	a	9	G
34	a	16	A
34	a	22	G
34	a	31	G
34	a	32	A
34	a	37	U
34	a	39	G
34	a	46	G
34	a	47	C
34	a	48	C
34	a	50	A
34	a	51	A
34	a	64	G
34	a	69	G
34	a	71	A
34	a	73	C
34	a	74	A
34	a	77	A
34	a	78	A
34	a	79	G

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Mol	Chain	Res	Type
34	a	80	A
34	a	81	A
34	a	83	C
34	a	84	U
34	a	85	U
34	a	86	G
34	a	88	U
34	a	89	U
34	a	90	C
34	a	92	U
34	a	94	G
34	a	97	G
34	a	114	U
34	a	121	U
34	a	131	A
34	a	133	U
34	a	140	U
34	a	141	G
34	a	144	G
34	a	145	G
34	a	146	G
34	a	148	G
34	a	155	A
34	a	156	C
34	a	157	U
34	a	158	G
34	a	159	G
34	a	160	A
34	a	161	A
34	a	162	A
34	a	163	C
34	a	164	G
34	a	165	G
34	a	167	A
34	a	169	C
34	a	170	U
34	a	171	A
34	a	173	U
34	a	174	A
34	a	179	A
34	a	180	U
34	a	182	A

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Mol	Chain	Res	Type
34	a	183	C
34	a	186	C
34	a	188	C
34	a	189	A
34	a	197	A
34	a	198	G
34	a	201	G
34	a	202	G
34	a	204	G
34	a	205	A
34	a	206	C
34	a	207	C
34	a	208	U
34	a	209	U
34	a	210	C
34	a	211	G
34	a	212	G
34	a	213	G
34	a	214	C
34	a	216	U
34	a	219	U
34	a	221	C
34	a	224	U
34	a	226	G
34	a	240	G
34	a	245	U
34	a	246	A
34	a	247	G
34	a	251	G
34	a	253	A
34	a	262	A
34	a	266	G
34	a	267	C
34	a	271	C
34	a	279	A
34	a	281	G
34	a	289	G
34	a	298	A
34	a	299	G
34	a	301	G
34	a	316	C
34	a	317	U

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Mol	Chain	Res	Type
34	a	321	A
34	a	322	C
34	a	328	C
34	a	330	C
34	a	342	C
34	a	344	A
34	a	345	C
34	a	346	G
34	a	347	G
34	a	351	G
34	a	352	C
34	a	354	G
34	a	363	A
34	a	367	U
34	a	372	C
34	a	373	A
34	a	374	A
34	a	375	U
34	a	376	G
34	a	384	G
34	a	388	G
34	a	392	C
34	a	397	A
34	a	405	U
34	a	406	G
34	a	411	A
34	a	414	A
34	a	415	A
34	a	421	U
34	a	422	C
34	a	423	G
34	a	428	G
34	a	429	U
34	a	430	A
34	a	435	A
34	a	436	C
34	a	439	U
34	a	442	G
34	a	443	C
34	a	447	G
34	a	448	A
34	a	454	G

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Mol	Chain	Res	Type
34	a	457	G
34	a	458	U
34	a	460	A
34	a	462	G
34	a	463	U
34	a	464	U
34	a	467	U
34	a	468	A
34	a	469	C
34	a	470	C
34	a	471	U
34	a	472	U
34	a	473	U
34	a	476	U
34	a	477	C
34	a	479	U
34	a	482	A
34	a	484	G
34	a	492	C
34	a	495	A
34	a	496	A
34	a	497	G
34	a	505	G
34	a	509	A
34	a	510	A
34	a	511	C
34	a	512	U
34	a	515	G
34	a	516	PSU
34	a	518	C
34	a	524	G
34	a	530	G
34	a	532	A
34	a	547	A
34	a	560	A
34	a	562	U
34	a	564	C
34	a	570	G
34	a	572	A
34	a	573	A
34	a	574	A
34	a	575	G

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Mol	Chain	Res	Type
34	a	576	C
34	a	577	G
34	a	583	A
34	a	596	A
34	a	607	A
34	a	614	C
34	a	618	C
34	a	620	C
34	a	623	C
34	a	624	C
34	a	633	G
34	a	635	A
34	a	636	U
34	a	639	G
34	a	641	U
34	a	650	G
34	a	661	G
34	a	662	U
34	a	665	A
34	a	676	A
34	a	686	U
34	a	687	A
34	a	690	G
34	a	693	G
34	a	695	A
34	a	700	G
34	a	702	A
34	a	703	G
34	a	710	G
34	a	721	G
34	a	723	U
34	a	724	G
34	a	731	G
34	a	733	G
34	a	734	G
34	a	736	C
34	a	739	C
34	a	753	A
34	a	755	G
34	a	777	A
34	a	781	A
34	a	782	A

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Mol	Chain	Res	Type
34	a	793	U
34	a	794	A
34	a	799	G
34	a	812	G
34	a	815	A
34	a	817	C
34	a	818	G
34	a	819	A
34	a	820	U
34	a	821	G
34	a	833	G
34	a	836	G
34	a	837	U
34	a	840	C
34	a	842	U
34	a	843	U
34	a	845	A
34	a	849	G
34	a	864	A
34	a	865	A
34	a	872	A
34	a	876	C
34	a	885	G
34	a	890	G
34	a	891	U
34	a	902	G
34	a	914	A
34	a	920	U
34	a	921	U
34	a	926	G
34	a	927	G
34	a	934	C
34	a	935	A
34	a	945	G
34	a	946	A
34	a	958	A
34	a	960	U
34	a	961	U
34	a	964	A
34	a	965	U
34	a	966	2MG
34	a	967	5MC

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Mol	Chain	Res	Type
34	a	969	A
34	a	975	A
34	a	976	G
34	a	977	A
34	a	979	C
34	a	980	C
34	a	982	U
34	a	984	C
34	a	989	U
34	a	992	U
34	a	993	G
34	a	994	A
34	a	995	C
34	a	996	A
34	a	997	U
34	a	1000	A
34	a	1002	G
34	a	1004	A
34	a	1009	U
34	a	1010	U
34	a	1011	C
34	a	1012	A
34	a	1022	A
34	a	1023	U
34	a	1026	G
34	a	1027	C
34	a	1028	C
34	a	1029	U
34	a	1030	U
34	a	1031	C
34	a	1032	G
34	a	1033	G
34	a	1034	G
34	a	1037	C
34	a	1041	G
34	a	1045	C
34	a	1049	U
34	a	1050	G
34	a	1064	G
34	a	1065	U
34	a	1075	U
34	a	1080	A

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Mol	Chain	Res	Type
34	a	1081	A
34	a	1082	A
34	a	1083	U
34	a	1084	G
34	a	1085	U
34	a	1086	U
34	a	1094	G
34	a	1100	C
34	a	1101	A
34	a	1102	A
34	a	1105	A
34	a	1108	G
34	a	1120	C
34	a	1124	G
34	a	1126	U
34	a	1127	G
34	a	1130	A
34	a	1131	G
34	a	1133	G
34	a	1134	G
34	a	1136	C
34	a	1137	C
34	a	1138	G
34	a	1140	C
34	a	1142	G
34	a	1143	G
34	a	1145	A
34	a	1146	A
34	a	1154	G
34	a	1159	U
34	a	1160	G
34	a	1167	A
34	a	1168	U
34	a	1169	A
34	a	1173	U
34	a	1176	A
34	a	1183	U
34	a	1184	G
34	a	1193	G
34	a	1196	A
34	a	1197	A
34	a	1200	C

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Mol	Chain	Res	Type
34	a	1201	A
34	a	1202	U
34	a	1210	C
34	a	1212	U
34	a	1213	A
34	a	1214	C
34	a	1227	A
34	a	1228	C
34	a	1236	A
34	a	1239	A
34	a	1242	G
34	a	1249	C
34	a	1250	A
34	a	1257	A
34	a	1260	G
34	a	1261	A
34	a	1262	C
34	a	1263	C
34	a	1264	U
34	a	1267	C
34	a	1269	A
34	a	1270	G
34	a	1274	A
34	a	1275	A
34	a	1280	A
34	a	1285	A
34	a	1287	A
34	a	1300	G
34	a	1301	U
34	a	1302	C
34	a	1303	C
34	a	1312	G
34	a	1317	C
34	a	1318	A
34	a	1319	A
34	a	1320	C
34	a	1322	C
34	a	1330	U
34	a	1331	G
34	a	1332	A
34	a	1333	A
34	a	1335	U

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Mol	Chain	Res	Type
34	a	1336	C
34	a	1338	G
34	a	1346	A
34	a	1347	G
34	a	1348	U
34	a	1349	A
34	a	1353	G
34	a	1360	A
34	a	1366	C
34	a	1370	G
34	a	1378	C
34	a	1381	U
34	a	1394	A
34	a	1395	C
34	a	1397	C
34	a	1398	A
34	a	1400	C
34	a	1408	A
34	a	1410	A
34	a	1419	G
34	a	1422	G
34	a	1441	A
34	a	1444	U
34	a	1446	A
34	a	1447	A
34	a	1450	U
34	a	1452	C
34	a	1453	G
34	a	1454	G
34	a	1456	A
34	a	1472	U
34	a	1492	A
34	a	1497	G
34	a	1499	A
34	a	1503	A
34	a	1506	U
34	a	1517	G
34	a	1520	C
34	a	1529	G
34	a	1530	G
34	a	1534	A
34	a	1536	C

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Mol	Chain	Res	Type
34	a	1538	C
34	a	1539	C
34	a	1540	U
55	v	9	G
55	v	17(A)	U
55	v	19	G
55	v	20	H2U
55	v	21	A
55	v	22	G
55	v	23	C
55	v	33	U
55	v	36	U
55	v	38	A
55	v	40	C
55	v	41	C
55	v	47	U
55	v	48	C
55	v	54	5MU
55	v	60	U
55	v	68	C
55	v	73	A
55	v	74	C
55	v	75	C
56	w	9	A
56	w	10	G
56	w	13	C
56	w	16	U
56	w	17	C
56	w	19	G
56	w	20	U
56	w	21	A
56	w	22	G
56	w	28	G
56	w	45	U
56	w	46	G7M
56	w	47	U
56	w	48	C
56	w	49	C
56	w	57	G
56	w	58	A
56	w	59	U
56	w	60	U

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Mol	Chain	Res	Type
56	w	61	C
56	w	69	G
56	w	73	A
56	w	76	A
59	z	2	U
59	z	4	U
59	z	9	U

All (42) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
8	A	102	U
8	A	141	G
8	A	160	A
8	A	162	U
8	A	242	G
8	A	310	A
8	A	555	G
8	A	733	G
8	A	746	PSU
8	A	784	G
8	A	882	G
8	A	885	C
8	A	1078	U
8	A	1085	A
8	A	1090	A
8	A	1091	G
8	A	1173	U
8	A	1178	C
8	A	1182	G
8	A	1200	C
8	A	1300	G
8	A	1358	G
8	A	1454	C
8	A	1490	A
8	A	1730	C
8	A	1789	A
8	A	1847	G
8	A	2192	U
8	A	2287	A
8	A	2308	G
8	A	2324	U

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Mol	Chain	Res	Type
8	A	2345	G
8	A	2346	A
8	A	2381	A
8	A	2405	G
8	A	2406	A
8	A	2728	U
8	A	2750	A
8	A	2820	A
9	B	44	G
9	B	52	A
9	B	66	A

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

46 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
8	PSU	A	1911	8	17,21,22	3.42	9 (52%)	20,30,33	3.24	6 (30%)
56	5MU	w	54	56	15,22,23	1.23	2 (13%)	16,32,35	2.15	2 (12%)
34	2MG	a	1207	34	19,26,27	3.53	7 (36%)	21,38,41	2.45	6 (28%)
34	G7M	a	527	34	20,26,27	3.10	6 (30%)	20,39,42	3.41	7 (35%)
34	MA6	a	1518	34	19,26,27	1.54	3 (15%)	18,38,41	3.47	3 (16%)
8	PSU	A	2604	8	17,21,22	3.56	9 (52%)	20,30,33	3.00	7 (35%)
56	PSU	w	32	56	17,21,22	3.49	9 (52%)	20,30,33	3.15	7 (35%)
56	4SU	w	8	56	14,21,22	1.46	3 (21%)	15,30,33	1.86	4 (26%)
55	PSU	v	55	55	17,21,22	3.55	9 (52%)	20,30,33	3.17	5 (25%)
8	3TD	A	1915	8	17,22,23	7.09	12 (70%)	19,32,35	2.22	5 (26%)
8	5MU	A	1939	8	15,22,23	2.84	3 (20%)	16,32,35	2.79	2 (12%)
56	MIA	w	37	56	24,31,32	2.44	4 (16%)	26,44,47	2.74	10 (38%)
8	OMG	A	2251	56,8	18,26,27	3.39	8 (44%)	20,38,41	3.22	7 (35%)
8	2MG	A	1835	8	19,26,27	3.64	7 (36%)	21,38,41	2.64	5 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
34	5MC	a	1407	34	15,22,23	2.58	5 (33%)	19,32,35	1.30	2 (10%)
34	UR3	a	1498	34	14,22,23	2.63	4 (28%)	15,32,35	0.88	1 (6%)
56	G7M	w	46	56	20,26,27	4.99	14 (70%)	20,39,42	2.65	6 (30%)
8	OMC	A	2498	8	15,22,23	3.44	6 (40%)	17,31,34	1.25	1 (5%)
8	PSU	A	2457	8	17,21,22	3.67	9 (52%)	20,30,33	3.35	6 (30%)
8	1MG	A	745	8	18,26,27	3.04	8 (44%)	19,39,42	2.67	3 (15%)
8	5MC	A	747	8	15,22,23	2.90	5 (33%)	19,32,35	1.32	3 (15%)
8	PSU	A	2504	8	17,21,22	3.57	9 (52%)	20,30,33	3.30	6 (30%)
8	5MC	A	1962	8	15,22,23	2.48	5 (33%)	19,32,35	1.09	2 (10%)
34	2MG	a	966	34	19,26,27	1.29	2 (10%)	21,38,41	2.43	9 (42%)
8	6MZ	A	1618	8	18,25,26	1.72	6 (33%)	16,36,39	2.94	4 (25%)
55	4SU	v	8	55	14,21,22	3.68	5 (35%)	15,30,33	1.32	2 (13%)
55	5MU	v	54	55	15,22,23	2.83	3 (20%)	16,32,35	2.84	3 (18%)
55	H2U	v	20	55	18,21,22	3.58	3 (16%)	21,30,33	2.03	5 (23%)
8	PSU	A	746	8	17,21,22	3.35	9 (52%)	20,30,33	3.52	7 (35%)
8	2MG	A	2445	8	19,26,27	3.27	8 (42%)	21,38,41	2.93	6 (28%)
58	FME	y	101	58	8,9,10	1.03	1 (12%)	7,9,11	1.05	1 (14%)
56	PSU	w	55	56	17,21,22	1.45	3 (17%)	20,30,33	3.17	8 (40%)
8	PSU	A	955	8	17,21,22	3.54	9 (52%)	20,30,33	3.33	6 (30%)
8	G7M	A	2069	8	20,26,27	2.78	6 (30%)	20,39,42	2.93	8 (40%)
34	2MG	a	1516	34	19,26,27	4.11	8 (42%)	21,38,41	2.43	8 (38%)
56	PSU	w	39	56	17,21,22	3.54	9 (52%)	20,30,33	3.05	7 (35%)
34	4OC	a	1402	34	16,23,24	3.25	6 (37%)	17,32,35	1.37	3 (17%)
34	5MC	a	967	34	15,22,23	2.80	5 (33%)	19,32,35	1.20	3 (15%)
34	PSU	a	516	34	17,21,22	3.41	9 (52%)	20,30,33	3.29	7 (35%)
8	6MZ	A	2030	8	18,25,26	1.80	6 (33%)	16,36,39	2.37	5 (31%)
8	OMU	A	2552	8	14,22,23	3.04	4 (28%)	14,31,34	1.15	1 (7%)
8	PSU	A	2580	8	17,21,22	3.68	9 (52%)	20,30,33	3.36	6 (30%)
8	PSU	A	1917	8	17,21,22	3.45	9 (52%)	20,30,33	3.15	6 (30%)
8	2MA	A	2503	8	17,25,26	3.55	6 (35%)	19,37,40	2.07	6 (31%)
8	PSU	A	2605	8	17,21,22	3.32	9 (52%)	20,30,33	2.79	6 (30%)
34	MA6	a	1519	34	19,26,27	1.53	3 (15%)	18,38,41	3.63	5 (27%)

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
8	PSU	A	1911	8	-	0/7/25/26	0/2/2/2
56	5MU	w	54	56	-	0/5/25/26	0/2/2/2
34	2MG	a	1207	34	-	0/5/27/28	0/3/3/3
34	G7M	a	527	34	-	2/3/25/26	0/3/3/3
34	MA6	a	1518	34	-	0/7/29/30	0/3/3/3
8	PSU	A	2604	8	-	2/7/25/26	0/2/2/2
56	PSU	w	32	56	-	2/7/25/26	0/2/2/2
56	4SU	w	8	56	-	0/5/25/26	0/2/2/2
55	PSU	v	55	55	-	2/7/25/26	0/2/2/2
8	3TD	A	1915	8	-	2/7/25/26	0/2/2/2
8	5MU	A	1939	8	-	4/5/25/26	0/2/2/2
56	MIA	w	37	56	-	3/11/33/34	0/3/3/3
8	OMG	A	2251	56,8	-	0/5/27/28	0/3/3/3
8	2MG	A	1835	8	-	2/5/27/28	0/3/3/3
34	5MC	a	1407	34	-	1/5/25/26	0/2/2/2
34	UR3	a	1498	34	-	0/5/25/26	0/2/2/2
56	G7M	w	46	56	-	1/3/25/26	0/3/3/3
8	OMC	A	2498	8	-	2/7/27/28	0/2/2/2
8	PSU	A	2457	8	-	0/7/25/26	0/2/2/2
8	1MG	A	745	8	-	0/3/25/26	0/3/3/3
8	5MC	A	747	8	-	2/5/25/26	0/2/2/2
8	PSU	A	2504	8	-	0/7/25/26	0/2/2/2
8	5MC	A	1962	8	-	2/5/25/26	0/2/2/2
34	2MG	a	966	34	-	3/5/27/28	0/3/3/3
8	6MZ	A	1618	8	-	2/5/27/28	0/3/3/3
55	4SU	v	8	55	-	0/5/25/26	0/2/2/2
55	5MU	v	54	55	-	3/5/25/26	0/2/2/2
55	H2U	v	20	55	-	1/7/38/39	0/2/2/2
8	PSU	A	746	8	-	4/7/25/26	0/2/2/2
8	2MG	A	2445	8	-	2/5/27/28	0/3/3/3
58	FME	y	101	58	-	4/7/9/11	-
56	PSU	w	55	56	-	0/7/25/26	0/2/2/2
8	PSU	A	955	8	-	0/7/25/26	0/2/2/2
8	G7M	A	2069	8	-	1/3/25/26	0/3/3/3
34	2MG	a	1516	34	-	0/5/27/28	0/3/3/3
56	PSU	w	39	56	-	2/7/25/26	0/2/2/2
34	4OC	a	1402	34	-	0/9/29/30	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	5MC	a	967	34	-	2/5/25/26	0/2/2/2
34	PSU	a	516	34	-	1/7/25/26	0/2/2/2
8	6MZ	A	2030	8	-	3/5/27/28	0/3/3/3
8	OMU	A	2552	8	-	0/7/27/28	0/2/2/2
8	PSU	A	2580	8	-	0/7/25/26	0/2/2/2
8	PSU	A	1917	8	-	0/7/25/26	0/2/2/2
8	2MA	A	2503	8	-	2/3/25/26	0/3/3/3
8	PSU	A	2605	8	-	0/7/25/26	0/2/2/2
34	MA6	a	1519	34	-	4/7/29/30	0/3/3/3

All (294) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	1915	3TD	C2'-C1'	-17.95	1.33	1.54
8	A	1915	3TD	O4'-C1'	15.25	1.67	1.44
55	v	20	H2U	C2-N1	12.16	1.53	1.35
34	a	1516	2MG	C2-N2	12.01	1.44	1.34
8	A	2580	PSU	C5-C1'	-10.29	1.43	1.52
56	w	46	G7M	C2'-C3'	-10.12	1.25	1.53
34	a	527	G7M	C4-N3	9.26	1.50	1.35
55	v	54	5MU	C4-C5	9.26	1.61	1.41
8	A	2457	PSU	C5-C1'	-9.15	1.44	1.52
34	a	1207	2MG	C2-N2	9.00	1.41	1.34
8	A	1835	2MG	C2-N2	8.95	1.41	1.34
8	A	1939	5MU	C4-C5	8.87	1.60	1.41
56	w	46	G7M	C4-N3	8.55	1.49	1.35
8	A	2251	OMG	C4-N3	8.51	1.49	1.35
8	A	2604	PSU	C5-C1'	-8.37	1.45	1.52
8	A	955	PSU	C5-C1'	-8.36	1.45	1.52
34	a	1516	2MG	C4-N3	8.32	1.48	1.35
8	A	1835	2MG	C4-N3	8.30	1.48	1.35
55	v	8	4SU	C5-C4	8.18	1.47	1.38
8	A	1915	3TD	C6-C5	8.01	1.50	1.38
8	A	2445	2MG	C2-N2	8.00	1.40	1.34
8	A	2445	2MG	C4-N3	7.58	1.47	1.35
8	A	2503	2MA	C4-N3	7.52	1.47	1.35
8	A	745	1MG	C4-N3	7.46	1.47	1.35
8	A	2503	2MA	C6-C5	7.41	1.52	1.41
8	A	2498	OMC	C6-N1	7.28	1.44	1.35
56	w	37	MIA	C13-C14	7.27	1.53	1.32
55	v	8	4SU	C6-N1	7.23	1.44	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	w	39	PSU	C5-C1'	-7.19	1.46	1.52
56	w	46	G7M	O4'-C1'	7.17	1.51	1.41
34	a	1207	2MG	C6-C5	6.92	1.53	1.41
56	w	46	G7M	C6-C5	6.88	1.53	1.41
8	A	1911	PSU	C5-C1'	-6.84	1.46	1.52
55	v	55	PSU	C4-N3	6.83	1.44	1.33
56	w	32	PSU	C4-N3	6.82	1.44	1.33
34	a	967	5MC	C4-N3	6.81	1.44	1.35
34	a	1207	2MG	C4-N3	6.79	1.46	1.35
8	A	2552	OMU	C4-N3	6.78	1.44	1.33
34	a	1498	UR3	C6-N1	6.76	1.44	1.35
55	v	20	H2U	C2-N3	6.75	1.50	1.38
8	A	1835	2MG	C6-C5	6.66	1.52	1.41
8	A	1915	3TD	C5-C1'	-6.61	1.46	1.52
8	A	2503	2MA	C2-N3	6.60	1.45	1.34
56	w	37	MIA	C2-S10	6.55	1.81	1.75
8	A	2504	PSU	C5-C1'	-6.51	1.46	1.52
8	A	2504	PSU	C4-N3	6.43	1.44	1.33
8	A	1917	PSU	C5-C1'	-6.35	1.46	1.52
34	a	1516	2MG	C6-C5	6.29	1.52	1.41
8	A	1915	3TD	O4'-C4'	-6.29	1.30	1.45
8	A	2069	G7M	C4-N3	6.28	1.45	1.35
8	A	1917	PSU	C4-N3	6.25	1.43	1.33
34	a	1402	4OC	C6-N1	6.21	1.43	1.35
8	A	2605	PSU	C5-C1'	-6.18	1.47	1.52
8	A	747	5MC	C4-N3	6.17	1.43	1.35
8	A	2605	PSU	C4-N3	6.17	1.43	1.33
8	A	1962	5MC	C4-N3	6.16	1.43	1.35
8	A	746	PSU	C4-N3	6.16	1.43	1.33
56	w	46	G7M	C3'-C4'	6.13	1.68	1.53
34	a	516	PSU	C5-C1'	-6.08	1.47	1.52
34	a	516	PSU	C4-N3	6.07	1.43	1.33
8	A	1911	PSU	C4-N3	6.07	1.43	1.33
55	v	55	PSU	C5-C1'	-6.05	1.47	1.52
8	A	2498	OMC	C4-N3	6.03	1.45	1.35
56	w	39	PSU	C4-N3	6.00	1.43	1.33
34	a	1402	4OC	C4-N3	5.98	1.46	1.34
8	A	2457	PSU	C4-N3	5.94	1.43	1.33
8	A	2251	OMG	C6-C5	5.93	1.51	1.41
8	A	2604	PSU	C4-N3	5.93	1.43	1.33
8	A	955	PSU	C4-N3	5.83	1.43	1.33
8	A	2504	PSU	C2-N1	5.81	1.49	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	w	46	G7M	C6-N1	5.81	1.43	1.33
8	A	1915	3TD	C2-N1	5.79	1.49	1.38
56	w	46	G7M	O4'-C4'	-5.76	1.32	1.45
8	A	2069	G7M	C6-N1	5.75	1.43	1.33
8	A	2445	2MG	C6-C5	5.70	1.51	1.41
34	a	1407	5MC	C4-N3	5.70	1.43	1.35
34	a	1516	2MG	C6-N1	5.68	1.42	1.33
56	w	32	PSU	C2-N1	5.65	1.49	1.38
8	A	1915	3TD	C4-N3	5.65	1.46	1.38
55	v	55	PSU	C2-N1	5.65	1.49	1.38
34	a	1402	4OC	C2-N3	5.65	1.49	1.38
55	v	55	PSU	C2-N3	5.64	1.49	1.38
8	A	747	5MC	C5-C4	5.56	1.50	1.41
8	A	2552	OMU	C6-N1	5.56	1.42	1.35
56	w	39	PSU	C2-N1	5.54	1.49	1.38
56	w	32	PSU	C2-N3	5.54	1.49	1.38
8	A	2503	2MA	C2-N1	5.53	1.43	1.34
8	A	1917	PSU	C2-N3	5.53	1.49	1.38
55	v	20	H2U	C4-N3	5.53	1.47	1.37
8	A	955	PSU	C2-N1	5.52	1.49	1.38
8	A	2604	PSU	C2-N1	5.51	1.49	1.38
8	A	746	PSU	C6-C5	5.50	1.46	1.38
8	A	746	PSU	C5-C1'	-5.46	1.47	1.52
8	A	2504	PSU	C2-N3	5.45	1.49	1.38
8	A	2580	PSU	C4-N3	5.44	1.42	1.33
8	A	1939	5MU	C4-N3	-5.38	1.23	1.33
34	a	516	PSU	C2-N3	5.38	1.48	1.38
8	A	2251	OMG	C2-N2	5.38	1.44	1.33
8	A	2605	PSU	C2-N3	5.37	1.48	1.38
8	A	2457	PSU	C2-N1	5.36	1.48	1.38
8	A	1915	3TD	C6-N1	5.36	1.45	1.34
34	a	1207	2MG	C6-N1	5.35	1.42	1.33
8	A	2498	OMC	C2-N3	5.34	1.48	1.38
56	w	32	PSU	C6-C5	5.32	1.46	1.38
55	v	8	4SU	C2-N3	5.31	1.48	1.38
8	A	1911	PSU	C2-N3	5.26	1.48	1.38
8	A	1917	PSU	C2-N1	5.26	1.48	1.38
8	A	1911	PSU	C2-N1	5.25	1.48	1.38
8	A	745	1MG	C6-C5	5.23	1.49	1.41
8	A	2498	OMC	C6-C5	5.22	1.49	1.38
56	w	39	PSU	C2-N3	5.21	1.48	1.38
8	A	2251	OMG	C6-N1	5.16	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	a	527	G7M	C6-C5	5.15	1.50	1.41
8	A	746	PSU	C2-N3	5.14	1.48	1.38
34	a	527	G7M	C6-N1	5.10	1.41	1.33
56	w	46	G7M	C2-N1	5.09	1.44	1.35
8	A	2552	OMU	C2-N3	5.08	1.48	1.38
8	A	746	PSU	C2-N1	5.06	1.48	1.38
56	w	46	G7M	C2-N2	5.04	1.44	1.33
8	A	2605	PSU	C2-N1	5.04	1.48	1.38
8	A	745	1MG	C2-N3	5.03	1.42	1.34
8	A	2580	PSU	C2-N3	5.01	1.48	1.38
8	A	1835	2MG	C6-N1	5.00	1.41	1.33
56	w	46	G7M	C2'-C1'	4.98	1.61	1.53
34	a	516	PSU	C2-N1	4.97	1.48	1.38
8	A	745	1MG	C2-N2	4.93	1.43	1.33
8	A	955	PSU	C2-N3	4.93	1.47	1.38
8	A	2457	PSU	C2-N3	4.92	1.47	1.38
34	a	967	5MC	C2-N3	4.86	1.47	1.38
55	v	54	5MU	C4-N3	-4.82	1.24	1.33
8	A	2604	PSU	C2-N3	4.81	1.47	1.38
8	A	2504	PSU	C6-N1	4.81	1.44	1.34
55	v	8	4SU	C4-S4	-4.78	1.58	1.67
55	v	55	PSU	C6-N1	4.76	1.44	1.34
8	A	747	5MC	C2-N3	4.75	1.47	1.38
56	w	39	PSU	C6-C5	4.75	1.45	1.38
56	w	32	PSU	C6-N1	4.72	1.44	1.34
8	A	2504	PSU	C6-C5	4.71	1.45	1.38
56	w	37	MIA	C6-N6	4.71	1.43	1.34
34	a	516	PSU	C6-C5	4.70	1.45	1.38
8	A	1915	3TD	O3'-C3'	-4.69	1.31	1.43
8	A	2069	G7M	C5-C4	-4.68	1.33	1.39
34	a	1402	4OC	C4-N4	4.68	1.46	1.36
56	w	32	PSU	C5-C1'	-4.65	1.48	1.52
34	a	527	G7M	C2-N2	4.64	1.43	1.33
8	A	1917	PSU	C6-C5	4.57	1.45	1.38
55	v	55	PSU	C6-C5	4.53	1.45	1.38
56	w	39	PSU	C6-N1	4.51	1.43	1.34
8	A	2580	PSU	C2-N1	4.49	1.47	1.38
34	a	1407	5MC	C5-C4	4.49	1.48	1.41
8	A	1915	3TD	C4-C5	4.44	1.51	1.41
34	a	967	5MC	C5-C4	4.43	1.48	1.41
34	a	1402	4OC	C6-C5	4.42	1.47	1.38
8	A	746	PSU	C6-N1	4.39	1.43	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	1962	5MC	C2-N3	4.33	1.46	1.38
34	a	1498	UR3	C4-N3	4.33	1.44	1.38
34	a	1498	UR3	C6-C5	4.32	1.47	1.38
8	A	1917	PSU	C6-N1	4.29	1.43	1.34
8	A	1911	PSU	C6-C5	4.28	1.45	1.38
8	A	2552	OMU	C6-C5	4.27	1.47	1.38
8	A	2069	G7M	C2-N1	4.27	1.43	1.35
8	A	2069	G7M	C6-C5	4.25	1.48	1.41
8	A	2503	2MA	C6-N1	4.22	1.43	1.35
34	a	1407	5MC	C2-N3	4.21	1.46	1.38
34	a	516	PSU	C6-N1	4.21	1.43	1.34
8	A	747	5MC	C4-N4	4.21	1.44	1.34
8	A	955	PSU	C6-N1	4.20	1.43	1.34
56	w	8	4SU	C4-S4	-4.17	1.59	1.67
55	v	8	4SU	C6-C5	4.17	1.47	1.38
8	A	2457	PSU	C6-N1	4.17	1.43	1.34
8	A	2251	OMG	C2-N1	4.14	1.42	1.35
8	A	1911	PSU	C6-N1	4.12	1.43	1.34
8	A	2069	G7M	C2-N2	4.08	1.42	1.33
34	a	966	2MG	C6-C5	4.06	1.48	1.41
8	A	2445	2MG	C6-N1	4.03	1.40	1.33
8	A	1618	6MZ	C6-N6	3.99	1.41	1.35
8	A	955	PSU	C6-C5	3.98	1.44	1.38
34	a	1402	4OC	C5-C4	3.97	1.48	1.39
8	A	2605	PSU	C6-C5	3.96	1.44	1.38
34	a	1519	MA6	C5-C4	-3.94	1.30	1.40
34	a	1407	5MC	C4-N4	3.90	1.43	1.34
34	a	967	5MC	C4-N4	3.90	1.43	1.34
34	a	1518	MA6	C5-C4	-3.89	1.30	1.40
8	A	2605	PSU	C6-N1	3.87	1.42	1.34
8	A	2498	OMC	C4-N4	3.87	1.46	1.35
8	A	2030	6MZ	C6-N6	3.86	1.41	1.35
8	A	2604	PSU	C6-N1	3.79	1.42	1.34
56	w	32	PSU	C4-C5	3.73	1.49	1.41
8	A	2604	PSU	C6-C5	3.71	1.44	1.38
8	A	1835	2MG	C2-N3	3.70	1.45	1.34
8	A	2457	PSU	C6-C5	3.68	1.44	1.38
8	A	1962	5MC	C5-C4	3.63	1.47	1.41
8	A	747	5MC	C6-C5	3.55	1.49	1.40
34	a	1516	2MG	C2-N3	3.55	1.45	1.34
56	w	46	G7M	O3'-C3'	3.50	1.51	1.43
8	A	2580	PSU	C6-C5	3.50	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	w	55	PSU	C4-C5	3.46	1.48	1.41
8	A	2605	PSU	C4-C5	3.41	1.48	1.41
34	a	527	G7M	C2-N1	3.36	1.41	1.35
56	w	55	PSU	C5-C1'	-3.34	1.49	1.52
56	w	37	MIA	C5-C4	-3.34	1.32	1.40
8	A	1618	6MZ	C5-C4	-3.32	1.32	1.40
8	A	2580	PSU	C6-N1	3.30	1.41	1.34
8	A	2498	OMC	C5-C4	3.26	1.49	1.41
34	a	516	PSU	O4'-C1'	-3.25	1.39	1.44
34	a	1518	MA6	C2-N3	3.22	1.37	1.32
8	A	2604	PSU	C4-C5	3.21	1.48	1.41
56	w	54	5MU	C4-C5	3.20	1.48	1.41
8	A	1962	5MC	C4-N4	3.17	1.42	1.34
55	v	55	PSU	C4-C5	3.15	1.48	1.41
56	w	46	G7M	O2'-C2'	3.11	1.50	1.43
8	A	1911	PSU	C4-C5	3.10	1.48	1.41
8	A	2445	2MG	C2-N3	3.10	1.44	1.34
8	A	1917	PSU	C4-C5	3.06	1.48	1.41
8	A	2030	6MZ	C5-C4	-3.05	1.32	1.40
8	A	2504	PSU	C4-C5	3.03	1.48	1.41
8	A	2580	PSU	O4'-C1'	-3.02	1.40	1.44
34	a	516	PSU	C4-C5	3.01	1.47	1.41
56	w	39	PSU	C4-C5	2.99	1.47	1.41
8	A	2604	PSU	O4'-C1'	-2.99	1.40	1.44
34	a	1407	5MC	C6-C5	2.95	1.48	1.40
8	A	2030	6MZ	C9-N6	-2.93	1.40	1.45
34	a	1207	2MG	C2-N3	2.90	1.43	1.34
34	a	967	5MC	C6-C5	2.85	1.48	1.40
8	A	746	PSU	C4-C5	2.79	1.47	1.41
8	A	745	1MG	C5-C4	-2.78	1.33	1.40
8	A	2457	PSU	C4-C5	2.71	1.47	1.41
56	w	46	G7M	C2-N3	2.71	1.47	1.34
8	A	745	1MG	O6-C6	-2.71	1.17	1.24
8	A	2030	6MZ	C6-N1	-2.70	1.30	1.34
8	A	1835	2MG	O6-C6	-2.69	1.17	1.24
34	a	1519	MA6	C2-N3	2.65	1.36	1.32
8	A	2605	PSU	O4'-C1'	-2.65	1.40	1.44
8	A	2457	PSU	O4'-C1'	-2.62	1.40	1.44
8	A	2251	OMG	O6-C6	-2.61	1.18	1.24
34	a	1207	2MG	C2-N1	2.60	1.42	1.34
8	A	1939	5MU	O4-C4	-2.59	1.18	1.24
8	A	2445	2MG	O6-C6	-2.59	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	955	PSU	C4-C5	2.58	1.47	1.41
8	A	745	1MG	CM1-N1	-2.58	1.41	1.47
56	w	46	G7M	O6-C6	-2.58	1.18	1.24
8	A	1911	PSU	O4'-C1'	-2.57	1.40	1.44
34	a	1498	UR3	O4-C4	-2.55	1.18	1.24
34	a	527	G7M	C5-C4	-2.53	1.36	1.39
8	A	745	1MG	C6-N1	2.53	1.42	1.38
34	a	1519	MA6	C10-N6	-2.52	1.39	1.45
8	A	2251	OMG	C5-C4	-2.50	1.34	1.40
8	A	1915	3TD	C3'-C4'	2.49	1.59	1.53
34	a	1516	2MG	C2-N1	2.48	1.42	1.34
34	a	1516	2MG	O6-C6	-2.47	1.18	1.24
55	v	55	PSU	O4-C4	-2.44	1.18	1.24
55	v	54	5MU	O4-C4	-2.40	1.18	1.24
8	A	2504	PSU	O4'-C1'	-2.38	1.41	1.44
34	a	1207	2MG	O6-C6	-2.36	1.18	1.24
8	A	1917	PSU	O4'-C1'	-2.35	1.41	1.44
8	A	1962	5MC	C6-C5	2.35	1.46	1.40
56	w	39	PSU	O4-C4	-2.30	1.18	1.24
8	A	2251	OMG	C2-N3	2.29	1.45	1.34
34	a	1516	2MG	C5-C4	-2.28	1.34	1.40
8	A	2030	6MZ	C5-N7	-2.27	1.31	1.39
8	A	1618	6MZ	C4-N3	-2.27	1.32	1.35
8	A	746	PSU	O4'-C1'	-2.25	1.41	1.44
8	A	2580	PSU	O4-C4	-2.25	1.18	1.24
8	A	2503	2MA	C5-C4	-2.23	1.35	1.40
8	A	1618	6MZ	C9-N6	-2.22	1.41	1.45
55	v	55	PSU	O4'-C1'	-2.22	1.41	1.44
56	w	32	PSU	O4'-C1'	-2.20	1.41	1.44
8	A	2605	PSU	O4-C4	-2.17	1.19	1.24
8	A	2445	2MG	CM2-N2	-2.16	1.41	1.45
8	A	2457	PSU	O4-C4	-2.16	1.19	1.24
56	w	8	4SU	C2-N3	-2.15	1.33	1.38
56	w	55	PSU	C2-N3	-2.15	1.33	1.38
34	a	966	2MG	C5-C4	2.14	1.46	1.40
8	A	955	PSU	O4-C4	-2.14	1.19	1.24
8	A	2445	2MG	C5-C4	-2.13	1.35	1.40
8	A	2580	PSU	C4-C5	2.13	1.46	1.41
8	A	746	PSU	O4-C4	-2.13	1.19	1.24
8	A	1618	6MZ	C6-N1	-2.12	1.31	1.34
8	A	955	PSU	O4'-C1'	-2.12	1.41	1.44
8	A	2030	6MZ	C2-N3	2.12	1.35	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	y	101	FME	CA-N	-2.11	1.43	1.46
8	A	1917	PSU	O4-C4	-2.11	1.19	1.24
34	a	1518	MA6	C10-N6	-2.10	1.40	1.45
56	w	39	PSU	O4'-C1'	-2.09	1.41	1.44
8	A	1618	6MZ	C5-N7	-2.08	1.32	1.39
8	A	1911	PSU	O4-C4	-2.08	1.19	1.24
34	a	516	PSU	O4-C4	-2.07	1.19	1.24
8	A	1835	2MG	C5-C4	-2.06	1.35	1.40
8	A	2604	PSU	O4-C4	-2.06	1.19	1.24
56	w	8	4SU	O4'-C1'	2.05	1.43	1.41
56	w	32	PSU	O4-C4	-2.05	1.19	1.24
8	A	2504	PSU	O4-C4	-2.05	1.19	1.24
56	w	54	5MU	C2-N3	-2.04	1.34	1.38
8	A	1915	3TD	O5'-C5'	-2.03	1.39	1.44

All (228) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	a	1519	MA6	N1-C6-N6	-12.93	103.44	117.06
34	a	1518	MA6	N1-C6-N6	-12.58	103.82	117.06
34	a	527	G7M	C1'-N9-C4	12.34	148.33	126.64
8	A	2504	PSU	N1-C2-N3	-11.40	119.37	128.43
8	A	746	PSU	N1-C2-N3	-11.36	119.40	128.43
55	v	55	PSU	N1-C2-N3	-11.26	119.48	128.43
8	A	2251	OMG	C1'-N9-C4	11.14	146.22	126.64
34	a	516	PSU	N1-C2-N3	-10.94	119.73	128.43
8	A	955	PSU	N1-C2-N3	-10.92	119.75	128.43
56	w	32	PSU	N1-C2-N3	-10.86	119.79	128.43
8	A	2457	PSU	N1-C2-N3	-10.86	119.80	128.43
8	A	1917	PSU	N1-C2-N3	-10.73	119.90	128.43
8	A	1911	PSU	N1-C2-N3	-10.50	120.08	128.43
8	A	1835	2MG	CM2-N2-C2	-9.75	111.83	123.59
56	w	39	PSU	N1-C2-N3	-9.63	120.77	128.43
8	A	2580	PSU	N1-C2-N3	-9.51	120.87	128.43
8	A	2604	PSU	N1-C2-N3	-9.42	120.94	128.43
8	A	745	1MG	C1'-N9-C4	-9.27	110.35	126.64
8	A	1939	5MU	C5-C6-N1	-9.08	112.41	122.19
8	A	2605	PSU	N1-C2-N3	-8.86	121.38	128.43
8	A	1618	6MZ	C9-N6-C6	-8.57	115.49	122.87
56	w	55	PSU	N1-C2-N3	-8.28	121.85	128.43
8	A	2069	G7M	C1'-N9-C4	8.21	141.06	126.64
55	v	54	5MU	C4-N3-C2	7.92	121.83	115.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	w	37	MIA	C12-C13-C14	-7.85	111.86	127.14
56	w	54	5MU	C4-N3-C2	7.45	121.43	115.14
8	A	2445	2MG	N2-C2-N3	7.37	124.04	116.96
8	A	746	PSU	C4-N3-C2	7.20	121.22	115.14
55	v	54	5MU	C5-C6-N1	-6.93	114.72	122.19
56	w	55	PSU	C4-N3-C2	6.85	120.92	115.14
55	v	20	H2U	C4-N3-C2	-6.84	120.11	125.79
8	A	2030	6MZ	C9-N6-C6	-6.57	117.22	122.87
8	A	2580	PSU	C5-C4-N3	-6.45	117.05	125.36
34	a	1207	2MG	CM2-N2-C2	-6.45	115.81	123.59
8	A	2445	2MG	CM2-N2-C2	-6.45	115.81	123.59
34	a	516	PSU	C4-N3-C2	6.37	120.52	115.14
34	a	1516	2MG	N2-C2-N3	6.10	122.82	116.96
8	A	2580	PSU	C4-N3-C2	6.08	120.27	115.14
8	A	2251	OMG	N3-C2-N1	-6.04	119.16	127.22
34	a	1518	MA6	N3-C2-N1	-5.97	119.34	128.68
8	A	1915	3TD	C5-C1'-C2'	-5.90	104.79	115.32
8	A	1618	6MZ	N3-C2-N1	-5.90	119.46	128.68
56	w	46	G7M	C2'-C3'-C4'	5.85	114.01	102.64
8	A	2069	G7M	N2-C2-N1	5.83	126.33	117.25
8	A	745	1MG	C6-C5-C4	-5.79	116.24	119.96
34	a	1519	MA6	N3-C2-N1	-5.75	119.69	128.68
8	A	1917	PSU	C4-N3-C2	5.74	119.99	115.14
8	A	2457	PSU	C4-N3-C2	5.72	119.97	115.14
8	A	1939	5MU	C4-N3-C2	5.67	119.93	115.14
8	A	2504	PSU	C4-N3-C2	5.54	119.82	115.14
56	w	32	PSU	C4-N3-C2	5.38	119.68	115.14
8	A	1911	PSU	C4-N3-C2	5.35	119.66	115.14
34	a	1516	2MG	C1'-N9-C4	-5.31	117.32	126.64
34	a	1207	2MG	C1'-N9-C4	-5.30	117.32	126.64
8	A	955	PSU	C4-N3-C2	5.27	119.59	115.14
8	A	2580	PSU	O4'-C1'-C5	-5.27	101.77	109.93
8	A	2457	PSU	C5-C4-N3	-5.26	118.58	125.36
56	w	37	MIA	C12-N6-C6	-5.26	114.76	122.55
34	a	966	2MG	C2-N3-C4	5.25	121.23	115.28
8	A	2030	6MZ	N3-C2-N1	-5.20	120.55	128.68
8	A	746	PSU	C5-C4-N3	-5.15	118.72	125.36
34	a	516	PSU	C5-C4-N3	-5.09	118.80	125.36
8	A	2445	2MG	C1'-N9-C4	-5.05	117.76	126.64
56	w	55	PSU	C5-C4-N3	-5.04	118.86	125.36
55	v	55	PSU	C4-N3-C2	5.03	119.39	115.14
8	A	1911	PSU	C5-C1'-C2'	-4.98	106.43	115.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	w	46	G7M	O3'-C3'-C4'	4.94	125.33	111.05
8	A	2604	PSU	C5-C4-N3	-4.92	119.02	125.36
56	w	39	PSU	C4-N3-C2	4.91	119.29	115.14
56	w	46	G7M	C1'-N9-C4	-4.91	118.02	126.64
8	A	2605	PSU	C5-C4-N3	-4.90	119.05	125.36
8	A	955	PSU	C5-C1'-C2'	-4.90	106.58	115.32
8	A	2445	2MG	N2-C2-N1	-4.80	112.35	116.96
8	A	1917	PSU	C5-C4-N3	-4.80	119.18	125.36
56	w	46	G7M	N3-C2-N1	-4.79	120.83	127.22
8	A	2503	2MA	C1'-N9-C4	-4.70	118.39	126.64
8	A	1911	PSU	C5-C4-N3	-4.70	119.31	125.36
56	w	39	PSU	C5-C4-N3	-4.66	119.36	125.36
8	A	2503	2MA	C2-N3-C4	4.65	119.30	115.52
34	a	527	G7M	N3-C2-N1	-4.65	121.03	127.22
56	w	8	4SU	C2-N3-C4	4.64	121.87	115.15
8	A	2604	PSU	C5-C6-N1	-4.58	118.81	124.44
8	A	2605	PSU	C4-N3-C2	4.57	119.00	115.14
56	w	37	MIA	C16-C14-C13	-4.49	109.67	122.65
8	A	955	PSU	C5-C4-N3	-4.44	119.64	125.36
8	A	1915	3TD	O4'-C1'-C5	4.41	116.77	109.93
56	w	37	MIA	C15-C14-C13	-4.40	109.94	122.65
8	A	2069	G7M	N3-C2-N1	-4.34	121.43	127.22
56	w	32	PSU	C5-C4-N3	-4.27	119.86	125.36
8	A	2504	PSU	C5-C4-N3	-4.25	119.89	125.36
56	w	39	PSU	C5-C1'-C2'	-4.19	107.85	115.32
8	A	2445	2MG	C5-C6-N1	-4.17	117.73	123.43
8	A	2457	PSU	C5-C6-N1	-4.14	119.35	124.44
8	A	2604	PSU	C4-N3-C2	4.12	118.62	115.14
56	w	37	MIA	N3-C2-N1	-4.11	119.42	126.98
34	a	966	2MG	C6-C5-C4	-4.10	116.88	120.80
55	v	55	PSU	C5-C4-N3	-4.08	120.10	125.36
34	a	1407	5MC	C2-N3-C4	4.08	120.94	116.02
56	w	55	PSU	C5-C1'-C2'	-4.07	108.07	115.32
34	a	1516	2MG	N3-C2-N1	-4.04	119.84	126.23
34	a	527	G7M	N2-C2-N3	4.02	124.34	117.79
34	a	1207	2MG	N2-C2-N1	4.00	120.81	116.96
56	w	55	PSU	C6-N1-C2	4.00	121.96	115.36
8	A	1618	6MZ	C1'-N9-C4	-4.00	119.62	126.64
56	w	46	G7M	C2-N3-C4	3.97	119.89	115.36
56	w	39	PSU	C5-C6-N1	-3.83	119.73	124.44
34	a	966	2MG	C5-C6-N1	-3.78	118.27	123.43
8	A	955	PSU	C5-C6-N1	-3.77	119.81	124.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	a	966	2MG	C6-N1-C2	3.73	121.85	115.18
56	w	55	PSU	C5-C6-N1	-3.72	119.87	124.44
8	A	2498	OMC	C2-N3-C4	3.71	120.10	116.34
56	w	54	5MU	C3'-C2'-C1'	3.61	106.41	100.98
8	A	2504	PSU	C5-C6-N1	-3.60	120.02	124.44
34	a	966	2MG	N2-C2-N1	3.60	120.41	116.96
56	w	37	MIA	C11-S10-C2	3.59	104.95	102.27
34	a	1207	2MG	C5-C6-N1	-3.58	118.54	123.43
34	a	1516	2MG	C2-N3-C4	3.56	119.32	115.28
55	v	8	4SU	C2-N3-C4	3.55	120.30	115.15
8	A	1835	2MG	N2-C2-N3	3.50	120.32	116.96
8	A	746	PSU	C5-C1'-C2'	-3.49	109.09	115.32
34	a	527	G7M	C2-N3-C4	3.49	119.34	115.36
56	w	8	4SU	C5-C4-N3	-3.47	119.19	123.83
8	A	2069	G7M	N2-C2-N3	-3.42	112.21	117.79
55	v	55	PSU	C5-C6-N1	-3.35	120.32	124.44
8	A	2069	G7M	C5-C6-N1	-3.35	118.85	123.43
34	a	1519	MA6	C10-N6-C9	3.34	126.90	116.12
34	a	966	2MG	CM2-N2-C2	-3.34	119.56	123.59
8	A	2604	PSU	C5-C1'-C2'	-3.33	109.38	115.32
8	A	1835	2MG	C1'-N9-C4	-3.32	120.81	126.64
8	A	2251	OMG	C6-N1-C2	3.27	121.12	115.93
8	A	2580	PSU	C5-C6-N1	-3.25	120.45	124.44
8	A	2503	2MA	CM2-C2-N1	3.23	122.19	117.15
56	w	32	PSU	C5-C6-N1	-3.22	120.48	124.44
34	a	967	5MC	C5-C6-N1	-3.22	118.72	122.19
34	a	1519	MA6	C1'-N9-C4	-3.19	121.03	126.64
8	A	1911	PSU	C5-C6-N1	-3.17	120.55	124.44
8	A	2445	2MG	C6-N1-C2	3.16	120.83	115.18
8	A	1835	2MG	C2-N3-C4	3.15	118.85	115.28
34	a	1518	MA6	C10-N6-C9	3.14	126.24	116.12
8	A	1915	3TD	C5-C6-N1	-3.13	120.59	124.44
34	a	527	G7M	CN7-N7-C8	-3.12	110.41	125.43
55	v	20	H2U	N3-C2-N1	3.12	119.95	116.65
8	A	747	5MC	C5-C6-N1	-3.11	118.84	122.19
8	A	2069	G7M	CN7-N7-C8	-3.11	110.48	125.43
8	A	746	PSU	O4'-C1'-C5	3.08	114.70	109.93
8	A	2605	PSU	O4'-C1'-C5	-3.06	105.18	109.93
56	w	37	MIA	S10-C2-N1	3.04	126.52	116.01
8	A	2504	PSU	C5-C1'-C2'	-3.02	109.94	115.32
55	v	54	5MU	C5M-C5-C4	2.99	126.72	121.37
55	v	8	4SU	C5-C4-N3	-2.98	119.84	123.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	a	966	2MG	C4-C5-N7	-2.98	106.30	109.40
34	a	1402	4OC	CM4-N4-C4	-2.93	120.45	122.97
8	A	2552	OMU	CM2-O2'-C2'	-2.90	106.92	114.52
8	A	1962	5MC	C5-C6-N1	-2.89	119.08	122.19
55	v	20	H2U	C5-C4-N3	2.89	119.89	116.65
8	A	2503	2MA	N3-C2-N1	-2.88	120.42	125.72
8	A	2503	2MA	C5-C6-N1	-2.88	120.04	123.06
55	v	20	H2U	O2-C2-N1	-2.87	119.50	123.11
8	A	747	5MC	C2-N3-C4	2.84	119.44	116.02
8	A	1917	PSU	C5-C6-N1	-2.83	120.97	124.44
55	v	55	PSU	C6-N1-C2	2.82	120.01	115.36
8	A	2251	OMG	C2-N3-C4	2.81	118.57	115.36
8	A	1915	3TD	C6-N1-C2	2.79	119.96	115.36
8	A	746	PSU	C5-C6-N1	-2.78	121.02	124.44
56	w	8	4SU	C3'-C2'-C1'	2.76	105.14	100.98
34	a	516	PSU	C5-C6-N1	-2.76	121.04	124.44
56	w	32	PSU	C6-N1-C2	2.76	119.91	115.36
8	A	2504	PSU	C6-N1-C2	2.75	119.90	115.36
8	A	1618	6MZ	C2-N1-C6	2.74	118.94	116.59
34	a	1516	2MG	CM2-N2-C2	-2.74	120.29	123.59
55	v	20	H2U	C5-C6-N1	2.73	120.59	111.61
34	a	1516	2MG	C6-N1-C2	2.72	120.05	115.18
8	A	2604	PSU	C6-N1-C2	2.71	119.83	115.36
8	A	2457	PSU	C5-C1'-C2'	-2.70	110.50	115.32
34	a	1407	5MC	C5-C6-N1	-2.70	119.28	122.19
8	A	2069	G7M	C6-C5-C4	-2.67	118.25	120.80
8	A	2457	PSU	C6-N1-C2	2.67	119.76	115.36
8	A	2580	PSU	O4'-C1'-C2'	2.66	108.97	104.66
8	A	2251	OMG	C6-C5-C4	-2.63	118.29	120.80
8	A	955	PSU	C6-N1-C2	2.61	119.66	115.36
34	a	966	2MG	C3'-C2'-C1'	2.59	104.88	100.98
34	a	1519	MA6	C9-N6-C6	-2.57	111.73	119.51
8	A	2251	OMG	C5-C6-N1	-2.50	120.01	123.43
56	w	55	PSU	O4'-C1'-C5	2.49	113.78	109.93
56	w	37	MIA	C1'-N9-C4	-2.45	122.34	126.64
56	w	37	MIA	C2-N3-C4	2.42	118.66	115.32
8	A	1911	PSU	C6-N1-C2	2.41	119.34	115.36
34	a	967	5MC	C2-N3-C4	2.41	118.92	116.02
8	A	1835	2MG	N3-C2-N1	-2.41	122.42	126.23
8	A	745	1MG	N2-C2-N1	2.39	121.47	118.47
8	A	2251	OMG	N2-C2-N3	2.39	121.68	117.79
34	a	527	G7M	C6-N1-C2	2.38	119.71	115.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	w	32	PSU	O4'-C1'-C2'	2.37	108.50	104.66
8	A	2605	PSU	O4'-C1'-C2'	2.36	108.48	104.66
8	A	1917	PSU	C5-C1'-C2'	-2.35	111.13	115.32
34	a	527	G7M	C5-C6-N1	-2.34	120.24	123.43
56	w	8	4SU	C6-N1-C2	-2.30	117.54	121.20
8	A	746	PSU	C6-N1-C2	2.29	119.14	115.36
8	A	2605	PSU	C5-C6-N1	-2.29	121.63	124.44
34	a	516	PSU	C6-N1-C2	2.28	119.12	115.36
8	A	1917	PSU	C6-N1-C2	2.28	119.11	115.36
34	a	1516	2MG	C6-C5-C4	-2.27	118.63	120.80
34	a	1498	UR3	C3U-N3-C4	2.27	121.12	118.12
8	A	1915	3TD	C4'-O4'-C1'	-2.26	106.64	109.42
8	A	2069	G7M	C6-N1-C2	2.26	119.51	115.93
34	a	1516	2MG	C5-C6-N1	-2.24	120.37	123.43
34	a	966	2MG	N3-C2-N1	-2.23	122.70	126.23
56	w	39	PSU	C6-N1-C2	2.23	119.04	115.36
34	a	1402	4OC	N4-C4-N3	2.22	122.04	116.37
58	y	101	FME	C-CA-N	2.21	113.73	109.73
34	a	1207	2MG	C6-N1-C2	2.21	119.13	115.18
56	w	37	MIA	C16-C14-C15	-2.20	109.74	114.60
56	w	32	PSU	C5-C1'-C2'	-2.18	111.42	115.32
34	a	1402	4OC	CM2-O2'-C2'	-2.16	108.85	114.52
8	A	747	5MC	C6-N1-C1'	2.15	124.07	119.24
34	a	1207	2MG	O3'-C3'-C2'	2.15	118.79	111.82
8	A	2030	6MZ	O3'-C3'-C4'	-2.13	104.90	111.05
8	A	2030	6MZ	C1'-N9-C4	-2.13	122.91	126.64
56	w	46	G7M	C5-C6-N1	-2.12	120.53	123.43
8	A	1962	5MC	C2-N3-C4	2.10	118.55	116.02
56	w	55	PSU	C3'-C2'-C1'	2.07	104.32	101.93
8	A	2503	2MA	O3'-C3'-C4'	-2.05	105.12	111.05
8	A	2030	6MZ	C2-N1-C6	2.04	118.34	116.59
34	a	516	PSU	O4'-C1'-C5	-2.03	106.79	109.93
34	a	967	5MC	N4-C4-N3	2.03	119.90	117.03
8	A	2604	PSU	O4'-C1'-C2'	2.02	107.93	104.66
34	a	516	PSU	C5-C1'-C2'	2.01	118.91	115.32
56	w	39	PSU	O4'-C1'-C2'	2.01	107.91	104.66

There are no chirality outliers.

All (61) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
34	a	967	5MC	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
34	a	967	5MC	C3'-C4'-C5'-O5'
34	a	1407	5MC	O4'-C1'-N1-C6
34	a	1519	MA6	C5-C6-N6-C9
34	a	1519	MA6	C5-C6-N6-C10
55	v	54	5MU	C2'-C1'-N1-C6
55	v	54	5MU	C3'-C4'-C5'-O5'
55	v	54	5MU	O4'-C4'-C5'-O5'
55	v	55	PSU	O4'-C1'-C5-C4
8	A	746	PSU	C2'-C1'-C5-C4
8	A	746	PSU	C2'-C1'-C5-C6
8	A	747	5MC	C2'-C1'-N1-C6
8	A	1618	6MZ	N1-C6-N6-C9
8	A	1915	3TD	O4'-C1'-C5-C4
8	A	1939	5MU	C2'-C1'-N1-C6
8	A	1939	5MU	O4'-C1'-N1-C6
8	A	1939	5MU	O4'-C4'-C5'-O5'
8	A	1962	5MC	O4'-C1'-N1-C6
8	A	1962	5MC	C2'-C1'-N1-C6
8	A	2030	6MZ	C3'-C4'-C5'-O5'
8	A	2445	2MG	C3'-C4'-C5'-O5'
8	A	2498	OMC	C1'-C2'-O2'-CM2
8	A	2503	2MA	O4'-C4'-C5'-O5'
56	w	32	PSU	O4'-C1'-C5-C4
56	w	37	MIA	C5-C6-N6-C12
56	w	37	MIA	C12-C13-C14-C16
56	w	39	PSU	O4'-C1'-C5-C4
58	y	101	FME	O1-CN-N-CA
58	y	101	FME	CB-CA-N-CN
34	a	966	2MG	O4'-C4'-C5'-O5'
34	a	966	2MG	C3'-C4'-C5'-O5'
8	A	1835	2MG	C3'-C4'-C5'-O5'
8	A	1939	5MU	C3'-C4'-C5'-O5'
8	A	2030	6MZ	O4'-C4'-C5'-O5'
34	a	1519	MA6	N1-C6-N6-C10
8	A	1835	2MG	O4'-C4'-C5'-O5'
58	y	101	FME	N-CA-CB-CG
56	w	37	MIA	N1-C6-N6-C12
8	A	2445	2MG	O4'-C4'-C5'-O5'
58	y	101	FME	CB-CG-SD-CE
8	A	2030	6MZ	N1-C6-N6-C9
34	a	527	G7M	C3'-C4'-C5'-O5'
55	v	55	PSU	O4'-C1'-C5-C6

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Mol	Chain	Res	Type	Atoms
8	A	746	PSU	O4'-C1'-C5-C6
8	A	1915	3TD	O4'-C1'-C5-C6
56	w	32	PSU	O4'-C1'-C5-C6
56	w	39	PSU	O4'-C1'-C5-C6
8	A	746	PSU	O4'-C1'-C5-C4
34	a	966	2MG	C4'-C5'-O5'-P
55	v	20	H2U	C4'-C5'-O5'-P
56	w	46	G7M	C4'-C5'-O5'-P
34	a	527	G7M	O4'-C4'-C5'-O5'
34	a	1519	MA6	C4'-C5'-O5'-P
8	A	747	5MC	C4'-C5'-O5'-P
8	A	2069	G7M	O4'-C4'-C5'-O5'
8	A	2503	2MA	C3'-C4'-C5'-O5'
8	A	2604	PSU	O4'-C4'-C5'-O5'
8	A	1618	6MZ	C5-C6-N6-C9
34	a	516	PSU	C2'-C1'-C5-C6
8	A	2604	PSU	C2'-C1'-C5-C6
8	A	2498	OMC	O4'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
61	AM2	a	2001	-	40,40,40	0.24	0	53,60,60	0.60	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
62	GDP	x	801	-	24,30,30	5.67	11 (45%)	31,47,47	2.22	12 (38%)

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
61	AM2	a	2001	-	-	4/12/84/84	0/4/4/4
62	GDP	x	801	-	-	7/12/32/32	0/3/3/3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
62	x	801	GDP	C2'-C1'	-17.38	1.27	1.53
62	x	801	GDP	O4'-C1'	10.27	1.55	1.41
62	x	801	GDP	C3'-C4'	-10.01	1.27	1.53
62	x	801	GDP	C4-N3	7.50	1.47	1.35
62	x	801	GDP	C6-C5	6.13	1.51	1.41
62	x	801	GDP	C2-N1	6.11	1.46	1.35
62	x	801	GDP	C2-N2	6.04	1.46	1.33
62	x	801	GDP	C6-N1	5.35	1.42	1.33
62	x	801	GDP	O4'-C4'	4.81	1.55	1.45
62	x	801	GDP	C2'-C3'	4.65	1.66	1.53
62	x	801	GDP	C5-C4	-2.11	1.35	1.40

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
62	x	801	GDP	N2-C2-N1	5.95	126.50	117.25
62	x	801	GDP	N3-C2-N1	-5.42	119.99	127.22
62	x	801	GDP	C5-C6-N1	-3.66	118.43	123.43
62	x	801	GDP	C3'-C2'-C1'	3.21	105.81	100.98
62	x	801	GDP	C6-N1-C2	3.20	121.01	115.93
62	x	801	GDP	N2-C2-N3	-2.63	113.50	117.79
62	x	801	GDP	C2'-C3'-C4'	2.63	107.75	102.64
62	x	801	GDP	PA-O3A-PB	-2.62	123.84	132.83
61	a	2001	AM2	CA1-OA4-CA5	2.47	117.04	113.06
62	x	801	GDP	C6-C5-C4	-2.15	118.74	120.80
62	x	801	GDP	C2-N3-C4	2.13	117.79	115.36
62	x	801	GDP	O3B-PB-O1B	2.08	118.84	110.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
62	x	801	GDP	O3B-PB-O3A	2.07	111.57	104.64
61	a	2001	AM2	OA4-CA1-CA2	2.07	114.86	110.25

There are no chirality outliers.

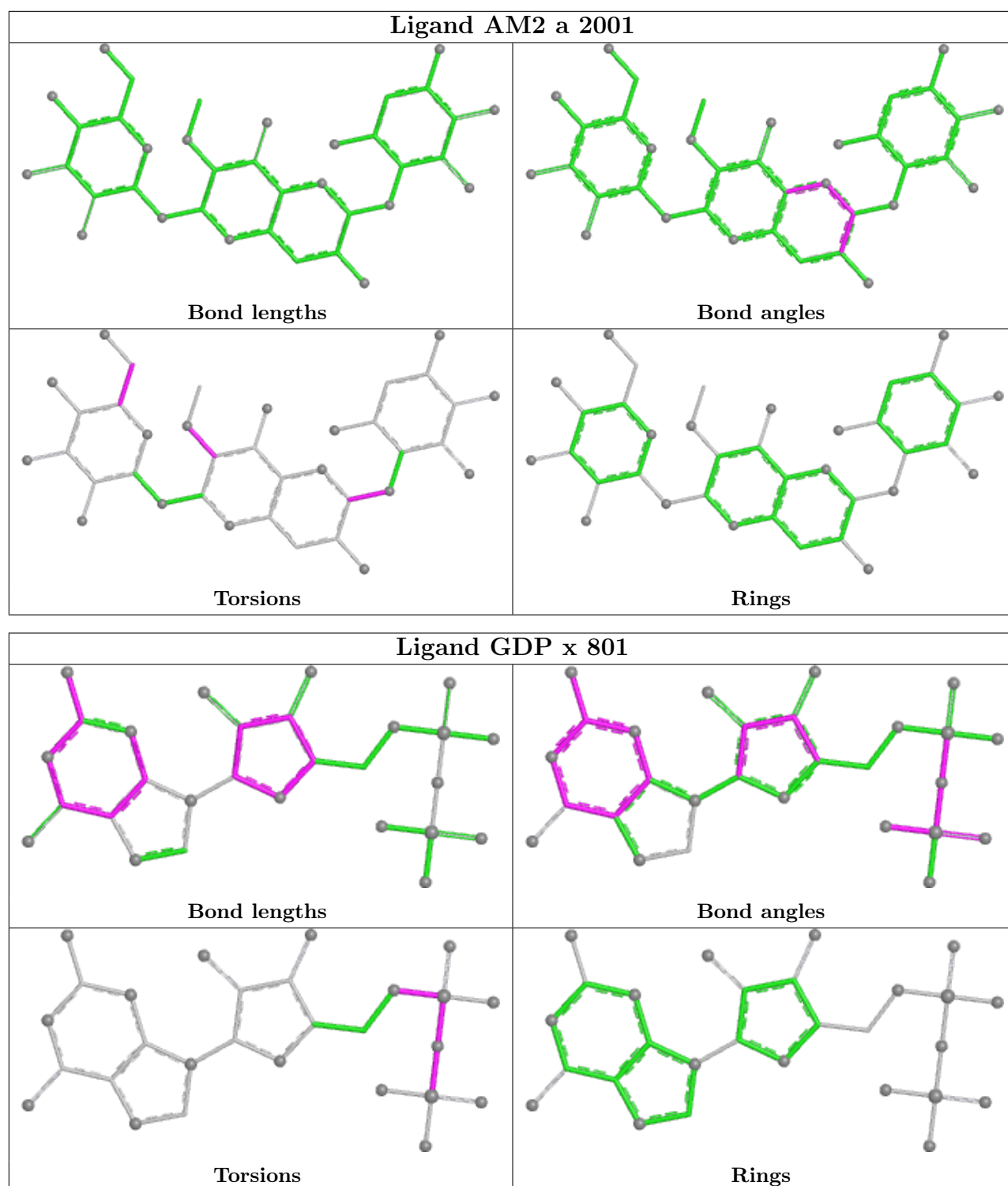
All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
61	a	2001	AM2	CA8-CA7-NA7-CA9
62	x	801	GDP	C5'-O5'-PA-O3A
61	a	2001	AM2	OB1-CB5-CB6-OB6
62	x	801	GDP	PA-O3A-PB-O3B
61	a	2001	AM2	OA4-CA1-OA1-CC1
62	x	801	GDP	C5'-O5'-PA-O1A
62	x	801	GDP	C5'-O5'-PA-O2A
61	a	2001	AM2	CA6-CA7-NA7-CA9
62	x	801	GDP	PA-O3A-PB-O2B
62	x	801	GDP	PB-O3A-PA-O1A
62	x	801	GDP	PB-O3A-PA-O2A

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

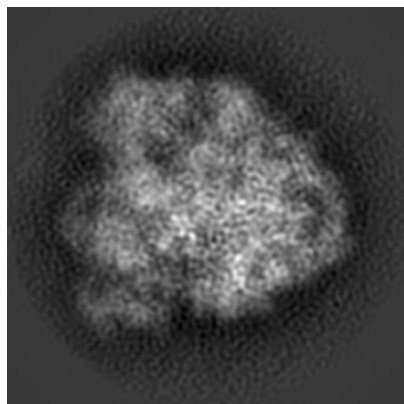
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-13465. These allow visual inspection of the internal detail of the map and identification of artifacts.

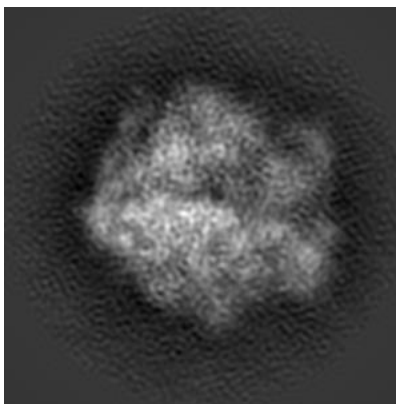
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

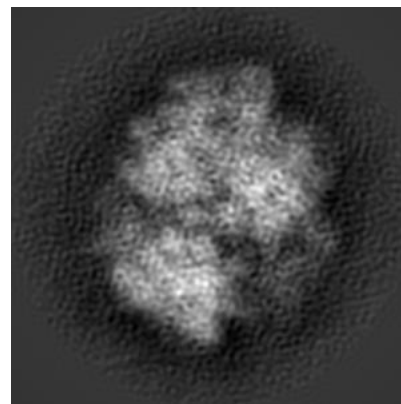
6.1.1 Primary map



X

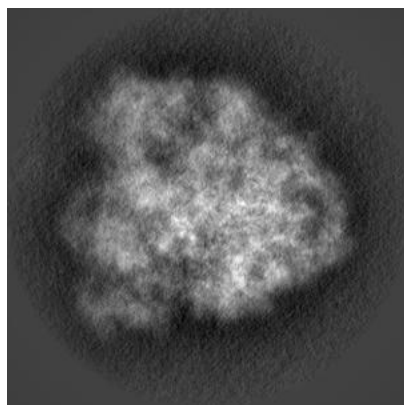


Y

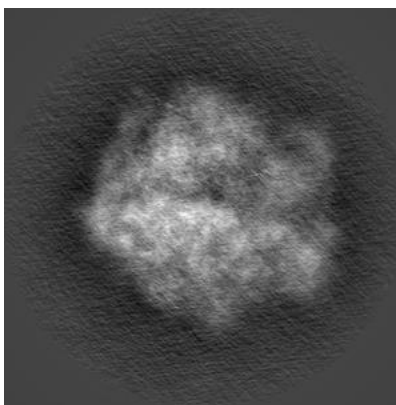


Z

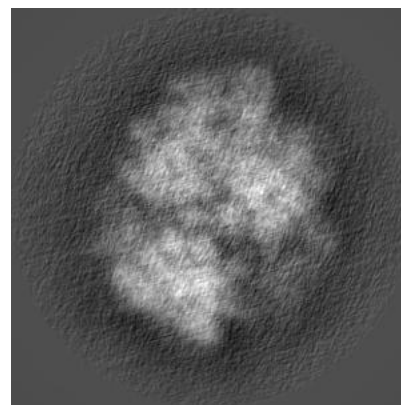
6.1.2 Raw map



X



Y

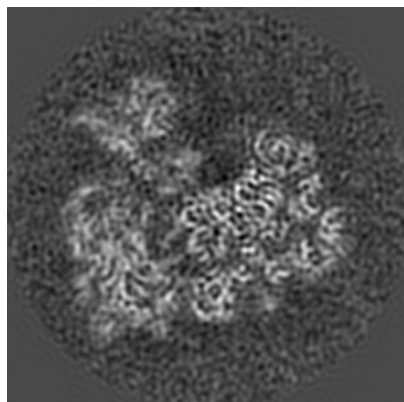


Z

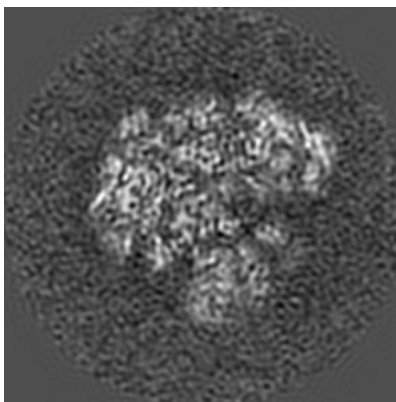
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

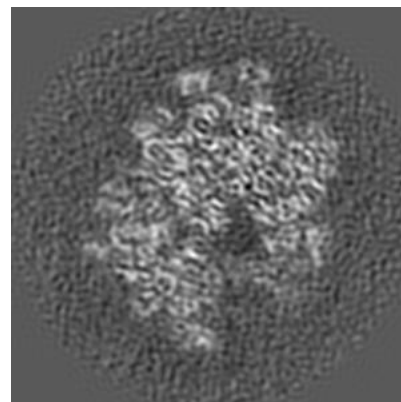
6.2.1 Primary map



X Index: 144

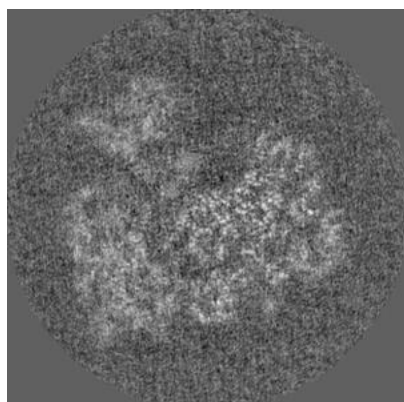


Y Index: 144

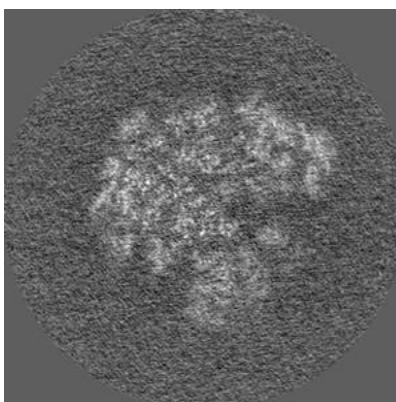


Z Index: 144

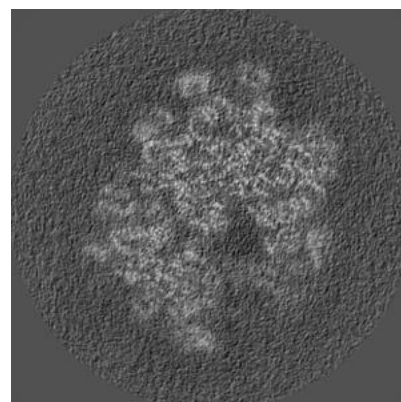
6.2.2 Raw map



X Index: 144



Y Index: 144

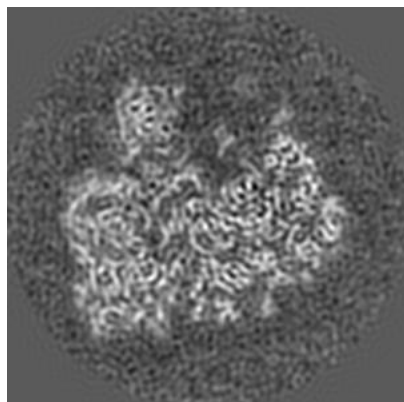


Z Index: 144

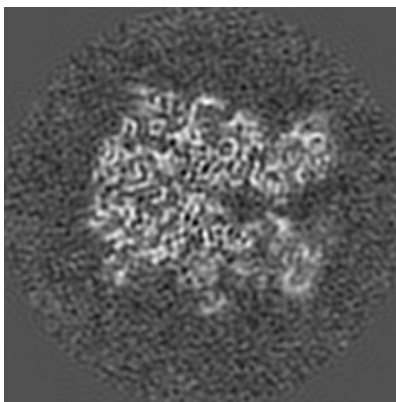
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

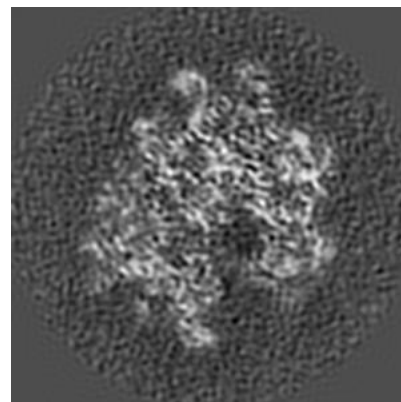
6.3.1 Primary map



X Index: 138

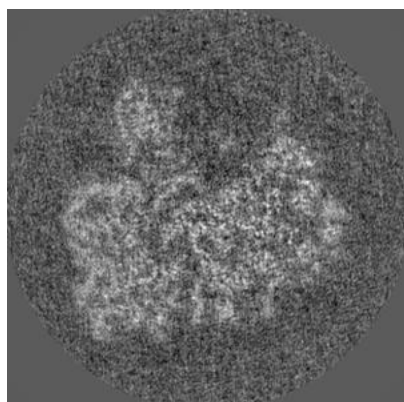


Y Index: 159

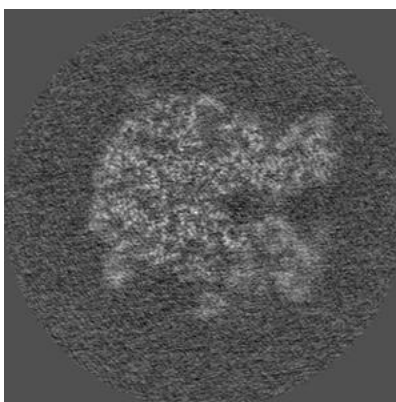


Z Index: 147

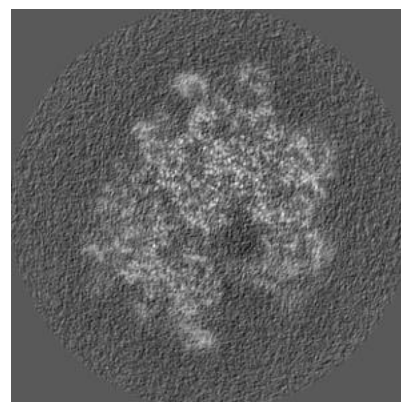
6.3.2 Raw map



X Index: 139



Y Index: 157

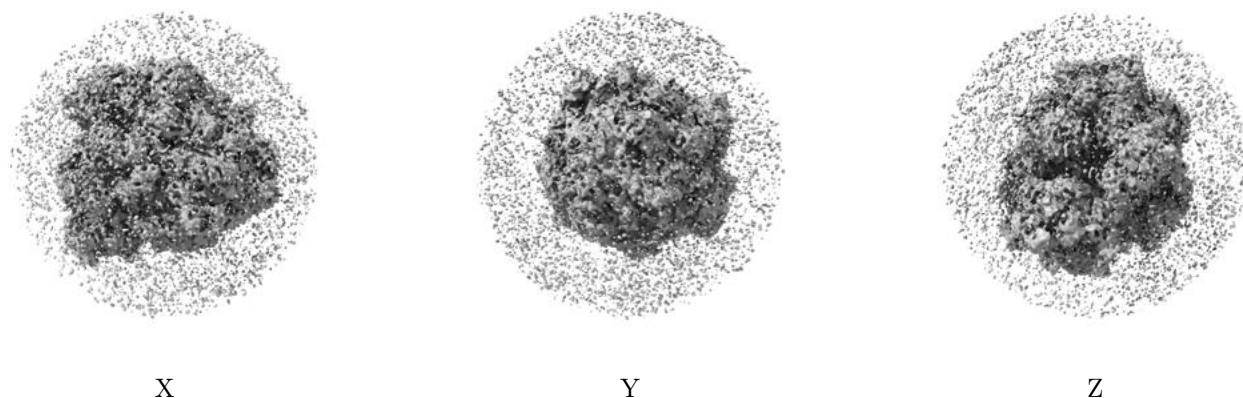


Z Index: 146

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

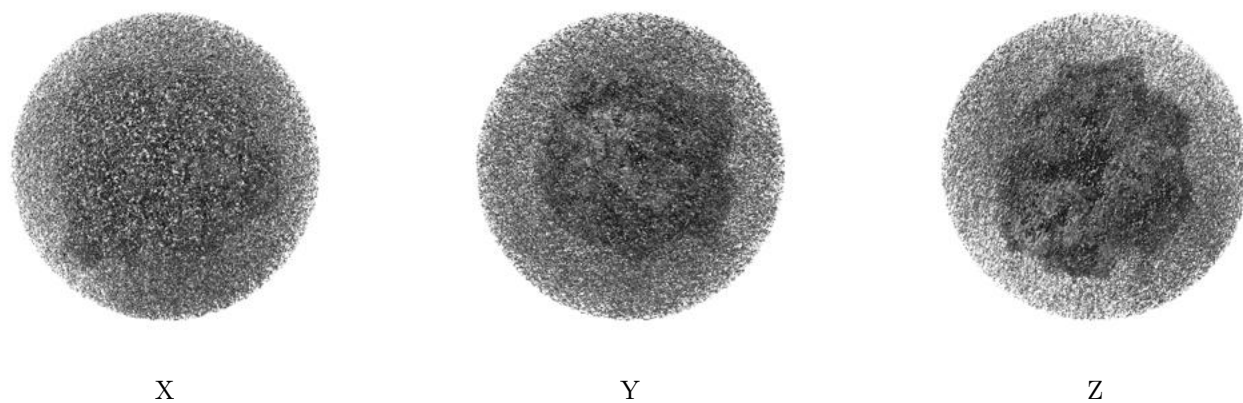
6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 1.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map



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

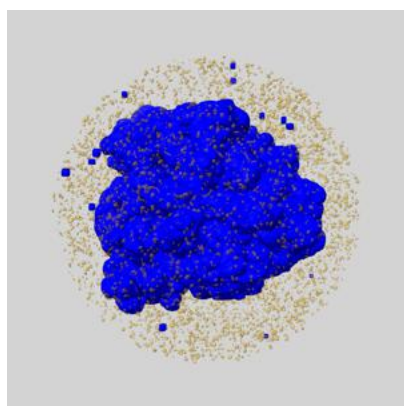
6.5 Mask visualisation [i](#)

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

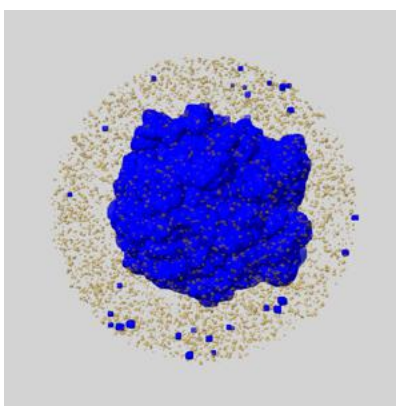
A mask typically either:

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

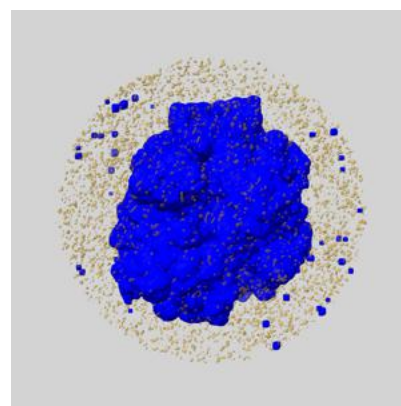
6.5.1 emd_13465_msk_1.map [i](#)



X



Y

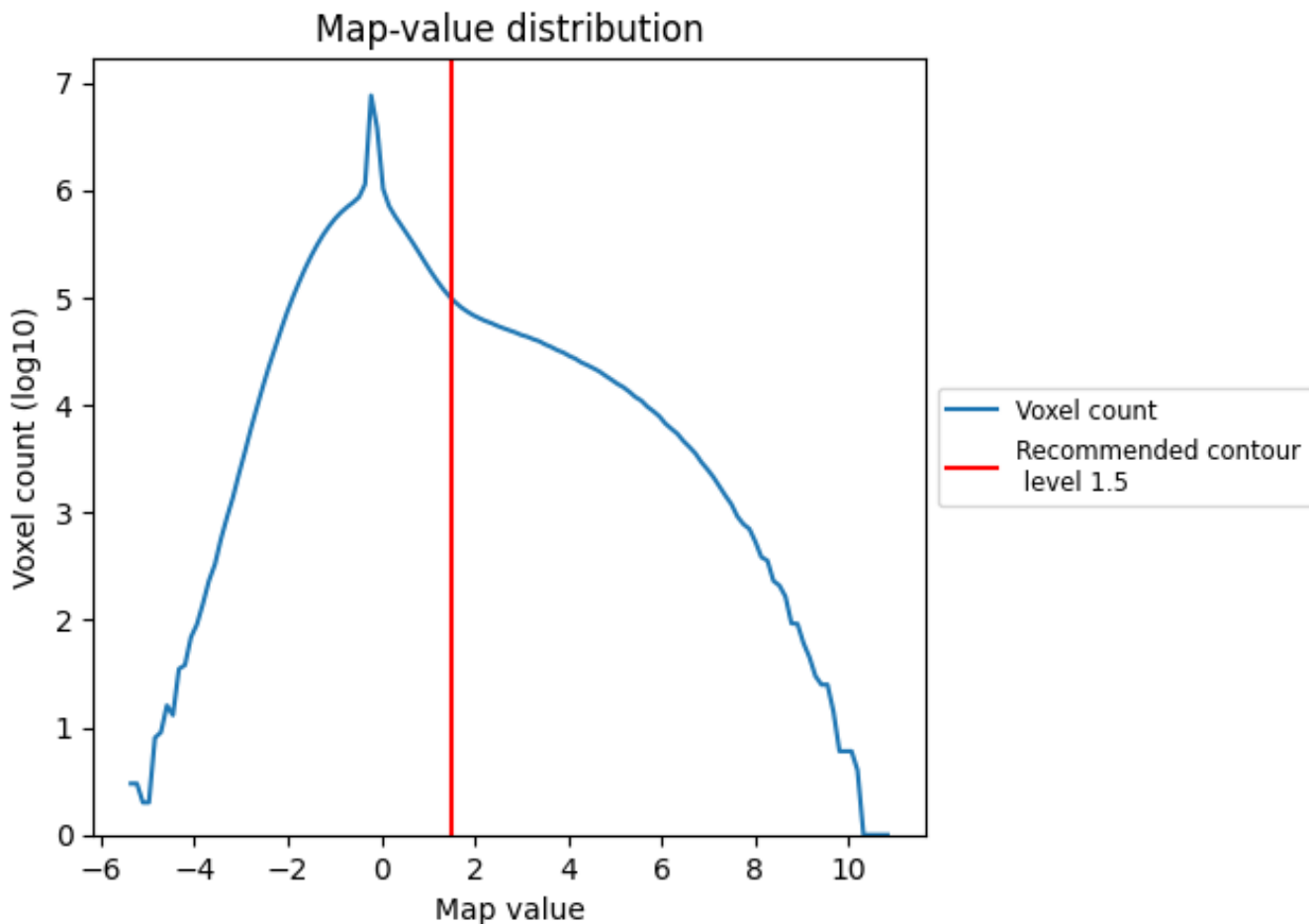


Z

7 Map analysis [i](#)

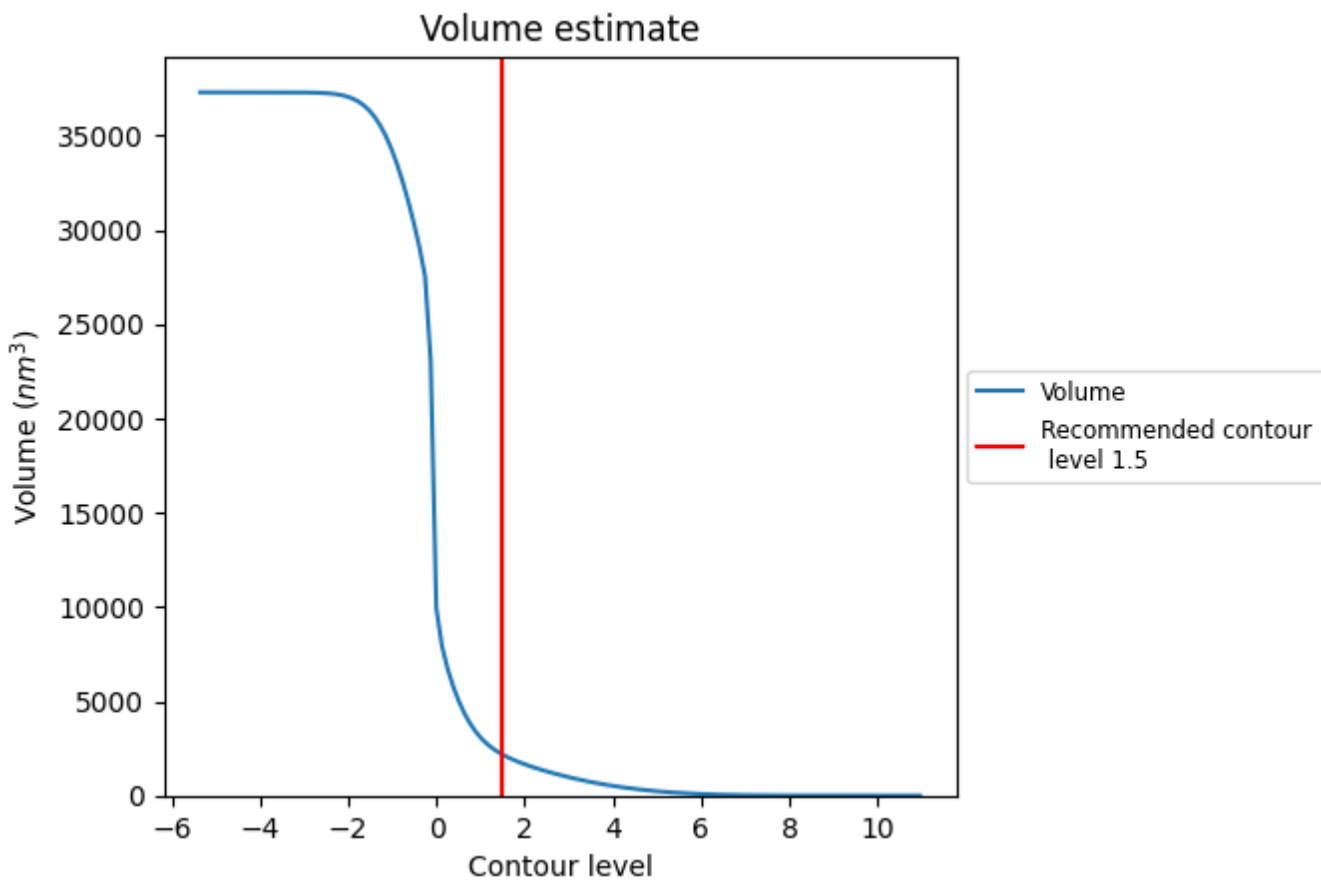
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

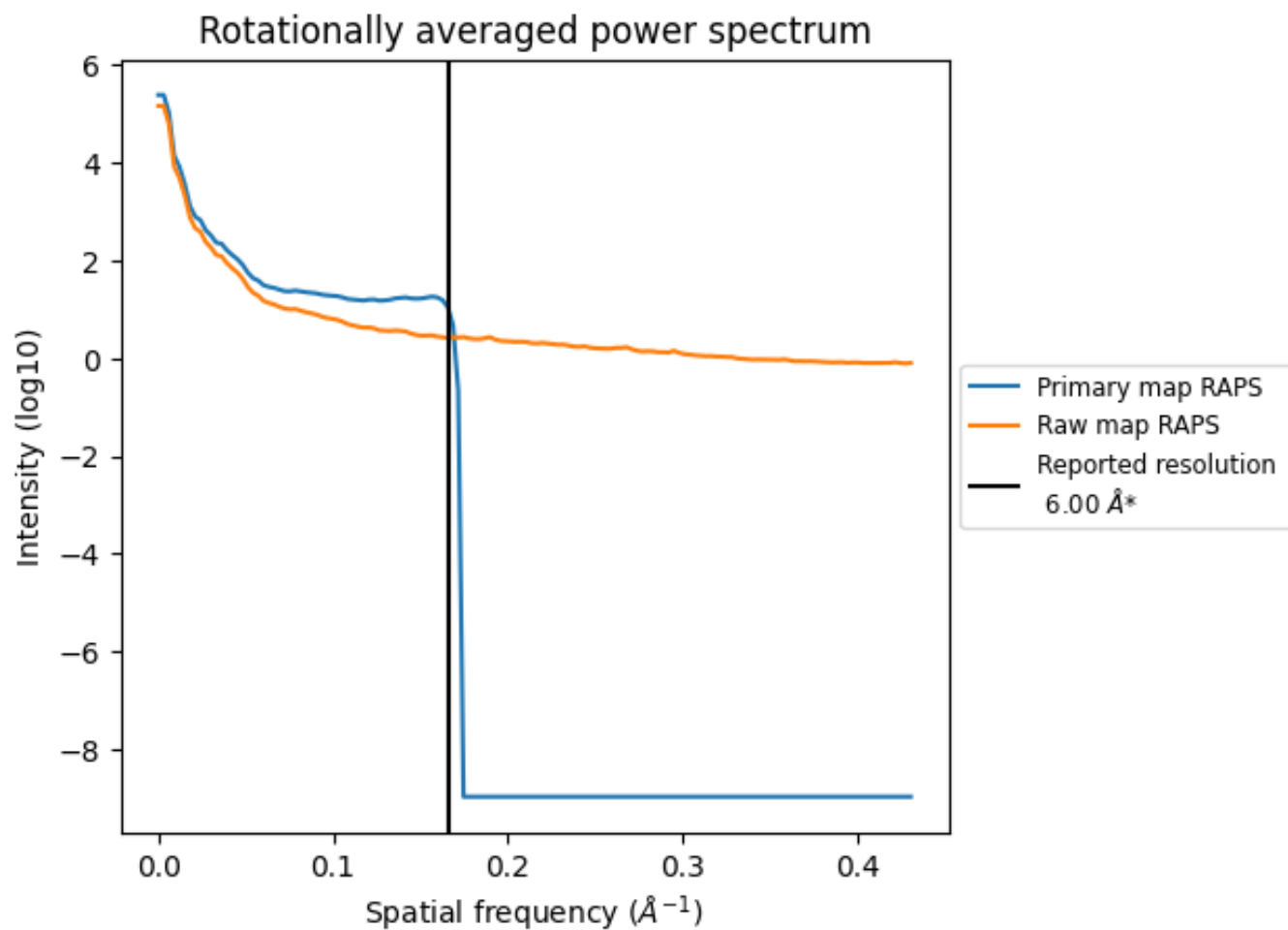
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2172 nm^3 ; this corresponds to an approximate mass of 1962 kDa.

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

7.3 Rotationally averaged power spectrum i

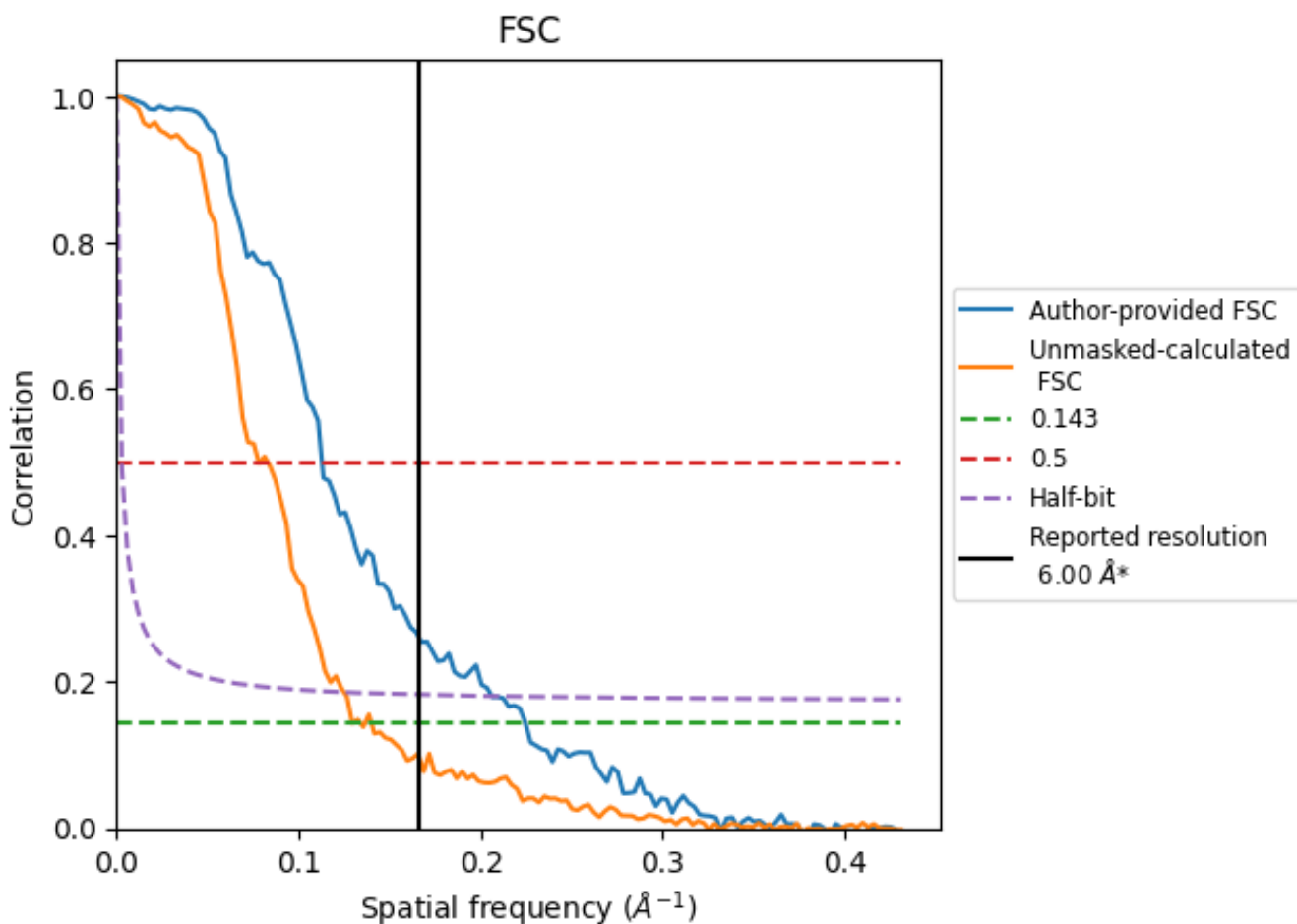


*Reported resolution corresponds to spatial frequency of 0.167 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.167 Å⁻¹

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	6.00	-	-
Author-provided FSC curve	4.45	8.86	4.85
Unmasked-calculated*	7.72	12.79	8.00

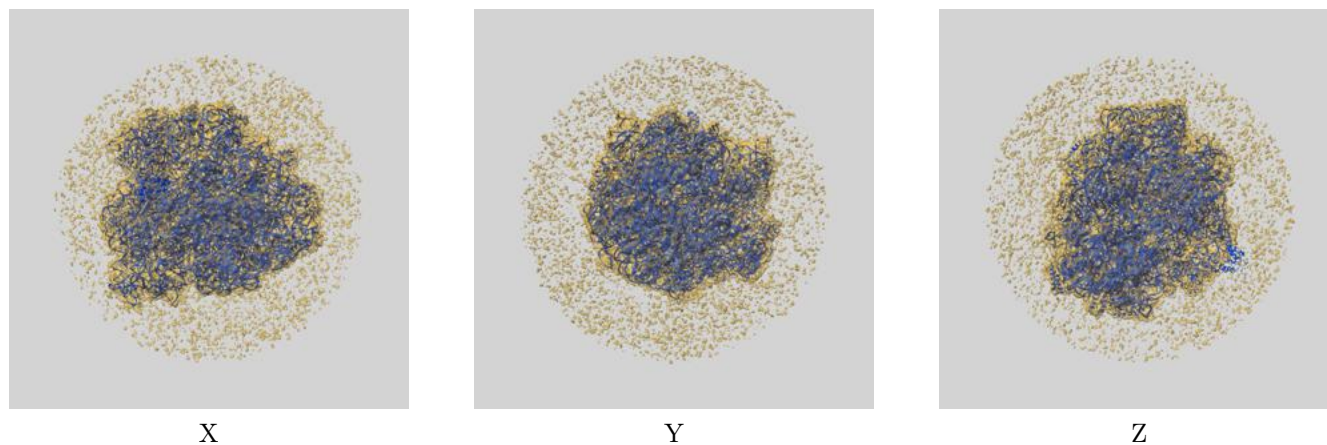
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 4.45 differs from the reported value 6.0 by more than 10 %

The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 7.72 differs from the reported value 6.0 by more than 10 %

9 Map-model fit [i](#)

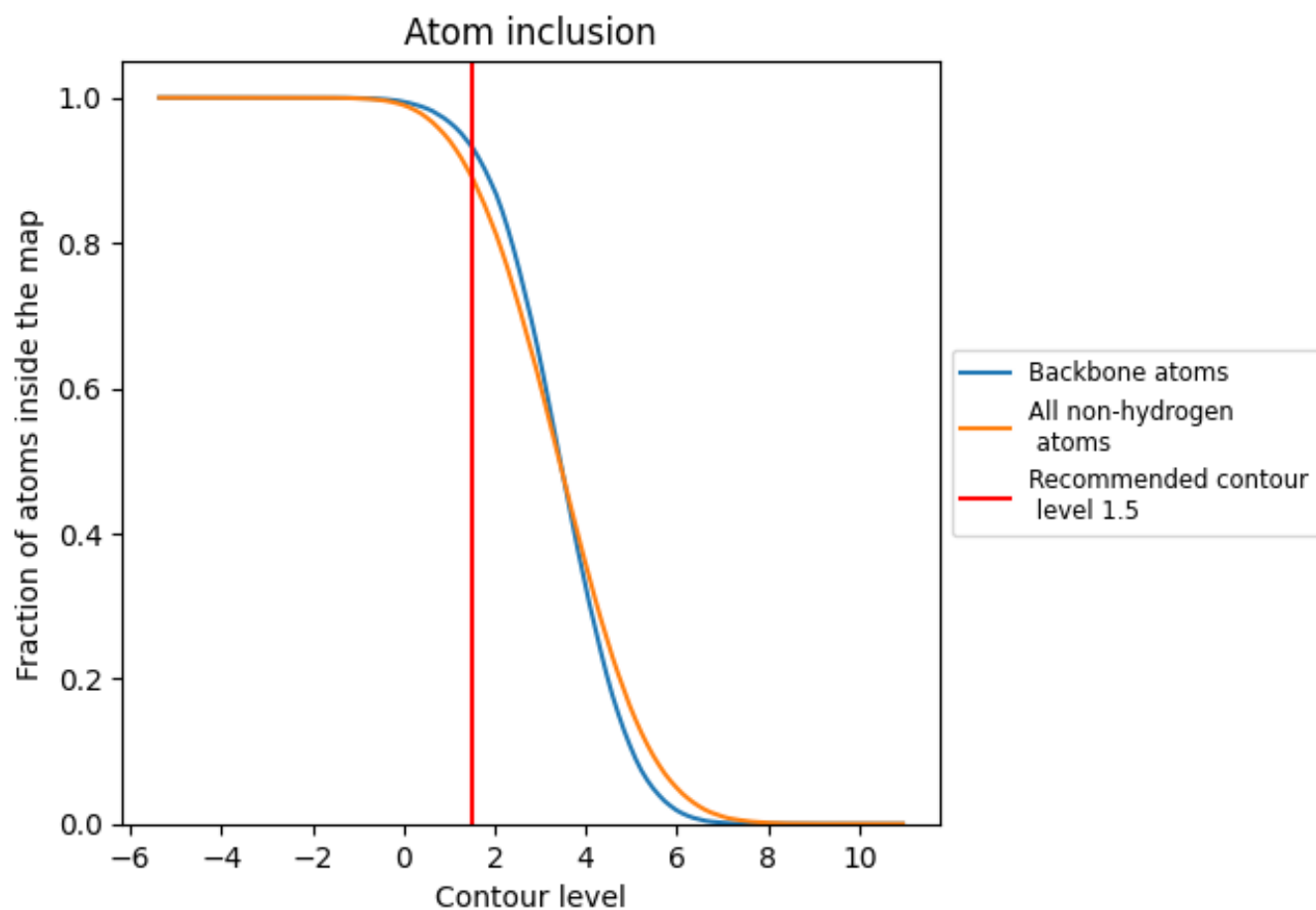
This section contains information regarding the fit between EMDB map EMD-13465 and PDB model 7PJZ. Per-residue inclusion information can be found in section 3 on page 16.

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 1.5 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 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 89% of all non-hydrogen atoms, are inside the map.