



Full wwPDB EM Validation Report ⓘ

Mar 6, 2025 – 06:38 pm GMT

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, 5LZD, 5J9Z, 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 types of validation reports are described at

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

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

EMDB validation analysis : **FAILED**
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.41

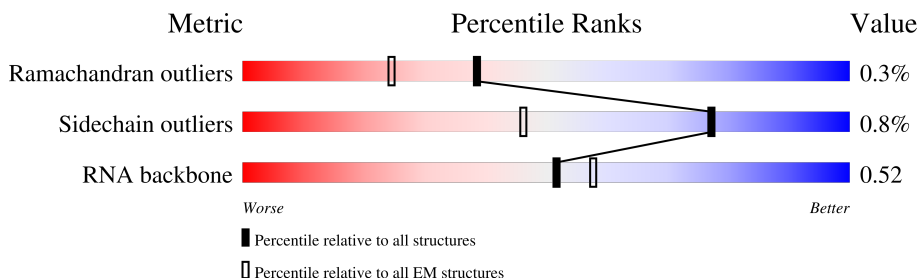
1 Overall quality at a glance

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	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 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 $\leq 5\%$.

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	
9	B	120	



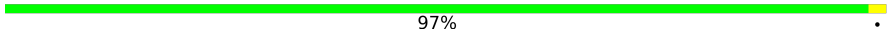
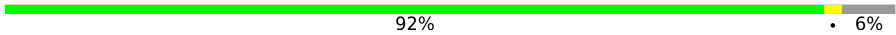


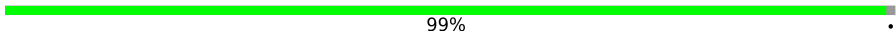
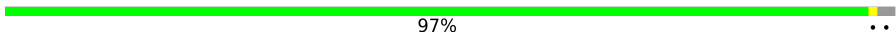
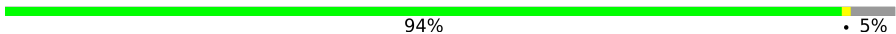

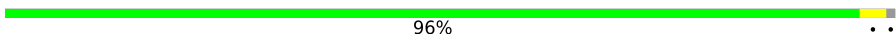
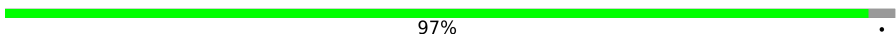
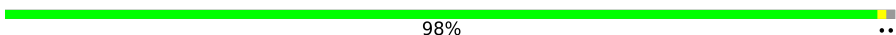
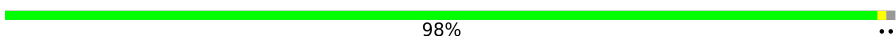

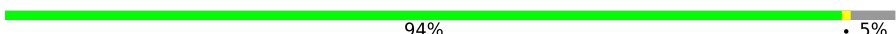


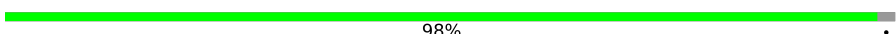






Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
10	C	273	96%
11	D	209	100%
12	E	201	100%
13	F	179	98%
14	G	177	97%
15	H	149	99%
16	I	142	99%
17	J	142	99%
18	K	123	96%
19	L	144	97%
20	M	136	97%
21	N	127	93%
22	O	117	97%
23	P	115	98%
24	Q	118	98%
25	R	103	98%
26	S	110	96%
27	T	100	90%
28	U	104	94%
29	V	94	99%
30	W	85	87%
31	X	78	94%
32	Y	63	98%
33	Z	59	98%
34	a	1542	39%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
35	b	240	 88% 9%
36	c	233	 88% 12%
37	d	206	 97%
38	e	167	 92% 6%
39	f	135	 74% 26%
40	g	179	 83% 16%
41	h	130	 99%
42	i	130	 97%
43	j	103	 94% 5%
44	k	129	 89% 10%
45	l	124	 96%
46	m	118	 97%
47	n	102	 98%
48	o	89	 98%
49	p	82	 99%
50	q	84	 94% 5%
51	r	75	 84% 13%
52	s	92	 86% 11%
53	t	87	 98%
54	u	71	 90% 8%
55	v	77	 43% 47% 10%
56	w	76	 46% 42% 12%
57	x	704	 92% 5%
58	y	2	 50% 50%
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
1	0	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- 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	S	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
21	N	120	Total	C	N	O	S	0	0
			960	593	196	166	5		

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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
55	v	77	Total	C	N	O	P	S	0	0
			1642	733	297	534	77	1		

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

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

- Molecule 57 is a protein called Elongation factor G.

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

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

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

- Molecule 59 is a RNA chain called mRNA.

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

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

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

- 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: $\text{C}_{10}\text{H}_{15}\text{N}_5\text{O}_{11}\text{P}_2$).



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. 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. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: 50S ribosomal protein L32

Chain 0:  98% .



- Molecule 2: 50S ribosomal protein L33

Chain 1:  91% 9%



- Molecule 3: 50S ribosomal protein L34

Chain 2:  96% .



- Molecule 4: 50S ribosomal protein L35

Chain 3:  95% . .




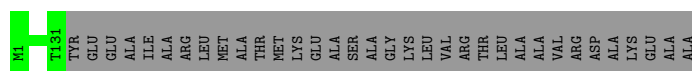
- Molecule 5: 50S ribosomal protein L36

Chain 4:  100%

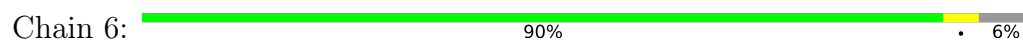
There are no outlier residues recorded for this chain.

- Molecule 6: 50S ribosomal protein L10

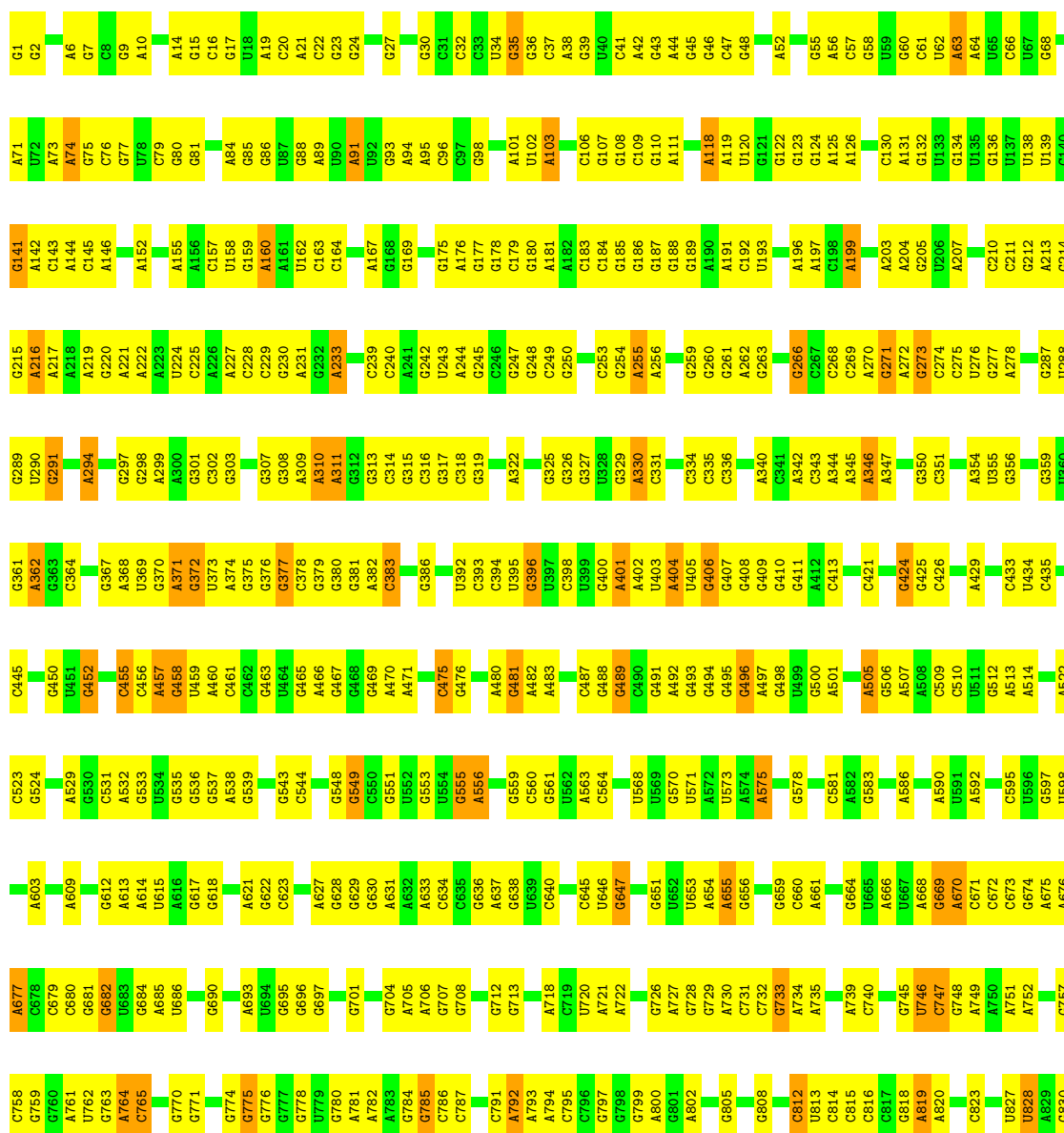
Chain 5:  79% 21%



• Molecule 7: 50S ribosomal protein L31

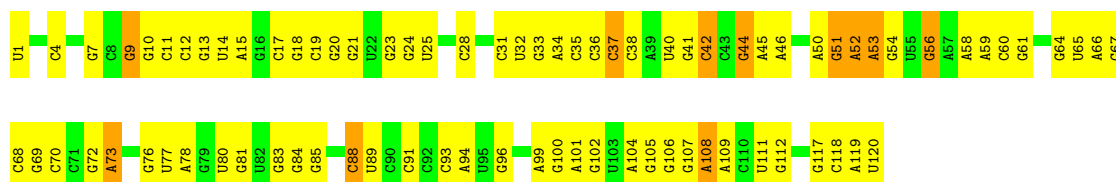


• Molecule 8: 23S ribosomal RNA









- Molecule 10: 50S ribosomal protein L2

Chain C: 96%



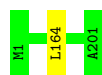
- Molecule 11: 50S ribosomal protein L3

Chain D: 100%

There are no outlier residues recorded for this chain.

- Molecule 12: 50S ribosomal protein L4

Chain E: 100%



- Molecule 13: 50S ribosomal protein L5

Chain F: 98%



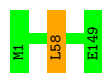
- Molecule 14: 50S ribosomal protein L6

Chain G: 97%



- Molecule 15: 50S ribosomal protein L9

Chain H: 99%



- Molecule 16: 50S ribosomal protein L11

Chain I: 99%



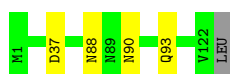
- Molecule 17: 50S ribosomal protein L13

Chain J: 99%



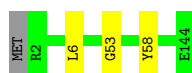
- Molecule 18: 50S ribosomal protein L14

Chain K: 96%



- Molecule 19: 50S ribosomal protein L15

Chain L: 97%



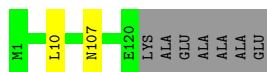
- Molecule 20: 50S ribosomal protein L16

Chain M: 97%



- Molecule 21: 50S ribosomal protein L17

Chain N: 93% 6%



- Molecule 22: 50S ribosomal protein L18

Chain O: 97%



- Molecule 23: 50S ribosomal protein L19

Chain P: 98%



- Molecule 24: 50S ribosomal protein L20

Chain Q: 98% ..



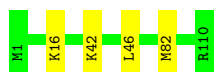
- Molecule 25: 50S ribosomal protein L21

Chain R: 98% .



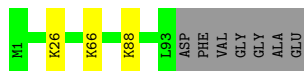
- Molecule 26: 50S ribosomal protein L22

Chain S: 96% .



- Molecule 27: 50S ribosomal protein L23

Chain T: 90% . 7%



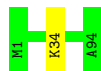
- Molecule 28: 50S ribosomal protein L24

Chain U: 94% . .



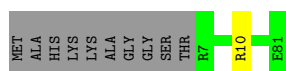
- Molecule 29: 50S ribosomal protein L25

Chain V: 99% .



- Molecule 30: 50S ribosomal protein L27

Chain W: 87% . 12%



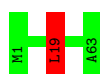
- Molecule 31: 50S ribosomal protein L28

Chain X: 94% 5%



- Molecule 32: 50S ribosomal protein L29

Chain Y: 98%



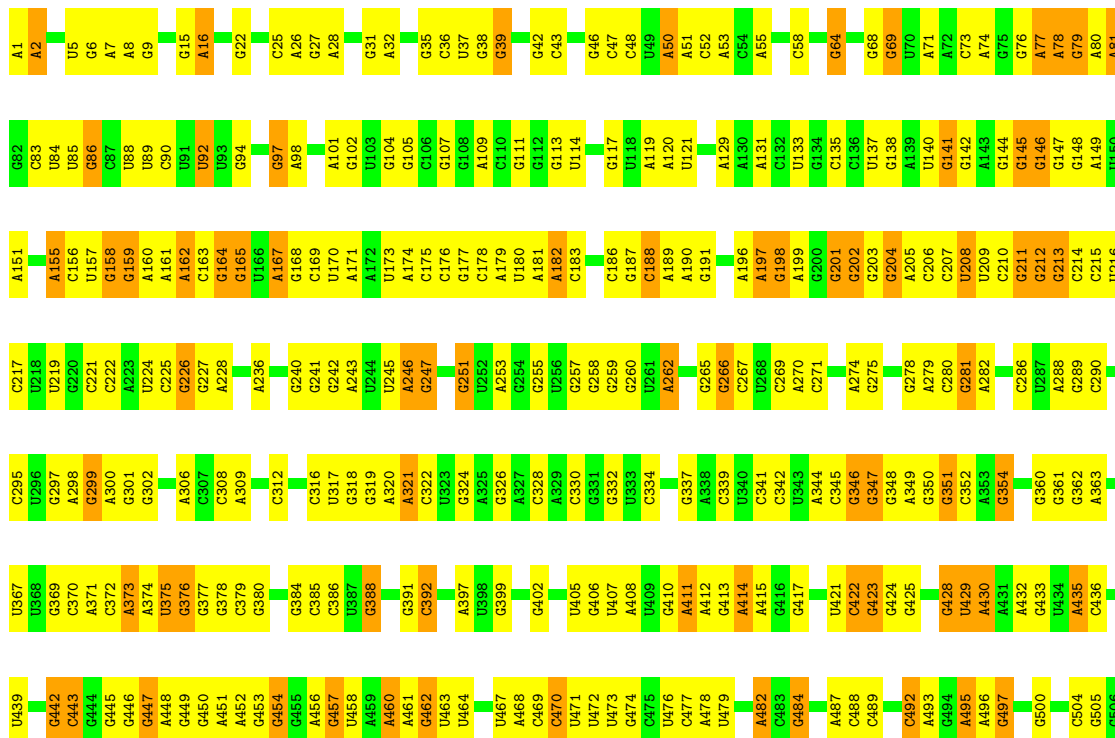
- Molecule 33: 50S ribosomal protein L30

Chain Z: 98%




- Molecule 34: 16S ribosomal RNA

Chain a: 39% 49% 11%




G1529	U1450	G1373	G1296	G1160	A1092	A1019	A946	A864	C796	A648		C507
G1530	U1451	A1374	A1227	C1161	A1093	G1020	G947	A865	C797	A649	G581	U508
A1534	C1452	A1375	C1228	A1162	G1094	A1021	C948	A872	U798	C650	C582	A509
C1535	G1453	A1376	A1229	A1163	U1095	A1022	A949	A873	G799	C651	A583	A510
C1536	G1454	A1377	C1230	U1164	C1096	U1023	U952		G800	G654	G584	C511
U1537	C1455	C1378	C1302	U1165	C1097	G1024	G953	C876	U801	A655	G585	U512
A1456	U1456	C1379	C1303	G1166	C1098	U1025	G954	A877	A802	A656	C586	G515
G1457	G1457	U1380	C1237	A1167	G1099	G1026		G878	G803	U659	C587	U516
C1458	U1458	U1381	A1238	U1168	C1100	C1027	G958	A879		U658	G588	C517
C1459	C1460	A1239	A1239	A1169	A1101	U1028	A958	C882	C806		G592	C518
G1461	G1461	U1240	A1240		A1102	C1029	U960		A807	G660		G521
C1462	G1309	G1241	G1241	U1173	C1103	U1030	U961	G885	G734	U662	A595	C522
	G1310	G1242	C1243	G1174	G1104	G1031		G886	G735	G661	A596	A523
A1465	U1395	C1243	G1243	G1175	A1105	G1032	A964	G887	C736	A663	G597	G524
C1466	A1394	A1244	G1244	A1176	G1106	C811	A965	G888	C737	G664	U598	C599
C1467	U1312	C1245	C1245	G1177	C1107	G1033	U966	G889	C738	A665	A600	C526
A1468	G1314	A1246	A1246	G1178	G1108	G1034	C967	G890	C739		G601	G527
	C1314			G1179	C1109	C1037	A968	U891	G742	G669	A602	
	C1317	C1249	C1249	A1180	A1110	G1038	A969		A743	G670	G603	G530
U1472	A1318	A1250	A1250	G1181	A1111	G1039		G894	C744	G671	U603	A531
G1475	A1319	A1251	A1251	G1182	C1112	U1040	G973	G895	G745	G674	G604	A532
A1476	C1320	A1252	A1252	U1183		G1041	A974	G896	G755	G675	U605	
	G1401	G1253	G1253	G1184	A1117	A1042	A975	G897		A676	A606	A535
C1402	U1321	G1254	A1254	G1185	U1118	G1043	G976	G898	G758		G615	
C1403	C1322	A1255	A1255	G1186	C1119	A1044	A977		A759	U686	G616	C545
C1404	G1323	A1256	A1256	G1187	C1120	C1045	U982	C910	G760	G687	G617	A546
G1405	A1324	A1257	A1257	G1190		A1046	G987	A912	G761	G688	U619	G547
U1481	C1325	G1258	C1259	G1191	G1124	G1047	G988	A913	G765	G689	C620	C548
G1482	C1328	C1259	C1259	G1193	U1126	U1048	U989	A914	G766	G690		G550
A1483	A1329	G1260	A1261	G1196	U1127	G1049	U991	A915	A767	U692	C624	A554
	U1330	A1261	C1262	A1197	G1128	G1050	C984	U916	G768	G691	G626	G558
G1486	G1331	C1262	C1262	A1198	C1129	G1051	G987	A917	G769	U693	G627	A559
G1487	A1332	U1264	U1264	U1199	G1130	C1059	U992	A918	C770	A694	U632	A560
G1488	G1333	C1265	C1265	U1200	G1131	C1059	A994	U920	G771	G700	A631	U662
G1489	U1334	U1264	U1264	U1201	G1132	U1060	C995	G922	G772	U701	A563	C564
A1492	C1335	G1267	G1267	A1202	G1133	G1061	U997	A923	G773	G702	G634	G567
G1497	U1336	C1268	C1268	A1203	U1135	U1065	C998	G926	G774	A704	A635	G568
U1498	C1337	A1269	A1269	U1204	G1136	G1065	C999	G927	G775	G705	G636	C569
A1499	G1338	G1270	G1270	A1205	C1137	U1065	A1000	G928	G776	A706	C637	G570
A1500	A1346	C1271	C1271	U1206	G1138	C1071	G1001	U929	G777	G710	G638	U571
C1501	U1347	G1272	G1272	U1207	U1139	G1072	G1002	G930	G778	G711	G639	A572
A1502	U1348	C1273	C1273	G1207	G1140	U1073	G1003	C931	G779	G712	U641	A573
A1503	A1349	A1274	A1274	U1208	C1141	G1074	G1004	A937	G780	G713	A642	A574
U1506	A1350	G1275	G1275	C1209	U1142	U1075	A1004	G933	G781	G714	G646	
	A1350	G1276	G1276	C1210	G1143	U1075	A1004	G934	G782	A715	C647	
	C1353	A1280	A1280	U1211	G1144	G1079	G1005	U1009	A783	G716		
	A1360	C1281	C1281	U1212	A1145	A1080	G1006	A935	G784	G717		
	C1361	C1282	C1282	A1213	A1146	A1081	G1007	G937	G785	G718		
	A1362			C1214	A1147	A1082	G1008	G938	G786			
	A1362	A1285	A1285	G1215	A1150	U1083	U1009	G939				
	G1365	U1286	U1286	A1216	G1153	U1084	U1009	G940				
	C1366	A1287	A1287	C1217	U1154	U1085	A936	G941				
	C1367	A1288	A1288	C1218	G1155	U1086	C936	G942				
	A1368	A1289	A1289	G1219	A1156	G1087	A937	G943				
	A1368			G1220	G1157	G1088	A1011	G944				
	G1369	G1221	G1221	G1222	U1159	G1089	A1012	G945				
	G1370	C1223	C1223	U1159	U1159	U1090	A1016					
	A1446	G1292	G1292	A1225		U1091						
	C1524	C1293	C1293									
	G1525	G1294	G1294									
		A1295	A1295									

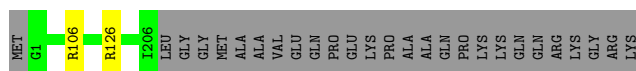
• Molecule 35: 30S ribosomal protein S2

Chain b:  88% 9%



- Molecule 36: 30S ribosomal protein S3

Chain c:  88% 12%



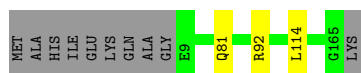
- Molecule 37: 30S ribosomal protein S4

Chain d:  97%



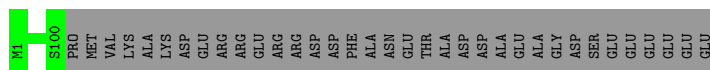
- Molecule 38: 30S ribosomal protein S5

Chain e:  92% 6%




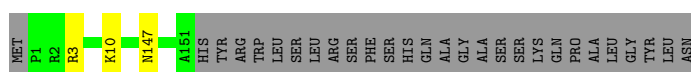
- Molecule 39: 30S ribosomal protein S6

Chain f:  74% 26%



- Molecule 40: 30S ribosomal protein S7

Chain g:  83% 16%



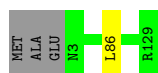
- Molecule 41: 30S ribosomal protein S8

Chain h:  99%



- Molecule 42: 30S ribosomal protein S9

Chain i:  97% ..




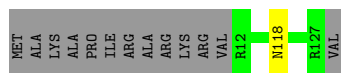
- Molecule 43: 30S ribosomal protein S10

Chain j:  94% • 5%



- Molecule 44: 30S ribosomal protein S11

Chain k:  89% • 10%



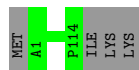
- Molecule 45: 30S ribosomal protein S12

Chain l:  96% ..



- Molecule 46: 30S ribosomal protein S13

Chain m:  97% •



- Molecule 47: 30S ribosomal protein S14

Chain n:  98% ..



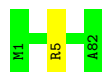
- Molecule 48: 30S ribosomal protein S15

Chain o:  98% ..



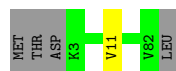
- Molecule 49: 30S ribosomal protein S16

Chain p:  99%




- Molecule 50: 30S ribosomal protein S17

Chain q:  94% 5%




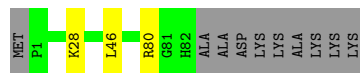
- Molecule 51: 30S ribosomal protein S18

Chain r:  84% 13%



- Molecule 52: 30S ribosomal protein S19

Chain s:  86% 11%




- Molecule 53: 30S ribosomal protein S20

Chain t:  98%



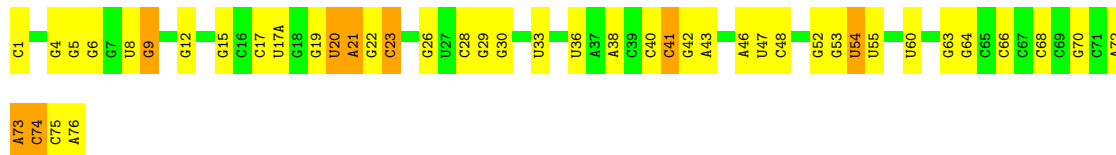
- Molecule 54: 30S ribosomal protein S21

Chain u:  90% 8%



- Molecule 55: P-site tRNA(fMet)

Chain v:  43% 47% 10%





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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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%)	8	38
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%)	3	22
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%)	19	57
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%)	13	49
26	S	108/110 (98%)	99 (92%)	9 (8%)	0	100	100
27	T	91/100 (91%)	81 (89%)	9 (10%)	1 (1%)	12	47
28	U	100/104 (96%)	89 (89%)	10 (10%)	1 (1%)	13	49
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%)	8	38

Continued on next page...

Continued from previous page...

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%)	25	65
36	c	204/233 (88%)	193 (95%)	11 (5%)	0	100	100
37	d	203/206 (98%)	172 (85%)	30 (15%)	1 (0%)	25	65
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%)	16	55
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%)	12	47
All	All	6516/6924 (94%)	5877 (90%)	621 (10%)	18 (0%)	38	73

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

Continued on next page...

Continued from previous page...

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 ⓘ

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%)	41	59
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%)	56	72
10	C	216/218 (99%)	213 (99%)	3 (1%)	62	75
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%)	60	75
15	H	114/114 (100%)	113 (99%)	1 (1%)	75	83
17	J	116/116 (100%)	116 (100%)	0	100	100
18	K	103/104 (99%)	99 (96%)	4 (4%)	27	48
19	L	102/103 (99%)	101 (99%)	1 (1%)	73	82

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	M	109/109 (100%)	108 (99%)	1 (1%)	75	83
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%)	70	80
27	T	80/84 (95%)	79 (99%)	1 (1%)	65	77
28	U	83/85 (98%)	83 (100%)	0	100	100
29	V	78/78 (100%)	77 (99%)	1 (1%)	65	77
30	W	57/63 (90%)	56 (98%)	1 (2%)	54	71
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%)	56	72
36	c	170/190 (90%)	169 (99%)	1 (1%)	84	88
37	d	172/173 (99%)	170 (99%)	2 (1%)	67	79
38	e	114/126 (90%)	112 (98%)	2 (2%)	54	71
39	f	87/116 (75%)	87 (100%)	0	100	100
40	g	124/147 (84%)	122 (98%)	2 (2%)	58	74
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%)	70	80
45	l	103/104 (99%)	101 (98%)	2 (2%)	52	69
46	m	92/96 (96%)	92 (100%)	0	100	100
47	n	79/84 (94%)	78 (99%)	1 (1%)	65	77
48	o	76/77 (99%)	75 (99%)	1 (1%)	65	77
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

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
52	s	72/79 (91%)	71 (99%)	1 (1%)	62	75
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%)	70	80
58	y	1/1 (100%)	1 (100%)	0	100	100
All	All	5178/5408 (96%)	5138 (99%)	40 (1%)	77	85

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

Continued on next page...

Continued from previous page...

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 ⓘ

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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	1MG	A	745	8	18,26,27	2.35	6 (33%)	19,39,42	1.58	5 (26%)
55	4SU	v	8	55	18,21,22	3.41	8 (44%)	26,30,33	2.15	4 (15%)
8	2MG	A	1835	8	18,26,27	2.08	7 (38%)	16,38,41	2.13	4 (25%)
8	5MU	A	1939	8	19,22,23	4.63	7 (36%)	28,32,35	3.83	9 (32%)
8	6MZ	A	2030	8	18,25,26	1.80	6 (33%)	16,36,39	2.37	5 (31%)
8	PSU	A	2604	8	18,21,22	3.51	8 (44%)	22,30,33	2.41	6 (27%)
34	2MG	a	966	34	18,26,27	0.99	1 (5%)	16,38,41	1.40	3 (18%)
55	PSU	v	55	55	18,21,22	3.82	6 (33%)	22,30,33	1.89	5 (22%)
56	G7M	w	46	56	20,26,27	4.39	14 (70%)	17,39,42	2.21	3 (17%)
8	PSU	A	1911	8	18,21,22	3.58	7 (38%)	22,30,33	1.96	5 (22%)
8	PSU	A	2605	8	18,21,22	3.48	7 (38%)	22,30,33	2.27	6 (27%)
8	5MC	A	747	8	18,22,23	3.41	7 (38%)	26,32,35	1.39	2 (7%)
8	OMU	A	2552	8	19,22,23	2.66	5 (26%)	26,31,34	2.07	6 (23%)
8	PSU	A	2457	8	18,21,22	3.52	8 (44%)	22,30,33	2.16	4 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
34	PSU	a	516	34	18,21,22	3.65	7 (38%)	22,30,33	1.90	5 (22%)
8	OMC	A	2498	8	19,22,23	3.08	8 (42%)	26,31,34	0.84	0
8	PSU	A	2504	8	18,21,22	3.85	7 (38%)	22,30,33	1.84	4 (18%)
8	PSU	A	2580	8	18,21,22	3.28	7 (38%)	22,30,33	2.54	6 (27%)
58	FME	y	101	58	8,9,10	1.03	1 (12%)	7,9,11	1.05	1 (14%)
34	MA6	a	1518	34	18,26,27	1.53	3 (16%)	19,38,41	3.38	3 (15%)
8	OMG	A	2251	56,8	18,26,27	2.49	8 (44%)	19,38,41	1.52	5 (26%)
8	5MC	A	1962	8	18,22,23	2.96	7 (38%)	26,32,35	1.34	2 (7%)
34	2MG	a	1516	34	18,26,27	2.32	7 (38%)	16,38,41	1.40	3 (18%)
56	5MU	w	54	56	19,22,23	1.38	6 (31%)	28,32,35	2.21	9 (32%)
8	3TD	A	1915	8	18,22,23	7.27	11 (61%)	22,32,35	1.73	2 (9%)
34	MA6	a	1519	34	18,26,27	1.53	3 (16%)	19,38,41	3.54	5 (26%)
8	PSU	A	955	8	18,21,22	3.55	7 (38%)	22,30,33	1.98	4 (18%)
55	5MU	v	54	55	19,22,23	4.60	7 (36%)	28,32,35	3.73	10 (35%)
8	G7M	A	2069	8	20,26,27	1.78	6 (30%)	17,39,42	1.85	4 (23%)
8	2MG	A	2445	8	18,26,27	1.89	5 (27%)	16,38,41	1.36	2 (12%)
56	PSU	w	32	56	18,21,22	3.91	6 (33%)	22,30,33	1.85	6 (27%)
34	2MG	a	1207	34	18,26,27	2.13	7 (38%)	16,38,41	1.50	4 (25%)
34	5MC	a	967	34	18,22,23	3.28	7 (38%)	26,32,35	1.29	4 (15%)
34	UR3	a	1498	34	19,22,23	2.46	6 (31%)	26,32,35	1.12	2 (7%)
55	H2U	v	20	55	18,21,22	3.58	3 (16%)	21,30,33	2.03	5 (23%)
8	PSU	A	746	8	18,21,22	3.74	6 (33%)	22,30,33	1.68	5 (22%)
56	PSU	w	55	56	18,21,22	1.43	3 (16%)	22,30,33	1.91	5 (22%)
8	6MZ	A	1618	8	18,25,26	1.72	6 (33%)	16,36,39	2.94	4 (25%)
56	MIA	w	37	56	24,31,32	2.44	4 (16%)	26,44,47	2.74	10 (38%)
34	4OC	a	1402	34	20,23,24	3.16	8 (40%)	26,32,35	1.13	3 (11%)
56	4SU	w	8	56	18,21,22	1.89	5 (27%)	26,30,33	2.11	6 (23%)
34	5MC	a	1407	34	18,22,23	3.16	7 (38%)	26,32,35	1.09	2 (7%)
56	PSU	w	39	56	18,21,22	3.75	6 (33%)	22,30,33	2.22	5 (22%)
34	G7M	a	527	34	20,26,27	2.07	4 (20%)	17,39,42	1.44	3 (17%)
8	PSU	A	1917	8	18,21,22	3.68	6 (33%)	22,30,33	1.92	5 (22%)
8	2MA	A	2503	8	19,25,26	3.11	7 (36%)	21,37,40	1.95	5 (23%)

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	1MG	A	745	8	-	0/3/25/26	0/3/3/3
55	4SU	v	8	55	-	0/7/25/26	0/2/2/2
8	2MG	A	1835	8	-	2/5/27/28	0/3/3/3
8	5MU	A	1939	8	-	2/7/25/26	0/2/2/2
8	6MZ	A	2030	8	-	3/5/27/28	0/3/3/3
8	PSU	A	2604	8	-	1/7/25/26	0/2/2/2
34	2MG	a	966	34	-	3/5/27/28	0/3/3/3
55	PSU	v	55	55	-	2/7/25/26	0/2/2/2
56	G7M	w	46	56	-	1/3/25/26	0/3/3/3
8	PSU	A	1911	8	-	0/7/25/26	0/2/2/2
8	PSU	A	2605	8	-	0/7/25/26	0/2/2/2
8	5MC	A	747	8	-	2/7/25/26	0/2/2/2
8	OMU	A	2552	8	-	2/9/27/28	0/2/2/2
8	PSU	A	2457	8	-	0/7/25/26	0/2/2/2
34	PSU	a	516	34	-	0/7/25/26	0/2/2/2
8	OMC	A	2498	8	-	2/9/27/28	0/2/2/2
8	PSU	A	2504	8	-	0/7/25/26	0/2/2/2
8	PSU	A	2580	8	-	0/7/25/26	0/2/2/2
58	FME	y	101	58	-	4/7/9/11	-
34	MA6	a	1518	34	-	0/7/29/30	0/3/3/3
8	OMG	A	2251	56,8	-	0/5/27/28	0/3/3/3
8	5MC	A	1962	8	-	0/7/25/26	0/2/2/2
34	2MG	a	1516	34	-	0/5/27/28	0/3/3/3
56	5MU	w	54	56	-	0/7/25/26	0/2/2/2
8	3TD	A	1915	8	-	2/7/25/26	0/2/2/2
34	MA6	a	1519	34	-	4/7/29/30	0/3/3/3
8	PSU	A	955	8	-	0/7/25/26	0/2/2/2
55	5MU	v	54	55	-	3/7/25/26	0/2/2/2
8	G7M	A	2069	8	-	1/3/25/26	0/3/3/3
8	2MG	A	2445	8	-	2/5/27/28	0/3/3/3
56	PSU	w	32	56	-	2/7/25/26	0/2/2/2
34	2MG	a	1207	34	-	0/5/27/28	0/3/3/3
34	5MC	a	967	34	-	2/7/25/26	0/2/2/2
34	UR3	a	1498	34	-	2/7/25/26	0/2/2/2
55	H2U	v	20	55	-	1/7/38/39	0/2/2/2
8	PSU	A	746	8	-	1/7/25/26	0/2/2/2
56	PSU	w	55	56	-	1/7/25/26	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	6MZ	A	1618	8	-	2/5/27/28	0/3/3/3
56	MIA	w	37	56	-	3/11/33/34	0/3/3/3
34	4OC	a	1402	34	-	0/9/29/30	0/2/2/2
56	4SU	w	8	56	-	0/7/25/26	0/2/2/2
34	5MC	a	1407	34	-	0/7/25/26	0/2/2/2
56	PSU	w	39	56	-	3/7/25/26	0/2/2/2
34	G7M	a	527	34	-	2/3/25/26	0/3/3/3
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

All (288) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	1915	3TD	O4'-C1'	17.31	1.67	1.43
8	A	1915	3TD	C2'-C1'	-15.67	1.33	1.53
8	A	1915	3TD	C6-C5	13.05	1.50	1.35
55	v	20	H2U	C2-N1	12.16	1.53	1.35
8	A	1939	5MU	C2-N1	10.72	1.55	1.38
55	v	54	5MU	C2-N1	10.49	1.55	1.38
56	w	46	G7M	C2'-C3'	-10.12	1.25	1.53
55	v	54	5MU	C4-C5	9.93	1.61	1.44
8	A	746	PSU	C6-C5	9.86	1.46	1.35
55	v	54	5MU	C6-N1	9.70	1.54	1.38
56	w	32	PSU	C6-C5	9.63	1.46	1.35
8	A	1915	3TD	C2-N1	9.58	1.49	1.37
8	A	2504	PSU	C2-N1	9.58	1.49	1.36
8	A	1939	5MU	C6-N1	9.55	1.54	1.38
8	A	1939	5MU	C4-C5	9.43	1.60	1.44
56	w	32	PSU	C2-N1	9.35	1.49	1.36
55	v	55	PSU	C2-N1	9.33	1.49	1.36
8	A	747	5MC	C6-C5	9.32	1.49	1.34
56	w	39	PSU	C2-N1	9.18	1.49	1.36
8	A	955	PSU	C2-N1	9.14	1.49	1.36
8	A	2604	PSU	C2-N1	9.14	1.49	1.36
8	A	2457	PSU	C2-N1	8.92	1.48	1.36
56	w	39	PSU	C6-C5	8.91	1.45	1.35
8	A	2504	PSU	C6-C5	8.86	1.45	1.35
34	a	516	PSU	C6-C5	8.85	1.45	1.35
8	A	1917	PSU	C2-N1	8.77	1.48	1.36
8	A	1911	PSU	C2-N1	8.75	1.48	1.36
8	A	1917	PSU	C6-C5	8.68	1.45	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	v	55	PSU	C6-C5	8.63	1.45	1.35
8	A	746	PSU	C2-N1	8.47	1.48	1.36
8	A	2605	PSU	C2-N1	8.45	1.48	1.36
34	a	516	PSU	C2-N1	8.35	1.48	1.36
34	a	1407	5MC	C6-C5	8.31	1.48	1.34
8	A	1911	PSU	C6-C5	8.31	1.45	1.35
8	A	1939	5MU	C4-N3	-8.18	1.23	1.38
34	a	967	5MC	C6-C5	8.14	1.48	1.34
55	v	8	4SU	C4-N3	7.99	1.46	1.37
8	A	955	PSU	C6-C5	7.93	1.44	1.35
8	A	2605	PSU	C6-C5	7.90	1.44	1.35
34	a	1402	4OC	C4-N3	7.71	1.46	1.32
55	v	54	5MU	C4-N3	-7.65	1.24	1.38
8	A	2580	PSU	C2-N1	7.64	1.47	1.36
8	A	2604	PSU	C6-C5	7.59	1.44	1.35
8	A	2457	PSU	C6-C5	7.55	1.44	1.35
8	A	2503	2MA	C4-N3	7.52	1.47	1.35
8	A	2580	PSU	C6-C5	7.32	1.43	1.35
8	A	1962	5MC	C6-C5	7.29	1.46	1.34
56	w	37	MIA	C13-C14	7.27	1.53	1.32
56	w	46	G7M	O4'-C1'	7.17	1.51	1.41
55	v	55	PSU	C2-N3	6.91	1.49	1.37
56	w	32	PSU	C2-N3	6.79	1.49	1.37
8	A	1917	PSU	C2-N3	6.78	1.49	1.37
55	v	20	H2U	C2-N3	6.75	1.50	1.38
8	A	2504	PSU	C2-N3	6.70	1.49	1.37
34	a	516	PSU	C2-N3	6.61	1.48	1.37
8	A	2605	PSU	C2-N3	6.60	1.48	1.37
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	1911	PSU	C2-N3	6.47	1.48	1.37
34	a	1402	4OC	C2-N3	6.41	1.49	1.36
56	w	39	PSU	C2-N3	6.41	1.48	1.37
8	A	2552	OMU	C2-N1	6.35	1.48	1.38
8	A	746	PSU	C2-N3	6.33	1.48	1.37
34	a	967	5MC	C4-N3	6.29	1.44	1.34
8	A	1915	3TD	O4'-C4'	-6.29	1.30	1.45
8	A	2498	OMC	C6-C5	6.25	1.49	1.35
8	A	2580	PSU	C2-N3	6.18	1.48	1.37
56	w	46	G7M	C3'-C4'	6.13	1.68	1.53
34	a	1498	UR3	C2-N1	6.12	1.47	1.38
8	A	2498	OMC	C2-N3	6.11	1.48	1.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	955	PSU	C2-N3	6.08	1.47	1.37
8	A	2457	PSU	C2-N3	6.07	1.47	1.37
55	v	8	4SU	C2-N3	6.01	1.48	1.38
8	A	2604	PSU	C2-N3	5.95	1.47	1.37
56	w	46	G7M	C2-N3	5.82	1.47	1.33
8	A	2552	OMU	C2-N3	5.77	1.48	1.38
56	w	46	G7M	O4'-C4'	-5.76	1.32	1.45
8	A	747	5MC	C4-N3	5.74	1.43	1.34
8	A	1962	5MC	C4-N3	5.74	1.43	1.34
8	A	1915	3TD	C6-N1	5.72	1.45	1.36
34	a	967	5MC	C2-N3	5.65	1.47	1.36
8	A	747	5MC	C2-N3	5.54	1.47	1.36
8	A	2503	2MA	C2-N1	5.53	1.43	1.34
55	v	20	H2U	C4-N3	5.53	1.47	1.37
34	a	1402	4OC	C6-C5	5.49	1.47	1.35
34	a	1498	UR3	C6-C5	5.40	1.47	1.35
8	A	2498	OMC	C4-N4	5.37	1.46	1.33
8	A	2498	OMC	C4-N3	5.36	1.45	1.34
8	A	2552	OMU	C6-C5	5.36	1.47	1.35
8	A	745	1MG	C2-N2	5.35	1.43	1.34
34	a	1407	5MC	C4-N3	5.34	1.43	1.34
8	A	1939	5MU	C6-C5	5.33	1.43	1.34
8	A	2503	2MA	C6-N1	5.28	1.43	1.33
34	a	527	G7M	C4-N3	5.28	1.50	1.37
55	v	8	4SU	C6-C5	5.26	1.47	1.35
8	A	1962	5MC	C2-N3	5.13	1.46	1.36
55	v	8	4SU	C4-S4	-5.09	1.58	1.68
8	A	2251	OMG	C2-N3	5.04	1.45	1.33
8	A	2504	PSU	C6-N1	5.02	1.44	1.36
34	a	1407	5MC	C2-N3	5.01	1.46	1.36
34	a	1402	4OC	C4-N4	4.99	1.46	1.35
56	w	46	G7M	C2'-C1'	4.98	1.61	1.53
55	v	8	4SU	C2-N1	4.98	1.46	1.38
8	A	1915	3TD	C2-N3	4.97	1.49	1.38
55	v	55	PSU	C6-N1	4.96	1.44	1.36
56	w	32	PSU	C6-N1	4.91	1.44	1.36
34	a	1516	2MG	C2-N2	4.88	1.44	1.33
56	w	46	G7M	C4-N3	4.83	1.49	1.37
8	A	2251	OMG	C4-N3	4.80	1.49	1.37
55	v	54	5MU	C6-C5	4.74	1.42	1.34
56	w	37	MIA	C6-N6	4.71	1.43	1.34
8	A	1915	3TD	O3'-C3'	-4.69	1.31	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	a	1516	2MG	C4-N3	4.67	1.48	1.37
8	A	1835	2MG	C4-N3	4.66	1.48	1.37
56	w	39	PSU	C6-N1	4.65	1.43	1.36
56	w	8	4SU	C4-S4	-4.49	1.59	1.68
8	A	746	PSU	C6-N1	4.49	1.43	1.36
8	A	2251	OMG	C2-N2	4.40	1.44	1.34
8	A	1917	PSU	C6-N1	4.36	1.43	1.36
34	a	1407	5MC	C6-N1	4.33	1.45	1.38
34	a	516	PSU	C6-N1	4.26	1.43	1.36
8	A	955	PSU	C6-N1	4.25	1.43	1.36
8	A	745	1MG	C2-N3	4.24	1.42	1.34
8	A	2457	PSU	C6-N1	4.21	1.43	1.36
34	a	527	G7M	C2-N3	4.21	1.43	1.33
8	A	2445	2MG	C4-N3	4.20	1.47	1.37
8	A	2498	OMC	C2-N1	4.16	1.49	1.40
8	A	1911	PSU	C6-N1	4.15	1.43	1.36
56	w	46	G7M	C2-N2	4.12	1.44	1.34
8	A	745	1MG	C4-N3	4.12	1.47	1.37
8	A	747	5MC	C4-N4	4.07	1.44	1.34
34	a	1498	UR3	C2-N3	4.06	1.46	1.39
8	A	1618	6MZ	C6-N6	3.99	1.41	1.35
56	w	8	4SU	C4-N3	-3.98	1.33	1.37
55	v	8	4SU	C5-C4	3.97	1.47	1.42
8	A	747	5MC	C2-N1	3.94	1.48	1.40
8	A	747	5MC	C6-N1	3.94	1.44	1.38
34	a	1519	MA6	C5-C4	-3.94	1.30	1.40
34	a	967	5MC	C2-N1	3.91	1.48	1.40
34	a	1518	MA6	C5-C4	-3.89	1.30	1.40
8	A	2030	6MZ	C6-N6	3.86	1.41	1.35
8	A	2605	PSU	C6-N1	3.83	1.42	1.36
34	a	967	5MC	C6-N1	3.79	1.44	1.38
34	a	1407	5MC	C4-N4	3.78	1.43	1.34
34	a	527	G7M	C2-N2	3.78	1.43	1.34
34	a	967	5MC	C4-N4	3.78	1.43	1.34
34	a	1207	2MG	C2-N2	3.76	1.41	1.33
8	A	1835	2MG	C2-N2	3.74	1.41	1.33
8	A	2604	PSU	C6-N1	3.73	1.42	1.36
8	A	745	1MG	C5-C4	-3.73	1.33	1.43
34	a	1207	2MG	C2-N1	3.71	1.42	1.36
34	a	1207	2MG	C4-N3	3.69	1.46	1.37
34	a	1402	4OC	C5-C4	3.67	1.48	1.40
56	w	55	PSU	C6-C5	3.61	1.39	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	w	46	G7M	C6-N1	3.55	1.43	1.37
34	a	1402	4OC	C2-N1	3.52	1.47	1.40
56	w	46	G7M	O3'-C3'	3.50	1.51	1.43
8	A	2552	OMU	C4-N3	3.50	1.44	1.38
34	a	1516	2MG	C2-N1	3.48	1.42	1.36
8	A	2069	G7M	C6-N1	3.47	1.43	1.37
34	a	1407	5MC	C2-N1	3.44	1.47	1.40
8	A	2251	OMG	C5-C4	-3.43	1.34	1.43
34	a	1516	2MG	C6-N1	3.39	1.42	1.37
8	A	2445	2MG	C2-N2	3.38	1.40	1.33
8	A	2069	G7M	C4-N3	3.36	1.45	1.37
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	2069	G7M	C2-N2	3.31	1.42	1.34
8	A	1962	5MC	C2-N1	3.29	1.47	1.40
55	v	55	PSU	C4-N3	3.28	1.44	1.38
56	w	32	PSU	C4-N3	3.28	1.44	1.38
8	A	1962	5MC	C6-N1	3.25	1.43	1.38
34	a	1518	MA6	C2-N3	3.22	1.37	1.32
34	a	1516	2MG	C5-C4	-3.20	1.34	1.43
56	w	46	G7M	O2'-C2'	3.11	1.50	1.43
8	A	2580	PSU	C6-N1	3.11	1.41	1.36
8	A	1962	5MC	C4-N4	3.07	1.42	1.34
56	w	8	4SU	C5-C4	-3.06	1.38	1.42
8	A	2445	2MG	C5-C4	-3.05	1.35	1.43
8	A	2030	6MZ	C5-C4	-3.05	1.32	1.40
56	w	46	G7M	C5-C6	3.01	1.53	1.45
34	a	1207	2MG	C6-N1	3.01	1.42	1.37
8	A	1835	2MG	C5-C4	-2.98	1.35	1.43
34	a	516	PSU	O4'-C1'	-2.96	1.39	1.43
8	A	2580	PSU	C1'-C5	-2.95	1.43	1.50
8	A	2030	6MZ	C9-N6	-2.93	1.40	1.45
8	A	1939	5MU	O4-C4	-2.92	1.18	1.23
8	A	1962	5MC	O2-C2	-2.92	1.18	1.23
8	A	2504	PSU	C4-N3	2.90	1.44	1.38
34	a	1207	2MG	C5-C6	2.90	1.53	1.47
8	A	2069	G7M	C5-C4	-2.88	1.33	1.39
56	w	54	5MU	C4-N3	-2.86	1.33	1.38
8	A	2498	OMC	C6-N1	2.83	1.44	1.38
56	w	55	PSU	C4-N3	-2.83	1.33	1.38
8	A	1915	3TD	C4-N3	2.82	1.46	1.40
55	v	8	4SU	C6-N1	2.80	1.44	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	747	5MC	O2-C2	-2.80	1.18	1.23
8	A	2251	OMG	C6-N1	2.79	1.42	1.37
8	A	745	1MG	CM1-N1	-2.78	1.41	1.47
34	a	1207	2MG	C5-C4	-2.77	1.36	1.43
8	A	1917	PSU	C4-N3	2.74	1.43	1.38
56	w	46	G7M	C2-N1	2.74	1.44	1.37
55	v	55	PSU	O4-C4	-2.72	1.18	1.23
8	A	1835	2MG	O6-C6	-2.71	1.17	1.23
34	a	527	G7M	C6-N1	2.71	1.41	1.37
8	A	2580	PSU	O4'-C1'	-2.70	1.40	1.43
8	A	2030	6MZ	C6-N1	-2.70	1.30	1.34
34	a	1407	5MC	O2-C2	-2.69	1.18	1.23
8	A	2498	OMC	C5-C4	2.68	1.49	1.42
8	A	1835	2MG	C5-C6	2.67	1.52	1.47
55	v	54	5MU	O4-C4	-2.67	1.18	1.23
8	A	2604	PSU	O4'-C1'	-2.67	1.40	1.43
8	A	2605	PSU	C4-N3	2.66	1.43	1.38
34	a	1519	MA6	C2-N3	2.65	1.36	1.32
8	A	746	PSU	C4-N3	2.65	1.43	1.38
34	a	967	5MC	O2-C2	-2.65	1.18	1.23
8	A	2251	OMG	O6-C6	-2.61	1.18	1.23
8	A	1835	2MG	C6-N1	2.60	1.41	1.37
8	A	2445	2MG	O6-C6	-2.59	1.18	1.23
34	a	1402	4OC	O2-C2	-2.58	1.18	1.23
56	w	46	G7M	O6-C6	-2.57	1.18	1.23
34	a	516	PSU	C4-N3	2.57	1.43	1.38
8	A	1911	PSU	C4-N3	2.57	1.43	1.38
34	a	1498	UR3	C6-N1	2.57	1.44	1.38
8	A	2503	2MA	C6-C5	2.56	1.52	1.43
56	w	39	PSU	O4-C4	-2.53	1.18	1.23
8	A	2457	PSU	C1'-C5	-2.52	1.44	1.50
8	A	1835	2MG	C2-N1	2.52	1.40	1.36
34	a	1519	MA6	C10-N6	-2.52	1.39	1.45
56	w	39	PSU	C4-N3	2.50	1.43	1.38
8	A	1915	3TD	C3'-C4'	2.49	1.59	1.53
8	A	1939	5MU	O2-C2	-2.48	1.18	1.23
34	a	1498	UR3	O4-C4	-2.48	1.18	1.23
8	A	2580	PSU	O4-C4	-2.47	1.18	1.23
55	v	8	4SU	O2-C2	-2.46	1.18	1.23
8	A	2498	OMC	O2-C2	-2.46	1.19	1.23
8	A	2457	PSU	C4-N3	2.44	1.43	1.38
34	a	1516	2MG	O6-C6	-2.44	1.18	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	2604	PSU	C4-N3	2.43	1.43	1.38
34	a	1498	UR3	O2-C2	-2.42	1.18	1.22
8	A	2069	G7M	C2-N3	2.42	1.39	1.33
8	A	745	1MG	O6-C6	-2.41	1.17	1.22
55	v	54	5MU	O2-C2	-2.41	1.18	1.23
8	A	2445	2MG	CM2-N2	-2.37	1.41	1.45
8	A	2605	PSU	O4-C4	-2.36	1.19	1.23
34	a	1516	2MG	C5-C6	2.36	1.52	1.47
8	A	955	PSU	C4-N3	2.35	1.43	1.38
8	A	2457	PSU	O4-C4	-2.34	1.19	1.23
8	A	955	PSU	O4-C4	-2.32	1.19	1.23
8	A	746	PSU	O4-C4	-2.31	1.19	1.23
34	a	1207	2MG	O6-C6	-2.30	1.18	1.23
8	A	2605	PSU	O4'-C1'	-2.29	1.40	1.43
8	A	1917	PSU	O4-C4	-2.29	1.19	1.23
34	a	1402	4OC	C6-N1	2.28	1.43	1.38
56	w	8	4SU	C2-N3	-2.28	1.33	1.38
34	a	966	2MG	C6-N1	-2.28	1.34	1.37
8	A	2030	6MZ	C5-N7	-2.27	1.31	1.39
8	A	2457	PSU	O4'-C1'	-2.27	1.40	1.43
8	A	1618	6MZ	C4-N3	-2.27	1.32	1.35
56	w	54	5MU	C6-N1	-2.25	1.34	1.38
8	A	1911	PSU	O4-C4	-2.24	1.19	1.23
8	A	2604	PSU	C1'-C5	-2.23	1.45	1.50
8	A	955	PSU	C1'-C5	-2.23	1.45	1.50
8	A	2503	2MA	C5-C4	-2.23	1.35	1.40
34	a	516	PSU	O4-C4	-2.22	1.19	1.23
8	A	1618	6MZ	C9-N6	-2.22	1.41	1.45
8	A	1911	PSU	O4'-C1'	-2.21	1.40	1.43
8	A	2604	PSU	O4-C4	-2.21	1.19	1.23
8	A	2552	OMU	O4-C4	-2.20	1.20	1.24
56	w	32	PSU	O4-C4	-2.20	1.19	1.23
8	A	2504	PSU	O4-C4	-2.20	1.19	1.23
56	w	54	5MU	C2-N1	2.20	1.42	1.38
56	w	54	5MU	C2-N3	-2.16	1.34	1.38
8	A	2069	G7M	C2-N1	2.15	1.43	1.37
56	w	54	5MU	C4-C5	2.14	1.48	1.44
56	w	8	4SU	C2-N1	2.13	1.41	1.38
8	A	1618	6MZ	C6-N1	-2.12	1.31	1.34
8	A	2030	6MZ	C2-N3	2.12	1.35	1.32
58	y	101	FME	CA-N	-2.11	1.43	1.46
34	a	1518	MA6	C10-N6	-2.10	1.40	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	w	54	5MU	C6-C5	2.10	1.38	1.34
56	w	55	PSU	C2-N3	-2.10	1.33	1.37
8	A	2503	2MA	C6-N6	-2.09	1.26	1.34
8	A	1618	6MZ	C5-N7	-2.08	1.32	1.39
8	A	2251	OMG	C2-N1	2.05	1.42	1.37
8	A	2251	OMG	C5-C6	2.05	1.51	1.47
8	A	1915	3TD	O5'-C5'	-2.03	1.39	1.44
8	A	2504	PSU	O4'-C1'	-2.01	1.41	1.43

All (206) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	1939	5MU	C5-C4-N3	13.01	126.41	115.31
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
55	v	54	5MU	C5-C4-N3	12.04	125.59	115.31
8	A	1939	5MU	C5-C6-N1	-10.62	112.41	123.34
8	A	1618	6MZ	C9-N6-C6	-8.57	115.49	122.87
55	v	54	5MU	C5-C6-N1	-8.38	114.72	123.34
56	w	37	MIA	C12-C13-C14	-7.85	111.86	127.14
55	v	8	4SU	C4-N3-C2	-7.25	120.30	127.34
55	v	54	5MU	C5M-C5-C4	7.23	126.72	118.77
8	A	2580	PSU	C6-C5-C4	7.12	123.17	118.20
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	2604	PSU	C6-C5-C4	6.52	122.76	118.20
8	A	2457	PSU	C6-C5-C4	6.21	122.54	118.20
8	A	2552	OMU	C4-N3-C2	-6.12	118.50	126.58
34	a	1518	MA6	N3-C2-N1	-5.97	119.34	128.68
56	w	55	PSU	N1-C2-N3	5.93	121.85	115.13
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	1939	5MU	O4-C4-C5	-5.84	118.13	124.90
55	v	54	5MU	C5M-C5-C6	-5.76	115.16	122.85
34	a	1519	MA6	N3-C2-N1	-5.75	119.69	128.68
8	A	1939	5MU	C4-N3-C2	-5.73	119.93	127.35
56	w	8	4SU	C4-N3-C2	-5.63	121.87	127.34
55	v	8	4SU	C5-C4-N3	5.55	119.84	114.69
8	A	2605	PSU	N1-C2-N3	5.52	121.38	115.13
8	A	1835	2MG	CM2-N2-C2	-5.44	111.83	123.86
8	A	2604	PSU	C4-N3-C2	-5.36	118.62	126.34
56	w	37	MIA	C12-N6-C6	-5.26	114.76	122.55

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	w	54	5MU	N3-C2-N1	5.26	121.87	114.89
8	A	2030	6MZ	N3-C2-N1	-5.20	120.55	128.68
56	w	39	PSU	C6-C5-C4	5.15	121.80	118.20
8	A	1915	3TD	N1-C2-N3	5.14	120.19	116.14
8	A	2604	PSU	N1-C2-N3	5.13	120.94	115.13
8	A	2605	PSU	C4-N3-C2	-5.09	119.00	126.34
8	A	2580	PSU	N1-C2-N3	5.07	120.87	115.13
56	w	39	PSU	N1-C2-N3	4.98	120.77	115.13
56	w	46	G7M	O3'-C3'-C4'	4.94	125.33	111.05
56	w	39	PSU	C4-N3-C2	-4.89	119.29	126.34
56	w	8	4SU	C5-C4-N3	4.85	119.19	114.69
55	v	55	PSU	C4-N3-C2	-4.82	119.39	126.34
55	v	54	5MU	O4-C4-C5	-4.80	119.34	124.90
8	A	955	PSU	C6-C5-C4	4.77	121.53	118.20
8	A	2503	2MA	C1'-N9-C4	-4.70	118.39	126.64
8	A	955	PSU	C4-N3-C2	-4.68	119.59	126.34
8	A	2503	2MA	C2-N3-C4	4.65	119.30	115.52
8	A	1911	PSU	C4-N3-C2	-4.64	119.66	126.34
8	A	1939	5MU	N3-C2-N1	4.64	121.04	114.89
56	w	32	PSU	C4-N3-C2	-4.62	119.68	126.34
56	w	54	5MU	C4-N3-C2	-4.57	121.43	127.35
8	A	2504	PSU	C4-N3-C2	-4.53	119.82	126.34
8	A	2605	PSU	C6-N1-C2	-4.52	118.06	122.68
8	A	2069	G7M	N2-C2-N1	4.52	126.33	116.71
56	w	37	MIA	C16-C14-C13	-4.49	109.67	122.65
34	a	967	5MC	C5-C6-N1	-4.49	118.72	123.34
8	A	2580	PSU	C6-N1-C2	-4.46	118.12	122.68
56	w	54	5MU	C5M-C5-C4	4.45	123.67	118.77
8	A	1835	2MG	C5-C6-N1	4.44	121.79	113.95
56	w	8	4SU	N3-C2-N1	4.44	120.78	114.89
8	A	2457	PSU	C4-N3-C2	-4.42	119.97	126.34
8	A	1917	PSU	C4-N3-C2	-4.41	119.99	126.34
56	w	37	MIA	C15-C14-C13	-4.40	109.94	122.65
8	A	1911	PSU	N1-C2-N3	4.37	120.08	115.13
8	A	747	5MC	C5-C6-N1	-4.37	118.84	123.34
55	v	54	5MU	C4-N3-C2	-4.27	121.83	127.35
55	v	8	4SU	C5-C4-S4	-4.27	118.97	124.47
8	A	1917	PSU	N1-C2-N3	4.21	119.90	115.13
8	A	2580	PSU	C4-N3-C2	-4.21	120.27	126.34
8	A	1915	3TD	C4-N3-C2	-4.19	120.06	124.61
8	A	1962	5MC	C5-C6-N1	-4.14	119.08	123.34
8	A	2457	PSU	N1-C2-N3	4.12	119.80	115.13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	w	32	PSU	N1-C2-N3	4.12	119.79	115.13
56	w	37	MIA	N3-C2-N1	-4.11	119.42	126.98
8	A	1911	PSU	C6-C5-C4	4.08	121.05	118.20
8	A	955	PSU	N1-C2-N3	4.08	119.75	115.13
34	a	516	PSU	N1-C2-N3	4.06	119.73	115.13
34	a	516	PSU	C4-N3-C2	-4.04	120.52	126.34
8	A	2504	PSU	C6-C5-C4	4.01	121.00	118.20
8	A	2552	OMU	C5-C4-N3	4.00	120.83	114.84
8	A	1618	6MZ	C1'-N9-C4	-4.00	119.62	126.64
34	a	1407	5MC	C5-C6-N1	-3.94	119.28	123.34
8	A	2069	G7M	N2-C2-N3	-3.87	112.21	119.74
55	v	55	PSU	N1-C2-N3	3.84	119.48	115.13
8	A	2605	PSU	C6-C5-C4	3.82	120.87	118.20
34	a	1498	UR3	C4-N3-C2	-3.81	120.97	124.56
8	A	1917	PSU	C6-C5-C4	3.79	120.85	118.20
8	A	746	PSU	N1-C2-N3	3.77	119.40	115.13
56	w	55	PSU	C4-N3-C2	-3.76	120.92	126.34
8	A	2504	PSU	N1-C2-N3	3.74	119.37	115.13
8	A	2552	OMU	N3-C2-N1	3.73	119.84	114.89
34	a	516	PSU	C6-C5-C4	3.68	120.77	118.20
8	A	745	1MG	CM1-N1-C2	-3.68	116.90	120.72
34	a	1207	2MG	CM2-N2-C2	-3.64	115.81	123.86
8	A	2445	2MG	CM2-N2-C2	-3.64	115.81	123.86
34	a	1516	2MG	C5-C6-N1	3.63	120.37	113.95
55	v	54	5MU	N3-C2-N1	3.61	119.69	114.89
55	v	55	PSU	C6-C5-C4	3.59	120.71	118.20
56	w	37	MIA	C11-S10-C2	3.59	104.95	102.27
56	w	54	5MU	C5-C4-N3	3.57	118.36	115.31
56	w	39	PSU	C6-N1-C2	-3.56	119.04	122.68
8	A	746	PSU	C4-N3-C2	-3.55	121.22	126.34
56	w	54	5MU	C5M-C5-C6	-3.55	118.10	122.85
56	w	46	G7M	C2-N1-C6	-3.53	118.60	125.10
8	A	1917	PSU	C6-N1-C2	-3.49	119.11	122.68
34	a	516	PSU	C6-N1-C2	-3.49	119.12	122.68
8	A	746	PSU	C6-N1-C2	-3.46	119.14	122.68
8	A	2251	OMG	C5-C6-N1	3.43	120.01	113.95
8	A	745	1MG	C5-C6-N1	3.43	119.06	113.90
8	A	2552	OMU	O4-C4-C5	-3.35	119.28	125.16
34	a	1519	MA6	C10-N6-C9	3.34	126.90	116.12
8	A	746	PSU	C6-C5-C4	3.28	120.49	118.20
8	A	1911	PSU	C6-N1-C2	-3.27	119.34	122.68
8	A	2503	2MA	CM2-C2-N1	3.23	122.19	117.15

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	a	1519	MA6	C1'-N9-C4	-3.19	121.03	126.64
56	w	8	4SU	C5-C4-S4	-3.19	120.36	124.47
34	a	1518	MA6	C10-N6-C9	3.14	126.24	116.12
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	2580	PSU	O2-C2-N1	-3.11	119.37	122.79
8	A	1962	5MC	C1'-N1-C6	-3.11	115.95	121.12
8	A	2069	G7M	CN7-N7-C8	-3.11	110.48	125.43
34	a	516	PSU	O2-C2-N1	-3.08	119.40	122.79
55	v	54	5MU	C1'-N1-C2	3.08	123.14	117.57
56	w	37	MIA	S10-C2-N1	3.04	126.52	116.01
8	A	2069	G7M	C2-N1-C6	-3.03	119.51	125.10
56	w	55	PSU	O2-C2-N1	-3.02	119.47	122.79
56	w	32	PSU	C6-C5-C4	2.98	120.28	118.20
8	A	1939	5MU	C5M-C5-C6	-2.97	118.88	122.85
8	A	955	PSU	C6-N1-C2	-2.95	119.66	122.68
8	A	1835	2MG	O6-C6-N1	-2.94	117.18	120.65
34	a	527	G7M	C2-N1-C6	-2.92	119.71	125.10
8	A	2503	2MA	N3-C2-N1	-2.91	120.42	125.73
55	v	8	4SU	N3-C2-N1	2.90	118.75	114.89
8	A	2552	OMU	CM2-O2'-C2'	-2.90	106.92	114.52
55	v	20	H2U	C5-C4-N3	2.89	119.89	116.65
55	v	20	H2U	O2-C2-N1	-2.87	119.50	123.11
8	A	2457	PSU	C6-N1-C2	-2.86	119.76	122.68
8	A	2604	PSU	C6-N1-C2	-2.79	119.83	122.68
56	w	54	5MU	O4-C4-C5	-2.78	121.68	124.90
8	A	1618	6MZ	C2-N1-C6	2.74	118.94	116.59
55	v	20	H2U	C5-C6-N1	2.73	120.59	111.61
8	A	2504	PSU	C6-N1-C2	-2.72	119.90	122.68
56	w	32	PSU	C6-N1-C2	-2.72	119.91	122.68
8	A	2580	PSU	O4'-C1'-C2'	2.72	108.97	105.14
56	w	8	4SU	C6-N1-C2	-2.70	117.54	120.99
8	A	2605	PSU	O2-C2-N1	-2.67	119.85	122.79
8	A	745	1MG	O6-C6-C5	-2.67	119.47	124.19
8	A	1911	PSU	O2-C2-N1	-2.64	119.88	122.79
56	w	54	5MU	C6-N1-C2	-2.64	118.63	121.30
55	v	54	5MU	O4-C4-N3	-2.63	115.07	120.12
56	w	54	5MU	C3'-C2'-C1'	2.62	106.41	101.43
55	v	55	PSU	C6-N1-C2	-2.62	120.01	122.68
8	A	747	5MC	CM5-C5-C6	-2.61	119.36	122.85
55	v	54	5MU	C1'-N1-C6	-2.61	116.79	121.12
34	a	1402	4OC	C5-C4-N4	-2.60	117.32	122.61

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	a	1207	2MG	C5-C6-N1	2.60	118.54	113.95
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	O6-C6-C5	-2.55	119.39	124.37
8	A	1835	2MG	C8-N7-C5	2.55	107.84	102.99
34	a	966	2MG	C8-N7-C5	2.54	107.82	102.99
8	A	1917	PSU	O2-C2-N1	-2.52	120.01	122.79
56	w	39	PSU	O2-C2-N1	-2.52	120.02	122.79
34	a	1516	2MG	O6-C6-C5	-2.51	119.48	124.37
8	A	1939	5MU	O2-C2-N1	-2.49	119.47	122.79
56	w	37	MIA	C1'-N9-C4	-2.45	122.34	126.64
34	a	966	2MG	C5-C6-N1	2.44	118.27	113.95
8	A	1939	5MU	O4-C4-N3	-2.44	115.44	120.12
8	A	1939	5MU	C5M-C5-C4	2.44	121.45	118.77
56	w	37	MIA	C2-N3-C4	2.42	118.66	115.32
8	A	2251	OMG	C8-N7-C5	2.41	107.58	102.99
34	a	1407	5MC	CM5-C5-C6	-2.39	119.65	122.85
56	w	32	PSU	O4'-C1'-C2'	2.38	108.50	105.14
34	a	967	5MC	C5-C4-N4	-2.37	117.93	121.48
56	w	55	PSU	C6-C5-C4	-2.37	116.54	118.20
34	a	527	G7M	N2-C2-N3	2.37	124.34	119.74
8	A	2605	PSU	O4'-C1'-C2'	2.36	108.48	105.14
8	A	2552	OMU	C2'-C1'-N1	-2.36	109.64	114.22
56	w	32	PSU	O2-C2-N1	-2.35	120.20	122.79
55	v	55	PSU	O2-C2-N1	-2.32	120.24	122.79
56	w	55	PSU	C3'-C2'-C1'	2.30	104.32	101.64
8	A	746	PSU	O2-C2-N1	-2.29	120.27	122.79
34	a	1516	2MG	C8-N7-C5	2.28	107.33	102.99
34	a	1498	UR3	C3U-N3-C4	2.26	121.12	117.89
8	A	745	1MG	C2-N1-C6	2.25	122.77	120.95
34	a	967	5MC	C1'-N1-C6	-2.24	117.39	121.12
8	A	2251	OMG	N1-C2-N3	-2.23	119.16	123.32
56	w	8	4SU	O4'-C1'-N1	2.22	113.43	108.36
58	y	101	FME	C-CA-N	2.21	113.73	109.73
56	w	37	MIA	C16-C14-C15	-2.20	109.74	114.60
8	A	2604	PSU	C5-C6-N1	-2.20	118.81	122.11
34	a	1402	4OC	CM2-O2'-C2'	-2.16	108.85	114.52
8	A	2251	OMG	C2-N1-C6	-2.16	121.12	125.10
34	a	1207	2MG	O3'-C3'-C2'	2.15	118.79	111.82
8	A	2445	2MG	C5-C6-N1	2.14	117.73	113.95
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	a	1402	4OC	C1'-N1-C6	-2.11	116.24	120.84
34	a	967	5MC	CM5-C5-C6	-2.08	120.07	122.85
8	A	2503	2MA	O3'-C3'-C4'	-2.05	105.12	111.05
8	A	2604	PSU	O2-C2-N3	-2.04	117.96	121.82
8	A	2030	6MZ	C2-N1-C6	2.04	118.34	116.59
56	w	54	5MU	O2-C2-N1	-2.04	120.08	122.79
34	a	1207	2MG	C8-N7-C5	2.03	106.87	102.99
8	A	745	1MG	CM1-N1-C6	2.03	120.32	117.55

There are no chirality outliers.

All (57) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
34	a	967	5MC	O4'-C4'-C5'-O5'
34	a	967	5MC	C3'-C4'-C5'-O5'
34	a	1498	UR3	O4'-C1'-N1-C6
34	a	1498	UR3	O4'-C1'-N1-C2
34	a	1519	MA6	C5-C6-N6-C9
34	a	1519	MA6	C5-C6-N6-C10
55	v	54	5MU	C3'-C4'-C5'-O5'
55	v	54	5MU	O4'-C4'-C5'-O5'
55	v	55	PSU	O4'-C1'-C5-C4
55	v	55	PSU	O4'-C1'-C5-C6
8	A	1618	6MZ	N1-C6-N6-C9
8	A	1915	3TD	O4'-C1'-C5-C4
8	A	1915	3TD	O4'-C1'-C5-C6
8	A	1939	5MU	O4'-C4'-C5'-O5'
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	32	PSU	O4'-C1'-C5-C6
56	w	37	MIA	C5-C6-N6-C12
56	w	37	MIA	C12-C13-C14-C16
56	w	39	PSU	C2'-C1'-C5-C4
56	w	39	PSU	O4'-C1'-C5-C4
56	w	39	PSU	O4'-C1'-C5-C6
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'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
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'
8	A	2552	OMU	O4'-C1'-N1-C6
58	y	101	FME	CB-CG-SD-CE
8	A	2552	OMU	O4'-C1'-N1-C2
8	A	2030	6MZ	N1-C6-N6-C9
34	a	527	G7M	C3'-C4'-C5'-O5'
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
55	v	54	5MU	C2'-C1'-N1-C2
8	A	746	PSU	O4'-C1'-C5-C6
56	w	55	PSU	O4'-C1'-C5-C6
8	A	747	5MC	C2'-C1'-N1-C2
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 oligosaccharides 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%)
62	GDP	x	801	-	24,30,30	5.24	12 (50%)	30,47,47	1.86	11 (36%)

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 (12) 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	C2-N2	4.96	1.46	1.34
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	C4-N3	4.14	1.47	1.37
62	x	801	GDP	C2-N3	4.06	1.43	1.33
62	x	801	GDP	C2-N1	3.48	1.46	1.37
62	x	801	GDP	C5-C4	-3.03	1.35	1.43
62	x	801	GDP	C6-N1	3.01	1.42	1.37
62	x	801	GDP	C5-C6	2.22	1.51	1.47

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
62	x	801	GDP	N2-C2-N1	4.60	126.50	116.71
62	x	801	GDP	C3'-C2'-C1'	3.21	105.81	100.98
62	x	801	GDP	N2-C2-N3	-3.20	113.50	119.74
62	x	801	GDP	C2'-C3'-C4'	2.63	107.75	102.64

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
62	x	801	GDP	PA-O3A-PB	-2.62	123.84	132.83
62	x	801	GDP	C5-C6-N1	2.54	118.43	113.95
61	a	2001	AM2	CA1-OA4-CA5	2.47	117.04	113.06
62	x	801	GDP	O6-C6-C5	-2.30	119.89	124.37
62	x	801	GDP	C2-N1-C6	-2.22	121.01	125.10
62	x	801	GDP	O3B-PB-O1B	2.08	118.84	110.68
62	x	801	GDP	C8-N7-C5	2.08	106.96	102.99
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.

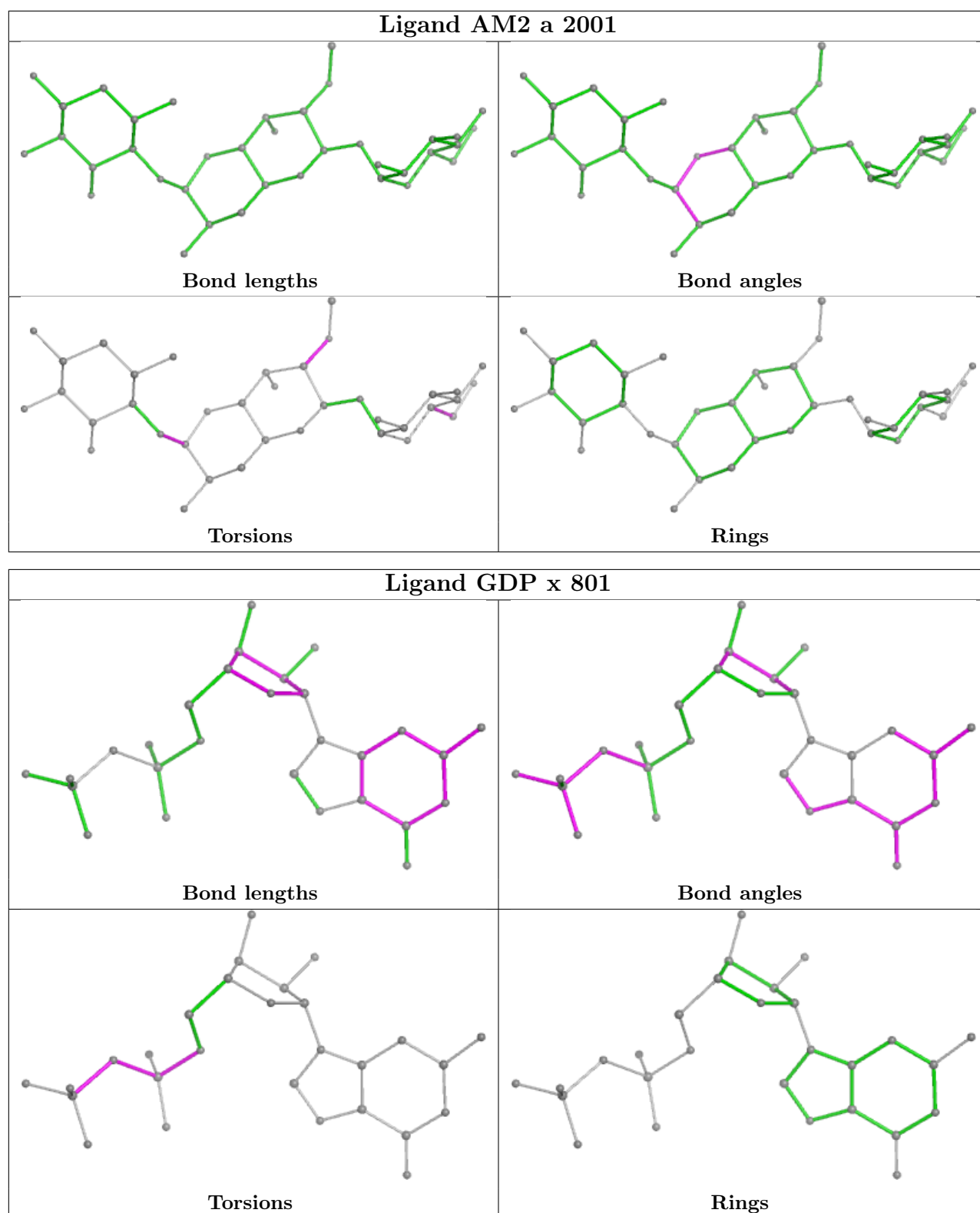
All (11) torsion outliers are listed below:

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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.