



Full wwPDB EM Validation Report ⓘ

Nov 20, 2022 – 11:21 AM EST

PDB ID : 4V6M
EMDB ID : EMD-1858
Title : Structure of the ribosome-SecYE complex in the membrane environment
Authors : Frauenfeld, J.; Gumbart, J.; van der Sluis, E.O.; Funes, S.; Gartmann, M.; Beatrix, B.; Mielke, T.; Berninghausen, O.; Becker, T.; Schulten, K.; Beckmann, R.
Deposited on : 2011-02-08
Resolution : 7.10 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

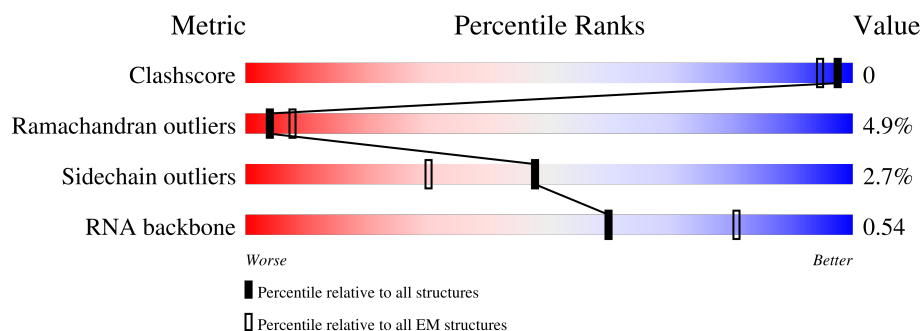
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 7.10 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.



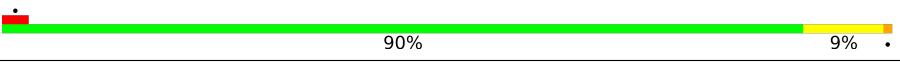
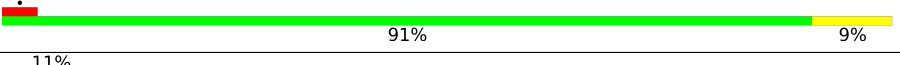
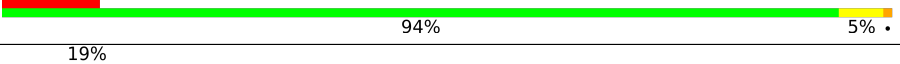
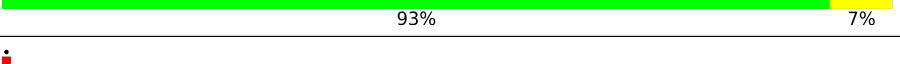
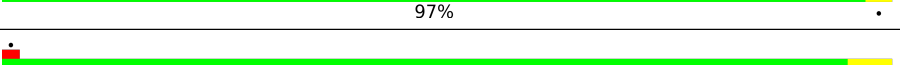
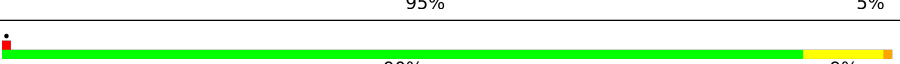
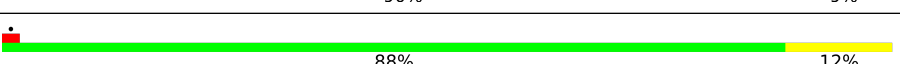
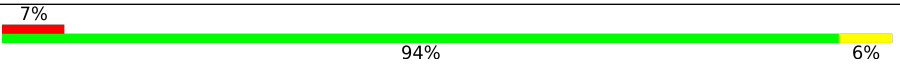
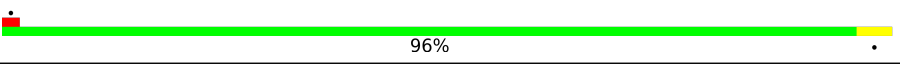
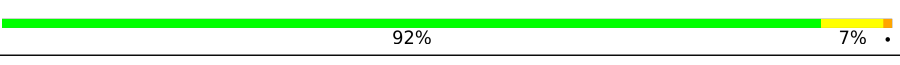
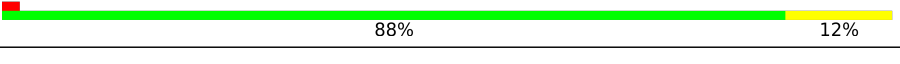
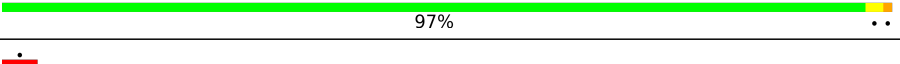
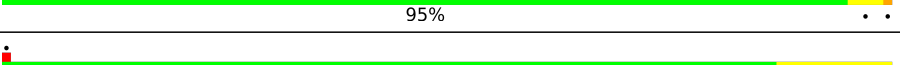
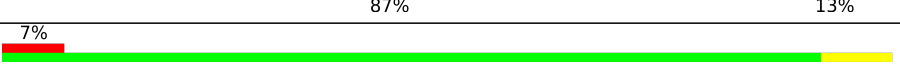
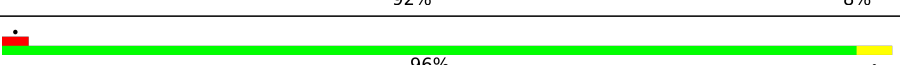
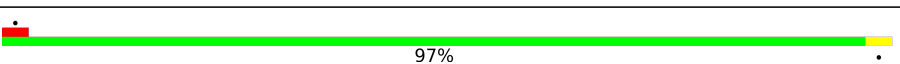
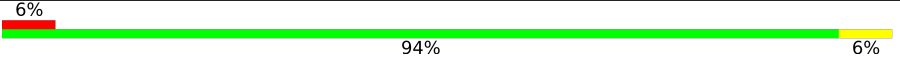
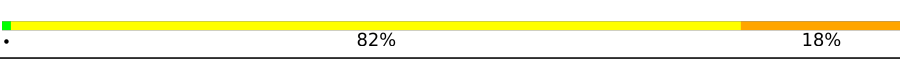
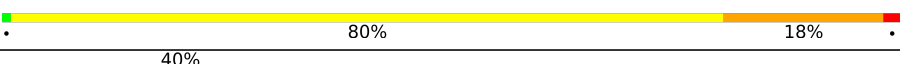

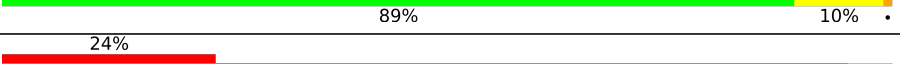
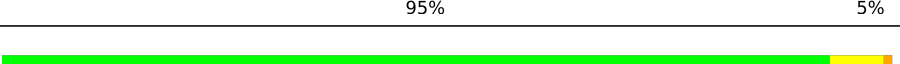
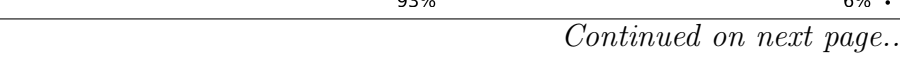


Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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

Mol	Chain	Length	Quality of chain
1	AA	1542	
2	AX	11	
3	AV	77	
4	AZ	98	
5	A0	200	
5	A1	200	
6	AB	240	


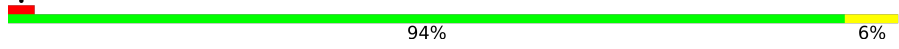
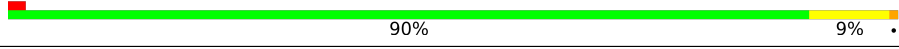
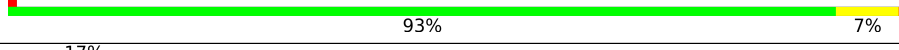

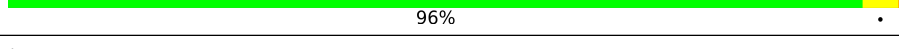
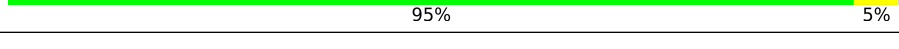
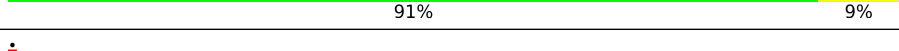
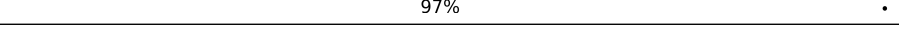
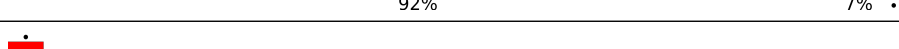
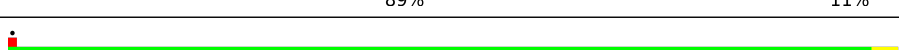
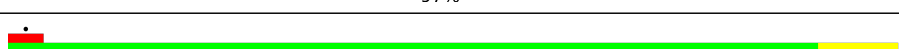
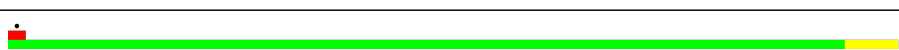
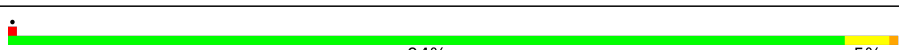
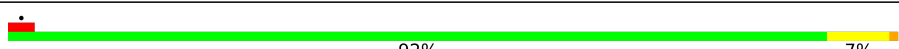

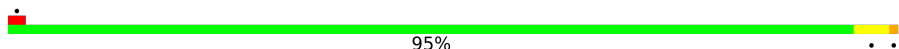
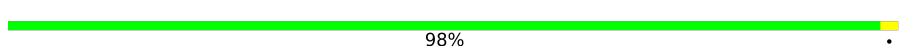
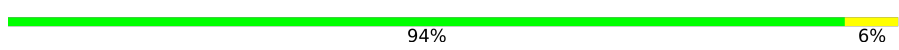

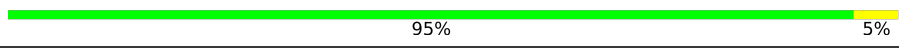
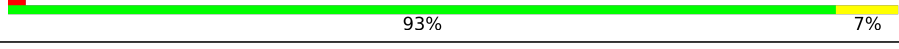
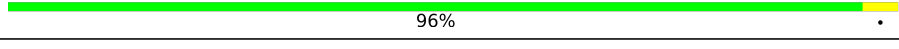


Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
7	AC	232	
8	AD	205	
9	AE	166	
10	AF	135	
11	AG	178	
12	AH	129	
13	AI	129	
14	AJ	103	
15	AK	128	
16	AL	123	
17	AM	117	
18	AN	100	
19	AO	88	
20	AP	82	
21	AQ	83	
22	AR	74	
23	AS	91	
24	AT	86	
25	AU	70	
26	B7	120	
27	B8	2904	
28	BA	435	
29	BB	116	
30	B5	234	
31	B6	272	


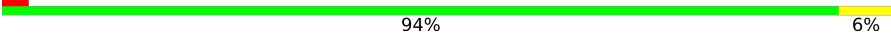

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
32	BD	209	
33	BE	201	
34	BF	178	
35	BG	176	
36	BH	149	
37	BI	141	
38	BJ	142	
39	BK	123	
40	BL	144	
41	BM	136	
42	BN	127	
43	BO	117	
44	BP	114	
45	BQ	117	
46	BR	103	
47	BS	110	
48	BT	100	
49	BU	103	
50	BV	94	
51	BW	84	
52	BX	77	
53	BY	63	
54	BZ	58	
55	B0	56	
56	B1	54	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
57	B2	46	
58	B3	64	
59	B4	38	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
60	PEV	A0	308	X	-	-	-
60	PEV	A0	314	X	-	-	-
60	PEV	A0	323	X	-	-	-
60	PEV	A1	301	X	-	-	-
60	PEV	A1	305	X	-	-	-
60	PEV	A1	313	X	-	-	-
60	PEV	A1	317	X	-	-	-
60	PEV	AZ	204	X	-	-	-
60	PEV	B8	3001	X	-	-	-
60	PEV	BA	502	X	-	-	-
60	PEV	BA	508	X	-	-	-
60	PEV	BA	526	X	-	-	-
60	PEV	BA	530	X	-	-	-
60	PEV	BA	533	-	-	X	-
60	PEV	BA	535	X	-	-	-
60	PEV	BA	537	X	-	-	-
60	PEV	BA	538	X	-	-	-
60	PEV	BB	202	X	-	-	-
60	PEV	BB	206	X	-	-	-
61	PGV	A0	304	X	-	-	-
61	PGV	A0	305	X	-	-	-
61	PGV	A0	306	X	-	-	-
61	PGV	A0	317	X	-	-	-
61	PGV	A0	318	X	-	-	-
61	PGV	A0	325	X	-	-	-
61	PGV	A0	327	X	-	-	-
61	PGV	A0	328	X	-	-	-
61	PGV	A0	331	X	-	-	-
61	PGV	A0	332	X	-	-	-
61	PGV	A1	303	X	-	-	-
61	PGV	A1	311	X	-	-	-
61	PGV	A1	315	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
61	PGV	A1	318	X	-	-	-
61	PGV	AZ	205	X	-	-	-
61	PGV	AZ	207	X	-	-	-
61	PGV	B8	3005	X	-	-	-
61	PGV	BA	501	X	-	-	-
61	PGV	BA	505	X	-	-	-
61	PGV	BA	512	X	-	-	-
61	PGV	BA	515	X	-	-	-
61	PGV	BA	516	X	-	-	-
61	PGV	BA	522	X	-	-	-
61	PGV	BA	536	X	-	-	-
61	PGV	BA	540	X	-	-	-
61	PGV	BB	203	X	-	-	-
61	PGV	BB	204	X	-	-	-
61	PGV	BB	205	X	-	-	-
61	PGV	BB	207	X	-	-	-
61	PGV	BB	208	X	-	-	-
61	PGV	BB	213	X	-	-	-
61	PGV	BB	217	X	-	-	-

2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 163040 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	AA	1542	Total	C	N	O	P	0	0
			33080	14754	6064	10720	1542		

- Molecule 2 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	AX	11	Total	C	N	O	P	0	0
			231	103	39	78	11		

- Molecule 3 is a RNA chain called FtsQ nascent chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	AV	77	Total	C	N	O	P	0	0
			1649	733	297	542	77		

- Molecule 4 is a protein called Cell division protein FtsQ.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	AZ	98	Total	C	N	O	S	0	0
			779	496	142	138	3		

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AZ	104	GLN	-	expression tag	UNP Q8X9Y5
AZ	105	HIS	-	expression tag	UNP Q8X9Y5
AZ	106	ALA	-	expression tag	UNP Q8X9Y5
AZ	107	ARG	-	expression tag	UNP Q8X9Y5
AZ	108	LEU	-	expression tag	UNP Q8X9Y5
AZ	109	ASP	-	expression tag	UNP Q8X9Y5
AZ	110	LYS	-	expression tag	UNP Q8X9Y5
AZ	111	PRO	-	expression tag	UNP Q8X9Y5
AZ	112	GLY	-	expression tag	UNP Q8X9Y5

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
AZ	113	ALA	-	expression tag	UNP Q8X9Y5
AZ	114	ARG	-	expression tag	UNP Q8X9Y5
AZ	115	HIS	-	expression tag	UNP Q8X9Y5
AZ	116	PRO	-	expression tag	UNP Q8X9Y5
AZ	117	CYS	-	expression tag	UNP Q8X9Y5
AZ	118	TRP	-	expression tag	UNP Q8X9Y5
AZ	119	PRO	-	expression tag	UNP Q8X9Y5

- Molecule 5 is a protein called Apolipoprotein A-I.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	A0	200	Total	C	N	O	S	0	0
			1640	1028	290	319	3		
5	A1	200	Total	C	N	O	S	0	0
			1640	1028	290	319	3		

- Molecule 6 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	AB	240	Total	C	N	O	S	0	0
			1872	1180	332	352	8		

- Molecule 7 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	AC	232	Total	C	N	O	S	0	0
			1822	1149	346	323	4		

- Molecule 8 is a protein called 30S ribosomal protein S4.

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

- Molecule 9 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	AE	166	Total	C	N	O	S	0	0
			1225	761	232	226	6		

- Molecule 10 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	AF	135	Total	C	N	O	S	0	0
			1101	677	198	219	7		

- Molecule 11 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	AG	178	Total	C	N	O	S	0	0
			1400	874	269	253	4		

- Molecule 12 is a protein called 30S ribosomal protein S8.

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

- Molecule 13 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	AI	129	Total	C	N	O	S	0	0
			1036	642	208	183	3		

- Molecule 14 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	AJ	103	Total	C	N	O	S	0	0
			825	514	158	151	2		

- Molecule 15 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	AK	128	Total	C	N	O	S	0	0
			965	595	196	171	3		

- Molecule 16 is a protein called 30S ribosomal protein S12.

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

- Molecule 17 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	AM	117	Total	C	N	O	S	0	0
			910	564	183	160	3		

- Molecule 18 is a protein called 30S ribosomal protein S14.

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

- Molecule 19 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	AO	88	Total	C	N	O	S	0	0
			716	440	146	129	1		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AO	79	ARG	GLN	conflict	UNP P0ADZ4

- Molecule 20 is a protein called 30S ribosomal protein S16.

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

- Molecule 21 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	AQ	83	Total	C	N	O	S	0	0
			672	425	124	120	3		

- Molecule 22 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	AR	74	Total	C	N	O	S	0	0
			626	395	123	107	1		

- Molecule 23 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	AS	91	Total	C	N	O	S	0	0
			727	464	139	122	2		

- Molecule 24 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	AT	86	Total	C	N	O	S	0	0
			670	414	138	115	3		

- Molecule 25 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	AU	70	Total	C	N	O	S	0	0
			590	366	125	98	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
26	B7	120	Total	C	N	O	P	0	0
			2570	1144	468	838	120		

- Molecule 27 is a RNA chain called 23S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	B8	2904	Total	C	N	O	P	0	0
			62341	27810	11469	20158	2904		

- Molecule 28 is a protein called Preprotein translocase secY subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	BA	435	Total	C	N	O	S	0	0
			3362	2221	553	571	17		

- Molecule 29 is a protein called Preprotein translocase secE subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	BB	116	Total	C	N	O	S	0	0
			889	587	154	145	3		

- Molecule 30 is a protein called 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	B5	234	Total	C	N	O	S	0	0
			1733	1081	315	330	7		

- Molecule 31 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	B6	272	Total	C	N	O	S	0	0
			2092	1294	425	366	7		

- Molecule 32 is a protein called 50S ribosomal protein L3.

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

- Molecule 33 is a protein called 50S ribosomal protein L4.

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

- Molecule 34 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	BF	178	Total	C	N	O	S	0	0
			1420	905	251	258	6		

- Molecule 35 is a protein called 50S ribosomal protein L6.

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

- Molecule 36 is a protein called 50S ribosomal protein L9.

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

- Molecule 37 is a protein called 50S ribosomal protein L11.

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

- Molecule 38 is a protein called 50S ribosomal protein L13.

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

- Molecule 39 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	BK	123	Total	C	N	O	S	0	0
			947	593	181	167	6		

- Molecule 40 is a protein called 50S ribosomal protein L15.

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

- Molecule 41 is a protein called 50S ribosomal protein L16.

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

- Molecule 42 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	BN	127	Total	C	N	O	S	0	0
			1008	621	204	178	5		

- Molecule 43 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	BO	117	Total	C	N	O	S	0	0
			900	557	179	163	1		

- Molecule 44 is a protein called 50S ribosomal protein L19.

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

- Molecule 45 is a protein called 50S ribosomal protein L20.

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

- Molecule 46 is a protein called 50S ribosomal protein L21.

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

- Molecule 47 is a protein called 50S ribosomal protein L22.

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

- Molecule 48 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	BT	100	Total	C	N	O	S	0	0
			787	496	146	143	2		

- Molecule 49 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	BU	103	Total	C	N	O		0	0
			789	498	148	143			

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

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

- Molecule 51 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	BW	84	Total	C	N	O	S	0	0
			634	391	129	113	1		

- Molecule 52 is a protein called 50S ribosomal protein L28.

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

- Molecule 53 is a protein called 50S ribosomal protein L29.

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

- Molecule 54 is a protein called 50S ribosomal protein L30.

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

- Molecule 55 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	B0	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

- Molecule 56 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
56	B1	54	Total	C	N	O	0	0
			441	284	81	76		

- Molecule 57 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	B2	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

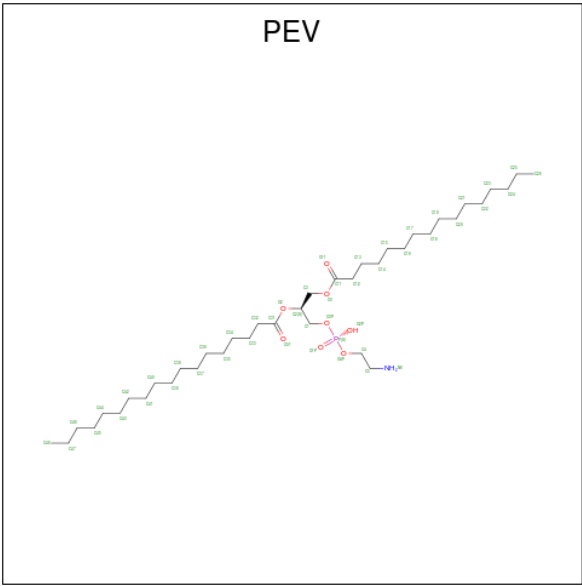
- Molecule 58 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	B3	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 59 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	B4	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 60 is (1S)-2-{[(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL STEARATE (three-letter code: PEV) (formula: C₃₉H₇₈NO₈P).



Mol	Chain	Residues	Atoms					AltConf
60	AZ	1	Total	C	N	O	P	0
			245	195	5	40	5	
60	AZ	1	Total	C	N	O	P	0
			245	195	5	40	5	
60	AZ	1	Total	C	N	O	P	0
			245	195	5	40	5	
60	AZ	1	Total	C	N	O	P	0
			245	195	5	40	5	
60	AZ	1	Total	C	N	O	P	0
			245	195	5	40	5	
60	A0	1	Total	C	N	O	P	0
			1078	858	22	176	22	
60	A0	1	Total	C	N	O	P	0
			1078	858	22	176	22	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
60	A0	1	Total	C	N	O	P	0
			1078	858	22	176	22	
60	A0	1	Total	C	N	O	P	0
			1078	858	22	176	22	
60	A0	1	Total	C	N	O	P	0
			1078	858	22	176	22	
60	A0	1	Total	C	N	O	P	0
			1078	858	22	176	22	
60	A0	1	Total	C	N	O	P	0
			1078	858	22	176	22	
60	A0	1	Total	C	N	O	P	0
			1078	858	22	176	22	
60	A0	1	Total	C	N	O	P	0
			1078	858	22	176	22	
60	A0	1	Total	C	N	O	P	0
			1078	858	22	176	22	
60	A0	1	Total	C	N	O	P	0
			1078	858	22	176	22	
60	A0	1	Total	C	N	O	P	0
			1078	858	22	176	22	
60	A0	1	Total	C	N	O	P	0
			1078	858	22	176	22	
60	A0	1	Total	C	N	O	P	0
			1078	858	22	176	22	
60	A0	1	Total	C	N	O	P	0
			1078	858	22	176	22	
60	A0	1	Total	C	N	O	P	0
			1078	858	22	176	22	
60	A0	1	Total	C	N	O	P	0
			1078	858	22	176	22	
60	A0	1	Total	C	N	O	P	0
			1078	858	22	176	22	
60	A1	1	Total	C	N	O	P	0
			1225	975	25	200	25	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
60	A1	1	Total	C	N	O	P	0
			1225	975	25	200	25	
60	A1	1	Total	C	N	O	P	0
			1225	975	25	200	25	
60	A1	1	Total	C	N	O	P	0
			1225	975	25	200	25	
60	A1	1	Total	C	N	O	P	0
			1225	975	25	200	25	
60	A1	1	Total	C	N	O	P	0
			1225	975	25	200	25	
60	A1	1	Total	C	N	O	P	0
			1225	975	25	200	25	
60	A1	1	Total	C	N	O	P	0
			1225	975	25	200	25	
60	A1	1	Total	C	N	O	P	0
			1225	975	25	200	25	
60	A1	1	Total	C	N	O	P	0
			1225	975	25	200	25	
60	A1	1	Total	C	N	O	P	0
			1225	975	25	200	25	
60	A1	1	Total	C	N	O	P	0
			1225	975	25	200	25	
60	A1	1	Total	C	N	O	P	0
			1225	975	25	200	25	
60	A1	1	Total	C	N	O	P	0
			1225	975	25	200	25	
60	A1	1	Total	C	N	O	P	0
			1225	975	25	200	25	
60	A1	1	Total	C	N	O	P	0
			1225	975	25	200	25	
60	A1	1	Total	C	N	O	P	0
			1225	975	25	200	25	
60	A1	1	Total	C	N	O	P	0
			1225	975	25	200	25	
60	A1	1	Total	C	N	O	P	0
			1225	975	25	200	25	
60	A1	1	Total	C	N	O	P	0
			1225	975	25	200	25	
60	A1	1	Total	C	N	O	P	0
			1225	975	25	200	25	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
60	A1	1	Total 1225	C 975	N 25	O 200	P 25	0
60	A1	1	Total 1225	C 975	N 25	O 200	P 25	0
60	A1	1	Total 1225	C 975	N 25	O 200	P 25	0
60	B8	1	Total 294	C 234	N 6	O 48	P 6	0
60	B8	1	Total 294	C 234	N 6	O 48	P 6	0
60	B8	1	Total 294	C 234	N 6	O 48	P 6	0
60	B8	1	Total 294	C 234	N 6	O 48	P 6	0
60	B8	1	Total 294	C 234	N 6	O 48	P 6	0
60	B8	1	Total 294	C 234	N 6	O 48	P 6	0
60	BA	1	Total 1568	C 1248	N 32	O 256	P 32	0
60	BA	1	Total 1568	C 1248	N 32	O 256	P 32	0
60	BA	1	Total 1568	C 1248	N 32	O 256	P 32	0
60	BA	1	Total 1568	C 1248	N 32	O 256	P 32	0
60	BA	1	Total 1568	C 1248	N 32	O 256	P 32	0
60	BA	1	Total 1568	C 1248	N 32	O 256	P 32	0
60	BA	1	Total 1568	C 1248	N 32	O 256	P 32	0
60	BA	1	Total 1568	C 1248	N 32	O 256	P 32	0
60	BA	1	Total 1568	C 1248	N 32	O 256	P 32	0
60	BA	1	Total 1568	C 1248	N 32	O 256	P 32	0
60	BA	1	Total 1568	C 1248	N 32	O 256	P 32	0
60	BA	1	Total 1568	C 1248	N 32	O 256	P 32	0

Continued on next page...

Continued from previous page...

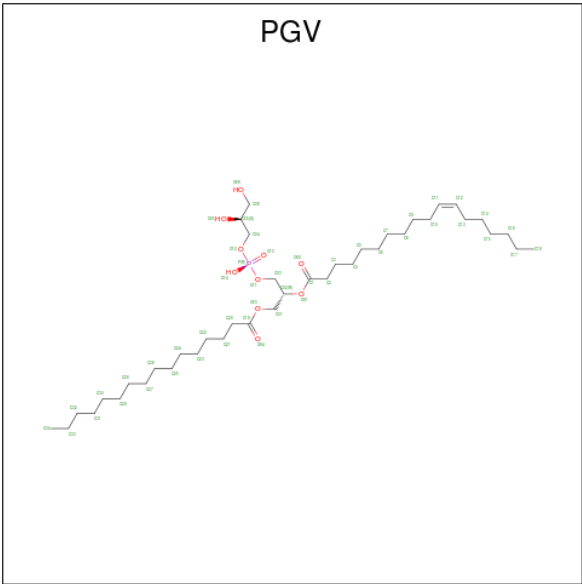
Mol	Chain	Residues	Atoms					AltConf
60	BA	1	Total	C	N	O	P	0
			1568	1248	32	256	32	
60	BA	1	Total	C	N	O	P	0
			1568	1248	32	256	32	
60	BA	1	Total	C	N	O	P	0
			1568	1248	32	256	32	
60	BA	1	Total	C	N	O	P	0
			1568	1248	32	256	32	
60	BA	1	Total	C	N	O	P	0
			1568	1248	32	256	32	
60	BA	1	Total	C	N	O	P	0
			1568	1248	32	256	32	
60	BA	1	Total	C	N	O	P	0
			1568	1248	32	256	32	
60	BA	1	Total	C	N	O	P	0
			1568	1248	32	256	32	
60	BA	1	Total	C	N	O	P	0
			1568	1248	32	256	32	
60	BA	1	Total	C	N	O	P	0
			1568	1248	32	256	32	
60	BA	1	Total	C	N	O	P	0
			1568	1248	32	256	32	
60	BA	1	Total	C	N	O	P	0
			1568	1248	32	256	32	
60	BA	1	Total	C	N	O	P	0
			1568	1248	32	256	32	
60	BA	1	Total	C	N	O	P	0
			1568	1248	32	256	32	
60	BA	1	Total	C	N	O	P	0
			1568	1248	32	256	32	
60	BA	1	Total	C	N	O	P	0
			1568	1248	32	256	32	
60	BB	1	Total	C	N	O	P	0
			539	429	11	88	11	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
60	BB	1	Total	C	N	O	P	0
			539	429	11	88	11	
60	BB	1	Total	C	N	O	P	0
			539	429	11	88	11	
60	BB	1	Total	C	N	O	P	0
			539	429	11	88	11	
60	BB	1	Total	C	N	O	P	0
			539	429	11	88	11	
60	BB	1	Total	C	N	O	P	0
			539	429	11	88	11	
60	BB	1	Total	C	N	O	P	0
			539	429	11	88	11	
60	BB	1	Total	C	N	O	P	0
			539	429	11	88	11	
60	BB	1	Total	C	N	O	P	0
			539	429	11	88	11	

- Molecule 61 is (1R)-2-{{[[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (three-letter code: PGV) (formula: C₄₀H₇₇O₁₀P).



Mol	Chain	Residues	Atoms				AltConf
61	AZ	1	Total	C	O	P	0
			102	80	20	2	
61	AZ	1	Total	C	O	P	0
			102	80	20	2	
61	A0	1	Total	C	O	P	0
			510	400	100	10	
61	A0	1	Total	C	O	P	0
			510	400	100	10	
61	A0	1	Total	C	O	P	0
			510	400	100	10	
61	A0	1	Total	C	O	P	0
			510	400	100	10	
61	A0	1	Total	C	O	P	0
			510	400	100	10	
61	A0	1	Total	C	O	P	0
			510	400	100	10	
61	A0	1	Total	C	O	P	0
			510	400	100	10	
61	A0	1	Total	C	O	P	0
			510	400	100	10	
61	A0	1	Total	C	O	P	0
			510	400	100	10	
61	A1	1	Total	C	O	P	0
			204	160	40	4	
61	A1	1	Total	C	O	P	0
			204	160	40	4	
61	A1	1	Total	C	O	P	0
			204	160	40	4	
61	A1	1	Total	C	O	P	0
			204	160	40	4	
61	B8	1	Total	C	O	P	0
			51	40	10	1	
61	BA	1	Total	C	O	P	0
			408	320	80	8	
61	BA	1	Total	C	O	P	0
			408	320	80	8	
61	BA	1	Total	C	O	P	0
			408	320	80	8	
61	BA	1	Total	C	O	P	0
			408	320	80	8	
61	BA	1	Total	C	O	P	0
			408	320	80	8	

Continued on next page...

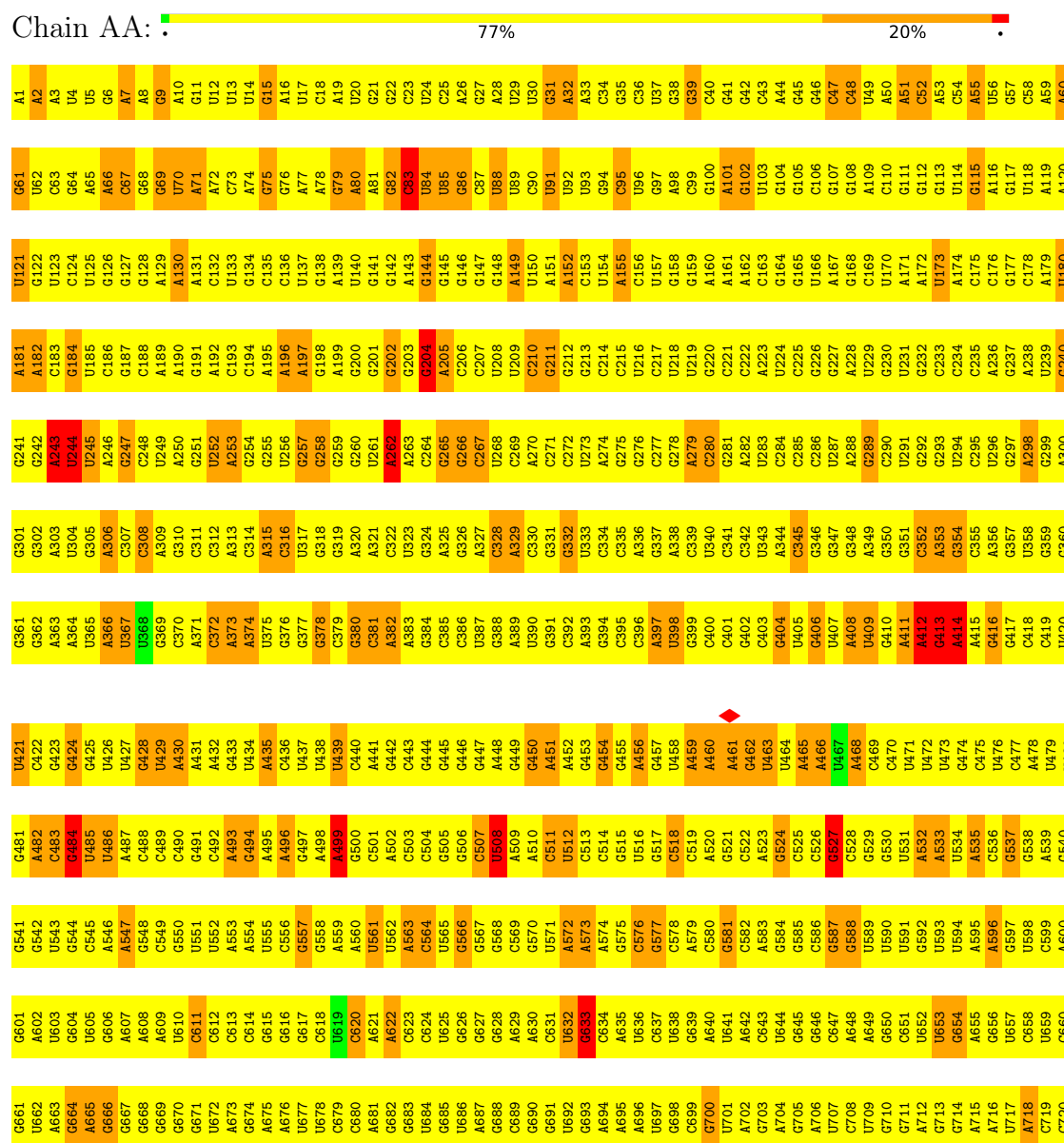
Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
61	BA	1	Total	C	O	P	0
			408	320	80	8	
61	BA	1	Total	C	O	P	0
			408	320	80	8	
61	BA	1	Total	C	O	P	0
			408	320	80	8	
61	BB	1	Total	C	O	P	0
			357	280	70	7	
61	BB	1	Total	C	O	P	0
			357	280	70	7	
61	BB	1	Total	C	O	P	0
			357	280	70	7	
61	BB	1	Total	C	O	P	0
			357	280	70	7	
61	BB	1	Total	C	O	P	0
			357	280	70	7	
61	BB	1	Total	C	O	P	0
			357	280	70	7	

3 Residue-property plots

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

• Molecule 1: 16S RIBOSOMAL RNA

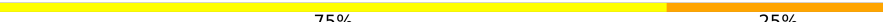


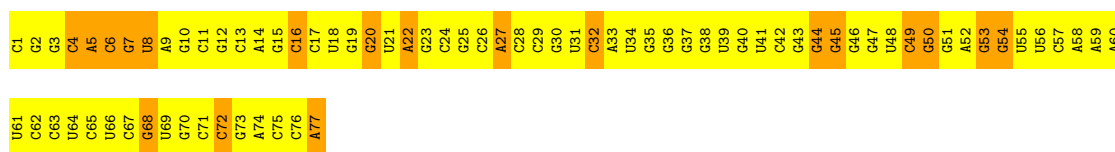
A1502	G1442	C1382	C1322	C1262	U1202	G1142	A1082	A1022	C962	G902	C841	A781	G721
A1503	C1443	C1383	C1323	C1263	C1203	G1143	U1083	U1023	G963	G903	U842	A782	G722
G1504	U1444	A1384	A1324	U1264	A1204	G1144	G1084	G1024	A964	U904	U843	A783	U723
G1505	U1445	G1385	C1325	C1265	U1205	G1145	U1085	U1025	U965	U905	G844	A784	G724
U1506	C1446	G1386	U1326	G1266	G1206	A1146	U1086	G1026	G966	A906	A845	G785	G725
A1507	A1447	G1387	C1327	C1267	G1207	G1147	G1087	G1027	C967	A907	G846	G786	G726
A1508	C1448	C1388	C1328	G1268	C1208	U1148	G1088	C1028	A968	A908	G847	A787	G727
C1509	U1449	C1389	A1329	G1269	C1209	C1149	G1089	U1029	A969	A909	C848	U788	A728
C1510	U1450	U1390	U1330	G1270	C1210	A1150	U1090	U1030	C970	C910	C849	U789	A729
G1511	U1451	U1391	G1331	A1271	U1211	A1151	U1091	C1031	G971	U911	U850	A790	G730
U1512	C1452	A1392	A1332	G1272	U1212	A1152	A1092	G1032	C972	C912	G851	G791	G731
A1513	G1453	U1393	C1333	C1273	A1213	G1153	G1093	G1033	A973	A913	G852	A792	G732
G1514	A1454	A1394	G1334	A1274	C1214	G1154	A1094	G1034	A974	A914	C853	U793	G733
G1515	G1455	C1395	U1385	A1275	G1215	A1155	U1095	A1035	A975	A915	U854	A794	G734
G1516	A1456	A1396	C1386	G1276	A1216	G1156	C1096	A1036	G976	U916	U855	C795	C735
G1517	A1457	G1397	G1337	C1277	C1217	A1157	C1097	C1037	A977	G917	C856	C796	C736
A1518	G1458	A1398	G1338	G1278	C1218	U1158	C1098	C1038	A978	A918	C857	C797	C737
A1519	G1459	C1399	A1339	G1279	A1219	U1159	G1099	G1039	C979	A919	G858	U798	C738
C1520	C1460	C1400	A1340	C1280	G1220	G1160	C1100	U1040	U980	U920	G859	C799	C739
C1521	G1461	G1401	U1341	C1281	G1221	C1161	A1101	G1041	U981	U921	A860	U800	U740
U1522	C1462	C1402	C1342	C1282	G1222	C1162	A1102	A1042	U982	G922	G861	U801	G741
G1523	U1463	G1403	G1343	C1283	C1223	A1163	C1103	G1043	A983	A923	C862	A802	G742
C1524	C1464	C1404	C1344	C1284	U1224	G1164	G1104	A1044	C984	C924	U863	G803	A743
G1525	A1465	G1405	U1345	A1285	C1225	U1165	A1105	C1045	C985	G925	A864	U804	C744
G1526	C1466	U1406	A1346	U1286	C1226	G1166	G1106	A1046	U986	G926	A865	C805	G745
U1527	C1467	C1407	G1347	A1287	A1227	A1167	C1107	G1047	G987	C927	C866	C806	A746
U1528	A1468	A1408	U1348	A1288	C1228	U1168	G1108	G1048	G988	G928	G867	A807	A747
G1529	C1469	A1409	A1349	A1289	C1229	U1169	C1109	U1049	U989	G929	C868	C808	G748
G1530	U1470	A1410	A1350	C1290	C1230	A1170	A1110	G1050	C990	C930	G869	C809	A749
A1531	U1471	C1411	U1351	U1291	G1231	A1171	A1111	C1051	U991	C931	C810	C750	C750
U1532	U1472	C1412	C1352	G1292	U1232	C1172	C1112	U1052	U992	C932	C811	U751	G751
C1533	G1473	A1413	G1353	C1293	G1233	U1173	C1113	G1053	G993	C933	A872	G752	G752
U1534	U1474	U1414	U1354	G1294	C1234	G1174	C1114	C1054	A994	C934	G873	A753	A753
C1535	G1475	G1415	G1355	U1295	U1235	G1175	U1115	U1055	A995	A935	U874	A814	G754
C1536	A1476	G1416	G1356	C1296	A1236	A1176	U1116	U1056	C996	C936	C875	A815	G755
U1537	G1477	G1417	A1357	G1297	C1237	G1177	A1117	G1057	U997	A937	G876	A816	C756
G1538	U1478	A1418	U1358	U1298	A1238	G1178	U1118	G1058	C998	A938	A877	C817	U757
C1539	C1479	G1419	C1359	A1299	A1239	A1179	C1119	C1059	C999	C939	C878	A818	C758
U1540	A1480	U1420	A1360	G1300	U1240	A1180	C1120	U1060	A1000	C940	C880	A819	A759
U1541	U1481	G1421	G1361	U1301	G1241	G1181	U1121	U1061	C1001	G941	G881	U820	G760
A1542	G1482	G1422	A1362	C1302	G1242	G1182	U1122	U1062	G1002	G942	C882	G821	G761
	A1483	G1423	A1363	C1303	C1243	U1183	U1123	C1063	G1003	U943	C883	U822	U762
	C1484	U1424	U1364	G1304	G1244	G1184	U1124	G1064	A1004	G944	U884	G823	G763
	U1485	U1425	G1365	G1305	C1245	G1185	U1125	U1065	A1005	G945	G885	G824	C764
	G1486	G1426	C1366	A1306	A1246	G1186	U1126	C1066	G1006	A946	G886	A825	G765
	G1487	C1427	C1367	U1307	U1247	G1187	G1127	U1067	U1007	G947	G887	C826	A766
	G1488	A1428	A1368	U1308	A1248	C1188	C1128	G1068	U1008	C948	G888	U827	A767
	G1489	A1429	C1369	G1309	C1249	U1189	C1129	C1069	U1009	A949	A889	U828	A768
	U1490	A1430	G1370	G1310	A1250	G1190	A1130	U1070	U1010	U950	G890	G829	C770
	G1491	A1431	G1371	A1311	A1251	A1191	G1131	C1071	C1011	G951	U891	G830	C771
	A1492	G1432	U1372	G1312	A1252	C1192	C1132	G1072	A1012	U952	A892	A831	G771
	A1493	A1433	G1373	U1313	G1253	G1193	G1133	U1073	G1013	G953	C893	G832	U772
	G1494	A1434	A1374	C1314	A1254	U1194	G1134	G1074	A1014	G954	G894	U833	G773
	U1495	G1435	A1375	U1315	G1255	U1195	U1135	U1075	G1015	U955	G895	U834	G774
	G1496	A1436	U1376	G1316	A1256	A1196	U1136	U1076	A1016	U956	C896	U835	G775
	G1497	A1437	C1377	C1317	A1257	A1197	G1137	G1077	U1017	U957	C897	G836	G776
	U1498	G1438	C1378	A1318	G1258	G1198	G1138	U1078	G1018	A958	G898	U837	A777
	A1499	G1439	G1379	A1319	C1259	U1199	G1139	G1079	A1019	A959	C899	G838	G778
	U1500	U1440	C1380	C1320	G1260	C1200	G1140	U1080	A1020	U960	A900	C839	G779
	C1501	A1441	U1381	U1321	A1261	A1201	C1141	A1081	A1021	U961	A901	C840	A780

● Molecule 2: mRNA




● Molecule 3: FtsQ nascent chain

Chain AV:  75% 25%



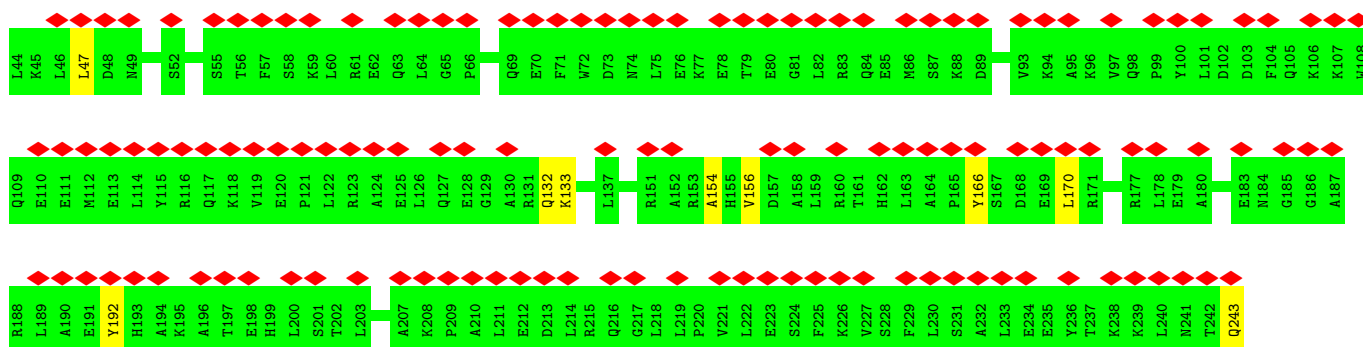
- Molecule 4: Cell division protein FtsQ

Chain AZ:  45% 76% 23%




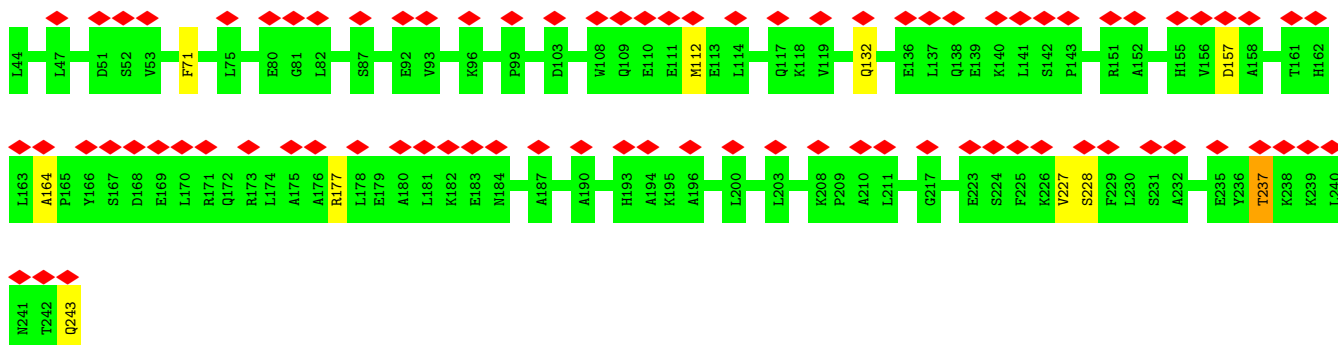
- Molecule 5: Apolipoprotein A-I

Chain A0:  65% 96%

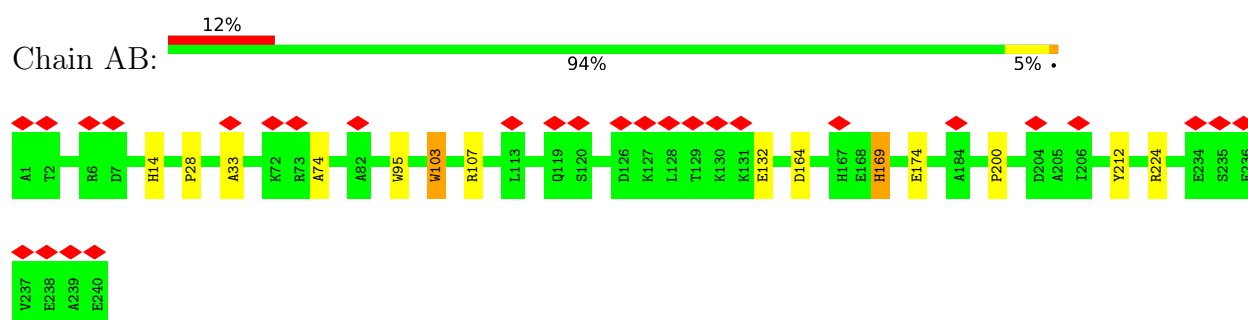


- Molecule 5: Apolipoprotein A-I

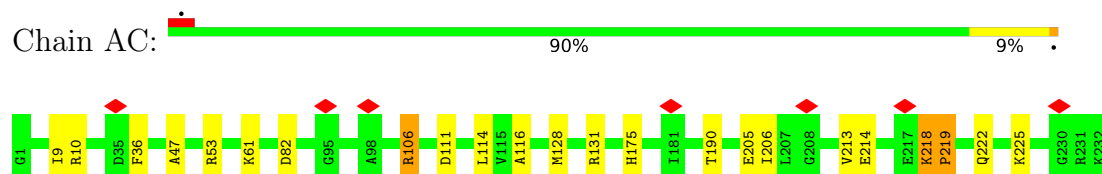
Chain A1:  41% 95%



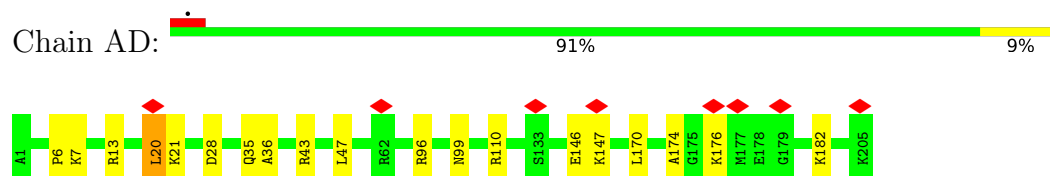
- Molecule 6: 30S ribosomal protein S2



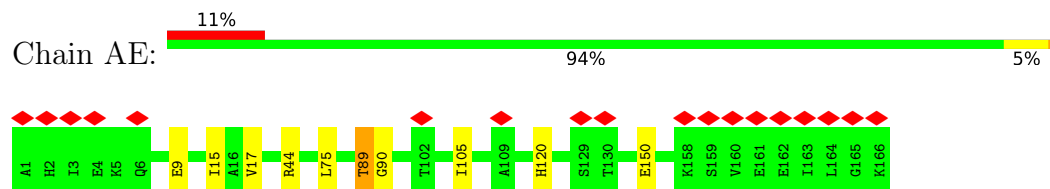
- Molecule 7: 30S ribosomal protein S3



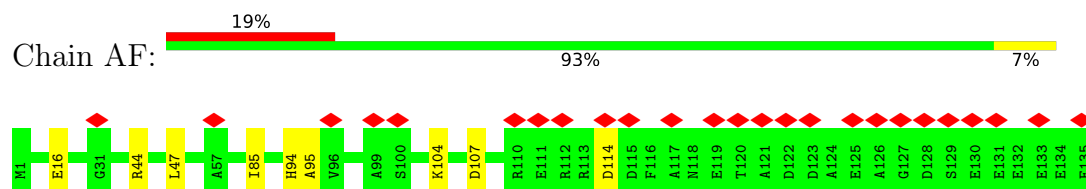
- Molecule 8: 30S ribosomal protein S4



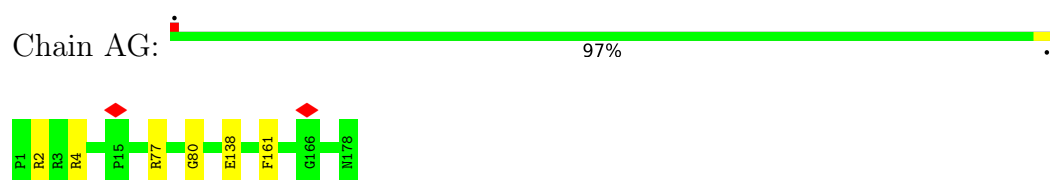
- Molecule 9: 30S ribosomal protein S5



- Molecule 10: 30S ribosomal protein S6

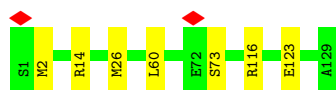


- Molecule 11: 30S ribosomal protein S7

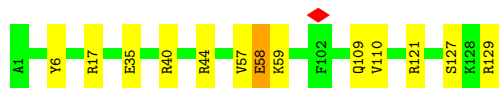


- Molecule 12: 30S ribosomal protein S8





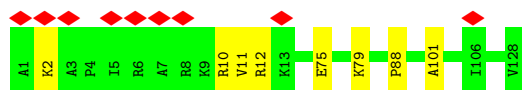
- Molecule 13: 30S ribosomal protein S9



- Molecule 14: 30S ribosomal protein S10



- Molecule 15: 30S ribosomal protein S11



- Molecule 16: 30S ribosomal protein S12



- Molecule 17: 30S ribosomal protein S13



- Molecule 18: 30S ribosomal protein S14



- Molecule 19: 30S ribosomal protein S15

Chain AO:  97% ..



- Molecule 20: 30S ribosomal protein S16

Chain AP:  95% ..



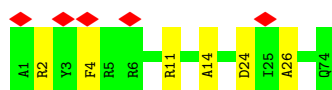
- Molecule 21: 30S ribosomal protein S17

Chain AQ:  87% 13%



- Molecule 22: 30S ribosomal protein S18

Chain AR:  7% 92% 8%



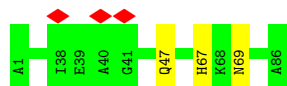
- Molecule 23: 30S ribosomal protein S19

Chain AS:  96% .



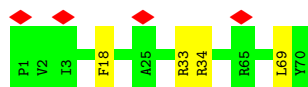
- Molecule 24: 30S ribosomal protein S20

Chain AT:  97% .



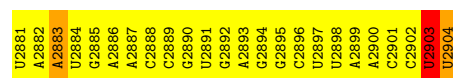
- Molecule 25: 30S ribosomal protein S21

Chain AU:  6% 94% 6%



A1801	G1741	G1681	U1821	C1561	G1501	G1441	G1381	A1321	G1261	U1201	U1141	U1081	A1021	C961	C841
A1802	U1742	G1682	G1622	U1562	A1502	U1442	G1382	A1322	A1262	G1202	A1142	U1082	G1022	G962	U842
A1803	G1743	U1683	G1623	U1563	A1503	U1443	A1383	C1323	U1263	U1203	A1143	U1083	U1023	G963	G843
C1804	U1744	G1684	G1624	U1564	A1504	U1444	A1384	A1264	A1204	A1204	A1144	A1084	G1024	G964	A844
A1805	A1745	C1685	G1625	C1565	A1505	U1445	A1385	U1325	A1265	A1205	C1145	A1085	G1025	C965	A845
C1806	A1746	U1686	A1626	U1566	U1506	U1446	C1386	U1326	G1266	C1206	C1146	A1086	G1026	G966	U846
G1807	U1747	G1687	G1627	G1567	C1507	C1447	A1387	A1327	U1267	C1207	A1147	G1087	A1027	G967	U847
A1808	U1748	U1688	G1628	G1568	A1508	U1448	A1388	A1328	A1268	C1208	U1148	A1088	A1028	C968	C848
A1809	A1749	U1689	U1629	U1569	A1509	U1449	A1389	U1329	A1269	U1209	U1149	A1089	A1029	C969	A849
A1810	A1750	A1690	A1630	A1570	G1510	C1450	U1390	C1330	G1270	C1210	A1150	G1090	C1030	G970	U850
A1811	U1751	C1691	G1631	A1571	G1511	C1451	U1391	G1331	G1271	C1211	A1151	G1091	G1031	G971	A851
U1812	C1752	U1692	A1632	A1572	C1512	G1452	A1392	G1332	A1272	G1212	C1152	C1092	A972	C912	U852
G1813	G1633	G1573	G1633	G1573	U1513	A1453	A1393	G1333	U1273	A1213	C1153	C1093	U1033	G913	C853
G1814	A1754	C1694	A1634	C1574	G1514	C1454	U1394	G1334	A1274	A1214	G1154	U1094	G1034	G914	C854
A1815	A1755	G1695	U1635	C1575	A1515	G1455	A1395	C1335	A1275	G1215	A1155	A1095	U1035	C915	G855
C1816	G1756	G1696	U1636	U1576	G1516	G1456	A1396	A1336	A1276	G1216	A1156	A1096	U1036	C916	G856
G1817	A1757	A1697	G1637	C1577	G1517	U1457	U1397	G1337	G1277	U1217	G1157	U1097	G1037	G917	G857
U1818	U1758	C1698	C1638	U1578	C1518	U1458	C1398	G1338	G1278	G1218	C1158	A1098	G1038	G918	G858
A1819	A1759	G1699	C1639	A1579	G1519	U1459	C1399	G1339	G1279	U1219	U1159	A1099	A1039	A919	G859
U1820	C1760	A1700	A1640	A1580	U1520	U1460	U1400	U1340	G1280	G1220	C1160	C1100	A1040	A920	U860
A1821	A1761	A1641	A1641	G1581	G1521	U1461	G1401	G1341	G1281	C1221	C1161	U1101	G1041	C921	A861
C1822	A1762	G1702	G1642	C1582	A1522	C1462	U1402	A1342	U1282	U1222	G1162	C1102	G1042	C922	G862
G1823	G1763	G1703	G1643	A1583	C1523	C1463	A1403	G1343	G1283	G1223	G1163	A1103	C1043	G923	A863
A1824	C1764	U1584	G1644	U1584	G1524	G1464	C1404	U1344	A1284	U1224	C1164	U1104	C1044	G924	G864
U1825	U1765	G1585	G1645	A1585	A1525	G1465	U1405	C1345	A1285	G1225	A1165	U1105	C1045	A925	G865
G1826	G1766	A1586	C1646	A1586	C1526	U1466	U1406	G1346	A1286	A1226	G1166	G1106	A1046	G926	A866
U1827	G1767	U1587	U1647	G1587	G1527	U1467	G1407	A1347	A1287	G1227	C1167	G1107	G1047	G927	C867
G1828	C1768	G1708	U1648	G1588	A1528	U1468	G1408	C1348	G1288	U1228	U1168	U1108	A1048	A928	U868
A1829	U1769	U1589	G1649	A1589	G1529	A1469	U1409	C1349	C1289	C1229	A1169	C1109	C1049	G929	G869
C1830	G1770	A1590	A1650	A1590	G1530	A1470	G1410	C1350	C1290	A1230	C1170	G1110	A1050	A930	U870
G1831	C1771	A1591	G1651	A1591	C1531	G1471	U1411	C1351	C1291	U1231	G1171	A1111	C1051	C931	U871
C1832	A1772	C1592	A1652	C1592	A1532	G1472	U1412	U1352	G1292	G1232	C1172	G1112	C1052	C932	U872
G1833	C1773	G1593	C1653	C1593	C1533	G1473	U1413	A1353	C1293	C1233	C1173	G1113	C1053	G933	C873
U1834	U1774	U1594	U1654	U1594	U1534	U1474	A1414	A1354	U1294	U1234	U1174	C1114	A1054	C934	G874
A1835	C1775	A1595	G1655	A1595	A1535	G1475	U1415	G1355	C1295	G1235	U1175	G1115	C1055	C935	G875
C1836	G1776	C1596	C1656	A1596	C1536	U1476	G1416	C1356	G1296	G1236	U1176	G1116	G1056	A936	C876
U1837	U1777	U1597	U1657	A1597	G1537	U1477	C1417	C1357	C1297	A1237	G1177	C1117	A1057	C937	A877
C1838	U1778	C1598	G1658	A1598	G1538	U1478	G1418	G1358	C1298	G1238	C1178	C1118	U1058	G938	A878
G1839	U1779	U1599	G1659	U1599	U1539	U1479	A1419	A1359	G1299	G1239	U1179	U1119	G1059	G939	G879
U1840	A1780	G1600	G1660	C1600	G1540	C1480	A1420	G1360	G1300	U1240	U1180	G1120	U1060	G940	G880
U1841	U1781	G1601	G1661	G1601	C1541	U1481	G1421	G1361	A1301	A1241	U1181	C1121	U1061	A1001	G881
G1842	U1782	U1602	U1662	U1602	U1542	U1482	G1422	C1362	A1302	A1242	G1182	G1122	G1062	A941	G882
C1843	G1723	G1603	G1663	A1603	C1543	G1483	G1423	C1363	G1303	C1243	U1183	G1123	G1063	A942	G883
A1844	A1784	C1604	U1664	C1604	A1544	U1484	G1424	G1364	A1304	A1244	U1184	G1124	C1064	C944	U884
G1845	A1785	C1605	A1665	C1605	A1545	U1485	G1425	A1365	C1305	G1245	G1185	G1125	U1065	A945	C885
A1846	A1786	C1606	G1666	C1606	G1546	U1486	A1426	A1366	C1306	A1246	G1186	A1126	U1066	C946	A886
A1847	A1787	G1607	G1667	C1607	C1547	U1487	A1427	A1367	A1307	A1247	G1187	A1127	A1067	C1007	U887
A1848	C1788	A1608	U1668	A1608	A1548	C1488	G1428	G1368	A1308	U1248	U1188	G1128	G1068	C948	C888
G1849	A1789	A1609	A1669	A1609	A1549	C1489	G1429	G1369	G1309	U1249	A1189	A1129	A1069	G949	C889
U1850	C1790	A1610	C1670	A1610	C1550	U1490	G1430	C1370	G1310	G1250	U1190	U1130	A1070	G950	C890
U1851	G1731	C1611	U1671	C1611	A1551	U1491	G1431	G1371	G1311	C1251	G1191	G1131	G1071	C951	G891
U1852	C1732	A1612	A1672	C1612	A1552	G1492	A1432	U1372	U1312	G1252	G1192	U1132	G1072	G952	A892
A1853	G1733	G1613	G1673	A1613	U1553	C1493	A1433	A1373	U1313	A1253	G1193	A1133	A1073	G953	C893
A1854	A1794	A1614	G1674	A1614	U1554	U1494	A1434	G1374	C1314	A1254	A1194	A1134	G1074	G954	U894
U1855	C1795	G1615	C1675	G1615	G1555	A1495	A1435	U1375	C1315	U1255	G1195	G1135	U1015	U955	U895
U1856	U1796	A1616	A1676	A1616	C1556	U1496	G1436	C1376	U1316	G1256	C1196	G1136	C1076	G956	A896
G1857	G1797	C1617	A1677	C1617	C1557	U1497	G1437	G1377	G1317	C1257	G1197	G1137	A1077	C957	C897
A1858	U1798	A1618	U1678	A1618	C1558	C1498	U1438	U1378	U1318	U1258	U1198	G1138	U1078	U958	C898
U1859	G1799	A1619	A1679	A1619	U1559	C1499	A1439	U1379	C1319	G1259	U1199	G1139	C1079	A959	A899
G1860	C1800	G1740	U1680	G1620	G1560	G1500	U1440	G1380	C1320	A1260	C1200	C1140	A1080	A960	A900

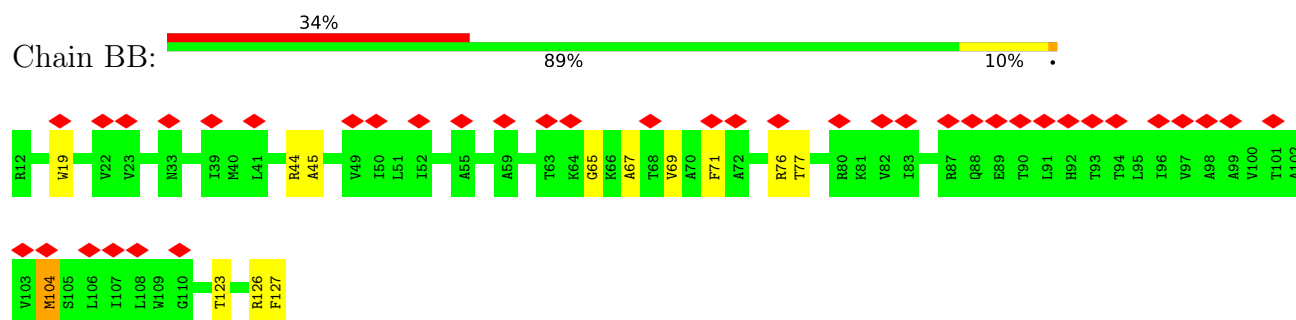
A2821	G2822	A2761	U2701	G2641	A2461	U2401	G2341	A2281	G2221	G2161	A2101	U2041	A1981	G1861
G2823	A2823	C2762	G2702	G2642	C2461	U2402	C2342	G2282	C2222	G2162	G2102	A2042	U1962	G1862
C2824	G2824	G2763	G2703	G2643	C2463	G2403	U2343	G2283	G2223	A2163	C2103	C2043	U1963	U1863
G2825	U2684	A2764	C2704	G2644	G2464	U2404	U2344	A2284	G2224	C2164	C2104	C2044	G1964	U1864
A2826	G2645	A2765	G2705	G2645	C2465	G2405	U2345	G2285	G2225	C2165	U2105	C2045	C1965	U1865
C2827	U2686	A2766	A2706	G2646	G2466	A2406	G2346	G2286	C2226	U2166	U2106	C2046	C1966	U1866
G2828	U2687	C2767	U2707	U2647	C2467	A2407	G2347	A2287	A2227	U2167	G2107	C2047	A1967	G1867
A2829	G2688	U2768	G2708	G2648	A2468	U2408	U2348	A2288	G2228	G2168	A2108	G2048	C1968	C1868
C2830	A2689	G2770	G2710	U2650	A2469	G2409	U2349	G2289	U2229	A2169	U2109	G2049	G1969	G1869
G2831	U2651	C2771	A2711	G2650	G2470	G2410	C2350	G2290	G2230	A2170	G2110	C2050	U1990	C1870
U2832	C2652	C2772	G2712	G2652	A2471	A2412	G2352	U2292	U2232	U2172	G2112	A2052	U1991	A1871
C2833	U2653	C2773	U2713	U2653	G2472	G2413	G2353	G2293	U2233	C2173	U2113	G2053	U1993	A1872
G2834	A2654	C2774	G2714	A2654	U2474	G2414	C2354	G2294	G2234	C2174	A2114	A2054	C1994	C1874
A2835	U2655	G2775	C2715	G2655	C2475	G2415	G2355	U2295	U2235	C2175	G2115	C2055	U1995	G1875
U2836	G2656	G2776	U2716	U2656	A2476	G2416	U2356	G2296	U2236	A2176	G2116	G2056	U1997	A1876
A2837	U2657	C2777	C2717	A2657	U2477	G2417	G2357	A2297	G2237	C2177	A2117	G2057	C1997	A1877
G2838	G2658	U2778	G2718	G2658	A2478	A2418	A2358	U2298	G2238	C2178	U2118	A2058	A1998	G1878
C2839	U2659	G2779	G2719	G2659	U2479	U2419	C2359	U2299	G2239	C2179	A2119	A2059	C1999	C1879
C2840	A2660	U2720	A2600	A2660	C2480	C2420	G2360	C2300	U2240	U2180	G2120	A2060	C2000	U1880
G2841	G2661	A2721	C2601	G2661	G2481	G2421	G2361	C2301	G2241	U2181	G2121	G2061	C2001	C1881
C2842	U2662	G2722	A2602	A2662	A2482	C2422	C2362	U2302	G2242	U2182	U2122	A2062	G2002	U1882
G2843	G2663	C2723	G2603	G2663	C2483	U2423	G2363	G2303	G2243	A2183	G2123	C2063	A2003	U1883
C2844	U2664	U2724	G2604	G2664	G2484	C2424	C2364	G2304	U2244	A2184	G2124	C2064	G2004	G1884
U2845	A2665	G2725	U2605	A2665	G2485	A2425	G2365	U2305	U2245	U2185	G2125	C2065	A2005	A1885
G2846	C2666	C2726	C2606	C2666	C2486	A2426	A2366	C2306	G2246	G2186	A2126	C2066	C2006	U1886
U2847	U2667	A2727	G2607	C2667	G2487	G2427	G2367	G2307	A2247	U2187	G2127	G2067	U2007	C1887
G2848	G2668	U2728	G2608	G2668	A2488	G2428	C2368	G2308	C2248	U2188	G2128	C2068	C2008	G1888
U2849	G2669	G2729	G2609	G2669	U2489	A2429	A2369	A2309	G2249	U2189	C2129	C2069	A2009	G1889
A2850	C2670	C2730	G2610	A2670	G2490	G2430	G2370	C2310	U2250	G2190	U2130	A2070	G2010	A1890
G2851	U2671	G2731	C2611	G2671	U2491	U2431	G2371	C2311	G2251	A2191	U2131	A2071	U2011	G1891
C2852	U2672	G2732	G2612	U2672	U2492	A2432	U2372	U2312	G2252	U2192	U2132	C2072	G2012	C1892
U2853	G2673	A2733	C2613	G2673	A2493	A2433	G2373	G2313	C2253	G2193	G2133	C2073	A2013	C1893
G2854	U2674	G2734	A2614	G2674	G2494	A2434	C2374	A2314	C2254	U2194	A2134	U2074	A2014	C1894
C2855	A2675	G2735	U2615	A2675	G2495	A2435	G2375	G2315	G2255	U2195	A2135	U2075	A2015	C1895
U2856	C2676	C2736	C2616	C2676	C2496	G2436	A2376	G2316	G2256	C2196	G2136	U2076	A2016	G1896
G2857	U2677	G2737	U2617	G2677	A2497	G2437	A2377	A2317	U2257	U2197	U2137	A2077	U2017	G1897
C2858	C2678	A2738	C2618	C2678	C2498	U2438	A2378	G2318	C2258	A2198	G2138	C2078	G2018	U1898
G2859	A2679	U2739	C2619	A2679	C2499	A2439	G2379	G2319	U2259	A2199	U2139	U2079	A2019	A1899
U2860	U2680	A2740	C2620	U2680	U2500	G2440	C2380	C2320	C2260	C2200	G2140	A2080	A2020	A1900
G2861	G2681	A2741	U2621	C2681	C2501	U2441	A2381	U2321	C2261	G2201	G2141	U2081	C2021	A1901
C2862	U2682	G2742	U2622	A2682	G2502	C2442	G2382	A2322	U2262	U2202	A2142	A2082	U2022	C1902
G2863	C2683	U2743	G2623	C2683	U2503	G2443	G2383	G2323	C2263	U2203	C2143	G2083	C2023	G1903
U2864	U2684	G2744	G2624	U2684	U2504	C2444	U2384	U2324	C2264	G2204	G2144	C2084	G2024	G1904
C2865	G2685	C2745	G2625	G2685	G2505	G2445	C2385	G2325	U2265	A2205	C2145	U2085	C2025	C1905
U2866	U2686	U2746	C2626	G2686	U2506	G2446	A2386	C2326	A2266	C2206	C2146	U2086	U2026	G1906
A2867	G2687	G2747	G2627	U2687	C2507	G2447	U2387	A2327	A2267	C2207	A2147	G2087	G2027	G1907
G2868	C2688	A2748	C2628	G2688	G2508	A2448	A2388	A2328	A2268	G2208	U2148	A2088	U2028	C1908
C2869	U2689	U2749	U2629	U2689	G2509	U2449	G2389	U2329	G2269	G2209	U2149	C2089	G2029	A1909
U2870	G2690	A2750	G2630	U2690	C2510	A2450	U2390	G2330	A2270	U2210	C2150	A2090	A2030	G1910
G2871	C2691	G2751	U2631	C2691	U2511	A2451	G2391	C2331	G2271	A2211	U2151	C2091	A2031	U1911
A2872	U2692	A2752	A2632	G2692	C2512	G2452	A2392	C2332	U2272	A2212	G2152	U2092	G2032	A1912
C2873	G2693	C2753	G2633	U2693	A2513	A2453	A2393	A2333	A2273	U2213	C2153	G2093	A2033	A1913
A2874	U2694	U2754	A2634	G2694	U2514	G2454	C2394	U2334	A2274	C2214	A2154	A2094	U2034	C1914
G2875	U2695	C2755	G2635	G2695	A2515	G2455	C2395	A2335	G2275	G2215	U2155	A2095	G2035	U1915
C2876	U2696	U2756	C2636	U2696	A2516	G2456	G2396	A2336	G2276	G2216	U2156	C2096	G2036	A1916
G2877	U2697	A2757	U2637	G2697	C2517	U2457	G2397	G2337	G2277	G2217	G2157	A2097	A2037	U1917
U2878	U2698	A2758	A2638	U2698	U2518	G2458	U2398	C2338	A2278	U2218	A2158	U2098	G2038	A1918
C2879	G2699	U2759	G2639	G2699	U2519	A2459	G2399	C2339	G2279	U2219	G2159	U2099	U2039	A1919
A2880	C2760	A2820	C2760	A2700	C2520	U2460	G2400	A2340	G2280	U2220	C2160	G2100	G2040	C1920



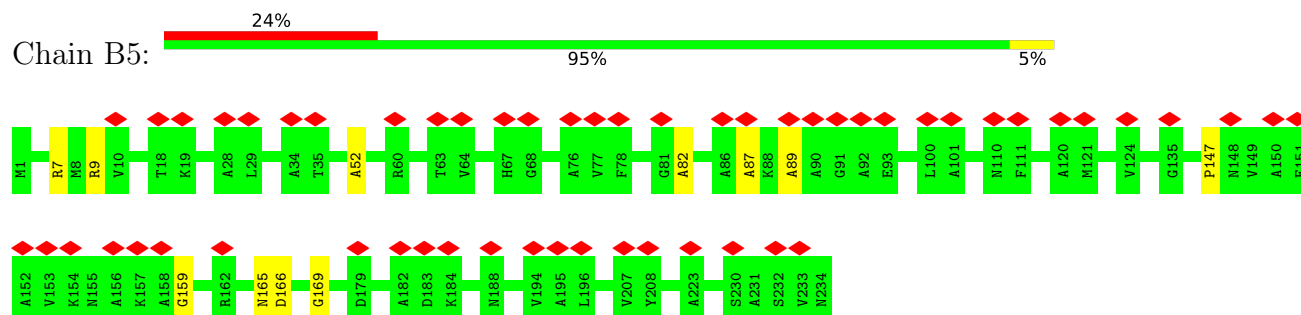
• Molecule 28: Preprotein translocase secY subunit



• Molecule 29: Preprotein translocase secE subunit

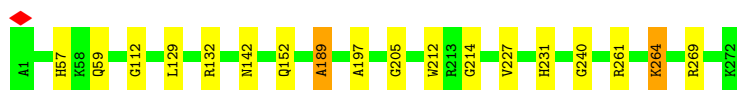


• Molecule 30: 50S ribosomal protein L1



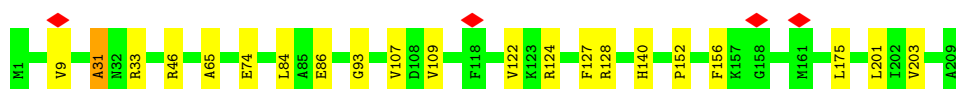
- Molecule 31: 50S ribosomal protein L2

Chain B6:  93% 6% .



- Molecule 32: 50S ribosomal protein L3

Chain BD:  90% 10% .



- Molecule 33: 50S ribosomal protein L4

Chain BE:  94% 6% .



- Molecule 34: 50S ribosomal protein L5

Chain BF:  90% 9% .




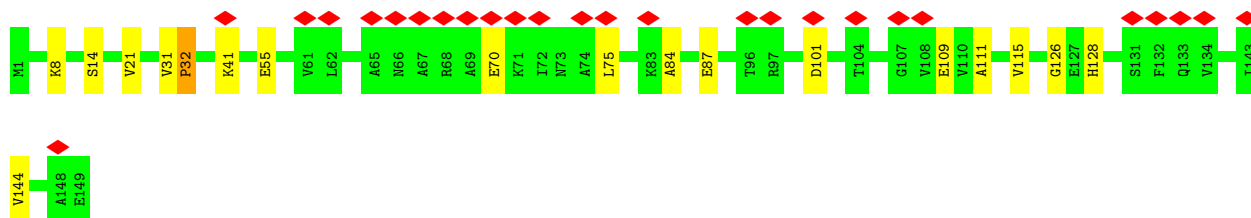
- Molecule 35: 50S ribosomal protein L6

Chain BG:  93% 7% .



- Molecule 36: 50S ribosomal protein L9

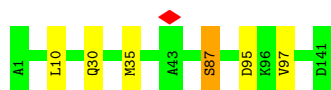
Chain BH:  17% 88% 11% .



- Molecule 37: 50S ribosomal protein L11



Chain BI:  96% . .



- Molecule 38: 50S ribosomal protein L13

Chain BJ:  95% 5%



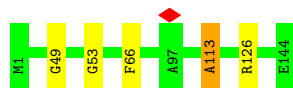
- Molecule 39: 50S ribosomal protein L14

Chain BK:  91% 9%



- Molecule 40: 50S ribosomal protein L15

Chain BL:  97% . .




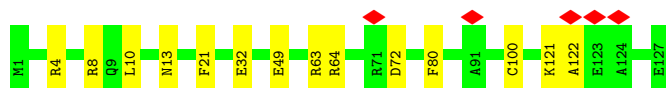
- Molecule 41: 50S ribosomal protein L16

Chain BM:  92% 7% .



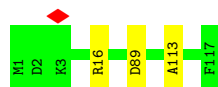
- Molecule 42: 50S ribosomal protein L17

Chain BN:  89% 11%



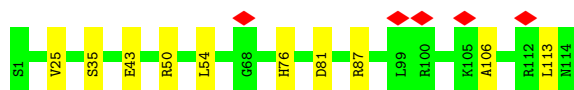
- Molecule 43: 50S ribosomal protein L18

Chain BO:  97% .



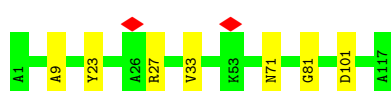
- Molecule 44: 50S ribosomal protein L19

Chain BP:  91% 9%



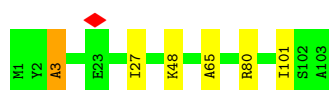
- Molecule 45: 50S ribosomal protein L20

Chain BQ:  94% 6%



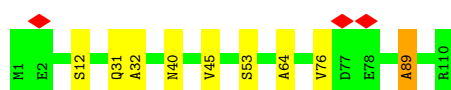
- Molecule 46: 50S ribosomal protein L21

Chain BR:  94% 5%




- Molecule 47: 50S ribosomal protein L22

Chain BS:  92% 7%



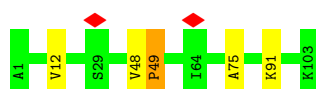
- Molecule 48: 50S ribosomal protein L23

Chain BT:  89% 9%



- Molecule 49: 50S ribosomal protein L24

Chain BU:  95%



- Molecule 50: 50S ribosomal protein L25

Chain BV:  98%



- Molecule 51: 50S ribosomal protein L27

Chain BW: 94% 6%



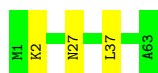
- Molecule 52: 50S ribosomal protein L28

Chain BX: 91% 9%



- Molecule 53: 50S ribosomal protein L29

Chain BY: 95% 5%



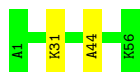
- Molecule 54: 50S ribosomal protein L30

Chain BZ: 93% 7%



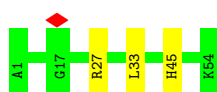
- Molecule 55: 50S ribosomal protein L32

Chain B0: 96% 4%



- Molecule 56: 50S ribosomal protein L33

Chain B1: 94% 6%



- Molecule 57: 50S ribosomal protein L34

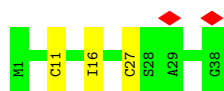
Chain B2: 87% 11% 2%



- Molecule 58: 50S ribosomal protein L35



- Molecule 59: 50S ribosomal protein L36



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	85664	Depositor
Resolution determination method	Not provided	
CTF correction method	DEFOCUS GROUP VOLUMES	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	22	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	4500	Depositor
Magnification	38000	Depositor
Image detector	KODAK SO-163 FILM	Depositor
Maximum map value	6.823	Depositor
Minimum map value	-3.534	Depositor
Average map value	0.051	Depositor
Map value standard deviation	0.456	Depositor
Recommended contour level	0.5	Depositor
Map size (\AA)	396, 396, 396	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90, 90, 90	wwPDB
Pixel spacing (\AA)	1.2375, 1.2375, 1.2375	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: PEV, PGV

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	AA	1.60	46/37039 (0.1%)	2.50	4339/57778 (7.5%)
2	AX	1.56	0/256	2.32	28/394 (7.1%)
3	AV	1.61	1/1842 (0.1%)	2.43	211/2870 (7.4%)
4	AZ	0.98	0/795	1.16	0/1082
5	A0	0.96	1/1667 (0.1%)	0.95	3/2240 (0.1%)
5	A1	0.97	1/1667 (0.1%)	0.95	0/2240
6	AB	0.92	0/1904	0.98	1/2565 (0.0%)
7	AC	1.00	0/1852	1.06	1/2490 (0.0%)
8	AD	1.04	0/1665	0.99	0/2227
9	AE	0.97	0/1239	1.03	0/1664
10	AF	0.99	0/1121	1.06	0/1509
11	AG	1.03	0/1422	1.01	2/1908 (0.1%)
12	AH	0.96	0/989	1.01	0/1326
13	AI	1.12	0/1048	1.01	0/1394
14	AJ	1.03	0/835	1.03	0/1127
15	AK	1.05	0/982	1.05	0/1323
16	AL	1.07	0/969	1.01	0/1300
17	AM	1.05	0/919	0.99	1/1226 (0.1%)
18	AN	1.07	0/817	1.05	1/1088 (0.1%)
19	AO	1.06	0/724	0.92	0/966
20	AP	1.07	0/659	1.03	0/884
21	AQ	0.99	0/681	1.05	0/913
22	AR	1.14	0/637	1.05	2/851 (0.2%)
23	AS	0.96	0/744	0.96	0/995
24	AT	0.96	0/676	0.94	0/895
25	AU	1.18	0/598	0.99	0/792
26	B7	1.59	2/2873 (0.1%)	2.49	325/4478 (7.3%)
27	B8	1.60	100/69822 (0.1%)	2.50	8171/108926 (7.5%)
28	BA	1.68	7/3439 (0.2%)	1.14	15/4662 (0.3%)
29	BB	0.98	1/902 (0.1%)	1.05	1/1228 (0.1%)
30	B5	0.92	0/1748	0.97	0/2355
31	B6	1.04	0/2131	1.03	1/2863 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	BD	0.97	0/1586	1.08	4/2134 (0.2%)
33	BE	0.95	0/1571	1.01	2/2113 (0.1%)
34	BF	1.01	0/1444	1.06	1/1937 (0.1%)
35	BG	0.96	0/1343	1.06	4/1816 (0.2%)
36	BH	0.93	0/1122	1.05	0/1515
37	BI	0.86	0/1046	1.00	1/1410 (0.1%)
38	BJ	0.97	0/1152	1.01	0/1551
39	BK	1.03	0/956	1.03	0/1279
40	BL	1.04	0/1062	0.98	1/1413 (0.1%)
41	BM	1.03	0/1093	1.06	2/1460 (0.1%)
42	BN	1.10	0/1021	1.03	1/1364 (0.1%)
43	BO	1.07	0/910	0.98	0/1219
44	BP	1.06	0/929	1.03	0/1242
45	BQ	1.09	0/960	1.00	2/1278 (0.2%)
46	BR	1.01	0/829	1.07	1/1107 (0.1%)
47	BS	0.99	0/864	1.04	1/1156 (0.1%)
48	BT	0.98	0/794	1.09	1/1060 (0.1%)
49	BU	0.96	0/797	1.04	0/1062
50	BV	0.96	0/766	1.02	0/1025
51	BW	1.04	0/642	1.05	0/848
52	BX	1.09	0/635	1.04	0/848
53	BY	1.00	0/510	0.90	0/677
54	BZ	0.99	0/453	0.99	0/605
55	B0	1.05	0/450	0.97	0/599
56	B1	0.93	0/448	1.01	0/594
57	B2	1.25	0/380	1.06	0/498
58	B3	0.98	0/513	0.98	0/676
59	B4	1.20	2/303 (0.7%)	1.03	0/397
All	All	1.44	161/169241 (0.1%)	2.16	13123/251442 (5.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	AA	0	72
3	AV	0	2
5	A1	0	1
7	AC	0	1
12	AH	0	1
13	AI	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
26	B7	0	2
27	B8	0	100
28	BA	0	5
34	BF	0	1
36	BH	0	1
49	BU	0	1
57	B2	0	1
All	All	0	189

All (161) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	BA	416	PHE	CG-CD2	41.52	2.01	1.38
28	BA	416	PHE	CG-CD1	39.62	1.98	1.38
28	BA	416	PHE	CE2-CZ	30.78	1.95	1.37
28	BA	416	PHE	CE1-CZ	30.54	1.95	1.37
28	BA	416	PHE	CD2-CE2	27.89	1.95	1.39
28	BA	416	PHE	CD1-CE1	26.46	1.92	1.39
27	B8	2860	A	N7-C5	-7.97	1.34	1.39
27	B8	2378	A	N7-C5	-7.45	1.34	1.39
1	AA	1016	A	N7-C5	-7.37	1.34	1.39
27	B8	2111	U	C2-N3	7.37	1.43	1.37
5	A0	243	GLN	C-OXT	7.34	1.37	1.23
28	BA	442	GLY	C-OXT	7.34	1.37	1.23
5	A1	243	GLN	C-OXT	7.32	1.37	1.23
29	BB	127	PHE	C-OXT	7.29	1.37	1.23
27	B8	1571	A	N7-C5	-7.16	1.34	1.39
27	B8	1213	A	N7-C5	-7.09	1.34	1.39
1	AA	190	A	N7-C5	-7.09	1.34	1.39
1	AA	162	A	N7-C5	-6.95	1.35	1.39
27	B8	633	A	N7-C5	-6.93	1.35	1.39
1	AA	487	A	N7-C5	-6.92	1.35	1.39
27	B8	1641	A	N7-C5	-6.54	1.35	1.39
1	AA	1005	A	N7-C5	-6.34	1.35	1.39
27	B8	705	A	N7-C5	-6.32	1.35	1.39
1	AA	1339	A	N7-C5	-6.25	1.35	1.39
1	AA	1468	A	N7-C5	-6.24	1.35	1.39
26	B7	73	A	N7-C5	-6.23	1.35	1.39
27	B8	1608	A	N7-C5	-6.18	1.35	1.39
27	B8	402	A	N7-C5	-6.18	1.35	1.39
27	B8	216	A	N7-C5	-6.17	1.35	1.39
27	B8	471	A	N7-C5	-6.08	1.35	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	B8	2225	A	N7-C5	-6.08	1.35	1.39
1	AA	495	A	N7-C5	-6.06	1.35	1.39
1	AA	119	A	N7-C5	-6.05	1.35	1.39
27	B8	820	A	N7-C5	-6.03	1.35	1.39
1	AA	1014	A	O3'-P	-6.01	1.53	1.61
27	B8	2412	A	N7-C5	-6.00	1.35	1.39
27	B8	1469	A	N7-C5	-5.99	1.35	1.39
27	B8	1722	A	N7-C5	-5.95	1.35	1.39
27	B8	2366	A	N7-C5	-5.95	1.35	1.39
27	B8	1029	A	N7-C5	-5.94	1.35	1.39
27	B8	374	A	N7-C5	-5.85	1.35	1.39
27	B8	2082	A	N7-C5	-5.84	1.35	1.39
27	B8	1001	A	N7-C5	-5.83	1.35	1.39
27	B8	877	A	N7-C5	-5.82	1.35	1.39
27	B8	2352	A	N7-C5	-5.82	1.35	1.39
27	B8	310	A	N7-C5	-5.82	1.35	1.39
27	B8	1866	A	N7-C5	-5.79	1.35	1.39
27	B8	513	A	N7-C5	-5.78	1.35	1.39
27	B8	52	A	N7-C5	-5.78	1.35	1.39
27	B8	1572	A	N7-C5	-5.75	1.35	1.39
27	B8	1744	A	N7-C5	-5.75	1.35	1.39
1	AA	533	A	N7-C5	-5.74	1.35	1.39
27	B8	2435	A	N7-C5	-5.70	1.35	1.39
1	AA	327	A	N7-C5	-5.69	1.35	1.39
1	AA	1375	A	N7-C5	-5.68	1.35	1.39
27	B8	2587	A	N7-C5	-5.67	1.35	1.39
27	B8	371	A	N7-C5	-5.66	1.35	1.39
1	AA	909	A	N7-C5	-5.64	1.35	1.39
1	AA	151	A	N7-C5	-5.63	1.35	1.39
27	B8	2013	A	N7-C5	-5.61	1.35	1.39
27	B8	2335	A	N7-C5	-5.60	1.35	1.39
27	B8	2662	A	N7-C5	-5.59	1.35	1.39
1	AA	1170	A	N7-C5	-5.58	1.35	1.39
59	B4	27	CYS	CB-SG	5.56	1.91	1.82
27	B8	1286	A	N7-C5	-5.55	1.35	1.39
27	B8	1477	A	N7-C5	-5.52	1.35	1.39
27	B8	340	A	N7-C5	-5.52	1.35	1.39
27	B8	190	A	N7-C5	-5.50	1.35	1.39
27	B8	2268	A	N7-C5	-5.50	1.35	1.39
27	B8	1021	A	N7-C5	-5.48	1.35	1.39
27	B8	256	A	N7-C5	-5.46	1.35	1.39
27	B8	1872	A	N7-C5	-5.46	1.35	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
59	B4	11	CYS	CB-SG	5.45	1.91	1.82
1	AA	873	A	N7-C5	-5.45	1.35	1.39
27	B8	191	A	N7-C5	-5.45	1.35	1.39
27	B8	251	A	N7-C5	-5.42	1.35	1.39
27	B8	2430	A	N7-C5	-5.42	1.35	1.39
27	B8	1373	A	N7-C5	-5.41	1.36	1.39
1	AA	468	A	N7-C5	-5.41	1.36	1.39
1	AA	1055	A	N7-C5	-5.41	1.36	1.39
1	AA	383	A	N7-C5	-5.39	1.36	1.39
27	B8	973	A	N7-C5	-5.39	1.36	1.39
27	B8	1717	A	N7-C5	-5.39	1.36	1.39
27	B8	609	A	N7-C5	-5.38	1.36	1.39
1	AA	919	A	N7-C5	-5.38	1.36	1.39
27	B8	278	A	N7-C5	-5.38	1.36	1.39
1	AA	781	A	N7-C5	-5.36	1.36	1.39
27	B8	1802	A	N7-C5	-5.36	1.36	1.39
27	B8	1378	A	N7-C5	-5.34	1.36	1.39
27	B8	918	A	N7-C5	-5.34	1.36	1.39
27	B8	447	A	N7-C5	-5.32	1.36	1.39
27	B8	1970	A	N7-C5	-5.32	1.36	1.39
1	AA	171	A	N7-C5	-5.31	1.36	1.39
27	B8	556	A	N7-C5	-5.30	1.36	1.39
27	B8	2297	A	N7-C5	-5.29	1.36	1.39
27	B8	279	A	N7-C5	-5.28	1.36	1.39
1	AA	908	A	N7-C5	-5.27	1.36	1.39
1	AA	439	U	C2-N3	5.26	1.41	1.37
27	B8	138	U	C2-N3	5.26	1.41	1.37
27	B8	266	G	C2-N3	5.26	1.36	1.32
27	B8	1439	A	N7-C5	-5.26	1.36	1.39
27	B8	1890	A	N7-C5	-5.26	1.36	1.39
27	B8	412	A	N7-C5	-5.25	1.36	1.39
27	B8	49	A	N7-C5	-5.25	1.36	1.39
27	B8	1470	A	N7-C5	-5.25	1.36	1.39
1	AA	55	A	N7-C5	-5.25	1.36	1.39
27	B8	917	A	N7-C5	-5.24	1.36	1.39
26	B7	99	A	N7-C5	-5.24	1.36	1.39
27	B8	1354	A	N7-C5	-5.24	1.36	1.39
27	B8	1237	A	N7-C5	-5.23	1.36	1.39
27	B8	428	A	N7-C5	-5.22	1.36	1.39
27	B8	2903	U	C2-N3	5.22	1.41	1.37
1	AA	262	A	N7-C5	-5.21	1.36	1.39
27	B8	975	A	N7-C5	-5.21	1.36	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	498	A	N7-C5	-5.21	1.36	1.39
1	AA	1401	G	C2-N3	5.20	1.36	1.32
1	AA	1306	A	N7-C5	-5.17	1.36	1.39
27	B8	879	G	C2-N3	5.17	1.36	1.32
27	B8	1419	A	N7-C5	-5.17	1.36	1.39
27	B8	1580	A	N7-C5	-5.16	1.36	1.39
27	B8	1254	A	N7-C5	-5.16	1.36	1.39
1	AA	696	A	N7-C5	-5.15	1.36	1.39
27	B8	1340	U	C2-N3	5.15	1.41	1.37
27	B8	2741	A	N7-C5	-5.14	1.36	1.39
1	AA	860	A	N7-C5	-5.14	1.36	1.39
27	B8	470	A	N7-C5	-5.13	1.36	1.39
1	AA	759	A	N7-C5	-5.13	1.36	1.39
27	B8	713	G	C2-N3	5.13	1.36	1.32
1	AA	69	G	N1-C2	5.13	1.41	1.37
1	AA	1483	A	N7-C5	-5.12	1.36	1.39
1	AA	753	A	N7-C5	-5.12	1.36	1.39
27	B8	2029	G	C2-N3	5.12	1.36	1.32
1	AA	653	U	C2-N3	5.12	1.41	1.37
1	AA	115	G	C2-N3	5.12	1.36	1.32
27	B8	1	G	C2-N3	5.12	1.36	1.32
27	B8	699	A	N7-C5	-5.11	1.36	1.39
27	B8	2748	A	N7-C5	-5.10	1.36	1.39
1	AA	1261	A	N7-C5	-5.10	1.36	1.39
27	B8	2171	A	N7-C5	-5.10	1.36	1.39
27	B8	2077	A	N7-C5	-5.10	1.36	1.39
1	AA	116	A	N7-C5	-5.09	1.36	1.39
27	B8	1690	A	N7-C5	-5.09	1.36	1.39
1	AA	1077	G	N1-C2	5.08	1.41	1.37
1	AA	1288	A	N7-C5	-5.08	1.36	1.39
27	B8	1395	A	N7-C5	-5.07	1.36	1.39
27	B8	1932	A	N7-C5	-5.07	1.36	1.39
1	AA	1255	G	C2-N3	5.07	1.36	1.32
27	B8	2511	U	C2-N3	5.06	1.41	1.37
1	AA	282	A	N7-C5	-5.06	1.36	1.39
27	B8	1634	A	N7-C5	-5.06	1.36	1.39
27	B8	1848	A	N7-C5	-5.05	1.36	1.39
1	AA	1316	G	C2-N3	5.05	1.36	1.32
27	B8	1027	A	N7-C5	-5.04	1.36	1.39
27	B8	2199	A	N7-C5	-5.03	1.36	1.39
27	B8	1803	A	N7-C5	-5.03	1.36	1.39
1	AA	1365	G	C2-N3	5.03	1.36	1.32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	B8	2566	A	N7-C5	-5.02	1.36	1.39
27	B8	2033	A	N7-C5	-5.01	1.36	1.39
3	AV	40	G	N1-C2	5.01	1.41	1.37
27	B8	2405	G	C2-N3	5.00	1.36	1.32
27	B8	2592	G	C2-N3	5.00	1.36	1.32

All (13123) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	85	U	P-O3'-C3'	19.51	143.11	119.70
27	B8	670	A	P-O3'-C3'	17.35	140.52	119.70
27	B8	2076	U	P-O3'-C3'	15.69	138.53	119.70
27	B8	6	A	N1-C6-N6	14.72	127.43	118.60
1	AA	1252	A	N1-C6-N6	14.43	127.26	118.60
27	B8	449	A	N1-C6-N6	14.43	127.26	118.60
1	AA	328	C	P-O3'-C3'	14.42	137.00	119.70
27	B8	2766	A	N1-C6-N6	14.36	127.21	118.60
27	B8	677	A	N1-C6-N6	14.21	127.12	118.60
27	B8	890	C	P-O3'-C3'	14.20	136.75	119.70
1	AA	1036	A	N1-C6-N6	14.12	127.07	118.60
27	B8	1977	A	N1-C6-N6	14.11	127.07	118.60
27	B8	2899	A	N1-C6-N6	14.10	127.06	118.60
27	B8	863	A	N1-C6-N6	14.04	127.02	118.60
1	AA	262	A	N1-C6-N6	14.02	127.01	118.60
1	AA	937	A	N1-C6-N6	14.01	127.01	118.60
27	B8	1745	A	N1-C6-N6	13.97	126.98	118.60
1	AA	1014	A	P-O3'-C3'	13.90	136.38	119.70
27	B8	880	G	P-O3'-C3'	13.88	136.36	119.70
27	B8	1784	A	N1-C6-N6	13.85	126.91	118.60
1	AA	174	A	N1-C6-N6	13.84	126.91	118.60
26	B7	66	A	N1-C6-N6	13.79	126.88	118.60
1	AA	780	A	N1-C6-N6	13.79	126.87	118.60
1	AA	16	A	N1-C6-N6	13.75	126.85	118.60
1	AA	181	A	N1-C6-N6	13.74	126.84	118.60
26	B7	109	A	N1-C6-N6	13.73	126.84	118.60
27	B8	959	A	N1-C6-N6	13.71	126.83	118.60
27	B8	1713	A	N1-C6-N6	13.71	126.82	118.60
27	B8	330	A	N1-C6-N6	13.68	126.81	118.60
1	AA	906	A	N1-C6-N6	13.66	126.80	118.60
27	B8	5	A	N1-C6-N6	13.64	126.78	118.60
27	B8	2171	A	N1-C6-N6	13.64	126.78	118.60
1	AA	1465	A	N1-C6-N6	13.62	126.77	118.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1500	A	N1-C6-N6	13.62	126.77	118.60
1	AA	1035	A	N1-C6-N6	13.61	126.77	118.60
27	B8	2662	A	N1-C6-N6	13.54	126.72	118.60
1	AA	1111	A	N1-C6-N6	13.54	126.72	118.60
27	B8	1598	A	N1-C6-N6	13.51	126.71	118.60
1	AA	71	A	N1-C6-N6	13.47	126.68	118.60
1	AA	288	A	N1-C6-N6	13.46	126.68	118.60
27	B8	689	A	N1-C6-N6	13.46	126.67	118.60
1	AA	901	A	N1-C6-N6	13.44	126.66	118.60
1	AA	1492	A	N1-C6-N6	13.44	126.66	118.60
1	AA	192	A	N1-C6-N6	13.43	126.66	118.60
27	B8	2163	A	N1-C6-N6	13.41	126.65	118.60
27	B8	2826	A	N1-C6-N6	13.39	126.64	118.60
1	AA	923	A	N1-C6-N6	13.38	126.63	118.60
27	B8	1205	A	P-O3'-C3'	13.38	135.75	119.70
27	B8	1899	A	N1-C6-N6	13.38	126.63	118.60
27	B8	2090	A	N1-C6-N6	13.37	126.62	118.60
27	B8	219	A	N1-C6-N6	13.36	126.61	118.60
26	B7	108	A	N1-C6-N6	13.34	126.60	118.60
27	B8	928	A	N1-C6-N6	13.33	126.60	118.60
27	B8	718	A	N1-C6-N6	13.32	126.59	118.60
27	B8	794	A	N1-C6-N6	13.32	126.59	118.60
27	B8	443	A	N1-C6-N6	13.31	126.59	118.60
27	B8	1532	A	N1-C6-N6	13.31	126.58	118.60
27	B8	1127	A	N1-C6-N6	13.29	126.57	118.60
27	B8	56	A	N1-C6-N6	13.28	126.57	118.60
1	AA	199	A	N1-C6-N6	13.26	126.56	118.60
27	B8	233	A	N1-C6-N6	13.25	126.55	118.60
3	AV	9	A	N1-C6-N6	13.24	126.54	118.60
27	B8	911	A	N1-C6-N6	13.24	126.54	118.60
1	AA	1437	A	N1-C6-N6	13.22	126.53	118.60
1	AA	595	A	N1-C6-N6	13.22	126.53	118.60
27	B8	734	A	N1-C6-N6	13.20	126.52	118.60
27	B8	2734	A	N1-C6-N6	13.20	126.52	118.60
1	AA	1236	A	N1-C6-N6	13.18	126.51	118.60
1	AA	996	A	N1-C6-N6	13.17	126.50	118.60
1	AA	1226	C	P-O3'-C3'	13.17	135.51	119.70
1	AA	1513	A	N1-C6-N6	13.17	126.50	118.60
27	B8	947	A	N1-C6-N6	13.16	126.50	118.60
1	AA	746	A	N1-C6-N6	13.16	126.50	118.60
1	AA	155	A	N1-C6-N6	13.13	126.48	118.60
27	B8	1027	A	N1-C6-N6	13.12	126.47	118.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	814	A	N1-C6-N6	13.11	126.47	118.60
27	B8	213	A	N1-C6-N6	13.11	126.47	118.60
1	AA	1360	A	N1-C6-N6	13.10	126.46	118.60
27	B8	19	A	N1-C6-N6	13.07	126.44	118.60
27	B8	2154	A	N1-C6-N6	13.07	126.44	118.60
1	AA	1014	A	N1-C6-N6	13.06	126.44	118.60
27	B8	1791	A	N1-C6-N6	13.06	126.44	118.60
27	B8	13	A	N1-C6-N6	13.06	126.43	118.60
27	B8	1431	A	N1-C6-N6	13.04	126.42	118.60
27	B8	1787	A	N1-C6-N6	13.03	126.42	118.60
27	B8	2051	A	N1-C6-N6	13.03	126.42	118.60
1	AA	1080	A	N1-C6-N6	13.03	126.42	118.60
27	B8	104	A	N1-C6-N6	13.03	126.42	118.60
27	B8	2453	A	N1-C6-N6	13.01	126.41	118.60
1	AA	1398	A	N1-C6-N6	13.01	126.41	118.60
27	B8	2879	A	N1-C6-N6	13.00	126.40	118.60
27	B8	2284	A	N1-C6-N6	13.00	126.40	118.60
27	B8	1144	A	N1-C6-N6	12.99	126.39	118.60
1	AA	1197	A	N1-C6-N6	12.99	126.39	118.60
27	B8	199	A	N1-C6-N6	12.98	126.39	118.60
27	B8	1700	A	N1-C6-N6	12.98	126.39	118.60
27	B8	1084	A	N1-C6-N6	12.97	126.38	118.60
27	B8	1603	A	N1-C6-N6	12.97	126.38	118.60
27	B8	1918	A	N1-C6-N6	12.97	126.38	118.60
27	B8	685	A	N1-C6-N6	12.96	126.38	118.60
27	B8	756	A	N1-C6-N6	12.95	126.37	118.60
1	AA	502	A	N1-C6-N6	12.95	126.37	118.60
27	B8	28	A	N1-C6-N6	12.95	126.37	118.60
27	B8	849	A	N1-C6-N6	12.94	126.37	118.60
26	B7	101	A	N1-C6-N6	12.94	126.36	118.60
27	B8	1590	A	N1-C6-N6	12.93	126.36	118.60
27	B8	599	A	N1-C6-N6	12.93	126.36	118.60
1	AA	451	A	N1-C6-N6	12.90	126.34	118.60
27	B8	152	A	N1-C6-N6	12.90	126.34	118.60
27	B8	1095	A	N1-C6-N6	12.89	126.33	118.60
27	B8	1927	A	N1-C6-N6	12.88	126.33	118.60
27	B8	322	A	N1-C6-N6	12.87	126.32	118.60
1	AA	563	A	N1-C6-N6	12.87	126.32	118.60
27	B8	2800	A	N1-C6-N6	12.84	126.30	118.60
27	B8	1269	A	N1-C6-N6	12.84	126.30	118.60
27	B8	1354	A	N1-C6-N6	12.83	126.30	118.60
27	B8	1061	U	P-O3'-C3'	12.82	135.09	119.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	503	A	N1-C6-N6	12.81	126.29	118.60
27	B8	582	A	N1-C6-N6	12.80	126.28	118.60
27	B8	221	A	N1-C6-N6	12.77	126.26	118.60
1	AA	1044	A	N1-C6-N6	12.77	126.26	118.60
27	B8	1677	A	N1-C6-N6	12.76	126.25	118.60
27	B8	2184	A	N1-C6-N6	12.75	126.25	118.60
1	AA	673	A	N1-C6-N6	12.75	126.25	118.60
27	B8	515	A	N1-C6-N6	12.75	126.25	118.60
27	B8	502	A	N1-C6-N6	12.74	126.25	118.60
27	B8	1275	A	N1-C6-N6	12.74	126.25	118.60
27	B8	2873	A	N1-C6-N6	12.74	126.25	118.60
27	B8	899	A	N1-C6-N6	12.74	126.24	118.60
1	AA	915	A	N1-C6-N6	12.73	126.24	118.60
27	B8	1433	A	N1-C6-N6	12.72	126.23	118.60
1	AA	320	A	N1-C6-N6	12.72	126.23	118.60
27	B8	1936	A	N1-C6-N6	12.72	126.23	118.60
27	B8	155	A	N1-C6-N6	12.71	126.23	118.60
27	B8	1496	A	N1-C6-N6	12.71	126.22	118.60
27	B8	429	A	N1-C6-N6	12.71	126.22	118.60
1	AA	81	A	N1-C6-N6	12.70	126.22	118.60
1	AA	1229	A	N1-C6-N6	12.70	126.22	118.60
27	B8	878	A	N1-C6-N6	12.69	126.22	118.60
1	AA	77	A	N1-C6-N6	12.69	126.22	118.60
27	B8	1634	A	N1-C6-N6	12.69	126.21	118.60
1	AA	478	A	N1-C6-N6	12.68	126.21	118.60
27	B8	1264	A	N1-C6-N6	12.68	126.21	118.60
1	AA	371	A	N1-C6-N6	12.67	126.20	118.60
27	B8	2430	A	N1-C6-N6	12.67	126.20	118.60
27	B8	262	A	N1-C6-N6	12.67	126.20	118.60
27	B8	182	A	N1-C6-N6	12.65	126.19	118.60
27	B8	226	A	N1-C6-N6	12.65	126.19	118.60
1	AA	98	A	N1-C6-N6	12.65	126.19	118.60
27	B8	522	A	N1-C6-N6	12.65	126.19	118.60
27	B8	2037	A	N1-C6-N6	12.65	126.19	118.60
27	B8	2042	A	N1-C6-N6	12.65	126.19	118.60
27	B8	2352	A	N1-C6-N6	12.65	126.19	118.60
27	B8	693	A	N1-C6-N6	12.65	126.19	118.60
1	AA	1269	A	N1-C6-N6	12.64	126.19	118.60
27	B8	532	A	N1-C6-N6	12.64	126.19	118.60
27	B8	255	A	N1-C6-N6	12.64	126.18	118.60
1	AA	10	A	N1-C6-N6	12.64	126.18	118.60
1	AA	1219	A	N1-C6-N6	12.64	126.18	118.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	B7	58	A	N1-C6-N6	12.63	126.18	118.60
1	AA	162	A	N1-C6-N6	12.63	126.18	118.60
1	AA	336	A	N1-C6-N6	12.63	126.17	118.60
1	AA	964	A	N1-C6-N6	12.62	126.17	118.60
27	B8	342	A	N1-C6-N6	12.62	126.17	118.60
1	AA	456	A	N1-C6-N6	12.62	126.17	118.60
27	B8	1244	A	N1-C6-N6	12.61	126.17	118.60
27	B8	2281	A	N1-C6-N6	12.61	126.17	118.60
3	AV	27	A	N1-C6-N6	12.61	126.17	118.60
27	B8	190	A	N1-C6-N6	12.61	126.17	118.60
27	B8	666	A	N1-C6-N6	12.61	126.16	118.60
26	B7	29	A	N1-C6-N6	12.60	126.16	118.60
27	B8	2267	A	N1-C6-N6	12.60	126.16	118.60
1	AA	1306	A	N1-C6-N6	12.60	126.16	118.60
1	AA	309	A	N1-C6-N6	12.60	126.16	118.60
27	B8	1773	A	N1-C6-N6	12.60	126.16	118.60
27	B8	2013	A	N1-C6-N6	12.60	126.16	118.60
27	B8	761	A	N1-C6-N6	12.59	126.16	118.60
27	B8	2369	A	N1-C6-N6	12.59	126.16	118.60
27	B8	347	A	N1-C6-N6	12.59	126.16	118.60
27	B8	655	A	N1-C6-N6	12.58	126.15	118.60
27	B8	1260	A	N1-C6-N6	12.58	126.15	118.60
1	AA	675	A	N1-C6-N6	12.58	126.15	118.60
27	B8	195	A	N1-C6-N6	12.58	126.15	118.60
27	B8	2600	A	N1-C6-N6	12.58	126.15	118.60
1	AA	139	A	N1-C6-N6	12.57	126.14	118.60
1	AA	205	A	N1-C6-N6	12.57	126.14	118.60
1	AA	1016	A	N1-C6-N6	12.57	126.14	118.60
26	B7	39	A	N1-C6-N6	12.57	126.14	118.60
27	B8	2336	A	P-O3'-C3'	12.57	134.78	119.70
27	B8	2412	A	N1-C6-N6	12.57	126.14	118.60
1	AA	974	A	N1-C6-N6	12.56	126.14	118.60
27	B8	1039	A	N1-C6-N6	12.56	126.14	118.60
27	B8	730	A	N1-C6-N6	12.56	126.14	118.60
1	AA	1167	A	N1-C6-N6	12.56	126.14	118.60
27	B8	83	A	N1-C6-N6	12.56	126.14	118.60
27	B8	592	A	N1-C6-N6	12.56	126.14	118.60
27	B8	637	A	N1-C6-N6	12.56	126.14	118.60
27	B8	2516	A	N1-C6-N6	12.56	126.14	118.60
27	B8	2278	A	N1-C6-N6	12.56	126.14	118.60
27	B8	1637	A	N1-C6-N6	12.56	126.13	118.60
27	B8	721	A	N1-C6-N6	12.54	126.13	118.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	33	A	N1-C6-N6	12.54	126.12	118.60
1	AA	300	A	N1-C6-N6	12.54	126.12	118.60
1	AA	1110	A	N1-C6-N6	12.54	126.13	118.60
1	AA	1151	A	N1-C6-N6	12.54	126.12	118.60
27	B8	492	A	N1-C6-N6	12.54	126.12	118.60
27	B8	1387	A	N1-C6-N6	12.54	126.12	118.60
27	B8	743	A	N1-C6-N6	12.54	126.12	118.60
27	B8	2311	A	N1-C6-N6	12.54	126.12	118.60
27	B8	749	A	N1-C6-N6	12.53	126.12	118.60
27	B8	1213	A	N1-C6-N6	12.53	126.12	118.60
1	AA	1000	A	N1-C6-N6	12.53	126.11	118.60
27	B8	497	A	N1-C6-N6	12.53	126.12	118.60
27	B8	2381	A	N1-C6-N6	12.52	126.11	118.60
27	B8	95	A	N1-C6-N6	12.52	126.11	118.60
1	AA	238	A	N1-C6-N6	12.52	126.11	118.60
1	AA	1081	A	N1-C6-N6	12.51	126.11	118.60
27	B8	2317	A	N1-C6-N6	12.51	126.10	118.60
27	B8	2333	A	N1-C6-N6	12.51	126.10	118.60
27	B8	2541	A	N1-C6-N6	12.51	126.10	118.60
27	B8	2274	A	N1-C6-N6	12.50	126.10	118.60
27	B8	2860	A	N1-C6-N6	12.50	126.10	118.60
27	B8	1551	A	N1-C6-N6	12.49	126.10	118.60
1	AA	655	A	N1-C6-N6	12.49	126.09	118.60
1	AA	468	A	N1-C6-N6	12.48	126.09	118.60
27	B8	644	A	N1-C6-N6	12.48	126.09	118.60
27	B8	2378	A	N1-C6-N6	12.48	126.09	118.60
27	B8	265	A	N1-C6-N6	12.48	126.09	118.60
27	B8	1204	A	N1-C6-N6	12.48	126.09	118.60
27	B8	1810	A	N1-C6-N6	12.48	126.09	118.60
27	B8	575	A	N1-C6-N6	12.48	126.08	118.60
27	B8	742	A	N1-C6-N6	12.47	126.08	118.60
1	AA	716	A	N1-C6-N6	12.47	126.08	118.60
1	AA	263	A	N1-C6-N6	12.47	126.08	118.60
1	AA	865	A	N1-C6-N6	12.47	126.08	118.60
1	AA	1171	A	N1-C6-N6	12.47	126.08	118.60
1	AA	53	A	N1-C6-N6	12.46	126.08	118.60
27	B8	2727	A	N1-C6-N6	12.46	126.08	118.60
1	AA	1357	A	N1-C6-N6	12.46	126.08	118.60
27	B8	2386	A	N1-C6-N6	12.46	126.08	118.60
1	AA	1434	A	N1-C6-N6	12.46	126.07	118.60
27	B8	1143	A	N1-C6-N6	12.46	126.07	118.60
1	AA	228	A	N1-C6-N6	12.45	126.07	118.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	B7	115	A	N1-C6-N6	12.45	126.07	118.60
27	B8	705	A	N1-C6-N6	12.45	126.07	118.60
27	B8	1794	A	N1-C6-N6	12.44	126.07	118.60
27	B8	127	A	N1-C6-N6	12.44	126.06	118.60
1	AA	629	A	N1-C6-N6	12.44	126.06	118.60
27	B8	2753	A	N1-C6-N6	12.44	126.06	118.60
1	AA	1065	U	P-O3'-C3'	12.43	134.62	119.70
27	B8	149	A	N1-C6-N6	12.43	126.06	118.60
27	B8	2482	A	N1-C6-N6	12.43	126.06	118.60
1	AA	482	A	N1-C6-N6	12.43	126.06	118.60
27	B8	299	A	N1-C6-N6	12.43	126.06	118.60
27	B8	382	A	N1-C6-N6	12.43	126.06	118.60
27	B8	300	A	N1-C6-N6	12.43	126.06	118.60
27	B8	466	A	N1-C6-N6	12.43	126.06	118.60
1	AA	270	A	N1-C6-N6	12.42	126.06	118.60
27	B8	633	A	N1-C6-N6	12.42	126.05	118.60
27	B8	2670	A	N1-C6-N6	12.42	126.05	118.60
27	B8	2598	A	N1-C6-N6	12.42	126.05	118.60
1	AA	223	A	N1-C6-N6	12.41	126.05	118.60
1	AA	1418	A	N1-C6-N6	12.41	126.05	118.60
1	AA	459	A	N1-C6-N6	12.41	126.05	118.60
27	B8	2094	A	N1-C6-N6	12.41	126.05	118.60
27	B8	415	A	N1-C6-N6	12.41	126.05	118.60
27	B8	1285	A	N1-C6-N6	12.41	126.05	118.60
27	B8	1654	A	N1-C6-N6	12.41	126.05	118.60
1	AA	960	U	P-O3'-C3'	12.40	134.59	119.70
27	B8	1664	A	N1-C6-N6	12.40	126.04	118.60
27	B8	89	A	N1-C6-N6	12.40	126.04	118.60
27	B8	2147	A	N1-C6-N6	12.40	126.04	118.60
1	AA	695	A	N1-C6-N6	12.40	126.04	118.60
1	AA	253	A	N1-C6-N6	12.39	126.04	118.60
27	B8	1579	A	N1-C6-N6	12.39	126.04	118.60
27	B8	84	A	N1-C6-N6	12.39	126.03	118.60
27	B8	2088	A	N1-C6-N6	12.38	126.03	118.60
1	AA	80	A	N1-C6-N6	12.38	126.03	118.60
1	AA	694	A	N1-C6-N6	12.38	126.03	118.60
1	AA	1155	A	N1-C6-N6	12.38	126.03	118.60
27	B8	1755	A	N1-C6-N6	12.38	126.03	118.60
27	B8	1194	A	N1-C6-N6	12.38	126.03	118.60
27	B8	2781	A	N1-C6-N6	12.38	126.03	118.60
1	AA	28	A	N1-C6-N6	12.38	126.03	118.60
26	B7	94	A	N1-C6-N6	12.38	126.03	118.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	2711	A	N1-C6-N6	12.38	126.03	118.60
1	AA	959	A	N1-C6-N6	12.37	126.02	118.60
27	B8	2031	A	N1-C6-N6	12.37	126.02	118.60
27	B8	943	A	N1-C6-N6	12.37	126.02	118.60
27	B8	1384	A	N1-C6-N6	12.37	126.02	118.60
26	B7	50	A	N1-C6-N6	12.36	126.02	118.60
27	B8	2900	A	N1-C6-N6	12.37	126.02	118.60
27	B8	368	A	N1-C6-N6	12.36	126.02	118.60
27	B8	513	A	N1-C6-N6	12.36	126.02	118.60
27	B8	1502	A	N1-C6-N6	12.36	126.02	118.60
1	AA	600	A	N1-C6-N6	12.36	126.02	118.60
27	B8	1640	A	N1-C6-N6	12.36	126.02	118.60
27	B8	2211	A	N1-C6-N6	12.36	126.02	118.60
27	B8	1253	A	N1-C6-N6	12.36	126.01	118.60
1	AA	768	A	N1-C6-N6	12.35	126.01	118.60
27	B8	111	A	N1-C6-N6	12.35	126.01	118.60
27	B8	1528	A	N1-C6-N6	12.35	126.01	118.60
1	AA	1105	A	N1-C6-N6	12.34	126.00	118.60
27	B8	227	A	N1-C6-N6	12.34	126.00	118.60
27	B8	1928	A	N1-C6-N6	12.34	126.00	118.60
1	AA	460	A	N1-C6-N6	12.34	126.00	118.60
1	AA	676	A	N1-C6-N6	12.34	126.00	118.60
27	B8	1366	A	N1-C6-N6	12.34	126.00	118.60
1	AA	994	A	N1-C6-N6	12.34	126.00	118.60
27	B8	2700	A	N1-C6-N6	12.34	126.00	118.60
27	B8	2411	A	N1-C6-N6	12.33	126.00	118.60
27	B8	626	A	N1-C6-N6	12.33	126.00	118.60
27	B8	1548	A	N1-C6-N6	12.33	126.00	118.60
27	B8	1705	A	N1-C6-N6	12.33	126.00	118.60
27	B8	2170	A	N1-C6-N6	12.32	125.99	118.60
27	B8	2665	A	N1-C6-N6	12.32	126.00	118.60
27	B8	716	A	N1-C6-N6	12.32	125.99	118.60
27	B8	1998	A	N1-C6-N6	12.32	125.99	118.60
27	B8	1525	A	N1-C6-N6	12.32	125.99	118.60
1	AA	236	A	N1-C6-N6	12.31	125.99	118.60
1	AA	573	A	N1-C6-N6	12.31	125.99	118.60
27	B8	1490	A	N1-C6-N6	12.31	125.99	118.60
27	B8	38	A	N1-C6-N6	12.31	125.99	118.60
27	B8	1969	A	N1-C6-N6	12.31	125.99	118.60
27	B8	2198	A	N1-C6-N6	12.31	125.98	118.60
27	B8	2434	A	N1-C6-N6	12.31	125.98	118.60
1	AA	1377	A	N1-C6-N6	12.30	125.98	118.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	251	A	N1-C6-N6	12.30	125.98	118.60
27	B8	1586	A	N1-C6-N6	12.30	125.98	118.60
27	B8	1757	A	N1-C6-N6	12.30	125.98	118.60
1	AA	784	A	N1-C6-N6	12.30	125.98	118.60
27	B8	167	A	N1-C6-N6	12.30	125.98	118.60
27	B8	1913	A	N1-C6-N6	12.30	125.98	118.60
1	AA	831	A	N1-C6-N6	12.30	125.98	118.60
27	B8	2589	A	N1-C6-N6	12.30	125.98	118.60
1	AA	8	A	N1-C6-N6	12.30	125.98	118.60
1	AA	32	A	N1-C6-N6	12.30	125.98	118.60
27	B8	2632	A	N1-C6-N6	12.30	125.98	118.60
27	B8	1669	A	N1-C6-N6	12.29	125.98	118.60
27	B8	1591	A	N1-C6-N6	12.29	125.97	118.60
1	AA	131	A	N1-C6-N6	12.29	125.97	118.60
1	AA	1004	A	N1-C6-N6	12.28	125.97	118.60
1	AA	1188	A	N1-C6-N6	12.28	125.97	118.60
27	B8	1077	A	N1-C6-N6	12.28	125.97	118.60
1	AA	1280	A	N1-C6-N6	12.28	125.97	118.60
27	B8	1650	A	N1-C6-N6	12.28	125.97	118.60
27	B8	1286	A	N1-C6-N6	12.28	125.97	118.60
27	B8	2887	A	N1-C6-N6	12.28	125.97	118.60
1	AA	935	A	N1-C6-N6	12.27	125.96	118.60
27	B8	1413	A	N1-C6-N6	12.27	125.96	118.60
1	AA	983	A	N1-C6-N6	12.27	125.96	118.60
27	B8	2183	A	N1-C6-N6	12.27	125.96	118.60
1	AA	574	A	N1-C6-N6	12.27	125.96	118.60
27	B8	2158	A	N1-C6-N6	12.27	125.96	118.60
1	AA	1287	A	N1-C6-N6	12.27	125.96	118.60
27	B8	782	A	N1-C6-N6	12.26	125.96	118.60
27	B8	632	A	N1-C6-N6	12.26	125.96	118.60
27	B8	1952	A	N1-C6-N6	12.26	125.96	118.60
1	AA	559	A	N1-C6-N6	12.26	125.95	118.60
1	AA	706	A	N1-C6-N6	12.26	125.95	118.60
1	AA	1374	A	N1-C6-N6	12.26	125.95	118.60
3	AV	22	A	N1-C6-N6	12.25	125.95	118.60
1	AA	182	A	N1-C6-N6	12.25	125.95	118.60
27	B8	1274	A	N1-C6-N6	12.25	125.95	118.60
27	B8	1819	A	N1-C6-N6	12.25	125.95	118.60
27	B8	2503	A	N1-C6-N6	12.25	125.95	118.60
1	AA	66	A	N1-C6-N6	12.25	125.95	118.60
3	AV	77	A	N1-C6-N6	12.24	125.95	118.60
27	B8	845	A	N1-C6-N6	12.24	125.95	118.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	2679	A	N1-C6-N6	12.24	125.95	118.60
27	B8	1226	A	N1-C6-N6	12.24	125.94	118.60
1	AA	907	A	N1-C6-N6	12.24	125.94	118.60
1	AA	1250	A	N1-C6-N6	12.24	125.94	118.60
27	B8	1735	A	N1-C6-N6	12.24	125.94	118.60
1	AA	3	A	N1-C6-N6	12.24	125.94	118.60
1	AA	1251	A	N1-C6-N6	12.24	125.94	118.60
27	B8	2439	A	N1-C6-N6	12.24	125.94	118.60
27	B8	1009	A	N1-C6-N6	12.23	125.94	118.60
27	B8	608	A	N1-C6-N6	12.23	125.94	118.60
27	B8	2328	A	N1-C6-N6	12.23	125.94	118.60
27	B8	203	A	N1-C6-N6	12.22	125.93	118.60
27	B8	996	A	N1-C6-N6	12.22	125.93	118.60
27	B8	2340	A	N1-C6-N6	12.22	125.93	118.60
27	B8	2660	A	N1-C6-N6	12.22	125.93	118.60
27	B8	1367	A	N1-C6-N6	12.22	125.93	118.60
27	B8	2837	A	N1-C6-N6	12.22	125.93	118.60
27	B8	354	A	N1-C6-N6	12.21	125.93	118.60
1	AA	190	A	N1-C6-N6	12.21	125.92	118.60
1	AA	787	A	N1-C6-N6	12.21	125.92	118.60
27	B8	2675	A	N1-C6-N6	12.21	125.92	118.60
3	AV	5	A	N1-C6-N6	12.21	125.92	118.60
27	B8	2738	A	N1-C6-N6	12.20	125.92	118.60
27	B8	91	A	N1-C6-N6	12.20	125.92	118.60
27	B8	892	A	N1-C6-N6	12.20	125.92	118.60
27	B8	925	A	N1-C6-N6	12.20	125.92	118.60
27	B8	2376	A	N1-C6-N6	12.20	125.92	118.60
27	B8	2406	A	N1-C6-N6	12.20	125.92	118.60
1	AA	919	A	N1-C6-N6	12.20	125.92	118.60
26	B7	119	A	N1-C6-N6	12.20	125.92	118.60
1	AA	383	A	N1-C6-N6	12.19	125.92	118.60
1	AA	1152	A	N1-C6-N6	12.19	125.92	118.60
1	AA	1447	A	N1-C6-N6	12.19	125.92	118.60
27	B8	2821	A	N1-C6-N6	12.19	125.92	118.60
1	AA	143	A	N1-C6-N6	12.19	125.91	118.60
27	B8	294	A	N1-C6-N6	12.19	125.91	118.60
27	B8	1618	A	N1-C6-N6	12.19	125.91	118.60
27	B8	2126	A	N1-C6-N6	12.19	125.91	118.60
1	AA	560	A	N1-C6-N6	12.18	125.91	118.60
27	B8	602	A	N1-C6-N6	12.18	125.91	118.60
27	B8	1134	A	N1-C6-N6	12.18	125.91	118.60
27	B8	2358	A	N1-C6-N6	12.18	125.91	118.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	120	A	N1-C6-N6	12.18	125.91	118.60
1	AA	1456	A	N1-C6-N6	12.18	125.91	118.60
27	B8	1866	A	N1-C6-N6	12.18	125.91	118.60
27	B8	1829	A	N1-C6-N6	12.18	125.91	118.60
1	AA	59	A	N1-C6-N6	12.18	125.91	118.60
27	B8	2314	A	N1-C6-N6	12.18	125.91	118.60
1	AA	648	A	N1-C6-N6	12.17	125.91	118.60
1	AA	1519	A	N1-C6-N6	12.17	125.90	118.60
27	B8	2893	A	N1-C6-N6	12.17	125.90	118.60
1	AA	1196	A	N1-C6-N6	12.16	125.90	118.60
27	B8	423	A	N1-C6-N6	12.16	125.90	118.60
27	B8	430	A	N1-C6-N6	12.16	125.90	118.60
27	B8	482	A	N1-C6-N6	12.16	125.90	118.60
1	AA	1396	A	N1-C6-N6	12.16	125.90	118.60
27	B8	53	A	N1-C6-N6	12.16	125.90	118.60
27	B8	1495	A	N1-C6-N6	12.16	125.89	118.60
1	AA	303	A	N1-C6-N6	12.15	125.89	118.60
27	B8	1953	A	N1-C6-N6	12.15	125.89	118.60
1	AA	366	A	N1-C6-N6	12.15	125.89	118.60
1	AA	546	A	N1-C6-N6	12.15	125.89	118.60
27	B8	332	A	N1-C6-N6	12.14	125.89	118.60
27	B8	789	A	N1-C6-N6	12.14	125.88	118.60
1	AA	630	A	N1-C6-N6	12.13	125.88	118.60
27	B8	1420	A	N1-C6-N6	12.13	125.88	118.60
27	B8	1609	A	N1-C6-N6	12.13	125.88	118.60
27	B8	1987	A	N1-C6-N6	12.13	125.88	118.60
27	B8	981	A	N1-C6-N6	12.13	125.88	118.60
27	B8	2792	A	N1-C6-N6	12.13	125.88	118.60
27	B8	2471	A	N1-C6-N6	12.13	125.88	118.60
27	B8	217	A	N1-C6-N6	12.13	125.88	118.60
1	AA	1201	A	N1-C6-N6	12.12	125.87	118.60
1	AA	149	A	N1-C6-N6	12.12	125.87	118.60
27	B8	14	A	N1-C6-N6	12.12	125.87	118.60
1	AA	349	A	N1-C6-N6	12.12	125.87	118.60
1	AA	635	A	N1-C6-N6	12.12	125.87	118.60
1	AA	1170	A	N1-C6-N6	12.12	125.87	118.60
1	AA	815	A	N1-C6-N6	12.12	125.87	118.60
1	AA	900	A	N1-C6-N6	12.12	125.87	118.60
27	B8	320	A	N1-C6-N6	12.12	125.87	118.60
1	AA	539	A	N1-C6-N6	12.12	125.87	118.60
1	AA	1507	A	N1-C6-N6	12.12	125.87	118.60
27	B8	2810	A	N1-C6-N6	12.11	125.87	118.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1324	A	N1-C6-N6	12.11	125.87	118.60
27	B8	146	A	N1-C6-N6	12.11	125.86	118.60
27	B8	2706	A	N1-C6-N6	12.11	125.86	118.60
1	AA	493	A	N1-C6-N6	12.10	125.86	118.60
1	AA	1274	A	N1-C6-N6	12.10	125.86	118.60
27	B8	1762	A	N1-C6-N6	12.10	125.86	118.60
27	B8	272	A	N1-C6-N6	12.10	125.86	118.60
27	B8	802	A	N1-C6-N6	12.10	125.86	118.60
27	B8	945	A	N1-C6-N6	12.10	125.86	118.60
1	AA	510	A	N1-C6-N6	12.10	125.86	118.60
1	AA	1169	A	N1-C6-N6	12.10	125.86	118.60
27	B8	352	A	N1-C6-N6	12.10	125.86	118.60
27	B8	1073	A	N1-C6-N6	12.10	125.86	118.60
27	B8	2518	A	N1-C6-N6	12.10	125.86	118.60
27	B8	2572	A	N1-C6-N6	12.10	125.86	118.60
1	AA	119	A	N1-C6-N6	12.09	125.86	118.60
27	B8	2823	A	N1-C6-N6	12.09	125.86	118.60
1	AA	873	A	N1-C6-N6	12.09	125.86	118.60
27	B8	833	A	N1-C6-N6	12.09	125.85	118.60
1	AA	499	A	N1-C6-N6	12.09	125.85	118.60
27	B8	2101	A	N1-C6-N6	12.09	125.85	118.60
27	B8	2191	A	N1-C6-N6	12.09	125.85	118.60
27	B8	2461	A	N1-C6-N6	12.09	125.85	118.60
27	B8	792	A	N1-C6-N6	12.09	125.85	118.60
1	AA	465	A	N1-C6-N6	12.09	125.85	118.60
27	B8	819	A	N1-C6-N6	12.09	125.85	118.60
27	B8	1085	A	N1-C6-N6	12.09	125.85	118.60
27	B8	1593	A	N1-C6-N6	12.09	125.85	118.60
1	AA	44	A	N1-C6-N6	12.08	125.85	118.60
27	B8	1978	A	N1-C6-N6	12.08	125.85	118.60
27	B8	160	A	N1-C6-N6	12.08	125.85	118.60
27	B8	1096	A	N1-C6-N6	12.08	125.85	118.60
27	B8	1877	A	N1-C6-N6	12.08	125.85	118.60
27	B8	2432	A	N1-C6-N6	12.08	125.85	118.60
27	B8	2682	A	N1-C6-N6	12.08	125.85	118.60
1	AA	1163	A	N1-C6-N6	12.07	125.84	118.60
27	B8	706	A	N1-C6-N6	12.07	125.84	118.60
27	B8	2377	A	N1-C6-N6	12.07	125.84	118.60
27	B8	1805	A	N1-C6-N6	12.07	125.84	118.60
27	B8	627	A	N1-C6-N6	12.06	125.84	118.60
27	B8	2142	A	N1-C6-N6	12.06	125.84	118.60
27	B8	2241	A	N1-C6-N6	12.06	125.84	118.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	2407	A	N1-C6-N6	12.06	125.84	118.60
1	AA	435	A	N1-C6-N6	12.06	125.84	118.60
1	AA	1022	A	N1-C6-N6	12.06	125.84	118.60
1	AA	496	A	N1-C6-N6	12.06	125.83	118.60
1	AA	1254	A	N1-C6-N6	12.06	125.84	118.60
27	B8	979	A	N1-C6-N6	12.06	125.84	118.60
27	B8	1069	A	N1-C6-N6	12.06	125.83	118.60
27	B8	1566	A	N1-C6-N6	12.06	125.83	118.60
27	B8	1403	A	N1-C6-N6	12.06	125.83	118.60
27	B8	1503	A	N1-C6-N6	12.06	125.83	118.60
27	B8	2560	A	N1-C6-N6	12.06	125.83	118.60
3	AV	14	A	N1-C6-N6	12.05	125.83	118.60
27	B8	1090	A	N1-C6-N6	12.05	125.83	118.60
1	AA	743	A	N1-C6-N6	12.05	125.83	118.60
27	B8	1676	A	N1-C6-N6	12.05	125.83	118.60
27	B8	2814	A	N1-C6-N6	12.05	125.83	118.60
1	AA	938	A	N1-C6-N6	12.05	125.83	118.60
27	B8	1050	A	N1-C6-N6	12.05	125.83	118.60
27	B8	1570	A	N1-C6-N6	12.04	125.83	118.60
27	B8	2602	A	N1-C6-N6	12.04	125.83	118.60
27	B8	1230	A	N1-C6-N6	12.04	125.83	118.60
27	B8	2850	A	N1-C6-N6	12.04	125.83	118.60
27	B8	590	A	N1-C6-N6	12.04	125.82	118.60
27	B8	804	A	N1-C6-N6	12.04	125.82	118.60
27	B8	1678	A	N1-C6-N6	12.04	125.82	118.60
27	B8	10	A	N1-C6-N6	12.03	125.82	118.60
27	B8	2005	A	N1-C6-N6	12.03	125.82	118.60
1	AA	321	A	N1-C6-N6	12.03	125.82	118.60
26	B7	46	A	N1-C6-N6	12.03	125.82	118.60
27	B8	1722	A	N1-C6-N6	12.03	125.82	118.60
1	AA	553	A	N1-C6-N6	12.03	125.82	118.60
27	B8	480	A	N1-C6-N6	12.03	125.81	118.60
27	B8	2388	A	N1-C6-N6	12.03	125.82	118.60
27	B8	1938	A	N1-C6-N6	12.02	125.81	118.60
1	AA	1311	A	N1-C6-N6	12.02	125.81	118.60
1	AA	306	A	N1-C6-N6	12.02	125.81	118.60
27	B8	1353	A	N1-C6-N6	12.02	125.81	118.60
27	B8	1014	A	N1-C6-N6	12.01	125.81	118.60
27	B8	2080	A	N1-C6-N6	12.01	125.81	118.60
27	B8	2346	A	N1-C6-N6	12.01	125.81	118.60
27	B8	2309	A	N1-C6-N6	12.01	125.80	118.60
27	B8	223	A	N1-C6-N6	12.00	125.80	118.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	1020	A	N1-C6-N6	12.00	125.80	118.60
27	B8	2448	A	N1-C6-N6	12.00	125.80	118.60
27	B8	764	A	N1-C6-N6	12.00	125.80	118.60
1	AA	958	A	N1-C6-N6	12.00	125.80	118.60
27	B8	2097	A	N1-C6-N6	12.00	125.80	118.60
1	AA	189	A	N1-C6-N6	12.00	125.80	118.60
1	AA	1350	A	N1-C6-N6	12.00	125.80	118.60
27	B8	563	A	N1-C6-N6	12.00	125.80	118.60
1	AA	579	A	N1-C6-N6	11.99	125.80	118.60
1	AA	363	A	N1-C6-N6	11.99	125.80	118.60
1	AA	1021	A	N1-C6-N6	11.99	125.80	118.60
27	B8	1008	A	N1-C6-N6	11.99	125.80	118.60
27	B8	1057	A	N1-C6-N6	11.99	125.80	118.60
27	B8	472	A	N1-C6-N6	11.99	125.79	118.60
27	B8	1970	A	N1-C6-N6	11.99	125.79	118.60
27	B8	2288	A	N1-C6-N6	11.99	125.79	118.60
27	B8	1754	A	N1-C6-N6	11.99	125.79	118.60
27	B8	2425	A	N1-C6-N6	11.98	125.79	118.60
1	AA	532	A	N1-C6-N6	11.98	125.79	118.60
27	B8	1029	A	N1-C6-N6	11.98	125.79	118.60
27	B8	1048	A	N1-C6-N6	11.98	125.79	118.60
27	B8	1241	A	N1-C6-N6	11.98	125.79	118.60
1	AA	1180	A	N1-C6-N6	11.98	125.79	118.60
27	B8	668	A	N1-C6-N6	11.98	125.79	118.60
27	B8	2019	A	N1-C6-N6	11.98	125.79	118.60
27	B8	311	A	N1-C6-N6	11.97	125.78	118.60
27	B8	345	A	N1-C6-N6	11.97	125.78	118.60
27	B8	1169	A	N1-C6-N6	11.97	125.78	118.60
27	B8	1665	A	N1-C6-N6	11.97	125.78	118.60
1	AA	1092	A	N1-C6-N6	11.97	125.78	118.60
27	B8	1246	A	N1-C6-N6	11.97	125.78	118.60
27	B8	1597	A	N1-C6-N6	11.97	125.78	118.60
27	B8	1802	A	N1-C6-N6	11.97	125.78	118.60
1	AA	728	A	N1-C6-N6	11.97	125.78	118.60
1	AA	1542	A	N1-C6-N6	11.97	125.78	118.60
27	B8	603	A	N1-C6-N6	11.96	125.78	118.60
27	B8	1262	A	N1-C6-N6	11.96	125.78	118.60
1	AA	781	A	N1-C6-N6	11.96	125.78	118.60
3	AV	52	A	N1-C6-N6	11.96	125.78	118.60
27	B8	2776	A	N1-C6-N6	11.96	125.78	118.60
27	B8	52	A	N1-C6-N6	11.96	125.78	118.60
27	B8	218	A	N1-C6-N6	11.96	125.78	118.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	1672	A	N1-C6-N6	11.96	125.77	118.60
27	B8	2426	A	N1-C6-N6	11.96	125.77	118.60
27	B8	2809	A	N1-C6-N6	11.96	125.77	118.60
27	B8	1327	A	N1-C6-N6	11.95	125.77	118.60
27	B8	1383	A	N1-C6-N6	11.95	125.77	118.60
27	B8	1385	A	N1-C6-N6	11.95	125.77	118.60
27	B8	1871	A	N1-C6-N6	11.95	125.77	118.60
1	AA	1493	A	N1-C6-N6	11.95	125.77	118.60
27	B8	980	A	N1-C6-N6	11.95	125.77	118.60
27	B8	1847	A	N1-C6-N6	11.95	125.77	118.60
27	B8	2740	A	N1-C6-N6	11.95	125.77	118.60
1	AA	101	A	N1-C6-N6	11.94	125.77	118.60
1	AA	816	A	N1-C6-N6	11.94	125.77	118.60
27	B8	2531	A	N1-C6-N6	11.94	125.77	118.60
27	B8	1046	A	N1-C6-N6	11.94	125.76	118.60
1	AA	602	A	N1-C6-N6	11.94	125.76	118.60
27	B8	905	A	N1-C6-N6	11.94	125.76	118.60
1	AA	621	A	N1-C6-N6	11.94	125.76	118.60
1	AA	1431	A	N1-C6-N6	11.94	125.76	118.60
27	B8	631	A	N1-C6-N6	11.94	125.76	118.60
1	AA	807	A	N1-C6-N6	11.93	125.76	118.60
27	B8	191	A	N1-C6-N6	11.93	125.76	118.60
27	B8	348	A	N1-C6-N6	11.93	125.76	118.60
27	B8	2205	A	N1-C6-N6	11.93	125.76	118.60
1	AA	1117	A	N1-C6-N6	11.93	125.76	118.60
1	AA	1271	A	N1-C6-N6	11.93	125.76	118.60
1	AA	1480	A	N1-C6-N6	11.93	125.76	118.60
27	B8	2247	A	N1-C6-N6	11.93	125.76	118.60
1	AA	338	A	N1-C6-N6	11.93	125.76	118.60
1	AA	596	A	N1-C6-N6	11.93	125.76	118.60
1	AA	946	A	N1-C6-N6	11.93	125.76	118.60
27	B8	572	A	N1-C6-N6	11.92	125.75	118.60
1	AA	1257	A	N1-C6-N6	11.92	125.75	118.60
27	B8	793	A	N1-C6-N6	11.92	125.75	118.60
27	B8	983	A	N1-C6-N6	11.92	125.75	118.60
27	B8	1966	A	N1-C6-N6	11.92	125.75	118.60
1	AA	1019	A	N1-C6-N6	11.91	125.75	118.60
27	B8	752	A	N1-C6-N6	11.91	125.75	118.60
27	B8	172	A	N1-C6-N6	11.91	125.75	118.60
1	AA	715	A	N1-C6-N6	11.91	125.75	118.60
27	B8	1759	A	N1-C6-N6	11.91	125.75	118.60
27	B8	739	A	N1-C6-N6	11.91	125.74	118.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	2071	A	N1-C6-N6	11.91	125.75	118.60
27	B8	2058	A	N1-C6-N6	11.91	125.74	118.60
1	AA	51	A	N1-C6-N6	11.90	125.74	118.60
1	AA	1067	A	N1-C6-N6	11.90	125.74	118.60
1	AA	1468	A	N1-C6-N6	11.90	125.74	118.60
27	B8	1504	A	N1-C6-N6	11.90	125.74	118.60
27	B8	1392	A	N1-C6-N6	11.90	125.74	118.60
1	AA	1093	A	N1-C6-N6	11.89	125.74	118.60
27	B8	173	A	N1-C6-N6	11.89	125.74	118.60
27	B8	1000	A	N1-C6-N6	11.89	125.74	118.60
27	B8	2565	A	N1-C6-N6	11.89	125.73	118.60
27	B8	2799	A	N1-C6-N6	11.89	125.73	118.60
1	AA	1394	A	N1-C6-N6	11.88	125.73	118.60
1	AA	1446	A	N1-C6-N6	11.88	125.73	118.60
27	B8	44	A	N1-C6-N6	11.88	125.73	118.60
27	B8	216	A	N1-C6-N6	11.88	125.73	118.60
27	B8	270	A	N1-C6-N6	11.88	125.73	118.60
27	B8	2322	A	N1-C6-N6	11.88	125.73	118.60
1	AA	1082	A	N1-C6-N6	11.88	125.73	118.60
1	AA	1430	A	N1-C6-N6	11.88	125.73	118.60
27	B8	1129	A	N1-C6-N6	11.88	125.73	118.60
27	B8	1470	A	N1-C6-N6	11.88	125.73	118.60
2	AX	21	A	N1-C6-N6	11.87	125.72	118.60
27	B8	125	A	N1-C6-N6	11.87	125.72	118.60
1	AA	918	A	N1-C6-N6	11.87	125.72	118.60
27	B8	2758	A	N1-C6-N6	11.87	125.72	118.60
1	AA	344	A	N1-C6-N6	11.87	125.72	118.60
1	AA	749	A	N1-C6-N6	11.87	125.72	118.60
27	B8	936	A	N1-C6-N6	11.87	125.72	118.60
27	B8	2003	A	N1-C6-N6	11.87	125.72	118.60
1	AA	1213	A	N1-C6-N6	11.87	125.72	118.60
1	AA	19	A	N1-C6-N6	11.86	125.72	118.60
1	AA	1499	A	N1-C6-N6	11.86	125.72	118.60
27	B8	788	A	N1-C6-N6	11.87	125.72	118.60
27	B8	960	A	N1-C6-N6	11.86	125.72	118.60
27	B8	984	A	N1-C6-N6	11.86	125.72	118.60
27	B8	877	A	N1-C6-N6	11.86	125.71	118.60
27	B8	861	A	N1-C6-N6	11.86	125.71	118.60
27	B8	197	A	N1-C6-N6	11.85	125.71	118.60
27	B8	1302	A	N1-C6-N6	11.85	125.71	118.60
27	B8	1151	A	N1-C6-N6	11.85	125.71	118.60
27	B8	2634	A	N1-C6-N6	11.85	125.71	118.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	572	A	N1-C6-N6	11.85	125.71	118.60
3	AV	59	A	N1-C6-N6	11.85	125.71	118.60
27	B8	1900	A	N1-C6-N6	11.85	125.71	118.60
1	AA	607	A	N1-C6-N6	11.84	125.71	118.60
1	AA	389	A	N1-C6-N6	11.84	125.70	118.60
27	B8	309	A	N1-C6-N6	11.84	125.70	118.60
27	B8	1549	A	N1-C6-N6	11.84	125.70	118.60
27	B8	1981	A	N1-C6-N6	11.84	125.70	118.60
27	B8	2459	A	N1-C6-N6	11.84	125.70	118.60
1	AA	1	A	N1-C6-N6	11.84	125.70	118.60
1	AA	161	A	N1-C6-N6	11.84	125.70	118.60
27	B8	1347	A	N1-C6-N6	11.84	125.70	118.60
1	AA	1476	A	N1-C6-N6	11.83	125.70	118.60
27	B8	1626	A	N1-C6-N6	11.83	125.70	118.60
27	B8	504	A	N1-C6-N6	11.83	125.70	118.60
27	B8	2547	A	N1-C6-N6	11.82	125.69	118.60
1	AA	851	G	N1-C6-O6	11.82	126.99	119.90
1	AA	1046	A	N1-C6-N6	11.82	125.69	118.60
27	B8	101	A	N1-C6-N6	11.82	125.69	118.60
27	B8	231	A	N1-C6-N6	11.82	125.69	118.60
27	B8	2813	A	N1-C6-N6	11.82	125.69	118.60
27	B8	49	A	N1-C6-N6	11.82	125.69	118.60
27	B8	384	A	N1-C6-N6	11.82	125.69	118.60
1	AA	197	A	N1-C6-N6	11.82	125.69	118.60
1	AA	2	A	N1-C6-N6	11.82	125.69	118.60
1	AA	415	A	N1-C6-N6	11.82	125.69	118.60
27	B8	844	A	N1-C6-N6	11.82	125.69	118.60
27	B8	1808	A	N1-C6-N6	11.81	125.69	118.60
1	AA	315	A	N1-C6-N6	11.81	125.69	118.60
1	AA	356	A	N1-C6-N6	11.81	125.69	118.60
27	B8	917	A	N1-C6-N6	11.81	125.69	118.60
2	AX	22	A	N1-C6-N6	11.80	125.68	118.60
27	B8	470	A	N1-C6-N6	11.80	125.68	118.60
1	AA	777	A	N1-C6-N6	11.80	125.68	118.60
26	B7	104	A	N1-C6-N6	11.80	125.68	118.60
27	B8	422	A	N1-C6-N6	11.80	125.68	118.60
1	AA	1216	A	N1-C6-N6	11.80	125.68	118.60
27	B8	1789	A	N1-C6-N6	11.80	125.68	118.60
27	B8	196	A	N1-C6-N6	11.80	125.68	118.60
27	B8	1328	A	N1-C6-N6	11.80	125.68	118.60
1	AA	466	A	N1-C6-N6	11.79	125.68	118.60
1	AA	1102	A	N1-C6-N6	11.79	125.68	118.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1518	A	N1-C6-N6	11.79	125.67	118.60
27	B8	1156	A	N1-C6-N6	11.79	125.67	118.60
27	B8	2009	A	N1-C6-N6	11.79	125.67	118.60
27	B8	1508	A	N1-C6-N6	11.79	125.67	118.60
27	B8	1632	A	N1-C6-N6	11.79	125.67	118.60
1	AA	495	A	N1-C6-N6	11.78	125.67	118.60
1	AA	1227	A	N1-C6-N6	11.78	125.67	118.60
27	B8	1175	A	N1-C6-N6	11.78	125.67	118.60
1	AA	767	A	N1-C6-N6	11.78	125.67	118.60
27	B8	507	A	N1-C6-N6	11.78	125.67	118.60
27	B8	972	A	N1-C6-N6	11.78	125.67	118.60
27	B8	1571	A	N1-C6-N6	11.78	125.67	118.60
27	B8	1505	A	N1-C6-N6	11.78	125.67	118.60
1	AA	640	A	N1-C6-N6	11.77	125.66	118.60
27	B8	344	A	N1-C6-N6	11.77	125.66	118.60
27	B8	439	A	N1-C6-N6	11.77	125.66	118.60
27	B8	1801	A	N1-C6-N6	11.77	125.66	118.60
27	B8	2270	A	N1-C6-N6	11.77	125.66	118.60
27	B8	2736	A	N1-C6-N6	11.77	125.66	118.60
1	AA	1503	A	N1-C6-N6	11.76	125.66	118.60
1	AA	712	A	N1-C6-N6	11.76	125.66	118.60
27	B8	1322	A	N1-C6-N6	11.76	125.66	118.60
27	B8	1821	A	N1-C6-N6	11.76	125.66	118.60
1	AA	1483	A	N1-C6-N6	11.76	125.66	118.60
27	B8	1635	A	N1-C6-N6	11.76	125.66	118.60
27	B8	1477	A	N1-C6-N6	11.76	125.66	118.60
1	AA	1375	A	N1-C6-N6	11.76	125.65	118.60
1	AA	622	A	N1-C6-N6	11.75	125.65	118.60
27	B8	156	A	N1-C6-N6	11.75	125.65	118.60
27	B8	1744	A	N1-C6-N6	11.75	125.65	118.60
1	AA	397	A	N1-C6-N6	11.75	125.65	118.60
1	AA	968	A	N1-C6-N6	11.75	125.65	118.60
27	B8	722	A	N1-C6-N6	11.74	125.64	118.60
27	B8	1054	A	N1-C6-N6	11.74	125.64	118.60
27	B8	1509	A	N1-C6-N6	11.74	125.64	118.60
27	B8	478	A	N1-C6-N6	11.74	125.64	118.60
27	B8	896	A	N1-C6-N6	11.74	125.64	118.60
1	AA	790	A	N1-C6-N6	11.74	125.64	118.60
27	B8	2266	A	N1-C6-N6	11.74	125.64	118.60
27	B8	1535	A	N1-C6-N6	11.73	125.64	118.60
1	AA	975	A	N1-C6-N6	11.73	125.64	118.60
1	AA	1179	A	N1-C6-N6	11.73	125.64	118.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1248	A	N1-C6-N6	11.73	125.64	118.60
27	B8	1080	A	N1-C6-N6	11.73	125.64	118.60
1	AA	729	A	N1-C6-N6	11.73	125.64	118.60
3	AV	58	A	N1-C6-N6	11.73	125.64	118.60
27	B8	975	A	N1-C6-N6	11.72	125.63	118.60
27	B8	1960	A	N1-C6-N6	11.72	125.63	118.60
27	B8	2577	A	N1-C6-N6	11.72	125.63	118.60
1	AA	243	A	N1-C6-N6	11.72	125.63	118.60
1	AA	250	A	N1-C6-N6	11.72	125.63	118.60
27	B8	715	A	N1-C6-N6	11.72	125.63	118.60
1	AA	74	A	N1-C6-N6	11.71	125.63	118.60
27	B8	1889	A	N1-C6-N6	11.71	125.63	118.60
27	B8	2614	A	N1-C6-N6	11.71	125.63	118.60
1	AA	845	A	N1-C6-N6	11.71	125.63	118.60
27	B8	176	A	N1-C6-N6	11.71	125.63	118.60
27	B8	1010	A	N1-C6-N6	11.71	125.63	118.60
27	B8	2327	A	N1-C6-N6	11.71	125.63	118.60
1	AA	1130	A	N1-C6-N6	11.71	125.62	118.60
27	B8	2820	A	N1-C6-N6	11.71	125.62	118.60
27	B8	282	A	N1-C6-N6	11.71	125.62	118.60
1	AA	484	G	P-O3'-C3'	11.70	133.74	119.70
27	B8	547	A	N1-C6-N6	11.70	125.62	118.60
1	AA	909	A	N1-C6-N6	11.70	125.62	118.60
1	AA	1408	A	N1-C6-N6	11.70	125.62	118.60
1	AA	1502	A	N1-C6-N6	11.70	125.62	118.60
27	B8	1419	A	N1-C6-N6	11.70	125.62	118.60
27	B8	2070	A	N1-C6-N6	11.70	125.62	118.60
27	B8	2534	A	N1-C6-N6	11.70	125.62	118.60
1	AA	78	A	N1-C6-N6	11.69	125.62	118.60
27	B8	1746	A	N1-C6-N6	11.69	125.62	118.60
27	B8	508	A	N1-C6-N6	11.69	125.62	118.60
27	B8	910	A	N1-C6-N6	11.69	125.62	118.60
1	AA	663	A	N1-C6-N6	11.69	125.61	118.60
1	AA	130	A	N1-C6-N6	11.69	125.61	118.60
27	B8	918	A	N1-C6-N6	11.69	125.61	118.60
27	B8	2433	A	N1-C6-N6	11.69	125.61	118.60
1	AA	167	A	N1-C6-N6	11.69	125.61	118.60
27	B8	1365	A	N1-C6-N6	11.69	125.61	118.60
1	AA	1363	A	N1-C6-N6	11.68	125.61	118.60
27	B8	1359	A	N1-C6-N6	11.68	125.61	118.60
27	B8	1772	A	N1-C6-N6	11.68	125.61	118.60
27	B8	2117	A	N1-C6-N6	11.68	125.61	118.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	2497	A	N1-C6-N6	11.68	125.61	118.60
27	B8	432	A	N1-C6-N6	11.68	125.61	118.60
27	B8	1608	A	N1-C6-N6	11.68	125.61	118.60
27	B8	310	A	N1-C6-N6	11.68	125.61	118.60
1	AA	461	A	N1-C6-N6	11.68	125.61	118.60
27	B8	73	A	N1-C6-N6	11.68	125.61	118.60
27	B8	661	A	N1-C6-N6	11.68	125.61	118.60
27	B8	2468	A	N1-C6-N6	11.68	125.61	118.60
1	AA	412	A	N1-C6-N6	11.67	125.60	118.60
1	AA	681	A	N1-C6-N6	11.67	125.60	118.60
1	AA	704	A	N1-C6-N6	11.67	125.60	118.60
1	AA	298	A	N1-C6-N6	11.67	125.60	118.60
27	B8	643	A	N1-C6-N6	11.67	125.60	118.60
27	B8	1284	A	N1-C6-N6	11.67	125.60	118.60
27	B8	2082	A	N1-C6-N6	11.67	125.60	118.60
27	B8	1572	A	N1-C6-N6	11.66	125.60	118.60
1	AA	747	A	N1-C6-N6	11.66	125.60	118.60
27	B8	866	A	N1-C6-N6	11.66	125.60	118.60
1	AA	1340	A	N1-C6-N6	11.66	125.59	118.60
27	B8	404	A	N1-C6-N6	11.66	125.59	118.60
27	B8	1912	A	N1-C6-N6	11.65	125.59	118.60
27	B8	2476	A	N1-C6-N6	11.65	125.59	118.60
27	B8	391	A	N1-C6-N6	11.65	125.59	118.60
27	B8	1089	A	N1-C6-N6	11.65	125.59	118.60
1	AA	1145	A	N1-C6-N6	11.64	125.59	118.60
27	B8	753	A	N1-C6-N6	11.64	125.58	118.60
26	B7	53	A	N1-C6-N6	11.64	125.58	118.60
27	B8	2513	A	N1-C6-N6	11.64	125.58	118.60
27	B8	2062	A	N1-C6-N6	11.63	125.58	118.60
1	AA	1410	A	N1-C6-N6	11.63	125.58	118.60
1	AA	1534	A	N1-C6-N6	11.63	125.58	118.60
27	B8	1916	A	N1-C6-N6	11.63	125.58	118.60
27	B8	2059	A	N1-C6-N6	11.63	125.58	118.60
27	B8	2590	A	N1-C6-N6	11.63	125.58	118.60
27	B8	2705	A	N1-C6-N6	11.63	125.58	118.60
27	B8	1749	A	N1-C6-N6	11.63	125.58	118.60
27	B8	144	A	N1-C6-N6	11.62	125.57	118.60
1	AA	374	A	N1-C6-N6	11.62	125.57	118.60
1	AA	977	A	N1-C6-N6	11.62	125.57	118.60
1	AA	1318	A	N1-C6-N6	11.62	125.57	118.60
1	AA	393	A	N1-C6-N6	11.62	125.57	118.60
27	B8	278	A	N1-C6-N6	11.61	125.57	118.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	408	A	N1-C6-N6	11.61	125.56	118.60
27	B8	131	A	N1-C6-N6	11.61	125.57	118.60
27	B8	1614	A	N1-C6-N6	11.60	125.56	118.60
27	B8	1265	A	N1-C6-N6	11.60	125.56	118.60
27	B8	1544	A	N1-C6-N6	11.60	125.56	118.60
1	AA	7	A	N1-C6-N6	11.60	125.56	118.60
1	AA	1042	A	N1-C6-N6	11.60	125.56	118.60
27	B8	2883	A	N1-C6-N6	11.60	125.56	118.60
27	B8	2418	A	N1-C6-N6	11.59	125.56	118.60
27	B8	2886	A	N1-C6-N6	11.59	125.55	118.60
27	B8	1247	A	N1-C6-N6	11.59	125.55	118.60
27	B8	1304	A	N1-C6-N6	11.59	125.55	118.60
1	AA	327	A	N1-C6-N6	11.58	125.55	118.60
27	B8	1254	A	N1-C6-N6	11.58	125.55	118.60
27	B8	1919	A	N1-C6-N6	11.58	125.55	118.60
27	B8	2287	A	N1-C6-N6	11.58	125.55	118.60
1	AA	50	A	N1-C6-N6	11.58	125.55	118.60
27	B8	71	A	N1-C6-N6	11.58	125.55	118.60
27	B8	165	A	N1-C6-N6	11.58	125.55	118.60
1	AA	72	A	N1-C6-N6	11.57	125.55	118.60
27	B8	1040	A	N1-C6-N6	11.57	125.54	118.60
27	B8	2114	A	N1-C6-N6	11.57	125.54	118.60
27	B8	2765	A	N1-C6-N6	11.57	125.54	118.60
1	AA	913	A	N1-C6-N6	11.57	125.54	118.60
27	B8	2176	A	N1-C6-N6	11.57	125.54	118.60
27	B8	2721	A	N1-C6-N6	11.57	125.54	118.60
1	AA	1246	A	N1-C6-N6	11.57	125.54	118.60
1	AA	1339	A	N1-C6-N6	11.56	125.54	118.60
27	B8	750	A	N1-C6-N6	11.56	125.54	118.60
27	B8	1336	A	N1-C6-N6	11.56	125.54	118.60
27	B8	2664	G	N1-C6-O6	11.56	126.84	119.90
27	B8	1133	A	N1-C6-N6	11.56	125.53	118.60
27	B8	2077	A	N1-C6-N6	11.56	125.53	118.60
1	AA	702	A	N1-C6-N6	11.55	125.53	118.60
1	AA	1531	A	N1-C6-N6	11.55	125.53	118.60
1	AA	452	A	N1-C6-N6	11.55	125.53	118.60
27	B8	1569	A	N1-C6-N6	11.55	125.53	118.60
27	B8	614	A	N1-C6-N6	11.54	125.53	118.60
27	B8	1711	A	N1-C6-N6	11.54	125.53	118.60
27	B8	1276	A	N1-C6-N6	11.54	125.53	118.60
27	B8	1434	A	N1-C6-N6	11.54	125.52	118.60
27	B8	2835	A	N1-C6-N6	11.54	125.52	118.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	160	A	N1-C6-N6	11.53	125.52	118.60
1	AA	411	A	N1-C6-N6	11.53	125.52	118.60
1	AA	1204	A	N1-C6-N6	11.53	125.52	118.60
27	B8	2733	A	N1-C6-N6	11.53	125.52	118.60
1	AA	523	A	N1-C6-N6	11.52	125.51	118.60
27	B8	2199	A	N1-C6-N6	11.52	125.51	118.60
27	B8	2566	A	N1-C6-N6	11.51	125.51	118.60
27	B8	2882	A	N1-C6-N6	11.51	125.51	118.60
1	AA	609	A	N1-C6-N6	11.51	125.51	118.60
27	B8	2095	A	N1-C6-N6	11.51	125.50	118.60
27	B8	1272	A	N1-C6-N6	11.51	125.50	118.60
27	B8	1583	A	N1-C6-N6	11.51	125.50	118.60
27	B8	74	A	N1-C6-N6	11.50	125.50	118.60
27	B8	1616	A	N1-C6-N6	11.50	125.50	118.60
1	AA	364	A	N1-C6-N6	11.50	125.50	118.60
27	B8	21	A	N1-C6-N6	11.50	125.50	118.60
27	B8	2030	A	N1-C6-N6	11.50	125.50	118.60
1	AA	1428	A	N1-C6-N6	11.49	125.50	118.60
27	B8	988	A	N1-C6-N6	11.49	125.50	118.60
1	AA	649	A	N1-C6-N6	11.48	125.49	118.60
27	B8	2530	A	N1-C6-N6	11.48	125.49	118.60
27	B8	920	A	N1-C6-N6	11.48	125.49	118.60
27	B8	927	A	N1-C6-N6	11.48	125.49	118.60
1	AA	313	A	N1-C6-N6	11.48	125.49	118.60
1	AA	819	A	N1-C6-N6	11.48	125.49	118.60
1	AA	1413	A	N1-C6-N6	11.47	125.48	118.60
1	AA	535	A	N1-C6-N6	11.47	125.48	118.60
1	AA	949	A	N1-C6-N6	11.47	125.48	118.60
27	B8	126	A	N1-C6-N6	11.47	125.48	118.60
27	B8	453	A	N1-C6-N6	11.47	125.48	118.60
27	B8	1067	A	N1-C6-N6	11.47	125.48	118.60
1	AA	382	A	N1-C6-N6	11.47	125.48	118.60
1	AA	449	G	N1-C6-O6	11.47	126.78	119.90
27	B8	2134	A	N1-C6-N6	11.46	125.48	118.60
1	AA	1225	A	N1-C6-N6	11.46	125.48	118.60
27	B8	2336	A	N1-C6-N6	11.46	125.48	118.60
1	AA	969	A	N1-C6-N6	11.46	125.47	118.60
1	AA	792	A	N1-C6-N6	11.46	125.47	118.60
1	AA	441	A	N1-C6-N6	11.45	125.47	118.60
27	B8	1321	A	N1-C6-N6	11.45	125.47	118.60
27	B8	1910	G	N1-C6-O6	11.45	126.77	119.90
1	AA	1256	A	N1-C6-N6	11.45	125.47	118.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	64	A	N1-C6-N6	11.44	125.47	118.60
27	B8	1395	A	N1-C6-N6	11.44	125.46	118.60
27	B8	2635	A	N1-C6-N6	11.44	125.46	118.60
1	AA	1508	A	N1-C6-N6	11.44	125.46	118.60
1	AA	547	A	N1-C6-N6	11.44	125.46	118.60
1	AA	878	A	N1-C6-N6	11.43	125.46	118.60
1	AA	1429	A	N1-C6-N6	11.43	125.46	118.60
27	B8	1510	G	N1-C6-O6	11.42	126.75	119.90
27	B8	2726	A	N1-C6-N6	11.42	125.45	118.60
27	B8	1147	A	N1-C6-N6	11.42	125.45	118.60
1	AA	1368	A	N1-C6-N6	11.42	125.45	118.60
3	AV	33	A	N1-C6-N6	11.42	125.45	118.60
27	B8	1469	A	N1-C6-N6	11.42	125.45	118.60
27	B8	340	A	N1-C6-N6	11.41	125.45	118.60
27	B8	613	A	N1-C6-N6	11.41	125.45	118.60
1	AA	1012	A	N1-C6-N6	11.41	125.45	118.60
27	B8	2020	A	N1-C6-N6	11.41	125.44	118.60
27	B8	526	A	N1-C6-N6	11.41	125.44	118.60
27	B8	781	A	N1-C6-N6	11.41	125.44	118.60
27	B8	2542	A	N1-C6-N6	11.41	125.44	118.60
1	AA	665	A	N1-C6-N6	11.40	125.44	118.60
27	B8	1103	A	N1-C6-N6	11.40	125.44	118.60
27	B8	751	A	N1-C6-N6	11.40	125.44	118.60
27	B8	1165	A	N1-C6-N6	11.40	125.44	118.60
3	AV	74	A	N1-C6-N6	11.40	125.44	118.60
27	B8	1237	A	N1-C6-N6	11.40	125.44	118.60
27	B8	2108	A	N1-C6-N6	11.40	125.44	118.60
26	B7	99	A	N1-C6-N6	11.39	125.44	118.60
27	B8	1142	A	N1-C6-N6	11.39	125.44	118.60
27	B8	1596	A	N1-C6-N6	11.39	125.44	118.60
1	AA	325	A	N1-C6-N6	11.39	125.43	118.60
27	B8	142	A	N1-C6-N6	11.39	125.43	118.60
27	B8	800	A	N1-C6-N6	11.39	125.43	118.60
27	B8	1373	A	N1-C6-N6	11.39	125.43	118.60
27	B8	42	A	N1-C6-N6	11.39	125.43	118.60
26	B7	52	A	N1-C6-N6	11.38	125.43	118.60
27	B8	1786	A	N1-C6-N6	11.38	125.43	118.60
1	AA	1332	A	N1-C6-N6	11.37	125.42	118.60
27	B8	2872	A	N1-C6-N6	11.37	125.42	118.60
26	B7	59	A	N1-C6-N6	11.36	125.42	118.60
27	B8	529	A	N1-C6-N6	11.36	125.42	118.60
27	B8	1494	A	N1-C6-N6	11.36	125.41	118.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	222	A	N1-C6-N6	11.35	125.41	118.60
1	AA	1346	A	N1-C6-N6	11.35	125.41	118.60
1	AA	825	A	N1-C6-N6	11.35	125.41	118.60
27	B8	783	A	N1-C6-N6	11.35	125.41	118.60
27	B8	1848	A	N1-C6-N6	11.34	125.41	118.60
27	B8	2425	A	P-O3'-C3'	11.34	133.31	119.70
3	AV	60	A	N1-C6-N6	11.34	125.40	118.60
27	B8	1086	A	N1-C6-N6	11.34	125.40	118.60
27	B8	1111	A	N1-C6-N6	11.34	125.40	118.60
27	B8	541	A	N1-C6-N6	11.33	125.40	118.60
1	AA	864	A	N1-C6-N6	11.33	125.40	118.60
27	B8	2029	G	N1-C6-O6	11.33	126.70	119.90
27	B8	941	A	N1-C6-N6	11.32	125.39	118.60
27	B8	2060	A	N1-C6-N6	11.31	125.39	118.60
27	B8	2451	A	N1-C6-N6	11.31	125.38	118.60
26	B7	73	A	N1-C6-N6	11.30	125.38	118.60
27	B8	2761	A	N1-C6-N6	11.31	125.38	118.60
1	AA	432	A	N1-C6-N6	11.30	125.38	118.60
27	B8	1189	A	N1-C6-N6	11.30	125.38	118.60
27	B8	479	A	N1-C6-N6	11.28	125.37	118.60
27	B8	63	A	N1-C6-N6	11.28	125.37	118.60
27	B8	362	A	N1-C6-N6	11.28	125.37	118.60
1	AA	794	A	N1-C6-N6	11.28	125.37	118.60
27	B8	1088	A	N1-C6-N6	11.28	125.37	118.60
27	B8	621	A	N1-C6-N6	11.27	125.36	118.60
27	B8	1580	A	N1-C6-N6	11.27	125.36	118.60
27	B8	886	A	N1-C6-N6	11.27	125.36	118.60
1	AA	60	A	P-O3'-C3'	11.27	133.22	119.70
27	B8	477	A	N1-C6-N6	11.27	125.36	118.60
1	AA	1362	A	N1-C6-N6	11.27	125.36	118.60
27	B8	574	A	N1-C6-N6	11.27	125.36	118.60
1	AA	1176	A	N1-C6-N6	11.26	125.36	118.60
27	B8	1287	A	N1-C6-N6	11.26	125.36	118.60
27	B8	2543	G	N1-C6-O6	11.26	126.66	119.90
26	B7	15	A	N1-C6-N6	11.26	125.35	118.60
27	B8	94	A	N1-C6-N6	11.26	125.35	118.60
1	AA	60	A	N1-C6-N6	11.25	125.35	118.60
27	B8	2856	A	N1-C6-N6	11.24	125.34	118.60
1	AA	908	A	N1-C6-N6	11.23	125.34	118.60
1	AA	1157	A	N1-C6-N6	11.23	125.34	118.60
1	AA	129	A	N1-C6-N6	11.22	125.33	118.60
1	AA	1150	A	N1-C6-N6	11.22	125.33	118.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	324	A	N1-C6-N6	11.22	125.33	118.60
27	B8	1679	A	N1-C6-N6	11.21	125.33	118.60
27	B8	1315	C	P-O3'-C3'	11.21	133.15	119.70
27	B8	1070	A	N1-C6-N6	11.21	125.32	118.60
1	AA	608	A	N1-C6-N6	11.20	125.32	118.60
27	B8	675	A	N1-C6-N6	11.20	125.32	118.60
27	B8	2750	A	N1-C6-N6	11.20	125.32	118.60
1	AA	1055	A	N1-C6-N6	11.19	125.32	118.60
1	AA	274	A	N1-C6-N6	11.18	125.31	118.60
27	B8	2829	A	N1-C6-N6	11.18	125.31	118.60
27	B8	118	A	N1-C6-N6	11.17	125.30	118.60
27	B8	1630	A	N1-C6-N6	11.16	125.30	118.60
1	AA	246	A	N1-C6-N6	11.16	125.30	118.60
27	B8	2564	A	N1-C6-N6	11.16	125.30	118.60
27	B8	1301	A	N1-C6-N6	11.15	125.29	118.60
27	B8	1307	A	N1-C6-N6	11.15	125.29	118.60
27	B8	1028	A	N1-C6-N6	11.15	125.29	118.60
27	B8	1690	A	N1-C6-N6	11.15	125.29	118.60
27	B8	727	A	N1-C6-N6	11.14	125.29	118.60
27	B8	1453	A	N1-C6-N6	11.14	125.29	118.60
1	AA	1206	G	N1-C6-O6	11.14	126.58	119.90
27	B8	2297	A	N1-C6-N6	11.13	125.28	118.60
27	B8	1021	A	N1-C6-N6	11.13	125.28	118.60
1	AA	1329	A	N1-C6-N6	11.13	125.28	118.60
1	AA	179	A	N1-C6-N6	11.12	125.27	118.60
27	B8	2764	A	N1-C6-N6	11.12	125.27	118.60
27	B8	2868	A	N1-C6-N6	11.12	125.27	118.60
27	B8	1853	A	N1-C6-N6	11.11	125.27	118.60
27	B8	2748	A	N1-C6-N6	11.11	125.27	118.60
27	B8	1854	A	N1-C6-N6	11.11	125.26	118.60
1	AA	554	A	N1-C6-N6	11.10	125.26	118.60
27	B8	279	A	N1-C6-N6	11.10	125.26	118.60
27	B8	1780	A	N1-C6-N6	11.10	125.26	118.60
27	B8	2015	A	N1-C6-N6	11.10	125.26	118.60
1	AA	1285	A	N1-C6-N6	11.10	125.26	118.60
27	B8	2119	A	N1-C6-N6	11.09	125.25	118.60
27	B8	1032	A	N1-C6-N6	11.08	125.25	118.60
1	AA	55	A	N1-C6-N6	11.07	125.24	118.60
27	B8	829	A	N1-C6-N6	11.07	125.24	118.60
1	AA	151	A	N1-C6-N6	11.05	125.23	118.60
3	AV	70	G	N1-C6-O6	11.05	126.53	119.90
27	B8	1126	A	N1-C6-N6	11.05	125.23	118.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	1439	A	N1-C6-N6	11.05	125.23	118.60
1	AA	148	G	N1-C6-O6	11.04	126.52	119.90
27	B8	1393	A	N1-C6-N6	11.04	125.22	118.60
1	AA	428	G	N1-C6-O6	11.04	126.52	119.90
1	AA	860	A	N1-C6-N6	11.04	125.22	118.60
1	AA	195	A	N1-C6-N6	11.03	125.22	118.60
27	B8	181	A	N1-C6-N6	11.02	125.21	118.60
27	B8	528	A	N1-C6-N6	11.01	125.21	118.60
1	AA	753	A	N1-C6-N6	11.01	125.21	118.60
27	B8	1872	A	N1-C6-N6	11.01	125.20	118.60
1	AA	171	A	N1-C6-N6	11.01	125.20	118.60
27	B8	1668	A	N1-C6-N6	11.01	125.20	118.60
27	B8	1641	A	N1-C6-N6	11.00	125.20	118.60
27	B8	1652	A	N1-C6-N6	11.00	125.20	118.60
27	B8	2225	A	N1-C6-N6	11.00	125.20	118.60
27	B8	825	A	N1-C6-N6	10.99	125.19	118.60
1	AA	696	A	N1-C6-N6	10.99	125.19	118.60
27	B8	900	A	N1-C6-N6	10.99	125.19	118.60
1	AA	26	A	N1-C6-N6	10.98	125.19	118.60
27	B8	2335	A	N1-C6-N6	10.97	125.18	118.60
1	AA	766	A	N1-C6-N6	10.95	125.17	118.60
1	AA	65	A	N1-C6-N6	10.94	125.16	118.60
27	B8	768	G	N1-C6-O6	10.94	126.46	119.90
27	B8	256	A	N1-C6-N6	10.94	125.16	118.60
27	B8	1803	A	N1-C6-N6	10.94	125.16	118.60
1	AA	533	A	N1-C6-N6	10.93	125.16	118.60
27	B8	1381	G	N1-C6-O6	10.93	126.46	119.90
27	B8	2273	A	N1-C6-N6	10.93	125.16	118.60
26	B7	57	A	N1-C6-N6	10.93	125.16	118.60
1	AA	520	A	N1-C6-N6	10.92	125.15	118.60
27	B8	2366	A	N1-C6-N6	10.92	125.15	118.60
1	AA	22	G	N1-C6-O6	10.90	126.44	119.90
1	AA	109	A	N1-C6-N6	10.90	125.14	118.60
1	AA	116	A	N1-C6-N6	10.90	125.14	118.60
1	AA	1333	A	N1-C6-N6	10.90	125.14	118.60
1	AA	914	A	N1-C6-N6	10.90	125.14	118.60
27	B8	1205	A	N1-C6-N6	10.90	125.14	118.60
27	B8	654	A	N1-C6-N6	10.89	125.14	118.60
27	B8	2435	A	N1-C6-N6	10.89	125.13	118.60
1	AA	76	G	N1-C6-O6	10.88	126.43	119.90
27	B8	1701	A	N1-C6-N6	10.87	125.12	118.60
1	AA	329	A	N1-C6-N6	10.86	125.11	118.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	933	A	N1-C6-N6	10.86	125.11	118.60
1	AA	301	G	N1-C6-O6	10.85	126.41	119.90
1	AA	509	A	N1-C6-N6	10.85	125.11	118.60
1	AA	1101	A	N1-C6-N6	10.85	125.11	118.60
26	B7	34	A	N1-C6-N6	10.83	125.10	118.60
27	B8	2747	G	N1-C6-O6	10.83	126.40	119.90
27	B8	556	A	N1-C6-N6	10.82	125.09	118.60
1	AA	1005	A	N1-C6-N6	10.81	125.08	118.60
27	B8	2135	A	N1-C6-N6	10.81	125.08	118.60
26	B7	78	A	N1-C6-N6	10.80	125.08	118.60
27	B8	1552	A	N1-C6-N6	10.80	125.08	118.60
27	B8	266	G	N1-C6-O6	10.80	126.38	119.90
27	B8	2014	A	N1-C6-N6	10.79	125.08	118.60
27	B8	559	G	N1-C6-O6	10.79	126.38	119.90
27	B8	990	A	N1-C6-N6	10.79	125.07	118.60
27	B8	670	A	N1-C6-N6	10.79	125.07	118.60
1	AA	487	A	N1-C6-N6	10.78	125.07	118.60
1	AA	1392	G	N1-C6-O6	10.76	126.36	119.90
1	AA	431	A	N1-C6-N6	10.75	125.05	118.60
1	AA	674	G	N1-C6-O6	10.75	126.35	119.90
1	AA	1486	G	N1-C6-O6	10.75	126.35	119.90
1	AA	1034	G	N1-C6-O6	10.74	126.34	119.90
27	B8	2169	A	N1-C6-N6	10.74	125.04	118.60
1	AA	414	A	N1-C6-N6	10.74	125.04	118.60
27	B8	663	G	N1-C6-O6	10.74	126.34	119.90
27	B8	2033	A	N1-C6-N6	10.73	125.04	118.60
27	B8	916	G	N1-C6-O6	10.73	126.34	119.90
27	B8	1445	G	N1-C6-O6	10.72	126.33	119.90
27	B8	161	A	N1-C6-N6	10.71	125.03	118.60
27	B8	374	A	N1-C6-N6	10.71	125.03	118.60
1	AA	184	G	N1-C6-O6	10.71	126.32	119.90
1	AA	718	A	N1-C6-N6	10.71	125.02	118.60
27	B8	1783	A	N1-C6-N6	10.70	125.02	118.60
27	B8	2124	G	N1-C6-O6	10.70	126.32	119.90
1	AA	366	A	P-O3'-C3'	10.69	132.53	119.70
27	B8	505	A	N1-C6-N6	10.69	125.02	118.60
27	B8	2201	G	N1-C6-O6	10.69	126.31	119.90
27	B8	194	G	N1-C6-O6	10.69	126.31	119.90
27	B8	2778	A	N1-C6-N6	10.67	125.00	118.60
1	AA	584	G	N1-C6-O6	10.66	126.30	119.90
1	AA	1319	A	N1-C6-N6	10.66	125.00	118.60
27	B8	1885	A	N1-C6-N6	10.66	125.00	118.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	353	A	N1-C6-N6	10.63	124.98	118.60
27	B8	1717	A	N1-C6-N6	10.63	124.98	118.60
27	B8	2469	A	N1-C6-N6	10.63	124.98	118.60
27	B8	2298	A	N1-C6-N6	10.62	124.97	118.60
27	B8	1378	A	N1-C6-N6	10.62	124.97	118.60
27	B8	1975	G	N1-C6-O6	10.62	126.27	119.90
27	B8	2903	U	O4'-C1'-N1	10.61	116.69	108.20
27	B8	248	G	N1-C6-O6	10.61	126.26	119.90
27	B8	616	A	N1-C6-N6	10.59	124.96	118.60
1	AA	258	G	N1-C6-O6	10.59	126.25	119.90
1	AA	1275	A	N1-C6-N6	10.58	124.95	118.60
27	B8	1907	G	N1-C6-O6	10.58	126.25	119.90
27	B8	2234	G	N1-C6-O6	10.58	126.25	119.90
1	AA	168	G	N1-C6-O6	10.57	126.24	119.90
1	AA	484	G	N1-C6-O6	10.56	126.23	119.90
27	B8	820	A	N1-C6-N6	10.56	124.93	118.60
27	B8	2212	A	N1-C6-N6	10.55	124.93	118.60
1	AA	1289	A	N1-C6-N6	10.55	124.93	118.60
1	AA	1290	G	N1-C6-O6	10.55	126.23	119.90
27	B8	2052	A	N1-C6-N6	10.55	124.93	118.60
1	AA	973	G	N1-C6-O6	10.55	126.23	119.90
27	B8	2268	A	N1-C6-N6	10.54	124.92	118.60
27	B8	1522	A	N1-C6-N6	10.53	124.92	118.60
1	AA	687	A	N1-C6-N6	10.53	124.92	118.60
27	B8	1001	A	N1-C6-N6	10.52	124.91	118.60
27	B8	2054	A	N1-C6-N6	10.52	124.91	118.60
27	B8	2535	G	N1-C6-O6	10.52	126.21	119.90
27	B8	2485	G	N1-C6-O6	10.51	126.21	119.90
1	AA	1435	G	N1-C6-O6	10.49	126.19	119.90
27	B8	2392	A	N1-C6-N6	10.49	124.89	118.60
1	AA	782	A	N1-C6-N6	10.48	124.89	118.60
27	B8	103	A	N1-C6-N6	10.48	124.89	118.60
27	B8	2447	G	N1-C6-O6	10.48	126.19	119.90
1	AA	99	C	O4'-C1'-N1	10.48	116.58	108.20
1	AA	570	G	N1-C6-O6	10.48	126.19	119.90
27	B8	350	G	N1-C6-O6	10.48	126.19	119.90
27	B8	2024	G	N1-C6-O6	10.48	126.19	119.90
1	AA	417	G	N1-C6-O6	10.47	126.19	119.90
27	B8	2587	A	N1-C6-N6	10.47	124.88	118.60
27	B8	2673	G	N1-C6-O6	10.47	126.18	119.90
27	B8	1342	A	N1-C6-N6	10.47	124.88	118.60
27	B8	514	A	N1-C6-N6	10.46	124.88	118.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	2741	A	N1-C6-N6	10.46	124.88	118.60
27	B8	1553	A	N1-C6-N6	10.46	124.88	118.60
27	B8	2027	G	N1-C6-O6	10.46	126.17	119.90
1	AA	275	G	N1-C6-O6	10.45	126.17	119.90
27	B8	1106	G	N1-C6-O6	10.45	126.17	119.90
27	B8	954	G	N1-C6-O6	10.45	126.17	119.90
27	B8	2624	G	N1-C6-O6	10.45	126.17	119.90
27	B8	346	A	N1-C6-N6	10.44	124.86	118.60
27	B8	2895	G	N1-C6-O6	10.43	126.16	119.90
1	AA	1033	G	N1-C6-O6	10.43	126.16	119.90
1	AA	1441	A	N1-C6-N6	10.43	124.86	118.60
1	AA	541	G	N1-C6-O6	10.42	126.15	119.90
27	B8	2227	A	N1-C6-N6	10.41	124.84	118.60
1	AA	1184	G	N1-C6-O6	10.40	126.14	119.90
27	B8	409	G	N1-C6-O6	10.40	126.14	119.90
27	B8	609	A	N1-C6-N6	10.40	124.84	118.60
1	AA	669	G	N1-C6-O6	10.39	126.13	119.90
27	B8	2279	G	N1-C6-O6	10.39	126.13	119.90
27	B8	424	G	N1-C6-O6	10.38	126.13	119.90
27	B8	538	A	N1-C6-N6	10.38	124.83	118.60
1	AA	454	G	N1-C6-O6	10.38	126.13	119.90
1	AA	259	G	N1-C6-O6	10.37	126.12	119.90
27	B8	2421	G	N1-C6-O6	10.37	126.12	119.90
26	B7	112	G	N1-C6-O6	10.36	126.12	119.90
27	B8	428	A	N1-C6-N6	10.36	124.82	118.60
1	AA	1191	A	N1-C6-N6	10.35	124.81	118.60
27	B8	1268	A	N1-C6-N6	10.35	124.81	118.60
1	AA	145	G	N1-C6-O6	10.34	126.11	119.90
27	B8	2304	G	N1-C6-O6	10.33	126.10	119.90
1	AA	457	G	N1-C6-O6	10.31	126.09	119.90
27	B8	757	G	N1-C6-O6	10.31	126.09	119.90
1	AA	616	G	N1-C6-O6	10.30	126.08	119.90
1	AA	1020	G	N1-C6-O6	10.30	126.08	119.90
27	B8	1743	G	N1-C6-O6	10.29	126.07	119.90
1	AA	1523	G	N1-C6-O6	10.28	126.07	119.90
27	B8	1422	G	N1-C6-O6	10.26	126.06	119.90
1	AA	778	G	N1-C6-O6	10.24	126.05	119.90
1	AA	1058	G	N1-C6-O6	10.24	126.05	119.90
1	AA	359	G	N1-C6-O6	10.24	126.04	119.90
27	B8	442	G	N1-C6-O6	10.24	126.04	119.90
1	AA	104	G	N1-C6-O6	10.23	126.04	119.90
27	B8	460	A	N1-C6-N6	10.23	124.74	118.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	628	G	N1-C6-O6	10.23	126.04	119.90
27	B8	1937	A	N1-C6-N6	10.23	124.74	118.60
1	AA	122	G	N1-C6-O6	10.22	126.03	119.90
27	B8	676	A	N1-C6-N6	10.22	124.73	118.60
26	B7	81	G	N1-C6-O6	10.21	126.03	119.90
27	B8	978	G	N1-C6-O6	10.21	126.03	119.90
1	AA	15	G	N1-C6-O6	10.21	126.03	119.90
1	AA	626	G	N1-C6-O6	10.21	126.03	119.90
27	B8	1492	G	N1-C6-O6	10.21	126.03	119.90
1	AA	1433	A	N1-C6-N6	10.19	124.72	118.60
27	B8	2363	G	N1-C6-O6	10.19	126.02	119.90
27	B8	1689	A	N1-C6-N6	10.19	124.71	118.60
1	AA	372	C	P-O3'-C3'	10.18	131.92	119.70
1	AA	1201	A	P-O3'-C3'	10.18	131.92	119.70
27	B8	735	A	N1-C6-N6	10.18	124.71	118.60
27	B8	1098	A	N1-C6-N6	10.18	124.70	118.60
27	B8	2601	C	P-O3'-C3'	10.18	131.91	119.70
27	B8	1785	A	N1-C6-N6	10.16	124.70	118.60
27	B8	1076	C	O4'-C1'-N1	10.15	116.32	108.20
27	B8	1627	G	N1-C6-O6	10.15	125.99	119.90
27	B8	2046	G	N1-C6-O6	10.15	125.99	119.90
27	B8	401	A	N1-C6-N6	10.15	124.69	118.60
27	B8	1655	A	N1-C6-N6	10.15	124.69	118.60
27	B8	2057	G	N1-C6-O6	10.15	125.99	119.90
27	B8	2714	G	N1-C6-O6	10.14	125.98	119.90
27	B8	244	A	N1-C6-N6	10.14	124.68	118.60
1	AA	164	G	N1-C6-O6	10.12	125.97	119.90
1	AA	1405	G	N1-C6-O6	10.12	125.97	119.90
27	B8	1157	G	N1-C6-O6	10.12	125.97	119.90
27	B8	2639	A	N1-C6-N6	10.12	124.67	118.60
1	AA	147	G	N1-C6-O6	10.12	125.97	119.90
27	B8	1649	G	N1-C6-O6	10.12	125.97	119.90
1	AA	933	G	N1-C6-O6	10.12	125.97	119.90
27	B8	501	A	N1-C6-N6	10.11	124.67	118.60
1	AA	601	G	N1-C6-O6	10.11	125.96	119.90
27	B8	784	G	N1-C6-O6	10.11	125.96	119.90
1	AA	1284	C	P-O3'-C3'	10.11	131.83	119.70
27	B8	1826	G	N1-C6-O6	10.11	125.96	119.90
1	AA	1048	G	N1-C6-O6	10.10	125.96	119.90
1	AA	424	G	N1-C6-O6	10.09	125.95	119.90
27	B8	2648	G	N1-C6-O6	10.09	125.95	119.90
1	AA	1338	G	O4'-C1'-N9	10.09	116.27	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	2544	G	N1-C6-O6	10.08	125.95	119.90
27	B8	2692	G	N1-C6-O6	10.08	125.95	119.90
1	AA	627	G	N1-C6-O6	10.08	125.95	119.90
1	AA	1455	G	N1-C6-O6	10.07	125.94	119.90
27	B8	1059	G	N1-C6-O6	10.07	125.94	119.90
27	B8	524	G	N1-C6-O6	10.07	125.94	119.90
1	AA	1006	G	N1-C6-O6	10.07	125.94	119.90
1	AA	279	A	P-O3'-C3'	10.06	131.78	119.70
27	B8	1038	G	N1-C6-O6	10.06	125.94	119.90
1	AA	1072	G	N1-C6-O6	10.05	125.93	119.90
27	B8	108	G	N1-C6-O6	10.05	125.93	119.90
27	B8	2409	G	N1-C6-O6	10.05	125.93	119.90
1	AA	413	G	N1-C6-O6	10.04	125.92	119.90
27	B8	701	G	N1-C6-O6	10.04	125.92	119.90
27	B8	1479	G	N1-C6-O6	10.04	125.92	119.90
27	B8	2839	G	N1-C6-O6	10.04	125.92	119.90
27	B8	496	G	N1-C6-O6	10.03	125.92	119.90
27	B8	1338	G	N1-C6-O6	10.03	125.92	119.90
27	B8	141	G	N1-C6-O6	10.03	125.92	119.90
27	B8	533	G	N1-C6-O6	10.03	125.92	119.90
1	AA	786	G	N1-C6-O6	10.03	125.92	119.90
1	AA	724	G	N1-C6-O6	10.03	125.92	119.90
27	B8	864	G	N1-C6-O6	10.03	125.92	119.90
27	B8	1421	G	N1-C6-O6	10.03	125.92	119.90
27	B8	2400	G	N1-C6-O6	10.03	125.92	119.90
1	AA	667	G	N1-C6-O6	10.02	125.91	119.90
27	B8	471	A	N1-C6-N6	10.02	124.61	118.60
27	B8	777	G	N1-C6-O6	10.02	125.91	119.90
27	B8	2819	G	N1-C6-O6	10.02	125.91	119.90
27	B8	953	G	N1-C6-O6	10.02	125.91	119.90
27	B8	2478	A	N1-C6-N6	10.02	124.61	118.60
1	AA	1497	G	N1-C6-O6	10.01	125.91	119.90
27	B8	699	A	N1-C6-N6	10.01	124.61	118.60
1	AA	450	G	N1-C6-O6	10.01	125.90	119.90
27	B8	2472	G	N1-C6-O6	10.01	125.90	119.90
26	B7	45	A	N1-C6-N6	10.00	124.60	118.60
27	B8	371	A	N1-C6-N6	10.00	124.60	118.60
27	B8	2056	G	N1-C6-O6	10.00	125.90	119.90
1	AA	302	G	N1-C6-O6	9.99	125.89	119.90
27	B8	412	A	N1-C6-N6	9.98	124.59	118.60
27	B8	2894	G	N1-C6-O6	9.98	125.89	119.90
27	B8	1901	A	N1-C6-N6	9.98	124.59	118.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	B7	54	G	N1-C6-O6	9.97	125.89	119.90
1	AA	75	G	N1-C6-O6	9.97	125.88	119.90
27	B8	662	G	N1-C6-O6	9.97	125.88	119.90
1	AA	849	G	N1-C6-O6	9.96	125.88	119.90
1	AA	889	A	N1-C6-N6	9.96	124.58	118.60
27	B8	81	G	N1-C6-O6	9.96	125.88	119.90
27	B8	2694	G	N1-C6-O6	9.96	125.88	119.90
27	B8	2147	A	P-O3'-C3'	9.96	131.65	119.70
27	B8	273	G	N1-C6-O6	9.96	125.87	119.90
1	AA	642	A	N1-C6-N6	9.96	124.57	118.60
1	AA	1323	G	N1-C6-O6	9.96	125.87	119.90
1	AA	951	G	N1-C6-O6	9.95	125.87	119.90
27	B8	1389	G	N1-C6-O6	9.95	125.87	119.90
1	AA	521	G	N1-C6-O6	9.95	125.87	119.90
27	B8	1465	G	N1-C6-O6	9.95	125.87	119.90
27	B8	1154	G	N1-C6-O6	9.95	125.87	119.90
27	B8	2414	G	N1-C6-O6	9.95	125.87	119.90
1	AA	138	G	N1-C6-O6	9.94	125.87	119.90
27	B8	1232	G	N1-C6-O6	9.94	125.87	119.90
27	B8	1515	A	O4'-C1'-N9	9.94	116.16	108.20
27	B8	1215	G	N1-C6-O6	9.94	125.87	119.90
1	AA	200	G	N1-C6-O6	9.94	125.86	119.90
26	B7	33	G	N1-C6-O6	9.94	125.86	119.90
26	B7	15	A	O4'-C1'-N9	9.94	116.15	108.20
1	AA	105	G	N1-C6-O6	9.94	125.86	119.90
1	AA	685	G	N1-C6-O6	9.92	125.86	119.90
27	B8	1815	A	N1-C6-N6	9.92	124.55	118.60
27	B8	2012	G	N1-C6-O6	9.92	125.85	119.90
27	B8	9	G	N1-C6-O6	9.92	125.85	119.90
27	B8	1896	G	N1-C6-O6	9.92	125.85	119.90
1	AA	279	A	N1-C6-N6	9.91	124.55	118.60
27	B8	1540	G	N1-C6-O6	9.91	125.85	119.90
27	B8	86	G	N1-C6-O6	9.91	125.84	119.90
1	AA	1133	G	N1-C6-O6	9.91	125.84	119.90
27	B8	2623	G	N1-C6-O6	9.91	125.84	119.90
27	B8	2583	G	N1-C6-O6	9.90	125.84	119.90
27	B8	2621	G	N1-C6-O6	9.90	125.84	119.90
27	B8	2383	G	N1-C6-O6	9.90	125.84	119.90
27	B8	520	G	N1-C6-O6	9.90	125.84	119.90
1	AA	39	G	N1-C6-O6	9.90	125.84	119.90
1	AA	1061	G	N1-C6-O6	9.90	125.84	119.90
27	B8	2803	G	N1-C6-O6	9.90	125.84	119.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	949	G	N1-C6-O6	9.89	125.84	119.90
27	B8	454	A	N1-C6-N6	9.89	124.54	118.60
27	B8	1182	G	N1-C6-O6	9.89	125.83	119.90
27	B8	2757	A	N1-C6-N6	9.89	124.53	118.60
1	AA	1164	G	N1-C6-O6	9.89	125.83	119.90
27	B8	875	G	N1-C6-O6	9.89	125.83	119.90
1	AA	57	G	N1-C6-O6	9.88	125.83	119.90
27	B8	659	G	N1-C6-O6	9.88	125.83	119.90
27	B8	2445	G	N1-C6-O6	9.88	125.83	119.90
26	B7	9	G	N1-C6-O6	9.88	125.83	119.90
27	B8	1435	G	N1-C6-O6	9.88	125.83	119.90
1	AA	838	G	N1-C6-O6	9.87	125.82	119.90
1	AA	711	G	N1-C6-O6	9.87	125.82	119.90
27	B8	2053	G	N1-C6-O6	9.87	125.82	119.90
27	B8	2574	G	N1-C6-O6	9.87	125.82	119.90
27	B8	2437	G	N1-C6-O6	9.87	125.82	119.90
27	B8	2140	G	N1-C6-O6	9.86	125.82	119.90
1	AA	812	G	N1-C6-O6	9.86	125.82	119.90
27	B8	291	G	N1-C6-O6	9.86	125.82	119.90
27	B8	1517	G	N1-C6-O6	9.86	125.82	119.90
27	B8	617	G	N1-C6-O6	9.86	125.82	119.90
1	AA	373	A	N1-C6-N6	9.86	124.51	118.60
27	B8	2709	G	N1-C6-O6	9.85	125.81	119.90
1	AA	617	G	N1-C6-O6	9.85	125.81	119.90
1	AA	1233	G	N1-C6-O6	9.85	125.81	119.90
1	AA	27	G	N1-C6-O6	9.85	125.81	119.90
1	AA	785	G	N1-C6-O6	9.85	125.81	119.90
27	B8	1034	G	N1-C6-O6	9.84	125.81	119.90
27	B8	1973	G	N1-C6-O6	9.84	125.81	119.90
1	AA	240	G	N1-C6-O6	9.84	125.81	119.90
1	AA	645	G	N1-C6-O6	9.84	125.80	119.90
1	AA	917	G	N1-C6-O6	9.84	125.80	119.90
27	B8	230	G	N1-C6-O6	9.83	125.80	119.90
27	B8	312	G	N1-C6-O6	9.83	125.80	119.90
27	B8	649	G	N1-C6-O6	9.83	125.80	119.90
1	AA	1419	G	N1-C6-O6	9.83	125.80	119.90
27	B8	2217	G	N1-C6-O6	9.83	125.80	119.90
27	B8	2702	G	N1-C6-O6	9.83	125.80	119.90
27	B8	1424	G	N1-C6-O6	9.82	125.80	119.90
27	B8	2631	G	N1-C6-O6	9.82	125.79	119.90
27	B8	483	A	N1-C6-N6	9.82	124.49	118.60
1	AA	117	G	N1-C6-O6	9.82	125.79	119.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	448	A	N1-C6-N6	9.82	124.49	118.60
27	B8	729	G	N1-C6-O6	9.82	125.79	119.90
1	AA	61	G	N1-C6-O6	9.81	125.79	119.90
27	B8	682	G	N1-C6-O6	9.81	125.79	119.90
27	B8	1193	G	N1-C6-O6	9.81	125.79	119.90
1	AA	115	G	N1-C6-O6	9.81	125.78	119.90
1	AA	1300	G	N1-C6-O6	9.81	125.78	119.90
27	B8	1809	A	N1-C6-N6	9.81	124.48	118.60
1	AA	1457	G	N1-C6-O6	9.81	125.78	119.90
27	B8	1538	G	N1-C6-O6	9.81	125.78	119.90
27	B8	1418	G	N1-C6-O6	9.80	125.78	119.90
27	B8	1797	G	N1-C6-O6	9.80	125.78	119.90
27	B8	2657	A	N1-C6-N6	9.80	124.48	118.60
27	B8	2221	G	N1-C6-O6	9.79	125.78	119.90
27	B8	1643	G	N1-C6-O6	9.79	125.78	119.90
1	AA	954	G	N1-C6-O6	9.79	125.77	119.90
26	B7	21	G	N1-C6-O6	9.78	125.77	119.90
27	B8	2722	G	N1-C6-O6	9.78	125.77	119.90
1	AA	45	G	N1-C6-O6	9.78	125.77	119.90
1	AA	1334	G	N1-C6-O6	9.78	125.77	119.90
27	B8	2093	G	N1-C6-O6	9.78	125.77	119.90
1	AA	1261	A	N1-C6-N6	9.77	124.46	118.60
27	B8	977	G	N1-C6-O6	9.77	125.76	119.90
27	B8	809	G	N1-C6-O6	9.77	125.76	119.90
27	B8	2654	A	N1-C6-N6	9.77	124.46	118.60
1	AA	1034	G	C5-C6-O6	-9.77	122.74	128.60
27	B8	2136	G	N1-C6-O6	9.77	125.76	119.90
1	AA	1511	G	N1-C6-O6	9.76	125.76	119.90
27	B8	123	G	N1-C6-O6	9.76	125.76	119.90
27	B8	2141	G	N1-C6-O6	9.76	125.76	119.90
27	B8	1239	G	N1-C6-O6	9.76	125.76	119.90
1	AA	1385	G	N1-C6-O6	9.76	125.75	119.90
27	B8	407	G	N1-C6-O6	9.76	125.75	119.90
1	AA	1193	G	N1-C6-O6	9.76	125.75	119.90
27	B8	400	G	N1-C6-O6	9.75	125.75	119.90
27	B8	2069	G	N1-C6-O6	9.75	125.75	119.90
27	B8	2123	G	N1-C6-O6	9.75	125.75	119.90
26	B7	10	G	N1-C6-O6	9.75	125.75	119.90
27	B8	1734	G	N1-C6-O6	9.75	125.75	119.90
27	B8	1218	G	N1-C6-O6	9.75	125.75	119.90
26	B7	86	G	N1-C6-O6	9.74	125.75	119.90
27	B8	1478	G	N1-C6-O6	9.74	125.75	119.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	2812	G	N1-C6-O6	9.74	125.75	119.90
27	B8	1099	G	N1-C6-O6	9.74	125.74	119.90
27	B8	1191	G	N1-C6-O6	9.74	125.74	119.90
1	AA	455	G	N1-C6-O6	9.74	125.74	119.90
27	B8	326	G	N1-C6-O6	9.74	125.74	119.90
1	AA	1220	G	N1-C6-O6	9.73	125.74	119.90
27	B8	2315	G	N1-C6-O6	9.73	125.74	119.90
1	AA	1423	G	N1-C6-O6	9.73	125.74	119.90
1	AA	402	G	N1-C6-O6	9.73	125.74	119.90
27	B8	260	G	N1-C6-O6	9.73	125.74	119.90
27	B8	1055	G	N1-C6-O6	9.73	125.74	119.90
1	AA	497	G	N1-C6-O6	9.73	125.74	119.90
26	B7	106	G	N1-C6-O6	9.73	125.74	119.90
27	B8	1107	G	N1-C6-O6	9.73	125.74	119.90
1	AA	668	G	N1-C6-O6	9.72	125.73	119.90
27	B8	1308	A	N1-C6-N6	9.72	124.43	118.60
1	AA	1353	G	N1-C6-O6	9.72	125.73	119.90
27	B8	1016	G	N1-C6-O6	9.72	125.73	119.90
27	B8	1682	G	N1-C6-O6	9.72	125.73	119.90
1	AA	142	G	N1-C6-O6	9.71	125.73	119.90
27	B8	285	G	N1-C6-O6	9.71	125.73	119.90
1	AA	734	G	N1-C6-O6	9.71	125.73	119.90
27	B8	1546	G	N1-C6-O6	9.71	125.73	119.90
27	B8	1964	G	N1-C6-O6	9.71	125.73	119.90
1	AA	318	G	N1-C6-O6	9.71	125.73	119.90
27	B8	2718	G	N1-C6-O6	9.71	125.73	119.90
27	B8	2557	G	N1-C6-O6	9.71	125.72	119.90
27	B8	2801	G	N1-C6-O6	9.71	125.72	119.90
27	B8	410	G	N1-C6-O6	9.71	125.72	119.90
1	AA	449	G	C5-C6-O6	-9.70	122.78	128.60
27	B8	2556	C	O4'-C1'-N1	9.70	115.96	108.20
1	AA	1349	A	N1-C6-N6	9.70	124.42	118.60
1	AA	755	G	N1-C6-O6	9.69	125.72	119.90
1	AA	1288	A	N1-C6-N6	9.70	124.42	118.60
27	B8	287	G	N1-C6-O6	9.70	125.72	119.90
27	B8	2630	G	N1-C6-O6	9.69	125.71	119.90
1	AA	293	G	N1-C6-O6	9.69	125.71	119.90
1	AA	416	G	N1-C6-O6	9.69	125.71	119.90
27	B8	1560	G	N1-C6-O6	9.69	125.71	119.90
27	B8	2640	G	N1-C6-O6	9.69	125.71	119.90
27	B8	2685	G	N1-C6-O6	9.69	125.71	119.90
27	B8	2592	G	N1-C6-O6	9.68	125.71	119.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1422	G	N1-C6-O6	9.68	125.71	119.90
27	B8	760	G	N1-C6-O6	9.68	125.71	119.90
27	B8	425	G	N1-C6-O6	9.68	125.70	119.90
1	AA	1030	U	O4'-C1'-N1	9.67	115.94	108.20
1	AA	9	G	N1-C6-O6	9.66	125.70	119.90
27	B8	185	G	N1-C6-O6	9.66	125.70	119.90
27	B8	1932	A	N1-C6-N6	9.66	124.40	118.60
27	B8	939	G	N1-C6-O6	9.66	125.70	119.90
27	B8	2508	G	N1-C6-O6	9.66	125.70	119.90
27	B8	1190	G	N1-C6-O6	9.66	125.69	119.90
27	B8	1206	G	N1-C6-O6	9.66	125.69	119.90
27	B8	2115	G	N1-C6-O6	9.66	125.69	119.90
27	B8	2484	G	N1-C6-O6	9.66	125.69	119.90
27	B8	2498	C	O4'-C1'-N1	9.66	115.92	108.20
1	AA	1343	G	N1-C6-O6	9.65	125.69	119.90
27	B8	2040	G	N1-C6-O6	9.65	125.69	119.90
1	AA	1050	G	N1-C6-O6	9.65	125.69	119.90
1	AA	1373	G	N1-C6-O6	9.65	125.69	119.90
1	AA	639	G	N1-C6-O6	9.65	125.69	119.90
27	B8	220	G	N1-C6-O6	9.65	125.69	119.90
27	B8	2208	C	O4'-C1'-N1	9.64	115.92	108.20
27	B8	579	G	N1-C6-O6	9.64	125.68	119.90
27	B8	1792	G	N1-C6-O6	9.64	125.68	119.90
26	B7	66	A	P-O3'-C3'	9.63	131.26	119.70
27	B8	1948	G	N1-C6-O6	9.63	125.68	119.90
1	AA	319	G	N1-C6-O6	9.63	125.68	119.90
1	AA	1154	G	N1-C6-O6	9.63	125.68	119.90
27	B8	759	G	N1-C6-O6	9.63	125.68	119.90
1	AA	1087	G	N1-C6-O6	9.63	125.68	119.90
27	B8	377	G	N1-C6-O6	9.63	125.68	119.90
27	B8	836	G	N1-C6-O6	9.63	125.68	119.90
1	AA	802	A	N1-C6-N6	9.63	124.38	118.60
1	AA	851	G	C5-C6-O6	-9.63	122.83	128.60
27	B8	2323	G	N1-C6-O6	9.62	125.67	119.90
27	B8	2419	U	O4'-C1'-N1	9.62	115.90	108.20
1	AA	1515	G	N1-C6-O6	9.61	125.67	119.90
1	AA	714	G	N1-C6-O6	9.61	125.67	119.90
1	AA	945	G	N1-C6-O6	9.61	125.67	119.90
27	B8	1138	G	N1-C6-O6	9.61	125.67	119.90
1	AA	861	G	N1-C6-O6	9.61	125.66	119.90
1	AA	894	G	N1-C6-O6	9.61	125.66	119.90
1	AA	1041	G	N1-C6-O6	9.61	125.66	119.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	107	G	N1-C6-O6	9.61	125.66	119.90
27	B8	1482	G	N1-C6-O6	9.61	125.66	119.90
27	B8	2209	G	N1-C6-O6	9.61	125.66	119.90
27	B8	2235	G	N1-C6-O6	9.61	125.66	119.90
27	B8	2570	G	N1-C6-O6	9.61	125.66	119.90
27	B8	1037	G	N1-C6-O6	9.60	125.66	119.90
27	B8	402	A	N1-C6-N6	9.60	124.36	118.60
27	B8	1163	G	N1-C6-O6	9.60	125.66	119.90
27	B8	1214	A	N1-C6-N6	9.60	124.36	118.60
1	AA	1143	G	N1-C6-O6	9.60	125.66	119.90
27	B8	2128	G	N1-C6-O6	9.60	125.66	119.90
1	AA	227	G	N1-C6-O6	9.60	125.66	119.90
27	B8	186	G	N1-C6-O6	9.59	125.66	119.90
27	B8	797	G	N1-C6-O6	9.59	125.66	119.90
27	B8	1698	A	N1-C6-N6	9.59	124.36	118.60
27	B8	2330	G	N1-C6-O6	9.59	125.66	119.90
1	AA	428	G	C5-C6-O6	-9.59	122.85	128.60
26	B7	23	G	N1-C6-O6	9.59	125.65	119.90
27	B8	363	G	N1-C6-O6	9.59	125.65	119.90
1	AA	939	G	N1-C6-O6	9.59	125.65	119.90
27	B8	1296	G	N1-C6-O6	9.59	125.65	119.90
27	B8	1511	G	N1-C6-O6	9.59	125.65	119.90
1	AA	148	G	C5-C6-O6	-9.58	122.85	128.60
1	AA	877	G	N1-C6-O6	9.58	125.65	119.90
27	B8	798	G	N1-C6-O6	9.58	125.65	119.90
27	B8	1306	C	O4'-C1'-N1	9.58	115.86	108.20
27	B8	2599	G	N1-C6-O6	9.58	125.65	119.90
27	B8	2603	G	N1-C6-O6	9.58	125.65	119.90
1	AA	763	G	N1-C6-O6	9.57	125.64	119.90
3	AV	3	G	N1-C6-O6	9.57	125.64	119.90
27	B8	924	G	N1-C6-O6	9.57	125.64	119.90
27	B8	1660	G	N1-C6-O6	9.57	125.64	119.90
27	B8	1162	G	N1-C6-O6	9.57	125.64	119.90
27	B8	1124	G	N1-C6-O6	9.57	125.64	119.90
27	B8	2487	G	N1-C6-O6	9.57	125.64	119.90
27	B8	1845	G	N1-C6-O6	9.57	125.64	119.90
27	B8	1238	G	N1-C6-O6	9.56	125.64	119.90
1	AA	1221	G	N1-C6-O6	9.56	125.64	119.90
27	B8	1309	G	N1-C6-O6	9.56	125.64	119.90
27	B8	2399	G	N1-C6-O6	9.56	125.64	119.90
27	B8	70	G	N1-C6-O6	9.56	125.64	119.90
27	B8	396	G	N1-C6-O6	9.56	125.63	119.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	1949	G	N1-C6-O6	9.56	125.64	119.90
1	AA	377	G	N1-C6-O6	9.55	125.63	119.90
27	B8	207	A	N1-C6-N6	9.55	124.33	118.60
27	B8	605	G	N1-C6-O6	9.55	125.63	119.90
27	B8	1545	A	N1-C6-N6	9.55	124.33	118.60
27	B8	1642	G	N1-C6-O6	9.55	125.63	119.90
27	B8	2664	G	C5-C6-O6	-9.55	122.87	128.60
27	B8	938	G	N1-C6-O6	9.55	125.63	119.90
27	B8	2588	G	N1-C6-O6	9.55	125.63	119.90
1	AA	1454	G	N1-C6-O6	9.54	125.63	119.90
1	AA	1494	G	N1-C6-O6	9.55	125.63	119.90
27	B8	122	G	N1-C6-O6	9.55	125.63	119.90
27	B8	1799	G	N1-C6-O6	9.55	125.63	119.90
27	B8	252	G	N1-C6-O6	9.54	125.63	119.90
27	B8	536	G	N1-C6-O6	9.54	125.63	119.90
1	AA	867	G	N1-C6-O6	9.54	125.62	119.90
27	B8	1510	G	C5-C6-O6	-9.54	122.88	128.60
1	AA	113	G	N1-C6-O6	9.54	125.62	119.90
27	B8	799	G	N1-C6-O6	9.54	125.62	119.90
27	B8	1179	G	N1-C6-O6	9.54	125.62	119.90
27	B8	1992	G	N1-C6-O6	9.54	125.62	119.90
27	B8	2641	G	N1-C6-O6	9.54	125.62	119.90
27	B8	550	C	O4'-C1'-N1	9.53	115.83	108.20
27	B8	976	G	N1-C6-O6	9.53	125.62	119.90
27	B8	1455	G	N1-C6-O6	9.53	125.62	119.90
27	B8	1651	G	N1-C6-O6	9.53	125.62	119.90
27	B8	2102	G	N1-C6-O6	9.53	125.62	119.90
27	B8	1093	G	N1-C6-O6	9.53	125.62	119.90
27	B8	1840	G	N1-C6-O6	9.53	125.62	119.90
27	B8	2464	G	N1-C6-O6	9.53	125.62	119.90
27	B8	2486	C	O4'-C1'-N1	9.53	115.82	108.20
27	B8	989	G	N1-C6-O6	9.52	125.61	119.90
27	B8	1137	G	N1-C6-O6	9.52	125.61	119.90
27	B8	2545	G	N1-C6-O6	9.52	125.61	119.90
1	AA	874	G	N1-C6-O6	9.52	125.61	119.90
27	B8	2677	G	N1-C6-O6	9.52	125.61	119.90
27	B8	1245	G	N1-C6-O6	9.51	125.61	119.90
1	AA	592	G	N1-C6-O6	9.51	125.61	119.90
27	B8	543	G	N1-C6-O6	9.51	125.61	119.90
27	B8	2643	G	N1-C6-O6	9.51	125.61	119.90
1	AA	892	A	N1-C6-N6	9.51	124.31	118.60
27	B8	1259	G	N1-C6-O6	9.51	125.61	119.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1292	G	N1-C6-O6	9.51	125.60	119.90
27	B8	2204	G	N1-C6-O6	9.51	125.60	119.90
27	B8	1954	G	N1-C6-O6	9.50	125.60	119.90
27	B8	212	G	N1-C6-O6	9.50	125.60	119.90
27	B8	1891	G	N1-C6-O6	9.50	125.60	119.90
1	AA	401	C	O4'-C1'-N1	9.50	115.80	108.20
1	AA	577	G	N1-C6-O6	9.50	125.60	119.90
27	B8	778	G	N1-C6-O6	9.50	125.60	119.90
27	B8	1659	G	N1-C6-O6	9.50	125.60	119.90
1	AA	725	G	N1-C6-O6	9.49	125.59	119.90
27	B8	1351	C	O4'-C1'-N1	9.49	115.79	108.20
1	AA	824	G	N1-C6-O6	9.49	125.59	119.90
1	AA	1174	G	N1-C6-O6	9.49	125.59	119.90
27	B8	2410	G	N1-C6-O6	9.49	125.59	119.90
27	B8	2674	G	N1-C6-O6	9.49	125.59	119.90
1	AA	779	C	O4'-C1'-N1	9.49	115.79	108.20
1	AA	846	G	N1-C6-O6	9.49	125.59	119.90
27	B8	121	G	N1-C6-O6	9.49	125.59	119.90
27	B8	2029	G	C5-C6-O6	-9.49	122.91	128.60
27	B8	1310	G	N1-C6-O6	9.49	125.59	119.90
1	AA	1310	G	N1-C6-O6	9.48	125.59	119.90
27	B8	408	G	N1-C6-O6	9.48	125.59	119.90
27	B8	1155	A	N1-C6-N6	9.48	124.29	118.60
27	B8	1707	G	N1-C6-O6	9.48	125.59	119.90
27	B8	245	G	N1-C6-O6	9.47	125.58	119.90
27	B8	1661	G	N1-C6-O6	9.47	125.58	119.90
1	AA	500	G	N1-C6-O6	9.47	125.58	119.90
27	B8	821	A	N1-C6-N6	9.47	124.28	118.60
27	B8	962	G	N1-C6-O6	9.47	125.58	119.90
27	B8	1906	G	N1-C6-O6	9.47	125.58	119.90
27	B8	2341	G	N1-C6-O6	9.47	125.58	119.90
1	AA	1127	G	N1-C6-O6	9.47	125.58	119.90
1	AA	198	G	N1-C6-O6	9.46	125.58	119.90
27	B8	77	G	N1-C6-O6	9.46	125.58	119.90
27	B8	2509	G	N1-C6-O6	9.46	125.58	119.90
27	B8	2716	C	O4'-C1'-N1	9.46	115.77	108.20
1	AA	615	G	N1-C6-O6	9.46	125.58	119.90
27	B8	1041	G	N1-C6-O6	9.46	125.58	119.90
27	B8	2078	C	O4'-C1'-N1	9.46	115.77	108.20
26	B7	83	G	N1-C6-O6	9.46	125.57	119.90
27	B8	2413	G	N1-C6-O6	9.46	125.57	119.90
1	AA	1386	G	N1-C6-O6	9.45	125.57	119.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	187	G	N1-C6-O6	9.45	125.57	119.90
27	B8	1256	G	N1-C6-O6	9.45	125.57	119.90
1	AA	791	G	N1-C6-O6	9.45	125.57	119.90
27	B8	2669	G	N1-C6-O6	9.45	125.57	119.90
27	B8	2731	G	N1-C6-O6	9.45	125.57	119.90
1	AA	347	G	N1-C6-O6	9.45	125.57	119.90
27	B8	717	C	O4'-C1'-N1	9.45	115.76	108.20
27	B8	1430	G	N1-C6-O6	9.45	125.57	119.90
27	B8	2355	G	N1-C6-O6	9.45	125.57	119.90
27	B8	2550	G	N1-C6-O6	9.45	125.57	119.90
27	B8	2732	G	N1-C6-O6	9.45	125.57	119.90
27	B8	998	C	O4'-C1'-N1	9.44	115.75	108.20
27	B8	1414	C	O4'-C1'-N1	9.44	115.75	108.20
1	AA	241	G	N1-C6-O6	9.44	125.56	119.90
27	B8	132	G	N1-C6-O6	9.44	125.56	119.90
27	B8	1601	G	N1-C6-O6	9.44	125.56	119.90
27	B8	1988	G	N1-C6-O6	9.44	125.56	119.90
27	B8	2782	G	N1-C6-O6	9.44	125.56	119.90
3	AV	23	G	N1-C6-O6	9.44	125.56	119.90
27	B8	585	G	N1-C6-O6	9.44	125.56	119.90
1	AA	213	G	N1-C6-O6	9.43	125.56	119.90
27	B8	258	G	N1-C6-O6	9.43	125.56	119.90
27	B8	319	G	N1-C6-O6	9.43	125.56	119.90
27	B8	966	G	N1-C6-O6	9.43	125.56	119.90
27	B8	2523	G	N1-C6-O6	9.43	125.56	119.90
1	AA	163	C	O4'-C1'-N1	9.43	115.74	108.20
27	B8	2110	G	N1-C6-O6	9.43	125.56	119.90
27	B8	1500	G	N1-C6-O6	9.43	125.56	119.90
27	B8	1904	G	N1-C6-O6	9.43	125.56	119.90
27	B8	914	G	N1-C6-O6	9.42	125.55	119.90
27	B8	1216	G	N1-C6-O6	9.42	125.55	119.90
27	B8	1429	G	N1-C6-O6	9.42	125.55	119.90
27	B8	1519	G	N1-C6-O6	9.42	125.56	119.90
27	B8	2276	G	N1-C6-O6	9.42	125.55	119.90
27	B8	1120	G	N1-C6-O6	9.42	125.55	119.90
27	B8	1731	G	N1-C6-O6	9.42	125.55	119.90
1	AA	666	G	N1-C6-O6	9.42	125.55	119.90
27	B8	1171	G	N1-C6-O6	9.41	125.55	119.90
27	B8	1448	G	N1-C6-O6	9.41	125.55	119.90
27	B8	1250	G	N1-C6-O6	9.41	125.55	119.90
27	B8	2838	G	N1-C6-O6	9.41	125.55	119.90
27	B8	792	A	P-O3'-C3'	9.41	130.99	119.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	1011	G	N1-C6-O6	9.41	125.55	119.90
27	B8	1862	G	N1-C6-O6	9.41	125.55	119.90
27	B8	2242	G	N1-C6-O6	9.41	125.55	119.90
1	AA	1026	G	N1-C6-O6	9.41	125.54	119.90
27	B8	259	G	N1-C6-O6	9.41	125.54	119.90
1	AA	141	G	N1-C6-O6	9.40	125.54	119.90
27	B8	1530	G	N1-C6-O6	9.40	125.54	119.90
1	AA	903	G	N1-C6-O6	9.40	125.54	119.90
27	B8	700	G	N1-C6-O6	9.40	125.54	119.90
27	B8	297	G	N1-C6-O6	9.40	125.54	119.90
27	B8	261	G	N1-C6-O6	9.40	125.54	119.90
27	B8	535	G	N1-C6-O6	9.40	125.54	119.90
27	B8	723	C	O4'-C1'-N1	9.39	115.72	108.20
1	AA	731	G	N1-C6-O6	9.39	125.53	119.90
27	B8	1984	G	N1-C6-O6	9.39	125.53	119.90
1	AA	111	G	N1-C6-O6	9.39	125.53	119.90
26	B7	18	G	N1-C6-O6	9.39	125.53	119.90
1	AA	1238	A	N1-C6-N6	9.39	124.23	118.60
27	B8	214	G	N1-C6-O6	9.39	125.53	119.90
27	B8	1031	G	N1-C6-O6	9.39	125.53	119.90
27	B8	1	G	N1-C6-O6	9.39	125.53	119.90
1	AA	1002	G	N1-C6-O6	9.38	125.53	119.90
26	B7	6	G	N1-C6-O6	9.38	125.53	119.90
27	B8	952	G	N1-C6-O6	9.38	125.53	119.90
1	AA	491	G	N1-C6-O6	9.38	125.53	119.90
27	B8	1192	G	N1-C6-O6	9.38	125.53	119.90
1	AA	1032	G	N1-C6-O6	9.38	125.53	119.90
27	B8	189	G	N1-C6-O6	9.38	125.53	119.90
27	B8	1850	G	N1-C6-O6	9.38	125.53	119.90
1	AA	1198	G	N1-C6-O6	9.38	125.53	119.90
1	AA	1234	C	O4'-C1'-N1	9.38	115.70	108.20
1	AA	585	G	N1-C6-O6	9.38	125.53	119.90
1	AA	774	G	N1-C6-O6	9.37	125.52	119.90
27	B8	956	G	N1-C6-O6	9.37	125.52	119.90
1	AA	242	G	N1-C6-O6	9.37	125.52	119.90
27	B8	1168	G	N1-C6-O6	9.37	125.52	119.90
27	B8	2502	G	N1-C6-O6	9.37	125.52	119.90
27	B8	2744	G	N1-C6-O6	9.37	125.52	119.90
1	AA	1206	G	C5-C6-O6	-9.37	122.98	128.60
27	B8	468	G	N1-C6-O6	9.37	125.52	119.90
27	B8	2828	G	N1-C6-O6	9.36	125.52	119.90
3	AV	54	G	N1-C6-O6	9.36	125.52	119.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	1388	G	N1-C6-O6	9.36	125.52	119.90
27	B8	1922	G	N1-C6-O6	9.36	125.52	119.90
27	B8	2846	G	N1-C6-O6	9.36	125.52	119.90
1	AA	314	C	O4'-C1'-N1	9.36	115.69	108.20
1	AA	929	G	N1-C6-O6	9.36	125.51	119.90
1	AA	604	G	N1-C6-O6	9.35	125.51	119.90
1	AA	671	G	N1-C6-O6	9.35	125.51	119.90
1	AA	1039	G	N1-C6-O6	9.35	125.51	119.90
27	B8	636	G	N1-C6-O6	9.35	125.51	119.90
27	B8	993	G	N1-C6-O6	9.35	125.51	119.90
27	B8	2107	G	N1-C6-O6	9.35	125.51	119.90
27	B8	2729	G	N1-C6-O6	9.35	125.51	119.90
1	AA	165	G	N1-C6-O6	9.35	125.51	119.90
27	B8	2895	G	C5-C6-O6	-9.35	122.99	128.60
27	B8	2759	G	N1-C6-O6	9.35	125.51	119.90
27	B8	424	G	C5-C6-O6	-9.35	122.99	128.60
27	B8	1358	G	N1-C6-O6	9.35	125.51	119.90
3	AV	47	G	N1-C6-O6	9.34	125.51	119.90
26	B7	7	G	N1-C6-O6	9.34	125.51	119.90
27	B8	2173	A	N1-C6-N6	9.34	124.20	118.60
27	B8	2325	G	N1-C6-O6	9.34	125.51	119.90
27	B8	2876	G	N1-C6-O6	9.34	125.50	119.90
1	AA	881	G	N1-C6-O6	9.34	125.50	119.90
26	B7	20	G	N1-C6-O6	9.34	125.50	119.90
3	AV	32	C	O4'-C1'-N1	9.34	115.67	108.20
27	B8	438	G	N1-C6-O6	9.34	125.50	119.90
1	AA	425	G	N1-C6-O6	9.33	125.50	119.90
27	B8	738	G	N1-C6-O6	9.33	125.50	119.90
27	B8	1724	G	N1-C6-O6	9.33	125.50	119.90
1	AA	836	G	N1-C6-O6	9.33	125.50	119.90
1	AA	902	G	N1-C6-O6	9.33	125.50	119.90
1	AA	1215	G	N1-C6-O6	9.33	125.50	119.90
27	B8	2490	G	N1-C6-O6	9.33	125.50	119.90
1	AA	548	G	N1-C6-O6	9.33	125.50	119.90
1	AA	1106	G	N1-C6-O6	9.32	125.49	119.90
26	B7	85	G	N1-C6-O6	9.32	125.49	119.90
27	B8	2582	G	N1-C6-O6	9.32	125.49	119.90
27	B8	215	G	N1-C6-O6	9.32	125.49	119.90
27	B8	1071	G	N1-C6-O6	9.32	125.49	119.90
27	B8	1281	G	N1-C6-O6	9.32	125.49	119.90
1	AA	203	G	N1-C6-O6	9.32	125.49	119.90
27	B8	2339	C	O4'-C1'-N1	9.32	115.66	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	2443	C	O4'-C1'-N1	9.32	115.66	108.20
27	B8	2671	G	N1-C6-O6	9.32	125.49	119.90
27	B8	638	G	N1-C6-O6	9.32	125.49	119.90
27	B8	827	U	P-O3'-C3'	9.32	130.88	119.70
27	B8	1813	G	N1-C6-O6	9.32	125.49	119.90
27	B8	2686	G	N1-C6-O6	9.31	125.49	119.90
26	B7	35	C	O4'-C1'-N1	9.31	115.65	108.20
27	B8	276	U	O4'-C1'-N1	9.31	115.65	108.20
27	B8	1921	G	N1-C6-O6	9.31	125.49	119.90
1	AA	184	G	C5-C6-O6	-9.31	123.01	128.60
26	B7	44	G	N1-C6-O6	9.31	125.49	119.90
27	B8	1221	C	O4'-C1'-N1	9.31	115.65	108.20
27	B8	75	G	N1-C6-O6	9.31	125.48	119.90
1	AA	925	G	N1-C6-O6	9.31	125.48	119.90
1	AA	1469	C	O4'-C1'-N1	9.30	115.64	108.20
27	B8	1610	A	N1-C6-N6	9.30	124.18	118.60
1	AA	610	U	O4'-C1'-N1	9.30	115.64	108.20
1	AA	821	G	N1-C6-O6	9.30	125.48	119.90
27	B8	266	G	C5-C6-O6	-9.30	123.02	128.60
27	B8	893	C	O4'-C1'-N1	9.30	115.64	108.20
27	B8	1444	G	N1-C6-O6	9.30	125.48	119.90
27	B8	1910	G	C5-C6-O6	-9.30	123.02	128.60
27	B8	2889	C	O4'-C1'-N1	9.30	115.64	108.20
27	B8	2316	G	N1-C6-O6	9.30	125.48	119.90
1	AA	885	G	N1-C6-O6	9.30	125.48	119.90
27	B8	856	G	N1-C6-O6	9.30	125.48	119.90
27	B8	2228	G	N1-C6-O6	9.30	125.48	119.90
27	B8	2567	G	N1-C6-O6	9.30	125.48	119.90
27	B8	2633	G	N1-C6-O6	9.30	125.48	119.90
27	B8	241	A	N1-C6-N6	9.29	124.18	118.60
27	B8	578	G	N1-C6-O6	9.29	125.48	119.90
27	B8	1625	C	O4'-C1'-N1	9.30	115.64	108.20
27	B8	1202	G	N1-C6-O6	9.29	125.48	119.90
27	B8	1357	C	O4'-C1'-N1	9.29	115.63	108.20
27	B8	1860	G	N1-C6-O6	9.29	125.47	119.90
27	B8	1766	G	N1-C6-O6	9.29	125.47	119.90
1	AA	953	G	N1-C6-O6	9.28	125.47	119.90
1	AA	1138	G	N1-C6-O6	9.29	125.47	119.90
1	AA	1242	G	N1-C6-O6	9.29	125.47	119.90
27	B8	674	G	N1-C6-O6	9.29	125.47	119.90
26	B7	75	G	N1-C6-O6	9.28	125.47	119.90
1	AA	1514	G	N1-C6-O6	9.28	125.47	119.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	301	G	C5-C6-O6	-9.28	123.03	128.60
1	AA	1435	G	C5-C6-O6	-9.28	123.03	128.60
27	B8	843	G	N1-C6-O6	9.28	125.47	119.90
27	B8	2495	G	N1-C6-O6	9.28	125.47	119.90
27	B8	2543	G	C5-C6-O6	-9.28	123.03	128.60
27	B8	2725	A	N1-C6-N6	9.28	124.17	118.60
27	B8	2802	G	N1-C6-O6	9.28	125.47	119.90
1	AA	230	G	N1-C6-O6	9.28	125.47	119.90
27	B8	629	G	N1-C6-O6	9.28	125.47	119.90
27	B8	1645	G	N1-C6-O6	9.28	125.47	119.90
27	B8	2087	G	N1-C6-O6	9.28	125.47	119.90
27	B8	2403	C	O4'-C1'-N1	9.28	115.62	108.20
1	AA	1458	G	N1-C6-O6	9.28	125.47	119.90
27	B8	313	G	N1-C6-O6	9.28	125.47	119.90
27	B8	1653	G	N1-C6-O6	9.28	125.47	119.90
27	B8	1666	G	N1-C6-O6	9.28	125.47	119.90
27	B8	1925	C	O4'-C1'-N1	9.28	115.62	108.20
27	B8	2454	G	N1-C6-O6	9.28	125.47	119.90
1	AA	102	G	N1-C6-O6	9.27	125.46	119.90
1	AA	1438	G	N1-C6-O6	9.27	125.47	119.90
27	B8	1723	G	N1-C6-O6	9.27	125.47	119.90
1	AA	1144	G	N1-C6-O6	9.27	125.46	119.90
27	B8	1185	G	N1-C6-O6	9.27	125.46	119.90
1	AA	1462	C	O4'-C1'-N1	9.27	115.61	108.20
1	AA	1529	G	N1-C6-O6	9.27	125.46	119.90
26	B7	16	G	N1-C6-O6	9.27	125.46	119.90
27	B8	681	G	N1-C6-O6	9.27	125.46	119.90
27	B8	697	G	N1-C6-O6	9.27	125.46	119.90
27	B8	1835	G	N1-C6-O6	9.27	125.46	119.90
27	B8	974	G	N1-C6-O6	9.27	125.46	119.90
1	AA	462	G	N1-C6-O6	9.26	125.46	119.90
27	B8	2666	C	O4'-C1'-N1	9.26	115.61	108.20
1	AA	332	G	N1-C6-O6	9.26	125.46	119.90
27	B8	380	G	N1-C6-O6	9.26	125.46	119.90
27	B8	2290	G	N1-C6-O6	9.26	125.46	119.90
27	B8	1441	G	N1-C6-O6	9.26	125.46	119.90
27	B8	2251	G	N1-C6-O6	9.26	125.45	119.90
1	AA	337	G	N1-C6-O6	9.26	125.45	119.90
1	AA	1043	G	N1-C6-O6	9.26	125.45	119.90
27	B8	604	G	N1-C6-O6	9.25	125.45	119.90
27	B8	1136	G	N1-C6-O6	9.25	125.45	119.90
27	B8	1628	G	N1-C6-O6	9.25	125.45	119.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	46	G	N1-C6-O6	9.25	125.45	119.90
27	B8	695	G	N1-C6-O6	9.25	125.45	119.90
27	B8	770	G	N1-C6-O6	9.25	125.45	119.90
1	AA	978	A	N1-C6-N6	9.24	124.14	118.60
27	B8	1416	G	N1-C6-O6	9.24	125.44	119.90
27	B8	1622	G	N1-C6-O6	9.24	125.44	119.90
27	B8	289	G	N1-C6-O6	9.24	125.44	119.90
27	B8	1343	G	N1-C6-O6	9.24	125.44	119.90
27	B8	2852	G	N1-C6-O6	9.24	125.44	119.90
1	AA	1356	G	N1-C6-O6	9.23	125.44	119.90
27	B8	796	C	O4'-C1'-N1	9.23	115.59	108.20
27	B8	2428	G	N1-C6-O6	9.23	125.44	119.90
1	AA	299	G	N1-C6-O6	9.23	125.44	119.90
26	B7	61	G	N1-C6-O6	9.23	125.44	119.90
27	B8	151	C	O4'-C1'-N1	9.23	115.59	108.20
1	AA	1294	G	N1-C6-O6	9.23	125.44	119.90
1	AA	1526	G	N1-C6-O6	9.23	125.44	119.90
27	B8	1878	G	N1-C6-O6	9.23	125.44	119.90
27	B8	774	G	N1-C6-O6	9.23	125.44	119.90
27	B8	2642	G	N1-C6-O6	9.23	125.44	119.90
27	B8	35	G	N1-C6-O6	9.23	125.44	119.90
1	AA	988	G	N1-C6-O6	9.22	125.44	119.90
1	AA	404	G	N1-C6-O6	9.22	125.43	119.90
27	B8	647	G	N1-C6-O6	9.22	125.43	119.90
1	AA	1088	G	N1-C6-O6	9.22	125.43	119.90
27	B8	134	G	N1-C6-O6	9.22	125.43	119.90
27	B8	907	G	N1-C6-O6	9.22	125.43	119.90
27	B8	1116	G	N1-C6-O6	9.22	125.43	119.90
1	AA	670	G	N1-C6-O6	9.21	125.43	119.90
27	B8	271	G	N1-C6-O6	9.21	125.43	119.90
27	B8	656	G	N1-C6-O6	9.21	125.43	119.90
27	B8	1106	G	C5-C6-O6	-9.21	123.07	128.60
1	AA	962	C	O4'-C1'-N1	9.21	115.57	108.20
27	B8	469	G	N1-C6-O6	9.21	125.43	119.90
27	B8	2752	C	O4'-C1'-N1	9.21	115.57	108.20
27	B8	1491	G	N1-C6-O6	9.21	125.43	119.90
27	B8	2256	G	N1-C6-O6	9.21	125.43	119.90
27	B8	2415	G	N1-C6-O6	9.21	125.43	119.90
26	B7	84	G	N1-C6-O6	9.20	125.42	119.90
27	B8	2002	G	N1-C6-O6	9.20	125.42	119.90
27	B8	2693	G	N1-C6-O6	9.20	125.42	119.90
27	B8	2854	G	N1-C6-O6	9.20	125.42	119.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	1087	G	N1-C6-O6	9.20	125.42	119.90
1	AA	1389	C	O4'-C1'-N1	9.20	115.56	108.20
27	B8	99	U	O4'-C1'-N1	9.20	115.56	108.20
27	B8	1361	G	N1-C6-O6	9.20	125.42	119.90
27	B8	1674	G	N1-C6-O6	9.19	125.42	119.90
1	AA	1415	G	N1-C6-O6	9.19	125.42	119.90
27	B8	2625	G	N1-C6-O6	9.19	125.41	119.90
1	AA	191	G	N1-C6-O6	9.19	125.41	119.90
27	B8	2777	G	N1-C6-O6	9.19	125.41	119.90
1	AA	538	G	N1-C6-O6	9.19	125.41	119.90
27	B8	1377	G	N1-C6-O6	9.19	125.41	119.90
27	B8	1450	G	N1-C6-O6	9.19	125.41	119.90
1	AA	529	G	N1-C6-O6	9.18	125.41	119.90
1	AA	1312	G	N1-C6-O6	9.18	125.41	119.90
27	B8	356	G	N1-C6-O6	9.18	125.41	119.90
27	B8	1842	G	N1-C6-O6	9.18	125.41	119.90
27	B8	1861	G	N1-C6-O6	9.18	125.41	119.90
1	AA	1124	G	N1-C6-O6	9.18	125.41	119.90
1	AA	1337	G	N1-C6-O6	9.18	125.41	119.90
27	B8	1261	C	O4'-C1'-N1	9.18	115.54	108.20
27	B8	2337	G	N1-C6-O6	9.18	125.41	119.90
27	B8	2763	G	N1-C6-O6	9.18	125.41	119.90
27	B8	325	G	N1-C6-O6	9.17	125.40	119.90
27	B8	733	G	N1-C6-O6	9.17	125.40	119.90
1	AA	31	G	N1-C6-O6	9.17	125.40	119.90
27	B8	1062	G	N1-C6-O6	9.17	125.40	119.90
27	B8	1730	C	P-O3'-C3'	9.17	130.70	119.70
27	B8	2246	G	N1-C6-O6	9.17	125.40	119.90
27	B8	2318	G	N1-C6-O6	9.17	125.40	119.90
26	B7	98	G	N1-C6-O6	9.16	125.40	119.90
27	B8	361	G	N1-C6-O6	9.16	125.40	119.90
27	B8	1410	G	N1-C6-O6	9.16	125.40	119.90
1	AA	688	G	N1-C6-O6	9.16	125.40	119.90
27	B8	1280	G	N1-C6-O6	9.16	125.40	119.90
1	AA	550	G	N1-C6-O6	9.16	125.39	119.90
1	AA	1255	G	N1-C6-O6	9.16	125.39	119.90
27	B8	768	G	C5-C6-O6	-9.16	123.11	128.60
27	B8	2405	G	N1-C6-O6	9.16	125.39	119.90
27	B8	205	G	N1-C6-O6	9.15	125.39	119.90
27	B8	1210	G	N1-C6-O6	9.15	125.39	119.90
27	B8	178	G	N1-C6-O6	9.15	125.39	119.90
27	B8	204	A	N1-C6-N6	9.15	124.09	118.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	2230	G	N1-C6-O6	9.15	125.39	119.90
27	B8	2367	G	N1-C6-O6	9.15	125.39	119.90
3	AV	10	G	N1-C6-O6	9.15	125.39	119.90
26	B7	64	G	N1-C6-O6	9.15	125.39	119.90
27	B8	175	G	N1-C6-O6	9.15	125.39	119.90
27	B8	179	C	O4'-C1'-N1	9.15	115.52	108.20
27	B8	874	G	N1-C6-O6	9.15	125.39	119.90
27	B8	1371	G	N1-C6-O6	9.15	125.39	119.90
27	B8	2373	G	N1-C6-O6	9.15	125.39	119.90
1	AA	348	G	N1-C6-O6	9.14	125.39	119.90
27	B8	909	A	N1-C6-N6	9.14	124.09	118.60
27	B8	2389	G	N1-C6-O6	9.14	125.39	119.90
27	B8	940	G	N1-C6-O6	9.14	125.39	119.90
1	AA	1272	G	N1-C6-O6	9.14	125.38	119.90
1	AA	1459	G	N1-C6-O6	9.14	125.38	119.90
27	B8	375	G	N1-C6-O6	9.14	125.38	119.90
1	AA	42	G	N1-C6-O6	9.13	125.38	119.90
1	AA	289	G	N1-C6-O6	9.13	125.38	119.90
3	AV	70	G	C5-C6-O6	-9.14	123.12	128.60
1	AA	11	G	N1-C6-O6	9.13	125.38	119.90
27	B8	2132	U	O4'-C1'-N1	9.13	115.51	108.20
27	B8	2526	G	N1-C6-O6	9.13	125.38	119.90
27	B8	2869	G	N1-C6-O6	9.13	125.38	119.90
27	B8	847	U	O4'-C1'-N1	9.13	115.50	108.20
1	AA	400	C	O4'-C1'-N1	9.13	115.50	108.20
27	B8	17	G	N1-C6-O6	9.13	125.38	119.90
27	B8	971	G	N1-C6-O6	9.13	125.38	119.90
27	B8	1997	C	O4'-C1'-N1	9.13	115.50	108.20
1	AA	126	G	N1-C6-O6	9.13	125.38	119.90
1	AA	567	G	N1-C6-O6	9.12	125.38	119.90
3	AV	51	G	N1-C6-O6	9.13	125.38	119.90
1	AA	927	G	N1-C6-O6	9.12	125.37	119.90
27	B8	1846	G	N1-C6-O6	9.12	125.37	119.90
1	AA	1187	G	N1-C6-O6	9.12	125.37	119.90
1	AA	588	G	N1-C6-O6	9.12	125.37	119.90
1	AA	1047	G	N1-C6-O6	9.12	125.37	119.90
1	AA	276	G	N1-C6-O6	9.12	125.37	119.90
1	AA	158	G	N1-C6-O6	9.11	125.37	119.90
1	AA	388	G	N1-C6-O6	9.11	125.37	119.90
1	AA	444	G	N1-C6-O6	9.12	125.37	119.90
1	AA	730	G	N1-C6-O6	9.11	125.37	119.90
27	B8	1036	G	N1-C6-O6	9.11	125.37	119.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	1220	G	N1-C6-O6	9.11	125.37	119.90
27	B8	1337	G	N1-C6-O6	9.11	125.37	119.90
1	AA	1033	G	C5-C6-O6	-9.11	123.14	128.60
1	AA	1153	G	N1-C6-O6	9.11	125.36	119.90
27	B8	785	G	N1-C6-O6	9.11	125.36	119.90
1	AA	542	G	N1-C6-O6	9.11	125.36	119.90
1	AA	1177	G	N1-C6-O6	9.11	125.36	119.90
26	B7	26	C	O4'-C1'-N1	9.11	115.48	108.20
27	B8	2396	G	N1-C6-O6	9.11	125.36	119.90
1	AA	196	A	N1-C6-N6	9.10	124.06	118.60
27	B8	930	G	N1-C6-O6	9.10	125.36	119.90
27	B8	2277	G	N1-C6-O6	9.10	125.36	119.90
1	AA	146	G	N1-C6-O6	9.10	125.36	119.90
1	AA	570	G	C5-C6-O6	-9.10	123.14	128.60
27	B8	283	G	N1-C6-O6	9.10	125.36	119.90
1	AA	1054	C	O4'-C1'-N1	9.10	115.48	108.20
27	B8	1177	G	N1-C6-O6	9.10	125.36	119.90
27	B8	1303	G	N1-C6-O6	9.10	125.36	119.90
27	B8	1751	U	O4'-C1'-N1	9.10	115.48	108.20
1	AA	887	G	N1-C6-O6	9.09	125.36	119.90
1	AA	1186	G	N1-C6-O6	9.09	125.36	119.90
1	AA	1309	G	N1-C6-O6	9.09	125.36	119.90
27	B8	584	C	O4'-C1'-N1	9.09	115.47	108.20
27	B8	841	G	N1-C6-O6	9.09	125.35	119.90
27	B8	2480	C	O4'-C1'-N1	9.09	115.47	108.20
27	B8	2862	G	N1-C6-O6	9.09	125.35	119.90
1	AA	361	G	N1-C6-O6	9.09	125.35	119.90
1	AA	872	A	N1-C6-N6	9.08	124.05	118.60
27	B8	712	G	N1-C6-O6	9.08	125.35	119.90
1	AA	776	G	N1-C6-O6	9.08	125.35	119.90
27	B8	1623	G	N1-C6-O6	9.08	125.35	119.90
27	B8	2488	G	N1-C6-O6	9.08	125.35	119.90
27	B8	1620	G	N1-C6-O6	9.07	125.34	119.90
1	AA	104	G	C5-C6-O6	-9.07	123.16	128.60
27	B8	1968	G	N1-C6-O6	9.07	125.34	119.90
1	AA	76	G	C5-C6-O6	-9.07	123.16	128.60
27	B8	406	G	N1-C6-O6	9.07	125.34	119.90
27	B8	1139	G	N1-C6-O6	9.07	125.34	119.90
27	B8	1369	G	N1-C6-O6	9.07	125.34	119.90
27	B8	1382	G	O4'-C1'-N9	9.07	115.45	108.20
27	B8	1719	G	N1-C6-O6	9.07	125.34	119.90
27	B8	992	C	O4'-C1'-N1	9.07	115.45	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	2569	G	N1-C6-O6	9.07	125.34	119.90
27	B8	2708	G	N1-C6-O6	9.07	125.34	119.90
1	AA	544	G	N1-C6-O6	9.07	125.34	119.90
27	B8	85	G	N1-C6-O6	9.07	125.34	119.90
27	B8	1480	C	O4'-C1'-N1	9.07	115.45	108.20
1	AA	597	G	N1-C6-O6	9.06	125.34	119.90
1	AA	1299	A	N1-C6-N6	9.06	124.04	118.60
27	B8	2100	G	N1-C6-O6	9.06	125.34	119.90
1	AA	442	G	N1-C6-O6	9.06	125.34	119.90
1	AA	540	G	N1-C6-O6	9.06	125.34	119.90
1	AA	987	G	N1-C6-O6	9.06	125.34	119.90
27	B8	2190	G	N1-C6-O6	9.06	125.34	119.90
27	B8	2691	C	O4'-C1'-N1	9.06	115.45	108.20
27	B8	771	G	N1-C6-O6	9.06	125.34	119.90
27	B8	1696	G	N1-C6-O6	9.06	125.34	119.90
1	AA	100	G	N1-C6-O6	9.06	125.34	119.90
27	B8	2474	U	O4'-C1'-N1	9.06	115.45	108.20
27	B8	2864	G	N1-C6-O6	9.06	125.34	119.90
1	AA	1185	G	N1-C6-O6	9.06	125.33	119.90
1	AA	1401	G	N1-C6-O6	9.06	125.33	119.90
1	AA	1486	G	C5-C6-O6	-9.06	123.17	128.60
27	B8	110	G	N1-C6-O6	9.06	125.33	119.90
27	B8	2004	G	N1-C6-O6	9.06	125.33	119.90
1	AA	1258	G	N1-C6-O6	9.06	125.33	119.90
1	AA	830	G	N1-C6-O6	9.05	125.33	119.90
27	B8	327	G	N1-C6-O6	9.05	125.33	119.90
27	B8	1128	G	N1-C6-O6	9.05	125.33	119.90
27	B8	1407	G	N1-C6-O6	9.05	125.33	119.90
27	B8	1740	G	N1-C6-O6	9.05	125.33	119.90
1	AA	46	G	N1-C6-O6	9.05	125.33	119.90
1	AA	1104	G	N1-C6-O6	9.05	125.33	119.90
27	B8	1849	G	N1-C6-O6	9.05	125.33	119.90
27	B8	692	C	O4'-C1'-N1	9.05	115.44	108.20
27	B8	1449	G	N1-C6-O6	9.05	125.33	119.90
1	AA	848	C	O4'-C1'-N1	9.05	115.44	108.20
1	AA	1270	G	N1-C6-O6	9.05	125.33	119.90
27	B8	2382	G	N1-C6-O6	9.05	125.33	119.90
27	B8	124	G	N1-C6-O6	9.04	125.33	119.90
27	B8	763	G	N1-C6-O6	9.04	125.33	119.90
27	B8	1149	G	N1-C6-O6	9.04	125.33	119.90
1	AA	41	G	N1-C6-O6	9.04	125.33	119.90
27	B8	1663	G	N1-C6-O6	9.04	125.33	119.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	474	G	N1-C6-O6	9.04	125.32	119.90
1	AA	799	G	N1-C6-O6	9.04	125.32	119.90
27	B8	301	G	N1-C6-O6	9.04	125.32	119.90
27	B8	728	G	N1-C6-O6	9.04	125.32	119.90
27	B8	1633	G	N1-C6-O6	9.04	125.32	119.90
1	AA	721	G	N1-C6-O6	9.04	125.32	119.90
27	B8	776	G	N1-C6-O6	9.04	125.32	119.90
27	B8	1266	G	N1-C6-O6	9.04	125.32	119.90
27	B8	1863	G	N1-C6-O6	9.04	125.32	119.90
27	B8	1972	G	N1-C6-O6	9.04	125.32	119.90
27	B8	708	G	N1-C6-O6	9.03	125.32	119.90
27	B8	1380	G	N1-C6-O6	9.03	125.32	119.90
27	B8	1125	G	N1-C6-O6	9.03	125.32	119.90
27	B8	1225	G	N1-C6-O6	9.03	125.32	119.90
27	B8	27	G	N1-C6-O6	9.03	125.32	119.90
27	B8	1750	G	N1-C6-O6	9.03	125.32	119.90
1	AA	1370	G	N1-C6-O6	9.03	125.32	119.90
27	B8	2216	G	N1-C6-O6	9.03	125.32	119.90
1	AA	1241	G	N1-C6-O6	9.03	125.32	119.90
27	B8	119	A	N1-C6-N6	9.03	124.02	118.60
1	AA	251	G	N1-C6-O6	9.02	125.31	119.90
1	AA	1244	G	N1-C6-O6	9.02	125.31	119.90
1	AA	391	G	N1-C6-O6	9.02	125.31	119.90
1	AA	748	G	N1-C6-O6	9.02	125.31	119.90
1	AA	1141	C	O4'-C1'-N1	9.02	115.42	108.20
27	B8	302	C	O4'-C1'-N1	9.02	115.42	108.20
27	B8	498	G	N1-C6-O6	9.02	125.31	119.90
27	B8	2770	G	N1-C6-O6	9.02	125.31	119.90
27	B8	1592	C	O4'-C1'-N1	9.02	115.42	108.20
27	B8	780	G	N1-C6-O6	9.02	125.31	119.90
1	AA	64	G	N1-C6-O6	9.02	125.31	119.90
27	B8	1332	G	N1-C6-O6	9.02	125.31	119.90
27	B8	1516	G	N1-C6-O6	9.01	125.31	119.90
27	B8	2223	G	N1-C6-O6	9.01	125.31	119.90
27	B8	2280	G	N1-C6-O6	9.01	125.31	119.90
27	B8	612	G	N1-C6-O6	9.01	125.31	119.90
27	B8	1291	C	O4'-C1'-N1	9.01	115.41	108.20
27	B8	1684	G	N1-C6-O6	9.01	125.31	119.90
27	B8	2525	G	N1-C6-O6	9.01	125.31	119.90
27	B8	92	U	O4'-C1'-N1	9.01	115.41	108.20
27	B8	822	G	N1-C6-O6	9.01	125.31	119.90
27	B8	1164	C	O4'-C1'-N1	9.01	115.41	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	247	G	N1-C6-O6	9.01	125.31	119.90
27	B8	834	G	N1-C6-O6	9.01	125.31	119.90
1	AA	292	G	N1-C6-O6	9.01	125.31	119.90
1	AA	144	G	N1-C6-O6	9.01	125.30	119.90
1	AA	362	G	N1-C6-O6	9.00	125.30	119.90
1	AA	212	G	N1-C6-O6	9.00	125.30	119.90
1	AA	421	U	O4'-C1'-N1	9.00	115.40	108.20
1	AA	445	G	N1-C6-O6	9.00	125.30	119.90
1	AA	993	G	N1-C6-O6	9.00	125.30	119.90
27	B8	1404	C	O4'-C1'-N1	9.00	115.40	108.20
27	B8	2458	G	N1-C6-O6	9.00	125.30	119.90
27	B8	2890	G	N1-C6-O6	9.00	125.30	119.90
27	B8	1606	C	O4'-C1'-N1	9.00	115.40	108.20
27	B8	2485	G	C5-C6-O6	-9.00	123.20	128.60
27	B8	2061	G	N1-C6-O6	9.00	125.30	119.90
27	B8	2747	G	C5-C6-O6	-9.00	123.20	128.60
27	B8	23	G	N1-C6-O6	9.00	125.30	119.90
1	AA	859	G	N1-C6-O6	8.99	125.30	119.90
1	AA	1253	G	N1-C6-O6	8.99	125.30	119.90
1	AA	1460	C	O4'-C1'-N1	8.99	115.39	108.20
27	B8	298	G	N1-C6-O6	8.99	125.30	119.90
27	B8	551	G	N1-C6-O6	8.99	125.30	119.90
27	B8	775	G	N1-C6-O6	8.99	125.30	119.90
27	B8	1588	G	N1-C6-O6	8.99	125.30	119.90
27	B8	2218	G	N1-C6-O6	8.99	125.30	119.90
27	B8	307	G	N1-C6-O6	8.99	125.30	119.90
1	AA	324	G	N1-C6-O6	8.99	125.29	119.90
27	B8	411	G	N1-C6-O6	8.99	125.29	119.90
27	B8	1452	G	N1-C6-O6	8.99	125.30	119.90
27	B8	2831	G	N1-C6-O6	8.99	125.29	119.90
27	B8	1828	G	N1-C6-O6	8.99	125.29	119.90
27	B8	2293	G	N1-C6-O6	8.99	125.29	119.90
1	AA	1146	A	N1-C6-N6	8.99	123.99	118.60
1	AA	82	G	N1-C6-O6	8.99	125.29	119.90
1	AA	1296	C	O4'-C1'-N1	8.99	115.39	108.20
27	B8	303	G	N1-C6-O6	8.99	125.29	119.90
27	B8	630	G	N1-C6-O6	8.99	125.29	119.90
27	B8	1195	G	N1-C6-O6	8.99	125.29	119.90
27	B8	2038	G	N1-C6-O6	8.99	125.29	119.90
27	B8	1212	G	N1-C6-O6	8.98	125.29	119.90
1	AA	928	G	N1-C6-O6	8.98	125.29	119.90
1	AA	226	G	N1-C6-O6	8.98	125.29	119.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	682	G	N1-C6-O6	8.98	125.29	119.90
1	AA	971	G	N1-C6-O6	8.98	125.29	119.90
1	AA	1084	G	N1-C6-O6	8.98	125.29	119.90
27	B8	277	G	N1-C6-O6	8.98	125.29	119.90
27	B8	2303	G	N1-C6-O6	8.98	125.29	119.90
1	AA	220	G	N1-C6-O6	8.98	125.29	119.90
1	AA	527	G	N1-C6-O6	8.98	125.29	119.90
27	B8	188	G	N1-C6-O6	8.98	125.29	119.90
3	AV	15	G	N1-C6-O6	8.98	125.29	119.90
1	AA	1304	G	N1-C6-O6	8.97	125.28	119.90
27	B8	537	G	N1-C6-O6	8.97	125.28	119.90
27	B8	2661	G	N1-C6-O6	8.97	125.28	119.90
27	B8	862	G	N1-C6-O6	8.97	125.28	119.90
27	B8	1150	C	O4'-C1'-N1	8.97	115.38	108.20
1	AA	1530	G	N1-C6-O6	8.97	125.28	119.90
27	B8	1897	G	N1-C6-O6	8.97	125.28	119.90
27	B8	359	G	N1-C6-O6	8.97	125.28	119.90
27	B8	2121	G	N1-C6-O6	8.97	125.28	119.90
27	B8	2732	G	C5-C6-O6	-8.97	123.22	128.60
27	B8	7	G	N1-C6-O6	8.97	125.28	119.90
27	B8	942	G	N1-C6-O6	8.96	125.28	119.90
27	B8	1324	G	N1-C6-O6	8.96	125.28	119.90
27	B8	1436	G	N1-C6-O6	8.96	125.28	119.90
27	B8	2578	G	N1-C6-O6	8.96	125.28	119.90
1	AA	1276	G	N1-C6-O6	8.96	125.28	119.90
1	AA	803	G	N1-C6-O6	8.96	125.27	119.90
27	B8	57	C	O4'-C1'-N1	8.96	115.37	108.20
27	B8	923	G	N1-C6-O6	8.96	125.28	119.90
27	B8	463	G	N1-C6-O6	8.96	125.27	119.90
27	B8	997	G	N1-C6-O6	8.96	125.27	119.90
27	B8	1333	G	P-O3'-C3'	8.96	130.45	119.70
27	B8	1381	G	C5-C6-O6	-8.96	123.22	128.60
1	AA	505	G	N1-C6-O6	8.96	125.27	119.90
27	B8	1537	G	N1-C6-O6	8.96	125.27	119.90
27	B8	31	C	O4'-C1'-N1	8.95	115.36	108.20
27	B8	1475	G	N1-C6-O6	8.95	125.27	119.90
27	B8	1514	G	N1-C6-O6	8.95	125.27	119.90
27	B8	2844	G	N1-C6-O6	8.95	125.27	119.90
1	AA	147	G	C5-C6-O6	-8.95	123.23	128.60
1	AA	773	G	N1-C6-O6	8.95	125.27	119.90
27	B8	1445	G	C5-C6-O6	-8.95	123.23	128.60
27	B8	1767	G	N1-C6-O6	8.95	125.27	119.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	1697	G	N1-C6-O6	8.95	125.27	119.90
27	B8	1063	G	N1-C6-O6	8.95	125.27	119.90
1	AA	1473	G	N1-C6-O6	8.95	125.27	119.90
27	B8	2857	G	N1-C6-O6	8.94	125.27	119.90
27	B8	2877	G	N1-C6-O6	8.95	125.27	119.90
1	AA	833	G	N1-C6-O6	8.94	125.27	119.90
27	B8	549	G	N1-C6-O6	8.94	125.27	119.90
1	AA	498	A	N1-C6-N6	8.94	123.96	118.60
27	B8	2697	G	N1-C6-O6	8.94	125.26	119.90
27	B8	916	G	C5-C6-O6	-8.94	123.24	128.60
27	B8	2867	G	N1-C6-O6	8.94	125.26	119.90
1	AA	1207	G	N1-C6-O6	8.94	125.26	119.90
27	B8	618	G	N1-C6-O6	8.94	125.26	119.90
27	B8	2717	C	O4'-C1'-N1	8.94	115.35	108.20
27	B8	736	C	O4'-C1'-N1	8.94	115.35	108.20
27	B8	1166	G	N1-C6-O6	8.94	125.26	119.90
1	AA	237	G	N1-C6-O6	8.93	125.26	119.90
1	AA	354	G	N1-C6-O6	8.93	125.26	119.90
1	AA	447	G	N1-C6-O6	8.93	125.26	119.90
27	B8	1811	G	N1-C6-O6	8.93	125.26	119.90
1	AA	944	G	N1-C6-O6	8.93	125.26	119.90
1	AA	1504	G	N1-C6-O6	8.93	125.26	119.90
3	AV	73	G	N1-C6-O6	8.93	125.26	119.90
27	B8	2645	G	N1-C6-O6	8.93	125.26	119.90
1	AA	710	G	N1-C6-O6	8.93	125.26	119.90
27	B8	518	G	N1-C6-O6	8.93	125.26	119.90
27	B8	1002	G	N1-C6-O6	8.93	125.26	119.90
27	B8	1160	G	N1-C6-O6	8.93	125.26	119.90
27	B8	2201	G	C5-C6-O6	-8.93	123.24	128.60
27	B8	24	G	N1-C6-O6	8.93	125.26	119.90
27	B8	1959	G	N1-C6-O6	8.93	125.26	119.90
27	B8	2773	C	O4'-C1'-N1	8.93	115.34	108.20
27	B8	2168	G	N1-C6-O6	8.92	125.25	119.90
27	B8	2730	C	O4'-C1'-N1	8.92	115.34	108.20
27	B8	2806	C	O4'-C1'-N1	8.92	115.34	108.20
1	AA	703	G	N1-C6-O6	8.92	125.25	119.90
27	B8	565	C	O4'-C1'-N1	8.92	115.34	108.20
27	B8	831	G	N1-C6-O6	8.92	125.25	119.90
27	B8	1442	U	O4'-C1'-N1	8.92	115.33	108.20
27	B8	2436	G	N1-C6-O6	8.92	125.25	119.90
27	B8	433	C	O4'-C1'-N1	8.92	115.33	108.20
27	B8	1334	G	N1-C6-O6	8.92	125.25	119.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	1568	G	N1-C6-O6	8.92	125.25	119.90
27	B8	1733	G	N1-C6-O6	8.92	125.25	119.90
27	B8	2892	G	N1-C6-O6	8.92	125.25	119.90
27	B8	1157	G	C5-C6-O6	-8.91	123.25	128.60
27	B8	1248	G	N1-C6-O6	8.91	125.25	119.90
27	B8	1567	G	N1-C6-O6	8.91	125.25	119.90
27	B8	1604	C	O4'-C1'-N1	8.91	115.33	108.20
26	B7	51	G	N1-C6-O6	8.91	125.25	119.90
27	B8	969	G	N1-C6-O6	8.91	125.24	119.90
1	AA	490	C	O4'-C1'-N1	8.90	115.32	108.20
1	AA	1442	G	N1-C6-O6	8.90	125.24	119.90
3	AV	25	G	N1-C6-O6	8.90	125.24	119.90
1	AA	115	G	C5-C6-O6	-8.90	123.26	128.60
27	B8	295	G	N1-C6-O6	8.90	125.24	119.90
27	B8	2409	G	C5-C6-O6	-8.90	123.26	128.60
1	AA	558	G	N1-C6-O6	8.90	125.24	119.90
27	B8	136	G	N1-C6-O6	8.90	125.24	119.90
27	B8	1577	C	O4'-C1'-N1	8.90	115.32	108.20
1	AA	1392	G	C5-C6-O6	-8.90	123.26	128.60
27	B8	1555	G	N1-C6-O6	8.90	125.24	119.90
26	B7	79	G	N1-C6-O6	8.90	125.24	119.90
27	B8	1425	G	N1-C6-O6	8.90	125.24	119.90
1	AA	127	G	N1-C6-O6	8.89	125.24	119.90
3	AV	2	G	N1-C6-O6	8.89	125.24	119.90
27	B8	60	G	N1-C6-O6	8.89	125.24	119.90
27	B8	1299	G	N1-C6-O6	8.89	125.24	119.90
1	AA	331	G	N1-C6-O6	8.89	125.23	119.90
27	B8	232	G	N1-C6-O6	8.89	125.23	119.90
27	B8	864	G	C5-C6-O6	-8.89	123.27	128.60
27	B8	2494	G	N1-C6-O6	8.89	125.23	119.90
1	AA	1139	G	N1-C6-O6	8.89	125.23	119.90
1	AA	433	G	N1-C6-O6	8.89	125.23	119.90
27	B8	926	G	N1-C6-O6	8.89	125.23	119.90
1	AA	742	G	N1-C6-O6	8.88	125.23	119.90
26	B7	27	C	O4'-C1'-N1	8.88	115.31	108.20
27	B8	2894	G	C5-C6-O6	-8.89	123.27	128.60
1	AA	94	G	N1-C6-O6	8.88	125.23	119.90
27	B8	389	G	N1-C6-O6	8.88	125.23	119.90
27	B8	648	G	N1-C6-O6	8.88	125.23	119.90
27	B8	1047	G	N1-C6-O6	8.88	125.23	119.90
27	B8	2186	G	N1-C6-O6	8.88	125.23	119.90
27	B8	553	G	N1-C6-O6	8.88	125.23	119.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	1368	G	N1-C6-O6	8.88	125.23	119.90
1	AA	1120	C	O4'-C1'-N1	8.88	115.30	108.20
27	B8	1814	G	N1-C6-O6	8.88	125.23	119.90
1	AA	69	G	N1-C6-O6	8.88	125.23	119.90
1	AA	399	G	N1-C6-O6	8.88	125.22	119.90
1	AA	1190	G	N1-C6-O6	8.88	125.22	119.90
26	B7	100	G	N1-C6-O6	8.87	125.22	119.90
27	B8	1223	G	N1-C6-O6	8.87	125.22	119.90
27	B8	2116	G	N1-C6-O6	8.88	125.22	119.90
1	AA	1290	G	C5-C6-O6	-8.87	123.28	128.60
26	B7	96	G	N1-C6-O6	8.87	125.22	119.90
27	B8	401	A	O4'-C1'-N9	8.87	115.30	108.20
27	B8	653	U	O4'-C1'-N1	8.87	115.30	108.20
27	B8	1681	G	N1-C6-O6	8.87	125.22	119.90
27	B8	1421	G	C5-C6-O6	-8.87	123.28	128.60
1	AA	973	G	C5-C6-O6	-8.87	123.28	128.60
1	AA	1439	G	N1-C6-O6	8.87	125.22	119.90
27	B8	1228	G	N1-C6-O6	8.87	125.22	119.90
27	B8	2724	U	O4'-C1'-N1	8.87	115.30	108.20
27	B8	1776	G	N1-C6-O6	8.87	125.22	119.90
27	B8	1824	G	N1-C6-O6	8.87	125.22	119.90
27	B8	2901	C	O4'-C1'-N1	8.87	115.29	108.20
1	AA	446	G	N1-C6-O6	8.86	125.22	119.90
1	AA	809	G	N1-C6-O6	8.87	125.22	119.90
1	AA	1426	G	N1-C6-O6	8.86	125.22	119.90
27	B8	254	G	N1-C6-O6	8.86	125.22	119.90
27	B8	885	C	O4'-C1'-N1	8.86	115.29	108.20
27	B8	1631	G	N1-C6-O6	8.86	125.22	119.90
27	B8	2028	U	O4'-C1'-N1	8.86	115.29	108.20
27	B8	2538	C	O4'-C1'-N1	8.87	115.29	108.20
1	AA	771	G	N1-C6-O6	8.86	125.22	119.90
1	AA	775	G	N1-C6-O6	8.86	125.22	119.90
1	AA	1305	G	N1-C6-O6	8.86	125.22	119.90
1	AA	1365	G	N1-C6-O6	8.86	125.22	119.90
27	B8	1945	G	N1-C6-O6	8.86	125.22	119.90
26	B7	107	G	N1-C6-O6	8.86	125.22	119.90
27	B8	15	G	N1-C6-O6	8.86	125.22	119.90
27	B8	2282	G	P-O3'-C3'	8.86	130.33	119.70
1	AA	369	G	N1-C6-O6	8.86	125.22	119.90
27	B8	458	G	N1-C6-O6	8.86	125.22	119.90
27	B8	467	G	N1-C6-O6	8.86	125.22	119.90
27	B8	622	G	N1-C6-O6	8.86	125.22	119.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	530	G	N1-C6-O6	8.86	125.21	119.90
1	AA	285	C	O4'-C1'-N1	8.86	115.28	108.20
1	AA	976	G	N1-C6-O6	8.86	125.21	119.90
3	AV	30	G	N1-C6-O6	8.86	125.21	119.90
27	B8	1524	G	N1-C6-O6	8.86	125.21	119.90
27	B8	1527	G	N1-C6-O6	8.86	125.21	119.90
1	AA	847	G	N1-C6-O6	8.85	125.21	119.90
27	B8	169	G	N1-C6-O6	8.85	125.21	119.90
27	B8	1152	C	O4'-C1'-N1	8.85	115.28	108.20
27	B8	1721	G	N1-C6-O6	8.85	125.21	119.90
1	AA	1064	G	N1-C6-O6	8.85	125.21	119.90
27	B8	859	G	N1-C6-O6	8.85	125.21	119.90
27	B8	1405	U	O4'-C1'-N1	8.85	115.28	108.20
27	B8	1581	G	N1-C6-O6	8.85	125.21	119.90
27	B8	1795	C	O4'-C1'-N1	8.85	115.28	108.20
27	B8	1933	G	N1-C6-O6	8.85	125.21	119.90
1	AA	79	G	N1-C6-O6	8.85	125.21	119.90
27	B8	45	G	N1-C6-O6	8.85	125.21	119.90
1	AA	880	C	O4'-C1'-N1	8.84	115.28	108.20
27	B8	2286	G	N1-C6-O6	8.84	125.21	119.90
27	B8	2371	G	N1-C6-O6	8.84	125.21	119.90
1	AA	424	G	C5-C6-O6	-8.84	123.30	128.60
1	AA	1108	G	N1-C6-O6	8.84	125.20	119.90
27	B8	263	G	N1-C6-O6	8.84	125.20	119.90
27	B8	524	G	C5-C6-O6	-8.84	123.30	128.60
27	B8	620	G	N1-C6-O6	8.84	125.20	119.90
27	B8	1994	C	O4'-C1'-N1	8.84	115.27	108.20
1	AA	423	G	N1-C6-O6	8.84	125.20	119.90
27	B8	1875	G	N1-C6-O6	8.84	125.20	119.90
27	B8	2529	G	N1-C6-O6	8.84	125.20	119.90
27	B8	2795	C	O4'-C1'-N1	8.84	115.27	108.20
1	AA	646	G	N1-C6-O6	8.83	125.20	119.90
1	AA	750	C	O4'-C1'-N1	8.83	115.27	108.20
27	B8	1753	G	N1-C6-O6	8.83	125.20	119.90
27	B8	2536	G	N1-C6-O6	8.83	125.20	119.90
27	B8	1283	G	N1-C6-O6	8.83	125.20	119.90
27	B8	2120	G	N1-C6-O6	8.83	125.20	119.90
27	B8	2843	G	N1-C6-O6	8.83	125.20	119.90
1	AA	674	G	C5-C6-O6	-8.83	123.30	128.60
27	B8	1903	G	N1-C6-O6	8.83	125.20	119.90
27	B8	2549	G	N1-C6-O6	8.83	125.20	119.90
27	B8	1374	G	N1-C6-O6	8.83	125.20	119.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	1884	G	N1-C6-O6	8.83	125.19	119.90
1	AA	1057	G	N1-C6-O6	8.82	125.19	119.90
27	B8	86	G	C5-C6-O6	-8.82	123.31	128.60
27	B8	2853	C	O4'-C1'-N1	8.82	115.26	108.20
1	AA	963	G	N1-C6-O6	8.82	125.19	119.90
26	B7	113	C	O4'-C1'-N1	8.82	115.26	108.20
27	B8	48	G	N1-C6-O6	8.82	125.19	119.90
27	B8	51	G	N1-C6-O6	8.82	125.19	119.90
27	B8	473	G	N1-C6-O6	8.82	125.19	119.90
27	B8	2357	G	N1-C6-O6	8.82	125.19	119.90
27	B8	2360	G	N1-C6-O6	8.82	125.19	119.90
1	AA	378	G	N1-C6-O6	8.82	125.19	119.90
1	AA	869	G	N1-C6-O6	8.82	125.19	119.90
26	B7	116	G	N1-C6-O6	8.82	125.19	119.90
27	B8	1277	G	N1-C6-O6	8.82	125.19	119.90
27	B8	1873	G	N1-C6-O6	8.82	125.19	119.90
27	B8	664	G	N1-C6-O6	8.82	125.19	119.90
27	B8	2239	G	N1-C6-O6	8.82	125.19	119.90
27	B8	2870	C	O4'-C1'-N1	8.82	115.25	108.20
1	AA	406	G	N1-C6-O6	8.81	125.19	119.90
1	AA	1209	C	O4'-C1'-N1	8.81	115.25	108.20
27	B8	1186	G	N1-C6-O6	8.81	125.19	119.90
1	AA	255	G	N1-C6-O6	8.81	125.19	119.90
27	B8	1888	G	N1-C6-O6	8.81	125.19	119.90
1	AA	469	C	O4'-C1'-N1	8.81	115.25	108.20
27	B8	338	G	N1-C6-O6	8.81	125.19	119.90
27	B8	1649	G	C5-C6-O6	-8.81	123.31	128.60
27	B8	1763	G	N1-C6-O6	8.81	125.19	119.90
27	B8	1869	G	N1-C6-O6	8.81	125.19	119.90
27	B8	80	G	N1-C6-O6	8.81	125.19	119.90
1	AA	278	G	N1-C6-O6	8.81	125.18	119.90
1	AA	1488	G	N1-C6-O6	8.81	125.18	119.90
3	AV	72	C	O4'-C1'-N1	8.80	115.24	108.20
27	B8	58	G	N1-C6-O6	8.80	125.18	119.90
27	B8	372	G	N1-C6-O6	8.80	125.18	119.90
27	B8	855	G	N1-C6-O6	8.80	125.18	119.90
1	AA	1013	G	N1-C6-O6	8.80	125.18	119.90
27	B8	2465	C	O4'-C1'-N1	8.80	115.24	108.20
3	AV	43	G	N1-C6-O6	8.80	125.18	119.90
26	B7	17	C	O4'-C1'-N1	8.80	115.24	108.20
27	B8	950	G	N1-C6-O6	8.80	125.18	119.90
27	B8	818	G	N1-C6-O6	8.80	125.18	119.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	1975	G	C5-C6-O6	-8.80	123.32	128.60
27	B8	2157	G	N1-C6-O6	8.80	125.18	119.90
27	B8	583	G	N1-C6-O6	8.79	125.18	119.90
27	B8	2455	G	N1-C6-O6	8.79	125.18	119.90
1	AA	584	G	C5-C6-O6	-8.79	123.32	128.60
26	B7	24	G	N1-C6-O6	8.79	125.18	119.90
27	B8	577	G	N1-C6-O6	8.79	125.18	119.90
1	AA	470	C	O4'-C1'-N1	8.79	115.23	108.20
27	B8	1243	C	O4'-C1'-N1	8.79	115.23	108.20
27	B8	2668	G	N1-C6-O6	8.79	125.17	119.90
3	AV	35	G	N1-C6-O6	8.79	125.17	119.90
26	B7	117	G	N1-C6-O6	8.79	125.17	119.90
27	B8	1288	G	N1-C6-O6	8.79	125.17	119.90
27	B8	1687	G	N1-C6-O6	8.79	125.17	119.90
27	B8	2049	G	N1-C6-O6	8.79	125.17	119.90
27	B8	418	C	O4'-C1'-N1	8.79	115.23	108.20
27	B8	2027	G	C5-C6-O6	-8.79	123.33	128.60
1	AA	1048	G	C5-C6-O6	-8.79	123.33	128.60
1	AA	581	G	N1-C6-O6	8.78	125.17	119.90
27	B8	157	C	O4'-C1'-N1	8.78	115.23	108.20
27	B8	2253	G	N1-C6-O6	8.78	125.17	119.90
27	B8	2446	G	N1-C6-O6	8.79	125.17	119.90
1	AA	350	G	N1-C6-O6	8.78	125.17	119.90
27	B8	248	G	C5-C6-O6	-8.78	123.33	128.60
27	B8	1074	G	N1-C6-O6	8.78	125.17	119.90
27	B8	1003	G	N1-C6-O6	8.78	125.17	119.90
27	B8	1110	G	N1-C6-O6	8.78	125.17	119.90
27	B8	1271	G	N1-C6-O6	8.78	125.17	119.90
27	B8	2524	G	N1-C6-O6	8.78	125.17	119.90
1	AA	481	G	N1-C6-O6	8.78	125.17	119.90
1	AA	966	G	N1-C6-O6	8.78	125.17	119.90
27	B8	1710	G	N1-C6-O6	8.78	125.17	119.90
27	B8	2592	G	C5-C6-O6	-8.78	123.33	128.60
1	AA	108	G	N1-C6-O6	8.78	125.17	119.90
1	AA	1387	G	N1-C6-O6	8.78	125.17	119.90
27	B8	2825	G	N1-C6-O6	8.78	125.17	119.90
27	B8	2834	G	N1-C6-O6	8.78	125.17	119.90
1	AA	394	G	N1-C6-O6	8.78	125.17	119.90
1	AA	1255	G	C5-C6-O6	-8.78	123.33	128.60
27	B8	2162	G	N1-C6-O6	8.78	125.17	119.90
1	AA	275	G	C5-C6-O6	-8.77	123.34	128.60
1	AA	656	G	N1-C6-O6	8.77	125.16	119.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1466	C	O4'-C1'-N1	8.77	115.22	108.20
27	B8	1839	G	N1-C6-O6	8.77	125.16	119.90
27	B8	2065	C	O4'-C1'-N1	8.77	115.22	108.20
27	B8	2623	G	C5-C6-O6	-8.77	123.34	128.60
1	AA	947	G	N1-C6-O6	8.77	125.16	119.90
27	B8	808	G	N1-C6-O6	8.77	125.16	119.90
27	B8	1619	G	N1-C6-O6	8.77	125.16	119.90
27	B8	1024	G	N1-C6-O6	8.77	125.16	119.90
27	B8	1356	G	N1-C6-O6	8.77	125.16	119.90
27	B8	1408	G	N1-C6-O6	8.77	125.16	119.90
27	B8	1986	C	O4'-C1'-N1	8.77	115.21	108.20
1	AA	713	G	N1-C6-O6	8.77	125.16	119.90
27	B8	69	C	O4'-C1'-N1	8.77	115.21	108.20
27	B8	257	C	O4'-C1'-N1	8.77	115.21	108.20
27	B8	857	G	N1-C6-O6	8.77	125.16	119.90
27	B8	1831	G	N1-C6-O6	8.77	125.16	119.90
1	AA	700	G	N1-C6-O6	8.76	125.16	119.90
1	AA	745	G	N1-C6-O6	8.76	125.16	119.90
27	B8	1051	G	N1-C6-O6	8.76	125.16	119.90
27	B8	2811	G	N1-C6-O6	8.76	125.16	119.90
27	B8	68	G	N1-C6-O6	8.76	125.16	119.90
27	B8	672	C	O4'-C1'-N1	8.76	115.21	108.20
27	B8	1049	C	O4'-C1'-N1	8.76	115.21	108.20
27	B8	2271	G	N1-C6-O6	8.76	125.16	119.90
27	B8	1823	G	N1-C6-O6	8.76	125.16	119.90
1	AA	281	G	N1-C6-O6	8.76	125.15	119.90
27	B8	117	G	N1-C6-O6	8.76	125.16	119.90
27	B8	1471	G	N1-C6-O6	8.76	125.15	119.90
1	AA	202	G	N1-C6-O6	8.75	125.15	119.90
1	AA	726	C	O4'-C1'-N1	8.75	115.20	108.20
27	B8	1346	G	N1-C6-O6	8.75	125.15	119.90
27	B8	1971	U	O4'-C1'-N1	8.75	115.20	108.20
27	B8	39	G	N1-C6-O6	8.75	125.15	119.90
27	B8	1702	G	N1-C6-O6	8.75	125.15	119.90
27	B8	555	G	N1-C6-O6	8.75	125.15	119.90
27	B8	663	G	C5-C6-O6	-8.75	123.35	128.60
27	B8	1292	G	N1-C6-O6	8.75	125.15	119.90
27	B8	2447	G	C5-C6-O6	-8.75	123.35	128.60
3	AV	45	G	N1-C6-O6	8.75	125.15	119.90
1	AA	661	G	N1-C6-O6	8.75	125.15	119.90
1	AA	852	G	N1-C6-O6	8.75	125.15	119.90
27	B8	130	C	O4'-C1'-N1	8.75	115.20	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	904	G	N1-C6-O6	8.75	125.15	119.90
27	B8	2780	G	N1-C6-O6	8.75	125.15	119.90
27	B8	334	C	O4'-C1'-N1	8.74	115.20	108.20
1	AA	858	G	N1-C6-O6	8.74	125.15	119.90
1	AA	1317	C	O4'-C1'-N1	8.74	115.19	108.20
26	B7	72	G	N1-C6-O6	8.74	125.15	119.90
27	B8	30	G	N1-C6-O6	8.74	125.15	119.90
27	B8	2237	G	N1-C6-O6	8.74	125.15	119.90
27	B8	2805	C	O4'-C1'-N1	8.74	115.20	108.20
27	B8	1025	G	N1-C6-O6	8.74	125.14	119.90
27	B8	1934	C	O4'-C1'-N1	8.74	115.19	108.20
27	B8	1699	G	N1-C6-O6	8.74	125.14	119.90
27	B8	1989	G	N1-C6-O6	8.74	125.14	119.90
27	B8	376	G	N1-C6-O6	8.74	125.14	119.90
1	AA	360	G	N1-C6-O6	8.73	125.14	119.90
1	AA	1024	G	N1-C6-O6	8.73	125.14	119.90
27	B8	379	G	N1-C6-O6	8.73	125.14	119.90
1	AA	844	G	N1-C6-O6	8.73	125.14	119.90
1	AA	1231	G	N1-C6-O6	8.73	125.14	119.90
27	B8	370	G	N1-C6-O6	8.73	125.14	119.90
27	B8	2553	G	N1-C6-O6	8.73	125.14	119.90
1	AA	575	G	N1-C6-O6	8.73	125.14	119.90
1	AA	1297	G	N1-C6-O6	8.73	125.14	119.90
1	AA	169	C	O4'-C1'-N1	8.73	115.18	108.20
27	B8	1627	G	C5-C6-O6	-8.73	123.36	128.60
27	B8	2368	C	O4'-C1'-N1	8.73	115.18	108.20
27	B8	2723	C	O4'-C1'-N1	8.73	115.18	108.20
1	AA	752	G	N1-C6-O6	8.72	125.14	119.90
1	AA	1003	G	N1-C6-O6	8.72	125.14	119.90
1	AA	193	C	O4'-C1'-N1	8.72	115.18	108.20
1	AA	616	G	C5-C6-O6	-8.72	123.37	128.60
1	AA	888	G	N1-C6-O6	8.72	125.13	119.90
27	B8	1311	G	N1-C6-O6	8.72	125.13	119.90
27	B8	489	G	N1-C6-O6	8.72	125.13	119.90
1	AA	346	G	N1-C6-O6	8.72	125.13	119.90
1	AA	606	G	N1-C6-O6	8.72	125.13	119.90
26	B7	102	G	N1-C6-O6	8.72	125.13	119.90
27	B8	517	C	O4'-C1'-N1	8.72	115.17	108.20
27	B8	891	G	O4'-C1'-N9	8.72	115.17	108.20
27	B8	98	G	N1-C6-O6	8.72	125.13	119.90
1	AA	769	G	N1-C6-O6	8.71	125.13	119.90
27	B8	1426	G	N1-C6-O6	8.71	125.13	119.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	517	G	N1-C6-O6	8.71	125.13	119.90
27	B8	2	G	N1-C6-O6	8.71	125.13	119.90
27	B8	1473	G	N1-C6-O6	8.71	125.13	119.90
27	B8	1756	G	N1-C6-O6	8.71	125.13	119.90
27	B8	2076	U	O4'-C1'-N1	8.71	115.17	108.20
27	B8	2532	G	N1-C6-O6	8.71	125.13	119.90
1	AA	112	G	N1-C6-O6	8.71	125.13	119.90
1	AA	398	U	O4'-C1'-N1	8.71	115.17	108.20
1	AA	419	C	O4'-C1'-N1	8.70	115.16	108.20
1	AA	1277	C	O4'-C1'-N1	8.71	115.16	108.20
27	B8	1827	U	O4'-C1'-N1	8.71	115.16	108.20
27	B8	2319	G	N1-C6-O6	8.71	125.12	119.90
27	B8	2379	G	N1-C6-O6	8.70	125.12	119.90
1	AA	357	G	N1-C6-O6	8.70	125.12	119.90
1	AA	524	G	N1-C6-O6	8.70	125.12	119.90
1	AA	1166	G	N1-C6-O6	8.70	125.12	119.90
27	B8	393	C	O4'-C1'-N1	8.70	115.16	108.20
27	B8	1703	G	N1-C6-O6	8.70	125.12	119.90
1	AA	1409	C	O4'-C1'-N1	8.70	115.16	108.20
27	B8	247	G	N1-C6-O6	8.70	125.12	119.90
27	B8	711	G	N1-C6-O6	8.70	125.12	119.90
1	AA	503	C	O4'-C1'-N1	8.69	115.16	108.20
1	AA	1316	G	N1-C6-O6	8.70	125.12	119.90
1	AA	1326	U	O4'-C1'-N1	8.69	115.16	108.20
27	B8	1432	G	N1-C6-O6	8.69	125.12	119.90
27	B8	2735	G	N1-C6-O6	8.69	125.12	119.90
1	AA	690	G	N1-C6-O6	8.69	125.11	119.90
1	AA	698	G	N1-C6-O6	8.69	125.11	119.90
1	AA	1099	G	N1-C6-O6	8.69	125.11	119.90
3	AV	44	G	N1-C6-O6	8.69	125.11	119.90
27	B8	725	G	N1-C6-O6	8.69	125.11	119.90
27	B8	1950	G	N1-C6-O6	8.69	125.11	119.90
27	B8	600	G	N1-C6-O6	8.69	125.11	119.90
27	B8	1542	U	O4'-C1'-N1	8.69	115.15	108.20
1	AA	172	A	N1-C6-N6	8.69	123.81	118.60
27	B8	704	G	N1-C6-O6	8.69	125.11	119.90
27	B8	805	G	N1-C6-O6	8.69	125.11	119.90
27	B8	2791	G	N1-C6-O6	8.69	125.11	119.90
1	AA	886	G	N1-C6-O6	8.69	125.11	119.90
1	AA	940	C	O4'-C1'-N1	8.69	115.15	108.20
27	B8	328	U	O4'-C1'-N1	8.69	115.15	108.20
27	B8	2144	G	N1-C6-O6	8.69	125.11	119.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	2676	C	O4'-C1'-N1	8.69	115.15	108.20
27	B8	548	G	N1-C6-O6	8.69	125.11	119.90
27	B8	671	C	O4'-C1'-N1	8.69	115.15	108.20
27	B8	2462	C	O4'-C1'-N1	8.69	115.15	108.20
1	AA	1087	G	C5-C6-O6	-8.68	123.39	128.60
26	B7	112	G	C5-C6-O6	-8.68	123.39	128.60
27	B8	1279	G	N1-C6-O6	8.68	125.11	119.90
27	B8	1667	G	N1-C6-O6	8.68	125.11	119.90
1	AA	637	C	O4'-C1'-N1	8.68	115.14	108.20
1	AA	1182	G	N1-C6-O6	8.68	125.11	119.90
1	AA	506	G	N1-C6-O6	8.68	125.11	119.90
1	AA	1475	G	N1-C6-O6	8.68	125.11	119.90
27	B8	273	G	C5-C6-O6	-8.68	123.39	128.60
27	B8	1237	A	O4'-C1'-N9	8.68	115.14	108.20
2	AX	14	G	N1-C6-O6	8.68	125.11	119.90
26	B7	62	C	O4'-C1'-N1	8.68	115.14	108.20
27	B8	1930	G	N1-C6-O6	8.67	125.10	119.90
27	B8	2193	G	N1-C6-O6	8.67	125.10	119.90
27	B8	2638	G	N1-C6-O6	8.67	125.10	119.90
1	AA	761	G	N1-C6-O6	8.67	125.10	119.90
27	B8	159	G	N1-C6-O6	8.67	125.10	119.90
27	B8	1770	G	N1-C6-O6	8.67	125.10	119.90
1	AA	568	G	N1-C6-O6	8.67	125.10	119.90
1	AA	1432	G	N1-C6-O6	8.67	125.10	119.90
26	B7	71	C	O4'-C1'-N1	8.67	115.13	108.20
27	B8	1437	C	O4'-C1'-N1	8.67	115.13	108.20
27	B8	2138	G	N1-C6-O6	8.67	125.10	119.90
27	B8	43	G	N1-C6-O6	8.66	125.10	119.90
1	AA	1074	G	N1-C6-O6	8.66	125.10	119.90
27	B8	488	G	N1-C6-O6	8.66	125.10	119.90
1	AA	515	G	N1-C6-O6	8.66	125.10	119.90
27	B8	2737	G	N1-C6-O6	8.66	125.10	119.90
27	B8	533	G	C5-C6-O6	-8.66	123.41	128.60
27	B8	1099	G	C5-C6-O6	-8.66	123.41	128.60
27	B8	2353	G	N1-C6-O6	8.66	125.09	119.90
27	B8	2429	G	N1-C6-O6	8.66	125.09	119.90
1	AA	113	G	C5-C6-O6	-8.65	123.41	128.60
1	AA	628	G	N1-C6-O6	8.65	125.09	119.90
1	AA	856	C	O4'-C1'-N1	8.65	115.12	108.20
27	B8	495	G	N1-C6-O6	8.65	125.09	119.90
3	AV	37	G	N1-C6-O6	8.65	125.09	119.90
27	B8	579	G	C5-C6-O6	-8.65	123.41	128.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	336	C	O4'-C1'-N1	8.65	115.12	108.20
27	B8	506	G	N1-C6-O6	8.65	125.09	119.90
27	B8	707	G	N1-C6-O6	8.65	125.09	119.90
27	B8	651	G	N1-C6-O6	8.65	125.09	119.90
27	B8	2535	G	C5-C6-O6	-8.65	123.41	128.60
27	B8	2775	G	N1-C6-O6	8.65	125.09	119.90
27	B8	876	C	O4'-C1'-N1	8.65	115.12	108.20
27	B8	2659	G	N1-C6-O6	8.65	125.09	119.90
1	AA	1134	G	N1-C6-O6	8.65	125.09	119.90
27	B8	601	C	O4'-C1'-N1	8.65	115.12	108.20
1	AA	1222	G	N1-C6-O6	8.64	125.09	119.90
1	AA	1489	G	N1-C6-O6	8.64	125.09	119.90
27	B8	2364	C	O4'-C1'-N1	8.64	115.12	108.20
3	AV	20	G	N1-C6-O6	8.64	125.09	119.90
27	B8	2673	G	C5-C6-O6	-8.64	123.41	128.60
1	AA	1113	C	O4'-C1'-N1	8.64	115.11	108.20
27	B8	1115	G	N1-C6-O6	8.64	125.08	119.90
27	B8	2699	C	O4'-C1'-N1	8.64	115.11	108.20
27	B8	2751	G	N1-C6-O6	8.64	125.08	119.90
1	AA	1455	G	C5-C6-O6	-8.64	123.42	128.60
27	B8	625	G	N1-C6-O6	8.64	125.08	119.90
27	B8	2255	G	N1-C6-O6	8.64	125.08	119.90
27	B8	2544	G	C5-C6-O6	-8.64	123.42	128.60
1	AA	187	G	N1-C6-O6	8.64	125.08	119.90
27	B8	713	G	N1-C6-O6	8.64	125.08	119.90
27	B8	882	G	N1-C6-O6	8.63	125.08	119.90
27	B8	2365	G	N1-C6-O6	8.63	125.08	119.90
27	B8	2808	G	N1-C6-O6	8.63	125.08	119.90
27	B8	2822	G	N1-C6-O6	8.63	125.08	119.90
1	AA	75	G	C5-C6-O6	-8.63	123.42	128.60
27	B8	2885	G	N1-C6-O6	8.63	125.08	119.90
1	AA	733	G	N1-C6-O6	8.63	125.08	119.90
1	AA	1417	G	N1-C6-O6	8.63	125.08	119.90
27	B8	426	C	O4'-C1'-N1	8.63	115.11	108.20
27	B8	2045	C	O4'-C1'-N1	8.63	115.11	108.20
27	B8	2663	G	N1-C6-O6	8.63	125.08	119.90
1	AA	1172	C	O4'-C1'-N1	8.63	115.10	108.20
1	AA	1398	A	O4'-C1'-N9	8.63	115.10	108.20
26	B7	4	C	O4'-C1'-N1	8.63	115.10	108.20
27	B8	474	G	N1-C6-O6	8.63	125.08	119.90
27	B8	2338	C	O4'-C1'-N1	8.63	115.10	108.20
1	AA	1347	G	N1-C6-O6	8.62	125.08	119.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	AV	12	G	N1-C6-O6	8.62	125.08	119.90
27	B8	493	G	N1-C6-O6	8.62	125.08	119.90
27	B8	1551	A	P-O3'-C3'	8.62	130.05	119.70
27	B8	2342	C	O4'-C1'-N1	8.63	115.10	108.20
27	B8	2289	G	N1-C6-O6	8.62	125.07	119.90
27	B8	2608	G	N1-C6-O6	8.62	125.08	119.90
1	AA	145	G	C5-C6-O6	-8.62	123.43	128.60
1	AA	310	G	N1-C6-O6	8.62	125.07	119.90
27	B8	757	G	C5-C6-O6	-8.62	123.43	128.60
1	AA	35	G	N1-C6-O6	8.62	125.07	119.90
1	AA	305	G	N1-C6-O6	8.62	125.07	119.90
1	AA	1331	G	N1-C6-O6	8.62	125.07	119.90
27	B8	1929	G	N1-C6-O6	8.62	125.07	119.90
27	B8	2127	G	N1-C6-O6	8.62	125.07	119.90
1	AA	297	G	N1-C6-O6	8.62	125.07	119.90
27	B8	1034	G	C5-C6-O6	-8.62	123.43	128.60
27	B8	143	C	O4'-C1'-N1	8.62	115.09	108.20
27	B8	1646	C	O4'-C1'-N1	8.62	115.09	108.20
27	B8	318	C	O4'-C1'-N1	8.62	115.09	108.20
27	B8	253	C	O4'-C1'-N1	8.62	115.09	108.20
27	B8	726	G	N1-C6-O6	8.62	125.07	119.90
27	B8	570	G	N1-C6-O6	8.61	125.07	119.90
27	B8	1092	C	O4'-C1'-N1	8.62	115.09	108.20
27	B8	1493	C	O4'-C1'-N1	8.62	115.09	108.20
27	B8	1538	G	C5-C6-O6	-8.62	123.43	128.60
1	AA	311	C	O4'-C1'-N1	8.61	115.09	108.20
1	AA	537	G	N1-C6-O6	8.61	125.07	119.90
27	B8	1333	G	N1-C6-O6	8.61	125.07	119.90
27	B8	1456	G	N1-C6-O6	8.61	125.07	119.90
1	AA	677	U	O4'-C1'-N1	8.61	115.09	108.20
1	AA	829	G	N1-C6-O6	8.61	125.07	119.90
1	AA	857	C	O4'-C1'-N1	8.61	115.09	108.20
1	AA	691	G	N1-C6-O6	8.61	125.06	119.90
27	B8	869	G	N1-C6-O6	8.61	125.07	119.90
27	B8	1364	G	N1-C6-O6	8.61	125.07	119.90
27	B8	2860	A	C4-C5-C6	8.61	121.31	117.00
27	B8	2863	C	O4'-C1'-N1	8.61	115.09	108.20
27	B8	623	C	O4'-C1'-N1	8.61	115.09	108.20
27	B8	891	G	N1-C6-O6	8.61	125.06	119.90
27	B8	1235	G	N1-C6-O6	8.61	125.06	119.90
27	B8	2331	G	N1-C6-O6	8.61	125.06	119.90
1	AA	370	C	O4'-C1'-N1	8.60	115.08	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	1718	G	N1-C6-O6	8.60	125.06	119.90
27	B8	1857	G	N1-C6-O6	8.60	125.06	119.90
1	AA	626	G	C5-C6-O6	-8.60	123.44	128.60
1	AA	351	G	N1-C6-O6	8.60	125.06	119.90
3	AV	40	G	N1-C6-O6	8.60	125.06	119.90
27	B8	1907	G	C5-C6-O6	-8.60	123.44	128.60
1	AA	1521	C	O4'-C1'-N1	8.60	115.08	108.20
27	B8	2159	G	N1-C6-O6	8.60	125.06	119.90
1	AA	107	G	N1-C6-O6	8.60	125.06	119.90
1	AA	1094	G	N1-C6-O6	8.60	125.06	119.90
27	B8	2607	G	N1-C6-O6	8.59	125.06	119.90
27	B8	1459	G	N1-C6-O6	8.59	125.05	119.90
27	B8	1956	U	O4'-C1'-N1	8.59	115.07	108.20
1	AA	83	C	O4'-C1'-N1	8.59	115.07	108.20
1	AA	647	C	O4'-C1'-N1	8.59	115.07	108.20
1	AA	1278	G	N1-C6-O6	8.59	125.05	119.90
2	AX	20	G	N1-C6-O6	8.59	125.05	119.90
27	B8	481	G	N1-C6-O6	8.59	125.05	119.90
27	B8	1807	G	N1-C6-O6	8.59	125.05	119.90
27	B8	341	C	O4'-C1'-N1	8.58	115.07	108.20
27	B8	669	G	N1-C6-O6	8.58	125.05	119.90
27	B8	2470	G	N1-C6-O6	8.58	125.05	119.90
27	B8	446	G	N1-C6-O6	8.58	125.05	119.90
27	B8	634	C	O4'-C1'-N1	8.58	115.06	108.20
27	B8	1726	C	O4'-C1'-N1	8.58	115.06	108.20
27	B8	1068	G	N1-C6-O6	8.58	125.05	119.90
1	AA	134	G	N1-C6-O6	8.58	125.05	119.90
1	AA	1193	G	C5-C6-O6	-8.58	123.45	128.60
27	B8	22	C	O4'-C1'-N1	8.58	115.06	108.20
1	AA	159	G	N1-C6-O6	8.57	125.05	119.90
3	AV	7	G	N1-C6-O6	8.57	125.05	119.90
26	B7	105	G	N1-C6-O6	8.57	125.05	119.90
27	B8	500	G	N1-C6-O6	8.57	125.05	119.90
27	B8	561	G	N1-C6-O6	8.57	125.05	119.90
27	B8	1005	C	O4'-C1'-N1	8.57	115.06	108.20
27	B8	1501	G	N1-C6-O6	8.57	125.04	119.90
27	B8	1879	C	O4'-C1'-N1	8.57	115.06	108.20
27	B8	2658	C	O4'-C1'-N1	8.57	115.06	108.20
1	AA	708	C	O4'-C1'-N1	8.57	115.06	108.20
1	AA	1178	G	N1-C6-O6	8.57	125.04	119.90
27	B8	1006	C	O4'-C1'-N1	8.57	115.06	108.20
27	B8	2018	G	N1-C6-O6	8.57	125.04	119.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	2206	C	O4'-C1'-N1	8.57	115.06	108.20
27	B8	2351	G	N1-C6-O6	8.57	125.04	119.90
27	B8	308	G	N1-C6-O6	8.57	125.04	119.90
27	B8	718	A	O4'-C1'-N9	8.57	115.06	108.20
27	B8	858	G	N1-C6-O6	8.57	125.04	119.90
27	B8	1339	G	N1-C6-O6	8.57	125.04	119.90
1	AA	290	C	O4'-C1'-N1	8.57	115.05	108.20
1	AA	501	C	O4'-C1'-N1	8.57	115.05	108.20
1	AA	1156	G	N1-C6-O6	8.57	125.04	119.90
3	AV	53	G	N1-C6-O6	8.57	125.04	119.90
27	B8	47	C	O4'-C1'-N1	8.57	115.05	108.20
27	B8	1844	C	O4'-C1'-N1	8.57	115.05	108.20
27	B8	2363	G	C5-C6-O6	-8.57	123.46	128.60
27	B8	1760	C	O4'-C1'-N1	8.57	115.05	108.20
27	B8	2787	C	O4'-C1'-N1	8.56	115.05	108.20
1	AA	359	G	C5-C6-O6	-8.56	123.46	128.60
3	AV	7	G	P-O3'-C3'	8.56	129.98	119.70
27	B8	381	G	N1-C6-O6	8.56	125.04	119.90
27	B8	417	C	O4'-C1'-N1	8.56	115.05	108.20
1	AA	1020	G	C5-C6-O6	-8.56	123.46	128.60
27	B8	367	G	N1-C6-O6	8.56	125.04	119.90
26	B7	114	C	O4'-C1'-N1	8.56	115.05	108.20
27	B8	1521	G	N1-C6-O6	8.56	125.04	119.90
27	B8	1550	C	O4'-C1'-N1	8.56	115.05	108.20
1	AA	128	G	N1-C6-O6	8.56	125.03	119.90
27	B8	2072	C	O4'-C1'-N1	8.56	115.05	108.20
27	B8	2156	G	N1-C6-O6	8.56	125.03	119.90
26	B7	91	C	O4'-C1'-N1	8.56	115.05	108.20
1	AA	667	G	C5-C6-O6	-8.55	123.47	128.60
26	B7	13	G	N1-C6-O6	8.55	125.03	119.90
27	B8	1715	G	N1-C6-O6	8.55	125.03	119.90
27	B8	2678	C	O4'-C1'-N1	8.55	115.04	108.20
27	B8	444	C	O4'-C1'-N1	8.55	115.04	108.20
27	B8	703	U	O4'-C1'-N1	8.55	115.04	108.20
27	B8	1812	U	O4'-C1'-N1	8.55	115.04	108.20
27	B8	2141	G	C5-C6-O6	-8.55	123.47	128.60
27	B8	2370	G	N1-C6-O6	8.55	125.03	119.90
27	B8	1	G	C5-C6-O6	-8.55	123.47	128.60
27	B8	2719	G	N1-C6-O6	8.55	125.03	119.90
1	AA	926	G	N1-C6-O6	8.54	125.03	119.90
27	B8	1483	G	N1-C6-O6	8.54	125.03	119.90
1	AA	272	C	O4'-C1'-N1	8.54	115.03	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	664	G	N1-C6-O6	8.54	125.03	119.90
27	B8	1298	C	O4'-C1'-N1	8.54	115.03	108.20
27	B8	2207	C	O4'-C1'-N1	8.54	115.03	108.20
27	B8	2688	G	N1-C6-O6	8.54	125.03	119.90
27	B8	1738	G	N1-C6-O6	8.54	125.02	119.90
1	AA	683	G	N1-C6-O6	8.54	125.02	119.90
26	B7	2	G	N1-C6-O6	8.54	125.02	119.90
27	B8	440	C	O4'-C1'-N1	8.54	115.03	108.20
27	B8	1227	G	N1-C6-O6	8.54	125.02	119.90
27	B8	2066	C	O4'-C1'-N1	8.54	115.03	108.20
27	B8	2749	A	N1-C6-N6	8.54	123.72	118.60
27	B8	2902	C	O4'-C1'-N1	8.54	115.03	108.20
1	AA	890	G	N1-C6-O6	8.54	125.02	119.90
1	AA	1079	G	N1-C6-O6	8.54	125.02	119.90
27	B8	619	G	N1-C6-O6	8.54	125.02	119.90
27	B8	817	C	O4'-C1'-N1	8.54	115.03	108.20
3	AV	46	G	N1-C6-O6	8.53	125.02	119.90
1	AA	417	G	C5-C6-O6	-8.53	123.48	128.60
1	AA	1089	G	N1-C6-O6	8.53	125.02	119.90
27	B8	1793	C	O4'-C1'-N1	8.53	115.03	108.20
27	B8	2252	G	N1-C6-O6	8.53	125.02	119.90
1	AA	1184	G	C5-C6-O6	-8.53	123.48	128.60
27	B8	1460	U	O4'-C1'-N1	8.53	115.03	108.20
1	AA	1068	G	N1-C6-O6	8.53	125.02	119.90
1	AA	1487	G	N1-C6-O6	8.53	125.02	119.90
1	AA	489	C	O4'-C1'-N1	8.53	115.02	108.20
27	B8	809	G	C5-C6-O6	-8.53	123.48	128.60
1	AA	972	C	O4'-C1'-N1	8.53	115.02	108.20
27	B8	168	G	N1-C6-O6	8.53	125.02	119.90
27	B8	512	G	N1-C6-O6	8.53	125.02	119.90
27	B8	180	G	N1-C6-O6	8.53	125.02	119.90
27	B8	559	G	C5-C6-O6	-8.53	123.48	128.60
27	B8	597	G	N1-C6-O6	8.53	125.02	119.90
27	B8	2848	G	N1-C6-O6	8.53	125.02	119.90
1	AA	124	C	O4'-C1'-N1	8.52	115.02	108.20
27	B8	557	C	O4'-C1'-N1	8.52	115.02	108.20
1	AA	639	G	C5-C6-O6	-8.52	123.49	128.60
1	AA	727	G	N1-C6-O6	8.52	125.01	119.90
27	B8	494	G	N1-C6-O6	8.52	125.01	119.90
27	B8	2816	G	N1-C6-O6	8.52	125.01	119.90
1	AA	122	G	C5-C6-O6	-8.52	123.49	128.60
1	AA	376	G	N1-C6-O6	8.52	125.01	119.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	657	U	O4'-C1'-N1	8.52	115.01	108.20
1	AA	1416	G	N1-C6-O6	8.52	125.01	119.90
27	B8	530	G	N1-C6-O6	8.52	125.01	119.90
26	B7	23	G	C5-C6-O6	-8.51	123.49	128.60
27	B8	881	G	N1-C6-O6	8.51	125.01	119.90
27	B8	1252	G	N1-C6-O6	8.51	125.01	119.90
1	AA	15	G	C5-C6-O6	-8.51	123.49	128.60
1	AA	741	G	N1-C6-O6	8.51	125.01	119.90
1	AA	1516	G	N1-C6-O6	8.51	125.01	119.90
26	B7	76	G	N1-C6-O6	8.51	125.01	119.90
27	B8	1741	C	O4'-C1'-N1	8.51	115.01	108.20
27	B8	1985	C	O4'-C1'-N1	8.51	115.01	108.20
27	B8	2324	U	O4'-C1'-N1	8.51	115.01	108.20
3	AV	1	C	O4'-C1'-N1	8.51	115.01	108.20
26	B7	41	G	N1-C6-O6	8.51	125.01	119.90
27	B8	2742	G	N1-C6-O6	8.51	125.01	119.90
27	B8	1146	C	O4'-C1'-N1	8.51	115.01	108.20
27	B8	2089	C	O4'-C1'-N1	8.51	115.00	108.20
27	B8	93	G	N1-C6-O6	8.51	125.00	119.90
1	AA	1279	G	N1-C6-O6	8.50	125.00	119.90
27	B8	242	G	N1-C6-O6	8.50	125.00	119.90
27	B8	366	C	O4'-C1'-N1	8.50	115.00	108.20
27	B8	1315	C	O4'-C1'-N1	8.50	115.00	108.20
1	AA	651	C	O4'-C1'-N1	8.50	115.00	108.20
27	B8	55	G	N1-C6-O6	8.50	125.00	119.90
27	B8	317	G	N1-C6-O6	8.50	125.00	119.90
27	B8	1038	G	C5-C6-O6	-8.50	123.50	128.60
1	AA	810	C	O4'-C1'-N1	8.50	115.00	108.20
27	B8	745	G	N1-C6-O6	8.50	125.00	119.90
1	AA	1260	G	N1-C6-O6	8.50	125.00	119.90
27	B8	413	C	O4'-C1'-N1	8.50	115.00	108.20
27	B8	1585	C	O4'-C1'-N1	8.50	115.00	108.20
27	B8	2032	G	N1-C6-O6	8.50	125.00	119.90
27	B8	2056	G	C5-C6-O6	-8.50	123.50	128.60
27	B8	2083	G	N1-C6-O6	8.50	125.00	119.90
27	B8	2466	C	O4'-C1'-N1	8.50	115.00	108.20
26	B7	54	G	C5-C6-O6	-8.49	123.50	128.60
27	B8	1892	C	O4'-C1'-N1	8.49	115.00	108.20
27	B8	2637	U	O4'-C1'-N1	8.49	115.00	108.20
27	B8	442	G	C5-C6-O6	-8.49	123.51	128.60
27	B8	1355	G	N1-C6-O6	8.49	124.99	119.90
1	AA	403	C	O4'-C1'-N1	8.49	114.99	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	388	G	N1-C6-O6	8.49	124.99	119.90
27	B8	737	C	O4'-C1'-N1	8.49	114.99	108.20
27	B8	2481	G	N1-C6-O6	8.49	124.99	119.90
1	AA	457	G	C5-C6-O6	-8.48	123.51	128.60
1	AA	879	C	O4'-C1'-N1	8.48	114.99	108.20
27	B8	1440	U	O4'-C1'-N1	8.48	114.99	108.20
1	AA	260	G	N1-C6-O6	8.48	124.99	119.90
27	B8	1197	G	N1-C6-O6	8.48	124.99	119.90
27	B8	1529	G	N1-C6-O6	8.48	124.99	119.90
1	AA	658	C	O4'-C1'-N1	8.48	114.98	108.20
1	AA	1524	C	O4'-C1'-N1	8.48	114.98	108.20
26	B7	33	G	C5-C6-O6	-8.48	123.51	128.60
1	AA	322	C	O4'-C1'-N1	8.48	114.98	108.20
1	AA	1405	G	C5-C6-O6	-8.48	123.51	128.60
27	B8	398	C	O4'-C1'-N1	8.48	114.98	108.20
1	AA	302	G	C5-C6-O6	-8.47	123.52	128.60
27	B8	1817	G	N1-C6-O6	8.47	124.98	119.90
1	AA	1421	G	N1-C6-O6	8.47	124.98	119.90
26	B7	56	G	N1-C6-O6	8.47	124.98	119.90
27	B8	2444	G	N1-C6-O6	8.47	124.98	119.90
1	AA	832	G	N1-C6-O6	8.47	124.98	119.90
1	AA	1077	G	N1-C6-O6	8.47	124.98	119.90
27	B8	1233	C	O4'-C1'-N1	8.47	114.98	108.20
27	B8	1867	G	N1-C6-O6	8.47	124.98	119.90
1	AA	22	G	C5-C6-O6	-8.47	123.52	128.60
27	B8	1447	C	O4'-C1'-N1	8.47	114.97	108.20
27	B8	333	G	N1-C6-O6	8.47	124.98	119.90
27	B8	1492	G	C5-C6-O6	-8.47	123.52	128.60
27	B8	1543	G	N1-C6-O6	8.47	124.98	119.90
27	B8	1686	C	O4'-C1'-N1	8.47	114.97	108.20
27	B8	2627	G	N1-C6-O6	8.47	124.98	119.90
1	AA	258	G	C5-C6-O6	-8.47	123.52	128.60
1	AA	942	G	N1-C6-O6	8.46	124.98	119.90
27	B8	2035	G	N1-C6-O6	8.46	124.98	119.90
1	AA	380	G	N1-C6-O6	8.46	124.98	119.90
27	B8	1515	A	N1-C6-N6	8.46	123.68	118.60
1	AA	1369	C	O4'-C1'-N1	8.46	114.97	108.20
27	B8	696	G	N1-C6-O6	8.46	124.97	119.90
27	B8	1236	G	N1-C6-O6	8.46	124.97	119.90
27	B8	1983	G	N1-C6-O6	8.46	124.97	119.90
1	AA	248	C	O4'-C1'-N1	8.46	114.96	108.20
27	B8	450	G	N1-C6-O6	8.45	124.97	119.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	777	G	C5-C6-O6	-8.46	123.53	128.60
27	B8	2694	G	C5-C6-O6	-8.46	123.53	128.60
27	B8	2378	A	C4-C5-C6	8.45	121.23	117.00
1	AA	785	G	C5-C6-O6	-8.45	123.53	128.60
1	AA	1453	G	N1-C6-O6	8.45	124.97	119.90
27	B8	1973	G	C5-C6-O6	-8.45	123.53	128.60
27	B8	2133	G	N1-C6-O6	8.45	124.97	119.90
1	AA	488	C	O4'-C1'-N1	8.45	114.96	108.20
27	B8	814	C	O4'-C1'-N1	8.45	114.96	108.20
27	B8	1896	G	C5-C6-O6	-8.45	123.53	128.60
27	B8	396	G	C5-C6-O6	-8.44	123.53	128.60
27	B8	1964	G	C5-C6-O6	-8.44	123.53	128.60
27	B8	1423	G	N1-C6-O6	8.44	124.97	119.90
27	B8	1401	G	N1-C6-O6	8.44	124.97	119.90
27	B8	1541	C	O4'-C1'-N1	8.44	114.95	108.20
27	B8	2624	G	C5-C6-O6	-8.44	123.53	128.60
1	AA	4	U	O4'-C1'-N1	8.44	114.95	108.20
27	B8	2269	G	N1-C6-O6	8.44	124.96	119.90
27	B8	2437	G	C5-C6-O6	-8.44	123.54	128.60
27	B8	2594	C	O4'-C1'-N1	8.44	114.95	108.20
27	B8	2597	G	N1-C6-O6	8.44	124.96	119.90
1	AA	235	C	O4'-C1'-N1	8.44	114.95	108.20
1	AA	486	U	O4'-C1'-N1	8.44	114.95	108.20
27	B8	1843	C	O4'-C1'-N1	8.44	114.95	108.20
27	B8	2512	C	O4'-C1'-N1	8.44	114.95	108.20
1	AA	1384	C	O4'-C1'-N1	8.44	114.95	108.20
3	AV	68	G	N1-C6-O6	8.44	124.96	119.90
27	B8	1682	G	C5-C6-O6	-8.44	123.54	128.60
27	B8	192	C	O4'-C1'-N1	8.43	114.94	108.20
27	B8	2214	C	O4'-C1'-N1	8.43	114.95	108.20
1	AA	168	G	C5-C6-O6	-8.43	123.54	128.60
1	AA	1505	G	N1-C6-O6	8.43	124.96	119.90
1	AA	1018	G	N1-C6-O6	8.43	124.96	119.90
1	AA	1265	C	O4'-C1'-N1	8.43	114.94	108.20
1	AA	259	G	C5-C6-O6	-8.43	123.55	128.60
1	AA	941	G	N1-C6-O6	8.43	124.95	119.90
1	AA	257	G	N1-C6-O6	8.42	124.95	119.90
1	AA	650	G	N1-C6-O6	8.42	124.95	119.90
1	AA	1175	G	N1-C6-O6	8.42	124.95	119.90
27	B8	16	C	O4'-C1'-N1	8.42	114.94	108.20
27	B8	679	C	O4'-C1'-N1	8.42	114.94	108.20
27	B8	1947	C	O4'-C1'-N1	8.42	114.94	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	38	G	N1-C6-O6	8.42	124.95	119.90
27	B8	2858	C	O4'-C1'-N1	8.42	114.94	108.20
1	AA	440	C	O4'-C1'-N1	8.42	114.94	108.20
1	AA	931	C	O4'-C1'-N1	8.42	114.94	108.20
1	AA	326	G	N1-C6-O6	8.41	124.95	119.90
1	AA	800	G	N1-C6-O6	8.41	124.95	119.90
27	B8	880	G	N1-C6-O6	8.41	124.95	119.90
27	B8	1180	U	O4'-C1'-N1	8.41	114.93	108.20
27	B8	935	C	O4'-C1'-N1	8.41	114.93	108.20
27	B8	2576	G	N1-C6-O6	8.41	124.95	119.90
1	AA	215	C	O4'-C1'-N1	8.41	114.93	108.20
1	AA	614	C	O4'-C1'-N1	8.41	114.93	108.20
26	B7	97	C	O4'-C1'-N1	8.41	114.93	108.20
27	B8	316	C	O4'-C1'-N1	8.41	114.93	108.20
27	B8	1017	G	N1-C6-O6	8.41	124.94	119.90
27	B8	1061	U	C2-N1-C1'	8.41	127.79	117.70
27	B8	1183	U	O4'-C1'-N1	8.41	114.93	108.20
27	B8	1239	G	C5-C6-O6	-8.41	123.55	128.60
1	AA	1058	G	C5-C6-O6	-8.41	123.56	128.60
27	B8	2361	G	N1-C6-O6	8.41	124.94	119.90
1	AA	86	G	N1-C6-O6	8.40	124.94	119.90
27	B8	1695	G	N1-C6-O6	8.40	124.94	119.90
27	B8	2874	C	O4'-C1'-N1	8.40	114.92	108.20
1	AA	812	G	C5-C6-O6	-8.40	123.56	128.60
1	AA	1338	G	N1-C6-O6	8.40	124.94	119.90
27	B8	315	G	N1-C6-O6	8.40	124.94	119.90
27	B8	486	C	O4'-C1'-N1	8.40	114.92	108.20
27	B8	2294	G	N1-C6-O6	8.40	124.94	119.90
27	B8	2414	G	C5-C6-O6	-8.40	123.56	128.60
27	B8	564	C	O4'-C1'-N1	8.40	114.92	108.20
27	B8	765	C	O4'-C1'-N1	8.40	114.92	108.20
27	B8	1957	C	O4'-C1'-N1	8.40	114.92	108.20
27	B8	491	G	N1-C6-O6	8.40	124.94	119.90
27	B8	948	C	O4'-C1'-N1	8.40	114.92	108.20
27	B8	2055	C	O4'-C1'-N1	8.40	114.92	108.20
27	B8	2332	C	O4'-C1'-N1	8.40	114.92	108.20
27	B8	2591	C	O4'-C1'-N1	8.39	114.92	108.20
27	B8	2644	G	N1-C6-O6	8.39	124.94	119.90
1	AA	201	G	N1-C6-O6	8.39	124.94	119.90
27	B8	2842	G	N1-C6-O6	8.39	124.94	119.90
1	AA	1154	G	C5-C6-O6	-8.39	123.56	128.60
27	B8	2421	G	C5-C6-O6	-8.39	123.56	128.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1217	C	O4'-C1'-N1	8.39	114.91	108.20
27	B8	2124	G	C5-C6-O6	-8.39	123.57	128.60
27	B8	2215	C	O4'-C1'-N1	8.39	114.91	108.20
26	B7	118	C	O4'-C1'-N1	8.39	114.91	108.20
27	B8	1587	G	N1-C6-O6	8.39	124.93	119.90
27	B8	1908	C	O4'-C1'-N1	8.39	114.91	108.20
27	B8	2177	C	O4'-C1'-N1	8.38	114.91	108.20
27	B8	2264	C	O4'-C1'-N1	8.38	114.91	108.20
1	AA	818	G	N1-C6-O6	8.38	124.93	119.90
3	AV	19	G	N1-C6-O6	8.38	124.93	119.90
27	B8	830	G	N1-C6-O6	8.38	124.93	119.90
27	B8	922	C	O4'-C1'-N1	8.38	114.91	108.20
27	B8	1187	G	N1-C6-O6	8.38	124.93	119.90
27	B8	1788	C	O4'-C1'-N1	8.38	114.91	108.20
27	B8	2618	G	N1-C6-O6	8.38	124.93	119.90
27	B8	2655	G	N1-C6-O6	8.38	124.93	119.90
1	AA	1273	C	O4'-C1'-N1	8.38	114.90	108.20
1	AA	693	G	N1-C6-O6	8.38	124.93	119.90
1	AA	90	C	O4'-C1'-N1	8.38	114.90	108.20
1	AA	1203	C	O4'-C1'-N1	8.38	114.90	108.20
27	B8	951	C	O4'-C1'-N1	8.37	114.90	108.20
27	B8	1743	G	C5-C6-O6	-8.37	123.58	128.60
27	B8	2774	C	O4'-C1'-N1	8.38	114.90	108.20
27	B8	836	G	C5-C6-O6	-8.37	123.58	128.60
27	B8	662	G	C5-C6-O6	-8.37	123.58	128.60
27	B8	1704	C	O4'-C1'-N1	8.37	114.90	108.20
27	B8	2048	G	N1-C6-O6	8.37	124.92	119.90
27	B8	2397	G	N1-C6-O6	8.37	124.92	119.90
1	AA	1382	C	O4'-C1'-N1	8.37	114.90	108.20
27	B8	1935	G	N1-C6-O6	8.37	124.92	119.90
27	B8	452	G	N1-C6-O6	8.37	124.92	119.90
27	B8	1685	C	O4'-C1'-N1	8.37	114.89	108.20
27	B8	1931	U	O4'-C1'-N1	8.36	114.89	108.20
1	AA	211	G	N1-C6-O6	8.36	124.92	119.90
27	B8	2683	C	O4'-C1'-N1	8.36	114.89	108.20
27	B8	329	G	N1-C6-O6	8.36	124.92	119.90
27	B8	1331	G	N1-C6-O6	8.36	124.92	119.90
27	B8	2507	C	O4'-C1'-N1	8.36	114.89	108.20
3	AV	36	G	N1-C6-O6	8.36	124.91	119.90
1	AA	895	G	N1-C6-O6	8.35	124.91	119.90
1	AA	1259	C	O4'-C1'-N1	8.35	114.88	108.20
26	B7	81	G	C5-C6-O6	-8.35	123.59	128.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	1464	G	N1-C6-O6	8.35	124.91	119.90
1	AA	97	G	N1-C6-O6	8.35	124.91	119.90
1	AA	1361	G	N1-C6-O6	8.35	124.91	119.90
27	B8	1967	C	O4'-C1'-N1	8.35	114.88	108.20
1	AA	1049	U	P-O3'-C3'	8.35	129.72	119.70
1	AA	1325	C	O4'-C1'-N1	8.35	114.88	108.20
27	B8	20	C	O4'-C1'-N1	8.34	114.87	108.20
27	B8	194	G	C5-C6-O6	-8.34	123.59	128.60
27	B8	795	C	O4'-C1'-N1	8.34	114.87	108.20
27	B8	1465	G	C5-C6-O6	-8.34	123.59	128.60
27	B8	2257	U	O4'-C1'-N1	8.34	114.87	108.20
27	B8	929	U	O4'-C1'-N1	8.34	114.87	108.20
27	B8	903	C	O4'-C1'-N1	8.34	114.87	108.20
27	B8	1140	C	O4'-C1'-N1	8.34	114.87	108.20
27	B8	1739	A	N1-C6-N6	8.34	123.60	118.60
1	AA	582	C	O4'-C1'-N1	8.34	114.87	108.20
1	AA	613	C	O4'-C1'-N1	8.34	114.87	108.20
1	AA	1016	A	C4-C5-C6	8.34	121.17	117.00
27	B8	2282	G	N1-C6-O6	8.34	124.90	119.90
27	B8	1184	U	O4'-C1'-N1	8.34	114.87	108.20
27	B8	846	U	O4'-C1'-N1	8.33	114.87	108.20
27	B8	1122	G	N1-C6-O6	8.33	124.90	119.90
27	B8	1026	G	N1-C6-O6	8.33	124.90	119.90
3	AV	65	C	O4'-C1'-N1	8.33	114.86	108.20
27	B8	1370	C	O4'-C1'-N1	8.33	114.86	108.20
27	B8	690	G	N1-C6-O6	8.33	124.90	119.90
1	AA	1461	G	N1-C6-O6	8.33	124.90	119.90
27	B8	260	G	C5-C6-O6	-8.33	123.60	128.60
27	B8	897	C	O4'-C1'-N1	8.33	114.86	108.20
26	B7	38	C	O4'-C1'-N1	8.32	114.86	108.20
27	B8	700	G	C5-C6-O6	-8.32	123.61	128.60
27	B8	748	G	N1-C6-O6	8.32	124.89	119.90
27	B8	1114	C	O4'-C1'-N1	8.32	114.86	108.20
1	AA	1164	G	C5-C6-O6	-8.32	123.61	128.60
27	B8	558	U	O4'-C1'-N1	8.32	114.86	108.20
27	B8	2410	G	C5-C6-O6	-8.32	123.61	128.60
27	B8	684	G	N1-C6-O6	8.32	124.89	119.90
3	AV	50	G	N1-C6-O6	8.32	124.89	119.90
27	B8	2140	G	C5-C6-O6	-8.32	123.61	128.60
1	AA	304	U	O4'-C1'-N1	8.31	114.85	108.20
1	AA	1148	U	O4'-C1'-N1	8.31	114.85	108.20
1	AA	1344	C	O4'-C1'-N1	8.31	114.85	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	1362	C	O4'-C1'-N1	8.31	114.85	108.20
1	AA	1268	G	N1-C6-O6	8.31	124.89	119.90
1	AA	842	U	O4'-C1'-N1	8.31	114.85	108.20
1	AA	1515	G	C5-C6-O6	-8.31	123.61	128.60
27	B8	2224	G	N1-C6-O6	8.31	124.89	119.90
27	B8	1769	U	O4'-C1'-N1	8.31	114.85	108.20
27	B8	2595	G	N1-C6-O6	8.31	124.89	119.90
1	AA	21	G	N1-C6-O6	8.30	124.88	119.90
1	AA	936	C	O4'-C1'-N1	8.30	114.84	108.20
27	B8	1153	C	O4'-C1'-N1	8.31	114.84	108.20
1	AA	1038	C	O4'-C1'-N1	8.30	114.84	108.20
1	AA	1355	G	N1-C6-O6	8.30	124.88	119.90
27	B8	97	C	O4'-C1'-N1	8.30	114.84	108.20
27	B8	112	U	O4'-C1'-N1	8.30	114.84	108.20
27	B8	210	C	O4'-C1'-N1	8.30	114.84	108.20
27	B8	350	G	C5-C6-O6	-8.30	123.62	128.60
27	B8	784	G	O4'-C1'-N9	8.30	114.84	108.20
27	B8	977	G	C5-C6-O6	-8.30	123.62	128.60
27	B8	1575	C	O4'-C1'-N1	8.30	114.84	108.20
27	B8	2010	G	N1-C6-O6	8.30	124.88	119.90
1	AA	6	G	N1-C6-O6	8.30	124.88	119.90
26	B7	10	G	C5-C6-O6	-8.30	123.62	128.60
27	B8	186	G	C5-C6-O6	-8.30	123.62	128.60
27	B8	1605	C	O4'-C1'-N1	8.30	114.84	108.20
27	B8	2839	G	C5-C6-O6	-8.30	123.62	128.60
27	B8	854	C	O4'-C1'-N1	8.30	114.84	108.20
27	B8	870	U	O4'-C1'-N1	8.30	114.84	108.20
27	B8	1874	C	O4'-C1'-N1	8.30	114.84	108.20
26	B7	60	C	O4'-C1'-N1	8.30	114.84	108.20
27	B8	1300	G	N1-C6-O6	8.30	124.88	119.90
27	B8	2067	G	N1-C6-O6	8.30	124.88	119.90
1	AA	268	U	O4'-C1'-N1	8.29	114.83	108.20
1	AA	45	G	C5-C6-O6	-8.29	123.62	128.60
1	AA	633	G	N1-C6-O6	8.29	124.88	119.90
1	AA	882	C	O4'-C1'-N1	8.29	114.83	108.20
1	AA	910	C	O4'-C1'-N1	8.29	114.83	108.20
1	AA	985	C	O4'-C1'-N1	8.29	114.83	108.20
27	B8	2350	C	O4'-C1'-N1	8.29	114.83	108.20
1	AA	379	C	O4'-C1'-N1	8.29	114.83	108.20
27	B8	1056	G	N1-C6-O6	8.29	124.87	119.90
27	B8	1737	G	N1-C6-O6	8.29	124.87	119.90
27	B8	2417	C	O4'-C1'-N1	8.29	114.83	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	2803	G	C5-C6-O6	-8.29	123.63	128.60
1	AA	594	U	O4'-C1'-N1	8.28	114.83	108.20
1	AA	216	U	O4'-C1'-N1	8.28	114.83	108.20
1	AA	519	C	O4'-C1'-N1	8.28	114.83	108.20
27	B8	1613	G	N1-C6-O6	8.28	124.87	119.90
1	AA	57	G	C5-C6-O6	-8.28	123.63	128.60
1	AA	1026	G	C5-C6-O6	-8.28	123.63	128.60
27	B8	1391	U	O4'-C1'-N1	8.28	114.82	108.20
27	B8	2222	C	O4'-C1'-N1	8.28	114.82	108.20
1	AA	838	G	C5-C6-O6	-8.28	123.64	128.60
27	B8	312	G	C5-C6-O6	-8.28	123.64	128.60
27	B8	875	G	C5-C6-O6	-8.28	123.64	128.60
27	B8	2023	C	O4'-C1'-N1	8.28	114.82	108.20
27	B8	2304	G	C5-C6-O6	-8.28	123.63	128.60
27	B8	2640	G	C5-C6-O6	-8.28	123.64	128.60
27	B8	2855	C	O4'-C1'-N1	8.28	114.82	108.20
1	AA	627	G	C5-C6-O6	-8.27	123.64	128.60
27	B8	185	G	C5-C6-O6	-8.27	123.64	128.60
27	B8	326	G	C5-C6-O6	-8.27	123.64	128.60
27	B8	2391	G	N1-C6-O6	8.27	124.86	119.90
1	AA	254	G	N1-C6-O6	8.27	124.86	119.90
27	B8	2400	G	C5-C6-O6	-8.27	123.64	128.60
27	B8	2649	C	O4'-C1'-N1	8.27	114.82	108.20
1	AA	557	G	N1-C6-O6	8.27	124.86	119.90
1	AA	1239	A	N1-C6-N6	8.27	123.56	118.60
27	B8	853	C	O4'-C1'-N1	8.27	114.82	108.20
27	B8	985	C	O4'-C1'-N1	8.27	114.82	108.20
27	B8	1167	C	O4'-C1'-N1	8.27	114.82	108.20
1	AA	689	C	O4'-C1'-N1	8.27	114.81	108.20
27	B8	816	C	O4'-C1'-N1	8.27	114.82	108.20
1	AA	1517	G	N1-C6-O6	8.27	124.86	119.90
1	AA	1520	C	O4'-C1'-N1	8.27	114.81	108.20
3	AV	75	C	O4'-C1'-N1	8.27	114.82	108.20
27	B8	208	C	O4'-C1'-N1	8.27	114.81	108.20
27	B8	2285	C	O4'-C1'-N1	8.27	114.81	108.20
27	B8	26	G	N1-C6-O6	8.27	124.86	119.90
27	B8	2620	C	O4'-C1'-N1	8.27	114.81	108.20
27	B8	987	C	O4'-C1'-N1	8.26	114.81	108.20
27	B8	2574	G	C5-C6-O6	-8.26	123.64	128.60
27	B8	137	U	O4'-C1'-N1	8.26	114.81	108.20
1	AA	385	C	O4'-C1'-N1	8.26	114.81	108.20
1	AA	1495	U	O4'-C1'-N1	8.26	114.81	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	409	U	O4'-C1'-N1	8.26	114.81	108.20
1	AA	1071	C	O4'-C1'-N1	8.26	114.81	108.20
27	B8	36	G	N1-C6-O6	8.26	124.86	119.90
27	B8	1826	G	C5-C6-O6	-8.26	123.64	128.60
1	AA	755	G	C5-C6-O6	-8.26	123.64	128.60
1	AA	1371	G	N1-C6-O6	8.26	124.85	119.90
26	B7	92	C	O4'-C1'-N1	8.26	114.81	108.20
1	AA	823	C	O4'-C1'-N1	8.25	114.80	108.20
27	B8	129	C	O4'-C1'-N1	8.25	114.80	108.20
27	B8	1573	G	N1-C6-O6	8.25	124.85	119.90
1	AA	756	C	O4'-C1'-N1	8.25	114.80	108.20
1	AA	898	G	N1-C6-O6	8.25	124.85	119.90
26	B7	63	C	O4'-C1'-N1	8.25	114.80	108.20
27	B8	1980	G	N1-C6-O6	8.25	124.85	119.90
1	AA	319	G	C5-C6-O6	-8.24	123.65	128.60
1	AA	455	G	C5-C6-O6	-8.24	123.65	128.60
1	AA	580	C	O4'-C1'-N1	8.24	114.80	108.20
27	B8	201	C	O4'-C1'-N1	8.24	114.80	108.20
1	AA	732	C	O4'-C1'-N1	8.24	114.79	108.20
27	B8	687	C	O4'-C1'-N1	8.24	114.79	108.20
27	B8	1547	C	O4'-C1'-N1	8.24	114.79	108.20
1	AA	999	C	O4'-C1'-N1	8.24	114.79	108.20
27	B8	121	G	C5-C6-O6	-8.24	123.66	128.60
27	B8	409	G	C5-C6-O6	-8.24	123.66	128.60
27	B8	1270	C	O4'-C1'-N1	8.24	114.79	108.20
27	B8	2217	G	C5-C6-O6	-8.24	123.66	128.60
26	B7	9	G	C5-C6-O6	-8.24	123.66	128.60
27	B8	539	G	N1-C6-O6	8.24	124.84	119.90
27	B8	2362	C	O4'-C1'-N1	8.24	114.79	108.20
27	B8	2704	C	O4'-C1'-N1	8.24	114.79	108.20
1	AA	778	G	C5-C6-O6	-8.23	123.66	128.60
3	AV	67	C	O4'-C1'-N1	8.23	114.79	108.20
27	B8	2559	C	O4'-C1'-N1	8.23	114.79	108.20
1	AA	105	G	C5-C6-O6	-8.23	123.66	128.60
27	B8	1191	G	C5-C6-O6	-8.23	123.66	128.60
1	AA	764	C	O4'-C1'-N1	8.23	114.78	108.20
27	B8	1540	G	C5-C6-O6	-8.23	123.66	128.60
1	AA	1266	G	N1-C6-O6	8.23	124.84	119.90
27	B8	109	C	O4'-C1'-N1	8.23	114.78	108.20
27	B8	968	C	O4'-C1'-N1	8.23	114.78	108.20
27	B8	2648	G	C5-C6-O6	-8.23	123.66	128.60
27	B8	2896	C	O4'-C1'-N1	8.23	114.78	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	899	C	O4'-C1'-N1	8.23	114.78	108.20
27	B8	954	G	C5-C6-O6	-8.23	123.66	128.60
27	B8	2715	C	O4'-C1'-N1	8.23	114.78	108.20
1	AA	269	C	O4'-C1'-N1	8.22	114.78	108.20
27	B8	355	U	O4'-C1'-N1	8.22	114.78	108.20
27	B8	1961	C	O4'-C1'-N1	8.22	114.78	108.20
1	AA	668	G	C5-C6-O6	-8.22	123.67	128.60
27	B8	2641	G	C5-C6-O6	-8.22	123.67	128.60
27	B8	465	G	N1-C6-O6	8.22	124.83	119.90
27	B8	673	C	O4'-C1'-N1	8.21	114.77	108.20
27	B8	2380	C	O4'-C1'-N1	8.21	114.77	108.20
1	AA	291	U	O4'-C1'-N1	8.21	114.77	108.20
1	AA	392	C	O4'-C1'-N1	8.21	114.77	108.20
27	B8	879	G	N1-C6-O6	8.21	124.83	119.90
26	B7	110	C	O4'-C1'-N1	8.21	114.77	108.20
1	AA	1002	G	C5-C6-O6	-8.21	123.67	128.60
26	B7	90	C	O4'-C1'-N1	8.21	114.77	108.20
27	B8	54	G	N1-C6-O6	8.21	124.83	119.90
27	B8	245	G	C5-C6-O6	-8.21	123.67	128.60
27	B8	1837	C	O4'-C1'-N1	8.21	114.77	108.20
1	AA	85	U	O4'-C1'-N1	8.20	114.76	108.20
1	AA	286	C	O4'-C1'-N1	8.20	114.76	108.20
1	AA	232	G	N1-C6-O6	8.20	124.82	119.90
1	AA	731	G	C5-C6-O6	-8.20	123.68	128.60
1	AA	1352	C	O4'-C1'-N1	8.20	114.76	108.20
27	B8	81	G	C5-C6-O6	-8.20	123.68	128.60
27	B8	2819	G	C5-C6-O6	-8.20	123.68	128.60
1	AA	138	G	C5-C6-O6	-8.20	123.68	128.60
1	AA	853	C	O4'-C1'-N1	8.20	114.76	108.20
27	B8	331	C	O4'-C1'-N1	8.20	114.76	108.20
27	B8	476	G	N1-C6-O6	8.20	124.82	119.90
27	B8	2057	G	C5-C6-O6	-8.19	123.68	128.60
27	B8	2185	U	O4'-C1'-N1	8.19	114.76	108.20
27	B8	2424	C	O4'-C1'-N1	8.19	114.75	108.20
27	B8	2801	G	C5-C6-O6	-8.20	123.68	128.60
27	B8	2588	G	C5-C6-O6	-8.19	123.68	128.60
1	AA	1328	C	O4'-C1'-N1	8.19	114.75	108.20
27	B8	1293	C	O4'-C1'-N1	8.19	114.75	108.20
27	B8	2557	G	C5-C6-O6	-8.19	123.69	128.60
27	B8	2722	G	C5-C6-O6	-8.19	123.69	128.60
1	AA	454	G	C5-C6-O6	-8.19	123.69	128.60
27	B8	611	C	O4'-C1'-N1	8.19	114.75	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	1341	G	N1-C6-O6	8.19	124.81	119.90
27	B8	2283	C	O4'-C1'-N1	8.19	114.75	108.20
1	AA	1132	C	O4'-C1'-N1	8.19	114.75	108.20
27	B8	2375	G	N1-C6-O6	8.19	124.81	119.90
1	AA	998	C	O4'-C1'-N1	8.18	114.75	108.20
1	AA	1320	C	O4'-C1'-N1	8.18	114.75	108.20
1	AA	1414	U	O4'-C1'-N1	8.18	114.75	108.20
1	AA	242	G	C5-C6-O6	-8.18	123.69	128.60
1	AA	786	G	C5-C6-O6	-8.18	123.69	128.60
3	AV	6	C	O4'-C1'-N1	8.18	114.75	108.20
27	B8	1435	G	C5-C6-O6	-8.18	123.69	128.60
1	AA	1454	G	C5-C6-O6	-8.18	123.69	128.60
27	B8	425	G	C5-C6-O6	-8.18	123.69	128.60
27	B8	2581	G	N1-C6-O6	8.18	124.81	119.90
27	B8	2631	G	C5-C6-O6	-8.18	123.69	128.60
1	AA	264	C	O4'-C1'-N1	8.18	114.74	108.20
1	AA	1136	C	O4'-C1'-N1	8.18	114.74	108.20
27	B8	496	G	C5-C6-O6	-8.18	123.69	128.60
27	B8	1858	A	N1-C6-N6	8.18	123.51	118.60
27	B8	1463	C	O4'-C1'-N1	8.18	114.74	108.20
27	B8	1734	G	C5-C6-O6	-8.17	123.70	128.60
1	AA	587	G	N1-C6-O6	8.17	124.80	119.90
1	AA	654	G	N1-C6-O6	8.17	124.80	119.90
27	B8	617	G	C5-C6-O6	-8.17	123.70	128.60
27	B8	754	U	O4'-C1'-N1	8.17	114.73	108.20
1	AA	475	C	O4'-C1'-N1	8.17	114.73	108.20
1	AA	1323	G	C5-C6-O6	-8.17	123.70	128.60
27	B8	784	G	C5-C6-O6	-8.17	123.70	128.60
1	AA	384	G	N1-C6-O6	8.16	124.80	119.90
1	AA	484	G	C5-C6-O6	-8.16	123.70	128.60
1	AA	426	U	O4'-C1'-N1	8.16	114.73	108.20
1	AA	578	C	O4'-C1'-N1	8.16	114.73	108.20
1	AA	722	G	N1-C6-O6	8.16	124.80	119.90
1	AA	1263	C	O4'-C1'-N1	8.16	114.73	108.20
1	AA	1283	U	O4'-C1'-N1	8.16	114.73	108.20
27	B8	88	G	N1-C6-O6	8.16	124.80	119.90
27	B8	105	C	O4'-C1'-N1	8.16	114.73	108.20
27	B8	236	C	O4'-C1'-N1	8.16	114.73	108.20
27	B8	386	G	N1-C6-O6	8.16	124.80	119.90
27	B8	2515	C	O4'-C1'-N1	8.16	114.73	108.20
1	AA	1484	C	O4'-C1'-N1	8.16	114.73	108.20
27	B8	1917	U	O4'-C1'-N1	8.16	114.72	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	1200	C	O4'-C1'-N1	8.15	114.72	108.20
1	AA	765	G	N1-C6-O6	8.15	124.79	119.90
1	AA	1343	G	C5-C6-O6	-8.15	123.71	128.60
27	B8	731	C	O4'-C1'-N1	8.15	114.72	108.20
27	B8	986	C	O4'-C1'-N1	8.15	114.72	108.20
27	B8	1561	C	O4'-C1'-N1	8.15	114.72	108.20
27	B8	2714	G	C5-C6-O6	-8.15	123.71	128.60
27	B8	2859	G	N1-C6-O6	8.15	124.79	119.90
1	AA	1525	G	N1-C6-O6	8.15	124.79	119.90
27	B8	2520	C	O4'-C1'-N1	8.15	114.72	108.20
1	AA	162	A	C4-C5-C6	8.15	121.07	117.00
27	B8	1949	G	C5-C6-O6	-8.15	123.71	128.60
27	B8	2483	C	O4'-C1'-N1	8.15	114.72	108.20
1	AA	948	C	O4'-C1'-N1	8.14	114.72	108.20
1	AA	1096	C	O4'-C1'-N1	8.14	114.71	108.20
27	B8	1488	C	O4'-C1'-N1	8.14	114.71	108.20
27	B8	2200	C	O4'-C1'-N1	8.14	114.71	108.20
1	AA	84	U	O4'-C1'-N1	8.13	114.71	108.20
27	B8	633	A	C4-C5-C6	8.13	121.07	117.00
27	B8	991	C	O4'-C1'-N1	8.13	114.71	108.20
27	B8	1171	G	C5-C6-O6	-8.13	123.72	128.60
27	B8	1424	G	C5-C6-O6	-8.13	123.72	128.60
27	B8	520	G	C5-C6-O6	-8.13	123.72	128.60
27	B8	724	U	O4'-C1'-N1	8.13	114.70	108.20
27	B8	1595	C	O4'-C1'-N1	8.13	114.71	108.20
27	B8	2248	C	O4'-C1'-N1	8.13	114.71	108.20
27	B8	628	G	C5-C6-O6	-8.13	123.72	128.60
1	AA	188	C	O4'-C1'-N1	8.13	114.70	108.20
27	B8	1213	A	C4-C5-C6	8.13	121.06	117.00
27	B8	2628	C	O4'-C1'-N1	8.13	114.70	108.20
27	B8	212	G	C5-C6-O6	-8.12	123.72	128.60
27	B8	1319	C	O4'-C1'-N1	8.12	114.70	108.20
27	B8	970	U	O4'-C1'-N1	8.12	114.70	108.20
1	AA	1037	C	O4'-C1'-N1	8.12	114.70	108.20
1	AA	1510	C	O4'-C1'-N1	8.12	114.70	108.20
27	B8	445	C	O4'-C1'-N1	8.12	114.70	108.20
1	AA	222	C	O4'-C1'-N1	8.12	114.69	108.20
1	AA	1109	C	O4'-C1'-N1	8.12	114.69	108.20
27	B8	801	G	N1-C6-O6	8.12	124.77	119.90
27	B8	1493	C	C2-N1-C1'	8.12	127.73	118.80
1	AA	1069	C	O4'-C1'-N1	8.12	114.69	108.20
27	B8	337	C	O4'-C1'-N1	8.12	114.69	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	556	C	O4'-C1'-N1	8.11	114.69	108.20
1	AA	883	C	O4'-C1'-N1	8.11	114.69	108.20
3	AV	26	C	O4'-C1'-N1	8.11	114.69	108.20
1	AA	51	A	P-O3'-C3'	8.11	129.43	119.70
1	AA	458	U	O4'-C1'-N1	8.11	114.69	108.20
1	AA	660	C	O4'-C1'-N1	8.11	114.69	108.20
26	B7	28	C	O4'-C1'-N1	8.11	114.69	108.20
27	B8	894	U	O4'-C1'-N1	8.11	114.69	108.20
27	B8	1102	C	O4'-C1'-N1	8.11	114.69	108.20
27	B8	1112	G	N1-C6-O6	8.11	124.77	119.90
27	B8	1990	C	O4'-C1'-N1	8.11	114.69	108.20
27	B8	2299	U	O4'-C1'-N1	8.11	114.69	108.20
1	AA	106	C	O4'-C1'-N1	8.11	114.69	108.20
1	AA	1143	G	C5-C6-O6	-8.11	123.74	128.60
27	B8	1108	U	O4'-C1'-N1	8.11	114.68	108.20
27	B8	1338	G	C5-C6-O6	-8.11	123.74	128.60
27	B8	1728	C	O4'-C1'-N1	8.11	114.69	108.20
1	AA	995	C	O4'-C1'-N1	8.10	114.68	108.20
1	AA	1449	C	O4'-C1'-N1	8.10	114.68	108.20
27	B8	163	C	O4'-C1'-N1	8.10	114.68	108.20
27	B8	2420	C	O4'-C1'-N1	8.10	114.68	108.20
1	AA	1523	G	C5-C6-O6	-8.10	123.74	128.60
27	B8	147	C	O4'-C1'-N1	8.10	114.68	108.20
27	B8	1075	C	O4'-C1'-N1	8.10	114.68	108.20
1	AA	27	G	C5-C6-O6	-8.10	123.74	128.60
27	B8	1100	C	O4'-C1'-N1	8.10	114.68	108.20
27	B8	1546	G	C5-C6-O6	-8.10	123.74	128.60
27	B8	2539	C	O4'-C1'-N1	8.10	114.68	108.20
1	AA	34	C	O4'-C1'-N1	8.10	114.68	108.20
1	AA	61	G	C5-C6-O6	-8.10	123.74	128.60
1	AA	190	A	C4-C5-C6	8.10	121.05	117.00
3	AV	21	U	O4'-C1'-N1	8.10	114.68	108.20
27	B8	598	U	O4'-C1'-N1	8.10	114.68	108.20
27	B8	2300	C	O4'-C1'-N1	8.10	114.68	108.20
27	B8	2794	C	O4'-C1'-N1	8.10	114.68	108.20
1	AA	1098	C	O4'-C1'-N1	8.09	114.67	108.20
27	B8	1835	G	C5-C6-O6	-8.09	123.75	128.60
1	AA	1051	C	O4'-C1'-N1	8.09	114.67	108.20
1	AA	1391	U	O4'-C1'-N1	8.09	114.67	108.20
27	B8	2046	G	C5-C6-O6	-8.09	123.75	128.60
27	B8	2226	C	O4'-C1'-N1	8.09	114.67	108.20
1	AA	1482	G	N1-C6-O6	8.09	124.75	119.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	1042	G	N1-C6-O6	8.09	124.75	119.90
27	B8	1658	C	O4'-C1'-N1	8.09	114.67	108.20
27	B8	1893	C	O4'-C1'-N1	8.09	114.67	108.20
27	B8	2523	G	C5-C6-O6	-8.09	123.75	128.60
27	B8	237	C	O4'-C1'-N1	8.09	114.67	108.20
27	B8	949	G	C5-C6-O6	-8.09	123.75	128.60
27	B8	283	G	O4'-C1'-N9	8.08	114.67	108.20
27	B8	1022	G	N1-C6-O6	8.08	124.75	119.90
1	AA	507	C	O4'-C1'-N1	8.08	114.66	108.20
1	AA	1379	G	N1-C6-O6	8.08	124.75	119.90
26	B7	8	C	O4'-C1'-N1	8.08	114.67	108.20
27	B8	2772	C	O4'-C1'-N1	8.08	114.66	108.20
27	B8	2812	G	C5-C6-O6	-8.08	123.75	128.60
27	B8	1059	G	C5-C6-O6	-8.08	123.75	128.60
27	B8	116	C	O4'-C1'-N1	8.07	114.66	108.20
27	B8	953	G	C5-C6-O6	-8.07	123.75	128.60
27	B8	2383	G	C5-C6-O6	-8.07	123.75	128.60
27	B8	6	A	C5-C6-N6	-8.07	117.24	123.70
27	B8	2345	G	N1-C6-O6	8.07	124.74	119.90
27	B8	2540	C	O4'-C1'-N1	8.07	114.66	108.20
1	AA	178	C	O4'-C1'-N1	8.07	114.65	108.20
27	B8	1822	C	O4'-C1'-N1	8.07	114.65	108.20
1	AA	525	C	O4'-C1'-N1	8.07	114.65	108.20
1	AA	1027	C	N3-C4-N4	8.07	123.65	118.00
27	B8	1386	C	O4'-C1'-N1	8.07	114.65	108.20
1	AA	150	U	O4'-C1'-N1	8.06	114.65	108.20
1	AA	1491	G	N1-C6-O6	8.06	124.74	119.90
27	B8	198	C	O4'-C1'-N1	8.06	114.65	108.20
27	B8	523	C	O4'-C1'-N1	8.06	114.65	108.20
27	B8	2148	G	N1-C6-O6	8.06	124.74	119.90
27	B8	973	A	N1-C6-N6	8.06	123.44	118.60
27	B8	2039	U	O4'-C1'-N1	8.06	114.65	108.20
1	AA	724	G	C5-C6-O6	-8.06	123.76	128.60
1	AA	868	C	O4'-C1'-N1	8.06	114.65	108.20
27	B8	1107	G	C5-C6-O6	-8.06	123.76	128.60
27	B8	1121	C	O4'-C1'-N1	8.06	114.65	108.20
27	B8	1259	G	C5-C6-O6	-8.06	123.76	128.60
27	B8	1642	G	C5-C6-O6	-8.06	123.76	128.60
26	B7	6	G	C5-C6-O6	-8.06	123.77	128.60
26	B7	85	G	C5-C6-O6	-8.06	123.77	128.60
27	B8	407	G	C5-C6-O6	-8.06	123.76	128.60
27	B8	1723	G	C5-C6-O6	-8.06	123.77	128.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	2301	C	O4'-C1'-N1	8.06	114.65	108.20
27	B8	9	G	C5-C6-O6	-8.06	123.77	128.60
1	AA	1388	C	O4'-C1'-N1	8.05	114.64	108.20
27	B8	719	C	O4'-C1'-N1	8.05	114.64	108.20
27	B8	1422	G	C5-C6-O6	-8.05	123.77	128.60
27	B8	2234	G	C5-C6-O6	-8.05	123.77	128.60
27	B8	2359	C	O4'-C1'-N1	8.05	114.64	108.20
1	AA	1385	G	C5-C6-O6	-8.05	123.77	128.60
27	B8	2450	A	N1-C6-N6	8.05	123.43	118.60
1	AA	504	C	O4'-C1'-N1	8.05	114.64	108.20
1	AA	1386	G	C5-C6-O6	-8.05	123.77	128.60
27	B8	183	C	O4'-C1'-N1	8.05	114.64	108.20
27	B8	540	C	O4'-C1'-N1	8.05	114.64	108.20
27	B8	1920	C	O4'-C1'-N1	8.05	114.64	108.20
1	AA	1090	U	O4'-C1'-N1	8.04	114.64	108.20
1	AA	1218	C	O4'-C1'-N1	8.04	114.64	108.20
1	AA	111	G	C5-C6-O6	-8.04	123.78	128.60
1	AA	522	C	O4'-C1'-N1	8.04	114.63	108.20
27	B8	729	G	C5-C6-O6	-8.04	123.77	128.60
27	B8	963	U	O4'-C1'-N1	8.04	114.63	108.20
27	B8	1123	C	O4'-C1'-N1	8.04	114.63	108.20
1	AA	1001	C	O4'-C1'-N1	8.04	114.63	108.20
27	B8	1345	C	O4'-C1'-N1	8.04	114.63	108.20
27	B8	1736	U	O4'-C1'-N1	8.04	114.63	108.20
27	B8	2666	C	C2-N1-C1'	8.04	127.64	118.80
27	B8	758	C	O4'-C1'-N1	8.04	114.63	108.20
27	B8	798	G	C5-C6-O6	-8.04	123.78	128.60
27	B8	2527	C	O4'-C1'-N1	8.04	114.63	108.20
27	B8	2667	C	O4'-C1'-N1	8.04	114.63	108.20
1	AA	861	G	C5-C6-O6	-8.04	123.78	128.60
27	B8	1415	U	O4'-C1'-N1	8.04	114.63	108.20
1	AA	468	A	O4'-C1'-N9	8.03	114.63	108.20
1	AA	808	C	O4'-C1'-N1	8.03	114.63	108.20
27	B8	1193	G	C5-C6-O6	-8.03	123.78	128.60
27	B8	2053	G	C5-C6-O6	-8.04	123.78	128.60
1	AA	1337	G	C5-C6-O6	-8.03	123.78	128.60
1	AA	601	G	C5-C6-O6	-8.03	123.78	128.60
1	AA	632	U	O4'-C1'-N1	8.03	114.63	108.20
27	B8	2295	C	O4'-C1'-N1	8.03	114.63	108.20
27	B8	66	C	O4'-C1'-N1	8.03	114.62	108.20
27	B8	2463	C	O4'-C1'-N1	8.03	114.62	108.20
1	AA	1509	C	O4'-C1'-N1	8.03	114.62	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	77	G	C5-C6-O6	-8.03	123.78	128.60
27	B8	2175	C	O4'-C1'-N1	8.03	114.62	108.20
27	B8	2276	G	C5-C6-O6	-8.03	123.78	128.60
1	AA	1262	C	O4'-C1'-N1	8.03	114.62	108.20
27	B8	1072	C	O4'-C1'-N1	8.03	114.62	108.20
27	B8	2260	C	O4'-C1'-N1	8.03	114.62	108.20
27	B8	732	C	O4'-C1'-N1	8.03	114.62	108.20
27	B8	1594	U	O4'-C1'-N1	8.03	114.62	108.20
1	AA	1045	C	O4'-C1'-N1	8.02	114.62	108.20
27	B8	976	G	C5-C6-O6	-8.02	123.79	128.60
27	B8	2261	C	O4'-C1'-N1	8.02	114.62	108.20
27	B8	2521	C	O4'-C1'-N1	8.02	114.62	108.20
1	AA	922	G	N1-C6-O6	8.02	124.71	119.90
27	B8	2830	C	O4'-C1'-N1	8.02	114.62	108.20
27	B8	2432	A	O4'-C1'-N9	8.02	114.61	108.20
27	B8	2625	G	C5-C6-O6	-8.02	123.79	128.60
1	AA	585	G	C5-C6-O6	-8.02	123.79	128.60
1	AA	636	U	O4'-C1'-N1	8.02	114.61	108.20
1	AA	1485	U	O4'-C1'-N1	8.02	114.61	108.20
26	B7	68	C	O4'-C1'-N1	8.02	114.61	108.20
27	B8	832	U	O4'-C1'-N1	8.02	114.61	108.20
27	B8	2841	C	O4'-C1'-N1	8.02	114.61	108.20
1	AA	623	C	O4'-C1'-N1	8.01	114.61	108.20
27	B8	1182	G	C5-C6-O6	-8.01	123.79	128.60
27	B8	2128	G	C5-C6-O6	-8.01	123.79	128.60
27	B8	2254	C	O4'-C1'-N1	8.01	114.61	108.20
1	AA	39	G	C5-C6-O6	-8.01	123.80	128.60
27	B8	682	G	C5-C6-O6	-8.01	123.79	128.60
27	B8	1905	C	O4'-C1'-N1	8.01	114.61	108.20
27	B8	2505	G	N1-C6-O6	8.01	124.71	119.90
27	B8	2744	G	C5-C6-O6	-8.01	123.79	128.60
1	AA	43	C	O4'-C1'-N1	8.01	114.61	108.20
1	AA	402	G	C5-C6-O6	-8.01	123.80	128.60
1	AA	1293	C	O4'-C1'-N1	8.01	114.61	108.20
27	B8	1571	A	C4-C5-C6	8.01	121.00	117.00
27	B8	978	G	C5-C6-O6	-8.01	123.80	128.60
27	B8	2347	C	O4'-C1'-N1	8.01	114.60	108.20
27	B8	457	A	N1-C6-N6	8.00	123.40	118.60
27	B8	2279	G	C5-C6-O6	-8.00	123.80	128.60
27	B8	2603	G	C5-C6-O6	-8.00	123.80	128.60
27	B8	2238	G	N1-C6-O6	8.00	124.70	119.90
1	AA	1245	C	O4'-C1'-N1	8.00	114.60	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	AV	31	U	O4'-C1'-N1	8.00	114.60	108.20
27	B8	1656	C	O4'-C1'-N1	8.00	114.60	108.20
1	AA	1300	G	P-O3'-C3'	8.00	129.30	119.70
1	AA	23	C	O4'-C1'-N1	8.00	114.60	108.20
1	AA	317	U	O4'-C1'-N1	8.00	114.60	108.20
1	AA	1086	U	O4'-C1'-N1	8.00	114.60	108.20
27	B8	1305	C	O4'-C1'-N1	8.00	114.60	108.20
27	B8	305	C	O4'-C1'-N1	8.00	114.60	108.20
1	AA	624	C	O4'-C1'-N1	7.99	114.59	108.20
1	AA	1411	C	O4'-C1'-N1	7.99	114.59	108.20
27	B8	153	U	O4'-C1'-N1	7.99	114.59	108.20
27	B8	238	C	O4'-C1'-N1	7.99	114.59	108.20
27	B8	566	U	O4'-C1'-N1	7.99	114.59	108.20
27	B8	1030	C	O4'-C1'-N1	7.99	114.59	108.20
27	B8	1651	G	C5-C6-O6	-7.99	123.80	128.60
27	B8	1924	C	O4'-C1'-N1	7.99	114.59	108.20
1	AA	551	U	O4'-C1'-N1	7.99	114.59	108.20
27	B8	1023	U	O4'-C1'-N1	7.99	114.59	108.20
27	B8	2081	U	O4'-C1'-N1	7.99	114.59	108.20
27	B8	106	C	O4'-C1'-N1	7.99	114.59	108.20
27	B8	1105	U	O4'-C1'-N1	7.99	114.59	108.20
27	B8	2508	G	C5-C6-O6	-7.99	123.81	128.60
1	AA	89	U	O4'-C1'-N1	7.99	114.59	108.20
3	AV	47	G	C5-C6-O6	-7.99	123.81	128.60
27	B8	1109	C	O4'-C1'-N1	7.99	114.59	108.20
27	B8	1124	G	C5-C6-O6	-7.99	123.81	128.60
1	AA	413	G	C5-C6-O6	-7.99	123.81	128.60
27	B8	938	G	C5-C6-O6	-7.99	123.81	128.60
27	B8	1135	C	O4'-C1'-N1	7.99	114.59	108.20
27	B8	1948	G	C5-C6-O6	-7.99	123.81	128.60
1	AA	876	C	O4'-C1'-N1	7.98	114.59	108.20
27	B8	1417	C	O4'-C1'-N1	7.98	114.59	108.20
27	B8	2024	G	C5-C6-O6	-7.98	123.81	128.60
3	AV	3	G	C5-C6-O6	-7.98	123.81	128.60
27	B8	351	C	O4'-C1'-N1	7.98	114.59	108.20
27	B8	1245	G	C5-C6-O6	-7.98	123.81	128.60
1	AA	300	A	O4'-C1'-N9	7.98	114.58	108.20
1	AA	1470	U	O4'-C1'-N1	7.98	114.58	108.20
27	B8	287	G	C5-C6-O6	-7.98	123.81	128.60
1	AA	740	U	O4'-C1'-N1	7.98	114.58	108.20
27	B8	170	U	O4'-C1'-N1	7.98	114.58	108.20
27	B8	1101	U	O4'-C1'-N1	7.98	114.58	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	701	G	C5-C6-O6	-7.98	123.81	128.60
27	B8	2596	U	O4'-C1'-N1	7.98	114.58	108.20
1	AA	867	G	C5-C6-O6	-7.97	123.81	128.60
1	AA	1050	G	C5-C6-O6	-7.97	123.81	128.60
1	AA	152	A	N1-C6-N6	7.97	123.38	118.60
27	B8	1232	G	C5-C6-O6	-7.97	123.82	128.60
27	B8	823	C	O4'-C1'-N1	7.97	114.58	108.20
1	AA	17	U	O4'-C1'-N1	7.97	114.58	108.20
27	B8	265	A	O4'-C1'-N9	7.97	114.58	108.20
27	B8	649	G	C5-C6-O6	-7.97	123.82	128.60
27	B8	1520	U	O4'-C1'-N1	7.97	114.58	108.20
27	B8	1562	U	O4'-C1'-N1	7.97	114.58	108.20
27	B8	2558	C	O4'-C1'-N1	7.97	114.58	108.20
1	AA	153	C	O4'-C1'-N1	7.97	114.57	108.20
1	AA	267	C	O4'-C1'-N1	7.97	114.57	108.20
27	B8	787	C	O4'-C1'-N1	7.97	114.57	108.20
27	B8	2157	G	O4'-C1'-N9	7.97	114.57	108.20
27	B8	2315	G	C5-C6-O6	-7.97	123.82	128.60
1	AA	1029	U	O4'-C1'-N1	7.96	114.57	108.20
26	B7	7	G	C5-C6-O6	-7.96	123.82	128.60
27	B8	177	G	N1-C6-O6	7.96	124.68	119.90
27	B8	919	U	O4'-C1'-N1	7.96	114.57	108.20
27	B8	2651	C	O4'-C1'-N1	7.96	114.57	108.20
27	B8	385	C	O4'-C1'-N1	7.96	114.57	108.20
1	AA	114	U	O4'-C1'-N1	7.96	114.56	108.20
1	AA	1133	G	C5-C6-O6	-7.96	123.83	128.60
27	B8	581	C	O4'-C1'-N1	7.96	114.57	108.20
27	B8	2195	U	O4'-C1'-N1	7.96	114.56	108.20
27	B8	1016	G	C5-C6-O6	-7.96	123.83	128.60
27	B8	1207	C	O4'-C1'-N1	7.96	114.56	108.20
27	B8	1661	G	C5-C6-O6	-7.96	123.83	128.60
27	B8	1162	G	C5-C6-O6	-7.95	123.83	128.60
27	B8	1278	C	O4'-C1'-N1	7.95	114.56	108.20
27	B8	2599	G	C5-C6-O6	-7.95	123.83	128.60
26	B7	22	U	O4'-C1'-N1	7.95	114.56	108.20
1	AA	142	G	C5-C6-O6	-7.95	123.83	128.60
27	B8	1518	C	O4'-C1'-N1	7.95	114.56	108.20
1	AA	1075	U	O4'-C1'-N1	7.95	114.56	108.20
27	B8	383	C	O4'-C1'-N1	7.95	114.56	108.20
27	B8	759	G	C5-C6-O6	-7.95	123.83	128.60
27	B8	1429	G	C5-C6-O6	-7.95	123.83	128.60
1	AA	52	C	O4'-C1'-N1	7.95	114.56	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	1479	G	C5-C6-O6	-7.95	123.83	128.60
1	AA	214	C	O4'-C1'-N1	7.95	114.56	108.20
1	AA	739	C	O4'-C1'-N1	7.95	114.56	108.20
27	B8	1816	C	O4'-C1'-N1	7.95	114.56	108.20
27	B8	1890	A	N1-C6-N6	7.94	123.37	118.60
27	B8	2250	G	N1-C6-O6	7.94	124.67	119.90
1	AA	1401	G	C5-C6-O6	-7.94	123.83	128.60
27	B8	1258	U	O4'-C1'-N1	7.94	114.55	108.20
27	B8	2484	G	C5-C6-O6	-7.94	123.83	128.60
27	B8	2804	U	O4'-C1'-N1	7.94	114.55	108.20
1	AA	1041	G	C5-C6-O6	-7.94	123.84	128.60
27	B8	1181	U	O4'-C1'-N1	7.94	114.55	108.20
27	B8	2096	C	O4'-C1'-N1	7.94	114.55	108.20
1	AA	798	U	O4'-C1'-N1	7.94	114.55	108.20
27	B8	680	C	O4'-C1'-N1	7.94	114.55	108.20
27	B8	1031	G	C5-C6-O6	-7.94	123.84	128.60
27	B8	2021	C	O4'-C1'-N1	7.94	114.55	108.20
1	AA	1061	G	C5-C6-O6	-7.94	123.84	128.60
1	AA	951	G	C5-C6-O6	-7.93	123.84	128.60
3	AV	39	U	O4'-C1'-N1	7.93	114.55	108.20
27	B8	164	C	O4'-C1'-N1	7.93	114.55	108.20
27	B8	1145	C	O4'-C1'-N1	7.93	114.55	108.20
27	B8	1206	G	C5-C6-O6	-7.93	123.84	128.60
27	B8	1389	G	C5-C6-O6	-7.93	123.84	128.60
27	B8	46	G	C5-C6-O6	-7.93	123.84	128.60
27	B8	131	A	O4'-C1'-N9	7.93	114.55	108.20
1	AA	1210	C	O4'-C1'-N1	7.93	114.54	108.20
27	B8	2643	G	C5-C6-O6	-7.93	123.84	128.60
27	B8	1131	G	N1-C6-O6	7.93	124.66	119.90
27	B8	1154	G	C5-C6-O6	-7.93	123.84	128.60
27	B8	2329	U	O4'-C1'-N1	7.93	114.54	108.20
26	B7	3	C	O4'-C1'-N1	7.93	114.54	108.20
1	AA	1039	G	C5-C6-O6	-7.92	123.84	128.60
27	B8	898	C	O4'-C1'-N1	7.92	114.54	108.20
27	B8	2390	U	O4'-C1'-N1	7.92	114.54	108.20
27	B8	2579	C	O4'-C1'-N1	7.92	114.54	108.20
27	B8	815	C	O4'-C1'-N1	7.92	114.54	108.20
27	B8	230	G	C5-C6-O6	-7.92	123.85	128.60
27	B8	363	G	C5-C6-O6	-7.92	123.85	128.60
1	AA	186	C	O4'-C1'-N1	7.92	114.53	108.20
1	AA	271	C	O4'-C1'-N1	7.92	114.53	108.20
1	AA	617	G	C5-C6-O6	-7.92	123.85	128.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	824	G	C5-C6-O6	-7.92	123.85	128.60
27	B8	799	G	C5-C6-O6	-7.92	123.85	128.60
27	B8	2458	G	O4'-C1'-N9	7.92	114.53	108.20
1	AA	518	C	O4'-C1'-N1	7.92	114.53	108.20
27	B8	288	U	O4'-C1'-N1	7.92	114.53	108.20
1	AA	1497	G	C5-C6-O6	-7.91	123.85	128.60
27	B8	414	C	O4'-C1'-N1	7.91	114.53	108.20
27	B8	1643	G	C5-C6-O6	-7.91	123.85	128.60
27	B8	2069	G	C5-C6-O6	-7.91	123.85	128.60
1	AA	538	G	C5-C6-O6	-7.91	123.85	128.60
27	B8	202	U	O4'-C1'-N1	7.91	114.53	108.20
27	B8	487	C	O4'-C1'-N1	7.91	114.53	108.20
1	AA	1010	U	O4'-C1'-N1	7.91	114.53	108.20
27	B8	1418	G	C5-C6-O6	-7.91	123.85	128.60
27	B8	2802	G	C5-C6-O6	-7.91	123.86	128.60
27	B8	1768	C	O4'-C1'-N1	7.91	114.53	108.20
27	B8	2785	C	O4'-C1'-N1	7.91	114.53	108.20
26	B7	111	U	O4'-C1'-N1	7.91	114.52	108.20
27	B8	1531	C	O4'-C1'-N1	7.91	114.52	108.20
1	AA	1366	C	O4'-C1'-N1	7.90	114.52	108.20
26	B7	88	C	O4'-C1'-N1	7.90	114.52	108.20
1	AA	135	C	O4'-C1'-N1	7.90	114.52	108.20
1	AA	821	G	C5-C6-O6	-7.90	123.86	128.60
1	AA	1478	U	O4'-C1'-N1	7.90	114.52	108.20
27	B8	2441	U	O4'-C1'-N1	7.90	114.52	108.20
27	B8	2464	G	C5-C6-O6	-7.90	123.86	128.60
27	B8	1914	C	O4'-C1'-N1	7.90	114.52	108.20
27	B8	2396	G	C5-C6-O6	-7.90	123.86	128.60
1	AA	234	C	O4'-C1'-N1	7.90	114.52	108.20
27	B8	946	C	O4'-C1'-N1	7.90	114.52	108.20
1	AA	450	G	C5-C6-O6	-7.90	123.86	128.60
27	B8	1706	C	O4'-C1'-N1	7.90	114.52	108.20
1	AA	241	G	C5-C6-O6	-7.89	123.86	128.60
26	B7	36	C	O4'-C1'-N1	7.89	114.51	108.20
27	B8	224	U	O4'-C1'-N1	7.89	114.51	108.20
27	B8	867	C	O4'-C1'-N1	7.89	114.51	108.20
27	B8	1462	C	O4'-C1'-N1	7.89	114.51	108.20
27	B8	2416	C	O4'-C1'-N1	7.89	114.51	108.20
27	B8	914	G	C5-C6-O6	-7.89	123.86	128.60
27	B8	1170	C	O4'-C1'-N1	7.89	114.51	108.20
1	AA	634	C	O4'-C1'-N1	7.89	114.51	108.20
27	B8	807	U	O4'-C1'-N1	7.89	114.51	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	1563	U	O4'-C1'-N1	7.89	114.51	108.20
1	AA	117	G	C5-C6-O6	-7.89	123.87	128.60
1	AA	146	G	C5-C6-O6	-7.89	123.87	128.60
1	AA	583	A	N1-C6-N6	7.89	123.33	118.60
1	AA	744	C	O4'-C1'-N1	7.89	114.51	108.20
1	AA	862	C	O4'-C1'-N1	7.89	114.51	108.20
1	AA	513	C	O4'-C1'-N1	7.88	114.51	108.20
27	B8	2063	C	O4'-C1'-N1	7.88	114.51	108.20
27	B8	797	G	C5-C6-O6	-7.88	123.87	128.60
27	B8	1093	G	C5-C6-O6	-7.88	123.87	128.60
27	B8	2867	G	O4'-C1'-N9	7.88	114.51	108.20
1	AA	849	G	C5-C6-O6	-7.88	123.87	128.60
3	AV	11	C	O4'-C1'-N1	7.88	114.50	108.20
27	B8	812	C	O4'-C1'-N1	7.88	114.50	108.20
27	B8	1343	G	C5-C6-O6	-7.88	123.87	128.60
27	B8	2146	C	O4'-C1'-N1	7.88	114.50	108.20
27	B8	2093	G	C5-C6-O6	-7.88	123.87	128.60
1	AA	986	U	O4'-C1'-N1	7.88	114.50	108.20
27	B8	924	G	C5-C6-O6	-7.88	123.87	128.60
27	B8	2630	G	C5-C6-O6	-7.88	123.87	128.60
1	AA	835	U	O4'-C1'-N1	7.87	114.50	108.20
1	AA	1006	G	C5-C6-O6	-7.87	123.88	128.60
27	B8	115	C	O4'-C1'-N1	7.87	114.50	108.20
27	B8	2824	C	O4'-C1'-N1	7.87	114.50	108.20
1	AA	500	G	C5-C6-O6	-7.87	123.88	128.60
1	AA	592	G	C5-C6-O6	-7.87	123.88	128.60
1	AA	1282	C	O4'-C1'-N1	7.87	114.50	108.20
27	B8	123	G	C5-C6-O6	-7.87	123.88	128.60
27	B8	1909	C	O4'-C1'-N1	7.87	114.50	108.20
27	B8	2880	C	O4'-C1'-N1	7.87	114.50	108.20
27	B8	1289	C	O4'-C1'-N1	7.87	114.50	108.20
27	B8	593	U	O4'-C1'-N1	7.87	114.50	108.20
27	B8	650	C	O4'-C1'-N1	7.87	114.49	108.20
27	B8	1530	G	C5-C6-O6	-7.87	123.88	128.60
27	B8	2189	U	O4'-C1'-N1	7.87	114.50	108.20
1	AA	334	C	O4'-C1'-N1	7.86	114.49	108.20
27	B8	509	C	O4'-C1'-N1	7.86	114.49	108.20
27	B8	534	U	O4'-C1'-N1	7.86	114.49	108.20
27	B8	1083	U	O4'-C1'-N1	7.86	114.49	108.20
27	B8	1238	G	C5-C6-O6	-7.86	123.88	128.60
27	B8	1691	C	O4'-C1'-N1	7.86	114.49	108.20
1	AA	9	G	C5-C6-O6	-7.86	123.88	128.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	599	C	O4'-C1'-N1	7.86	114.49	108.20
27	B8	234	U	O4'-C1'-N1	7.86	114.49	108.20
27	B8	252	G	C5-C6-O6	-7.86	123.88	128.60
27	B8	902	C	O4'-C1'-N1	7.86	114.49	108.20
27	B8	1297	C	O4'-C1'-N1	7.86	114.49	108.20
27	B8	2041	U	O4'-C1'-N1	7.86	114.49	108.20
1	AA	487	A	C4-C5-C6	7.86	120.93	117.00
27	B8	1752	C	O4'-C1'-N1	7.86	114.49	108.20
27	B8	2698	U	O4'-C1'-N1	7.86	114.49	108.20
27	B8	325	G	C5-C6-O6	-7.86	123.89	128.60
27	B8	2782	G	C5-C6-O6	-7.85	123.89	128.60
1	AA	1425	U	O4'-C1'-N1	7.85	114.48	108.20
3	AV	62	C	O4'-C1'-N1	7.85	114.48	108.20
27	B8	1888	G	O4'-C1'-N9	7.85	114.48	108.20
1	AA	191	G	C5-C6-O6	-7.85	123.89	128.60
1	AA	225	C	O4'-C1'-N1	7.85	114.48	108.20
1	AA	970	C	O4'-C1'-N1	7.85	114.48	108.20
3	AV	23	G	C5-C6-O6	-7.85	123.89	128.60
27	B8	209	C	O4'-C1'-N1	7.85	114.48	108.20
1	AA	308	C	O4'-C1'-N1	7.85	114.48	108.20
1	AA	1220	G	C5-C6-O6	-7.85	123.89	128.60
1	AA	176	C	O4'-C1'-N1	7.84	114.48	108.20
1	AA	207	C	O4'-C1'-N1	7.84	114.48	108.20
27	B8	2221	G	C5-C6-O6	-7.84	123.89	128.60
27	B8	2467	C	O4'-C1'-N1	7.84	114.48	108.20
1	AA	1540	U	O4'-C1'-N1	7.84	114.47	108.20
1	AA	25	C	O4'-C1'-N1	7.84	114.47	108.20
1	AA	917	G	C5-C6-O6	-7.84	123.90	128.60
26	B7	117	G	P-O3'-C3'	7.84	129.11	119.70
27	B8	605	G	C5-C6-O6	-7.84	123.89	128.60
27	B8	822	G	C5-C6-O6	-7.84	123.89	128.60
27	B8	2232	C	O4'-C1'-N1	7.84	114.47	108.20
26	B7	106	G	C5-C6-O6	-7.84	123.90	128.60
27	B8	141	G	C5-C6-O6	-7.84	123.90	128.60
27	B8	1455	G	C5-C6-O6	-7.84	123.90	128.60
27	B8	1727	C	O4'-C1'-N1	7.84	114.47	108.20
27	B8	1850	G	C5-C6-O6	-7.84	123.90	128.60
1	AA	1230	C	O4'-C1'-N1	7.84	114.47	108.20
27	B8	552	U	O4'-C1'-N1	7.84	114.47	108.20
27	B8	2104	C	O4'-C1'-N1	7.84	114.47	108.20
1	AA	543	U	O4'-C1'-N1	7.84	114.47	108.20
1	AA	748	G	C5-C6-O6	-7.84	123.90	128.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1149	C	O4'-C1'-N1	7.84	114.47	108.20
26	B7	86	G	C5-C6-O6	-7.84	123.90	128.60
27	B8	1673	G	N1-C6-O6	7.84	124.60	119.90
27	B8	2209	G	C5-C6-O6	-7.84	123.90	128.60
1	AA	266	G	N1-C6-O6	7.83	124.60	119.90
27	B8	485	C	O4'-C1'-N1	7.83	114.47	108.20
27	B8	2530	A	O4'-C1'-N9	7.83	114.47	108.20
1	AA	1072	G	C5-C6-O6	-7.83	123.90	128.60
1	AA	1147	C	O4'-C1'-N1	7.83	114.47	108.20
26	B7	84	G	C5-C6-O6	-7.83	123.90	128.60
27	B8	1427	A	N1-C6-N6	7.83	123.30	118.60
27	B8	1816	C	C2-N1-C1'	7.83	127.42	118.80
27	B8	2355	G	C5-C6-O6	-7.83	123.90	128.60
27	B8	1806	C	O4'-C1'-N1	7.83	114.47	108.20
27	B8	2323	G	C5-C6-O6	-7.83	123.90	128.60
27	B8	2325	G	C5-C6-O6	-7.83	123.90	128.60
1	AA	361	G	C5-C6-O6	-7.83	123.90	128.60
27	B8	767	U	O4'-C1'-N1	7.83	114.46	108.20
27	B8	834	G	C5-C6-O6	-7.83	123.90	128.60
27	B8	1448	G	C5-C6-O6	-7.83	123.90	128.60
27	B8	1196	C	O4'-C1'-N1	7.83	114.46	108.20
27	B8	1902	C	O4'-C1'-N1	7.83	114.46	108.20
1	AA	335	C	O4'-C1'-N1	7.83	114.46	108.20
27	B8	267	C	O4'-C1'-N1	7.83	114.46	108.20
27	B8	1517	G	C5-C6-O6	-7.83	123.91	128.60
27	B8	2548	U	O4'-C1'-N1	7.83	114.46	108.20
27	B8	1832	C	O4'-C1'-N1	7.82	114.46	108.20
27	B8	1188	U	O4'-C1'-N1	7.82	114.46	108.20
27	B8	1472	C	O4'-C1'-N1	7.82	114.46	108.20
27	B8	1612	C	O4'-C1'-N1	7.82	114.46	108.20
27	B8	1636	U	O4'-C1'-N1	7.82	114.46	108.20
27	B8	1766	G	C5-C6-O6	-7.82	123.91	128.60
27	B8	1999	C	O4'-C1'-N1	7.82	114.46	108.20
27	B8	2861	U	O4'-C1'-N1	7.82	114.46	108.20
27	B8	274	C	O4'-C1'-N1	7.82	114.45	108.20
27	B8	467	G	C5-C6-O6	-7.82	123.91	128.60
27	B8	995	C	O4'-C1'-N1	7.82	114.45	108.20
27	B8	1372	U	O4'-C1'-N1	7.82	114.45	108.20
27	B8	2677	G	C5-C6-O6	-7.82	123.91	128.60
1	AA	36	C	O4'-C1'-N1	7.82	114.45	108.20
27	B8	1256	G	C5-C6-O6	-7.82	123.91	128.60
27	B8	2382	G	C5-C6-O6	-7.81	123.91	128.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	140	C	O4'-C1'-N1	7.81	114.45	108.20
27	B8	778	G	C5-C6-O6	-7.81	123.91	128.60
27	B8	61	C	O4'-C1'-N1	7.81	114.45	108.20
27	B8	1323	C	O4'-C1'-N1	7.81	114.45	108.20
27	B8	2718	G	C5-C6-O6	-7.81	123.91	128.60
1	AA	492	C	O4'-C1'-N1	7.81	114.45	108.20
1	AA	645	G	C5-C6-O6	-7.81	123.92	128.60
1	AA	1531	A	O4'-C1'-N9	7.81	114.45	108.20
1	AA	428	G	P-O3'-C3'	7.81	129.07	119.70
27	B8	214	G	C5-C6-O6	-7.81	123.92	128.60
27	B8	850	U	O4'-C1'-N1	7.81	114.45	108.20
27	B8	1601	G	C5-C6-O6	-7.81	123.92	128.60
27	B8	2827	C	O4'-C1'-N1	7.81	114.45	108.20
1	AA	425	G	C5-C6-O6	-7.80	123.92	128.60
1	AA	1272	G	C5-C6-O6	-7.80	123.92	128.60
3	AV	71	C	O4'-C1'-N1	7.80	114.44	108.20
27	B8	246	C	O4'-C1'-N1	7.80	114.44	108.20
27	B8	1058	U	O4'-C1'-N1	7.80	114.44	108.20
27	B8	1904	G	C5-C6-O6	-7.80	123.92	128.60
1	AA	725	G	C5-C6-O6	-7.80	123.92	128.60
1	AA	738	C	O4'-C1'-N1	7.80	114.44	108.20
27	B8	108	G	C5-C6-O6	-7.80	123.92	128.60
1	AA	933	G	C5-C6-O6	-7.80	123.92	128.60
27	B8	851	C	O4'-C1'-N1	7.80	114.44	108.20
27	B8	1119	U	O4'-C1'-N1	7.80	114.44	108.20
1	AA	165	G	C5-C6-O6	-7.79	123.92	128.60
1	AA	439	U	O4'-C1'-N1	7.79	114.44	108.20
27	B8	1192	G	C5-C6-O6	-7.79	123.92	128.60
27	B8	239	C	O4'-C1'-N1	7.79	114.43	108.20
27	B8	1796	U	O4'-C1'-N1	7.79	114.44	108.20
1	AA	341	C	O4'-C1'-N1	7.79	114.43	108.20
1	AA	620	C	O4'-C1'-N1	7.79	114.43	108.20
27	B8	2228	G	C5-C6-O6	-7.79	123.92	128.60
27	B8	2703	C	O4'-C1'-N1	7.79	114.43	108.20
27	B8	1457	U	O4'-C1'-N1	7.79	114.43	108.20
1	AA	1494	G	C5-C6-O6	-7.79	123.93	128.60
27	B8	468	G	C5-C6-O6	-7.79	123.93	128.60
27	B8	2120	G	P-O3'-C3'	7.79	129.04	119.70
1	AA	1190	G	P-O3'-C3'	7.79	129.04	119.70
27	B8	2652	C	O4'-C1'-N1	7.79	114.43	108.20
1	AA	1276	G	C5-C6-O6	-7.79	123.93	128.60
27	B8	2509	G	C5-C6-O6	-7.79	123.93	128.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	894	G	C5-C6-O6	-7.78	123.93	128.60
1	AA	1310	G	C5-C6-O6	-7.78	123.93	128.60
27	B8	2153	C	O4'-C1'-N1	7.78	114.43	108.20
1	AA	164	G	C5-C6-O6	-7.78	123.93	128.60
1	AA	567	G	C5-C6-O6	-7.78	123.93	128.60
26	B7	73	A	C4-C5-C6	7.78	120.89	117.00
27	B8	1094	U	O4'-C1'-N1	7.78	114.42	108.20
27	B8	806	C	O4'-C1'-N1	7.78	114.42	108.20
27	B8	1954	G	C5-C6-O6	-7.78	123.93	128.60
1	AA	1334	G	C5-C6-O6	-7.78	123.93	128.60
1	AA	1471	U	O4'-C1'-N1	7.78	114.42	108.20
27	B8	1534	U	O4'-C1'-N1	7.78	114.42	108.20
27	B8	2731	G	C5-C6-O6	-7.78	123.93	128.60
1	AA	87	C	O4'-C1'-N1	7.78	114.42	108.20
1	AA	377	G	C5-C6-O6	-7.78	123.93	128.60
27	B8	678	C	O4'-C1'-N1	7.78	114.42	108.20
27	B8	2502	G	C5-C6-O6	-7.77	123.94	128.60
1	AA	289	G	C5-C6-O6	-7.77	123.94	128.60
1	AA	669	G	C5-C6-O6	-7.77	123.94	128.60
1	AA	763	G	C5-C6-O6	-7.77	123.94	128.60
27	B8	1784	A	C5-C6-N6	-7.77	117.48	123.70
1	AA	797	C	O4'-C1'-N1	7.77	114.42	108.20
1	AA	1018	G	O4'-C1'-N9	7.77	114.42	108.20
1	AA	1407	C	O4'-C1'-N1	7.77	114.41	108.20
27	B8	394	C	O4'-C1'-N1	7.77	114.42	108.20
27	B8	2134	A	O4'-C1'-N9	7.77	114.41	108.20
27	B8	2550	G	C5-C6-O6	-7.77	123.94	128.60
1	AA	1162	C	O4'-C1'-N1	7.76	114.41	108.20
27	B8	416	U	O4'-C1'-N1	7.76	114.41	108.20
27	B8	2854	G	C5-C6-O6	-7.76	123.94	128.60
1	AA	527	G	C5-C6-O6	-7.76	123.94	128.60
1	AA	586	C	O4'-C1'-N1	7.76	114.41	108.20
1	AA	685	G	C5-C6-O6	-7.76	123.94	128.60
1	AA	1336	C	O4'-C1'-N1	7.76	114.41	108.20
27	B8	1044	C	O4'-C1'-N1	7.76	114.41	108.20
27	B8	1348	C	O4'-C1'-N1	7.76	114.41	108.20
27	B8	2263	C	O4'-C1'-N1	7.76	114.41	108.20
1	AA	284	C	O4'-C1'-N1	7.76	114.41	108.20
27	B8	2838	G	C5-C6-O6	-7.76	123.94	128.60
27	B8	2011	U	O4'-C1'-N1	7.76	114.41	108.20
1	AA	477	C	O4'-C1'-N1	7.76	114.41	108.20
1	AA	1205	U	O4'-C1'-N1	7.76	114.41	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1443	C	O4'-C1'-N1	7.76	114.41	108.20
27	B8	2084	C	O4'-C1'-N1	7.76	114.41	108.20
27	B8	843	G	C5-C6-O6	-7.75	123.95	128.60
27	B8	1731	G	C5-C6-O6	-7.75	123.95	128.60
27	B8	1790	C	O4'-C1'-N1	7.75	114.40	108.20
1	AA	156	C	O4'-C1'-N1	7.75	114.40	108.20
1	AA	1181	G	N1-C6-O6	7.75	124.55	119.90
3	AV	54	G	C5-C6-O6	-7.75	123.95	128.60
27	B8	1804	C	O4'-C1'-N1	7.75	114.40	108.20
1	AA	312	C	O4'-C1'-N1	7.75	114.40	108.20
1	AA	347	G	C5-C6-O6	-7.75	123.95	128.60
27	B8	964	C	O4'-C1'-N1	7.75	114.40	108.20
27	B8	2040	G	C5-C6-O6	-7.75	123.95	128.60
1	AA	544	G	C5-C6-O6	-7.75	123.95	128.60
27	B8	883	G	N1-C6-O6	7.75	124.55	119.90
1	AA	707	U	O4'-C1'-N1	7.75	114.40	108.20
27	B8	32	C	O4'-C1'-N1	7.75	114.40	108.20
27	B8	128	C	O4'-C1'-N1	7.75	114.40	108.20
1	AA	897	C	O4'-C1'-N1	7.75	114.40	108.20
1	AA	924	C	O4'-C1'-N1	7.75	114.40	108.20
1	AA	1040	U	O4'-C1'-N1	7.75	114.40	108.20
1	AA	939	G	C5-C6-O6	-7.74	123.95	128.60
1	AA	541	G	C5-C6-O6	-7.74	123.95	128.60
1	AA	1121	U	O4'-C1'-N1	7.74	114.39	108.20
27	B8	2582	G	C5-C6-O6	-7.74	123.96	128.60
27	B8	2692	G	C5-C6-O6	-7.74	123.96	128.60
1	AA	1195	C	O4'-C1'-N1	7.74	114.39	108.20
27	B8	2472	G	C5-C6-O6	-7.74	123.96	128.60
27	B8	2510	C	O4'-C1'-N1	7.74	114.39	108.20
27	B8	1670	C	O4'-C1'-N1	7.73	114.39	108.20
27	B8	2136	G	C5-C6-O6	-7.73	123.96	128.60
27	B8	1375	U	O4'-C1'-N1	7.73	114.39	108.20
1	AA	404	G	C5-C6-O6	-7.73	123.96	128.60
1	AA	1031	C	O4'-C1'-N1	7.73	114.38	108.20
1	AA	1427	C	O4'-C1'-N1	7.73	114.38	108.20
27	B8	2155	U	O4'-C1'-N1	7.73	114.38	108.20
27	B8	811	U	O4'-C1'-N1	7.73	114.38	108.20
27	B8	2098	U	O4'-C1'-N1	7.73	114.38	108.20
1	AA	58	C	O4'-C1'-N1	7.72	114.38	108.20
27	B8	7	G	C5-C6-O6	-7.72	123.97	128.60
27	B8	921	C	O4'-C1'-N1	7.72	114.38	108.20
27	B8	2233	U	O4'-C1'-N1	7.72	114.38	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	1519	G	C5-C6-O6	-7.72	123.97	128.60
27	B8	2851	A	N1-C6-N6	7.72	123.23	118.60
27	B8	1056	G	O4'-C1'-N9	7.72	114.38	108.20
27	B8	1792	G	C5-C6-O6	-7.72	123.97	128.60
27	B8	2125	G	N1-C6-O6	7.72	124.53	119.90
27	B8	2739	U	O4'-C1'-N1	7.72	114.38	108.20
1	AA	175	C	O4'-C1'-N1	7.72	114.37	108.20
1	AA	1059	C	O4'-C1'-N1	7.72	114.38	108.20
1	AA	1053	G	N1-C6-O6	7.72	124.53	119.90
27	B8	813	U	O4'-C1'-N1	7.72	114.37	108.20
27	B8	1478	G	C5-C6-O6	-7.72	123.97	128.60
27	B8	2404	U	O4'-C1'-N1	7.71	114.37	108.20
26	B7	1	U	O4'-C1'-N1	7.71	114.37	108.20
27	B8	2091	C	O4'-C1'-N1	7.71	114.37	108.20
1	AA	240	G	C5-C6-O6	-7.71	123.97	128.60
1	AA	806	C	O4'-C1'-N1	7.71	114.37	108.20
1	AA	1383	C	O4'-C1'-N1	7.71	114.37	108.20
27	B8	1296	G	C5-C6-O6	-7.71	123.97	128.60
27	B8	41	C	O4'-C1'-N1	7.71	114.37	108.20
27	B8	1988	G	C5-C6-O6	-7.71	123.97	128.60
1	AA	217	C	O4'-C1'-N1	7.71	114.37	108.20
1	AA	997	U	O4'-C1'-N1	7.71	114.37	108.20
3	AV	10	G	C5-C6-O6	-7.71	123.97	128.60
27	B8	1799	G	C5-C6-O6	-7.71	123.97	128.60
27	B8	2230	G	C5-C6-O6	-7.71	123.97	128.60
27	B8	2729	G	C5-C6-O6	-7.71	123.97	128.60
27	B8	1215	G	C5-C6-O6	-7.71	123.98	128.60
27	B8	2573	C	O4'-C1'-N1	7.71	114.36	108.20
27	B8	291	G	C5-C6-O6	-7.71	123.98	128.60
27	B8	2343	U	O4'-C1'-N1	7.71	114.36	108.20
27	B8	2240	U	O4'-C1'-N1	7.70	114.36	108.20
27	B8	2766	A	C5-C6-N6	-7.70	117.54	123.70
26	B7	49	C	O4'-C1'-N1	7.70	114.36	108.20
27	B8	211	C	O4'-C1'-N1	7.70	114.36	108.20
27	B8	240	C	O4'-C1'-N1	7.70	114.36	108.20
27	B8	2777	G	C5-C6-O6	-7.70	123.98	128.60
1	AA	497	G	C5-C6-O6	-7.70	123.98	128.60
1	AA	604	G	C5-C6-O6	-7.70	123.98	128.60
1	AA	788	U	O4'-C1'-N1	7.70	114.36	108.20
1	AA	1128	C	O4'-C1'-N1	7.70	114.36	108.20
27	B8	835	C	O4'-C1'-N1	7.70	114.36	108.20
27	B8	1281	G	C5-C6-O6	-7.70	123.98	128.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	2789	C	O4'-C1'-N1	7.70	114.36	108.20
1	AA	1097	C	O4'-C1'-N1	7.70	114.36	108.20
1	AA	930	C	O4'-C1'-N1	7.70	114.36	108.20
27	B8	2554	U	O4'-C1'-N1	7.70	114.36	108.20
27	B8	1118	C	O4'-C1'-N1	7.69	114.36	108.20
27	B8	436	C	O4'-C1'-N1	7.69	114.36	108.20
27	B8	1218	G	C5-C6-O6	-7.69	123.98	128.60
1	AA	443	C	O4'-C1'-N1	7.69	114.35	108.20
27	B8	319	G	C5-C6-O6	-7.69	123.99	128.60
27	B8	659	G	C5-C6-O6	-7.69	123.99	128.60
27	B8	1906	G	C5-C6-O6	-7.69	123.98	128.60
27	B8	2161	C	P-O3'-C3'	7.69	128.93	119.70
27	B8	292	U	O4'-C1'-N1	7.69	114.35	108.20
27	B8	635	C	O4'-C1'-N1	7.69	114.35	108.20
1	AA	136	C	O4'-C1'-N1	7.69	114.35	108.20
1	AA	1253	G	C5-C6-O6	-7.69	123.99	128.60
26	B7	67	G	N1-C6-O6	7.69	124.51	119.90
1	AA	1174	G	C5-C6-O6	-7.69	123.99	128.60
27	B8	18	U	O4'-C1'-N1	7.69	114.35	108.20
1	AA	1292	G	C5-C6-O6	-7.68	123.99	128.60
27	B8	2202	U	O4'-C1'-N1	7.68	114.35	108.20
1	AA	18	C	O4'-C1'-N1	7.68	114.35	108.20
1	AA	680	C	O4'-C1'-N1	7.68	114.35	108.20
27	B8	85	G	C5-C6-O6	-7.68	123.99	128.60
27	B8	1830	C	O4'-C1'-N1	7.68	114.35	108.20
27	B8	2899	A	C5-C6-N6	-7.68	117.55	123.70
27	B8	1511	G	C5-C6-O6	-7.68	123.99	128.60
27	B8	1684	G	C5-C6-O6	-7.68	123.99	128.60
26	B7	93	C	O4'-C1'-N1	7.68	114.34	108.20
1	AA	552	U	O4'-C1'-N1	7.68	114.34	108.20
1	AA	1309	G	C5-C6-O6	-7.68	123.99	128.60
1	AA	1511	G	C5-C6-O6	-7.68	123.99	128.60
27	B8	1277	G	O4'-C1'-N9	7.68	114.34	108.20
27	B8	1657	U	O4'-C1'-N1	7.68	114.34	108.20
27	B8	2506	U	O4'-C1'-N1	7.68	114.34	108.20
1	AA	859	G	C5-C6-O6	-7.67	124.00	128.60
1	AA	1215	G	C5-C6-O6	-7.67	124.00	128.60
3	AV	42	C	O4'-C1'-N1	7.67	114.34	108.20
27	B8	17	G	C5-C6-O6	-7.67	124.00	128.60
27	B8	1979	U	O4'-C1'-N1	7.67	114.34	108.20
27	B8	2743	U	O4'-C1'-N1	7.67	114.34	108.20
1	AA	41	G	C5-C6-O6	-7.67	124.00	128.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	184	C	O4'-C1'-N1	7.67	114.34	108.20
1	AA	774	G	C5-C6-O6	-7.67	124.00	128.60
27	B8	1104	C	O4'-C1'-N1	7.67	114.33	108.20
27	B8	1113	U	O4'-C1'-N1	7.67	114.33	108.20
27	B8	2277	G	C5-C6-O6	-7.67	124.00	128.60
1	AA	1514	G	C5-C6-O6	-7.67	124.00	128.60
27	B8	285	G	C5-C6-O6	-7.67	124.00	128.60
27	B8	1432	G	O4'-C1'-N9	7.67	114.33	108.20
27	B8	1526	C	O4'-C1'-N1	7.67	114.33	108.20
1	AA	62	U	O4'-C1'-N1	7.66	114.33	108.20
1	AA	494	G	N1-C6-O6	7.66	124.50	119.90
1	AA	1364	U	O4'-C1'-N1	7.66	114.33	108.20
27	B8	2229	U	O4'-C1'-N1	7.66	114.33	108.20
27	B8	2308	G	N1-C6-O6	7.66	124.50	119.90
1	AA	418	C	O4'-C1'-N1	7.66	114.33	108.20
1	AA	203	G	O4'-C1'-N9	7.66	114.33	108.20
27	B8	2636	C	O4'-C1'-N1	7.66	114.33	108.20
2	AX	17	C	O4'-C1'-N1	7.66	114.33	108.20
3	AV	57	C	O4'-C1'-N1	7.66	114.33	108.20
27	B8	1317	G	N1-C6-O6	7.66	124.50	119.90
27	B8	2460	U	O4'-C1'-N1	7.66	114.33	108.20
27	B8	400	G	C5-C6-O6	-7.66	124.01	128.60
27	B8	937	C	O4'-C1'-N1	7.66	114.33	108.20
27	B8	2043	C	O4'-C1'-N1	7.66	114.33	108.20
27	B8	258	G	C5-C6-O6	-7.66	124.01	128.60
27	B8	1250	G	C5-C6-O6	-7.66	124.01	128.60
27	B8	838	C	O4'-C1'-N1	7.65	114.32	108.20
27	B8	1581	G	C5-C6-O6	-7.65	124.01	128.60
1	AA	734	G	C5-C6-O6	-7.65	124.01	128.60
1	AA	758	C	O4'-C1'-N1	7.65	114.32	108.20
1	AA	1107	C	O4'-C1'-N1	7.65	114.32	108.20
27	B8	40	U	O4'-C1'-N1	7.65	114.32	108.20
27	B8	966	G	C5-C6-O6	-7.65	124.01	128.60
27	B8	1921	G	C5-C6-O6	-7.65	124.01	128.60
27	B8	2671	G	C5-C6-O6	-7.65	124.01	128.60
1	AA	170	U	O4'-C1'-N1	7.65	114.32	108.20
1	AA	954	G	C5-C6-O6	-7.65	124.01	128.60
1	AA	1424	U	O4'-C1'-N1	7.65	114.32	108.20
27	B8	290	U	O4'-C1'-N1	7.65	114.32	108.20
1	AA	337	G	C5-C6-O6	-7.65	124.01	128.60
1	AA	1448	C	O4'-C1'-N1	7.65	114.32	108.20
26	B7	47	C	O4'-C1'-N1	7.65	114.32	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	1930	G	O4'-C1'-N9	7.65	114.32	108.20
1	AA	1237	C	O4'-C1'-N1	7.65	114.32	108.20
1	AA	1161	C	O4'-C1'-N1	7.64	114.31	108.20
1	AA	476	U	O4'-C1'-N1	7.64	114.31	108.20
27	B8	2626	C	O4'-C1'-N1	7.64	114.31	108.20
1	AA	679	C	O4'-C1'-N1	7.64	114.31	108.20
27	B8	624	C	O4'-C1'-N1	7.64	114.31	108.20
27	B8	763	G	C5-C6-O6	-7.64	124.02	128.60
27	B8	901	C	O4'-C1'-N1	7.64	114.31	108.20
27	B8	940	G	C5-C6-O6	-7.64	124.02	128.60
1	AA	902	G	C5-C6-O6	-7.64	124.02	128.60
1	AA	1252	A	C5-C6-N6	-7.64	117.59	123.70
27	B8	779	U	O4'-C1'-N1	7.64	114.31	108.20
27	B8	2430	A	C4-C5-C6	7.64	120.82	117.00
1	AA	1247	U	O4'-C1'-N1	7.63	114.31	108.20
27	B8	27	G	O4'-C1'-N9	7.63	114.31	108.20
27	B8	250	G	N1-C6-O6	7.63	124.48	119.90
27	B8	2783	U	O4'-C1'-N1	7.63	114.31	108.20
1	AA	540	G	C5-C6-O6	-7.63	124.02	128.60
27	B8	2306	C	O4'-C1'-N1	7.63	114.31	108.20
3	AV	66	U	O4'-C1'-N1	7.63	114.30	108.20
27	B8	110	G	C5-C6-O6	-7.63	124.02	128.60
27	B8	1201	U	O4'-C1'-N1	7.63	114.30	108.20
1	AA	688	G	C5-C6-O6	-7.63	124.02	128.60
27	B8	2798	U	O4'-C1'-N1	7.63	114.30	108.20
27	B8	2876	G	C5-C6-O6	-7.63	124.02	128.60
27	B8	261	G	C5-C6-O6	-7.62	124.03	128.60
27	B8	1179	G	C5-C6-O6	-7.62	124.03	128.60
1	AA	854	U	O4'-C1'-N1	7.62	114.30	108.20
27	B8	1290	C	O4'-C1'-N1	7.62	114.30	108.20
1	AA	846	G	C5-C6-O6	-7.62	124.03	128.60
1	AA	1390	U	O4'-C1'-N1	7.62	114.30	108.20
27	B8	275	C	O4'-C1'-N1	7.62	114.30	108.20
27	B8	1399	C	O4'-C1'-N1	7.62	114.30	108.20
27	B8	1482	G	C5-C6-O6	-7.62	124.03	128.60
1	AA	206	C	O4'-C1'-N1	7.62	114.30	108.20
27	B8	1977	A	C5-C6-N6	-7.62	117.60	123.70
1	AA	141	G	C5-C6-O6	-7.62	124.03	128.60
1	AA	1140	C	O4'-C1'-N1	7.62	114.29	108.20
27	B8	677	A	C5-C6-N6	-7.62	117.61	123.70
27	B8	863	A	C5-C6-N6	-7.62	117.61	123.70
27	B8	2686	G	C5-C6-O6	-7.62	124.03	128.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	BG	93	TYR	CB-CG-CD1	-7.62	116.43	121.00
27	B8	1499	C	O4'-C1'-N1	7.61	114.29	108.20
27	B8	2394	C	O4'-C1'-N1	7.61	114.29	108.20
27	B8	2165	C	P-O3'-C3'	7.61	128.83	119.70
27	B8	2442	C	O4'-C1'-N1	7.61	114.29	108.20
27	B8	2844	G	O4'-C1'-N9	7.61	114.29	108.20
1	AA	348	G	C5-C6-O6	-7.61	124.03	128.60
27	B8	1416	G	C5-C6-O6	-7.61	124.03	128.60
27	B8	1992	G	C5-C6-O6	-7.61	124.04	128.60
1	AA	1070	U	O4'-C1'-N1	7.61	114.28	108.20
27	B8	698	C	O4'-C1'-N1	7.61	114.28	108.20
27	B8	1411	U	O4'-C1'-N1	7.61	114.28	108.20
27	B8	79	C	O4'-C1'-N1	7.60	114.28	108.20
27	B8	1096	A	O4'-C1'-N9	7.60	114.28	108.20
27	B8	2330	G	C5-C6-O6	-7.60	124.04	128.60
1	AA	929	G	C5-C6-O6	-7.60	124.04	128.60
1	AA	1356	G	C5-C6-O6	-7.60	124.04	128.60
1	AA	1481	U	O4'-C1'-N1	7.60	114.28	108.20
27	B8	959	A	C5-C6-N6	-7.60	117.62	123.70
27	B8	1062	G	C5-C6-O6	-7.60	124.04	128.60
27	B8	1007	C	O4'-C1'-N1	7.60	114.28	108.20
27	B8	1708	C	O4'-C1'-N1	7.60	114.28	108.20
27	B8	2123	G	C5-C6-O6	-7.60	124.04	128.60
1	AA	277	C	O4'-C1'-N1	7.60	114.28	108.20
27	B8	122	G	C5-C6-O6	-7.60	124.04	128.60
1	AA	1183	U	O4'-C1'-N1	7.59	114.28	108.20
27	B8	810	U	O4'-C1'-N1	7.59	114.28	108.20
27	B8	1641	A	C4-C5-C6	7.59	120.80	117.00
27	B8	2514	U	O4'-C1'-N1	7.59	114.28	108.20
1	AA	659	U	O4'-C1'-N1	7.59	114.27	108.20
27	B8	2427	C	O4'-C1'-N1	7.59	114.27	108.20
1	AA	1353	G	C5-C6-O6	-7.59	124.05	128.60
1	AA	1536	C	O4'-C1'-N1	7.59	114.27	108.20
27	B8	674	G	C5-C6-O6	-7.59	124.05	128.60
27	B8	1064	C	O4'-C1'-N1	7.59	114.27	108.20
27	B8	1974	C	O4'-C1'-N1	7.59	114.27	108.20
27	B8	2875	C	O4'-C1'-N1	7.59	114.27	108.20
1	AA	474	G	C5-C6-O6	-7.59	124.05	128.60
1	AA	1373	G	C5-C6-O6	-7.59	124.05	128.60
27	B8	1052	C	O4'-C1'-N1	7.59	114.27	108.20
27	B8	1933	G	C5-C6-O6	-7.59	124.05	128.60
1	AA	29	U	O4'-C1'-N1	7.59	114.27	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	123	U	O4'-C1'-N1	7.59	114.27	108.20
26	B7	19	C	O4'-C1'-N1	7.59	114.27	108.20
27	B8	2621	G	C5-C6-O6	-7.59	124.05	128.60
1	AA	1341	U	O4'-C1'-N1	7.59	114.27	108.20
1	AA	1367	C	O4'-C1'-N1	7.59	114.27	108.20
27	B8	441	U	O4'-C1'-N1	7.59	114.27	108.20
1	AA	1100	C	O4'-C1'-N1	7.58	114.27	108.20
27	B8	1833	C	O4'-C1'-N1	7.58	114.27	108.20
27	B8	1861	G	C5-C6-O6	-7.58	124.05	128.60
27	B8	314	C	O4'-C1'-N1	7.58	114.27	108.20
27	B8	1019	U	O4'-C1'-N1	7.58	114.27	108.20
27	B8	1190	G	C5-C6-O6	-7.58	124.05	128.60
1	AA	671	G	C5-C6-O6	-7.58	124.05	128.60
27	B8	1675	C	O4'-C1'-N1	7.58	114.26	108.20
27	B8	2047	C	O4'-C1'-N1	7.58	114.26	108.20
1	AA	342	C	O4'-C1'-N1	7.58	114.26	108.20
1	AA	1027	C	O4'-C1'-N1	7.58	114.26	108.20
1	AA	1114	C	O4'-C1'-N1	7.58	114.26	108.20
27	B8	1771	C	O4'-C1'-N1	7.58	114.26	108.20
1	AA	615	G	O4'-C1'-N9	7.58	114.26	108.20
27	B8	1097	U	O4'-C1'-N1	7.58	114.26	108.20
27	B8	2840	C	O4'-C1'-N1	7.58	114.26	108.20
1	AA	233	C	O4'-C1'-N1	7.58	114.26	108.20
27	B8	1707	G	C5-C6-O6	-7.58	124.06	128.60
27	B8	2672	U	O4'-C1'-N1	7.58	114.26	108.20
1	AA	811	C	O4'-C1'-N1	7.57	114.26	108.20
27	B8	1537	G	C5-C6-O6	-7.57	124.06	128.60
27	B8	1941	C	O4'-C1'-N1	7.57	114.26	108.20
1	AA	1457	G	C5-C6-O6	-7.57	124.06	128.60
27	B8	2012	G	C5-C6-O6	-7.57	124.06	128.60
27	B8	406	G	C5-C6-O6	-7.57	124.06	128.60
27	B8	994	C	O4'-C1'-N1	7.57	114.26	108.20
27	B8	2702	G	C5-C6-O6	-7.57	124.06	128.60
1	AA	396	C	O4'-C1'-N1	7.57	114.25	108.20
1	AA	1119	C	O4'-C1'-N1	7.57	114.25	108.20
1	AA	436	C	O4'-C1'-N1	7.57	114.25	108.20
26	B7	64	G	C5-C6-O6	-7.57	124.06	128.60
27	B8	560	C	O4'-C1'-N1	7.57	114.25	108.20
27	B8	2878	U	O4'-C1'-N1	7.57	114.25	108.20
27	B8	760	G	C5-C6-O6	-7.57	124.06	128.60
27	B8	1241	A	O4'-C1'-N9	7.57	114.25	108.20
27	B8	1533	C	O4'-C1'-N1	7.57	114.25	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	1984	G	C5-C6-O6	-7.57	124.06	128.60
27	B8	2456	C	O4'-C1'-N1	7.57	114.25	108.20
27	B8	420	C	O4'-C1'-N1	7.56	114.25	108.20
27	B8	2313	C	O4'-C1'-N1	7.56	114.25	108.20
27	B8	2440	C	O4'-C1'-N1	7.56	114.25	108.20
1	AA	545	C	O4'-C1'-N1	7.56	114.25	108.20
27	B8	2888	C	O4'-C1'-N1	7.56	114.25	108.20
1	AA	1412	C	O4'-C1'-N1	7.56	114.25	108.20
27	B8	1624	U	O4'-C1'-N1	7.56	114.25	108.20
27	B8	2150	C	O4'-C1'-N1	7.56	114.25	108.20
27	B8	2235	G	C5-C6-O6	-7.56	124.06	128.60
1	AA	221	C	O4'-C1'-N1	7.56	114.25	108.20
3	AV	41	U	O4'-C1'-N1	7.56	114.25	108.20
27	B8	1081	U	O4'-C1'-N1	7.56	114.25	108.20
27	B8	2247	A	O4'-C1'-N9	7.56	114.25	108.20
27	B8	2293	G	C5-C6-O6	-7.56	124.06	128.60
27	B8	1158	C	O4'-C1'-N1	7.56	114.25	108.20
1	AA	249	U	O4'-C1'-N1	7.55	114.24	108.20
27	B8	873	C	O4'-C1'-N1	7.55	114.24	108.20
27	B8	2004	G	C5-C6-O6	-7.55	124.07	128.60
1	AA	786	G	O4'-C1'-N9	7.55	114.24	108.20
27	B8	1808	A	O4'-C1'-N9	7.55	114.24	108.20
27	B8	1976	U	O4'-C1'-N1	7.55	114.24	108.20
1	AA	395	C	O4'-C1'-N1	7.55	114.24	108.20
3	AV	24	C	O4'-C1'-N1	7.55	114.24	108.20
26	B7	16	G	O4'-C1'-N9	7.55	114.24	108.20
26	B7	83	G	C5-C6-O6	-7.55	124.07	128.60
27	B8	786	C	O4'-C1'-N1	7.55	114.24	108.20
1	AA	737	C	O4'-C1'-N1	7.55	114.24	108.20
1	AA	766	A	O4'-C1'-N9	7.55	114.24	108.20
1	AA	805	C	O4'-C1'-N1	7.55	114.24	108.20
26	B7	108	A	C5-C6-N6	-7.55	117.66	123.70
27	B8	738	G	C5-C6-O6	-7.55	124.07	128.60
27	B8	2026	U	O4'-C1'-N1	7.55	114.24	108.20
27	B8	2650	U	O4'-C1'-N1	7.55	114.24	108.20
1	AA	656	G	O4'-C1'-N9	7.54	114.23	108.20
1	AA	1468	A	C4-C5-C6	7.54	120.77	117.00
27	B8	1220	G	O4'-C1'-N9	7.54	114.23	108.20
27	B8	1438	U	O4'-C1'-N1	7.54	114.23	108.20
27	B8	1560	G	C5-C6-O6	-7.54	124.07	128.60
27	B8	1564	C	O4'-C1'-N1	7.54	114.24	108.20
27	B8	1881	C	O4'-C1'-N1	7.54	114.23	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	2322	A	O4'-C1'-N9	7.54	114.23	108.20
27	B8	1430	G	C5-C6-O6	-7.54	124.08	128.60
35	BG	93	TYR	CB-CG-CD2	7.54	125.52	121.00
1	AA	1444	U	O4'-C1'-N1	7.54	114.23	108.20
27	B8	1535	A	O4'-C1'-N9	7.54	114.23	108.20
27	B8	2567	G	C5-C6-O6	-7.54	124.08	128.60
1	AA	795	C	O4'-C1'-N1	7.54	114.23	108.20
1	AA	984	C	O4'-C1'-N1	7.54	114.23	108.20
1	AA	1078	U	O4'-C1'-N1	7.54	114.23	108.20
27	B8	2903	U	C2-N1-C1'	7.54	126.74	117.70
1	AA	1232	U	O4'-C1'-N1	7.53	114.23	108.20
27	B8	1195	G	C5-C6-O6	-7.53	124.08	128.60
27	B8	1330	C	O4'-C1'-N1	7.53	114.23	108.20
1	AA	916	U	O4'-C1'-N1	7.53	114.22	108.20
27	B8	1653	G	C5-C6-O6	-7.53	124.08	128.60
27	B8	2569	G	C5-C6-O6	-7.53	124.08	128.60
27	B8	2583	G	C5-C6-O6	-7.53	124.08	128.60
27	B8	2303	G	C5-C6-O6	-7.53	124.08	128.60
1	AA	110	C	O4'-C1'-N1	7.53	114.22	108.20
1	AA	709	U	O4'-C1'-N1	7.53	114.22	108.20
1	AA	1351	U	O4'-C1'-N1	7.53	114.22	108.20
27	B8	358	U	O4'-C1'-N1	7.53	114.22	108.20
27	B8	380	G	C5-C6-O6	-7.53	124.08	128.60
27	B8	681	G	C5-C6-O6	-7.53	124.08	128.60
27	B8	865	C	O4'-C1'-N1	7.53	114.22	108.20
27	B8	908	C	O4'-C1'-N1	7.53	114.22	108.20
1	AA	1056	U	O4'-C1'-N1	7.53	114.22	108.20
27	B8	1764	C	O4'-C1'-N1	7.53	114.22	108.20
27	B8	45	G	C5-C6-O6	-7.52	124.09	128.60
27	B8	281	C	O4'-C1'-N1	7.52	114.22	108.20
27	B8	554	U	O4'-C1'-N1	7.52	114.22	108.20
27	B8	1486	U	O4'-C1'-N1	7.52	114.22	108.20
1	AA	1348	U	O4'-C1'-N1	7.52	114.22	108.20
27	B8	2087	G	C5-C6-O6	-7.52	124.09	128.60
1	AA	1472	U	O4'-C1'-N1	7.52	114.22	108.20
27	B8	2006	C	O4'-C1'-N1	7.52	114.22	108.20
27	B8	2316	G	C5-C6-O6	-7.52	124.09	128.60
1	AA	521	G	C5-C6-O6	-7.52	124.09	128.60
27	B8	906	U	O4'-C1'-N1	7.52	114.21	108.20
27	B8	1043	C	O4'-C1'-N1	7.52	114.21	108.20
1	AA	953	G	C5-C6-O6	-7.52	124.09	128.60
27	B8	145	C	O4'-C1'-N1	7.52	114.21	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	1441	G	C5-C6-O6	-7.52	124.09	128.60
1	AA	720	C	O4'-C1'-N1	7.51	114.21	108.20
1	AA	1207	G	C5-C6-O6	-7.51	124.09	128.60
27	B8	271	G	C5-C6-O6	-7.51	124.09	128.60
27	B8	2413	G	C5-C6-O6	-7.51	124.09	128.60
1	AA	200	G	C5-C6-O6	-7.51	124.09	128.60
3	AV	28	C	O4'-C1'-N1	7.51	114.21	108.20
1	AA	276	G	C5-C6-O6	-7.51	124.09	128.60
27	B8	691	C	O4'-C1'-N1	7.51	114.21	108.20
27	B8	1500	G	C5-C6-O6	-7.51	124.09	128.60
27	B8	2428	G	C5-C6-O6	-7.51	124.09	128.60
27	B8	141	G	O4'-C1'-N9	7.51	114.21	108.20
27	B8	1216	G	C5-C6-O6	-7.51	124.10	128.60
27	B8	2606	C	O4'-C1'-N1	7.51	114.20	108.20
27	B8	498	G	C5-C6-O6	-7.50	124.10	128.60
27	B8	588	U	O4'-C1'-N1	7.50	114.20	108.20
27	B8	1175	A	O4'-C1'-N9	7.50	114.20	108.20
27	B8	1208	C	O4'-C1'-N1	7.50	114.20	108.20
1	AA	1043	G	C5-C6-O6	-7.50	124.10	128.60
1	AA	1187	G	C5-C6-O6	-7.50	124.10	128.60
1	AA	1370	G	C5-C6-O6	-7.50	124.10	128.60
27	B8	60	G	C5-C6-O6	-7.50	124.10	128.60
27	B8	2341	G	C5-C6-O6	-7.50	124.10	128.60
27	B8	2389	G	C5-C6-O6	-7.50	124.10	128.60
27	B8	335	C	O4'-C1'-N1	7.50	114.20	108.20
27	B8	2788	C	O4'-C1'-N1	7.50	114.20	108.20
27	B8	1337	G	C5-C6-O6	-7.50	124.10	128.60
27	B8	1368	G	C5-C6-O6	-7.50	124.10	128.60
27	B8	1382	G	N1-C6-O6	7.50	124.40	119.90
27	B8	2246	G	C5-C6-O6	-7.50	124.10	128.60
1	AA	1423	G	C5-C6-O6	-7.50	124.10	128.60
27	B8	2619	C	O4'-C1'-N1	7.50	114.20	108.20
27	B8	2126	A	O4'-C1'-N9	7.50	114.20	108.20
1	AA	804	U	O4'-C1'-N1	7.49	114.19	108.20
1	AA	885	G	C5-C6-O6	-7.49	124.11	128.60
27	B8	2633	G	C5-C6-O6	-7.49	124.11	128.60
1	AA	548	G	C5-C6-O6	-7.49	124.11	128.60
1	AA	643	C	O4'-C1'-N1	7.49	114.19	108.20
27	B8	229	C	O4'-C1'-N1	7.49	114.19	108.20
27	B8	839	U	O4'-C1'-N1	7.49	114.19	108.20
27	B8	1017	G	O4'-C1'-N9	7.49	114.19	108.20
27	B8	1185	G	C5-C6-O6	-7.49	124.11	128.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	1663	G	C5-C6-O6	-7.49	124.11	128.60
1	AA	293	G	C5-C6-O6	-7.49	124.11	128.60
1	AA	937	A	C5-C6-N6	-7.49	117.71	123.70
27	B8	944	C	O4'-C1'-N1	7.49	114.19	108.20
27	B8	1390	U	O4'-C1'-N1	7.49	114.19	108.20
27	B8	2709	G	C5-C6-O6	-7.49	124.11	128.60
27	B8	1303	G	C5-C6-O6	-7.49	124.11	128.60
27	B8	1555	G	C5-C6-O6	-7.49	124.11	128.60
27	B8	2661	G	C5-C6-O6	-7.49	124.11	128.60
26	B7	65	U	O4'-C1'-N1	7.49	114.19	108.20
27	B8	1491	G	C5-C6-O6	-7.49	124.11	128.60
27	B8	2337	G	C5-C6-O6	-7.49	124.11	128.60
1	AA	611	C	O4'-C1'-N1	7.48	114.19	108.20
1	AA	943	U	O4'-C1'-N1	7.48	114.19	108.20
27	B8	82	U	O4'-C1'-N1	7.48	114.19	108.20
27	B8	2064	C	O4'-C1'-N1	7.48	114.19	108.20
27	B8	2167	U	O4'-C1'-N1	7.48	114.19	108.20
1	AA	493	A	O4'-C1'-N9	7.48	114.18	108.20
3	AV	17	C	O4'-C1'-N1	7.48	114.19	108.20
27	B8	1873	G	C5-C6-O6	-7.48	124.11	128.60
27	B8	640	C	O4'-C1'-N1	7.48	114.18	108.20
1	AA	227	G	C5-C6-O6	-7.48	124.11	128.60
27	B8	132	G	C5-C6-O6	-7.48	124.11	128.60
27	B8	2454	G	C5-C6-O6	-7.47	124.12	128.60
1	AA	911	U	O4'-C1'-N1	7.47	114.18	108.20
1	AA	1327	C	O4'-C1'-N1	7.47	114.18	108.20
27	B8	2272	U	O4'-C1'-N1	7.47	114.18	108.20
27	B8	2642	G	C5-C6-O6	-7.47	124.12	128.60
27	B8	76	C	O4'-C1'-N1	7.47	114.17	108.20
27	B8	553	G	C5-C6-O6	-7.47	124.12	128.60
27	B8	2152	G	N1-C6-O6	7.47	124.38	119.90
27	B8	2334	U	O4'-C1'-N1	7.47	114.18	108.20
1	AA	37	U	O4'-C1'-N1	7.47	114.17	108.20
1	AA	68	G	N1-C6-O6	7.47	124.38	119.90
27	B8	410	G	C5-C6-O6	-7.47	124.12	128.60
1	AA	697	U	O4'-C1'-N1	7.47	114.17	108.20
1	AA	1442	G	C5-C6-O6	-7.47	124.12	128.60
26	B7	89	U	O4'-C1'-N1	7.47	114.17	108.20
27	B8	848	C	O4'-C1'-N1	7.47	114.17	108.20
27	B8	697	G	C5-C6-O6	-7.46	124.12	128.60
27	B8	1202	G	C5-C6-O6	-7.46	124.12	128.60
27	B8	2669	G	C5-C6-O6	-7.46	124.12	128.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	2710	C	O4'-C1'-N1	7.46	114.17	108.20
1	AA	590	U	O4'-C1'-N1	7.46	114.17	108.20
26	B7	117	G	C5-C6-O6	-7.46	124.12	128.60
27	B8	1443	U	O4'-C1'-N1	7.46	114.17	108.20
27	B8	1474	U	O4'-C1'-N1	7.46	114.17	108.20
27	B8	2818	U	O4'-C1'-N1	7.46	114.17	108.20
1	AA	903	G	C5-C6-O6	-7.46	124.12	128.60
1	AA	955	U	O4'-C1'-N1	7.46	114.17	108.20
1	AA	1339	A	C4-C5-C6	7.46	120.73	117.00
27	B8	1868	C	O4'-C1'-N1	7.46	114.17	108.20
27	B8	484	C	O4'-C1'-N1	7.46	114.17	108.20
27	B8	1894	C	O4'-C1'-N1	7.46	114.17	108.20
27	B8	536	G	C5-C6-O6	-7.46	124.12	128.60
1	AA	485	U	O4'-C1'-N1	7.46	114.17	108.20
27	B8	1295	C	O4'-C1'-N1	7.46	114.17	108.20
27	B8	1112	G	O4'-C1'-N9	7.46	114.16	108.20
26	B7	48	U	O4'-C1'-N1	7.45	114.16	108.20
27	B8	1740	G	C5-C6-O6	-7.45	124.13	128.60
1	AA	678	U	O4'-C1'-N1	7.45	114.16	108.20
1	AA	1186	G	C5-C6-O6	-7.45	124.13	128.60
1	AA	1208	C	O4'-C1'-N1	7.45	114.16	108.20
1	AA	1376	U	O4'-C1'-N1	7.45	114.16	108.20
26	B7	116	G	C5-C6-O6	-7.45	124.13	128.60
27	B8	134	G	C5-C6-O6	-7.45	124.13	128.60
27	B8	2180	U	O4'-C1'-N1	7.45	114.16	108.20
27	B8	2495	G	C5-C6-O6	-7.45	124.13	128.60
27	B8	2528	U	O4'-C1'-N1	7.45	114.16	108.20
27	B8	80	G	C5-C6-O6	-7.45	124.13	128.60
27	B8	2762	C	O4'-C1'-N1	7.45	114.16	108.20
1	AA	73	C	O4'-C1'-N1	7.45	114.16	108.20
27	B8	1761	C	O4'-C1'-N1	7.45	114.16	108.20
1	AA	372	C	O4'-C1'-N1	7.44	114.16	108.20
27	B8	1576	U	O4'-C1'-N1	7.44	114.16	108.20
27	B8	2241	A	O4'-C1'-N9	7.44	114.16	108.20
27	B8	856	G	C5-C6-O6	-7.44	124.13	128.60
27	B8	1409	U	O4'-C1'-N1	7.44	114.15	108.20
1	AA	1131	G	N1-C6-O6	7.44	124.36	119.90
27	B8	852	U	O4'-C1'-N1	7.44	114.15	108.20
27	B8	2395	C	O4'-C1'-N1	7.44	114.15	108.20
27	B8	2525	G	C5-C6-O6	-7.44	124.14	128.60
1	AA	877	G	C5-C6-O6	-7.44	124.14	128.60
1	AA	1354	U	O4'-C1'-N1	7.44	114.15	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	1335	C	O4'-C1'-N1	7.44	114.15	108.20
27	B8	510	C	O4'-C1'-N1	7.44	114.15	108.20
27	B8	1660	G	C5-C6-O6	-7.44	124.14	128.60
1	AA	391	G	C5-C6-O6	-7.43	124.14	128.60
1	AA	847	G	O4'-C1'-N9	7.43	114.15	108.20
27	B8	774	G	C5-C6-O6	-7.43	124.14	128.60
1	AA	920	U	O4'-C1'-N1	7.43	114.15	108.20
26	B7	21	G	C5-C6-O6	-7.43	124.14	128.60
27	B8	70	G	C5-C6-O6	-7.43	124.14	128.60
27	B8	1813	G	C5-C6-O6	-7.43	124.14	128.60
27	B8	2367	G	C5-C6-O6	-7.43	124.14	128.60
1	AA	1264	U	O4'-C1'-N1	7.43	114.14	108.20
27	B8	37	C	O4'-C1'-N1	7.43	114.14	108.20
27	B8	702	U	O4'-C1'-N1	7.43	114.14	108.20
27	B8	1923	U	O4'-C1'-N1	7.43	114.14	108.20
27	B8	993	G	C5-C6-O6	-7.43	124.14	128.60
27	B8	1055	G	C5-C6-O6	-7.43	124.14	128.60
1	AA	577	G	C5-C6-O6	-7.42	124.14	128.60
26	B7	98	G	C5-C6-O6	-7.42	124.14	128.60
1	AA	1342	C	O4'-C1'-N1	7.42	114.14	108.20
26	B7	32	U	O4'-C1'-N1	7.42	114.14	108.20
27	B8	304	U	O4'-C1'-N1	7.42	114.14	108.20
27	B8	1722	A	C4-C5-C6	7.42	120.71	117.00
27	B8	35	G	C5-C6-O6	-7.42	124.15	128.60
27	B8	2212	A	O4'-C1'-N9	7.42	114.14	108.20
27	B8	2219	U	O4'-C1'-N1	7.42	114.14	108.20
1	AA	453	G	N1-C6-O6	7.42	124.35	119.90
1	AA	1300	G	C5-C6-O6	-7.42	124.15	128.60
27	B8	1282	U	O4'-C1'-N1	7.42	114.13	108.20
27	B8	2290	G	C5-C6-O6	-7.42	124.15	128.60
1	AA	144	G	C5-C6-O6	-7.41	124.15	128.60
1	AA	40	C	O4'-C1'-N1	7.41	114.13	108.20
1	AA	837	U	O4'-C1'-N1	7.41	114.13	108.20
1	AA	1198	G	C5-C6-O6	-7.41	124.15	128.60
27	B8	1449	G	C5-C6-O6	-7.41	124.15	128.60
1	AA	1233	G	C5-C6-O6	-7.41	124.16	128.60
27	B8	178	G	C5-C6-O6	-7.41	124.16	128.60
27	B8	683	U	O4'-C1'-N1	7.41	114.13	108.20
27	B8	1887	C	O4'-C1'-N1	7.41	114.12	108.20
1	AA	1314	C	O4'-C1'-N1	7.41	114.12	108.20
27	B8	877	A	C4-C5-C6	7.41	120.70	117.00
27	B8	1011	G	C5-C6-O6	-7.41	124.16	128.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	1574	C	O4'-C1'-N1	7.41	114.12	108.20
27	B8	2487	G	C5-C6-O6	-7.41	124.16	128.60
1	AA	491	G	C5-C6-O6	-7.40	124.16	128.60
1	AA	791	G	C5-C6-O6	-7.40	124.16	128.60
1	AA	1243	C	O4'-C1'-N1	7.40	114.12	108.20
27	B8	296	U	O4'-C1'-N1	7.40	114.12	108.20
27	B8	708	G	C5-C6-O6	-7.40	124.16	128.60
27	B8	1846	G	C5-C6-O6	-7.40	124.16	128.60
27	B8	1867	G	C5-C6-O6	-7.40	124.16	128.60
1	AA	550	G	C5-C6-O6	-7.40	124.16	128.60
1	AA	1538	C	O4'-C1'-N1	7.40	114.12	108.20
27	B8	884	U	O4'-C1'-N1	7.40	114.12	108.20
1	AA	1307	U	O4'-C1'-N1	7.40	114.12	108.20
27	B8	934	U	O4'-C1'-N1	7.40	114.12	108.20
27	B8	1053	C	O4'-C1'-N1	7.40	114.12	108.20
27	B8	1628	G	C5-C6-O6	-7.40	124.16	128.60
1	AA	896	C	O4'-C1'-N1	7.39	114.11	108.20
1	AA	1159	U	O4'-C1'-N1	7.39	114.11	108.20
26	B7	70	C	O4'-C1'-N1	7.39	114.11	108.20
27	B8	378	C	O4'-C1'-N1	7.39	114.12	108.20
27	B8	449	A	C5-C6-N6	-7.39	117.79	123.70
27	B8	2251	G	C5-C6-O6	-7.39	124.17	128.60
1	AA	967	C	O4'-C1'-N1	7.39	114.11	108.20
27	B8	301	G	C5-C6-O6	-7.39	124.17	128.60
1	AA	119	A	C4-C5-C6	7.39	120.69	117.00
27	B8	1897	G	C5-C6-O6	-7.39	124.17	128.60
1	AA	212	G	C5-C6-O6	-7.39	124.17	128.60
27	B8	464	U	O4'-C1'-N1	7.39	114.11	108.20
27	B8	773	U	O4'-C1'-N1	7.39	114.11	108.20
26	B7	30	C	O4'-C1'-N1	7.39	114.11	108.20
27	B8	805	G	C5-C6-O6	-7.39	124.17	128.60
27	B8	1136	G	C5-C6-O6	-7.39	124.17	128.60
27	B8	1388	G	C5-C6-O6	-7.39	124.17	128.60
27	B8	1747	U	O4'-C1'-N1	7.39	114.11	108.20
1	AA	410	G	N1-C6-O6	7.38	124.33	119.90
27	B8	1013	C	O4'-C1'-N1	7.38	114.11	108.20
27	B8	2187	U	O4'-C1'-N1	7.38	114.11	108.20
27	B8	585	G	C5-C6-O6	-7.38	124.17	128.60
1	AA	316	C	O4'-C1'-N1	7.38	114.11	108.20
1	AA	1535	C	O4'-C1'-N1	7.38	114.11	108.20
27	B8	1161	C	O4'-C1'-N1	7.38	114.10	108.20
27	B8	1659	G	C5-C6-O6	-7.38	124.17	128.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	1725	U	O4'-C1'-N1	7.38	114.10	108.20
27	B8	2555	U	O4'-C1'-N1	7.38	114.10	108.20
1	AA	783	C	O4'-C1'-N1	7.37	114.10	108.20
1	AA	836	G	C5-C6-O6	-7.37	124.18	128.60
27	B8	392	U	O4'-C1'-N1	7.37	114.10	108.20
1	AA	1270	G	C5-C6-O6	-7.37	124.18	128.60
27	B8	1037	G	C5-C6-O6	-7.37	124.18	128.60
27	B8	2036	C	O4'-C1'-N1	7.37	114.10	108.20
1	AA	154	U	O4'-C1'-N1	7.37	114.10	108.20
1	AA	1142	G	P-O3'-C3'	7.37	128.54	119.70
27	B8	1666	G	C5-C6-O6	-7.37	124.18	128.60
1	AA	406	G	C5-C6-O6	-7.37	124.18	128.60
1	AA	723	U	O4'-C1'-N1	7.37	114.09	108.20
1	AA	893	C	O4'-C1'-N1	7.37	114.09	108.20
1	AA	765	G	O4'-C1'-N9	7.37	114.09	108.20
27	B8	2445	G	C5-C6-O6	-7.37	124.18	128.60
1	AA	515	G	C5-C6-O6	-7.37	124.18	128.60
1	AA	1316	G	N3-C2-N2	7.37	125.06	119.90
27	B8	656	G	C5-C6-O6	-7.37	124.18	128.60
27	B8	1608	A	C4-C5-C6	7.37	120.68	117.00
1	AA	839	C	O4'-C1'-N1	7.36	114.09	108.20
1	AA	1312	G	C5-C6-O6	-7.36	124.18	128.60
27	B8	1360	G	N1-C6-O6	7.36	124.32	119.90
27	B8	1444	G	C5-C6-O6	-7.36	124.18	128.60
27	B8	1450	G	C5-C6-O6	-7.36	124.18	128.60
1	AA	1228	C	O4'-C1'-N1	7.36	114.09	108.20
27	B8	1228	G	C5-C6-O6	-7.36	124.18	128.60
27	B8	1446	C	O4'-C1'-N1	7.36	114.09	108.20
27	B8	1748	C	O4'-C1'-N1	7.36	114.09	108.20
1	AA	665	A	O4'-C1'-N9	7.36	114.09	108.20
1	AA	612	C	O4'-C1'-N1	7.36	114.09	108.20
27	B8	1050	A	O4'-C1'-N9	7.36	114.09	108.20
27	B8	1645	G	C5-C6-O6	-7.36	124.19	128.60
27	B8	2815	C	O4'-C1'-N1	7.36	114.09	108.20
1	AA	388	G	C5-C6-O6	-7.36	124.19	128.60
1	AA	529	G	C5-C6-O6	-7.36	124.19	128.60
1	AA	813	U	O4'-C1'-N1	7.36	114.08	108.20
1	AA	1329	A	O4'-C1'-N9	7.36	114.08	108.20
27	B8	2687	U	O4'-C1'-N1	7.36	114.08	108.20
27	B8	2760	C	O4'-C1'-N1	7.36	114.08	108.20
27	B8	2862	G	C5-C6-O6	-7.36	124.19	128.60
27	B8	1139	G	C5-C6-O6	-7.35	124.19	128.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	444	G	C5-C6-O6	-7.35	124.19	128.60
1	AA	863	U	O4'-C1'-N1	7.35	114.08	108.20
1	AA	925	G	C5-C6-O6	-7.35	124.19	128.60
26	B7	16	G	C5-C6-O6	-7.35	124.19	128.60
27	B8	890	C	O4'-C1'-N1	7.35	114.08	108.20
27	B8	2373	G	C5-C6-O6	-7.35	124.19	128.60
1	AA	69	G	C5-C6-O6	-7.35	124.19	128.60
27	B8	840	C	O4'-C1'-N1	7.35	114.08	108.20
27	B8	862	G	C5-C6-O6	-7.35	124.19	128.60
27	B8	2401	U	O4'-C1'-N1	7.35	114.08	108.20
27	B8	2892	G	C5-C6-O6	-7.35	124.19	128.60
1	AA	254	G	O4'-C1'-N9	7.35	114.08	108.20
1	AA	698	G	C5-C6-O6	-7.35	124.19	128.60
1	AA	987	G	C5-C6-O6	-7.35	124.19	128.60
27	B8	967	U	O4'-C1'-N1	7.35	114.08	108.20
27	B8	1003	G	C5-C6-O6	-7.35	124.19	128.60
1	AA	355	C	O4'-C1'-N1	7.35	114.08	108.20
27	B8	1995	U	O4'-C1'-N1	7.34	114.08	108.20
27	B8	2178	C	O4'-C1'-N1	7.34	114.08	108.20
27	B8	2585	U	P-O3'-C3'	7.34	128.51	119.70
1	AA	776	G	C5-C6-O6	-7.34	124.19	128.60
27	B8	657	U	O4'-C1'-N1	7.34	114.07	108.20
27	B8	1172	C	O4'-C1'-N1	7.34	114.07	108.20
27	B8	171	U	O4'-C1'-N1	7.34	114.07	108.20
1	AA	423	G	O4'-C1'-N9	7.34	114.07	108.20
1	AA	631	C	O4'-C1'-N1	7.34	114.07	108.20
1	AA	1522	U	O4'-C1'-N1	7.34	114.07	108.20
3	AV	13	C	O4'-C1'-N1	7.34	114.07	108.20
2	AX	16	C	O4'-C1'-N1	7.34	114.07	108.20
27	B8	364	C	O4'-C1'-N1	7.34	114.07	108.20
27	B8	2008	C	O4'-C1'-N1	7.34	114.07	108.20
27	B8	2845	U	O4'-C1'-N1	7.33	114.07	108.20
26	B7	43	C	O4'-C1'-N1	7.33	114.07	108.20
27	B8	516	C	O4'-C1'-N1	7.33	114.07	108.20
3	AV	48	U	O4'-C1'-N1	7.33	114.06	108.20
27	B8	187	G	C5-C6-O6	-7.33	124.20	128.60
27	B8	694	U	O4'-C1'-N1	7.33	114.06	108.20
27	B8	1638	C	O4'-C1'-N1	7.33	114.06	108.20
1	AA	1073	U	O4'-C1'-N1	7.33	114.06	108.20
27	B8	2001	C	O4'-C1'-N1	7.33	114.06	108.20
1	AA	1315	U	O4'-C1'-N1	7.33	114.06	108.20
27	B8	1688	U	O4'-C1'-N1	7.33	114.06	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1479	C	O4'-C1'-N1	7.33	114.06	108.20
1	AA	213	G	C5-C6-O6	-7.32	124.21	128.60
1	AA	549	C	O4'-C1'-N1	7.32	114.06	108.20
27	B8	408	G	C5-C6-O6	-7.32	124.21	128.60
27	B8	2755	C	O4'-C1'-N1	7.32	114.06	108.20
1	AA	56	U	O4'-C1'-N1	7.32	114.06	108.20
1	AA	140	U	O4'-C1'-N1	7.32	114.06	108.20
1	AA	770	C	O4'-C1'-N1	7.32	114.06	108.20
27	B8	259	G	C5-C6-O6	-7.32	124.21	128.60
27	B8	1280	G	C5-C6-O6	-7.32	124.21	128.60
27	B8	1423	G	O4'-C1'-N9	7.32	114.06	108.20
27	B8	837	C	O4'-C1'-N1	7.32	114.06	108.20
26	B7	44	G	C5-C6-O6	-7.32	124.21	128.60
27	B8	154	U	O4'-C1'-N1	7.32	114.05	108.20
27	B8	2616	C	O4'-C1'-N1	7.32	114.06	108.20
27	B8	1336	A	O4'-C1'-N9	7.32	114.05	108.20
1	AA	358	U	O4'-C1'-N1	7.31	114.05	108.20
27	B8	235	U	O4'-C1'-N1	7.31	114.05	108.20
27	B8	2869	G	C5-C6-O6	-7.31	124.21	128.60
1	AA	330	C	O4'-C1'-N1	7.31	114.05	108.20
1	AA	828	U	O4'-C1'-N1	7.31	114.05	108.20
1	AA	1153	G	C5-C6-O6	-7.31	124.21	128.60
27	B8	518	G	C5-C6-O6	-7.31	124.21	128.60
27	B8	826	U	O4'-C1'-N1	7.31	114.05	108.20
1	AA	670	G	C5-C6-O6	-7.31	124.21	128.60
1	AA	218	U	O4'-C1'-N1	7.31	114.05	108.20
1	AA	1459	G	C5-C6-O6	-7.31	124.22	128.60
27	B8	196	A	O4'-C1'-N9	7.31	114.05	108.20
27	B8	1863	G	C5-C6-O6	-7.31	124.22	128.60
1	AA	1301	U	O4'-C1'-N1	7.31	114.05	108.20
27	B8	494	G	O4'-C1'-N9	7.31	114.05	108.20
27	B8	638	G	C5-C6-O6	-7.31	124.22	128.60
27	B8	771	G	O4'-C1'-N9	7.31	114.05	108.20
27	B8	2225	A	C4-C5-C6	7.31	120.65	117.00
27	B8	2256	G	C5-C6-O6	-7.31	124.22	128.60
27	B8	2352	A	C4-C5-C6	7.31	120.65	117.00
27	B8	2674	G	C5-C6-O6	-7.31	124.22	128.60
27	B8	2836	U	O4'-C1'-N1	7.31	114.05	108.20
26	B7	80	U	O4'-C1'-N1	7.31	114.05	108.20
27	B8	567	U	O4'-C1'-N1	7.31	114.05	108.20
27	B8	2646	C	O4'-C1'-N1	7.31	114.05	108.20
1	AA	516	U	O4'-C1'-N1	7.30	114.04	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	638	U	O4'-C1'-N1	7.30	114.04	108.20
27	B8	11	C	O4'-C1'-N1	7.30	114.04	108.20
27	B8	1623	G	C5-C6-O6	-7.30	124.22	128.60
27	B8	1943	U	O4'-C1'-N1	7.30	114.04	108.20
27	B8	2196	C	O4'-C1'-N1	7.30	114.04	108.20
27	B8	135	U	O4'-C1'-N1	7.30	114.04	108.20
1	AA	666	G	C5-C6-O6	-7.30	124.22	128.60
3	AV	63	C	O4'-C1'-N1	7.30	114.04	108.20
27	B8	2552	U	O4'-C1'-N1	7.30	114.04	108.20
1	AA	801	U	O4'-C1'-N1	7.30	114.04	108.20
1	AA	1465	A	C5-C6-N6	-7.30	117.86	123.70
27	B8	1063	G	C5-C6-O6	-7.30	124.22	128.60
1	AA	506	G	C5-C6-O6	-7.30	124.22	128.60
27	B8	320	A	P-O3'-C3'	7.30	128.46	119.70
27	B8	2103	C	O4'-C1'-N1	7.30	114.04	108.20
27	B8	2143	C	O4'-C1'-N1	7.30	114.04	108.20
1	AA	562	U	P-O3'-C3'	7.30	128.46	119.70
1	AA	347	G	O4'-C1'-N9	7.29	114.04	108.20
1	AA	371	A	O4'-C1'-N9	7.29	114.04	108.20
26	B7	95	U	O4'-C1'-N1	7.29	114.03	108.20
27	B8	658	U	O4'-C1'-N1	7.29	114.03	108.20
27	B8	939	G	C5-C6-O6	-7.29	124.23	128.60
27	B8	1453	A	O4'-C1'-N9	7.29	114.03	108.20
1	AA	971	G	C5-C6-O6	-7.29	124.23	128.60
27	B8	1016	G	O4'-C1'-N9	7.29	114.03	108.20
27	B8	1035	U	O4'-C1'-N1	7.29	114.03	108.20
27	B8	1847	A	O4'-C1'-N9	7.29	114.03	108.20
27	B8	2585	U	O4'-C1'-N1	7.29	114.03	108.20
1	AA	833	G	C5-C6-O6	-7.29	124.23	128.60
1	AA	887	G	C5-C6-O6	-7.29	124.23	128.60
26	B7	2	G	C5-C6-O6	-7.29	124.23	128.60
1	AA	103	U	O4'-C1'-N1	7.29	114.03	108.20
1	AA	526	C	O4'-C1'-N1	7.29	114.03	108.20
27	B8	962	G	C5-C6-O6	-7.29	124.23	128.60
27	B8	1292	G	C5-C6-O6	-7.29	124.23	128.60
27	B8	1484	U	O4'-C1'-N1	7.29	114.03	108.20
1	AA	11	G	C5-C6-O6	-7.29	124.23	128.60
1	AA	93	U	O4'-C1'-N1	7.29	114.03	108.20
27	B8	177	G	O4'-C1'-N9	7.29	114.03	108.20
27	B8	289	G	C5-C6-O6	-7.29	124.23	128.60
27	B8	1220	G	C5-C6-O6	-7.28	124.23	128.60
27	B8	1859	U	O4'-C1'-N1	7.28	114.02	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	133	U	O4'-C1'-N1	7.28	114.02	108.20
27	B8	156	A	O4'-C1'-N9	7.28	114.02	108.20
27	B8	375	G	C5-C6-O6	-7.28	124.23	128.60
27	B8	2242	G	C5-C6-O6	-7.28	124.23	128.60
27	B8	220	G	C5-C6-O6	-7.28	124.23	128.60
27	B8	370	G	C5-C6-O6	-7.28	124.23	128.60
27	B8	660	C	O4'-C1'-N1	7.28	114.02	108.20
27	B8	2511	U	O4'-C1'-N1	7.28	114.02	108.20
27	B8	2617	U	O4'-C1'-N1	7.28	114.02	108.20
1	AA	318	G	C5-C6-O6	-7.27	124.24	128.60
27	B8	297	G	C5-C6-O6	-7.27	124.24	128.60
27	B8	768	G	O4'-C1'-N9	7.27	114.02	108.20
27	B8	2573	C	C2-N1-C1'	7.27	126.80	118.80
1	AA	21	G	O4'-C1'-N9	7.27	114.02	108.20
27	B8	8	C	N3-C4-N4	7.27	123.09	118.00
27	B8	193	U	O4'-C1'-N1	7.27	114.02	108.20
27	B8	2860	A	C5-C6-N1	-7.27	114.06	117.70
27	B8	249	C	O4'-C1'-N1	7.27	114.02	108.20
27	B8	1041	G	C5-C6-O6	-7.27	124.24	128.60
1	AA	230	G	C5-C6-O6	-7.27	124.24	128.60
27	B8	543	G	C5-C6-O6	-7.27	124.24	128.60
27	B8	610	C	O4'-C1'-N1	7.27	114.02	108.20
27	B8	874	G	C5-C6-O6	-7.27	124.24	128.60
27	B8	1234	U	O4'-C1'-N1	7.27	114.02	108.20
27	B8	1487	U	O4'-C1'-N1	7.27	114.02	108.20
1	AA	94	G	C5-C6-O6	-7.27	124.24	128.60
1	AA	830	G	C5-C6-O6	-7.27	124.24	128.60
27	B8	1719	G	C5-C6-O6	-7.27	124.24	128.60
27	B8	2062	A	O4'-C1'-N9	7.27	114.01	108.20
27	B8	2455	G	C5-C6-O6	-7.27	124.24	128.60
27	B8	4	U	O4'-C1'-N1	7.27	114.01	108.20
27	B8	1696	G	C5-C6-O6	-7.26	124.24	128.60
27	B8	1878	G	C5-C6-O6	-7.26	124.24	128.60
27	B8	2767	C	O4'-C1'-N1	7.26	114.01	108.20
1	AA	564	C	O4'-C1'-N1	7.26	114.01	108.20
1	AA	1124	G	C5-C6-O6	-7.26	124.24	128.60
1	AA	1175	G	C5-C6-O6	-7.26	124.24	128.60
1	AA	1221	G	C5-C6-O6	-7.26	124.24	128.60
27	B8	965	C	O4'-C1'-N1	7.26	114.01	108.20
27	B8	1617	C	O4'-C1'-N1	7.26	114.01	108.20
27	B8	2110	G	C5-C6-O6	-7.26	124.24	128.60
1	AA	1527	U	O4'-C1'-N1	7.26	114.01	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	712	G	C5-C6-O6	-7.26	124.24	128.60
27	B8	1117	C	O4'-C1'-N1	7.26	114.01	108.20
27	B8	2561	U	O4'-C1'-N1	7.26	114.01	108.20
1	AA	1106	G	C5-C6-O6	-7.26	124.25	128.60
27	B8	377	G	C5-C6-O6	-7.26	124.25	128.60
27	B8	1895	C	O4'-C1'-N1	7.26	114.00	108.20
27	B8	923	G	C5-C6-O6	-7.25	124.25	128.60
27	B8	2458	G	C5-C6-O6	-7.25	124.25	128.60
1	AA	625	U	O4'-C1'-N1	7.25	114.00	108.20
27	B8	1744	A	C4-C5-C6	7.25	120.63	117.00
27	B8	2137	U	O4'-C1'-N1	7.25	114.00	108.20
1	AA	126	G	C5-C6-O6	-7.25	124.25	128.60
1	AA	719	C	O4'-C1'-N1	7.25	114.00	108.20
1	AA	912	C	O4'-C1'-N1	7.25	114.00	108.20
27	B8	419	U	O4'-C1'-N1	7.25	114.00	108.20
27	B8	2106	U	O4'-C1'-N1	7.25	114.00	108.20
27	B8	2492	U	O4'-C1'-N1	7.25	114.00	108.20
27	B8	2707	U	O4'-C1'-N1	7.25	114.00	108.20
1	AA	751	U	O4'-C1'-N1	7.25	114.00	108.20
1	AA	1241	G	C5-C6-O6	-7.25	124.25	128.60
1	AA	684	U	O4'-C1'-N1	7.25	114.00	108.20
1	AA	866	C	O4'-C1'-N1	7.25	114.00	108.20
27	B8	1922	G	C5-C6-O6	-7.25	124.25	128.60
26	B7	103	U	O4'-C1'-N1	7.25	114.00	108.20
27	B8	1702	G	C5-C6-O6	-7.25	124.25	128.60
27	B8	2102	G	C5-C6-O6	-7.25	124.25	128.60
1	AA	947	G	C5-C6-O6	-7.25	124.25	128.60
27	B8	1137	G	C5-C6-O6	-7.25	124.25	128.60
1	AA	224	U	O4'-C1'-N1	7.24	113.99	108.20
3	AV	53	G	O4'-C1'-N9	7.24	114.00	108.20
27	B8	646	U	O4'-C1'-N1	7.24	113.99	108.20
27	B8	1078	U	O4'-C1'-N1	7.24	113.99	108.20
27	B8	216	A	C4-C5-C6	7.24	120.62	117.00
1	AA	980	C	O4'-C1'-N1	7.24	113.99	108.20
1	AA	1419	G	C5-C6-O6	-7.24	124.25	128.60
26	B7	105	G	C5-C6-O6	-7.24	124.26	128.60
27	B8	283	G	C5-C6-O6	-7.24	124.25	128.60
27	B8	591	U	O4'-C1'-N1	7.24	113.99	108.20
27	B8	710	U	O4'-C1'-N1	7.24	113.99	108.20
27	B8	1074	G	C5-C6-O6	-7.24	124.26	128.60
27	B8	1963	U	O4'-C1'-N1	7.24	113.99	108.20
27	B8	2112	G	N1-C6-O6	7.24	124.24	119.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	780	A	C5-C6-N6	-7.24	117.91	123.70
1	AA	1036	A	C5-C6-N6	-7.24	117.91	123.70
27	B8	2415	G	C5-C6-O6	-7.24	124.26	128.60
1	AA	157	U	O4'-C1'-N1	7.24	113.99	108.20
27	B8	1797	G	C5-C6-O6	-7.24	124.26	128.60
1	AA	874	G	C5-C6-O6	-7.24	124.26	128.60
27	B8	993	G	O4'-C1'-N9	7.24	113.99	108.20
27	B8	1229	C	O4'-C1'-N1	7.24	113.99	108.20
27	B8	1834	U	O4'-C1'-N1	7.24	113.99	108.20
1	AA	941	G	C5-C6-O6	-7.23	124.26	128.60
1	AA	1467	C	O4'-C1'-N1	7.23	113.99	108.20
1	AA	1496	C	O4'-C1'-N1	7.23	113.99	108.20
26	B7	31	C	O4'-C1'-N1	7.23	113.99	108.20
1	AA	31	G	C5-C6-O6	-7.23	124.26	128.60
1	AA	288	A	C5-C6-N6	-7.23	117.91	123.70
1	AA	757	U	O4'-C1'-N1	7.23	113.98	108.20
27	B8	1506	U	O4'-C1'-N1	7.23	113.99	108.20
27	B8	1840	G	C5-C6-O6	-7.23	124.26	128.60
27	B8	2179	C	O4'-C1'-N1	7.23	113.99	108.20
1	AA	841	C	O4'-C1'-N1	7.23	113.98	108.20
1	AA	873	A	C4-C5-C6	7.23	120.61	117.00
27	B8	2399	G	C5-C6-O6	-7.23	124.26	128.60
1	AA	1402	C	O4'-C1'-N1	7.23	113.98	108.20
27	B8	2549	G	C5-C6-O6	-7.23	124.26	128.60
1	AA	615	G	C5-C6-O6	-7.23	124.26	128.60
1	AA	1116	U	O4'-C1'-N1	7.23	113.98	108.20
27	B8	1279	G	C5-C6-O6	-7.23	124.26	128.60
27	B8	766	U	O4'-C1'-N1	7.23	113.98	108.20
1	AA	399	G	C5-C6-O6	-7.22	124.27	128.60
27	B8	549	G	C5-C6-O6	-7.22	124.27	128.60
27	B8	808	G	C5-C6-O6	-7.22	124.27	128.60
27	B8	1377	G	C5-C6-O6	-7.22	124.27	128.60
27	B8	1662	U	O4'-C1'-N1	7.22	113.98	108.20
1	AA	1083	U	O4'-C1'-N1	7.22	113.98	108.20
26	B7	61	G	C5-C6-O6	-7.22	124.27	128.60
27	B8	447	A	N1-C6-N6	7.22	122.93	118.60
27	B8	2236	U	O4'-C1'-N1	7.22	113.98	108.20
1	AA	1313	U	O4'-C1'-N1	7.22	113.97	108.20
27	B8	1346	G	C5-C6-O6	-7.22	124.27	128.60
27	B8	2412	A	C4-C5-C6	7.22	120.61	117.00
27	B8	2470	G	C5-C6-O6	-7.22	124.27	128.60
3	AV	29	C	O4'-C1'-N1	7.22	113.97	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	2578	G	C5-C6-O6	-7.22	124.27	128.60
1	AA	46	G	C5-C6-O6	-7.22	124.27	128.60
1	AA	1104	G	C5-C6-O6	-7.22	124.27	128.60
1	AA	1244	G	C5-C6-O6	-7.22	124.27	128.60
27	B8	29	U	O4'-C1'-N1	7.22	113.97	108.20
27	B8	439	A	O4'-C1'-N9	7.22	113.97	108.20
27	B8	500	G	C5-C6-O6	-7.22	124.27	128.60
27	B8	542	C	O4'-C1'-N1	7.22	113.97	108.20
27	B8	868	U	O4'-C1'-N1	7.22	113.97	108.20
1	AA	1168	U	O4'-C1'-N1	7.21	113.97	108.20
27	B8	52	A	C4-C5-C6	7.21	120.61	117.00
27	B8	2305	U	O4'-C1'-N1	7.21	113.97	108.20
27	B8	2536	G	C5-C6-O6	-7.21	124.27	128.60
27	B8	2759	G	C5-C6-O6	-7.21	124.27	128.60
27	B8	962	G	O4'-C1'-N9	7.21	113.97	108.20
27	B8	1469	A	C4-C5-C6	7.21	120.61	117.00
1	AA	1047	G	C5-C6-O6	-7.21	124.27	128.60
1	AA	1182	G	C5-C6-O6	-7.21	124.28	128.60
27	B8	1310	G	C5-C6-O6	-7.21	124.28	128.60
1	AA	1202	U	O4'-C1'-N1	7.21	113.97	108.20
1	AA	1360	A	C4-C5-C6	7.21	120.60	117.00
1	AA	1518	A	O4'-C1'-N9	7.21	113.97	108.20
27	B8	629	G	C5-C6-O6	-7.21	124.28	128.60
27	B8	1410	G	C5-C6-O6	-7.21	124.28	128.60
27	B8	438	G	C5-C6-O6	-7.21	124.28	128.60
27	B8	2087	G	O4'-C1'-N9	7.21	113.96	108.20
1	AA	255	G	C5-C6-O6	-7.20	124.28	128.60
1	AA	289	G	O4'-C1'-N9	7.20	113.96	108.20
1	AA	537	G	C5-C6-O6	-7.20	124.28	128.60
1	AA	1192	C	O4'-C1'-N1	7.20	113.96	108.20
27	B8	124	G	C5-C6-O6	-7.20	124.28	128.60
27	B8	346	A	O4'-C1'-N9	7.20	113.96	108.20
27	B8	1324	G	C5-C6-O6	-7.20	124.28	128.60
27	B8	1393	A	O4'-C1'-N9	7.20	113.96	108.20
27	B8	2061	G	C5-C6-O6	-7.20	124.28	128.60
1	AA	881	G	C5-C6-O6	-7.20	124.28	128.60
27	B8	1959	G	C5-C6-O6	-7.20	124.28	128.60
27	B8	2109	U	O4'-C1'-N1	7.20	113.96	108.20
1	AA	736	C	O4'-C1'-N1	7.20	113.96	108.20
1	AA	923	A	C5-C6-N6	-7.20	117.94	123.70
27	B8	189	G	C5-C6-O6	-7.20	124.28	128.60
27	B8	647	G	C5-C6-O6	-7.20	124.28	128.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	734	A	C5-C6-N6	-7.20	117.94	123.70
27	B8	841	G	C5-C6-O6	-7.20	124.28	128.60
27	B8	1165	A	O4'-C1'-N9	7.20	113.96	108.20
27	B8	30	G	C5-C6-O6	-7.20	124.28	128.60
27	B8	1160	G	C5-C6-O6	-7.20	124.28	128.60
1	AA	1135	U	O4'-C1'-N1	7.20	113.96	108.20
27	B8	1899	A	C5-C6-N6	-7.20	117.94	123.70
27	B8	2223	G	C5-C6-O6	-7.20	124.28	128.60
27	B8	2385	C	O4'-C1'-N1	7.20	113.96	108.20
27	B8	1588	G	C5-C6-O6	-7.19	124.28	128.60
27	B8	1620	G	C5-C6-O6	-7.19	124.28	128.60
27	B8	1720	U	O4'-C1'-N1	7.19	113.95	108.20
27	B8	2044	C	O4'-C1'-N1	7.19	113.95	108.20
27	B8	956	G	C5-C6-O6	-7.19	124.28	128.60
27	B8	2318	G	C5-C6-O6	-7.19	124.28	128.60
27	B8	2869	G	O4'-C1'-N9	7.19	113.95	108.20
1	AA	333	U	O4'-C1'-N1	7.19	113.95	108.20
1	AA	1532	U	O4'-C1'-N1	7.19	113.95	108.20
27	B8	201	C	N3-C4-N4	7.19	123.03	118.00
27	B8	206	U	O4'-C1'-N1	7.19	113.95	108.20
1	AA	1322	C	O4'-C1'-N1	7.19	113.95	108.20
27	B8	926	G	C5-C6-O6	-7.19	124.29	128.60
1	AA	929	G	O4'-C1'-N9	7.19	113.95	108.20
1	AA	1249	C	O4'-C1'-N1	7.19	113.95	108.20
27	B8	1379	U	O4'-C1'-N1	7.19	113.95	108.20
27	B8	1459	G	O4'-C1'-N9	7.19	113.95	108.20
27	B8	2218	G	C5-C6-O6	-7.19	124.29	128.60
27	B8	2490	G	C5-C6-O6	-7.19	124.29	128.60
1	AA	952	U	O4'-C1'-N1	7.19	113.95	108.20
27	B8	989	G	C5-C6-O6	-7.19	124.29	128.60
27	B8	2737	G	C5-C6-O6	-7.19	124.29	128.60
27	B8	1513	U	O4'-C1'-N1	7.18	113.95	108.20
27	B8	1095	A	O4'-C1'-N9	7.18	113.95	108.20
27	B8	1742	U	O4'-C1'-N1	7.18	113.95	108.20
27	B8	1750	G	O4'-C1'-N9	7.18	113.95	108.20
27	B8	1849	G	C5-C6-O6	-7.18	124.29	128.60
27	B8	2354	C	O4'-C1'-N1	7.18	113.95	108.20
27	B8	2457	U	O4'-C1'-N1	7.18	113.95	108.20
1	AA	95	C	N3-C4-N4	7.18	123.03	118.00
27	B8	1836	C	O4'-C1'-N1	7.18	113.94	108.20
1	AA	137	U	O4'-C1'-N1	7.18	113.94	108.20
1	AA	181	A	C5-C6-N6	-7.18	117.96	123.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	B7	5	U	O4'-C1'-N1	7.18	113.94	108.20
26	B7	18	G	C5-C6-O6	-7.18	124.29	128.60
27	B8	437	U	O4'-C1'-N1	7.18	113.94	108.20
27	B8	643	A	O4'-C1'-N9	7.18	113.94	108.20
27	B8	740	C	O4'-C1'-N1	7.18	113.94	108.20
1	AA	108	G	O4'-C1'-N9	7.18	113.94	108.20
27	B8	2696	U	O4'-C1'-N1	7.18	113.94	108.20
27	B8	1309	G	C5-C6-O6	-7.17	124.30	128.60
27	B8	1373	A	C4-C5-C6	7.17	120.59	117.00
1	AA	957	U	O4'-C1'-N1	7.17	113.94	108.20
1	AA	423	G	C5-C6-O6	-7.17	124.30	128.60
27	B8	107	G	C5-C6-O6	-7.17	124.30	128.60
27	B8	578	G	C5-C6-O6	-7.17	124.30	128.60
27	B8	2398	U	O4'-C1'-N1	7.17	113.94	108.20
27	B8	2693	G	C5-C6-O6	-7.17	124.30	128.60
26	B7	12	C	O4'-C1'-N1	7.17	113.94	108.20
1	AA	299	G	C5-C6-O6	-7.17	124.30	128.60
1	AA	1084	G	C5-C6-O6	-7.17	124.30	128.60
27	B8	2605	U	O4'-C1'-N1	7.17	113.94	108.20
1	AA	906	A	C5-C6-N6	-7.17	117.97	123.70
26	B7	120	U	O4'-C1'-N1	7.17	113.93	108.20
27	B8	27	G	C5-C6-O6	-7.17	124.30	128.60
27	B8	771	G	C5-C6-O6	-7.17	124.30	128.60
27	B8	2586	U	O4'-C1'-N1	7.17	113.93	108.20
27	B8	2881	U	O4'-C1'-N1	7.17	113.93	108.20
27	B8	96	C	O4'-C1'-N1	7.17	113.93	108.20
27	B8	1209	U	O4'-C1'-N1	7.17	113.93	108.20
1	AA	569	C	O4'-C1'-N1	7.16	113.93	108.20
1	AA	979	C	O4'-C1'-N1	7.16	113.93	108.20
1	AA	132	C	O4'-C1'-N1	7.16	113.93	108.20
1	AA	462	G	C5-C6-O6	-7.16	124.30	128.60
1	AA	900	A	O4'-C1'-N9	7.16	113.93	108.20
27	B8	24	G	C5-C6-O6	-7.16	124.30	128.60
27	B8	636	G	C5-C6-O6	-7.16	124.30	128.60
27	B8	2245	U	O4'-C1'-N1	7.16	113.93	108.20
1	AA	514	C	O4'-C1'-N1	7.16	113.93	108.20
1	AA	1404	C	O4'-C1'-N1	7.16	113.93	108.20
27	B8	2000	C	O4'-C1'-N1	7.16	113.93	108.20
27	B8	2259	U	O4'-C1'-N1	7.16	113.93	108.20
27	B8	2846	G	C5-C6-O6	-7.16	124.31	128.60
1	AA	295	C	O4'-C1'-N1	7.16	113.93	108.20
27	B8	136	G	C5-C6-O6	-7.16	124.31	128.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	357	C	O4'-C1'-N1	7.16	113.93	108.20
1	AA	442	G	C5-C6-O6	-7.16	124.31	128.60
3	AV	51	G	C5-C6-O6	-7.16	124.31	128.60
27	B8	511	U	O4'-C1'-N1	7.16	113.92	108.20
27	B8	1053	C	N3-C4-N4	7.16	123.01	118.00
27	B8	2204	G	C5-C6-O6	-7.15	124.31	128.60
1	AA	210	C	O4'-C1'-N1	7.15	113.92	108.20
1	AA	1463	U	O4'-C1'-N1	7.15	113.92	108.20
1	AA	445	G	C5-C6-O6	-7.15	124.31	128.60
27	B8	1148	U	O4'-C1'-N1	7.15	113.92	108.20
27	B8	2668	G	C5-C6-O6	-7.15	124.31	128.60
1	AA	24	U	O4'-C1'-N1	7.15	113.92	108.20
27	B8	1249	U	O4'-C1'-N1	7.15	113.92	108.20
27	B8	2685	G	C5-C6-O6	-7.15	124.31	128.60
1	AA	79	G	C5-C6-O6	-7.15	124.31	128.60
1	AA	799	G	C5-C6-O6	-7.15	124.31	128.60
1	AA	1138	G	C5-C6-O6	-7.15	124.31	128.60
1	AA	42	G	C5-C6-O6	-7.14	124.31	128.60
1	AA	644	U	O4'-C1'-N1	7.14	113.92	108.20
1	AA	711	G	C5-C6-O6	-7.14	124.31	128.60
1	AA	904	U	O4'-C1'-N1	7.14	113.92	108.20
27	B8	1509	A	O4'-C1'-N9	7.14	113.92	108.20
27	B8	1680	U	O4'-C1'-N1	7.14	113.92	108.20
27	B8	2243	U	O4'-C1'-N1	7.14	113.92	108.20
27	B8	2680	U	O4'-C1'-N1	7.14	113.92	108.20
1	AA	39	G	O4'-C1'-N9	7.14	113.92	108.20
26	B7	75	G	C5-C6-O6	-7.14	124.31	128.60
27	B8	1380	G	C5-C6-O6	-7.14	124.31	128.60
27	B8	2496	C	O4'-C1'-N1	7.14	113.91	108.20
1	AA	375	U	O4'-C1'-N1	7.14	113.91	108.20
27	B8	2593	U	O4'-C1'-N1	7.14	113.91	108.20
27	B8	269	C	O4'-C1'-N1	7.14	113.91	108.20
27	B8	1632	A	O4'-C1'-N9	7.14	113.91	108.20
27	B8	2216	G	C5-C6-O6	-7.14	124.32	128.60
27	B8	2277	G	O4'-C1'-N9	7.14	113.91	108.20
1	AA	741	G	O4'-C1'-N9	7.14	113.91	108.20
1	AA	1308	U	O4'-C1'-N1	7.14	113.91	108.20
27	B8	1222	U	O4'-C1'-N1	7.14	113.91	108.20
27	B8	1714	U	O4'-C1'-N1	7.14	113.91	108.20
27	B8	2826	A	C5-C6-N6	-7.14	117.99	123.70
1	AA	1397	C	O4'-C1'-N1	7.13	113.91	108.20
26	B7	109	A	C5-C6-N6	-7.13	117.99	123.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	23	G	C5-C6-O6	-7.13	124.32	128.60
27	B8	705	A	C4-C5-C6	7.13	120.57	117.00
27	B8	1993	U	O4'-C1'-N1	7.13	113.91	108.20
1	AA	524	G	C5-C6-O6	-7.13	124.32	128.60
1	AA	425	G	O4'-C1'-N9	7.13	113.91	108.20
1	AA	921	U	O4'-C1'-N1	7.13	113.91	108.20
27	B8	150	U	O4'-C1'-N1	7.13	113.91	108.20
27	B8	1266	G	C5-C6-O6	-7.13	124.32	128.60
27	B8	1891	G	C5-C6-O6	-7.13	124.32	128.60
27	B8	2387	U	O4'-C1'-N1	7.13	113.90	108.20
27	B8	2884	U	O4'-C1'-N1	7.13	113.90	108.20
1	AA	993	G	O4'-C1'-N9	7.13	113.90	108.20
27	B8	618	G	C5-C6-O6	-7.13	124.32	128.60
27	B8	1128	G	C5-C6-O6	-7.13	124.32	128.60
27	B8	1231	U	O4'-C1'-N1	7.13	113.90	108.20
27	B8	2293	G	O4'-C1'-N9	7.13	113.90	108.20
1	AA	1005	A	C4-C5-C6	7.12	120.56	117.00
27	B8	205	G	C5-C6-O6	-7.12	124.33	128.60
27	B8	1199	U	O4'-C1'-N1	7.12	113.90	108.20
27	B8	1451	C	O4'-C1'-N1	7.12	113.90	108.20
1	AA	64	G	C5-C6-O6	-7.12	124.33	128.60
1	AA	468	A	C4-C5-C6	7.12	120.56	117.00
1	AA	682	G	C5-C6-O6	-7.12	124.33	128.60
1	AA	961	U	O4'-C1'-N1	7.12	113.90	108.20
27	B8	1036	G	O4'-C1'-N9	7.12	113.90	108.20
27	B8	1862	G	C5-C6-O6	-7.12	124.33	128.60
1	AA	533	A	C4-C5-C6	7.12	120.56	117.00
27	B8	49	A	C4-C5-C6	7.12	120.56	117.00
27	B8	89	A	O4'-C1'-N9	7.12	113.89	108.20
27	B8	1137	G	O4'-C1'-N9	7.12	113.89	108.20
1	AA	674	G	O4'-C1'-N9	7.11	113.89	108.20
1	AA	762	U	O4'-C1'-N1	7.11	113.89	108.20
1	AA	809	G	C5-C6-O6	-7.11	124.33	128.60
27	B8	614	A	O4'-C1'-N9	7.11	113.89	108.20
27	B8	1257	C	O4'-C1'-N1	7.11	113.89	108.20
1	AA	121	U	O4'-C1'-N1	7.11	113.89	108.20
1	AA	1464	U	O4'-C1'-N1	7.11	113.89	108.20
1	AA	505	G	C5-C6-O6	-7.11	124.33	128.60
26	B7	79	G	C5-C6-O6	-7.11	124.34	128.60
27	B8	34	U	O4'-C1'-N1	7.11	113.89	108.20
1	AA	1160	G	N1-C6-O6	7.11	124.16	119.90
27	B8	315	G	O4'-C1'-N9	7.11	113.89	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	639	U	O4'-C1'-N1	7.11	113.89	108.20
27	B8	1004	U	O4'-C1'-N1	7.11	113.89	108.20
27	B8	2074	U	O4'-C1'-N1	7.11	113.89	108.20
1	AA	292	G	C5-C6-O6	-7.10	124.34	128.60
1	AA	353	A	O4'-C1'-N9	7.10	113.88	108.20
1	AA	1361	G	O4'-C1'-N9	7.10	113.88	108.20
3	AV	55	U	O4'-C1'-N1	7.10	113.88	108.20
27	B8	2085	U	O4'-C1'-N1	7.10	113.88	108.20
1	AA	891	U	O4'-C1'-N1	7.10	113.88	108.20
27	B8	1079	C	O4'-C1'-N1	7.10	113.88	108.20
27	B8	1582	C	O4'-C1'-N1	7.10	113.88	108.20
27	B8	2580	U	O4'-C1'-N1	7.10	113.88	108.20
1	AA	661	G	C5-C6-O6	-7.10	124.34	128.60
27	B8	1711	A	O4'-C1'-N9	7.10	113.88	108.20
27	B8	1882	U	O4'-C1'-N1	7.10	113.88	108.20
27	B8	2231	U	O4'-C1'-N1	7.10	113.88	108.20
27	B8	2800	A	C4-C5-C6	7.10	120.55	117.00
1	AA	88	U	O4'-C1'-N1	7.10	113.88	108.20
27	B8	860	U	O4'-C1'-N1	7.10	113.88	108.20
27	B8	686	U	O4'-C1'-N1	7.09	113.88	108.20
1	AA	809	G	O4'-C1'-N9	7.09	113.87	108.20
1	AA	1504	G	C5-C6-O6	-7.09	124.34	128.60
26	B7	102	G	C5-C6-O6	-7.09	124.34	128.60
27	B8	5	A	C5-C6-N6	-7.09	118.03	123.70
27	B8	495	G	C5-C6-O6	-7.09	124.34	128.60
27	B8	2612	C	O4'-C1'-N1	7.09	113.87	108.20
1	AA	982	U	O4'-C1'-N1	7.09	113.87	108.20
1	AA	1387	G	C5-C6-O6	-7.09	124.35	128.60
27	B8	323	C	C2-N1-C1'	7.09	126.60	118.80
27	B8	1255	U	O4'-C1'-N1	7.09	113.87	108.20
27	B8	2366	A	C4-C5-C6	7.09	120.54	117.00
27	B8	2768	U	O4'-C1'-N1	7.09	113.87	108.20
3	AV	15	G	C5-C6-O6	-7.09	124.35	128.60
1	AA	1194	U	O4'-C1'-N1	7.09	113.87	108.20
1	AA	1448	C	N3-C4-N4	7.09	122.96	118.00
3	AV	40	G	C5-C6-O6	-7.09	124.35	128.60
27	B8	59	U	O4'-C1'-N1	7.09	113.87	108.20
1	AA	672	U	O4'-C1'-N1	7.08	113.87	108.20
27	B8	1926	U	O4'-C1'-N1	7.08	113.87	108.20
27	B8	2186	G	C5-C6-O6	-7.08	124.35	128.60
1	AA	605	U	O4'-C1'-N1	7.08	113.87	108.20
27	B8	612	G	C5-C6-O6	-7.08	124.35	128.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	915	C	O4'-C1'-N1	7.08	113.87	108.20
1	AA	446	G	C5-C6-O6	-7.08	124.35	128.60
1	AA	1526	G	C5-C6-O6	-7.08	124.35	128.60
27	B8	459	U	O4'-C1'-N1	7.08	113.86	108.20
27	B8	952	G	C5-C6-O6	-7.08	124.35	128.60
27	B8	1475	G	C5-C6-O6	-7.08	124.35	128.60
27	B8	2771	C	O4'-C1'-N1	7.08	113.86	108.20
27	B8	310	A	C4-C5-C6	7.08	120.54	117.00
27	B8	1069	A	O4'-C1'-N9	7.08	113.86	108.20
27	B8	1358	G	C5-C6-O6	-7.08	124.35	128.60
27	B8	1398	C	O4'-C1'-N1	7.08	113.86	108.20
27	B8	1765	U	O4'-C1'-N1	7.08	113.86	108.20
27	B8	1845	G	C5-C6-O6	-7.08	124.35	128.60
27	B8	2107	G	C5-C6-O6	-7.08	124.35	128.60
1	AA	495	A	C4-C5-C6	7.08	120.54	117.00
27	B8	1225	G	C5-C6-O6	-7.08	124.36	128.60
27	B8	1709	U	O4'-C1'-N1	7.08	113.86	108.20
27	B8	864	G	O4'-C1'-N9	7.07	113.86	108.20
27	B8	2647	U	O4'-C1'-N1	7.07	113.86	108.20
1	AA	460	A	O4'-C1'-N9	7.07	113.86	108.20
27	B8	1210	G	C5-C6-O6	-7.07	124.36	128.60
27	B8	1767	G	C5-C6-O6	-7.07	124.36	128.60
27	B8	2286	G	C5-C6-O6	-7.07	124.36	128.60
27	B8	2405	G	C5-C6-O6	-7.07	124.36	128.60
1	AA	1393	U	O4'-C1'-N1	7.07	113.86	108.20
1	AA	1378	C	O4'-C1'-N1	7.07	113.85	108.20
27	B8	2541	A	C4-C5-C6	7.07	120.53	117.00
1	AA	198	G	C5-C6-O6	-7.07	124.36	128.60
1	AA	1306	A	O4'-C1'-N9	7.07	113.85	108.20
27	B8	8	C	O4'-C1'-N1	7.07	113.85	108.20
27	B8	1431	A	C5-C6-N6	-7.07	118.05	123.70
1	AA	1422	G	C5-C6-O6	-7.06	124.36	128.60
27	B8	2452	C	O4'-C1'-N1	7.06	113.85	108.20
1	AA	1365	G	C5-C6-O6	-7.06	124.36	128.60
27	B8	803	U	O4'-C1'-N1	7.06	113.85	108.20
27	B8	1350	C	O4'-C1'-N1	7.06	113.85	108.20
27	B8	1633	G	C5-C6-O6	-7.06	124.36	128.60
27	B8	1842	G	C5-C6-O6	-7.06	124.36	128.60
27	B8	2489	U	O4'-C1'-N1	7.06	113.85	108.20
1	AA	331	G	C5-C6-O6	-7.06	124.36	128.60
27	B8	169	G	C5-C6-O6	-7.06	124.36	128.60
27	B8	463	G	C5-C6-O6	-7.06	124.36	128.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	776	G	C5-C6-O6	-7.06	124.36	128.60
1	AA	745	G	C5-C6-O6	-7.06	124.36	128.60
27	B8	576	U	O4'-C1'-N1	7.06	113.84	108.20
27	B8	695	G	C5-C6-O6	-7.06	124.36	128.60
27	B8	769	U	O4'-C1'-N1	7.06	113.84	108.20
1	AA	127	G	C5-C6-O6	-7.06	124.37	128.60
1	AA	193	C	N3-C4-N4	7.05	122.94	118.00
1	AA	274	A	P-O3'-C3'	7.05	128.16	119.70
1	AA	822	U	O4'-C1'-N1	7.05	113.84	108.20
3	AV	8	U	O4'-C1'-N1	7.05	113.84	108.20
3	AV	44	G	C5-C6-O6	-7.05	124.37	128.60
1	AA	1529	G	O4'-C1'-N9	7.05	113.84	108.20
1	AA	381	C	O4'-C1'-N1	7.05	113.84	108.20
27	B8	688	U	O4'-C1'-N1	7.05	113.84	108.20
1	AA	773	G	C5-C6-O6	-7.05	124.37	128.60
1	AA	945	G	C5-C6-O6	-7.05	124.37	128.60
27	B8	78	U	O4'-C1'-N1	7.05	113.84	108.20
27	B8	323	C	O4'-C1'-N1	7.05	113.84	108.20
27	B8	583	G	C5-C6-O6	-7.05	124.37	128.60
27	B8	1930	G	P-O3'-C3'	7.05	128.16	119.70
27	B8	2378	A	C5-C6-N1	-7.05	114.17	117.70
1	AA	571	U	O4'-C1'-N1	7.05	113.84	108.20
1	AA	1525	G	O4'-C1'-N9	7.05	113.84	108.20
27	B8	1507	C	O4'-C1'-N1	7.05	113.84	108.20
1	AA	1258	G	C5-C6-O6	-7.05	124.37	128.60
27	B8	1982	U	O4'-C1'-N1	7.05	113.84	108.20
27	B8	2852	G	O4'-C1'-N9	7.05	113.84	108.20
1	AA	1023	U	O4'-C1'-N1	7.04	113.84	108.20
1	AA	416	G	C5-C6-O6	-7.04	124.37	128.60
1	AA	993	G	C5-C6-O6	-7.04	124.37	128.60
27	B8	2	G	C5-C6-O6	-7.04	124.37	128.60
27	B8	265	A	C5-C6-N6	-7.04	118.06	123.70
26	B7	56	G	C5-C6-O6	-7.04	124.38	128.60
27	B8	90	U	O4'-C1'-N1	7.04	113.83	108.20
27	B8	295	G	C5-C6-O6	-7.04	124.38	128.60
27	B8	1125	G	C5-C6-O6	-7.04	124.38	128.60
27	B8	1292	G	O4'-C1'-N9	7.04	113.83	108.20
27	B8	1401	G	C5-C6-O6	-7.04	124.38	128.60
1	AA	1474	U	O4'-C1'-N1	7.04	113.83	108.20
27	B8	469	G	C5-C6-O6	-7.04	124.38	128.60
27	B8	1116	G	C5-C6-O6	-7.04	124.38	128.60
27	B8	2335	A	C4-C5-C6	7.04	120.52	117.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	2669	G	O4'-C1'-N9	7.04	113.83	108.20
27	B8	926	G	O4'-C1'-N9	7.04	113.83	108.20
27	B8	942	G	C5-C6-O6	-7.04	124.38	128.60
27	B8	969	G	C5-C6-O6	-7.04	124.38	128.60
27	B8	975	A	C4-C5-C6	7.04	120.52	117.00
1	AA	72	A	O4'-C1'-N9	7.04	113.83	108.20
1	AA	1359	C	O4'-C1'-N1	7.04	113.83	108.20
27	B8	620	G	C5-C6-O6	-7.04	124.38	128.60
1	AA	1242	G	C5-C6-O6	-7.03	124.38	128.60
1	AA	905	U	O4'-C1'-N1	7.03	113.83	108.20
1	AA	339	C	O4'-C1'-N1	7.03	113.83	108.20
27	B8	427	U	O4'-C1'-N1	7.03	113.83	108.20
27	B8	1825	U	O4'-C1'-N1	7.03	113.82	108.20
27	B8	2326	C	O4'-C1'-N1	7.03	113.82	108.20
1	AA	203	G	C5-C6-O6	-7.03	124.38	128.60
1	AA	597	G	C5-C6-O6	-7.03	124.38	128.60
1	AA	1064	G	C5-C6-O6	-7.03	124.38	128.60
3	AV	69	U	O4'-C1'-N1	7.03	113.82	108.20
27	B8	1024	G	C5-C6-O6	-7.03	124.38	128.60
27	B8	535	G	C5-C6-O6	-7.03	124.39	128.60
27	B8	1831	G	C5-C6-O6	-7.03	124.39	128.60
1	AA	310	G	O4'-C1'-N9	7.02	113.82	108.20
1	AA	829	G	C5-C6-O6	-7.02	124.39	128.60
27	B8	303	G	C5-C6-O6	-7.02	124.39	128.60
27	B8	930	G	C5-C6-O6	-7.02	124.39	128.60
27	B8	974	G	C5-C6-O6	-7.02	124.39	128.60
27	B8	1456	G	C5-C6-O6	-7.02	124.39	128.60
27	B8	1860	G	C5-C6-O6	-7.02	124.39	128.60
27	B8	2244	U	O4'-C1'-N1	7.02	113.82	108.20
1	AA	802	A	O4'-C1'-N9	7.02	113.82	108.20
26	B7	37	C	O4'-C1'-N1	7.02	113.82	108.20
27	B8	514	A	O4'-C1'-N9	7.02	113.82	108.20
27	B8	2645	G	C5-C6-O6	-7.02	124.39	128.60
3	AV	35	G	C5-C6-O6	-7.02	124.39	128.60
27	B8	573	U	O4'-C1'-N1	7.02	113.82	108.20
27	B8	891	G	C1'-O4'-C4'	-7.02	104.28	109.90
27	B8	2848	G	O4'-C1'-N9	7.02	113.82	108.20
1	AA	699	C	O4'-C1'-N1	7.02	113.82	108.20
27	B8	188	G	C5-C6-O6	-7.02	124.39	128.60
27	B8	1018	U	O4'-C1'-N1	7.02	113.82	108.20
27	B8	1441	G	O4'-C1'-N9	7.02	113.82	108.20
27	B8	2695	U	O4'-C1'-N1	7.02	113.81	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	770	G	C5-C6-O6	-7.02	124.39	128.60
27	B8	1567	G	C5-C6-O6	-7.02	124.39	128.60
27	B8	2002	G	C5-C6-O6	-7.02	124.39	128.60
27	B8	2543	G	O4'-C1'-N9	7.02	113.81	108.20
1	AA	1530	G	C5-C6-O6	-7.02	124.39	128.60
27	B8	2307	G	N1-C6-O6	7.02	124.11	119.90
27	B8	2584	U	O4'-C1'-N1	7.02	113.81	108.20
27	B8	2828	G	C5-C6-O6	-7.02	124.39	128.60
1	AA	542	G	C5-C6-O6	-7.01	124.39	128.60
27	B8	1349	C	O4'-C1'-N1	7.01	113.81	108.20
27	B8	1219	U	O4'-C1'-N1	7.01	113.81	108.20
27	B8	1699	G	C5-C6-O6	-7.01	124.39	128.60
27	B8	2267	A	C4-C5-C6	7.01	120.50	117.00
27	B8	2292	U	O4'-C1'-N1	7.01	113.81	108.20
27	B8	2488	G	C5-C6-O6	-7.01	124.39	128.60
1	AA	775	G	C5-C6-O6	-7.01	124.39	128.60
1	AA	1032	G	C5-C6-O6	-7.01	124.39	128.60
27	B8	361	G	C5-C6-O6	-7.01	124.39	128.60
27	B8	475	C	O4'-C1'-N1	7.01	113.81	108.20
27	B8	2697	G	C5-C6-O6	-7.01	124.39	128.60
1	AA	928	G	C5-C6-O6	-7.01	124.39	128.60
27	B8	2547	A	O4'-C1'-N9	7.01	113.81	108.20
1	AA	451	A	C5-C6-N6	-7.01	118.09	123.70
27	B8	364	C	N3-C4-N4	7.01	122.90	118.00
27	B8	1516	G	C5-C6-O6	-7.01	124.40	128.60
27	B8	1070	A	O4'-C1'-N9	7.00	113.80	108.20
27	B8	1410	G	O4'-C1'-N9	7.00	113.80	108.20
27	B8	2082	A	C4-C5-C6	7.00	120.50	117.00
26	B7	66	A	C5-C6-N6	-7.00	118.10	123.70
27	B8	521	U	O4'-C1'-N1	7.00	113.80	108.20
27	B8	1286	A	C4-C5-C6	7.00	120.50	117.00
27	B8	1374	G	C5-C6-O6	-7.00	124.40	128.60
1	AA	725	G	O4'-C1'-N9	7.00	113.80	108.20
1	AA	1304	G	C5-C6-O6	-7.00	124.40	128.60
1	AA	48	C	O4'-C1'-N1	7.00	113.80	108.20
27	B8	254	G	C5-C6-O6	-7.00	124.40	128.60
27	B8	2406	A	O4'-C1'-N9	7.00	113.80	108.20
1	AA	447	G	N3-C2-N2	7.00	124.80	119.90
1	AA	792	A	O4'-C1'-N9	7.00	113.80	108.20
1	AA	1252	A	C4-C5-C6	7.00	120.50	117.00
27	B8	457	A	O4'-C1'-N9	7.00	113.80	108.20
27	B8	630	G	C5-C6-O6	-7.00	124.40	128.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	1149	G	C5-C6-O6	-7.00	124.40	128.60
27	B8	2545	G	C5-C6-O6	-7.00	124.40	128.60
1	AA	155	A	C5-C6-N6	-7.00	118.10	123.70
1	AA	1439	G	C5-C6-O6	-7.00	124.40	128.60
27	B8	1402	U	O4'-C1'-N1	7.00	113.80	108.20
27	B8	1823	G	O4'-C1'-N9	7.00	113.80	108.20
1	AA	237	G	C5-C6-O6	-6.99	124.40	128.60
27	B8	1432	G	C5-C6-O6	-6.99	124.40	128.60
27	B8	2700	A	O4'-C1'-N9	6.99	113.80	108.20
1	AA	1295	U	O4'-C1'-N1	6.99	113.79	108.20
26	B7	51	G	C5-C6-O6	-6.99	124.41	128.60
1	AA	327	A	C4-C5-C6	6.99	120.50	117.00
1	AA	713	G	C5-C6-O6	-6.99	124.41	128.60
1	AA	1190	G	C5-C6-O6	-6.99	124.41	128.60
27	B8	785	G	C5-C6-O6	-6.99	124.41	128.60
27	B8	1466	U	O4'-C1'-N1	6.99	113.79	108.20
27	B8	2188	U	O4'-C1'-N1	6.99	113.79	108.20
26	B7	96	G	C5-C6-O6	-6.99	124.41	128.60
27	B8	1407	G	O4'-C1'-N9	6.99	113.79	108.20
1	AA	273	U	O4'-C1'-N1	6.99	113.79	108.20
3	AV	2	G	C5-C6-O6	-6.99	124.41	128.60
27	B8	753	A	C4-C5-C6	6.99	120.49	117.00
27	B8	1767	G	O4'-C1'-N9	6.99	113.79	108.20
27	B8	2393	U	O4'-C1'-N1	6.99	113.79	108.20
1	AA	251	G	C5-C6-O6	-6.98	124.41	128.60
1	AA	100	G	C5-C6-O6	-6.98	124.41	128.60
1	AA	1035	A	C5-C6-N6	-6.98	118.11	123.70
1	AA	1477	U	O4'-C1'-N1	6.98	113.79	108.20
27	B8	306	U	O4'-C1'-N1	6.98	113.79	108.20
27	B8	770	G	O4'-C1'-N9	6.98	113.79	108.20
27	B8	997	G	C5-C6-O6	-6.98	124.41	128.60
27	B8	1087	G	C5-C6-O6	-6.98	124.41	128.60
27	B8	1120	G	C5-C6-O6	-6.98	124.41	128.60
27	B8	1332	G	C5-C6-O6	-6.98	124.41	128.60
27	B8	2877	G	C5-C6-O6	-6.98	124.41	128.60
1	AA	383	A	C4-C5-C6	6.98	120.49	117.00
27	B8	263	G	C5-C6-O6	-6.98	124.41	128.60
27	B8	918	A	C4-C5-C6	6.98	120.49	117.00
27	B8	1619	G	C5-C6-O6	-6.98	124.41	128.60
27	B8	2471	A	O4'-C1'-N9	6.98	113.78	108.20
27	B8	327	G	C5-C6-O6	-6.98	124.41	128.60
1	AA	55	A	C4-C5-C6	6.98	120.49	117.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1255	G	O4'-C1'-N9	6.98	113.78	108.20
27	B8	1163	G	C5-C6-O6	-6.98	124.41	128.60
27	B8	2049	G	C5-C6-O6	-6.98	124.41	128.60
1	AA	72	A	C4-C5-C6	6.98	120.49	117.00
27	B8	1666	G	O4'-C1'-N9	6.98	113.78	108.20
27	B8	1848	A	C4-C5-C6	6.98	120.49	117.00
27	B8	648	G	C5-C6-O6	-6.97	124.42	128.60
27	B8	2148	G	C5-C6-O6	-6.97	124.42	128.60
1	AA	530	G	C5-C6-O6	-6.97	124.42	128.60
1	AA	402	G	O4'-C1'-N9	6.97	113.77	108.20
1	AA	1200	C	N3-C4-N4	6.97	122.88	118.00
27	B8	396	G	O4'-C1'-N9	6.97	113.77	108.20
27	B8	525	U	O4'-C1'-N1	6.97	113.77	108.20
27	B8	537	G	C5-C6-O6	-6.97	124.42	128.60
27	B8	2174	C	O4'-C1'-N1	6.97	113.77	108.20
1	AA	710	G	O4'-C1'-N9	6.96	113.77	108.20
27	B8	215	G	C5-C6-O6	-6.96	124.42	128.60
27	B8	1363	C	O4'-C1'-N1	6.96	113.77	108.20
1	AA	265	G	N1-C6-O6	6.96	124.08	119.90
27	B8	431	U	O4'-C1'-N1	6.96	113.77	108.20
27	B8	397	U	O4'-C1'-N1	6.96	113.77	108.20
27	B8	1029	A	C4-C5-C6	6.96	120.48	117.00
1	AA	932	C	O4'-C1'-N1	6.96	113.77	108.20
27	B8	407	G	O4'-C1'-N9	6.96	113.77	108.20
1	AA	54	C	O4'-C1'-N1	6.96	113.77	108.20
1	AA	491	G	O4'-C1'-N9	6.96	113.77	108.20
27	B8	1147	A	O4'-C1'-N9	6.96	113.77	108.20
27	B8	1733	G	C5-C6-O6	-6.96	124.42	128.60
1	AA	771	G	C5-C6-O6	-6.96	124.43	128.60
1	AA	1134	G	C5-C6-O6	-6.96	124.43	128.60
27	B8	1205	A	O4'-C1'-N9	6.96	113.77	108.20
27	B8	1371	G	C5-C6-O6	-6.96	124.43	128.60
27	B8	1621	U	O4'-C1'-N1	6.96	113.77	108.20
27	B8	2152	G	O4'-C1'-N9	6.96	113.77	108.20
27	B8	2852	G	C5-C6-O6	-6.96	124.43	128.60
1	AA	1024	G	O4'-C1'-N9	6.96	113.76	108.20
27	B8	506	G	C5-C6-O6	-6.96	124.43	128.60
27	B8	733	G	C5-C6-O6	-6.96	124.43	128.60
26	B7	77	U	O4'-C1'-N1	6.95	113.76	108.20
27	B8	1056	G	C5-C6-O6	-6.95	124.43	128.60
27	B8	2297	A	C4-C5-C6	6.95	120.48	117.00
27	B8	2484	G	O4'-C1'-N9	6.95	113.76	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AX	18	C	O4'-C1'-N1	6.95	113.76	108.20
27	B8	2111	U	O4'-C1'-N1	6.95	113.76	108.20
1	AA	1400	C	O4'-C1'-N1	6.95	113.76	108.20
27	B8	2493	U	O4'-C1'-N1	6.95	113.76	108.20
1	AA	278	G	C5-C6-O6	-6.95	124.43	128.60
27	B8	551	G	C5-C6-O6	-6.95	124.43	128.60
27	B8	877	A	C5-C6-N1	-6.95	114.22	117.70
27	B8	1568	G	C5-C6-O6	-6.95	124.43	128.60
27	B8	2291	U	O4'-C1'-N1	6.95	113.76	108.20
27	B8	2379	G	C5-C6-O6	-6.95	124.43	128.60
27	B8	2633	G	O4'-C1'-N9	6.95	113.76	108.20
1	AA	729	A	O4'-C1'-N9	6.95	113.76	108.20
27	B8	580	U	O4'-C1'-N1	6.95	113.76	108.20
1	AA	1379	G	O4'-C1'-N9	6.94	113.75	108.20
3	AV	30	G	C5-C6-O6	-6.94	124.43	128.60
1	AA	966	G	C5-C6-O6	-6.94	124.44	128.60
1	AA	1267	C	O4'-C1'-N1	6.94	113.75	108.20
27	B8	2786	U	O4'-C1'-N1	6.94	113.75	108.20
1	AA	1235	U	O4'-C1'-N1	6.94	113.75	108.20
1	AA	46	G	O4'-C1'-N9	6.94	113.75	108.20
1	AA	656	G	C5-C6-O6	-6.94	124.44	128.60
1	AA	1395	C	O4'-C1'-N1	6.94	113.75	108.20
27	B8	794	A	C5-C6-N6	-6.94	118.15	123.70
1	AA	716	A	O4'-C1'-N9	6.94	113.75	108.20
27	B8	519	U	O4'-C1'-N1	6.94	113.75	108.20
27	B8	1866	A	C4-C5-C6	6.94	120.47	117.00
27	B8	2361	G	O4'-C1'-N9	6.94	113.75	108.20
27	B8	278	A	C4-C5-C6	6.93	120.47	117.00
27	B8	2193	G	C5-C6-O6	-6.93	124.44	128.60
27	B8	2571	U	O4'-C1'-N1	6.93	113.75	108.20
27	B8	2663	G	C5-C6-O6	-6.93	124.44	128.60
1	AA	175	C	N3-C4-N4	6.93	122.85	118.00
1	AA	1468	A	O4'-C1'-N9	6.93	113.75	108.20
27	B8	1473	G	C5-C6-O6	-6.93	124.44	128.60
27	B8	628	G	O4'-C1'-N9	6.93	113.75	108.20
27	B8	2864	G	C5-C6-O6	-6.93	124.44	128.60
27	B8	471	A	C4-C5-C6	6.93	120.46	117.00
27	B8	780	G	C5-C6-O6	-6.93	124.44	128.60
27	B8	928	A	C5-C6-N6	-6.93	118.16	123.70
27	B8	1750	G	C5-C6-O6	-6.93	124.44	128.60
27	B8	2077	A	C4-C5-C6	6.93	120.47	117.00
1	AA	703	G	C5-C6-O6	-6.93	124.44	128.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	1177	G	C5-C6-O6	-6.93	124.44	128.60
1	AA	563	A	C4-C5-C6	6.93	120.46	117.00
27	B8	494	G	C5-C6-O6	-6.93	124.44	128.60
27	B8	2834	G	C5-C6-O6	-6.93	124.44	128.60
1	AA	71	A	C5-C6-N6	-6.92	118.16	123.70
1	AA	796	C	O4'-C1'-N1	6.92	113.74	108.20
1	AA	1139	G	C5-C6-O6	-6.92	124.45	128.60
1	AA	1438	G	C5-C6-O6	-6.92	124.44	128.60
27	B8	286	U	O4'-C1'-N1	6.92	113.74	108.20
27	B8	1753	G	C5-C6-O6	-6.92	124.44	128.60
27	B8	1903	G	C5-C6-O6	-6.92	124.44	128.60
1	AA	603	U	O4'-C1'-N1	6.92	113.74	108.20
1	AA	1088	G	C5-C6-O6	-6.92	124.45	128.60
1	AA	1241	G	O4'-C1'-N9	6.92	113.74	108.20
1	AA	310	G	C5-C6-O6	-6.92	124.45	128.60
27	B8	2157	G	C5-C6-O6	-6.92	124.45	128.60
27	B8	2371	G	C5-C6-O6	-6.92	124.45	128.60
27	B8	474	G	C5-C6-O6	-6.92	124.45	128.60
27	B8	1322	A	O4'-C1'-N9	6.92	113.74	108.20
27	B8	1814	G	C5-C6-O6	-6.92	124.45	128.60
27	B8	2178	C	C2-N1-C1'	6.92	126.41	118.80
1	AA	721	G	C5-C6-O6	-6.92	124.45	128.60
26	B7	100	G	C5-C6-O6	-6.92	124.45	128.60
27	B8	373	U	O4'-C1'-N1	6.92	113.73	108.20
27	B8	1816	C	C6-N1-C1'	-6.92	112.50	120.80
27	B8	2499	C	O4'-C1'-N1	6.92	113.73	108.20
27	B8	2770	G	C5-C6-O6	-6.92	124.45	128.60
27	B8	667	U	O4'-C1'-N1	6.92	113.73	108.20
27	B8	1425	G	C5-C6-O6	-6.92	124.45	128.60
27	B8	2161	C	O4'-C1'-N1	6.92	113.73	108.20
1	AA	91	U	O4'-C1'-N1	6.91	113.73	108.20
27	B8	889	C	O4'-C1'-N1	6.91	113.73	108.20
27	B8	1178	C	O4'-C1'-N1	6.91	113.73	108.20
27	B8	2570	G	C5-C6-O6	-6.91	124.45	128.60
1	AA	194	C	O4'-C1'-N1	6.91	113.73	108.20
27	B8	1133	A	P-O3'-C3'	6.91	127.99	119.70
27	B8	1369	G	C5-C6-O6	-6.91	124.45	128.60
27	B8	51	G	C5-C6-O6	-6.91	124.45	128.60
27	B8	1516	G	O4'-C1'-N9	6.91	113.73	108.20
27	B8	1763	G	C5-C6-O6	-6.91	124.45	128.60
27	B8	1841	U	O4'-C1'-N1	6.91	113.73	108.20
27	B8	2135	A	O4'-C1'-N9	6.91	113.73	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1156	G	C5-C6-O6	-6.91	124.45	128.60
1	AA	1492	A	C5-C6-N6	-6.91	118.17	123.70
26	B7	7	G	O4'-C1'-N9	6.91	113.73	108.20
27	B8	191	A	C4-C5-C6	6.91	120.45	117.00
27	B8	586	A	N1-C6-N6	6.91	122.75	118.60
27	B8	2372	U	O4'-C1'-N1	6.91	113.73	108.20
27	B8	1361	G	C5-C6-O6	-6.91	124.46	128.60
27	B8	1851	U	O4'-C1'-N1	6.90	113.72	108.20
1	AA	384	G	C5-C6-O6	-6.90	124.46	128.60
1	AA	601	G	O4'-C1'-N9	6.90	113.72	108.20
1	AA	753	A	C4-C5-C6	6.90	120.45	117.00
1	AA	860	A	O4'-C1'-N9	6.90	113.72	108.20
1	AA	1473	G	C5-C6-O6	-6.90	124.46	128.60
27	B8	2429	G	C5-C6-O6	-6.90	124.46	128.60
27	B8	2662	A	C4-C5-C6	6.90	120.45	117.00
27	B8	904	G	C5-C6-O6	-6.90	124.46	128.60
27	B8	1355	G	O4'-C1'-N9	6.90	113.72	108.20
27	B8	2697	G	O4'-C1'-N9	6.90	113.72	108.20
1	AA	287	U	O4'-C1'-N1	6.90	113.72	108.20
1	AA	988	G	C5-C6-O6	-6.90	124.46	128.60
1	AA	1185	G	C5-C6-O6	-6.90	124.46	128.60
27	B8	214	G	O4'-C1'-N9	6.90	113.72	108.20
27	B8	1168	G	C5-C6-O6	-6.90	124.46	128.60
1	AA	568	G	C5-C6-O6	-6.90	124.46	128.60
27	B8	1400	U	O4'-C1'-N1	6.90	113.72	108.20
27	B8	515	A	O4'-C1'-N9	6.89	113.72	108.20
27	B8	545	U	O4'-C1'-N1	6.89	113.72	108.20
27	B8	1776	G	C5-C6-O6	-6.89	124.46	128.60
1	AA	714	G	C5-C6-O6	-6.89	124.47	128.60
26	B7	96	G	O4'-C1'-N9	6.89	113.71	108.20
27	B8	15	G	C5-C6-O6	-6.89	124.46	128.60
27	B8	1831	G	O4'-C1'-N9	6.89	113.72	108.20
27	B8	2374	C	O4'-C1'-N1	6.89	113.71	108.20
27	B8	389	G	C5-C6-O6	-6.89	124.47	128.60
27	B8	2031	A	O4'-C1'-N9	6.89	113.71	108.20
1	AA	683	G	O4'-C1'-N9	6.89	113.71	108.20
27	B8	158	U	O4'-C1'-N1	6.89	113.71	108.20
27	B8	718	A	C5-C6-N6	-6.89	118.19	123.70
27	B8	2162	G	C5-C6-O6	-6.89	124.47	128.60
27	B8	2302	U	O4'-C1'-N1	6.89	113.71	108.20
27	B8	1830	C	N3-C4-N4	6.89	122.82	118.00
27	B8	651	G	C5-C6-O6	-6.89	124.47	128.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	1958	C	O4'-C1'-N1	6.89	113.71	108.20
1	AA	151	A	C4-C5-C6	6.88	120.44	117.00
27	B8	1721	G	C5-C6-O6	-6.88	124.47	128.60
1	AA	1322	C	C2-N1-C1'	6.88	126.37	118.80
27	B8	1143	A	O4'-C1'-N9	6.88	113.71	108.20
27	B8	2751	G	C5-C6-O6	-6.88	124.47	128.60
27	B8	2763	G	C5-C6-O6	-6.88	124.47	128.60
1	AA	618	C	O4'-C1'-N1	6.88	113.71	108.20
1	AA	1310	G	O4'-C1'-N9	6.88	113.70	108.20
27	B8	268	C	N3-C4-N4	6.88	122.82	118.00
27	B8	2016	U	O4'-C1'-N1	6.88	113.71	108.20
27	B8	2340	A	O4'-C1'-N9	6.88	113.71	108.20
27	B8	2900	A	O4'-C1'-N9	6.88	113.71	108.20
1	AA	1512	U	O4'-C1'-N1	6.88	113.70	108.20
27	B8	727	A	O4'-C1'-N9	6.88	113.70	108.20
27	B8	1789	A	C4-C5-C6	6.88	120.44	117.00
1	AA	1505	G	C5-C6-O6	-6.88	124.47	128.60
1	AA	1529	G	C5'-C4'-O4'	6.88	117.35	109.10
1	AA	430	A	N1-C6-N6	6.88	122.73	118.60
1	AA	1137	C	O4'-C1'-N1	6.88	113.70	108.20
1	AA	1368	A	O4'-C1'-N9	6.88	113.70	108.20
27	B8	169	G	O4'-C1'-N9	6.88	113.70	108.20
27	B8	1888	G	C5-C6-O6	-6.88	124.47	128.60
27	B8	2116	G	C5-C6-O6	-6.88	124.47	128.60
1	AA	903	G	O4'-C1'-N9	6.88	113.70	108.20
27	B8	353	C	O4'-C1'-N1	6.88	113.70	108.20
27	B8	2163	A	C4-C5-C6	6.88	120.44	117.00
1	AA	340	U	O4'-C1'-N1	6.87	113.70	108.20
1	AA	673	A	C4-C5-C6	6.87	120.44	117.00
1	AA	1108	G	C5-C6-O6	-6.87	124.47	128.60
27	B8	251	A	C4-C5-C6	6.87	120.44	117.00
27	B8	1777	U	O4'-C1'-N1	6.87	113.70	108.20
27	B8	2159	G	C5-C6-O6	-6.87	124.48	128.60
27	B8	2181	U	O4'-C1'-N1	6.87	113.70	108.20
27	B8	67	U	O4'-C1'-N1	6.87	113.70	108.20
27	B8	411	G	C5-C6-O6	-6.87	124.48	128.60
27	B8	604	G	C5-C6-O6	-6.87	124.48	128.60
27	B8	1730	C	O4'-C1'-N1	6.87	113.70	108.20
27	B8	2721	A	O4'-C1'-N9	6.87	113.70	108.20
27	B8	1600	C	O4'-C1'-N1	6.87	113.70	108.20
27	B8	1757	A	O4'-C1'-N9	6.87	113.70	108.20
1	AA	558	G	C5-C6-O6	-6.87	124.48	128.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1000	A	O4'-C1'-N9	6.87	113.69	108.20
27	B8	2811	G	C5-C6-O6	-6.87	124.48	128.60
1	AA	71	A	O4'-C1'-N9	6.87	113.69	108.20
1	AA	346	G	C5-C6-O6	-6.87	124.48	128.60
1	AA	464	U	O4'-C1'-N1	6.87	113.69	108.20
1	AA	803	G	C5-C6-O6	-6.87	124.48	128.60
1	AA	824	G	O4'-C1'-N9	6.87	113.69	108.20
27	B8	544	C	O4'-C1'-N1	6.87	113.69	108.20
27	B8	2615	U	O4'-C1'-N1	6.87	113.69	108.20
27	B8	2734	A	C5-C6-N6	-6.87	118.21	123.70
1	AA	220	G	C5-C6-O6	-6.86	124.48	128.60
1	AA	1294	G	C5-C6-O6	-6.86	124.48	128.60
27	B8	2587	A	C4-C5-C6	6.86	120.43	117.00
27	B8	2871	U	O4'-C1'-N1	6.86	113.69	108.20
1	AA	1044	A	C5-C6-N6	-6.86	118.21	123.70
3	AV	36	G	C5-C6-O6	-6.86	124.48	128.60
27	B8	75	G	C5-C6-O6	-6.86	124.48	128.60
27	B8	330	A	C5-C6-N6	-6.86	118.21	123.70
27	B8	625	G	C5-C6-O6	-6.86	124.48	128.60
1	AA	593	U	O4'-C1'-N1	6.86	113.69	108.20
27	B8	917	A	C4-C5-C6	6.86	120.43	117.00
27	B8	1198	U	O4'-C1'-N1	6.86	113.69	108.20
27	B8	2097	A	O4'-C1'-N9	6.86	113.69	108.20
1	AA	95	C	O4'-C1'-N1	6.86	113.69	108.20
27	B8	824	U	O4'-C1'-N1	6.86	113.69	108.20
27	B8	1551	A	O4'-C1'-N9	6.86	113.69	108.20
27	B8	2139	U	O4'-C1'-N1	6.86	113.69	108.20
27	B8	2728	U	O4'-C1'-N1	6.86	113.69	108.20
1	AA	174	A	C5-C6-N6	-6.86	118.22	123.70
27	B8	1782	U	O4'-C1'-N1	6.86	113.68	108.20
27	B8	2601	C	N3-C4-N4	6.86	122.80	118.00
1	AA	116	A	C4-C5-C6	6.85	120.43	117.00
1	AA	610	U	C2-N1-C1'	6.85	125.92	117.70
1	AA	935	A	C4-C5-C6	6.85	120.43	117.00
27	B8	912	C	O4'-C1'-N1	6.85	113.68	108.20
27	B8	2217	G	O4'-C1'-N9	6.85	113.68	108.20
27	B8	2532	G	C5-C6-O6	-6.85	124.49	128.60
27	B8	2575	C	O4'-C1'-N1	6.85	113.68	108.20
27	B8	2825	G	C5-C6-O6	-6.85	124.49	128.60
27	B8	48	G	C5-C6-O6	-6.85	124.49	128.60
27	B8	1598	A	C5-C6-N6	-6.85	118.22	123.70
1	AA	1115	U	O4'-C1'-N1	6.85	113.68	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	242	G	O4'-C1'-N9	6.85	113.68	108.20
27	B8	744	U	O4'-C1'-N1	6.85	113.68	108.20
27	B8	1556	C	O4'-C1'-N1	6.85	113.68	108.20
27	B8	1603	A	C5-C6-N6	-6.85	118.22	123.70
27	B8	2129	C	O4'-C1'-N1	6.85	113.68	108.20
1	AA	924	C	N3-C4-N4	6.85	122.79	118.00
1	AA	1294	G	O4'-C1'-N9	6.85	113.68	108.20
27	B8	340	A	C4-C5-C6	6.85	120.42	117.00
27	B8	1369	G	O4'-C1'-N9	6.85	113.68	108.20
27	B8	2438	U	O4'-C1'-N1	6.85	113.68	108.20
1	AA	591	U	O4'-C1'-N1	6.85	113.68	108.20
27	B8	1984	G	O4'-C1'-N9	6.85	113.68	108.20
1	AA	1453	G	C5-C6-O6	-6.84	124.49	128.60
27	B8	489	G	C5-C6-O6	-6.84	124.49	128.60
27	B8	971	G	C5-C6-O6	-6.84	124.49	128.60
27	B8	1539	U	O4'-C1'-N1	6.84	113.67	108.20
27	B8	277	G	C5-C6-O6	-6.84	124.49	128.60
27	B8	704	G	C5-C6-O6	-6.84	124.49	128.60
1	AA	437	U	O4'-C1'-N1	6.84	113.67	108.20
26	B7	24	G	C5-C6-O6	-6.84	124.50	128.60
26	B7	33	G	O4'-C1'-N9	6.84	113.67	108.20
27	B8	2025	C	O4'-C1'-N1	6.84	113.67	108.20
27	B8	2067	G	C5-C6-O6	-6.84	124.50	128.60
1	AA	107	G	C5-C6-O6	-6.84	124.50	128.60
1	AA	710	G	C5-C6-O6	-6.84	124.50	128.60
1	AA	1489	G	C5-C6-O6	-6.84	124.50	128.60
1	AA	1003	G	C5-C6-O6	-6.84	124.50	128.60
1	AA	1177	G	C5-C6-O6	-6.84	124.50	128.60
27	B8	356	G	C5-C6-O6	-6.84	124.50	128.60
27	B8	1120	G	O4'-C1'-N9	6.84	113.67	108.20
27	B8	2253	G	C5-C6-O6	-6.84	124.50	128.60
1	AA	1131	G	O4'-C1'-N9	6.84	113.67	108.20
27	B8	2280	G	C5-C6-O6	-6.84	124.50	128.60
27	B8	2604	U	O4'-C1'-N1	6.84	113.67	108.20
1	AA	606	G	C5-C6-O6	-6.83	124.50	128.60
27	B8	221	A	C4-C5-C6	6.83	120.42	117.00
27	B8	367	G	C5-C6-O6	-6.83	124.50	128.60
1	AA	528	C	O4'-C1'-N1	6.83	113.67	108.20
1	AA	1046	A	O4'-C1'-N9	6.83	113.67	108.20
27	B8	178	G	O4'-C1'-N9	6.83	113.67	108.20
27	B8	190	A	C4-C5-C6	6.83	120.42	117.00
27	B8	279	A	C4-C5-C6	6.83	120.42	117.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	939	G	O4'-C1'-N9	6.83	113.67	108.20
1	AA	2	A	O4'-C1'-N9	6.83	113.67	108.20
27	B8	1915	U	O4'-C1'-N1	6.83	113.67	108.20
27	B8	2479	U	O4'-C1'-N1	6.83	113.67	108.20
1	AA	20	U	O4'-C1'-N1	6.83	113.66	108.20
27	B8	303	G	O4'-C1'-N9	6.83	113.66	108.20
27	B8	787	C	N3-C4-N4	6.83	122.78	118.00
27	B8	1277	G	C5-C6-O6	-6.83	124.50	128.60
1	AA	67	C	O4'-C1'-N1	6.83	113.66	108.20
1	AA	690	G	C5-C6-O6	-6.83	124.50	128.60
27	B8	971	G	O4'-C1'-N9	6.83	113.66	108.20
1	AA	420	U	O4'-C1'-N1	6.83	113.66	108.20
1	AA	730	G	O4'-C1'-N9	6.83	113.66	108.20
27	B8	1027	A	C4-C5-C6	6.83	120.41	117.00
27	B8	2110	G	O4'-C1'-N9	6.83	113.66	108.20
1	AA	976	G	C5-C6-O6	-6.82	124.50	128.60
27	B8	12	U	O4'-C1'-N1	6.82	113.66	108.20
27	B8	669	G	C5-C6-O6	-6.82	124.51	128.60
27	B8	1464	G	C5-C6-O6	-6.82	124.51	128.60
27	B8	1853	A	O4'-C1'-N9	6.82	113.66	108.20
27	B8	2018	G	C5-C6-O6	-6.82	124.51	128.60
27	B8	2242	G	O4'-C1'-N9	6.82	113.66	108.20
27	B8	2271	G	C5-C6-O6	-6.82	124.51	128.60
27	B8	2813	A	O4'-C1'-N9	6.82	113.66	108.20
1	AA	589	U	O4'-C1'-N1	6.82	113.66	108.20
27	B8	2867	G	C5-C6-O6	-6.82	124.51	128.60
27	B8	1104	C	N3-C4-N4	6.82	122.78	118.00
27	B8	2249	U	O4'-C1'-N1	6.82	113.66	108.20
27	B8	2789	C	N3-C4-N4	6.82	122.77	118.00
1	AA	350	G	C5-C6-O6	-6.82	124.51	128.60
27	B8	1807	G	C5-C6-O6	-6.82	124.51	128.60
27	B8	1968	G	C5-C6-O6	-6.82	124.51	128.60
3	AV	53	G	C5-C6-O6	-6.82	124.51	128.60
27	B8	1110	G	C5-C6-O6	-6.82	124.51	128.60
27	B8	1989	G	C5-C6-O6	-6.82	124.51	128.60
27	B8	2255	G	C5-C6-O6	-6.82	124.51	128.60
27	B8	2163	A	C5-C6-N6	-6.81	118.25	123.70
27	B8	2769	U	O4'-C1'-N1	6.81	113.65	108.20
1	AA	761	G	C5-C6-O6	-6.81	124.51	128.60
3	AV	38	G	N1-C6-O6	6.81	123.99	119.90
26	B7	55	U	O4'-C1'-N1	6.81	113.65	108.20
27	B8	39	G	C5-C6-O6	-6.81	124.51	128.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	596	U	O4'-C1'-N1	6.81	113.65	108.20
27	B8	1149	G	O4'-C1'-N9	6.81	113.65	108.20
27	B8	1407	G	C5-C6-O6	-6.81	124.51	128.60
27	B8	2847	U	O4'-C1'-N1	6.81	113.65	108.20
1	AA	1111	A	C5-C6-N6	-6.81	118.25	123.70
27	B8	2169	A	O4'-C1'-N9	6.81	113.65	108.20
1	AA	257	G	C5-C6-O6	-6.81	124.51	128.60
1	AA	1016	A	C5-C6-N1	-6.81	114.30	117.70
27	B8	376	G	C5-C6-O6	-6.81	124.52	128.60
27	B8	555	G	C5-C6-O6	-6.81	124.51	128.60
27	B8	1364	G	C5-C6-O6	-6.81	124.51	128.60
1	AA	814	A	C5-C6-N6	-6.81	118.25	123.70
1	AA	1379	G	C5-C6-O6	-6.81	124.52	128.60
27	B8	98	G	C5-C6-O6	-6.81	124.52	128.60
27	B8	859	G	C5-C6-O6	-6.81	124.52	128.60
27	B8	1112	G	C5-C6-O6	-6.81	124.52	128.60
27	B8	1217	U	O4'-C1'-N1	6.81	113.65	108.20
27	B8	1333	G	C5-C6-O6	-6.81	124.52	128.60
27	B8	1452	G	C5-C6-O6	-6.81	124.52	128.60
27	B8	2168	G	C5-C6-O6	-6.81	124.52	128.60
27	B8	2661	G	O4'-C1'-N9	6.81	113.65	108.20
27	B8	2898	U	O4'-C1'-N1	6.81	113.64	108.20
1	AA	479	U	O4'-C1'-N1	6.81	113.64	108.20
27	B8	1354	A	C4-C5-C6	6.81	120.40	117.00
27	B8	2120	G	C5-C6-O6	-6.81	124.52	128.60
1	AA	229	U	O4'-C1'-N1	6.80	113.64	108.20
1	AA	296	U	O4'-C1'-N1	6.80	113.64	108.20
3	AV	73	G	C5-C6-O6	-6.80	124.52	128.60
27	B8	595	C	O4'-C1'-N1	6.80	113.64	108.20
27	B8	1481	U	O4'-C1'-N1	6.80	113.64	108.20
27	B8	1552	A	C4-C5-C6	6.80	120.40	117.00
27	B8	1883	U	O4'-C1'-N1	6.80	113.64	108.20
27	B8	2607	G	C5-C6-O6	-6.80	124.52	128.60
27	B8	2784	U	O4'-C1'-N1	6.80	113.64	108.20
1	AA	250	A	O4'-C1'-N9	6.80	113.64	108.20
3	AV	43	G	C5-C6-O6	-6.80	124.52	128.60
27	B8	2348	U	O4'-C1'-N1	6.80	113.64	108.20
1	AA	41	G	O4'-C1'-N9	6.80	113.64	108.20
1	AA	844	G	C5-C6-O6	-6.80	124.52	128.60
1	AA	1403	C	N3-C4-N4	6.80	122.76	118.00
27	B8	1212	G	C5-C6-O6	-6.80	124.52	128.60
27	B8	1710	G	C5-C6-O6	-6.80	124.52	128.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	1794	A	O4'-C1'-N9	6.80	113.64	108.20
27	B8	1884	G	C5-C6-O6	-6.80	124.52	128.60
27	B8	772	C	O4'-C1'-N1	6.80	113.64	108.20
27	B8	1684	G	O4'-C1'-N9	6.80	113.64	108.20
27	B8	2644	G	C5-C6-O6	-6.80	124.52	128.60
27	B8	2848	G	C5-C6-O6	-6.80	124.52	128.60
1	AA	319	G	O4'-C1'-N9	6.80	113.64	108.20
1	AA	1036	A	C4-C5-C6	6.80	120.40	117.00
27	B8	512	G	C5-C6-O6	-6.80	124.52	128.60
27	B8	1025	G	C5-C6-O6	-6.80	124.52	128.60
27	B8	1598	A	C4-C5-C6	6.80	120.40	117.00
27	B8	1784	A	P-O3'-C3'	6.80	127.86	119.70
27	B8	2868	A	C4-C5-C6	6.80	120.40	117.00
27	B8	911	A	C5-C6-N6	-6.79	118.26	123.70
1	AA	362	G	C5-C6-O6	-6.79	124.52	128.60
1	AA	1231	G	O4'-C1'-N9	6.79	113.64	108.20
27	B8	462	C	O4'-C1'-N1	6.79	113.64	108.20
27	B8	775	G	C5-C6-O6	-6.79	124.52	128.60
27	B8	1461	C	O4'-C1'-N1	6.79	113.63	108.20
1	AA	1260	G	C5-C6-O6	-6.79	124.53	128.60
27	B8	1138	G	C5-C6-O6	-6.79	124.53	128.60
27	B8	1420	A	O4'-C1'-N9	6.79	113.63	108.20
1	AA	850	U	O4'-C1'-N1	6.79	113.63	108.20
1	AA	1330	U	O4'-C1'-N1	6.79	113.63	108.20
27	B8	1743	G	N3-C2-N2	6.79	124.65	119.90
27	B8	2214	C	N3-C4-N4	6.79	122.75	118.00
1	AA	1401	G	O4'-C1'-N9	6.79	113.63	108.20
27	B8	2144	G	C5-C6-O6	-6.79	124.53	128.60
1	AA	380	G	C5-C6-O6	-6.79	124.53	128.60
1	AA	1436	U	O4'-C1'-N1	6.79	113.63	108.20
1	AA	1273	C	N3-C4-N4	6.79	122.75	118.00
27	B8	199	A	C5-C6-N6	-6.79	118.27	123.70
27	B8	313	G	C5-C6-O6	-6.79	124.53	128.60
27	B8	1681	G	C5-C6-O6	-6.79	124.53	128.60
27	B8	1745	A	C5-C6-N6	-6.79	118.27	123.70
1	AA	652	U	O4'-C1'-N1	6.78	113.63	108.20
1	AA	1024	G	C5-C6-O6	-6.78	124.53	128.60
1	AA	1297	G	C5-C6-O6	-6.78	124.53	128.60
27	B8	2459	A	C4-C5-C6	6.78	120.39	117.00
27	B8	2897	U	O4'-C1'-N1	6.78	113.63	108.20
1	AA	901	A	C4-C5-C6	6.78	120.39	117.00
27	B8	955	U	O4'-C1'-N1	6.78	113.62	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	338	G	C5-C6-O6	-6.78	124.53	128.60
27	B8	947	A	C5-C6-N6	-6.78	118.28	123.70
27	B8	1869	G	C5-C6-O6	-6.78	124.53	128.60
27	B8	1904	G	O4'-C1'-N9	6.78	113.62	108.20
27	B8	2102	G	O4'-C1'-N9	6.78	113.62	108.20
27	B8	2553	G	C5-C6-O6	-6.78	124.53	128.60
27	B8	1533	C	N3-C4-N4	6.78	122.75	118.00
27	B8	2204	G	O4'-C1'-N9	6.78	113.62	108.20
1	AA	134	G	C5-C6-O6	-6.78	124.53	128.60
1	AA	390	U	O4'-C1'-N1	6.78	113.62	108.20
1	AA	496	A	C5-C6-N6	-6.78	118.28	123.70
26	B7	20	G	C5-C6-O6	-6.78	124.53	128.60
27	B8	219	A	C5-C6-N6	-6.78	118.28	123.70
27	B8	1115	G	C5-C6-O6	-6.78	124.53	128.60
27	B8	1467	U	O4'-C1'-N1	6.78	113.62	108.20
27	B8	1584	U	O4'-C1'-N1	6.78	113.62	108.20
1	AA	875	U	O4'-C1'-N1	6.78	113.62	108.20
1	AA	1278	G	C5-C6-O6	-6.78	124.53	128.60
27	B8	443	A	O4'-C1'-N9	6.78	113.62	108.20
27	B8	1051	G	C5-C6-O6	-6.78	124.53	128.60
27	B8	1775	U	O4'-C1'-N1	6.78	113.62	108.20
1	AA	1017	U	O4'-C1'-N1	6.77	113.62	108.20
27	B8	569	U	O4'-C1'-N1	6.77	113.62	108.20
1	AA	303	A	O4'-C1'-N9	6.77	113.62	108.20
1	AA	354	G	C5-C6-O6	-6.77	124.54	128.60
1	AA	817	C	O4'-C1'-N1	6.77	113.62	108.20
27	B8	175	G	C5-C6-O6	-6.77	124.54	128.60
27	B8	232	G	C5-C6-O6	-6.77	124.54	128.60
27	B8	1159	U	O4'-C1'-N1	6.77	113.62	108.20
27	B8	1423	G	C5-C6-O6	-6.77	124.54	128.60
27	B8	1842	G	O4'-C1'-N9	6.77	113.62	108.20
2	AX	14	G	C5-C6-O6	-6.77	124.54	128.60
27	B8	1202	G	O4'-C1'-N9	6.77	113.62	108.20
27	B8	1644	C	O4'-C1'-N1	6.77	113.62	108.20
27	B8	899	A	O4'-C1'-N9	6.77	113.61	108.20
27	B8	997	G	O4'-C1'-N9	6.77	113.62	108.20
27	B8	2171	A	C5-C6-N6	-6.77	118.28	123.70
1	AA	500	G	O4'-C1'-N9	6.77	113.61	108.20
27	B8	1622	G	C5-C6-O6	-6.77	124.54	128.60
27	B8	1687	G	O4'-C1'-N9	6.77	113.61	108.20
27	B8	1872	A	O4'-C1'-N9	6.77	113.61	108.20
27	B8	372	G	C5-C6-O6	-6.77	124.54	128.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1355	G	O4'-C1'-N9	6.76	113.61	108.20
2	AX	20	G	C5-C6-O6	-6.76	124.54	128.60
27	B8	1245	G	O4'-C1'-N9	6.76	113.61	108.20
27	B8	1734	G	O4'-C1'-N9	6.76	113.61	108.20
27	B8	2049	G	O4'-C1'-N9	6.76	113.61	108.20
27	B8	2748	A	C4-C5-C6	6.76	120.38	117.00
27	B8	561	G	C5-C6-O6	-6.76	124.54	128.60
27	B8	2825	G	O4'-C1'-N9	6.76	113.61	108.20
1	AA	847	G	C5-C6-O6	-6.76	124.54	128.60
1	AA	827	U	O4'-C1'-N1	6.76	113.61	108.20
1	AA	1197	A	C5-C6-N6	-6.76	118.29	123.70
1	AA	1454	G	O4'-C1'-N9	6.76	113.61	108.20
27	B8	470	A	C4-C5-C6	6.76	120.38	117.00
27	B8	2357	G	C5-C6-O6	-6.76	124.55	128.60
1	AA	1381	U	O4'-C1'-N1	6.76	113.61	108.20
27	B8	1857	G	C5-C6-O6	-6.76	124.55	128.60
27	B8	2395	C	N3-C4-N4	6.76	122.73	118.00
1	AA	1375	A	C4-C5-C6	6.76	120.38	117.00
27	B8	1703	G	C5-C6-O6	-6.76	124.55	128.60
27	B8	1873	G	O4'-C1'-N9	6.76	113.61	108.20
27	B8	56	A	C5-C6-N6	-6.75	118.30	123.70
27	B8	458	G	C5-C6-O6	-6.75	124.55	128.60
27	B8	2435	A	C4-C5-C6	6.75	120.38	117.00
3	AV	14	A	C4-C5-C6	6.75	120.38	117.00
27	B8	2360	G	C5-C6-O6	-6.75	124.55	128.60
27	B8	2656	U	O4'-C1'-N1	6.75	113.60	108.20
27	B8	2844	G	C5-C6-O6	-6.75	124.55	128.60
27	B8	2857	G	C5-C6-O6	-6.75	124.55	128.60
1	AA	205	A	C5-C6-N6	-6.75	118.30	123.70
1	AA	561	U	O4'-C1'-N1	6.75	113.60	108.20
1	AA	642	A	C4-C5-C6	6.75	120.38	117.00
27	B8	221	A	C5-C6-N6	-6.75	118.30	123.70
27	B8	371	A	C4-C5-C6	6.75	120.38	117.00
27	B8	2073	C	O4'-C1'-N1	6.75	113.60	108.20
1	AA	881	G	O4'-C1'-N9	6.75	113.60	108.20
1	AA	1529	G	C5-C6-O6	-6.75	124.55	128.60
27	B8	2083	G	C5-C6-O6	-6.75	124.55	128.60
1	AA	148	G	O4'-C1'-N9	6.75	113.60	108.20
1	AA	714	G	O4'-C1'-N9	6.75	113.60	108.20
1	AA	752	G	C5-C6-O6	-6.75	124.55	128.60
1	AA	781	A	C4-C5-C6	6.75	120.38	117.00
27	B8	473	G	C5-C6-O6	-6.75	124.55	128.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	2893	A	C4-C5-C6	6.75	120.37	117.00
1	AA	230	G	O4'-C1'-N9	6.75	113.60	108.20
1	AA	919	A	C4-C5-C6	6.75	120.37	117.00
27	B8	49	A	O4'-C1'-N9	6.75	113.60	108.20
27	B8	456	C	O4'-C1'-N1	6.75	113.60	108.20
27	B8	513	A	C4-C5-C6	6.75	120.37	117.00
27	B8	1697	G	C5-C6-O6	-6.75	124.55	128.60
1	AA	1398	A	C5-C6-N6	-6.75	118.30	123.70
3	AV	45	G	C5-C6-O6	-6.74	124.55	128.60
27	B8	633	A	C5-C6-N1	-6.74	114.33	117.70
27	B8	1498	C	O4'-C1'-N1	6.74	113.59	108.20
27	B8	2100	G	C5-C6-O6	-6.74	124.55	128.60
1	AA	332	G	C5-C6-O6	-6.74	124.56	128.60
1	AA	555	U	O4'-C1'-N1	6.74	113.59	108.20
27	B8	256	A	C4-C5-C6	6.74	120.37	117.00
27	B8	1468	U	O4'-C1'-N1	6.74	113.59	108.20
27	B8	1977	A	C4-C5-C6	6.74	120.37	117.00
1	AA	735	C	O4'-C1'-N1	6.74	113.59	108.20
1	AA	950	U	O4'-C1'-N1	6.74	113.59	108.20
1	AA	1060	U	O4'-C1'-N1	6.74	113.59	108.20
1	AA	1516	G	C5-C6-O6	-6.74	124.56	128.60
27	B8	1071	G	C5-C6-O6	-6.74	124.56	128.60
27	B8	2349	G	N1-C6-O6	6.74	123.94	119.90
1	AA	108	G	C5-C6-O6	-6.74	124.56	128.60
1	AA	412	A	O4'-C1'-N9	6.74	113.59	108.20
1	AA	1094	G	C5-C6-O6	-6.74	124.56	128.60
1	AA	1316	G	C5-C6-O6	-6.74	124.56	128.60
27	B8	491	G	C5-C6-O6	-6.74	124.56	128.60
27	B8	835	C	N3-C4-N4	6.74	122.72	118.00
1	AA	282	A	N1-C6-N6	6.74	122.64	118.60
1	AA	700	G	C5-C6-O6	-6.74	124.56	128.60
1	AA	1068	G	C5-C6-O6	-6.74	124.56	128.60
1	AA	1458	G	C5-C6-O6	-6.74	124.56	128.60
27	B8	1339	G	C5-C6-O6	-6.74	124.56	128.60
27	B8	2754	U	O4'-C1'-N1	6.74	113.59	108.20
27	B8	2810	A	O4'-C1'-N9	6.74	113.59	108.20
1	AA	907	A	C4-C5-C6	6.74	120.37	117.00
27	B8	1091	G	N1-C6-O6	6.74	123.94	119.90
27	B8	2476	A	C4-C5-C6	6.74	120.37	117.00
1	AA	769	G	C5-C6-O6	-6.73	124.56	128.60
27	B8	446	G	C5-C6-O6	-6.73	124.56	128.60
27	B8	819	A	C4-C5-C6	6.73	120.37	117.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	281	G	C5-C6-O6	-6.73	124.56	128.60
3	AV	20	G	C5-C6-O6	-6.73	124.56	128.60
27	B8	363	G	O4'-C1'-N9	6.73	113.59	108.20
27	B8	2341	G	O4'-C1'-N9	6.73	113.58	108.20
27	B8	2701	U	O4'-C1'-N1	6.73	113.58	108.20
27	B8	1593	A	O4'-C1'-N9	6.73	113.58	108.20
27	B8	1865	U	O4'-C1'-N1	6.73	113.58	108.20
27	B8	2319	G	C5-C6-O6	-6.73	124.56	128.60
27	B8	2436	G	C5-C6-O6	-6.73	124.56	128.60
27	B8	2831	G	C5-C6-O6	-6.73	124.56	128.60
27	B8	652	U	O4'-C1'-N1	6.73	113.58	108.20
27	B8	1311	G	C5-C6-O6	-6.73	124.56	128.60
1	AA	1103	C	O4'-C1'-N1	6.73	113.58	108.20
27	B8	359	G	C5-C6-O6	-6.73	124.56	128.60
27	B8	608	A	C4-C5-C6	6.73	120.36	117.00
27	B8	1067	A	O4'-C1'-N9	6.73	113.58	108.20
27	B8	1227	G	O4'-C1'-N9	6.73	113.58	108.20
27	B8	1313	U	C2-N1-C1'	6.73	125.77	117.70
27	B8	1955	U	O4'-C1'-N1	6.73	113.58	108.20
27	B8	1715	G	C5-C6-O6	-6.73	124.56	128.60
27	B8	2090	A	C5-C6-N6	-6.73	118.32	123.70
1	AA	352	C	O4'-C1'-N1	6.72	113.58	108.20
26	B7	107	G	C5-C6-O6	-6.72	124.56	128.60
27	B8	426	C	N3-C4-N4	6.72	122.71	118.00
27	B8	747	U	O4'-C1'-N1	6.72	113.58	108.20
27	B8	1434	A	O4'-C1'-N9	6.72	113.58	108.20
27	B8	1807	G	O4'-C1'-N9	6.72	113.58	108.20
27	B8	2742	G	C5-C6-O6	-6.72	124.56	128.60
27	B8	704	G	O4'-C1'-N9	6.72	113.58	108.20
1	AA	1076	U	O4'-C1'-N1	6.72	113.58	108.20
1	AA	405	U	O4'-C1'-N1	6.72	113.58	108.20
1	AA	1066	C	O4'-C1'-N1	6.72	113.58	108.20
1	AA	1397	C	C2-N1-C1'	6.72	126.19	118.80
27	B8	332	A	C4-C5-C6	6.72	120.36	117.00
27	B8	381	G	C5-C6-O6	-6.72	124.57	128.60
27	B8	642	U	O4'-C1'-N1	6.72	113.58	108.20
27	B8	1382	G	C5-C6-O6	-6.72	124.57	128.60
27	B8	2408	U	O4'-C1'-N1	6.72	113.58	108.20
1	AA	211	G	O4'-C1'-N9	6.72	113.57	108.20
1	AA	262	A	C4-C5-C6	6.72	120.36	117.00
27	B8	720	U	O4'-C1'-N1	6.72	113.57	108.20
27	B8	1746	A	O4'-C1'-N9	6.72	113.58	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	2670	A	O4'-C1'-N9	6.72	113.57	108.20
1	AA	102	G	C5-C6-O6	-6.72	124.57	128.60
1	AA	1165	U	O4'-C1'-N1	6.72	113.57	108.20
27	B8	280	U	O4'-C1'-N1	6.72	113.57	108.20
27	B8	480	A	C4-C5-C6	6.72	120.36	117.00
27	B8	594	U	O4'-C1'-N1	6.72	113.57	108.20
27	B8	842	U	O4'-C1'-N1	6.72	113.57	108.20
1	AA	297	G	C5-C6-O6	-6.71	124.57	128.60
1	AA	453	G	C5-C6-O6	-6.71	124.57	128.60
1	AA	834	U	O4'-C1'-N1	6.71	113.57	108.20
1	AA	1261	A	C4-C5-C6	6.71	120.36	117.00
27	B8	721	A	C5-C6-N1	-6.71	114.34	117.70
27	B8	2353	G	C5-C6-O6	-6.71	124.57	128.60
27	B8	2373	G	O4'-C1'-N9	6.71	113.57	108.20
1	AA	10	A	O4'-C1'-N9	6.71	113.57	108.20
27	B8	551	G	O4'-C1'-N9	6.71	113.57	108.20
27	B8	556	A	C4-C5-C6	6.71	120.36	117.00
27	B8	2465	C	N3-C4-N4	6.71	122.70	118.00
1	AA	369	G	C5-C6-O6	-6.71	124.57	128.60
3	AV	25	G	C5-C6-O6	-6.71	124.57	128.60
27	B8	741	U	O4'-C1'-N1	6.71	113.57	108.20
27	B8	1001	A	C4-C5-C6	6.71	120.36	117.00
27	B8	1573	G	O4'-C1'-N9	6.71	113.57	108.20
27	B8	1724	G	C5-C6-O6	-6.71	124.57	128.60
27	B8	2708	G	C5-C6-O6	-6.71	124.57	128.60
27	B8	2199	A	C4-C5-C6	6.71	120.36	117.00
1	AA	662	U	O4'-C1'-N1	6.71	113.57	108.20
1	AA	1013	G	C5-C6-O6	-6.71	124.57	128.60
27	B8	96	C	N3-C4-N4	6.71	122.70	118.00
27	B8	527	C	O4'-C1'-N1	6.71	113.57	108.20
27	B8	1002	G	C5-C6-O6	-6.71	124.58	128.60
27	B8	2517	C	O4'-C1'-N1	6.71	113.57	108.20
1	AA	746	A	C5-C6-N6	-6.71	118.33	123.70
3	AV	68	G	C5-C6-O6	-6.71	124.58	128.60
27	B8	374	A	C4-C5-C6	6.71	120.35	117.00
27	B8	467	G	O4'-C1'-N9	6.71	113.57	108.20
27	B8	1254	A	C4-C5-C6	6.71	120.35	117.00
27	B8	1267	U	O4'-C1'-N1	6.71	113.56	108.20
27	B8	2886	A	C4-C5-C6	6.71	120.35	117.00
1	AA	1028	C	O4'-C1'-N1	6.71	113.56	108.20
27	B8	1130	U	O4'-C1'-N1	6.71	113.56	108.20
27	B8	2356	U	O4'-C1'-N1	6.71	113.56	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	575	G	C5-C6-O6	-6.70	124.58	128.60
27	B8	1839	G	C5-C6-O6	-6.70	124.58	128.60
1	AA	76	G	O4'-C1'-N9	6.70	113.56	108.20
26	B7	25	U	O4'-C1'-N1	6.70	113.56	108.20
27	B8	175	G	O4'-C1'-N9	6.70	113.56	108.20
27	B8	1248	G	C5-C6-O6	-6.70	124.58	128.60
27	B8	1501	G	C5-C6-O6	-6.70	124.58	128.60
27	B8	1664	A	C4-C5-C6	6.70	120.35	117.00
27	B8	1669	A	C4-C5-C6	6.70	120.35	117.00
1	AA	772	U	O4'-C1'-N1	6.70	113.56	108.20
1	AA	909	A	C4-C5-C6	6.70	120.35	117.00
26	B7	52	A	O4'-C1'-N9	6.70	113.56	108.20
27	B8	547	A	O4'-C1'-N9	6.70	113.56	108.20
27	B8	2526	G	C5-C6-O6	-6.70	124.58	128.60
27	B8	2808	G	C5-C6-O6	-6.70	124.58	128.60
1	AA	1500	A	C5-C6-N6	-6.70	118.34	123.70
27	B8	1096	A	C4-C5-C6	6.70	120.35	117.00
27	B8	1674	G	C5-C6-O6	-6.70	124.58	128.60
27	B8	1269	A	C5-C6-N6	-6.69	118.34	123.70
27	B8	2017	U	O4'-C1'-N1	6.69	113.56	108.20
27	B8	2086	U	O4'-C1'-N1	6.69	113.56	108.20
1	AA	1439	G	O4'-C1'-N9	6.69	113.55	108.20
27	B8	2720	U	O4'-C1'-N1	6.69	113.55	108.20
27	B8	2007	U	O4'-C1'-N1	6.69	113.55	108.20
27	B8	2803	G	O4'-C1'-N9	6.69	113.55	108.20
27	B8	2843	G	C5-C6-O6	-6.69	124.58	128.60
1	AA	1252	A	O4'-C1'-N9	6.69	113.55	108.20
27	B8	256	A	O4'-C1'-N9	6.69	113.55	108.20
27	B8	1310	G	O4'-C1'-N9	6.69	113.55	108.20
1	AA	324	G	C5-C6-O6	-6.69	124.59	128.60
26	B7	41	G	C5-C6-O6	-6.69	124.59	128.60
27	B8	820	A	C4-C5-C6	6.69	120.34	117.00
27	B8	1347	A	O4'-C1'-N9	6.69	113.55	108.20
27	B8	1802	A	C4-C5-C6	6.69	120.34	117.00
1	AA	653	U	O4'-C1'-N1	6.69	113.55	108.20
27	B8	308	G	C5-C6-O6	-6.69	124.59	128.60
27	B8	941	A	O4'-C1'-N9	6.69	113.55	108.20
1	AA	1129	C	O4'-C1'-N1	6.68	113.55	108.20
27	B8	1683	U	O4'-C1'-N1	6.68	113.55	108.20
1	AA	927	G	C5-C6-O6	-6.68	124.59	128.60
27	B8	907	G	C5-C6-O6	-6.68	124.59	128.60
27	B8	1355	G	C5-C6-O6	-6.68	124.59	128.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	787	A	O4'-C1'-N9	6.68	113.54	108.20
1	AA	944	G	N3-C2-N2	6.68	124.58	119.90
1	AA	1089	G	C5-C6-O6	-6.68	124.59	128.60
27	B8	622	G	C5-C6-O6	-6.68	124.59	128.60
27	B8	1068	G	C5-C6-O6	-6.68	124.59	128.60
28	BA	79	ALA	N-CA-CB	6.68	119.45	110.10
1	AA	539	A	O4'-C1'-N9	6.68	113.54	108.20
27	B8	1439	A	C4-C5-C6	6.68	120.34	117.00
27	B8	2797	U	O4'-C1'-N1	6.68	113.54	108.20
1	AA	923	A	C4-C5-C6	6.68	120.34	117.00
26	B7	13	G	C5-C6-O6	-6.68	124.59	128.60
27	B8	1036	G	C5-C6-O6	-6.68	124.59	128.60
1	AA	563	A	C5-C6-N6	-6.67	118.36	123.70
27	B8	830	G	C5-C6-O6	-6.67	124.60	128.60
27	B8	1395	A	C4-C5-C6	6.67	120.34	117.00
27	B8	1572	A	C4-C5-C6	6.67	120.34	117.00
27	B8	1920	C	N3-C4-N4	6.67	122.67	118.00
1	AA	1528	U	O4'-C1'-N1	6.67	113.54	108.20
27	B8	2618	G	C5-C6-O6	-6.67	124.60	128.60
1	AA	81	A	C5-C6-N6	-6.67	118.36	123.70
27	B8	2775	G	C5-C6-O6	-6.67	124.60	128.60
27	B8	2885	G	C5-C6-O6	-6.67	124.60	128.60
1	AA	1452	C	O4'-C1'-N1	6.67	113.54	108.20
27	B8	709	U	O4'-C1'-N1	6.67	113.54	108.20
27	B8	2566	A	C4-C5-C6	6.67	120.33	117.00
1	AA	534	U	O4'-C1'-N1	6.67	113.53	108.20
1	AA	963	G	C5-C6-O6	-6.67	124.60	128.60
27	B8	924	G	O4'-C1'-N9	6.67	113.53	108.20
27	B8	2416	C	N3-C4-N4	6.67	122.67	118.00
27	B8	2809	A	O4'-C1'-N9	6.67	113.53	108.20
27	B8	725	G	C5-C6-O6	-6.67	124.60	128.60
27	B8	1242	U	O4'-C1'-N1	6.67	113.53	108.20
27	B8	2133	G	C5-C6-O6	-6.67	124.60	128.60
27	B8	2239	G	C5-C6-O6	-6.67	124.60	128.60
1	AA	1166	G	C5-C6-O6	-6.67	124.60	128.60
1	AA	717	U	O4'-C1'-N1	6.66	113.53	108.20
1	AA	888	G	C5-C6-O6	-6.66	124.60	128.60
1	AA	1065	U	O4'-C1'-N1	6.66	113.53	108.20
1	AA	1374	A	O4'-C1'-N9	6.66	113.53	108.20
1	AA	1453	G	O4'-C1'-N9	6.66	113.53	108.20
27	B8	950	G	C5-C6-O6	-6.66	124.60	128.60
27	B8	1360	G	O4'-C1'-N9	6.66	113.53	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	1459	G	C5-C6-O6	-6.66	124.60	128.60
27	B8	2524	G	C5-C6-O6	-6.66	124.60	128.60
1	AA	1431	A	P-O3'-C3'	6.66	127.69	119.70
1	AA	1534	A	O4'-C1'-N9	6.66	113.53	108.20
27	B8	126	A	O4'-C1'-N9	6.66	113.53	108.20
27	B8	665	U	O4'-C1'-N1	6.66	113.53	108.20
27	B8	2780	G	C5-C6-O6	-6.66	124.60	128.60
1	AA	621	A	O4'-C1'-N9	6.66	113.53	108.20
1	AA	673	A	C5-C6-N6	-6.66	118.37	123.70
26	B7	105	G	O4'-C1'-N9	6.66	113.53	108.20
27	B8	159	G	C5-C6-O6	-6.66	124.61	128.60
27	B8	528	A	O4'-C1'-N9	6.66	113.53	108.20
27	B8	2192	U	O4'-C1'-N1	6.66	113.53	108.20
1	AA	506	G	O4'-C1'-N9	6.66	113.53	108.20
1	AA	646	G	C5-C6-O6	-6.66	124.61	128.60
27	B8	161	A	O4'-C1'-N9	6.66	113.52	108.20
27	B8	969	G	O4'-C1'-N9	6.66	113.53	108.20
27	B8	1824	G	C5-C6-O6	-6.66	124.61	128.60
27	B8	1970	A	C4-C5-C6	6.66	120.33	117.00
1	AA	1009	U	O4'-C1'-N1	6.65	113.52	108.20
1	AA	696	A	C4-C5-C6	6.65	120.33	117.00
1	AA	733	G	C5-C6-O6	-6.65	124.61	128.60
27	B8	1057	A	C4-C5-C6	6.65	120.33	117.00
27	B8	2284	A	C4-C5-C6	6.65	120.33	117.00
1	AA	63	C	N3-C4-N4	6.65	122.66	118.00
1	AA	520	A	C4-C5-C6	6.65	120.33	117.00
27	B8	1631	G	C5-C6-O6	-6.65	124.61	128.60
1	AA	1170	A	C4-C5-C6	6.65	120.32	117.00
27	B8	2227	A	O4'-C1'-N9	6.65	113.52	108.20
1	AA	444	G	O4'-C1'-N9	6.65	113.52	108.20
26	B7	99	A	C4-C5-C6	6.65	120.32	117.00
1	AA	991	U	O4'-C1'-N1	6.65	113.52	108.20
27	B8	548	G	C5-C6-O6	-6.65	124.61	128.60
27	B8	664	G	C5-C6-O6	-6.65	124.61	128.60
1	AA	797	C	N3-C4-N4	6.64	122.65	118.00
26	B7	72	G	C5-C6-O6	-6.64	124.61	128.60
27	B8	2569	G	O4'-C1'-N9	6.64	113.52	108.20
27	B8	99	U	C2-N1-C1'	6.64	125.67	117.70
27	B8	425	G	O4'-C1'-N9	6.64	113.51	108.20
27	B8	821	A	O4'-C1'-N9	6.64	113.51	108.20
27	B8	1015	U	O4'-C1'-N1	6.64	113.51	108.20
27	B8	1026	G	C5-C6-O6	-6.64	124.61	128.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	1559	U	O4'-C1'-N1	6.64	113.52	108.20
27	B8	1634	A	C4-C5-C6	6.64	120.32	117.00
27	B8	1643	G	O4'-C1'-N9	6.64	113.51	108.20
1	AA	1483	A	C4-C5-C6	6.64	120.32	117.00
1	AA	1057	G	O4'-C1'-N9	6.64	113.51	108.20
1	AA	1312	G	O4'-C1'-N9	6.64	113.51	108.20
27	B8	869	G	C5-C6-O6	-6.64	124.62	128.60
1	AA	194	C	N3-C4-N4	6.64	122.64	118.00
1	AA	270	A	O4'-C1'-N9	6.64	113.51	108.20
1	AA	1400	C	C2-N1-C1'	6.64	126.10	118.80
26	B7	110	C	N3-C4-N4	6.64	122.64	118.00
27	B8	1828	G	C5-C6-O6	-6.64	124.62	128.60
27	B8	2285	C	N3-C4-N4	6.64	122.65	118.00
1	AA	254	G	C5-C6-O6	-6.63	124.62	128.60
27	B8	166	U	O4'-C1'-N1	6.63	113.51	108.20
27	B8	1935	G	C5-C6-O6	-6.63	124.62	128.60
27	B8	2477	U	O4'-C1'-N1	6.63	113.51	108.20
27	B8	2638	G	C5-C6-O6	-6.63	124.62	128.60
1	AA	1178	G	C5-C6-O6	-6.63	124.62	128.60
1	AA	1362	A	O4'-C1'-N9	6.63	113.51	108.20
1	AA	1531	A	C4-C5-C6	6.63	120.32	117.00
27	B8	1791	A	C5-C6-N6	-6.63	118.39	123.70
27	B8	900	A	O4'-C1'-N9	6.63	113.50	108.20
27	B8	2032	G	C5-C6-O6	-6.63	124.62	128.60
27	B8	2351	G	C5-C6-O6	-6.63	124.62	128.60
27	B8	2890	G	C5-C6-O6	-6.63	124.62	128.60
1	AA	180	U	O4'-C1'-N1	6.63	113.50	108.20
1	AA	394	G	C5-C6-O6	-6.63	124.62	128.60
27	B8	2551	C	O4'-C1'-N1	6.63	113.50	108.20
27	B8	247	G	C5-C6-O6	-6.63	124.62	128.60
27	B8	1017	G	C5-C6-O6	-6.63	124.62	128.60
27	B8	1528	A	C4-C5-C6	6.63	120.31	117.00
27	B8	2800	A	C5-C6-N6	-6.63	118.40	123.70
1	AA	270	A	C4-C5-C6	6.63	120.31	117.00
1	AA	908	A	C4-C5-C6	6.63	120.31	117.00
27	B8	3	U	O4'-C1'-N1	6.63	113.50	108.20
27	B8	1406	U	O4'-C1'-N1	6.63	113.50	108.20
27	B8	379	G	C5-C6-O6	-6.62	124.62	128.60
27	B8	2044	C	N3-C4-N4	6.62	122.64	118.00
27	B8	1089	A	C4-C5-C6	6.62	120.31	117.00
27	B8	2118	U	O4'-C1'-N1	6.62	113.50	108.20
1	AA	480	U	O4'-C1'-N1	6.62	113.50	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1282	C	N3-C4-N4	6.62	122.64	118.00
27	B8	2648	G	O4'-C1'-N9	6.62	113.50	108.20
27	B8	413	C	N3-C4-N4	6.62	122.63	118.00
27	B8	1326	U	O4'-C1'-N1	6.62	113.50	108.20
1	AA	818	G	O4'-C1'-N9	6.62	113.49	108.20
26	B7	69	G	N1-C6-O6	6.62	123.87	119.90
27	B8	1473	G	O4'-C1'-N9	6.62	113.49	108.20
27	B8	2684	U	O4'-C1'-N1	6.62	113.49	108.20
1	AA	429	U	P-O3'-C3'	6.62	127.64	119.70
27	B8	1271	G	C5-C6-O6	-6.62	124.63	128.60
27	B8	1426	G	C5-C6-O6	-6.62	124.63	128.60
1	AA	596	A	O4'-C1'-N9	6.62	113.49	108.20
1	AA	1517	G	C5-C6-O6	-6.62	124.63	128.60
3	AV	5	A	O4'-C1'-N9	6.62	113.49	108.20
27	B8	493	G	C5-C6-O6	-6.62	124.63	128.60
27	B8	343	C	O4'-C1'-N1	6.61	113.49	108.20
27	B8	1832	C	N3-C4-N4	6.61	122.63	118.00
27	B8	2435	A	C5-C6-N1	-6.61	114.39	117.70
27	B8	2608	G	C5-C6-O6	-6.61	124.63	128.60
1	AA	1035	A	O4'-C1'-N9	6.61	113.49	108.20
27	B8	2315	G	O4'-C1'-N9	6.61	113.49	108.20
1	AA	49	U	O4'-C1'-N1	6.61	113.49	108.20
1	AA	231	U	O4'-C1'-N1	6.61	113.49	108.20
1	AA	587	G	C5-C6-O6	-6.61	124.63	128.60
1	AA	1370	G	O4'-C1'-N9	6.61	113.49	108.20
27	B8	176	A	O4'-C1'-N9	6.61	113.49	108.20
27	B8	745	G	C5-C6-O6	-6.61	124.63	128.60
27	B8	1611	C	O4'-C1'-N1	6.61	113.49	108.20
1	AA	481	G	C5-C6-O6	-6.61	124.64	128.60
1	AA	628	G	O4'-C1'-N9	6.61	113.49	108.20
27	B8	1376	C	O4'-C1'-N1	6.61	113.49	108.20
27	B8	1852	U	O4'-C1'-N1	6.61	113.49	108.20
1	AA	1413	A	O4'-C1'-N9	6.61	113.49	108.20
27	B8	228	C	O4'-C1'-N1	6.61	113.48	108.20
27	B8	849	A	C5-C6-N6	-6.61	118.41	123.70
27	B8	1100	C	N3-C4-N4	6.61	122.63	118.00
27	B8	1387	A	O4'-C1'-N9	6.61	113.49	108.20
27	B8	1470	A	C4-C5-C6	6.61	120.30	117.00
27	B8	1543	G	C5-C6-O6	-6.61	124.64	128.60
27	B8	597	G	C5-C6-O6	-6.61	124.64	128.60
27	B8	1965	C	O4'-C1'-N1	6.61	113.48	108.20
1	AA	1213	A	C4-C5-C6	6.60	120.30	117.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	149	A	C4-C5-C6	6.60	120.30	117.00
27	B8	1501	G	O4'-C1'-N9	6.60	113.48	108.20
27	B8	2842	G	C5-C6-O6	-6.60	124.64	128.60
1	AA	145	G	O4'-C1'-N9	6.60	113.48	108.20
1	AA	1014	A	C5-C6-N6	-6.60	118.42	123.70
1	AA	1259	C	N3-C4-N4	6.60	122.62	118.00
27	B8	159	G	O4'-C1'-N9	6.60	113.48	108.20
27	B8	522	A	C5-C6-N6	-6.60	118.42	123.70
27	B8	728	G	C5-C6-O6	-6.60	124.64	128.60
27	B8	1690	A	C4-C5-C6	6.60	120.30	117.00
27	B8	1798	U	O4'-C1'-N1	6.60	113.48	108.20
27	B8	2220	U	O4'-C1'-N1	6.60	113.48	108.20
27	B8	2533	U	O4'-C1'-N1	6.60	113.48	108.20
1	AA	1171	A	O4'-C1'-N9	6.60	113.48	108.20
27	B8	180	G	C5-C6-O6	-6.60	124.64	128.60
27	B8	1032	A	O4'-C1'-N9	6.60	113.48	108.20
1	AA	118	U	O4'-C1'-N1	6.60	113.48	108.20
27	B8	2289	G	C5-C6-O6	-6.60	124.64	128.60
1	AA	96	U	O4'-C1'-N1	6.60	113.48	108.20
1	AA	478	A	O4'-C1'-N9	6.60	113.48	108.20
1	AA	502	A	C5-C6-N6	-6.60	118.42	123.70
1	AA	843	U	O4'-C1'-N1	6.59	113.47	108.20
1	AA	927	G	O4'-C1'-N9	6.59	113.48	108.20
1	AA	1490	U	O4'-C1'-N1	6.59	113.47	108.20
27	B8	998	C	N3-C4-N4	6.59	122.62	118.00
27	B8	1493	C	C6-N1-C1'	-6.59	112.89	120.80
27	B8	2877	G	O4'-C1'-N9	6.59	113.47	108.20
27	B8	2879	A	C5-C6-N6	-6.59	118.42	123.70
1	AA	1347	G	C5-C6-O6	-6.59	124.64	128.60
27	B8	327	G	O4'-C1'-N9	6.59	113.47	108.20
27	B8	756	A	C5-C6-N6	-6.59	118.43	123.70
27	B8	891	G	C5-C6-O6	-6.59	124.64	128.60
27	B8	1477	A	C4-C5-C6	6.59	120.30	117.00
27	B8	1549	A	O4'-C1'-N9	6.59	113.47	108.20
27	B8	2504	U	O4'-C1'-N1	6.59	113.47	108.20
1	AA	1197	A	C4-C5-C6	6.59	120.30	117.00
27	B8	2048	G	C5-C6-O6	-6.59	124.65	128.60
1	AA	696	A	O4'-C1'-N9	6.59	113.47	108.20
1	AA	860	A	C4-C5-C6	6.59	120.30	117.00
1	AA	1418	A	C4-C5-C6	6.59	120.30	117.00
27	B8	1716	U	O4'-C1'-N1	6.59	113.47	108.20
27	B8	2478	A	C4-C5-C6	6.59	120.30	117.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	2668	G	O4'-C1'-N9	6.59	113.47	108.20
27	B8	530	G	C5-C6-O6	-6.59	124.65	128.60
27	B8	1182	G	O4'-C1'-N9	6.59	113.47	108.20
27	B8	2149	U	O4'-C1'-N1	6.59	113.47	108.20
27	B8	2865	U	O4'-C1'-N1	6.59	113.47	108.20
1	AA	126	G	O4'-C1'-N9	6.59	113.47	108.20
1	AA	158	G	C5-C6-O6	-6.59	124.65	128.60
1	AA	1279	G	C5-C6-O6	-6.59	124.65	128.60
27	B8	408	G	O4'-C1'-N9	6.59	113.47	108.20
27	B8	827	U	O4'-C1'-N1	6.59	113.47	108.20
27	B8	1283	G	C5-C6-O6	-6.59	124.65	128.60
27	B8	1299	G	C5-C6-O6	-6.59	124.65	128.60
27	B8	1383	A	O4'-C1'-N9	6.59	113.47	108.20
27	B8	1485	U	O4'-C1'-N1	6.59	113.47	108.20
27	B8	1514	G	C5-C6-O6	-6.59	124.65	128.60
27	B8	1590	A	O4'-C1'-N9	6.59	113.47	108.20
27	B8	2444	G	O4'-C1'-N9	6.59	113.47	108.20
27	B8	1420	A	C4-C5-C6	6.58	120.29	117.00
27	B8	1774	C	O4'-C1'-N1	6.58	113.47	108.20
1	AA	377	G	O4'-C1'-N9	6.58	113.47	108.20
1	AA	588	G	C5-C6-O6	-6.58	124.65	128.60
27	B8	74	A	C4-C5-C6	6.58	120.29	117.00
27	B8	443	A	C4-C5-C6	6.58	120.29	117.00
27	B8	577	G	C5-C6-O6	-6.58	124.65	128.60
1	AA	595	A	C5-C6-N6	-6.58	118.43	123.70
1	AA	1144	G	C5-C6-O6	-6.58	124.65	128.60
27	B8	2119	A	C4-C5-C6	6.58	120.29	117.00
27	B8	2121	G	C5-C6-O6	-6.58	124.65	128.60
27	B8	2194	U	O4'-C1'-N1	6.58	113.47	108.20
27	B8	2294	G	C5-C6-O6	-6.58	124.65	128.60
1	AA	730	G	C5-C6-O6	-6.58	124.65	128.60
1	AA	971	G	O4'-C1'-N9	6.58	113.46	108.20
1	AA	1225	A	C4-C5-C6	6.58	120.29	117.00
3	AV	13	C	N3-C4-N4	6.58	122.61	118.00
27	B8	307	G	C5-C6-O6	-6.58	124.65	128.60
27	B8	2494	G	C5-C6-O6	-6.58	124.65	128.60
1	AA	267	C	N3-C4-N4	6.58	122.60	118.00
27	B8	198	C	N3-C4-N4	6.58	122.61	118.00
27	B8	402	A	C4-C5-C6	6.58	120.29	117.00
27	B8	493	G	O4'-C1'-N9	6.58	113.46	108.20
27	B8	1223	G	C5-C6-O6	-6.58	124.65	128.60
27	B8	1352	U	O4'-C1'-N1	6.58	113.46	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	1521	G	C5-C6-O6	-6.58	124.65	128.60
27	B8	2370	G	C5-C6-O6	-6.58	124.65	128.60
1	AA	1258	G	O4'-C1'-N9	6.58	113.46	108.20
27	B8	1936	A	C4-C5-C6	6.58	120.29	117.00
1	AA	253	A	O4'-C1'-N9	6.58	113.46	108.20
27	B8	1047	G	C5-C6-O6	-6.58	124.65	128.60
27	B8	1213	A	C5-C6-N1	-6.58	114.41	117.70
27	B8	1766	G	O4'-C1'-N9	6.58	113.46	108.20
27	B8	2092	U	O4'-C1'-N1	6.58	113.46	108.20
27	B8	2802	G	O4'-C1'-N9	6.58	113.46	108.20
1	AA	149	A	C4-C5-C6	6.57	120.29	117.00
1	AA	865	A	C4-C5-C6	6.57	120.29	117.00
1	AA	1416	G	C5-C6-O6	-6.57	124.66	128.60
27	B8	443	A	C5-C6-N6	-6.57	118.44	123.70
27	B8	1031	G	O4'-C1'-N9	6.57	113.46	108.20
27	B8	983	A	C4-C5-C6	6.57	120.29	117.00
27	B8	1045	C	N3-C4-N4	6.57	122.60	118.00
1	AA	315	A	O4'-C1'-N9	6.57	113.46	108.20
1	AA	566	G	N1-C6-O6	6.57	123.84	119.90
1	AA	890	G	C5-C6-O6	-6.57	124.66	128.60
1	AA	1432	G	C5-C6-O6	-6.57	124.66	128.60
27	B8	359	G	O4'-C1'-N9	6.57	113.46	108.20
27	B8	879	G	C5-C6-O6	-6.57	124.66	128.60
27	B8	1604	C	N3-C4-N4	6.57	122.60	118.00
27	B8	2529	G	C5-C6-O6	-6.57	124.66	128.60
27	B8	36	G	C5-C6-O6	-6.57	124.66	128.60
27	B8	117	G	C5-C6-O6	-6.57	124.66	128.60
27	B8	233	A	C4-C5-C6	6.57	120.28	117.00
27	B8	333	G	C5-C6-O6	-6.57	124.66	128.60
27	B8	1378	A	C4-C5-C6	6.57	120.28	117.00
3	AV	7	G	C5-C6-O6	-6.57	124.66	128.60
27	B8	388	G	C5-C6-O6	-6.57	124.66	128.60
27	B8	696	G	O4'-C1'-N9	6.57	113.45	108.20
27	B8	2817	U	O4'-C1'-N1	6.57	113.45	108.20
1	AA	360	G	C5-C6-O6	-6.56	124.66	128.60
1	AA	3	A	C4-C5-C6	6.56	120.28	117.00
1	AA	768	A	O4'-C1'-N9	6.56	113.45	108.20
1	AA	994	A	C4-C5-C6	6.56	120.28	117.00
3	AV	49	C	O4'-C1'-N1	6.56	113.45	108.20
27	B8	488	G	C5-C6-O6	-6.56	124.66	128.60
27	B8	1186	G	O4'-C1'-N9	6.56	113.45	108.20
27	B8	1508	A	O4'-C1'-N9	6.56	113.45	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	1571	A	C5-C6-N1	-6.56	114.42	117.70
27	B8	2174	C	N3-C4-N4	6.56	122.59	118.00
27	B8	2190	G	O4'-C1'-N9	6.56	113.45	108.20
27	B8	2740	A	O4'-C1'-N9	6.56	113.45	108.20
1	AA	338	A	O4'-C1'-N9	6.56	113.45	108.20
1	AA	780	A	O4'-C1'-N9	6.56	113.45	108.20
1	AA	1440	U	O4'-C1'-N1	6.56	113.45	108.20
1	AA	14	U	O4'-C1'-N1	6.56	113.45	108.20
1	AA	1001	C	N3-C4-N4	6.56	122.59	118.00
27	B8	53	A	C4-C5-C6	6.56	120.28	117.00
27	B8	113	U	O4'-C1'-N1	6.56	113.45	108.20
27	B8	195	A	C4-C5-C6	6.56	120.28	117.00
27	B8	2659	G	C5-C6-O6	-6.56	124.66	128.60
1	AA	63	C	O4'-C1'-N1	6.56	113.45	108.20
1	AA	1355	G	C5-C6-O6	-6.56	124.67	128.60
27	B8	664	G	O4'-C1'-N9	6.56	113.45	108.20
27	B8	1073	A	C5-C6-N6	-6.56	118.45	123.70
1	AA	16	A	C5-C6-N6	-6.55	118.46	123.70
1	AA	504	C	N3-C4-N4	6.55	122.59	118.00
1	AA	598	U	O4'-C1'-N1	6.55	113.44	108.20
1	AA	1303	C	O4'-C1'-N1	6.55	113.44	108.20
27	B8	225	C	O4'-C1'-N1	6.55	113.44	108.20
27	B8	2115	G	C5-C6-O6	-6.55	124.67	128.60
27	B8	2862	G	O4'-C1'-N9	6.55	113.44	108.20
27	B8	414	C	N3-C4-N4	6.55	122.59	118.00
27	B8	421	C	O4'-C1'-N1	6.55	113.44	108.20
1	AA	1426	G	C5-C6-O6	-6.55	124.67	128.60
27	B8	233	A	C5-C6-N6	-6.55	118.46	123.70
27	B8	399	U	O4'-C1'-N1	6.55	113.44	108.20
27	B8	503	A	C5-C6-N6	-6.55	118.46	123.70
27	B8	1021	A	C4-C5-C6	6.55	120.28	117.00
27	B8	2822	G	C5-C6-O6	-6.55	124.67	128.60
27	B8	1987	A	O4'-C1'-N9	6.55	113.44	108.20
27	B8	95	A	C4-C5-C6	6.55	120.27	117.00
27	B8	298	G	C5-C6-O6	-6.55	124.67	128.60
27	B8	880	G	C5-C6-O6	-6.55	124.67	128.60
27	B8	1945	G	C5-C6-O6	-6.55	124.67	128.60
27	B8	2237	G	C5-C6-O6	-6.55	124.67	128.60
27	B8	2311	A	C4-C5-C6	6.55	120.27	117.00
27	B8	2400	G	O4'-C1'-N9	6.55	113.44	108.20
27	B8	2597	G	C5-C6-O6	-6.55	124.67	128.60
1	AA	944	G	C5-C6-O6	-6.54	124.67	128.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1305	G	C5-C6-O6	-6.54	124.67	128.60
1	AA	1386	G	O4'-C1'-N9	6.54	113.44	108.20
1	AA	1542	A	C4-C5-C6	6.54	120.27	117.00
27	B8	191	A	O4'-C1'-N9	6.54	113.44	108.20
27	B8	2842	G	O4'-C1'-N9	6.54	113.44	108.20
27	B8	1175	A	C4-C5-C6	6.54	120.27	117.00
27	B8	1419	A	C4-C5-C6	6.54	120.27	117.00
27	B8	2328	A	C4-C5-C6	6.54	120.27	117.00
1	AA	35	G	C5-C6-O6	-6.54	124.67	128.60
1	AA	307	C	O4'-C1'-N1	6.54	113.43	108.20
27	B8	831	G	O4'-C1'-N9	6.54	113.43	108.20
27	B8	1671	U	O4'-C1'-N1	6.54	113.43	108.20
27	B8	2681	C	O4'-C1'-N1	6.54	113.43	108.20
1	AA	1222	G	C5-C6-O6	-6.54	124.68	128.60
3	AV	9	A	C4-C5-C6	6.54	120.27	117.00
27	B8	619	G	C5-C6-O6	-6.54	124.68	128.60
27	B8	2872	A	C4-C5-C6	6.54	120.27	117.00
1	AA	226	G	C5-C6-O6	-6.54	124.68	128.60
1	AA	691	G	C5-C6-O6	-6.54	124.68	128.60
1	AA	693	G	C5-C6-O6	-6.54	124.68	128.60
1	AA	1055	A	C4-C5-C6	6.54	120.27	117.00
1	AA	1149	C	N3-C4-N4	6.54	122.58	118.00
26	B7	15	A	C4-C5-C6	6.54	120.27	117.00
27	B8	731	C	N3-C4-N4	6.54	122.58	118.00
27	B8	927	A	O4'-C1'-N9	6.54	113.43	108.20
27	B8	1252	G	C5-C6-O6	-6.54	124.68	128.60
27	B8	1946	U	O4'-C1'-N1	6.54	113.43	108.20
27	B8	253	C	N3-C4-N4	6.54	122.58	118.00
27	B8	434	U	O4'-C1'-N1	6.54	113.43	108.20
27	B8	1226	A	C4-C5-C6	6.54	120.27	117.00
27	B8	2112	G	O4'-C1'-N9	6.54	113.43	108.20
1	AA	1077	G	C5-C6-O6	-6.54	124.68	128.60
27	B8	174	U	O4'-C1'-N1	6.54	113.43	108.20
27	B8	1412	U	O4'-C1'-N1	6.54	113.43	108.20
27	B8	2010	G	C5-C6-O6	-6.54	124.68	128.60
27	B8	2040	G	O4'-C1'-N9	6.54	113.43	108.20
27	B8	2068	U	O4'-C1'-N1	6.54	113.43	108.20
27	B8	2268	A	C4-C5-C6	6.54	120.27	117.00
27	B8	2611	C	O4'-C1'-N1	6.54	113.43	108.20
1	AA	190	A	C5-C6-N1	-6.53	114.43	117.70
1	AA	260	G	C5-C6-O6	-6.53	124.68	128.60
27	B8	1911	U	O4'-C1'-N1	6.53	113.43	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	43	G	C5-C6-O6	-6.53	124.68	128.60
1	AA	86	G	C5-C6-O6	-6.53	124.68	128.60
1	AA	92	U	O4'-C1'-N1	6.53	113.42	108.20
1	AA	141	G	O4'-C1'-N9	6.53	113.42	108.20
1	AA	412	A	C4-C5-C6	6.53	120.27	117.00
1	AA	947	G	O4'-C1'-N9	6.53	113.42	108.20
1	AA	1426	G	O4'-C1'-N9	6.53	113.42	108.20
3	AV	50	G	C5-C6-O6	-6.53	124.68	128.60
26	B7	119	A	O4'-C1'-N9	6.53	113.42	108.20
1	AA	283	U	O4'-C1'-N1	6.53	113.42	108.20
3	AV	33	A	O4'-C1'-N9	6.53	113.42	108.20
27	B8	2677	G	O4'-C1'-N9	6.53	113.42	108.20
3	AV	37	G	C5-C6-O6	-6.53	124.68	128.60
27	B8	35	G	O4'-C1'-N9	6.53	113.42	108.20
27	B8	458	G	O4'-C1'-N9	6.53	113.42	108.20
1	AA	512	U	O4'-C1'-N1	6.53	113.42	108.20
27	B8	93	G	C5-C6-O6	-6.53	124.69	128.60
27	B8	476	G	C5-C6-O6	-6.53	124.68	128.60
27	B8	888	C	O4'-C1'-N1	6.53	113.42	108.20
27	B8	1811	G	C5-C6-O6	-6.53	124.69	128.60
27	B8	2034	U	O4'-C1'-N1	6.53	113.42	108.20
1	AA	183	C	O4'-C1'-N1	6.52	113.42	108.20
1	AA	220	G	O4'-C1'-N9	6.52	113.42	108.20
1	AA	996	A	C5-C6-N6	-6.52	118.48	123.70
27	B8	2060	A	O4'-C1'-N9	6.52	113.42	108.20
27	B8	2779	U	O4'-C1'-N1	6.52	113.42	108.20
1	AA	654	G	C5-C6-O6	-6.52	124.69	128.60
27	B8	609	A	C4-C5-C6	6.52	120.26	117.00
1	AA	901	A	C5-C6-N6	-6.52	118.48	123.70
27	B8	2873	A	C4-C5-C6	6.52	120.26	117.00
1	AA	313	A	C4-C5-C6	6.52	120.26	117.00
1	AA	351	G	C5-C6-O6	-6.52	124.69	128.60
1	AA	1002	G	O4'-C1'-N9	6.52	113.42	108.20
26	B7	58	A	C4-C5-C6	6.52	120.26	117.00
27	B8	1408	G	C5-C6-O6	-6.52	124.69	128.60
27	B8	1876	A	N1-C6-N6	6.52	122.51	118.60
1	AA	583	A	O4'-C1'-N9	6.52	113.41	108.20
1	AA	592	G	O4'-C1'-N9	6.52	113.42	108.20
1	AA	1387	G	O4'-C1'-N9	6.52	113.41	108.20
26	B7	64	G	O4'-C1'-N9	6.52	113.41	108.20
27	B8	1668	A	P-O3'-C3'	6.52	127.52	119.70
27	B8	2766	A	C4-C5-C6	6.52	120.26	117.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	776	G	O4'-C1'-N9	6.52	113.41	108.20
27	B8	1577	C	N3-C4-N4	6.52	122.56	118.00
27	B8	544	C	C2-N1-C1'	6.51	125.97	118.80
27	B8	1002	G	O4'-C1'-N9	6.51	113.41	108.20
27	B8	1532	A	C5-C6-N6	-6.51	118.49	123.70
26	B7	76	G	C5-C6-O6	-6.51	124.69	128.60
27	B8	2627	G	C5-C6-O6	-6.51	124.69	128.60
1	AA	44	A	O4'-C1'-N9	6.51	113.41	108.20
1	AA	250	A	C4-C5-C6	6.51	120.25	117.00
1	AA	532	A	C4-C5-C6	6.51	120.26	117.00
1	AA	1222	G	O4'-C1'-N9	6.51	113.41	108.20
1	AA	1434	A	O4'-C1'-N9	6.51	113.41	108.20
27	B8	58	G	C5-C6-O6	-6.51	124.69	128.60
27	B8	708	G	O4'-C1'-N9	6.51	113.41	108.20
1	AA	782	A	O4'-C1'-N9	6.51	113.41	108.20
27	B8	213	A	C5-C6-N6	-6.51	118.49	123.70
27	B8	315	G	C5-C6-O6	-6.51	124.69	128.60
27	B8	855	G	C5-C6-O6	-6.51	124.69	128.60
27	B8	95	A	C5-C6-N6	-6.51	118.49	123.70
27	B8	424	G	O4'-C1'-N9	6.51	113.41	108.20
27	B8	515	A	C5-C6-N6	-6.51	118.49	123.70
27	B8	2524	G	O4'-C1'-N9	6.51	113.41	108.20
1	AA	12	U	O4'-C1'-N1	6.51	113.41	108.20
27	B8	1334	G	C5-C6-O6	-6.51	124.70	128.60
27	B8	1564	C	N3-C4-N4	6.51	122.56	118.00
27	B8	1756	G	C5-C6-O6	-6.51	124.70	128.60
1	AA	38	G	C5-C6-O6	-6.50	124.70	128.60
27	B8	391	A	C4-C5-C6	6.50	120.25	117.00
1	AA	1063	C	N3-C4-N4	6.50	122.55	118.00
1	AA	1219	A	C4-C5-C6	6.50	120.25	117.00
1	AA	1417	G	C5-C6-O6	-6.50	124.70	128.60
1	AA	259	G	O4'-C1'-N9	6.50	113.40	108.20
1	AA	731	G	O4'-C1'-N9	6.50	113.40	108.20
27	B8	1026	G	O4'-C1'-N9	6.50	113.40	108.20
27	B8	1531	C	N3-C4-N4	6.50	122.55	118.00
27	B8	2138	G	C5-C6-O6	-6.50	124.70	128.60
1	AA	712	A	O4'-C1'-N9	6.50	113.40	108.20
27	B8	400	G	N3-C2-N2	6.50	124.45	119.90
27	B8	2212	A	C4-C5-C6	6.50	120.25	117.00
27	B8	2508	G	O4'-C1'-N9	6.50	113.40	108.20
1	AA	256	U	O4'-C1'-N1	6.50	113.40	108.20
1	AA	1262	C	N3-C4-N4	6.50	122.55	118.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	871	U	O4'-C1'-N1	6.50	113.40	108.20
27	B8	1948	G	O4'-C1'-N9	6.50	113.40	108.20
1	AA	376	G	C5-C6-O6	-6.50	124.70	128.60
27	B8	230	G	O4'-C1'-N9	6.50	113.40	108.20
27	B8	1088	A	O4'-C1'-N9	6.50	113.40	108.20
27	B8	1702	G	O4'-C1'-N9	6.50	113.40	108.20
1	AA	472	U	O4'-C1'-N1	6.50	113.40	108.20
1	AA	1263	C	N3-C4-N4	6.50	122.55	118.00
27	B8	560	C	N3-C4-N4	6.50	122.55	118.00
27	B8	1700	A	C4-C5-C6	6.50	120.25	117.00
27	B8	2282	G	C5-C6-O6	-6.50	124.70	128.60
1	AA	82	G	C5-C6-O6	-6.49	124.70	128.60
1	AA	262	A	C5-C6-N6	-6.49	118.50	123.70
1	AA	305	G	C5-C6-O6	-6.49	124.70	128.60
1	AA	926	G	C5-C6-O6	-6.49	124.70	128.60
27	B8	689	A	C5-C6-N6	-6.49	118.50	123.70
27	B8	872	U	O4'-C1'-N1	6.49	113.39	108.20
27	B8	876	C	C5'-C4'-O4'	6.49	116.89	109.10
27	B8	1471	G	C5-C6-O6	-6.49	124.70	128.60
27	B8	2432	A	C4-C5-C6	6.49	120.25	117.00
27	B8	2611	C	N3-C4-N4	6.49	122.55	118.00
27	B8	412	A	C4-C5-C6	6.49	120.25	117.00
27	B8	1819	A	C4-C5-C6	6.49	120.25	117.00
1	AA	475	C	N3-C4-N4	6.49	122.54	118.00
1	AA	694	A	C4-C5-C6	6.49	120.25	117.00
1	AA	789	U	O4'-C1'-N1	6.49	113.39	108.20
27	B8	973	A	C4-C5-C6	6.49	120.25	117.00
27	B8	1237	A	C4-C5-C6	6.49	120.25	117.00
27	B8	1613	G	O4'-C1'-N9	6.49	113.39	108.20
27	B8	2051	A	C5-C6-N6	-6.49	118.51	123.70
27	B8	2537	U	O4'-C1'-N1	6.49	113.39	108.20
27	B8	2774	C	N3-C4-N4	6.49	122.54	118.00
27	B8	2821	A	C4-C5-C6	6.49	120.25	117.00
27	B8	2573	C	C6-N1-C1'	-6.49	113.01	120.80
1	AA	1079	G	C5-C6-O6	-6.49	124.71	128.60
27	B8	2127	G	C5-C6-O6	-6.49	124.71	128.60
27	B8	2816	G	C5-C6-O6	-6.49	124.71	128.60
27	B8	2863	C	N3-C4-N4	6.49	122.54	118.00
1	AA	597	G	O4'-C1'-N9	6.49	113.39	108.20
27	B8	305	C	N3-C4-N4	6.49	122.54	118.00
27	B8	1527	G	C5-C6-O6	-6.49	124.71	128.60
1	AA	410	G	O4'-C1'-N9	6.48	113.39	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	1938	A	O4'-C1'-N9	6.48	113.39	108.20
1	AA	187	G	C5-C6-O6	-6.48	124.71	128.60
1	AA	208	U	O4'-C1'-N1	6.48	113.39	108.20
27	B8	532	A	C5-C6-N6	-6.48	118.51	123.70
27	B8	712	G	O4'-C1'-N9	6.48	113.39	108.20
27	B8	1524	G	C5-C6-O6	-6.48	124.71	128.60
27	B8	1580	A	C4-C5-C6	6.48	120.24	117.00
27	B8	2014	A	C4-C5-C6	6.48	120.24	117.00
27	B8	2665	A	C4-C5-C6	6.48	120.24	117.00
27	B8	2887	A	C4-C5-C6	6.48	120.24	117.00
1	AA	574	A	C4-C5-C6	6.48	120.24	117.00
1	AA	1123	U	O4'-C1'-N1	6.48	113.39	108.20
1	AA	1415	G	C5-C6-O6	-6.48	124.71	128.60
27	B8	1263	U	O4'-C1'-N1	6.48	113.38	108.20
27	B8	1371	G	O4'-C1'-N9	6.48	113.39	108.20
27	B8	2154	A	C4-C5-C6	6.48	120.24	117.00
1	AA	1111	A	C4-C5-C6	6.48	120.24	117.00
3	AV	9	A	C5-C6-N6	-6.48	118.52	123.70
26	B7	46	A	C5-C6-N1	-6.48	114.46	117.70
27	B8	889	C	C2-N1-C1'	6.48	125.93	118.80
1	AA	550	G	O4'-C1'-N9	6.48	113.38	108.20
1	AA	737	C	N3-C4-N4	6.48	122.53	118.00
27	B8	365	U	O4'-C1'-N1	6.48	113.38	108.20
27	B8	570	G	C5-C6-O6	-6.48	124.71	128.60
27	B8	1578	U	O4'-C1'-N1	6.48	113.38	108.20
27	B8	1648	U	O4'-C1'-N1	6.48	113.38	108.20
27	B8	2568	U	O4'-C1'-N1	6.48	113.38	108.20
27	B8	1066	U	O4'-C1'-N1	6.48	113.38	108.20
27	B8	1483	G	C5-C6-O6	-6.48	124.71	128.60
27	B8	1872	A	C4-C5-C6	6.48	120.24	117.00
1	AA	768	A	C4-C5-C6	6.47	120.24	117.00
1	AA	1541	U	P-O3'-C3'	6.47	127.47	119.70
27	B8	582	A	C5-C6-N6	-6.47	118.52	123.70
27	B8	1314	C	O4'-C1'-N1	6.47	113.38	108.20
27	B8	2256	G	O4'-C1'-N9	6.47	113.38	108.20
27	B8	2560	A	C5-C6-N1	-6.47	114.46	117.70
1	AA	133	U	O4'-C1'-N1	6.47	113.38	108.20
1	AA	159	G	C5-C6-O6	-6.47	124.72	128.60
27	B8	982	C	C2-N1-C1'	6.47	125.92	118.80
27	B8	1048	A	C4-C5-C6	6.47	120.24	117.00
27	B8	1392	A	C4-C5-C6	6.47	120.24	117.00
27	B8	2721	A	C4-C5-C6	6.47	120.24	117.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1306	A	C4-C5-C6	6.47	120.23	117.00
27	B8	1121	C	N3-C4-N4	6.47	122.53	118.00
27	B8	1166	G	C5-C6-O6	-6.47	124.72	128.60
1	AA	1434	A	C4-C5-C6	6.47	120.23	117.00
26	B7	74	U	O4'-C1'-N1	6.47	113.38	108.20
27	B8	882	G	C5-C6-O6	-6.47	124.72	128.60
27	B8	2662	A	C5-C6-N6	-6.47	118.52	123.70
1	AA	263	A	C4-C5-C6	6.47	120.23	117.00
1	AA	541	G	O4'-C1'-N9	6.47	113.38	108.20
1	AA	1324	A	C4-C5-C6	6.47	120.23	117.00
1	AA	1459	G	O4'-C1'-N9	6.47	113.37	108.20
27	B8	212	G	O4'-C1'-N9	6.47	113.37	108.20
27	B8	1667	G	C5-C6-O6	-6.47	124.72	128.60
1	AA	6	G	C5-C6-O6	-6.47	124.72	128.60
1	AA	139	A	O4'-C1'-N9	6.47	113.37	108.20
1	AA	886	G	C5-C6-O6	-6.47	124.72	128.60
1	AA	1488	G	C5-C6-O6	-6.47	124.72	128.60
27	B8	19	A	C5-C6-N6	-6.47	118.53	123.70
27	B8	2122	U	O4'-C1'-N1	6.47	113.37	108.20
1	AA	477	C	N3-C4-N4	6.46	122.53	118.00
27	B8	54	G	C5-C6-O6	-6.46	124.72	128.60
27	B8	207	A	O4'-C1'-N9	6.46	113.37	108.20
27	B8	752	A	C4-C5-C6	6.46	120.23	117.00
27	B8	1453	A	C4-C5-C6	6.46	120.23	117.00
27	B8	1700	A	C5-C6-N6	-6.46	118.53	123.70
27	B8	277	G	O4'-C1'-N9	6.46	113.37	108.20
27	B8	2735	G	C5-C6-O6	-6.46	124.72	128.60
1	AA	125	U	O4'-C1'-N1	6.46	113.37	108.20
1	AA	247	G	C5-C6-O6	-6.46	124.72	128.60
27	B8	600	G	C5-C6-O6	-6.46	124.72	128.60
27	B8	1020	A	O4'-C1'-N9	6.46	113.37	108.20
27	B8	2033	A	C4-C5-C6	6.46	120.23	117.00
27	B8	2271	G	O4'-C1'-N9	6.46	113.37	108.20
27	B8	2838	G	O4'-C1'-N9	6.46	113.37	108.20
1	AA	540	G	O4'-C1'-N9	6.46	113.37	108.20
1	AA	894	G	O4'-C1'-N9	6.46	113.37	108.20
3	AV	19	G	C5-C6-O6	-6.46	124.72	128.60
5	A0	166	TYR	CB-CG-CD2	-6.46	117.12	121.00
27	B8	503	A	C4-C5-C6	6.46	120.23	117.00
27	B8	1713	A	C4-C5-C6	6.46	120.23	117.00
27	B8	2499	C	N3-C4-N4	6.46	122.52	118.00
1	AA	138	G	O4'-C1'-N9	6.46	113.37	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	337	G	O4'-C1'-N9	6.46	113.37	108.20
1	AA	756	C	N3-C4-N4	6.46	122.52	118.00
27	B8	452	G	C5-C6-O6	-6.46	124.72	128.60
27	B8	1875	G	C5-C6-O6	-6.46	124.72	128.60
27	B8	2482	A	C4-C5-C6	6.46	120.23	117.00
27	B8	2595	G	C5-C6-O6	-6.46	124.72	128.60
1	AA	19	A	C4-C5-C6	6.46	120.23	117.00
1	AA	262	A	C5-C6-N1	-6.46	114.47	117.70
1	AA	818	G	C5-C6-O6	-6.46	124.73	128.60
1	AA	826	C	O4'-C1'-N1	6.46	113.37	108.20
27	B8	110	G	O4'-C1'-N9	6.46	113.36	108.20
27	B8	352	A	C4-C5-C6	6.46	120.23	117.00
27	B8	592	A	O4'-C1'-N9	6.46	113.36	108.20
27	B8	1189	A	C4-C5-C6	6.46	120.23	117.00
27	B8	1589	U	O4'-C1'-N1	6.46	113.37	108.20
27	B8	662	G	O4'-C1'-N9	6.46	113.36	108.20
1	AA	1248	A	O4'-C1'-N9	6.45	113.36	108.20
27	B8	2729	G	O4'-C1'-N9	6.45	113.36	108.20
1	AA	557	G	C5-C6-O6	-6.45	124.73	128.60
27	B8	167	A	C4-C5-C6	6.45	120.23	117.00
27	B8	1178	C	N3-C4-N4	6.45	122.52	118.00
1	AA	628	G	C5-C6-O6	-6.45	124.73	128.60
27	B8	1283	G	O4'-C1'-N9	6.45	113.36	108.20
27	B8	2190	G	C5-C6-O6	-6.45	124.73	128.60
1	AA	682	G	O4'-C1'-N9	6.45	113.36	108.20
1	AA	1438	G	O4'-C1'-N9	6.45	113.36	108.20
26	B7	119	A	C4-C5-C6	6.45	120.22	117.00
27	B8	104	A	C5-C6-N6	-6.45	118.54	123.70
27	B8	114	U	O4'-C1'-N1	6.45	113.36	108.20
27	B8	1535	A	C4-C5-C6	6.45	120.22	117.00
27	B8	1862	G	O4'-C1'-N9	6.45	113.36	108.20
27	B8	2811	G	O4'-C1'-N9	6.45	113.36	108.20
27	B8	2895	G	O4'-C1'-N9	6.45	113.36	108.20
1	AA	1441	A	O4'-C1'-N9	6.45	113.36	108.20
26	B7	35	C	C2-N1-C1'	6.45	125.89	118.80
27	B8	1235	G	C5-C6-O6	-6.45	124.73	128.60
27	B8	1315	C	N3-C4-N4	6.45	122.51	118.00
27	B8	2544	G	O4'-C1'-N9	6.45	113.36	108.20
27	B8	713	G	C5-C6-O6	-6.44	124.73	128.60
27	B8	866	A	C4-C5-C6	6.44	120.22	117.00
27	B8	1930	G	C5-C6-O6	-6.44	124.73	128.60
1	AA	419	C	N3-C4-N4	6.44	122.51	118.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1127	G	C5-C6-O6	-6.44	124.73	128.60
27	B8	196	A	C4-C5-C6	6.44	120.22	117.00
27	B8	801	G	C5-C6-O6	-6.44	124.73	128.60
27	B8	2464	G	O4'-C1'-N9	6.44	113.35	108.20
1	AA	128	G	C5-C6-O6	-6.44	124.74	128.60
1	AA	498	A	C4-C5-C6	6.44	120.22	117.00
1	AA	915	A	C5-C6-N6	-6.44	118.55	123.70
1	AA	1039	G	O4'-C1'-N9	6.44	113.35	108.20
1	AA	1173	U	O4'-C1'-N1	6.44	113.35	108.20
27	B8	782	A	C4-C5-C6	6.44	120.22	117.00
27	B8	1703	G	O4'-C1'-N9	6.44	113.35	108.20
27	B8	2706	A	C4-C5-C6	6.44	120.22	117.00
1	AA	1062	U	O4'-C1'-N1	6.44	113.35	108.20
27	B8	264	C	O4'-C1'-N1	6.44	113.35	108.20
27	B8	406	G	O4'-C1'-N9	6.44	113.35	108.20
27	B8	2130	U	O4'-C1'-N1	6.44	113.35	108.20
1	AA	459	A	C4-C5-C6	6.44	120.22	117.00
1	AA	865	A	O4'-C1'-N9	6.44	113.35	108.20
1	AA	1406	U	O4'-C1'-N1	6.44	113.35	108.20
27	B8	37	C	N3-C4-N4	6.43	122.50	118.00
27	B8	522	A	O4'-C1'-N9	6.43	113.35	108.20
27	B8	716	A	C4-C5-C6	6.43	120.22	117.00
27	B8	2546	U	O4'-C1'-N1	6.43	113.35	108.20
1	AA	536	C	O4'-C1'-N1	6.43	113.35	108.20
27	B8	330	A	C4-C5-C6	6.43	120.22	117.00
27	B8	1730	C	C2-N1-C1'	6.43	125.88	118.80
27	B8	2150	C	N3-C4-N4	6.43	122.50	118.00
27	B8	2269	G	C5-C6-O6	-6.43	124.74	128.60
1	AA	355	C	N3-C4-N4	6.43	122.50	118.00
27	B8	1170	C	N3-C4-N4	6.43	122.50	118.00
27	B8	1773	A	C5-C6-N6	-6.43	118.56	123.70
1	AA	371	A	C5-C6-N6	-6.43	118.56	123.70
1	AA	376	G	O4'-C1'-N9	6.43	113.34	108.20
1	AA	974	A	C4-C5-C6	6.43	120.22	117.00
1	AA	1324	A	O4'-C1'-N9	6.43	113.34	108.20
27	B8	975	A	O4'-C1'-N9	6.43	113.34	108.20
27	B8	1436	G	C5-C6-O6	-6.43	124.74	128.60
27	B8	1922	G	O4'-C1'-N9	6.43	113.34	108.20
27	B8	2035	G	C5-C6-O6	-6.43	124.74	128.60
27	B8	2309	A	C4-C5-C6	6.43	120.22	117.00
27	B8	2444	G	C5-C6-O6	-6.43	124.74	128.60
1	AA	1172	C	N3-C4-N4	6.43	122.50	118.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	AV	46	G	C5-C6-O6	-6.43	124.74	128.60
1	AA	1	A	C4-C5-C6	6.43	120.21	117.00
1	AA	692	U	O4'-C1'-N1	6.43	113.34	108.20
27	B8	581	C	N3-C4-N4	6.43	122.50	118.00
27	B8	1565	C	O4'-C1'-N1	6.43	113.34	108.20
27	B8	1755	A	O4'-C1'-N9	6.43	113.34	108.20
27	B8	2793	C	O4'-C1'-N1	6.43	113.34	108.20
1	AA	695	A	C4-C5-C6	6.42	120.21	117.00
1	AA	1018	G	C5-C6-O6	-6.42	124.75	128.60
1	AA	1403	C	O4'-C1'-N1	6.42	113.34	108.20
27	B8	107	G	O4'-C1'-N9	6.42	113.34	108.20
27	B8	1275	A	C4-C5-C6	6.42	120.21	117.00
27	B8	2365	G	C5-C6-O6	-6.42	124.75	128.60
1	AA	581	G	O4'-C1'-N9	6.42	113.34	108.20
1	AA	389	A	C4-C5-C6	6.42	120.21	117.00
1	AA	581	G	C5-C6-O6	-6.42	124.75	128.60
27	B8	276	U	C2-N1-C1'	6.42	125.41	117.70
27	B8	1211	C	C2-N1-C1'	6.42	125.86	118.80
27	B8	1300	G	C5-C6-O6	-6.42	124.75	128.60
27	B8	1898	U	O4'-C1'-N1	6.42	113.34	108.20
1	AA	309	A	O4'-C1'-N9	6.42	113.34	108.20
3	AV	64	U	O4'-C1'-N1	6.42	113.34	108.20
27	B8	189	G	O4'-C1'-N9	6.42	113.34	108.20
27	B8	324	A	O4'-C1'-N9	6.42	113.34	108.20
27	B8	1717	A	C4-C5-C6	6.42	120.21	117.00
27	B8	2899	A	O4'-C1'-N9	6.42	113.34	108.20
1	AA	2	A	C4-C5-C6	6.42	120.21	117.00
1	AA	219	U	O4'-C1'-N1	6.42	113.33	108.20
1	AA	433	G	C5-C6-O6	-6.42	124.75	128.60
27	B8	105	C	N3-C4-N4	6.42	122.49	118.00
27	B8	685	A	C5-C6-N6	-6.42	118.56	123.70
27	B8	802	A	C4-C5-C6	6.42	120.21	117.00
27	B8	1787	A	C5-C6-N6	-6.42	118.56	123.70
1	AA	447	G	C5-C6-O6	-6.42	124.75	128.60
1	AA	448	A	O4'-C1'-N9	6.42	113.33	108.20
3	AV	22	A	C4-C5-C6	6.42	120.21	117.00
27	B8	300	A	C4-C5-C6	6.42	120.21	117.00
1	AA	1266	G	C5-C6-O6	-6.42	124.75	128.60
3	AV	56	U	O4'-C1'-N1	6.42	113.33	108.20
27	B8	28	A	C5-C6-N6	-6.42	118.57	123.70
27	B8	349	U	O4'-C1'-N1	6.42	113.33	108.20
27	B8	1086	A	C5-C6-N1	-6.42	114.49	117.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	38	G	O4'-C1'-N9	6.41	113.33	108.20
27	B8	1599	U	O4'-C1'-N1	6.41	113.33	108.20
27	B8	1770	G	C5-C6-O6	-6.41	124.75	128.60
27	B8	2265	U	O4'-C1'-N1	6.41	113.33	108.20
27	B8	2505	G	O4'-C1'-N9	6.41	113.33	108.20
1	AA	1179	A	C4-C5-C6	6.41	120.21	117.00
27	B8	10	A	C4-C5-C6	6.41	120.21	117.00
27	B8	1260	A	C5-C6-N6	-6.41	118.57	123.70
1	AA	192	A	C5-C6-N6	-6.41	118.57	123.70
27	B8	1916	A	O4'-C1'-N9	6.41	113.33	108.20
26	B7	2	G	O4'-C1'-N9	6.41	113.33	108.20
27	B8	755	U	O4'-C1'-N1	6.41	113.33	108.20
27	B8	899	A	C5-C6-N6	-6.41	118.57	123.70
27	B8	1000	A	C4-C5-C6	6.41	120.20	117.00
27	B8	2045	C	N3-C4-N4	6.41	122.49	118.00
27	B8	2791	G	C5-C6-O6	-6.41	124.75	128.60
3	AV	27	A	C4-C5-C6	6.41	120.20	117.00
27	B8	356	G	O4'-C1'-N9	6.41	113.33	108.20
27	B8	1476	U	O4'-C1'-N1	6.41	113.33	108.20
1	AA	1191	A	C4-C5-C6	6.41	120.20	117.00
27	B8	1639	C	N3-C4-N4	6.41	122.48	118.00
27	B8	1757	A	C4-C5-C6	6.41	120.20	117.00
27	B8	1259	G	O4'-C1'-N9	6.40	113.32	108.20
27	B8	1808	A	C4-C5-C6	6.40	120.20	117.00
27	B8	2170	A	C4-C5-C6	6.40	120.20	117.00
1	AA	21	G	C5-C6-O6	-6.40	124.76	128.60
1	AA	399	G	O4'-C1'-N9	6.40	113.32	108.20
27	B8	299	A	C4-C5-C6	6.40	120.20	117.00
27	B8	2284	A	C5-C6-N6	-6.40	118.58	123.70
1	AA	482	A	C5-C6-N6	-6.40	118.58	123.70
1	AA	1138	G	O4'-C1'-N9	6.40	113.32	108.20
1	AA	1268	G	C5-C6-O6	-6.40	124.76	128.60
26	B7	42	C	O4'-C1'-N1	6.40	113.32	108.20
27	B8	1642	G	O4'-C1'-N9	6.40	113.32	108.20
27	B8	1713	A	C5-C6-N6	-6.40	118.58	123.70
27	B8	1929	G	C5-C6-O6	-6.40	124.76	128.60
27	B8	2013	A	C4-C5-C6	6.40	120.20	117.00
27	B8	707	G	O4'-C1'-N9	6.40	113.32	108.20
27	B8	711	G	O4'-C1'-N9	6.40	113.32	108.20
27	B8	1874	C	N3-C4-N4	6.40	122.48	118.00
1	AA	228	A	C4-C5-C6	6.40	120.20	117.00
1	AA	421	U	C2-N1-C1'	6.40	125.38	117.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	556	C	N3-C4-N4	6.40	122.48	118.00
1	AA	893	C	N3-C4-N4	6.40	122.48	118.00
1	AA	1399	C	O4'-C1'-N1	6.40	113.32	108.20
3	AV	77	A	C4-C5-C6	6.40	120.20	117.00
27	B8	55	G	C5-C6-O6	-6.40	124.76	128.60
27	B8	1285	A	C4-C5-C6	6.40	120.20	117.00
27	B8	1787	A	C4-C5-C6	6.40	120.20	117.00
27	B8	2175	C	P-O3'-C3'	6.40	127.38	119.70
1	AA	608	A	O4'-C1'-N9	6.40	113.32	108.20
27	B8	1103	A	C4-C5-C6	6.40	120.20	117.00
1	AA	1011	C	O4'-C1'-N1	6.39	113.31	108.20
1	AA	1331	G	C5-C6-O6	-6.39	124.76	128.60
27	B8	28	A	O4'-C1'-N9	6.39	113.32	108.20
27	B8	317	G	C5-C6-O6	-6.39	124.76	128.60
27	B8	1027	A	C5-C6-N6	-6.39	118.58	123.70
27	B8	1132	U	O4'-C1'-N1	6.39	113.32	108.20
27	B8	1781	U	O4'-C1'-N1	6.39	113.31	108.20
27	B8	2655	G	C5-C6-O6	-6.39	124.76	128.60
1	AA	378	G	C5-C6-O6	-6.39	124.76	128.60
1	AA	1491	G	C5-C6-O6	-6.39	124.76	128.60
27	B8	1309	G	O4'-C1'-N9	6.39	113.31	108.20
27	B8	2446	G	C5-C6-O6	-6.39	124.76	128.60
27	B8	1953	A	C4-C5-C6	6.39	120.19	117.00
27	B8	2793	C	N3-C4-N4	6.39	122.47	118.00
1	AA	52	C	N3-C4-N4	6.39	122.47	118.00
1	AA	343	U	O4'-C1'-N1	6.39	113.31	108.20
1	AA	990	C	O4'-C1'-N1	6.39	113.31	108.20
26	B7	112	G	O4'-C1'-N9	6.39	113.31	108.20
27	B8	418	C	N3-C4-N4	6.39	122.47	118.00
27	B8	449	A	C4-C5-C6	6.39	120.19	117.00
27	B8	748	G	C5-C6-O6	-6.39	124.77	128.60
27	B8	1346	G	O4'-C1'-N9	6.39	113.31	108.20
27	B8	2800	A	O4'-C1'-N9	6.39	113.31	108.20
1	AA	1507	A	C4-C5-C6	6.39	120.19	117.00
1	AA	1493	A	C4-C5-C6	6.39	120.19	117.00
27	B8	1341	G	C5-C6-O6	-6.39	124.77	128.60
27	B8	1980	G	C5-C6-O6	-6.39	124.77	128.60
1	AA	147	G	O4'-C1'-N9	6.38	113.31	108.20
27	B8	595	C	N3-C4-N4	6.38	122.47	118.00
27	B8	1712	U	O4'-C1'-N1	6.38	113.31	108.20
27	B8	2901	C	N3-C4-N4	6.38	122.47	118.00
1	AA	202	G	C5-C6-O6	-6.38	124.77	128.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	629	A	C4-C5-C6	6.38	120.19	117.00
1	AA	1499	A	C4-C5-C6	6.38	120.19	117.00
27	B8	2776	A	C4-C5-C6	6.38	120.19	117.00
1	AA	109	A	C4-C5-C6	6.38	120.19	117.00
1	AA	495	A	C5-C6-N1	-6.38	114.51	117.70
1	AA	1423	G	O4'-C1'-N9	6.38	113.31	108.20
27	B8	64	A	C5-C6-N1	-6.38	114.51	117.70
27	B8	655	A	O4'-C1'-N9	6.38	113.31	108.20
27	B8	1122	G	C5-C6-O6	-6.38	124.77	128.60
27	B8	1359	A	O4'-C1'-N9	6.38	113.31	108.20
27	B8	2062	A	C4-C5-C6	6.38	120.19	117.00
27	B8	2258	C	O4'-C1'-N1	6.38	113.31	108.20
27	B8	2686	G	O4'-C1'-N9	6.38	113.31	108.20
1	AA	987	G	O4'-C1'-N9	6.38	113.30	108.20
1	AA	1110	A	C4-C5-C6	6.38	120.19	117.00
27	B8	260	G	O4'-C1'-N9	6.38	113.30	108.20
1	AA	1112	C	O4'-C1'-N1	6.38	113.30	108.20
3	AV	30	G	O4'-C1'-N9	6.38	113.30	108.20
1	AA	77	A	C5-C6-N6	-6.38	118.60	123.70
1	AA	270	A	C5-C6-N6	-6.38	118.60	123.70
27	B8	219	A	C4-C5-C6	6.38	120.19	117.00
27	B8	329	G	C5-C6-O6	-6.38	124.77	128.60
27	B8	2602	A	C4-C5-C6	6.38	120.19	117.00
27	B8	2606	C	N3-C4-N4	6.38	122.46	118.00
27	B8	2900	A	C5-C6-N6	-6.38	118.60	123.70
1	AA	28	A	O4'-C1'-N9	6.38	113.30	108.20
27	B8	2406	A	C4-C5-C6	6.38	120.19	117.00
1	AA	53	A	O4'-C1'-N9	6.37	113.30	108.20
1	AA	776	G	O4'-C1'-N9	6.37	113.30	108.20
1	AA	1095	U	O4'-C1'-N1	6.37	113.30	108.20
27	B8	243	U	O4'-C1'-N1	6.37	113.30	108.20
27	B8	1664	A	C5-C6-N6	-6.37	118.60	123.70
27	B8	2632	A	C5-C6-N6	-6.37	118.60	123.70
1	AA	176	C	N3-C4-N4	6.37	122.46	118.00
1	AA	742	G	C5-C6-O6	-6.37	124.78	128.60
27	B8	571	U	O4'-C1'-N1	6.37	113.30	108.20
27	B8	1921	G	O4'-C1'-N9	6.37	113.30	108.20
27	B8	2297	A	C5-C6-N1	-6.37	114.51	117.70
41	BM	43	ALA	N-CA-CB	6.37	119.02	110.10
1	AA	386	C	O4'-C1'-N1	6.37	113.30	108.20
1	AA	455	G	O4'-C1'-N9	6.37	113.30	108.20
1	AA	941	G	O4'-C1'-N9	6.37	113.29	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1244	G	O4'-C1'-N9	6.37	113.30	108.20
1	AA	1534	A	C4-C5-C6	6.37	120.18	117.00
27	B8	13	A	C5-C6-N6	-6.37	118.61	123.70
27	B8	2442	C	N3-C4-N4	6.37	122.46	118.00
27	B8	2451	A	O4'-C1'-N9	6.37	113.30	108.20
27	B8	2113	U	O4'-C1'-N1	6.37	113.29	108.20
26	B7	101	A	C5-C6-N6	-6.37	118.61	123.70
27	B8	1098	A	C4-C5-C6	6.37	120.18	117.00
27	B8	1692	U	O4'-C1'-N1	6.37	113.29	108.20
27	B8	1745	A	C4-C5-C6	6.37	120.18	117.00
27	B8	2079	U	O4'-C1'-N1	6.37	113.29	108.20
1	AA	1496	C	N3-C4-N4	6.36	122.45	118.00
27	B8	420	C	N3-C4-N4	6.36	122.45	118.00
27	B8	1861	G	O4'-C1'-N9	6.36	113.29	108.20
27	B8	1880	U	O4'-C1'-N1	6.36	113.29	108.20
27	B8	2434	A	C4-C5-C6	6.36	120.18	117.00
27	B8	881	G	C5-C6-O6	-6.36	124.78	128.60
27	B8	1823	G	C5-C6-O6	-6.36	124.78	128.60
27	B8	2030	A	C4-C5-C6	6.36	120.18	117.00
27	B8	2358	A	C4-C5-C6	6.36	120.18	117.00
1	AA	1105	A	O4'-C1'-N9	6.36	113.29	108.20
1	AA	1480	A	O4'-C1'-N9	6.36	113.29	108.20
27	B8	284	U	O4'-C1'-N1	6.36	113.29	108.20
27	B8	403	U	O4'-C1'-N1	6.36	113.29	108.20
27	B8	1061	U	C6-N1-C1'	-6.36	112.30	121.20
27	B8	1317	G	O4'-C1'-N9	6.36	113.29	108.20
27	B8	1689	A	C4-C5-C6	6.36	120.18	117.00
1	AA	312	C	N3-C4-N4	6.36	122.45	118.00
1	AA	1332	A	O4'-C1'-N9	6.36	113.29	108.20
1	AA	1338	G	C5-C6-O6	-6.36	124.78	128.60
1	AA	1456	A	C4-C5-C6	6.36	120.18	117.00
26	B7	39	A	C5-C6-N6	-6.36	118.61	123.70
27	B8	16	C	N3-C4-N4	6.36	122.45	118.00
27	B8	45	G	O4'-C1'-N9	6.36	113.29	108.20
27	B8	428	A	C4-C5-C6	6.36	120.18	117.00
27	B8	547	A	C4-C5-C6	6.36	120.18	117.00
27	B8	2732	G	O4'-C1'-N9	6.36	113.29	108.20
1	AA	1072	G	O4'-C1'-N9	6.36	113.28	108.20
3	AV	12	G	C5-C6-O6	-6.36	124.79	128.60
27	B8	1347	A	C5-C6-N1	-6.36	114.52	117.70
27	B8	2076	U	C2-N1-C1'	6.36	125.33	117.70
1	AA	1074	G	C5-C6-O6	-6.35	124.79	128.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	1207	C	N3-C4-N4	6.35	122.45	118.00
27	B8	2850	A	C4-C5-C6	6.35	120.18	117.00
1	AA	595	A	C4-C5-C6	6.35	120.18	117.00
1	AA	777	A	C4-C5-C6	6.35	120.18	117.00
1	AA	989	U	O4'-C1'-N1	6.35	113.28	108.20
27	B8	255	A	C4-C5-C6	6.35	120.18	117.00
27	B8	390	U	O4'-C1'-N1	6.35	113.28	108.20
27	B8	999	U	O4'-C1'-N1	6.35	113.28	108.20
27	B8	2517	C	N3-C4-N4	6.35	122.45	118.00
1	AA	517	G	C5-C6-O6	-6.35	124.79	128.60
27	B8	101	A	C4-C5-C6	6.35	120.18	117.00
27	B8	1187	G	C5-C6-O6	-6.35	124.79	128.60
27	B8	1203	U	O4'-C1'-N1	6.35	113.28	108.20
1	AA	676	A	C5-C6-N1	-6.35	114.53	117.70
1	AA	866	C	N3-C4-N4	6.35	122.44	118.00
1	AA	1206	G	O4'-C1'-N9	6.35	113.28	108.20
27	B8	575	A	C5-C6-N1	-6.35	114.53	117.70
27	B8	607	U	O4'-C1'-N1	6.35	113.28	108.20
27	B8	863	A	C4-C5-C6	6.35	120.17	117.00
27	B8	1163	G	O4'-C1'-N9	6.35	113.28	108.20
27	B8	2006	C	N3-C4-N4	6.35	122.44	118.00
1	AA	128	G	O4'-C1'-N9	6.35	113.28	108.20
1	AA	318	G	O4'-C1'-N9	6.35	113.28	108.20
1	AA	367	U	O4'-C1'-N1	6.35	113.28	108.20
27	B8	217	A	C4-C5-C6	6.35	120.17	117.00
27	B8	242	G	C5-C6-O6	-6.35	124.79	128.60
27	B8	2173	A	C4-C5-C6	6.35	120.17	117.00
1	AA	146	G	O4'-C1'-N9	6.35	113.28	108.20
1	AA	1219	A	C5-C6-N6	-6.35	118.62	123.70
27	B8	417	C	N3-C4-N4	6.35	122.44	118.00
27	B8	752	A	O4'-C1'-N9	6.35	113.28	108.20
27	B8	1288	G	C5-C6-O6	-6.35	124.79	128.60
27	B8	2261	C	N3-C4-N4	6.35	122.44	118.00
27	B8	2425	A	C4-C5-C6	6.35	120.17	117.00
1	AA	155	A	O4'-C1'-N9	6.34	113.28	108.20
1	AA	162	A	C5-C6-N1	-6.34	114.53	117.70
1	AA	1475	G	C5-C6-O6	-6.34	124.79	128.60
27	B8	227	A	C4-C5-C6	6.34	120.17	117.00
27	B8	1669	A	C5-C6-N1	-6.34	114.53	117.70
27	B8	1802	A	C5-C6-N1	-6.34	114.53	117.70
27	B8	268	C	O4'-C1'-N1	6.34	113.27	108.20
27	B8	1197	G	C5-C6-O6	-6.34	124.79	128.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	1754	A	C4-C5-C6	6.34	120.17	117.00
27	B8	2127	G	O4'-C1'-N9	6.34	113.27	108.20
32	BD	31	ALA	N-CA-CB	6.34	118.98	110.10
1	AA	1530	G	O4'-C1'-N9	6.34	113.27	108.20
27	B8	635	C	N3-C4-N4	6.34	122.44	118.00
27	B8	938	G	O4'-C1'-N9	6.34	113.27	108.20
27	B8	1368	G	O4'-C1'-N9	6.34	113.27	108.20
27	B8	1886	U	O4'-C1'-N1	6.34	113.27	108.20
27	B8	1962	C	N3-C4-N4	6.34	122.44	118.00
27	B8	492	A	C4-C5-C6	6.34	120.17	117.00
27	B8	1465	G	O4'-C1'-N9	6.34	113.27	108.20
27	B8	1548	A	O4'-C1'-N9	6.34	113.27	108.20
27	B8	2015	A	O4'-C1'-N9	6.34	113.27	108.20
27	B8	2072	C	N3-C4-N4	6.34	122.44	118.00
27	B8	857	G	C5-C6-O6	-6.34	124.80	128.60
27	B8	1573	G	C5-C6-O6	-6.34	124.80	128.60
27	B8	2262	U	O4'-C1'-N1	6.34	113.27	108.20
1	AA	47	C	N3-C4-N4	6.34	122.44	118.00
1	AA	74	A	O4'-C1'-N9	6.34	113.27	108.20
1	AA	1180	A	C4-C5-C6	6.34	120.17	117.00
1	AA	1199	U	O4'-C1'-N1	6.34	113.27	108.20
27	B8	142	A	O4'-C1'-N9	6.34	113.27	108.20
27	B8	186	G	O4'-C1'-N9	6.34	113.27	108.20
27	B8	728	G	O4'-C1'-N9	6.34	113.27	108.20
27	B8	1498	C	N3-C4-N4	6.34	122.44	118.00
27	B8	1860	G	O4'-C1'-N9	6.34	113.27	108.20
27	B8	1918	A	C5-C6-N6	-6.34	118.63	123.70
27	B8	1996	C	N3-C4-N4	6.33	122.43	118.00
27	B8	2575	C	N3-C4-N4	6.33	122.43	118.00
3	AV	71	C	N3-C4-N4	6.33	122.43	118.00
27	B8	1613	G	C5-C6-O6	-6.33	124.80	128.60
27	B8	2352	A	C5-C6-N1	-6.33	114.53	117.70
1	AA	408	A	C4-C5-C6	6.33	120.17	117.00
1	AA	1030	U	C2-N1-C1'	6.33	125.30	117.70
27	B8	138	U	O4'-C1'-N1	6.33	113.27	108.20
27	B8	237	C	N3-C4-N4	6.33	122.43	118.00
27	B8	2165	C	O4'-C1'-N1	6.33	113.27	108.20
27	B8	2168	G	O4'-C1'-N9	6.33	113.27	108.20
27	B8	2322	A	C4-C5-C6	6.33	120.17	117.00
27	B8	91	A	C4-C5-C6	6.33	120.17	117.00
27	B8	529	A	C4-C5-C6	6.33	120.17	117.00
27	B8	1780	A	O4'-C1'-N9	6.33	113.26	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	2666	C	C6-N1-C1'	-6.33	113.20	120.80
1	AA	869	G	C5-C6-O6	-6.33	124.80	128.60
27	B8	54	G	O4'-C1'-N9	6.33	113.26	108.20
27	B8	185	G	O4'-C1'-N9	6.33	113.26	108.20
27	B8	216	A	O4'-C1'-N9	6.33	113.26	108.20
27	B8	1557	C	O4'-C1'-N1	6.33	113.26	108.20
27	B8	1724	G	O4'-C1'-N9	6.33	113.26	108.20
27	B8	2787	C	N3-C4-N4	6.33	122.43	118.00
1	AA	284	C	N3-C4-N4	6.33	122.43	118.00
1	AA	586	C	N3-C4-N4	6.33	122.43	118.00
1	AA	727	G	C5-C6-O6	-6.33	124.80	128.60
1	AA	1189	U	O4'-C1'-N1	6.33	113.26	108.20
27	B8	699	A	C4-C5-C6	6.33	120.16	117.00
1	AA	461	A	C4-C5-C6	6.33	120.16	117.00
1	AA	814	A	C4-C5-C6	6.33	120.16	117.00
1	AA	1360	A	C5-C6-N6	-6.33	118.64	123.70
26	B7	75	G	O4'-C1'-N9	6.33	113.26	108.20
27	B8	619	G	O4'-C1'-N9	6.33	113.26	108.20
1	AA	204	G	O4'-C1'-N9	6.32	113.26	108.20
27	B8	87	U	O4'-C1'-N1	6.32	113.26	108.20
27	B8	909	A	O4'-C1'-N9	6.32	113.26	108.20
27	B8	1264	A	C5-C6-N6	-6.32	118.64	123.70
27	B8	2065	C	N3-C4-N4	6.32	122.43	118.00
1	AA	830	G	O4'-C1'-N9	6.32	113.26	108.20
27	B8	750	A	C4-C5-C6	6.32	120.16	117.00
27	B8	644	A	C4-C5-C6	6.32	120.16	117.00
1	AA	70	U	O4'-C1'-N1	6.32	113.25	108.20
27	B8	577	G	O4'-C1'-N9	6.32	113.25	108.20
1	AA	738	C	N3-C4-N4	6.32	122.42	118.00
1	AA	1513	A	C5-C6-N6	-6.32	118.65	123.70
27	B8	732	C	N3-C4-N4	6.32	122.42	118.00
27	B8	1496	A	C5-C6-N6	-6.32	118.65	123.70
27	B8	2101	A	O4'-C1'-N9	6.32	113.25	108.20
27	B8	2134	A	C4-C5-C6	6.32	120.16	117.00
1	AA	892	A	O4'-C1'-N9	6.32	113.25	108.20
1	AA	1501	C	O4'-C1'-N1	6.32	113.25	108.20
27	B8	479	A	C4-C5-C6	6.32	120.16	117.00
27	B8	1509	A	C4-C5-C6	6.32	120.16	117.00
27	B8	1738	G	C5-C6-O6	-6.32	124.81	128.60
27	B8	2733	A	C4-C5-C6	6.31	120.16	117.00
1	AA	177	G	N1-C6-O6	6.31	123.69	119.90
1	AA	803	G	O4'-C1'-N9	6.31	113.25	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1119	C	N3-C4-N4	6.31	122.42	118.00
1	AA	1489	G	O4'-C1'-N9	6.31	113.25	108.20
27	B8	726	G	C5-C6-O6	-6.31	124.81	128.60
27	B8	1227	G	C5-C6-O6	-6.31	124.81	128.60
27	B8	1345	C	N3-C4-N4	6.31	122.42	118.00
27	B8	2033	A	O4'-C1'-N9	6.31	113.25	108.20
27	B8	656	G	O4'-C1'-N9	6.31	113.25	108.20
27	B8	1635	A	C4-C5-C6	6.31	120.16	117.00
27	B8	2215	C	N3-C4-N4	6.31	122.42	118.00
27	B8	2709	G	O4'-C1'-N9	6.31	113.25	108.20
1	AA	573	A	C4-C5-C6	6.31	120.16	117.00
1	AA	614	C	N3-C4-N4	6.31	122.42	118.00
1	AA	1455	G	O4'-C1'-N9	6.31	113.25	108.20
1	AA	1498	U	O4'-C1'-N1	6.31	113.25	108.20
3	AV	34	U	O4'-C1'-N1	6.31	113.25	108.20
27	B8	881	G	O4'-C1'-N9	6.31	113.25	108.20
27	B8	1737	G	C5-C6-O6	-6.31	124.81	128.60
1	AA	245	U	O4'-C1'-N1	6.31	113.25	108.20
27	B8	684	G	C5-C6-O6	-6.31	124.81	128.60
27	B8	797	G	O4'-C1'-N9	6.31	113.25	108.20
26	B7	53	A	O4'-C1'-N9	6.31	113.25	108.20
27	B8	1269	A	C4-C5-C6	6.31	120.15	117.00
1	AA	101	A	C4-C5-C6	6.30	120.15	117.00
1	AA	247	G	O4'-C1'-N9	6.30	113.24	108.20
1	AA	868	C	N3-C4-N4	6.30	122.41	118.00
27	B8	294	A	C5-C6-N6	-6.30	118.66	123.70
27	B8	2331	G	C5-C6-O6	-6.30	124.82	128.60
27	B8	2788	C	N3-C4-N4	6.30	122.41	118.00
1	AA	468	A	C5-C6-N1	-6.30	114.55	117.70
26	B7	94	A	O4'-C1'-N9	6.30	113.24	108.20
27	B8	109	C	N3-C4-N4	6.30	122.41	118.00
27	B8	2154	A	C5-C6-N6	-6.30	118.66	123.70
27	B8	2899	A	C4-C5-C6	6.30	120.15	117.00
1	AA	739	C	N3-C4-N4	6.30	122.41	118.00
1	AA	859	G	O4'-C1'-N9	6.30	113.24	108.20
1	AA	895	G	C5-C6-O6	-6.30	124.82	128.60
1	AA	1291	U	O4'-C1'-N1	6.30	113.24	108.20
3	AV	74	A	O4'-C1'-N9	6.30	113.24	108.20
27	B8	2089	C	N3-C4-N4	6.30	122.41	118.00
27	B8	2551	C	N3-C4-N4	6.30	122.41	118.00
27	B8	2667	C	N3-C4-N4	6.30	122.41	118.00
27	B8	2682	A	C4-C5-C6	6.30	120.15	117.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	2904	U	O4'-C1'-N1	6.30	113.24	108.20
1	AA	1345	U	O4'-C1'-N1	6.30	113.24	108.20
27	B8	1041	G	O4'-C1'-N9	6.30	113.24	108.20
27	B8	2675	A	C5-C6-N1	-6.30	114.55	117.70
1	AA	205	A	C4-C5-C6	6.30	120.15	117.00
27	B8	132	G	O4'-C1'-N9	6.30	113.24	108.20
1	AA	1447	A	C5-C6-N1	-6.30	114.55	117.70
27	B8	111	A	C4-C5-C6	6.30	120.15	117.00
27	B8	535	G	O4'-C1'-N9	6.30	113.24	108.20
27	B8	1287	A	O4'-C1'-N9	6.30	113.24	108.20
27	B8	1972	G	C5-C6-O6	-6.30	124.82	128.60
1	AA	106	C	N3-C4-N4	6.29	122.41	118.00
1	AA	675	A	C4-C5-C6	6.29	120.15	117.00
27	B8	936	A	C4-C5-C6	6.29	120.15	117.00
27	B8	2151	U	O4'-C1'-N1	6.29	113.24	108.20
27	B8	2591	C	N3-C4-N4	6.29	122.41	118.00
1	AA	81	A	C4-C5-C6	6.29	120.15	117.00
1	AA	432	A	C4-C5-C6	6.29	120.15	117.00
1	AA	937	A	C4-C5-C6	6.29	120.15	117.00
27	B8	1469	A	O4'-C1'-N9	6.29	113.23	108.20
27	B8	2216	G	O4'-C1'-N9	6.29	113.23	108.20
1	AA	397	A	C4-C5-C6	6.29	120.15	117.00
1	AA	509	A	C4-C5-C6	6.29	120.15	117.00
1	AA	932	C	N3-C4-N4	6.29	122.40	118.00
26	B7	8	C	N3-C4-N4	6.29	122.40	118.00
27	B8	711	G	C5-C6-O6	-6.29	124.83	128.60
27	B8	1847	A	C4-C5-C6	6.29	120.15	117.00
1	AA	299	G	O4'-C1'-N9	6.29	113.23	108.20
1	AA	320	A	C5-C6-N6	-6.29	118.67	123.70
1	AA	1437	A	C5-C6-N6	-6.29	118.67	123.70
27	B8	1698	A	C4-C5-C6	6.29	120.14	117.00
27	B8	2430	A	C5-C6-N6	-6.29	118.67	123.70
1	AA	1000	A	C5-C6-N6	-6.29	118.67	123.70
1	AA	1028	C	N3-C4-N4	6.29	122.40	118.00
3	AV	76	C	N3-C4-N4	6.29	122.40	118.00
27	B8	298	G	N3-C2-N2	6.29	124.30	119.90
27	B8	438	G	O4'-C1'-N9	6.29	113.23	108.20
27	B8	641	U	O4'-C1'-N1	6.29	113.23	108.20
27	B8	1117	C	N3-C4-N4	6.29	122.40	118.00
27	B8	1214	A	O4'-C1'-N9	6.29	113.23	108.20
27	B8	1279	G	O4'-C1'-N9	6.29	113.23	108.20
27	B8	2042	A	C4-C5-C6	6.29	120.14	117.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	2353	G	O4'-C1'-N9	6.29	113.23	108.20
1	AA	645	G	O4'-C1'-N9	6.29	113.23	108.20
27	B8	2218	G	O4'-C1'-N9	6.29	113.23	108.20
27	B8	2266	A	C4-C5-C6	6.29	120.14	117.00
1	AA	199	A	C5-C6-N6	-6.29	118.67	123.70
1	AA	255	G	O4'-C1'-N9	6.29	113.23	108.20
1	AA	765	G	C5-C6-O6	-6.29	124.83	128.60
1	AA	886	G	O4'-C1'-N9	6.29	113.23	108.20
1	AA	934	C	N3-C4-C5	-6.29	119.39	121.90
1	AA	1397	C	N3-C4-N4	6.29	122.40	118.00
27	B8	25	U	O4'-C1'-N1	6.29	113.23	108.20
27	B8	484	C	N3-C4-N4	6.29	122.40	118.00
27	B8	675	A	C4-C5-C6	6.29	120.14	117.00
27	B8	681	G	O4'-C1'-N9	6.29	113.23	108.20
1	AA	161	A	C4-C5-C6	6.28	120.14	117.00
1	AA	1102	A	C4-C5-C6	6.28	120.14	117.00
1	AA	1488	G	O4'-C1'-N9	6.28	113.23	108.20
27	B8	886	A	C4-C5-C6	6.28	120.14	117.00
27	B8	982	C	O4'-C1'-N1	6.28	113.23	108.20
27	B8	1244	A	O4'-C1'-N9	6.28	113.23	108.20
27	B8	1593	A	C4-C5-C6	6.28	120.14	117.00
27	B8	2050	C	O4'-C1'-N1	6.28	113.23	108.20
27	B8	2827	C	N3-C4-N4	6.28	122.40	118.00
27	B8	125	A	C4-C5-C6	6.28	120.14	117.00
27	B8	1928	A	C4-C5-C6	6.28	120.14	117.00
27	B8	2205	A	O4'-C1'-N9	6.28	113.23	108.20
27	B8	2738	A	C5-C6-N1	-6.28	114.56	117.70
27	B8	379	G	O4'-C1'-N9	6.28	113.22	108.20
27	B8	482	A	C4-C5-C6	6.28	120.14	117.00
27	B8	505	A	C4-C5-C6	6.28	120.14	117.00
27	B8	572	A	C4-C5-C6	6.28	120.14	117.00
27	B8	1104	C	N3-C4-C5	-6.28	119.39	121.90
27	B8	2407	A	C4-C5-C6	6.28	120.14	117.00
27	B8	2612	C	N3-C4-N4	6.28	122.40	118.00
27	B8	2008	C	N3-C4-N4	6.28	122.39	118.00
1	AA	214	C	N3-C4-N4	6.28	122.39	118.00
1	AA	1398	A	C4-C5-C6	6.28	120.14	117.00
27	B8	1695	G	C5-C6-O6	-6.28	124.83	128.60
27	B8	2351	G	N3-C2-N2	6.28	124.30	119.90
27	B8	2745	C	N3-C4-N4	6.28	122.39	118.00
27	B8	2748	A	O4'-C1'-N9	6.28	113.22	108.20
1	AA	1415	G	O4'-C1'-N9	6.28	113.22	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	6	A	C4-C5-C6	6.28	120.14	117.00
27	B8	188	G	O4'-C1'-N9	6.28	113.22	108.20
27	B8	251	A	C5-C6-N1	-6.28	114.56	117.70
27	B8	1246	A	O4'-C1'-N9	6.28	113.22	108.20
27	B8	1579	A	C5-C6-N6	-6.28	118.68	123.70
27	B8	1596	A	O4'-C1'-N9	6.28	113.22	108.20
27	B8	1668	A	C4-C5-C6	6.28	120.14	117.00
27	B8	1864	U	O4'-C1'-N1	6.28	113.22	108.20
3	AV	68	G	O4'-C1'-N9	6.27	113.22	108.20
26	B7	50	A	O4'-C1'-N9	6.27	113.22	108.20
27	B8	1124	G	O4'-C1'-N9	6.27	113.22	108.20
27	B8	1353	A	O4'-C1'-N9	6.27	113.22	108.20
27	B8	1813	G	O4'-C1'-N9	6.27	113.22	108.20
27	B8	1988	G	O4'-C1'-N9	6.27	113.22	108.20
27	B8	2745	C	O4'-C1'-N1	6.27	113.22	108.20
1	AA	179	A	C4-C5-C6	6.27	120.14	117.00
1	AA	670	G	O4'-C1'-N9	6.27	113.22	108.20
1	AA	1525	G	C5-C6-O6	-6.27	124.84	128.60
2	AX	22	A	C4-C5-C6	6.27	120.14	117.00
27	B8	671	C	N3-C4-N4	6.27	122.39	118.00
27	B8	2518	A	C5-C6-N6	-6.27	118.68	123.70
27	B8	2558	C	N3-C4-N4	6.27	122.39	118.00
1	AA	334	C	N3-C4-N4	6.27	122.39	118.00
1	AA	990	C	N3-C4-N4	6.27	122.39	118.00
1	AA	1066	C	N3-C4-N4	6.27	122.39	118.00
27	B8	136	G	O4'-C1'-N9	6.27	113.22	108.20
27	B8	707	G	C5-C6-O6	-6.27	124.84	128.60
1	AA	40	C	N3-C4-N4	6.27	122.39	118.00
1	AA	958	A	C4-C5-C6	6.27	120.14	117.00
1	AA	1361	G	C5-C6-O6	-6.27	124.84	128.60
27	B8	892	A	C4-C5-C6	6.27	120.14	117.00
27	B8	1582	C	N3-C4-N4	6.27	122.39	118.00
27	B8	2335	A	O4'-C1'-N9	6.27	113.22	108.20
27	B8	2391	G	C5-C6-O6	-6.27	124.84	128.60
27	B8	2855	C	N3-C4-N4	6.27	122.39	118.00
1	AA	1145	A	C5-C6-N1	-6.27	114.57	117.70
27	B8	1127	A	C5-C6-N6	-6.27	118.69	123.70
27	B8	1673	G	C5-C6-O6	-6.27	124.84	128.60
27	B8	2715	C	N3-C4-N4	6.27	122.39	118.00
1	AA	357	G	C5-C6-O6	-6.27	124.84	128.60
27	B8	1085	A	C5-C6-N6	-6.27	118.69	123.70
27	B8	1433	A	O4'-C1'-N9	6.27	113.21	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	2579	C	N3-C4-N4	6.27	122.39	118.00
1	AA	130	A	C4-C5-C6	6.26	120.13	117.00
1	AA	1357	A	C4-C5-C6	6.26	120.13	117.00
26	B7	20	G	O4'-C1'-N9	6.26	113.21	108.20
27	B8	583	G	O4'-C1'-N9	6.26	113.21	108.20
27	B8	861	A	C5-C6-N6	-6.26	118.69	123.70
27	B8	1927	A	C5-C6-N1	-6.26	114.57	117.70
27	B8	1969	A	C4-C5-C6	6.26	120.13	117.00
27	B8	2274	A	C5-C6-N6	-6.26	118.69	123.70
27	B8	2516	A	O4'-C1'-N9	6.26	113.21	108.20
1	AA	313	A	O4'-C1'-N9	6.26	113.21	108.20
1	AA	1422	G	O4'-C1'-N9	6.26	113.21	108.20
27	B8	1705	A	C5-C6-N6	-6.26	118.69	123.70
1	AA	266	G	C5-C6-O6	-6.26	124.84	128.60
1	AA	838	G	O4'-C1'-N9	6.26	113.21	108.20
1	AA	962	C	N3-C4-N4	6.26	122.38	118.00
1	AA	1363	A	C4-C5-C6	6.26	120.13	117.00
27	B8	651	G	O4'-C1'-N9	6.26	113.21	108.20
27	B8	1957	C	N3-C4-N4	6.26	122.38	118.00
27	B8	2771	C	N3-C4-N4	6.26	122.38	118.00
1	AA	576	C	O4'-C1'-N1	6.26	113.21	108.20
27	B8	38	A	C4-C5-C6	6.26	120.13	117.00
27	B8	177	G	C5-C6-O6	-6.26	124.84	128.60
27	B8	2736	A	C4-C5-C6	6.26	120.13	117.00
1	AA	300	A	C5-C6-N6	-6.26	118.69	123.70
27	B8	1434	A	C5-C6-N6	-6.26	118.69	123.70
27	B8	2513	A	C5-C6-N1	-6.26	114.57	117.70
1	AA	338	A	C4-C5-C6	6.26	120.13	117.00
1	AA	746	A	C4-C5-C6	6.26	120.13	117.00
1	AA	1014	A	C4-C5-C6	6.26	120.13	117.00
1	AA	1420	U	O4'-C1'-N1	6.26	113.20	108.20
26	B7	115	A	C5-C6-N6	-6.26	118.69	123.70
27	B8	1143	A	C5-C6-N6	-6.26	118.69	123.70
27	B8	2253	G	O4'-C1'-N9	6.26	113.20	108.20
27	B8	2274	A	C4-C5-C6	6.26	120.13	117.00
1	AA	1129	C	N3-C4-N4	6.25	122.38	118.00
27	B8	2631	G	O4'-C1'-N9	6.25	113.20	108.20
27	B8	2778	A	C4-C5-C6	6.25	120.13	117.00
1	AA	758	C	N3-C4-N4	6.25	122.38	118.00
27	B8	1187	G	O4'-C1'-N9	6.25	113.20	108.20
27	B8	1228	G	O4'-C1'-N9	6.25	113.20	108.20
1	AA	23	C	N3-C4-N4	6.25	122.38	118.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	98	A	C4-C5-C6	6.25	120.13	117.00
27	B8	1088	A	C4-C5-C6	6.25	120.13	117.00
27	B8	1901	A	C4-C5-C6	6.25	120.13	117.00
27	B8	2222	C	N3-C4-N4	6.25	122.38	118.00
27	B8	2843	G	O4'-C1'-N9	6.25	113.20	108.20
27	B8	1900	A	C5-C6-N1	-6.25	114.58	117.70
1	AA	988	G	O4'-C1'-N9	6.25	113.20	108.20
1	AA	1038	C	N3-C4-N4	6.25	122.38	118.00
26	B7	27	C	N3-C4-N4	6.25	122.37	118.00
27	B8	182	A	C4-C5-C6	6.25	120.12	117.00
27	B8	246	C	N3-C4-N4	6.25	122.37	118.00
27	B8	966	G	O4'-C1'-N9	6.25	113.20	108.20
27	B8	1867	G	O4'-C1'-N9	6.25	113.20	108.20
27	B8	2043	C	N3-C4-N4	6.25	122.37	118.00
28	BA	314	GLN	CB-CA-C	6.25	122.89	110.40
1	AA	51	A	C4-C5-C6	6.25	120.12	117.00
1	AA	848	C	N3-C4-N4	6.25	122.37	118.00
1	AA	1269	A	C5-C6-N6	-6.25	118.70	123.70
27	B8	1367	A	O4'-C1'-N9	6.25	113.20	108.20
27	B8	2316	G	O4'-C1'-N9	6.25	113.20	108.20
28	BA	401	PHE	N-CA-CB	6.25	121.84	110.60
1	AA	1022	A	C5-C6-N1	-6.25	114.58	117.70
27	B8	33	C	N3-C4-N4	6.25	122.37	118.00
27	B8	2105	U	O4'-C1'-N1	6.25	113.20	108.20
27	B8	2439	A	C4-C5-C6	6.25	120.12	117.00
1	AA	9	G	O4'-C1'-N9	6.24	113.19	108.20
1	AA	607	A	C4-C5-C6	6.24	120.12	117.00
1	AA	858	G	C5-C6-O6	-6.24	124.85	128.60
1	AA	1053	G	C5-C6-O6	-6.24	124.85	128.60
26	B7	84	G	O4'-C1'-N9	6.24	113.19	108.20
27	B8	378	C	N3-C4-N4	6.24	122.37	118.00
27	B8	402	A	O4'-C1'-N9	6.24	113.19	108.20
27	B8	509	C	N3-C4-C5	-6.24	119.40	121.90
27	B8	1482	G	O4'-C1'-N9	6.24	113.19	108.20
27	B8	2613	U	O4'-C1'-N1	6.24	113.19	108.20
27	B8	2646	C	N3-C4-N4	6.24	122.37	118.00
1	AA	864	A	C4-C5-C6	6.24	120.12	117.00
27	B8	1557	C	N3-C4-N4	6.24	122.37	118.00
27	B8	1871	A	C4-C5-C6	6.24	120.12	117.00
1	AA	1445	U	O4'-C1'-N1	6.24	113.19	108.20
27	B8	42	A	O4'-C1'-N9	6.24	113.19	108.20
27	B8	670	A	C4-C5-C6	6.24	120.12	117.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	759	G	O4'-C1'-N9	6.24	113.19	108.20
27	B8	1240	U	O4'-C1'-N1	6.24	113.19	108.20
27	B8	1620	G	O4'-C1'-N9	6.24	113.19	108.20
27	B8	1659	G	O4'-C1'-N9	6.24	113.19	108.20
1	AA	1048	G	O4'-C1'-N9	6.24	113.19	108.20
1	AA	1231	G	C5-C6-O6	-6.24	124.86	128.60
27	B8	984	A	C4-C5-C6	6.24	120.12	117.00
27	B8	1510	G	O4'-C1'-N9	6.24	113.19	108.20
27	B8	1687	G	C5-C6-O6	-6.24	124.86	128.60
27	B8	2726	A	C4-C5-C6	6.24	120.12	117.00
1	AA	624	C	N3-C4-N4	6.24	122.37	118.00
1	AA	675	A	O4'-C1'-N9	6.24	113.19	108.20
1	AA	845	A	C4-C5-C6	6.24	120.12	117.00
27	B8	195	A	C5-C6-N6	-6.24	118.71	123.70
27	B8	986	C	N3-C4-N4	6.24	122.37	118.00
27	B8	1638	C	N3-C4-N4	6.24	122.37	118.00
27	B8	1885	A	C4-C5-C6	6.24	120.12	117.00
27	B8	2719	G	C5-C6-O6	-6.24	124.86	128.60
1	AA	415	A	C4-C5-C6	6.24	120.12	117.00
1	AA	1288	A	C4-C5-C6	6.24	120.12	117.00
1	AA	1385	G	O4'-C1'-N9	6.24	113.19	108.20
26	B7	53	A	C4-C5-C6	6.24	120.12	117.00
27	B8	415	A	C5-C6-N6	-6.24	118.71	123.70
27	B8	1356	G	C5-C6-O6	-6.24	124.86	128.60
26	B7	3	C	N3-C4-N4	6.23	122.36	118.00
27	B8	123	G	O4'-C1'-N9	6.23	113.19	108.20
27	B8	705	A	C5-C6-N6	-6.23	118.71	123.70
27	B8	1131	G	C5-C6-O6	-6.23	124.86	128.60
27	B8	1275	A	C5-C6-N6	-6.23	118.71	123.70
27	B8	1490	A	C4-C5-C6	6.23	120.12	117.00
27	B8	1793	C	N3-C4-N4	6.23	122.36	118.00
1	AA	887	G	O4'-C1'-N9	6.23	113.19	108.20
1	AA	1080	A	C5-C6-N6	-6.23	118.71	123.70
27	B8	210	C	N3-C4-N4	6.23	122.36	118.00
27	B8	696	G	C5-C6-O6	-6.23	124.86	128.60
27	B8	1144	A	C4-C5-C6	6.23	120.12	117.00
27	B8	1726	C	N3-C4-N4	6.23	122.36	118.00
27	B8	2088	A	O4'-C1'-N9	6.23	113.19	108.20
27	B8	2178	C	P-O3'-C3'	6.23	127.18	119.70
27	B8	2463	C	N3-C4-N4	6.23	122.36	118.00
27	B8	2495	G	O4'-C1'-N9	6.23	113.19	108.20
1	AA	27	G	O4'-C1'-N9	6.23	113.19	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	316	C	N3-C4-N4	6.23	122.36	118.00
1	AA	435	A	C4-C5-C6	6.23	120.11	117.00
1	AA	626	G	O4'-C1'-N9	6.23	113.18	108.20
3	AV	27	A	C5-C6-N6	-6.23	118.72	123.70
27	B8	77	G	O4'-C1'-N9	6.23	113.18	108.20
27	B8	429	A	C4-C5-C6	6.23	120.11	117.00
27	B8	718	A	C4-C5-C6	6.23	120.11	117.00
27	B8	2660	A	C4-C5-C6	6.23	120.11	117.00
1	AA	139	A	C5-C6-N6	-6.23	118.72	123.70
27	B8	126	A	C4-C5-C6	6.23	120.11	117.00
27	B8	565	C	N3-C4-N4	6.23	122.36	118.00
27	B8	2886	A	O4'-C1'-N9	6.23	113.18	108.20
1	AA	171	A	C4-C5-C6	6.23	120.11	117.00
1	AA	852	G	C5-C6-O6	-6.23	124.86	128.60
1	AA	1482	G	C5-C6-O6	-6.23	124.86	128.60
1	AA	1502	A	C4-C5-C6	6.23	120.11	117.00
27	B8	2795	C	N3-C4-N4	6.23	122.36	118.00
28	BA	249	ALA	N-CA-CB	6.23	118.82	110.10
27	B8	152	A	C5-C6-N6	-6.23	118.72	123.70
27	B8	2018	G	O4'-C1'-N9	6.23	113.18	108.20
1	AA	77	A	C4-C5-C6	6.22	120.11	117.00
1	AA	474	G	O4'-C1'-N9	6.22	113.18	108.20
27	B8	52	A	C5-C6-N1	-6.22	114.59	117.70
27	B8	621	A	O4'-C1'-N9	6.22	113.18	108.20
27	B8	1317	G	C5-C6-O6	-6.22	124.86	128.60
27	B8	1387	A	C5-C6-N6	-6.22	118.72	123.70
27	B8	1618	A	C4-C5-C6	6.22	120.11	117.00
27	B8	2632	A	C4-C5-C6	6.22	120.11	117.00
1	AA	98	A	C5-C6-N6	-6.22	118.72	123.70
1	AA	1281	C	O4'-C1'-N1	6.22	113.18	108.20
27	B8	111	A	O4'-C1'-N9	6.22	113.18	108.20
27	B8	822	G	O4'-C1'-N9	6.22	113.18	108.20
27	B8	831	G	C5-C6-O6	-6.22	124.87	128.60
27	B8	878	A	C4-C5-C6	6.22	120.11	117.00
27	B8	2225	A	C5-C6-N1	-6.22	114.59	117.70
1	AA	32	A	C4-C5-C6	6.22	120.11	117.00
1	AA	33	A	C4-C5-C6	6.22	120.11	117.00
1	AA	623	C	N3-C4-N4	6.22	122.36	118.00
27	B8	377	G	O4'-C1'-N9	6.22	113.18	108.20
27	B8	1084	A	C4-C5-C6	6.22	120.11	117.00
27	B8	1464	G	O4'-C1'-N9	6.22	113.18	108.20
27	B8	2003	A	C4-C5-C6	6.22	120.11	117.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	15	G	O4'-C1'-N9	6.22	113.17	108.20
1	AA	326	G	C5-C6-O6	-6.22	124.87	128.60
1	AA	1158	C	C2-N1-C1'	6.22	125.64	118.80
5	A0	166	TYR	CB-CG-CD1	6.22	124.73	121.00
27	B8	347	A	C5-C6-N6	-6.22	118.72	123.70
27	B8	1331	G	C5-C6-O6	-6.22	124.87	128.60
27	B8	1696	G	O4'-C1'-N9	6.22	113.18	108.20
27	B8	1934	C	N3-C4-N4	6.22	122.35	118.00
27	B8	2392	A	C4-C5-C6	6.22	120.11	117.00
27	B8	2577	A	C4-C5-C6	6.22	120.11	117.00
27	B8	2753	A	C4-C5-C6	6.22	120.11	117.00
27	B8	2816	G	O4'-C1'-N9	6.22	113.18	108.20
1	AA	144	G	O4'-C1'-N9	6.22	113.17	108.20
1	AA	1274	A	O4'-C1'-N9	6.22	113.17	108.20
1	AA	1276	G	O4'-C1'-N9	6.22	113.17	108.20
27	B8	629	G	O4'-C1'-N9	6.22	113.17	108.20
27	B8	1762	A	C4-C5-C6	6.22	120.11	117.00
27	B8	2704	C	N3-C4-N4	6.22	122.35	118.00
1	AA	192	A	C4-C5-C6	6.22	120.11	117.00
1	AA	713	G	O4'-C1'-N9	6.22	113.17	108.20
1	AA	732	C	N3-C4-N4	6.22	122.35	118.00
1	AA	1046	A	C5-C6-N6	-6.22	118.73	123.70
1	AA	1526	G	O4'-C1'-N9	6.22	113.17	108.20
27	B8	386	G	C5-C6-O6	-6.22	124.87	128.60
27	B8	1205	A	C4-C5-C6	6.22	120.11	117.00
1	AA	10	A	C4-C5-C6	6.21	120.11	117.00
1	AA	16	A	C4-C5-C6	6.21	120.11	117.00
1	AA	463	U	O4'-C1'-N1	6.21	113.17	108.20
1	AA	1224	U	O4'-C1'-N1	6.21	113.17	108.20
27	B8	267	C	N3-C4-N4	6.21	122.35	118.00
27	B8	323	C	C6-N1-C1'	-6.21	113.34	120.80
27	B8	454	A	C4-C5-C6	6.21	120.11	117.00
27	B8	1722	A	C5-C6-N1	-6.21	114.59	117.70
27	B8	1892	C	N3-C4-N4	6.21	122.35	118.00
27	B8	1966	A	C4-C5-C6	6.21	120.11	117.00
1	AA	621	A	C4-C5-C6	6.21	120.11	117.00
2	AX	21	A	C4-C5-C6	6.21	120.11	117.00
27	B8	1244	A	C5-C6-N6	-6.21	118.73	123.70
1	AA	681	A	C5-C6-N1	-6.21	114.59	117.70
1	AA	745	G	O4'-C1'-N9	6.21	113.17	108.20
1	AA	964	A	C4-C5-C6	6.21	120.11	117.00
27	B8	680	C	N3-C4-N4	6.21	122.35	118.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	925	A	C5-C6-N1	-6.21	114.59	117.70
27	B8	1054	A	C4-C5-C6	6.21	120.11	117.00
27	B8	1321	A	C4-C5-C6	6.21	120.11	117.00
27	B8	2126	A	C4-C5-C6	6.21	120.11	117.00
27	B8	2738	A	C4-C5-C6	6.21	120.11	117.00
27	B8	2792	A	C4-C5-C6	6.21	120.11	117.00
27	B8	360	U	O4'-C1'-N1	6.21	113.17	108.20
27	B8	1713	A	C5-C6-N1	-6.21	114.60	117.70
27	B8	2879	A	C4-C5-C6	6.21	120.11	117.00
1	AA	227	G	O4'-C1'-N9	6.21	113.17	108.20
1	AA	359	G	O4'-C1'-N9	6.21	113.17	108.20
1	AA	1057	G	C5-C6-O6	-6.21	124.88	128.60
1	AA	1092	A	C4-C5-C6	6.21	120.10	117.00
27	B8	563	A	C4-C5-C6	6.21	120.10	117.00
27	B8	1969	A	O4'-C1'-N9	6.21	113.17	108.20
27	B8	2071	A	C4-C5-C6	6.21	120.10	117.00
27	B8	2114	A	C4-C5-C6	6.21	120.10	117.00
27	B8	2223	G	O4'-C1'-N9	6.21	113.17	108.20
27	B8	2649	C	N3-C4-N4	6.21	122.34	118.00
1	AA	599	C	N3-C4-N4	6.21	122.34	118.00
1	AA	855	U	O4'-C1'-N1	6.21	113.16	108.20
27	B8	117	G	O4'-C1'-N9	6.21	113.16	108.20
27	B8	119	A	O4'-C1'-N9	6.21	113.16	108.20
27	B8	840	C	N3-C4-N4	6.21	122.34	118.00
27	B8	1052	C	N3-C4-N4	6.21	122.34	118.00
1	AA	285	C	N3-C4-N4	6.20	122.34	118.00
1	AA	349	A	C5-C6-N1	-6.20	114.60	117.70
1	AA	524	G	O4'-C1'-N9	6.20	113.16	108.20
27	B8	1301	A	C4-C5-C6	6.20	120.10	117.00
27	B8	1316	U	O4'-C1'-N1	6.20	113.16	108.20
27	B8	2038	G	C5-C6-O6	-6.20	124.88	128.60
27	B8	2273	A	C4-C5-C6	6.20	120.10	117.00
1	AA	363	A	C4-C5-C6	6.20	120.10	117.00
27	B8	384	A	C4-C5-C6	6.20	120.10	117.00
27	B8	2764	A	C4-C5-C6	6.20	120.10	117.00
1	AA	112	G	C5-C6-O6	-6.20	124.88	128.60
27	B8	1586	A	C4-C5-C6	6.20	120.10	117.00
27	B8	1916	A	C4-C5-C6	6.20	120.10	117.00
27	B8	2491	U	O4'-C1'-N1	6.20	113.16	108.20
1	AA	186	C	N3-C4-N4	6.20	122.34	118.00
1	AA	494	G	C5-C6-O6	-6.20	124.88	128.60
1	AA	895	G	O4'-C1'-N9	6.20	113.16	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	964	A	C5-C6-N6	-6.20	118.74	123.70
1	AA	1236	A	C5-C6-N6	-6.20	118.74	123.70
27	B8	326	G	O4'-C1'-N9	6.20	113.16	108.20
1	AA	1256	A	C4-C5-C6	6.20	120.10	117.00
1	AA	1357	A	C5-C6-N6	-6.20	118.74	123.70
27	B8	1253	A	C4-C5-C6	6.20	120.10	117.00
1	AA	1421	G	C5-C6-O6	-6.20	124.88	128.60
1	AA	1457	G	O4'-C1'-N9	6.20	113.16	108.20
27	B8	26	G	C5-C6-O6	-6.20	124.88	128.60
27	B8	2614	A	C4-C5-C6	6.20	120.10	117.00
27	B8	2706	A	O4'-C1'-N9	6.20	113.16	108.20
1	AA	538	G	O4'-C1'-N9	6.19	113.16	108.20
1	AA	741	G	C5-C6-O6	-6.19	124.88	128.60
27	B8	21	A	C4-C5-C6	6.19	120.10	117.00
27	B8	1022	G	O4'-C1'-N9	6.19	113.16	108.20
1	AA	129	A	O4'-C1'-N9	6.19	113.16	108.20
1	AA	1122	U	O4'-C1'-N1	6.19	113.15	108.20
27	B8	160	A	C4-C5-C6	6.19	120.10	117.00
27	B8	461	C	N3-C4-N4	6.19	122.33	118.00
27	B8	1737	G	P-O3'-C3'	6.19	127.13	119.70
27	B8	2168	G	N3-C2-N2	6.19	124.23	119.90
27	B8	2354	C	N3-C4-N4	6.19	122.33	118.00
27	B8	2557	G	O4'-C1'-N9	6.19	113.15	108.20
1	AA	622	A	O4'-C1'-N9	6.19	113.15	108.20
1	AA	777	A	O4'-C1'-N9	6.19	113.15	108.20
1	AA	940	C	N3-C4-N4	6.19	122.33	118.00
26	B7	49	C	N3-C4-N4	6.19	122.33	118.00
27	B8	730	A	C4-C5-C6	6.19	120.09	117.00
27	B8	1704	C	N3-C4-N4	6.19	122.33	118.00
1	AA	86	G	O4'-C1'-N9	6.19	113.15	108.20
1	AA	577	G	O4'-C1'-N9	6.19	113.15	108.20
27	B8	661	A	C4-C5-C6	6.19	120.09	117.00
27	B8	1095	A	C5-C6-N6	-6.19	118.75	123.70
27	B8	2080	A	C4-C5-C6	6.19	120.09	117.00
27	B8	2184	A	C5-C6-N6	-6.19	118.75	123.70
1	AA	865	A	C5-C6-N6	-6.19	118.75	123.70
27	B8	1042	G	O4'-C1'-N9	6.19	113.15	108.20
27	B8	2741	A	C4-C5-C6	6.19	120.09	117.00
1	AA	460	A	C5-C6-N1	-6.19	114.61	117.70
27	B8	1413	A	C5-C6-N6	-6.19	118.75	123.70
27	B8	1422	G	O4'-C1'-N9	6.19	113.15	108.20
27	B8	1544	A	C4-C5-C6	6.19	120.09	117.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	1644	C	N3-C4-N4	6.19	122.33	118.00
27	B8	2453	A	C5-C6-N6	-6.19	118.75	123.70
1	AA	66	A	C4-C5-C6	6.18	120.09	117.00
26	B7	29	A	C5-C6-N6	-6.18	118.75	123.70
27	B8	68	G	O4'-C1'-N9	6.18	113.15	108.20
27	B8	168	G	O4'-C1'-N9	6.18	113.15	108.20
27	B8	491	G	C5'-C4'-O4'	6.18	116.52	109.10
27	B8	1818	U	O4'-C1'-N1	6.18	113.15	108.20
27	B8	1900	A	C4-C5-C6	6.18	120.09	117.00
1	AA	35	G	O4'-C1'-N9	6.18	113.15	108.20
1	AA	373	A	C4-C5-C6	6.18	120.09	117.00
1	AA	1418	A	C5-C6-N6	-6.18	118.75	123.70
27	B8	415	A	C4-C5-C6	6.18	120.09	117.00
27	B8	465	G	C5-C6-O6	-6.18	124.89	128.60
27	B8	1144	A	C5-C6-N6	-6.18	118.75	123.70
27	B8	165	A	C4-C5-C6	6.18	120.09	117.00
27	B8	1504	A	C4-C5-C6	6.18	120.09	117.00
27	B8	2025	C	N3-C4-C5	-6.18	119.43	121.90
1	AA	431	A	O4'-C1'-N9	6.18	113.14	108.20
1	AA	1153	G	O4'-C1'-N9	6.18	113.14	108.20
27	B8	71	A	C4-C5-C6	6.18	120.09	117.00
27	B8	1008	A	C4-C5-C6	6.18	120.09	117.00
1	AA	1344	C	N3-C4-N4	6.18	122.32	118.00
27	B8	2	G	O4'-C1'-N9	6.18	113.14	108.20
27	B8	293	U	O4'-C1'-N1	6.18	113.14	108.20
27	B8	2330	G	O4'-C1'-N9	6.18	113.14	108.20
27	B8	2746	U	O4'-C1'-N1	6.18	113.14	108.20
1	AA	181	A	O4'-C1'-N9	6.18	113.14	108.20
1	AA	466	A	C4-C5-C6	6.18	120.09	117.00
27	B8	33	C	O4'-C1'-N1	6.18	113.14	108.20
27	B8	197	A	C4-C5-C6	6.18	120.09	117.00
27	B8	655	A	C5-C6-N6	-6.18	118.76	123.70
27	B8	816	C	N3-C4-N4	6.18	122.32	118.00
27	B8	1069	A	C4-C5-C6	6.18	120.09	117.00
27	B8	1810	A	C4-C5-C6	6.18	120.09	117.00
27	B8	2488	G	O4'-C1'-N9	6.18	113.14	108.20
1	AA	236	A	C4-C5-C6	6.17	120.09	117.00
1	AA	1044	A	C4-C5-C6	6.17	120.09	117.00
1	AA	1309	G	O4'-C1'-N9	6.17	113.14	108.20
27	B8	172	A	O4'-C1'-N9	6.17	113.14	108.20
27	B8	368	A	C4-C5-C6	6.17	120.09	117.00
27	B8	620	G	O4'-C1'-N9	6.17	113.14	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	1543	G	O4'-C1'-N9	6.17	113.14	108.20
27	B8	2375	G	C5-C6-O6	-6.17	124.89	128.60
27	B8	2461	A	C4-C5-C6	6.17	120.09	117.00
27	B8	2512	C	N3-C4-N4	6.17	122.32	118.00
27	B8	2810	A	C4-C5-C6	6.17	120.09	117.00
1	AA	872	A	C4-C5-C6	6.17	120.09	117.00
1	AA	879	C	N3-C4-N4	6.17	122.32	118.00
1	AA	1093	A	C4-C5-C6	6.17	120.09	117.00
1	AA	1099	G	C5-C6-O6	-6.17	124.90	128.60
27	B8	389	G	O4'-C1'-N9	6.17	113.14	108.20
27	B8	947	A	C4-C5-C6	6.17	120.09	117.00
27	B8	2047	C	N3-C4-N4	6.17	122.32	118.00
1	AA	294	U	O4'-C1'-N1	6.17	113.14	108.20
1	AA	1449	C	N3-C4-N4	6.17	122.32	118.00
27	B8	282	A	C5-C6-N1	-6.17	114.61	117.70
27	B8	689	A	C4-C5-C6	6.17	120.09	117.00
27	B8	815	C	N3-C4-N4	6.17	122.32	118.00
27	B8	876	C	N3-C4-N4	6.17	122.32	118.00
27	B8	1755	A	C5-C6-N6	-6.17	118.76	123.70
27	B8	2428	G	O4'-C1'-N9	6.17	113.14	108.20
1	AA	749	A	O4'-C1'-N9	6.17	113.14	108.20
27	B8	730	A	C5-C6-N6	-6.17	118.76	123.70
1	AA	265	G	O4'-C1'-N9	6.17	113.13	108.20
1	AA	650	G	C5-C6-O6	-6.17	124.90	128.60
1	AA	664	G	C5-C6-O6	-6.17	124.90	128.60
1	AA	1359	C	N3-C4-N4	6.17	122.32	118.00
27	B8	1039	A	C4-C5-C6	6.17	120.08	117.00
27	B8	1425	G	O4'-C1'-N9	6.17	113.14	108.20
27	B8	2402	U	O4'-C1'-N1	6.17	113.13	108.20
1	AA	328	C	O4'-C1'-N1	6.17	113.13	108.20
1	AA	456	A	C5-C6-N1	-6.17	114.62	117.70
1	AA	630	A	C4-C5-C6	6.17	120.08	117.00
11	AG	161	PHE	CB-CG-CD2	-6.17	116.48	120.80
26	B7	11	C	O4'-C1'-N1	6.17	113.13	108.20
27	B8	606	U	O4'-C1'-N1	6.17	113.13	108.20
27	B8	614	A	C4-C5-C6	6.17	120.08	117.00
27	B8	2386	A	C5-C6-N6	-6.17	118.77	123.70
27	B8	2403	C	N3-C4-N4	6.17	122.32	118.00
27	B8	2765	A	C4-C5-C6	6.17	120.08	117.00
1	AA	442	G	O4'-C1'-N9	6.17	113.13	108.20
18	AN	52	ARG	NE-CZ-NH1	6.17	123.38	120.30
27	B8	492	A	O4'-C1'-N9	6.17	113.13	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	2420	C	N3-C4-N4	6.17	122.31	118.00
26	B7	85	G	O4'-C1'-N9	6.16	113.13	108.20
26	B7	104	A	C5-C6-N6	-6.16	118.77	123.70
27	B8	690	G	C5-C6-O6	-6.16	124.90	128.60
27	B8	1022	G	C5-C6-O6	-6.16	124.90	128.60
27	B8	1885	A	O4'-C1'-N9	6.16	113.13	108.20
27	B8	2152	G	C5-C6-O6	-6.16	124.90	128.60
27	B8	2581	G	C5-C6-O6	-6.16	124.90	128.60
1	AA	1377	A	C4-C5-C6	6.16	120.08	117.00
1	AA	36	C	N3-C4-N4	6.16	122.31	118.00
1	AA	754	C	C2-N1-C1'	6.16	125.58	118.80
1	AA	981	U	O4'-C1'-N1	6.16	113.13	108.20
1	AA	1297	G	O4'-C1'-N9	6.16	113.13	108.20
27	B8	833	A	C4-C5-C6	6.16	120.08	117.00
27	B8	1062	G	O4'-C1'-N9	6.16	113.13	108.20
27	B8	2147	A	C4-C5-C6	6.16	120.08	117.00
1	AA	142	G	O4'-C1'-N9	6.16	113.13	108.20
1	AA	306	A	C4-C5-C6	6.16	120.08	117.00
1	AA	313	A	C5-C6-N6	-6.16	118.77	123.70
1	AA	832	G	O4'-C1'-N9	6.16	113.13	108.20
1	AA	937	A	O4'-C1'-N9	6.16	113.13	108.20
1	AA	956	U	O4'-C1'-N1	6.16	113.13	108.20
1	AA	1022	A	C4-C5-C6	6.16	120.08	117.00
27	B8	663	G	O4'-C1'-N9	6.16	113.13	108.20
27	B8	2166	U	O4'-C1'-N1	6.16	113.13	108.20
27	B8	2882	A	C5-C6-N1	-6.16	114.62	117.70
1	AA	1251	A	O4'-C1'-N9	6.16	113.13	108.20
27	B8	988	A	C4-C5-C6	6.16	120.08	117.00
27	B8	1133	A	C4-C5-C6	6.16	120.08	117.00
27	B8	1251	C	N3-C4-N4	6.16	122.31	118.00
1	AA	33	A	C5-C6-N6	-6.16	118.78	123.70
1	AA	410	G	N3-C2-N2	6.16	124.21	119.90
1	AA	1096	C	N3-C4-N4	6.16	122.31	118.00
1	AA	1339	A	C5-C6-N1	-6.16	114.62	117.70
27	B8	1918	A	C4-C5-C6	6.16	120.08	117.00
27	B8	2267	A	C5-C6-N6	-6.16	118.78	123.70
1	AA	862	C	N3-C4-N4	6.15	122.31	118.00
27	B8	644	A	C5-C6-N6	-6.15	118.78	123.70
27	B8	789	A	C4-C5-C6	6.15	120.08	117.00
1	AA	764	C	N3-C4-N4	6.15	122.31	118.00
1	AA	1098	C	N3-C4-N4	6.15	122.31	118.00
1	AA	1242	G	O4'-C1'-N9	6.15	113.12	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1434	A	C5-C6-N6	-6.15	118.78	123.70
27	B8	1608	A	C5-C6-N1	-6.15	114.62	117.70
27	B8	2531	A	C5-C6-N1	-6.15	114.62	117.70
1	AA	908	A	O4'-C1'-N9	6.15	113.12	108.20
1	AA	1128	C	N3-C4-C5	-6.15	119.44	121.90
26	B7	34	A	O4'-C1'-N9	6.15	113.12	108.20
27	B8	342	A	C4-C5-C6	6.15	120.08	117.00
27	B8	472	A	C4-C5-C6	6.15	120.08	117.00
27	B8	927	A	C4-C5-C6	6.15	120.08	117.00
27	B8	1307	A	O4'-C1'-N9	6.15	113.12	108.20
27	B8	1417	C	N3-C4-N4	6.15	122.31	118.00
27	B8	1897	G	O4'-C1'-N9	6.15	113.12	108.20
27	B8	2037	A	O4'-C1'-N9	6.15	113.12	108.20
27	B8	2388	A	C4-C5-C6	6.15	120.08	117.00
27	B8	2481	G	C5-C6-O6	-6.15	124.91	128.60
1	AA	1061	G	O4'-C1'-N9	6.15	113.12	108.20
27	B8	792	A	C4-C5-C6	6.15	120.07	117.00
27	B8	953	G	O4'-C1'-N9	6.15	113.12	108.20
27	B8	1805	A	O4'-C1'-N9	6.15	113.12	108.20
27	B8	2717	C	N3-C4-N4	6.15	122.30	118.00
1	AA	311	C	N3-C4-N4	6.15	122.30	118.00
26	B7	91	C	N3-C4-N4	6.15	122.30	118.00
27	B8	1204	A	C4-C5-C6	6.15	120.07	117.00
27	B8	1950	G	C5-C6-O6	-6.15	124.91	128.60
27	B8	2228	G	O4'-C1'-N9	6.15	113.12	108.20
27	B8	2873	A	C5-C6-N6	-6.15	118.78	123.70
1	AA	80	A	C4-C5-C6	6.15	120.07	117.00
27	B8	122	G	O4'-C1'-N9	6.15	113.12	108.20
1	AA	211	G	C5-C6-O6	-6.14	124.91	128.60
1	AA	898	G	C5-C6-O6	-6.14	124.91	128.60
27	B8	146	A	O4'-C1'-N9	6.14	113.12	108.20
27	B8	258	G	O4'-C1'-N9	6.14	113.11	108.20
27	B8	325	G	O4'-C1'-N9	6.14	113.11	108.20
27	B8	1063	G	O4'-C1'-N9	6.14	113.11	108.20
27	B8	1603	A	C4-C5-C6	6.14	120.07	117.00
27	B8	2411	A	C4-C5-C6	6.14	120.07	117.00
1	AA	321	A	O4'-C1'-N9	6.14	113.11	108.20
1	AA	779	C	N3-C4-N4	6.14	122.30	118.00
1	AA	1156	G	N3-C2-N2	6.14	124.20	119.90
1	AA	1435	G	O4'-C1'-N9	6.14	113.11	108.20
27	B8	218	A	C4-C5-C6	6.14	120.07	117.00
27	B8	367	G	O4'-C1'-N9	6.14	113.11	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	160	A	C4-C5-C6	6.14	120.07	117.00
1	AA	743	A	C4-C5-C6	6.14	120.07	117.00
1	AA	790	A	C4-C5-C6	6.14	120.07	117.00
1	AA	1374	A	C5-C6-N6	-6.14	118.79	123.70
26	B7	27	C	P-O5'-C5'	6.14	130.72	120.90
27	B8	309	A	C4-C5-C6	6.14	120.07	117.00
27	B8	354	A	C5-C6-N1	-6.14	114.63	117.70
27	B8	910	A	C4-C5-C6	6.14	120.07	117.00
1	AA	297	G	O4'-C1'-N9	6.14	113.11	108.20
27	B8	73	A	O4'-C1'-N9	6.14	113.11	108.20
27	B8	144	A	C4-C5-C6	6.14	120.07	117.00
27	B8	226	A	C5-C6-N6	-6.14	118.79	123.70
27	B8	920	A	O4'-C1'-N9	6.14	113.11	108.20
27	B8	1561	C	N3-C4-N4	6.14	122.30	118.00
27	B8	1924	C	N3-C4-N4	6.14	122.30	118.00
1	AA	393	A	C4-C5-C6	6.13	120.07	117.00
1	AA	873	A	C5-C6-N1	-6.13	114.63	117.70
26	B7	86	G	O4'-C1'-N9	6.13	113.11	108.20
26	B7	87	U	O4'-C1'-N1	6.13	113.11	108.20
27	B8	585	G	N3-C2-N2	6.13	124.19	119.90
27	B8	1287	A	C4-C5-C6	6.13	120.07	117.00
27	B8	1358	G	O4'-C1'-N9	6.13	113.11	108.20
27	B8	1495	A	C4-C5-C6	6.13	120.07	117.00
1	AA	572	A	C4-C5-C6	6.13	120.07	117.00
1	AA	675	A	C5-C6-N6	-6.13	118.79	123.70
27	B8	152	A	C4-C5-C6	6.13	120.07	117.00
27	B8	1877	A	C4-C5-C6	6.13	120.07	117.00
1	AA	189	A	C4-C5-C6	6.13	120.07	117.00
1	AA	471	U	O4'-C1'-N1	6.13	113.11	108.20
1	AA	763	G	O4'-C1'-N9	6.13	113.11	108.20
1	AA	817	C	N3-C4-C5	-6.13	119.45	121.90
1	AA	1088	G	O4'-C1'-N9	6.13	113.11	108.20
27	B8	353	C	N3-C4-N4	6.13	122.29	118.00
27	B8	592	A	C5-C6-N1	-6.13	114.63	117.70
27	B8	1134	A	C4-C5-C6	6.13	120.06	117.00
27	B8	1253	A	C5-C6-N1	-6.13	114.63	117.70
27	B8	1431	A	C4-C5-C6	6.13	120.07	117.00
27	B8	1994	C	N3-C4-N4	6.13	122.29	118.00
27	B8	896	A	C4-C5-C6	6.13	120.06	117.00
1	AA	560	A	C4-C5-C6	6.13	120.06	117.00
3	AV	58	A	C4-C5-C6	6.13	120.06	117.00
26	B7	92	C	N3-C4-N4	6.13	122.29	118.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	510	C	N3-C4-N4	6.13	122.29	118.00
27	B8	915	C	N3-C4-N4	6.13	122.29	118.00
27	B8	1752	C	N3-C4-C5	-6.13	119.45	121.90
27	B8	2688	G	C5-C6-O6	-6.13	124.92	128.60
1	AA	724	G	O4'-C1'-N9	6.13	113.10	108.20
1	AA	968	A	C4-C5-C6	6.13	120.06	117.00
1	AA	1318	A	C4-C5-C6	6.13	120.06	117.00
27	B8	743	A	C5-C6-N6	-6.13	118.80	123.70
27	B8	1574	C	N3-C4-N4	6.13	122.29	118.00
27	B8	1654	A	C4-C5-C6	6.13	120.06	117.00
27	B8	1673	G	O4'-C1'-N9	6.13	113.10	108.20
27	B8	2470	G	O4'-C1'-N9	6.13	113.10	108.20
27	B8	30	G	O4'-C1'-N9	6.12	113.10	108.20
27	B8	409	G	O4'-C1'-N9	6.12	113.10	108.20
27	B8	2405	G	N3-C2-N2	6.12	124.19	119.90
1	AA	206	C	N3-C4-N4	6.12	122.29	118.00
1	AA	536	C	N3-C4-N4	6.12	122.29	118.00
1	AA	629	A	O4'-C1'-N9	6.12	113.10	108.20
1	AA	742	G	O4'-C1'-N9	6.12	113.10	108.20
1	AA	1319	A	C4-C5-C6	6.12	120.06	117.00
1	AA	1408	A	O4'-C1'-N9	6.12	113.10	108.20
1	AA	1479	C	N3-C4-C5	-6.12	119.45	121.90
27	B8	584	C	N3-C4-N4	6.12	122.29	118.00
27	B8	858	G	C5-C6-O6	-6.12	124.92	128.60
27	B8	911	A	C4-C5-C6	6.12	120.06	117.00
27	B8	1039	A	O4'-C1'-N9	6.12	113.10	108.20
1	AA	1275	A	C4-C5-C6	6.12	120.06	117.00
1	AA	1441	A	C4-C5-C6	6.12	120.06	117.00
3	AV	70	G	O4'-C1'-N9	6.12	113.10	108.20
27	B8	93	G	O4'-C1'-N9	6.12	113.10	108.20
27	B8	795	C	N3-C4-N4	6.12	122.28	118.00
27	B8	1262	A	C4-C5-C6	6.12	120.06	117.00
27	B8	1529	G	C5-C6-O6	-6.12	124.93	128.60
27	B8	1876	A	O4'-C1'-N9	6.12	113.10	108.20
27	B8	2095	A	C4-C5-C6	6.12	120.06	117.00
1	AA	909	A	O4'-C1'-N9	6.12	113.10	108.20
27	B8	666	A	C5-C6-N6	-6.12	118.80	123.70
1	AA	173	U	O4'-C1'-N1	6.12	113.09	108.20
1	AA	201	G	C5-C6-O6	-6.12	124.93	128.60
1	AA	416	G	O4'-C1'-N9	6.12	113.09	108.20
1	AA	1019	A	C4-C5-C6	6.12	120.06	117.00
27	B8	94	A	O4'-C1'-N9	6.12	113.09	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	1186	G	C5-C6-O6	-6.12	124.93	128.60
27	B8	1288	G	O4'-C1'-N9	6.12	113.09	108.20
27	B8	1393	A	C4-C5-C6	6.12	120.06	117.00
27	B8	1517	G	O4'-C1'-N9	6.12	113.09	108.20
27	B8	1579	A	C4-C5-C6	6.12	120.06	117.00
1	AA	131	A	C4-C5-C6	6.12	120.06	117.00
27	B8	65	U	O4'-C1'-N1	6.12	113.09	108.20
27	B8	1299	G	O4'-C1'-N9	6.12	113.09	108.20
27	B8	1991	U	O4'-C1'-N1	6.12	113.09	108.20
1	AA	238	A	C4-C5-C6	6.12	120.06	117.00
1	AA	295	C	N3-C4-N4	6.12	122.28	118.00
1	AA	309	A	C5-C6-N6	-6.12	118.81	123.70
1	AA	579	A	C4-C5-C6	6.12	120.06	117.00
1	AA	784	A	C4-C5-C6	6.12	120.06	117.00
27	B8	1072	C	N3-C4-N4	6.12	122.28	118.00
27	B8	1354	A	C5-C6-N6	-6.12	118.81	123.70
27	B8	2773	C	N3-C4-N4	6.12	122.28	118.00
1	AA	119	A	C5-C6-N1	-6.11	114.64	117.70
1	AA	942	G	C5-C6-O6	-6.11	124.93	128.60
1	AA	1167	A	C5-C6-N6	-6.11	118.81	123.70
1	AA	1254	A	C5-C6-N1	-6.11	114.64	117.70
27	B8	73	A	C4-C5-C6	6.11	120.06	117.00
27	B8	1366	A	C4-C5-C6	6.11	120.06	117.00
27	B8	2227	A	C4-C5-C6	6.11	120.06	117.00
27	B8	2711	A	C5-C6-N6	-6.11	118.81	123.70
1	AA	545	C	N3-C4-N4	6.11	122.28	118.00
1	AA	953	G	O4'-C1'-N9	6.11	113.09	108.20
27	B8	1215	G	O4'-C1'-N9	6.11	113.09	108.20
27	B8	1590	A	C5-C6-N6	-6.11	118.81	123.70
27	B8	2333	A	C5-C6-N6	-6.11	118.81	123.70
27	B8	2700	A	C5-C6-N6	-6.11	118.81	123.70
1	AA	404	G	O4'-C1'-N9	6.11	113.09	108.20
1	AA	1131	G	C5-C6-O6	-6.11	124.93	128.60
1	AA	1150	A	C4-C5-C6	6.11	120.06	117.00
1	AA	1451	U	O4'-C1'-N1	6.11	113.09	108.20
27	B8	19	A	O4'-C1'-N9	6.11	113.09	108.20
27	B8	127	A	C5-C6-N6	-6.11	118.81	123.70
27	B8	200	U	O4'-C1'-N1	6.11	113.09	108.20
27	B8	502	A	C5-C6-N6	-6.11	118.81	123.70
27	B8	1505	A	C4-C5-C6	6.11	120.06	117.00
27	B8	2361	G	C5-C6-O6	-6.11	124.93	128.60
27	B8	996	A	C4-C5-C6	6.11	120.06	117.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	1168	G	O4'-C1'-N9	6.11	113.09	108.20
27	B8	1179	G	O4'-C1'-N9	6.11	113.09	108.20
27	B8	1359	A	C4-C5-C6	6.11	120.05	117.00
26	B7	62	C	N3-C4-N4	6.11	122.28	118.00
27	B8	151	C	N3-C4-C5	-6.11	119.46	121.90
27	B8	155	A	C5-C6-N1	-6.11	114.65	117.70
27	B8	1718	G	C5-C6-O6	-6.11	124.94	128.60
27	B8	1739	A	O4'-C1'-N9	6.11	113.09	108.20
27	B8	2037	A	C5-C6-N6	-6.11	118.81	123.70
27	B8	2237	G	N3-C2-N2	6.11	124.17	119.90
27	B8	2336	A	C4-C5-C6	6.11	120.05	117.00
27	B8	2622	U	O4'-C1'-N1	6.11	113.09	108.20
27	B8	2799	A	C4-C5-C6	6.11	120.05	117.00
1	AA	8	A	C4-C5-C6	6.11	120.05	117.00
1	AA	8	A	O4'-C1'-N9	6.11	113.08	108.20
1	AA	42	G	O4'-C1'-N9	6.11	113.08	108.20
1	AA	1052	U	O4'-C1'-N1	6.11	113.08	108.20
1	AA	1487	G	C5-C6-O6	-6.11	124.94	128.60
26	B7	78	A	C5-C6-N6	-6.11	118.81	123.70
27	B8	575	A	C4-C5-C6	6.11	120.05	117.00
27	B8	616	A	C4-C5-C6	6.11	120.05	117.00
27	B8	845	A	C4-C5-C6	6.11	120.05	117.00
27	B8	1365	A	C4-C5-C6	6.11	120.05	117.00
27	B8	2042	A	C5-C6-N6	-6.11	118.81	123.70
27	B8	2576	G	C5-C6-O6	-6.11	124.94	128.60
1	AA	1074	G	O4'-C1'-N9	6.10	113.08	108.20
27	B8	1433	A	C4-C5-C6	6.10	120.05	117.00
27	B8	2864	G	O4'-C1'-N9	6.10	113.08	108.20
1	AA	238	A	C5-C6-N6	-6.10	118.82	123.70
27	B8	372	G	O4'-C1'-N9	6.10	113.08	108.20
27	B8	613	A	C4-C5-C6	6.10	120.05	117.00
27	B8	637	A	C4-C5-C6	6.10	120.05	117.00
27	B8	793	A	C4-C5-C6	6.10	120.05	117.00
27	B8	885	C	N3-C4-N4	6.10	122.27	118.00
27	B8	960	A	C4-C5-C6	6.10	120.05	117.00
27	B8	1192	G	O4'-C1'-N9	6.10	113.08	108.20
27	B8	1318	U	O4'-C1'-N1	6.10	113.08	108.20
27	B8	1583	A	O4'-C1'-N9	6.10	113.08	108.20
27	B8	2598	A	C5-C6-N6	-6.10	118.82	123.70
26	B7	58	A	C5-C6-N6	-6.10	118.82	123.70
27	B8	1550	C	N3-C4-N4	6.10	122.27	118.00
27	B8	1868	C	N3-C4-N4	6.10	122.27	118.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	252	U	O4'-C1'-N1	6.10	113.08	108.20
1	AA	722	G	C5-C6-O6	-6.10	124.94	128.60
1	AA	918	A	C4-C5-C6	6.10	120.05	117.00
26	B7	101	A	O4'-C1'-N9	6.10	113.08	108.20
27	B8	474	G	O4'-C1'-N9	6.10	113.08	108.20
27	B8	859	G	N3-C2-N2	6.10	124.17	119.90
27	B8	988	A	O4'-C1'-N9	6.10	113.08	108.20
1	AA	202	G	O4'-C1'-N9	6.10	113.08	108.20
1	AA	840	C	O4'-C1'-N1	6.10	113.08	108.20
27	B8	342	A	C5-C6-N6	-6.10	118.82	123.70
27	B8	825	A	O4'-C1'-N9	6.10	113.08	108.20
27	B8	861	A	O4'-C1'-N9	6.10	113.08	108.20
27	B8	1640	A	C5-C6-N6	-6.10	118.82	123.70
27	B8	1932	A	O4'-C1'-N9	6.10	113.08	108.20
27	B8	2885	G	O4'-C1'-N9	6.10	113.08	108.20
1	AA	18	C	N3-C4-N4	6.10	122.27	118.00
1	AA	718	A	C4-C5-C6	6.10	120.05	117.00
1	AA	726	C	N3-C4-N4	6.10	122.27	118.00
27	B8	630	G	O4'-C1'-N9	6.10	113.08	108.20
1	AA	360	G	O4'-C1'-N9	6.09	113.08	108.20
1	AA	975	A	C4-C5-C6	6.09	120.05	117.00
1	AA	975	A	O4'-C1'-N9	6.09	113.08	108.20
1	AA	1514	G	O4'-C1'-N9	6.09	113.08	108.20
27	B8	883	G	C5-C6-O6	-6.09	124.94	128.60
27	B8	1373	A	O4'-C1'-N9	6.09	113.08	108.20
27	B8	1512	C	N3-C4-N4	6.09	122.27	118.00
27	B8	1973	G	O4'-C1'-N9	6.09	113.08	108.20
27	B8	2589	A	C4-C5-C6	6.09	120.05	117.00
27	B8	2896	C	N3-C4-N4	6.09	122.27	118.00
27	B8	2252	G	C5-C6-O6	-6.09	124.94	128.60
1	AA	761	G	O4'-C1'-N9	6.09	113.07	108.20
1	AA	919	A	C5-C6-N1	-6.09	114.66	117.70
1	AA	1476	A	C5-C6-N1	-6.09	114.65	117.70
27	B8	626	A	C4-C5-C6	6.09	120.05	117.00
27	B8	818	G	C5-C6-O6	-6.09	124.95	128.60
27	B8	2186	G	O4'-C1'-N9	6.09	113.07	108.20
27	B8	2727	A	C4-C5-C6	6.09	120.05	117.00
1	AA	427	U	O4'-C1'-N1	6.09	113.07	108.20
1	AA	1195	C	N3-C4-N4	6.09	122.26	118.00
27	B8	964	C	N3-C4-N4	6.09	122.26	118.00
27	B8	1512	C	O4'-C1'-N1	6.09	113.07	108.20
27	B8	1525	A	C4-C5-C6	6.09	120.04	117.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	2117	A	C4-C5-C6	6.09	120.05	117.00
27	B8	2283	C	N3-C4-N4	6.09	122.26	118.00
27	B8	2288	A	C4-C5-C6	6.09	120.05	117.00
45	BQ	23	TYR	CB-CG-CD1	-6.09	117.35	121.00
1	AA	596	A	C4-C5-C6	6.09	120.04	117.00
1	AA	831	A	O4'-C1'-N9	6.09	113.07	108.20
1	AA	1437	A	C4-C5-C6	6.09	120.04	117.00
1	AA	1458	G	O4'-C1'-N9	6.09	113.07	108.20
26	B7	113	C	N3-C4-N4	6.09	122.26	118.00
27	B8	337	C	N3-C4-N4	6.09	122.26	118.00
27	B8	722	A	C4-C5-C6	6.09	120.04	117.00
27	B8	1014	A	O4'-C1'-N9	6.09	113.07	108.20
27	B8	2207	C	N3-C4-N4	6.09	122.26	118.00
1	AA	649	A	O4'-C1'-N9	6.09	113.07	108.20
27	B8	761	A	C5-C6-N6	-6.09	118.83	123.70
27	B8	1061	U	O4'-C1'-N1	6.09	113.07	108.20
27	B8	1080	A	O4'-C1'-N9	6.09	113.07	108.20
27	B8	2345	G	C5-C6-O6	-6.09	124.95	128.60
1	AA	1185	G	O4'-C1'-N9	6.08	113.07	108.20
27	B8	2670	A	C4-C5-C6	6.08	120.04	117.00
1	AA	527	G	O4'-C1'-N9	6.08	113.07	108.20
1	AA	1508	A	O4'-C1'-N9	6.08	113.07	108.20
27	B8	435	C	O4'-C1'-N1	6.08	113.07	108.20
27	B8	790	U	O4'-C1'-N1	6.08	113.07	108.20
27	B8	918	A	C5-C6-N1	-6.08	114.66	117.70
27	B8	1156	A	C4-C5-C6	6.08	120.04	117.00
27	B8	2566	A	C5-C6-N1	-6.08	114.66	117.70
27	B8	2658	C	N3-C4-N4	6.08	122.26	118.00
1	AA	53	A	C5-C6-N6	-6.08	118.84	123.70
1	AA	221	C	N3-C4-N4	6.08	122.26	118.00
1	AA	403	C	N3-C4-N4	6.08	122.26	118.00
1	AA	483	C	N3-C4-N4	6.08	122.26	118.00
1	AA	539	A	C4-C5-C6	6.08	120.04	117.00
1	AA	1229	A	C4-C5-C6	6.08	120.04	117.00
27	B8	362	A	C4-C5-C6	6.08	120.04	117.00
27	B8	858	G	O4'-C1'-N9	6.08	113.06	108.20
27	B8	1626	A	C4-C5-C6	6.08	120.04	117.00
27	B8	1630	A	O4'-C1'-N9	6.08	113.07	108.20
1	AA	151	A	C5-C6-N1	-6.08	114.66	117.70
27	B8	925	A	C4-C5-C6	6.08	120.04	117.00
27	B8	1566	A	C4-C5-C6	6.08	120.04	117.00
27	B8	2627	G	O4'-C1'-N9	6.08	113.06	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	155	A	C4-C5-C6	6.08	120.04	117.00
1	AA	695	A	C5-C6-N6	-6.08	118.84	123.70
1	AA	1245	C	N3-C4-N4	6.08	122.25	118.00
1	AA	1285	A	C4-C5-C6	6.08	120.04	117.00
27	B8	477	A	C4-C5-C6	6.08	120.04	117.00
27	B8	985	C	N3-C4-N4	6.08	122.25	118.00
27	B8	1151	A	C4-C5-C6	6.08	120.04	117.00
27	B8	1268	A	C4-C5-C6	6.08	120.04	117.00
27	B8	1846	G	O4'-C1'-N9	6.08	113.06	108.20
27	B8	2300	C	N3-C4-N4	6.08	122.25	118.00
27	B8	2494	G	O4'-C1'-N9	6.08	113.06	108.20
27	B8	2792	A	P-O3'-C3'	6.08	127.00	119.70
27	B8	1020	A	C4-C5-C6	6.08	120.04	117.00
27	B8	1735	A	C4-C5-C6	6.08	120.04	117.00
27	B8	2156	G	O4'-C1'-N9	6.08	113.06	108.20
27	B8	2826	A	C4-C5-C6	6.08	120.04	117.00
1	AA	1146	A	C4-C5-C6	6.08	120.04	117.00
1	AA	1226	C	O4'-C1'-N1	6.08	113.06	108.20
1	AA	1314	C	N3-C4-N4	6.08	122.25	118.00
11	AG	161	PHE	CB-CG-CD1	6.08	125.05	120.80
27	B8	1298	C	N3-C4-N4	6.08	122.25	118.00
27	B8	1424	G	O4'-C1'-N9	6.08	113.06	108.20
27	B8	1551	A	C5-C6-N1	-6.08	114.66	117.70
27	B8	2433	A	C4-C5-C6	6.08	120.04	117.00
27	B8	2560	A	C4-C5-C6	6.08	120.04	117.00
1	AA	683	G	C5-C6-O6	-6.07	124.95	128.60
1	AA	1151	A	C4-C5-C6	6.07	120.04	117.00
1	AA	1503	A	C4-C5-C6	6.07	120.04	117.00
26	B7	45	A	O4'-C1'-N9	6.07	113.06	108.20
27	B8	262	A	C4-C5-C6	6.07	120.04	117.00
27	B8	450	G	C5-C6-O6	-6.07	124.96	128.60
27	B8	2323	G	O4'-C1'-N9	6.07	113.06	108.20
1	AA	445	G	O4'-C1'-N9	6.07	113.06	108.20
27	B8	676	A	O4'-C1'-N9	6.07	113.06	108.20
27	B8	2572	A	C4-C5-C6	6.07	120.04	117.00
1	AA	1102	A	C5-C6-N1	-6.07	114.67	117.70
1	AA	1287	A	C4-C5-C6	6.07	120.03	117.00
1	AA	1299	A	C4-C5-C6	6.07	120.03	117.00
1	AA	1372	U	O4'-C1'-N1	6.07	113.06	108.20
1	AA	1407	C	N3-C4-N4	6.07	122.25	118.00
27	B8	513	A	C5-C6-N6	-6.07	118.84	123.70
27	B8	829	A	P-O3'-C3'	6.07	126.98	119.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	1206	G	O4'-C1'-N9	6.07	113.06	108.20
27	B8	2513	A	C4-C5-C6	6.07	120.03	117.00
1	AA	1	A	O4'-C1'-N9	6.07	113.06	108.20
1	AA	116	A	O4'-C1'-N9	6.07	113.06	108.20
1	AA	531	U	O4'-C1'-N1	6.07	113.06	108.20
27	B8	255	A	C5-C6-N6	-6.07	118.84	123.70
27	B8	263	G	O4'-C1'-N9	6.07	113.06	108.20
27	B8	2370	G	O4'-C1'-N9	6.07	113.06	108.20
1	AA	182	A	C4-C5-C6	6.07	120.03	117.00
1	AA	514	C	N3-C4-N4	6.07	122.25	118.00
1	AA	1201	A	C4-C5-C6	6.07	120.03	117.00
26	B7	29	A	C4-C5-C6	6.07	120.03	117.00
27	B8	737	C	N3-C4-N4	6.07	122.25	118.00
27	B8	1470	A	C5-C6-N6	-6.07	118.85	123.70
27	B8	1829	A	C5-C6-N6	-6.07	118.85	123.70
27	B8	2238	G	C5-C6-O6	-6.07	124.96	128.60
27	B8	2287	A	C4-C5-C6	6.07	120.03	117.00
1	AA	473	U	O4'-C1'-N1	6.07	113.05	108.20
1	AA	501	C	N3-C4-N4	6.07	122.25	118.00
1	AA	1188	A	C4-C5-C6	6.07	120.03	117.00
27	B8	168	G	C5-C6-O6	-6.07	124.96	128.60
27	B8	182	A	C5-C6-N1	-6.07	114.67	117.70
27	B8	1640	A	C4-C5-C6	6.07	120.03	117.00
27	B8	1672	A	C4-C5-C6	6.07	120.03	117.00
27	B8	2376	A	C4-C5-C6	6.07	120.03	117.00
1	AA	28	A	C4-C5-C6	6.06	120.03	117.00
1	AA	181	A	C4-C5-C6	6.06	120.03	117.00
1	AA	1487	G	O4'-C1'-N9	6.06	113.05	108.20
27	B8	725	G	O4'-C1'-N9	6.06	113.05	108.20
27	B8	1641	A	C5-C6-N1	-6.06	114.67	117.70
27	B8	2084	C	N3-C4-N4	6.06	122.25	118.00
27	B8	2158	A	C4-C5-C6	6.06	120.03	117.00
1	AA	253	A	C5-C6-N6	-6.06	118.85	123.70
27	B8	381	G	O4'-C1'-N9	6.06	113.05	108.20
27	B8	788	A	C4-C5-C6	6.06	120.03	117.00
27	B8	2380	C	N3-C4-N4	6.06	122.24	118.00
27	B8	2503	A	C4-C5-C6	6.06	120.03	117.00
27	B8	2742	G	O4'-C1'-N9	6.06	113.05	108.20
1	AA	1468	A	C5-C6-N1	-6.06	114.67	117.70
27	B8	631	A	C4-C5-C6	6.06	120.03	117.00
27	B8	2399	G	O4'-C1'-N9	6.06	113.05	108.20
1	AA	1397	C	C6-N1-C1'	-6.06	113.53	120.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	451	U	O4'-C1'-N1	6.06	113.05	108.20
27	B8	1229	C	N3-C4-N4	6.06	122.24	118.00
27	B8	1285	A	C5-C6-N6	-6.06	118.85	123.70
27	B8	2230	G	O4'-C1'-N9	6.06	113.05	108.20
27	B8	2346	A	C4-C5-C6	6.06	120.03	117.00
27	B8	2437	G	O4'-C1'-N9	6.06	113.05	108.20
27	B8	2565	A	C4-C5-C6	6.06	120.03	117.00
1	AA	235	C	N3-C4-N4	6.06	122.24	118.00
1	AA	470	C	N3-C4-N4	6.06	122.24	118.00
1	AA	831	A	C4-C5-C6	6.06	120.03	117.00
26	B7	60	C	N3-C4-N4	6.06	122.24	118.00
27	B8	461	C	O4'-C1'-N1	6.06	113.05	108.20
27	B8	1095	A	C4-C5-C6	6.06	120.03	117.00
27	B8	1755	A	C4-C5-C6	6.06	120.03	117.00
1	AA	385	C	N3-C4-N4	6.06	122.24	118.00
1	AA	782	A	C4-C5-C6	6.06	120.03	117.00
27	B8	1560	G	O4'-C1'-N9	6.06	113.05	108.20
27	B8	2629	U	O4'-C1'-N1	6.06	113.05	108.20
27	B8	2760	C	N3-C4-N4	6.06	122.24	118.00
1	AA	502	A	C4-C5-C6	6.05	120.03	117.00
1	AA	1164	G	O4'-C1'-N9	6.05	113.04	108.20
1	AA	1207	G	O4'-C1'-N9	6.05	113.04	108.20
3	AV	60	A	O4'-C1'-N9	6.05	113.04	108.20
27	B8	248	G	O4'-C1'-N9	6.05	113.04	108.20
27	B8	1508	A	C4-C5-C6	6.05	120.03	117.00
27	B8	1597	A	C4-C5-C6	6.05	120.03	117.00
27	B8	1849	G	O4'-C1'-N9	6.05	113.04	108.20
27	B8	2562	U	O4'-C1'-N1	6.05	113.04	108.20
1	AA	816	A	C4-C5-C6	6.05	120.03	117.00
26	B7	39	A	C4-C5-C6	6.05	120.03	117.00
27	B8	28	A	C4-C5-C6	6.05	120.03	117.00
27	B8	818	G	N3-C2-N2	6.05	124.14	119.90
1	AA	1152	A	C4-C5-C6	6.05	120.03	117.00
1	AA	1257	A	C4-C5-C6	6.05	120.03	117.00
26	B7	59	A	C4-C5-C6	6.05	120.03	117.00
26	B7	63	C	N3-C4-C5	-6.05	119.48	121.90
27	B8	216	A	C5-C6-N1	-6.05	114.67	117.70
27	B8	734	A	C4-C5-C6	6.05	120.03	117.00
27	B8	1067	A	C4-C5-C6	6.05	120.03	117.00
27	B8	1268	A	O4'-C1'-N9	6.05	113.04	108.20
27	B8	2144	G	O4'-C1'-N9	6.05	113.04	108.20
1	AA	679	C	N3-C4-C5	-6.05	119.48	121.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	996	A	C4-C5-C6	6.05	120.03	117.00
27	B8	149	A	C5-C6-N6	-6.05	118.86	123.70
27	B8	1918	A	O4'-C1'-N9	6.05	113.04	108.20
27	B8	2730	C	N3-C4-N4	6.05	122.23	118.00
1	AA	883	C	N3-C4-N4	6.05	122.23	118.00
1	AA	1465	A	C4-C5-C6	6.05	120.02	117.00
27	B8	1983	G	C5-C6-O6	-6.05	124.97	128.60
27	B8	2070	A	O4'-C1'-N9	6.05	113.04	108.20
27	B8	2692	G	O4'-C1'-N9	6.05	113.04	108.20
1	AA	977	A	C4-C5-C6	6.05	120.02	117.00
27	B8	1077	A	C4-C5-C6	6.05	120.02	117.00
27	B8	1336	A	C4-C5-C6	6.05	120.02	117.00
27	B8	1811	G	O4'-C1'-N9	6.05	113.04	108.20
27	B8	1942	C	O4'-C1'-N1	6.05	113.04	108.20
27	B8	2197	U	O4'-C1'-N1	6.05	113.04	108.20
1	AA	515	G	O4'-C1'-N9	6.04	113.04	108.20
1	AA	1004	A	C4-C5-C6	6.04	120.02	117.00
27	B8	184	C	N3-C4-N4	6.04	122.23	118.00
27	B8	781	A	C4-C5-C6	6.04	120.02	117.00
1	AA	30	U	O4'-C1'-N1	6.04	113.03	108.20
27	B8	13	A	C4-C5-C6	6.04	120.02	117.00
27	B8	751	A	C4-C5-C6	6.04	120.02	117.00
27	B8	1385	A	C5-C6-N1	-6.04	114.68	117.70
27	B8	1677	A	C5-C6-N6	-6.04	118.87	123.70
27	B8	1803	A	C4-C5-C6	6.04	120.02	117.00
1	AA	440	C	N3-C4-N4	6.04	122.23	118.00
1	AA	794	A	O4'-C1'-N9	6.04	113.03	108.20
27	B8	56	A	C4-C5-C6	6.04	120.02	117.00
27	B8	167	A	C5-C6-N6	-6.04	118.87	123.70
27	B8	508	A	C4-C5-C6	6.04	120.02	117.00
27	B8	987	C	N3-C4-N4	6.04	122.23	118.00
27	B8	1038	G	O4'-C1'-N9	6.04	113.03	108.20
27	B8	1304	A	O4'-C1'-N9	6.04	113.03	108.20
27	B8	1855	U	O4'-C1'-N1	6.04	113.03	108.20
27	B8	2184	A	C4-C5-C6	6.04	120.02	117.00
27	B8	2270	A	C4-C5-C6	6.04	120.02	117.00
27	B8	2505	G	C5-C6-O6	-6.04	124.97	128.60
1	AA	10	A	C5-C6-N6	-6.04	118.87	123.70
1	AA	97	G	C5-C6-O6	-6.04	124.98	128.60
1	AA	663	A	C5-C6-N1	-6.04	114.68	117.70
1	AA	718	A	O4'-C1'-N9	6.04	113.03	108.20
27	B8	324	A	C4-C5-C6	6.04	120.02	117.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	34	C	N3-C4-N4	6.04	122.23	118.00
1	AA	1091	U	O4'-C1'-N1	6.04	113.03	108.20
1	AA	1316	G	P-O3'-C3'	6.04	126.95	119.70
2	AX	18	C	N3-C4-N4	6.04	122.23	118.00
27	B8	344	A	O4'-C1'-N9	6.04	113.03	108.20
27	B8	1526	C	N3-C4-N4	6.04	122.23	118.00
27	B8	2171	A	C4-C5-C6	6.04	120.02	117.00
27	B8	2183	A	C4-C5-C6	6.04	120.02	117.00
27	B8	2263	C	N3-C4-N4	6.04	122.23	118.00
27	B8	2385	C	N3-C4-N4	6.04	122.23	118.00
1	AA	315	A	C5-C6-N1	-6.04	114.68	117.70
27	B8	957	C	N3-C4-N4	6.04	122.23	118.00
27	B8	1055	G	O4'-C1'-N9	6.04	113.03	108.20
27	B8	1204	A	C5-C6-N6	-6.04	118.87	123.70
1	AA	53	A	C4-C5-C6	6.04	120.02	117.00
1	AA	365	U	O4'-C1'-N1	6.04	113.03	108.20
1	AA	459	A	C5-C6-N1	-6.04	114.68	117.70
27	B8	439	A	C5-C6-N1	-6.04	114.68	117.70
27	B8	1236	G	C5-C6-O6	-6.04	124.98	128.60
27	B8	1344	U	O4'-C1'-N1	6.04	113.03	108.20
27	B8	1383	A	C4-C5-C6	6.04	120.02	117.00
27	B8	2048	G	O4'-C1'-N9	6.04	113.03	108.20
27	B8	2281	A	C5-C6-N6	-6.04	118.87	123.70
27	B8	2507	C	N3-C4-N4	6.04	122.22	118.00
27	B8	2634	A	C4-C5-C6	6.04	120.02	117.00
28	BA	383	PHE	CB-CG-CD2	6.04	125.02	120.80
1	AA	223	A	C4-C5-C6	6.03	120.02	117.00
1	AA	383	A	C5-C6-N1	-6.03	114.68	117.70
1	AA	435	A	O4'-C1'-N9	6.03	113.03	108.20
1	AA	755	G	O4'-C1'-N9	6.03	113.03	108.20
1	AA	1167	A	O4'-C1'-N9	6.03	113.03	108.20
1	AA	1404	C	N3-C4-N4	6.03	122.22	118.00
1	AA	1473	G	O4'-C1'-N9	6.03	113.03	108.20
27	B8	187	G	O4'-C1'-N9	6.03	113.03	108.20
27	B8	291	G	O4'-C1'-N9	6.03	113.03	108.20
27	B8	432	A	C4-C5-C6	6.03	120.02	117.00
27	B8	945	A	C4-C5-C6	6.03	120.02	117.00
27	B8	1190	G	O4'-C1'-N9	6.03	113.03	108.20
27	B8	1532	A	C4-C5-C6	6.03	120.02	117.00
27	B8	1894	C	N3-C4-N4	6.03	122.22	118.00
27	B8	2279	G	O4'-C1'-N9	6.03	113.03	108.20
27	B8	2471	A	C5-C6-N6	-6.03	118.87	123.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	2900	A	C4-C5-C6	6.03	120.02	117.00
1	AA	228	A	C5-C6-N6	-6.03	118.87	123.70
27	B8	1233	C	N3-C4-N4	6.03	122.22	118.00
27	B8	2117	A	O4'-C1'-N9	6.03	113.03	108.20
1	AA	493	A	C5-C6-N6	-6.03	118.88	123.70
1	AA	979	C	N3-C4-N4	6.03	122.22	118.00
27	B8	320	A	C4-C5-C6	6.03	120.02	117.00
27	B8	453	A	C4-C5-C6	6.03	120.02	117.00
27	B8	541	A	C4-C5-C6	6.03	120.02	117.00
1	AA	1114	C	N3-C4-N4	6.03	122.22	118.00
1	AA	1140	C	N3-C4-C5	-6.03	119.49	121.90
27	B8	1314	C	N3-C4-N4	6.03	122.22	118.00
27	B8	1524	G	O4'-C1'-N9	6.03	113.02	108.20
27	B8	2369	A	C5-C6-N6	-6.03	118.88	123.70
1	AA	16	A	C5-C6-N1	-6.03	114.69	117.70
1	AA	706	A	C4-C5-C6	6.03	120.01	117.00
1	AA	1209	C	N3-C4-N4	6.03	122.22	118.00
27	B8	572	A	C5-C6-N6	-6.03	118.88	123.70
27	B8	991	C	N3-C4-C5	-6.03	119.49	121.90
27	B8	1591	A	O4'-C1'-N9	6.03	113.02	108.20
27	B8	1735	A	O4'-C1'-N9	6.03	113.02	108.20
27	B8	1791	A	C4-C5-C6	6.03	120.01	117.00
27	B8	2031	A	C4-C5-C6	6.03	120.01	117.00
27	B8	2534	A	C4-C5-C6	6.03	120.01	117.00
27	B8	2541	A	C5-C6-N6	-6.03	118.88	123.70
3	AV	75	C	N3-C4-C5	-6.03	119.49	121.90
27	B8	94	A	C4-C5-C6	6.03	120.01	117.00
27	B8	222	A	C4-C5-C6	6.03	120.01	117.00
27	B8	522	A	C4-C5-C6	6.03	120.01	117.00
27	B8	678	C	N3-C4-N4	6.03	122.22	118.00
27	B8	937	C	N3-C4-N4	6.03	122.22	118.00
27	B8	1084	A	C5-C6-N1	-6.03	114.69	117.70
27	B8	1261	C	N3-C4-N4	6.03	122.22	118.00
27	B8	2138	G	O4'-C1'-N9	6.03	113.02	108.20
1	AA	179	A	C5-C6-N1	-6.02	114.69	117.70
1	AA	499	A	C4-C5-C6	6.02	120.01	117.00
1	AA	519	C	N3-C4-C5	-6.02	119.49	121.90
27	B8	68	G	C5-C6-O6	-6.02	124.99	128.60
1	AA	336	A	C5-C6-N1	-6.02	114.69	117.70
1	AA	493	A	C4-C5-C6	6.02	120.01	117.00
1	AA	892	A	C4-C5-C6	6.02	120.01	117.00
1	AA	1443	C	N3-C4-N4	6.02	122.22	118.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	736	C	N3-C4-N4	6.02	122.22	118.00
27	B8	892	A	C5-C6-N6	-6.02	118.88	123.70
27	B8	2371	G	O4'-C1'-N9	6.02	113.02	108.20
1	AA	984	C	N3-C4-N4	6.02	122.22	118.00
27	B8	786	C	N3-C4-N4	6.02	122.22	118.00
27	B8	1676	A	C5-C6-N6	-6.02	118.88	123.70
1	AA	59	A	C4-C5-C6	6.02	120.01	117.00
1	AA	320	A	O4'-C1'-N9	6.02	113.02	108.20
1	AA	1542	A	O4'-C1'-N9	6.02	113.02	108.20
3	AV	33	A	C4-C5-C6	6.02	120.01	117.00
26	B7	38	C	N3-C4-N4	6.02	122.21	118.00
27	B8	172	A	C4-C5-C6	6.02	120.01	117.00
27	B8	322	A	C5-C6-N1	-6.02	114.69	117.70
27	B8	1084	A	C5-C6-N6	-6.02	118.89	123.70
27	B8	2054	A	C4-C5-C6	6.02	120.01	117.00
27	B8	2679	A	O4'-C1'-N9	6.02	113.02	108.20
1	AA	547	A	C4-C5-C6	6.02	120.01	117.00
1	AA	1246	A	O4'-C1'-N9	6.02	113.01	108.20
27	B8	173	A	O4'-C1'-N9	6.02	113.01	108.20
27	B8	468	G	O4'-C1'-N9	6.02	113.01	108.20
27	B8	743	A	O4'-C1'-N9	6.02	113.01	108.20
27	B8	1571	A	O4'-C1'-N9	6.02	113.02	108.20
27	B8	2516	A	C5-C6-N6	-6.02	118.89	123.70
1	AA	329	A	C4-C5-C6	6.02	120.01	117.00
3	AV	16	C	O4'-C1'-N1	6.02	113.01	108.20
27	B8	231	A	C4-C5-C6	6.02	120.01	117.00
27	B8	726	G	O4'-C1'-N9	6.02	113.01	108.20
27	B8	2178	C	C6-N1-C1'	-6.02	113.58	120.80
1	AA	356	A	C5-C6-N6	-6.01	118.89	123.70
1	AA	1130	A	C5-C6-N6	-6.01	118.89	123.70
3	AV	4	C	N3-C4-N4	6.01	122.21	118.00
27	B8	20	C	N3-C4-N4	6.01	122.21	118.00
27	B8	148	U	O4'-C1'-N1	6.01	113.01	108.20
27	B8	231	A	C5-C6-N1	-6.01	114.69	117.70
27	B8	341	C	N3-C4-N4	6.01	122.21	118.00
27	B8	506	G	O4'-C1'-N9	6.01	113.01	108.20
27	B8	1029	A	C5-C6-N1	-6.01	114.69	117.70
27	B8	1336	A	C5-C6-N6	-6.01	118.89	123.70
27	B8	1632	A	C4-C5-C6	6.01	120.01	117.00
27	B8	1913	A	C4-C5-C6	6.01	120.01	117.00
27	B8	2224	G	C5-C6-O6	-6.01	124.99	128.60
3	AV	50	G	O4'-C1'-N9	6.01	113.01	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	760	G	O4'-C1'-N9	6.01	113.01	108.20
27	B8	1384	A	C5-C6-N6	-6.01	118.89	123.70
27	B8	2531	A	C4-C5-C6	6.01	120.01	117.00
1	AA	400	C	N3-C4-N4	6.01	122.21	118.00
1	AA	969	A	O4'-C1'-N9	6.01	113.01	108.20
27	B8	262	A	C5-C6-N1	-6.01	114.69	117.70
27	B8	979	A	C4-C5-C6	6.01	120.01	117.00
27	B8	1302	A	C5-C6-N1	-6.01	114.69	117.70
27	B8	1541	C	N3-C4-N4	6.01	122.21	118.00
27	B8	1665	A	C4-C5-C6	6.01	120.01	117.00
27	B8	1998	A	C4-C5-C6	6.01	120.00	117.00
27	B8	2327	A	C4-C5-C6	6.01	120.01	117.00
27	B8	2377	A	C4-C5-C6	6.01	120.01	117.00
27	B8	2453	A	C4-C5-C6	6.01	120.01	117.00
1	AA	82	G	O4'-C1'-N9	6.01	113.01	108.20
1	AA	120	A	C4-C5-C6	6.01	120.00	117.00
1	AA	237	G	O4'-C1'-N9	6.01	113.01	108.20
27	B8	599	A	C5-C6-N6	-6.01	118.89	123.70
27	B8	975	A	C5-C6-N1	-6.01	114.69	117.70
27	B8	2278	A	C5-C6-N6	-6.01	118.89	123.70
27	B8	2475	C	N3-C4-C5	-6.01	119.50	121.90
27	B8	2653	U	O4'-C1'-N1	6.01	113.01	108.20
27	B8	742	A	C5-C6-N6	-6.01	118.89	123.70
27	B8	1086	A	O4'-C1'-N9	6.01	113.01	108.20
27	B8	1678	A	C4-C5-C6	6.01	120.00	117.00
27	B8	2349	G	O4'-C1'-N9	6.01	113.01	108.20
27	B8	2678	C	N3-C4-N4	6.01	122.21	118.00
27	B8	2831	G	O4'-C1'-N9	6.01	113.01	108.20
1	AA	1200	C	O4'-C1'-N1	6.01	113.01	108.20
1	AA	1521	C	N3-C4-N4	6.01	122.20	118.00
27	B8	259	G	O4'-C1'-N9	6.01	113.01	108.20
27	B8	1297	C	N3-C4-N4	6.01	122.20	118.00
27	B8	1821	A	O4'-C1'-N9	6.01	113.00	108.20
28	BA	383	PHE	CB-CG-CD1	-6.01	116.59	120.80
1	AA	174	A	C4-C5-C6	6.00	120.00	117.00
27	B8	921	C	N3-C4-N4	6.00	122.20	118.00
27	B8	1822	C	N3-C4-N4	6.00	122.20	118.00
27	B8	1958	C	N3-C4-N4	6.00	122.20	118.00
27	B8	2635	A	C4-C5-C6	6.00	120.00	117.00
1	AA	704	A	C4-C5-C6	6.00	120.00	117.00
27	B8	236	C	N3-C4-N4	6.00	122.20	118.00
27	B8	311	A	C4-C5-C6	6.00	120.00	117.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	698	C	N3-C4-N4	6.00	122.20	118.00
27	B8	991	C	N3-C4-N4	6.00	122.20	118.00
27	B8	1174	U	O4'-C1'-N1	6.00	113.00	108.20
27	B8	2381	A	C5-C6-N6	-6.00	118.90	123.70
27	B8	2679	A	C5-C6-N6	-6.00	118.90	123.70
1	AA	143	A	C4-C5-C6	6.00	120.00	117.00
1	AA	418	C	N3-C4-N4	6.00	122.20	118.00
1	AA	502	A	O4'-C1'-N9	6.00	113.00	108.20
1	AA	602	A	O4'-C1'-N9	6.00	113.00	108.20
1	AA	1502	A	O4'-C1'-N9	6.00	113.00	108.20
27	B8	83	A	C4-C5-C6	6.00	120.00	117.00
27	B8	213	A	C4-C5-C6	6.00	120.00	117.00
27	B8	492	A	C5-C6-N6	-6.00	118.90	123.70
27	B8	504	A	C4-C5-C6	6.00	120.00	117.00
27	B8	820	A	O4'-C1'-N9	6.00	113.00	108.20
27	B8	995	C	C2-N1-C1'	6.00	125.40	118.80
27	B8	2094	A	C4-C5-C6	6.00	120.00	117.00
1	AA	831	A	C5-C6-N6	-6.00	118.90	123.70
27	B8	2142	A	C5-C6-N6	-6.00	118.90	123.70
27	B8	2301	C	N3-C4-N4	6.00	122.20	118.00
27	B8	2486	C	N3-C4-N4	6.00	122.20	118.00
1	AA	374	A	C4-C5-C6	6.00	120.00	117.00
26	B7	35	C	C6-N1-C1'	-6.00	113.60	120.80
27	B8	289	G	O4'-C1'-N9	6.00	113.00	108.20
27	B8	423	A	C5-C6-N6	-6.00	118.90	123.70
27	B8	677	A	O4'-C1'-N9	6.00	113.00	108.20
27	B8	808	G	O4'-C1'-N9	6.00	113.00	108.20
27	B8	2211	A	C5-C6-N6	-6.00	118.90	123.70
27	B8	2485	G	O4'-C1'-N9	6.00	113.00	108.20
27	B8	2814	A	C4-C5-C6	6.00	120.00	117.00
1	AA	286	C	N3-C4-N4	6.00	122.20	118.00
1	AA	364	A	C4-C5-C6	6.00	120.00	117.00
1	AA	422	C	O4'-C1'-N1	6.00	113.00	108.20
1	AA	715	A	C4-C5-C6	6.00	120.00	117.00
1	AA	1394	A	C4-C5-C6	6.00	120.00	117.00
27	B8	447	A	C4-C5-C6	6.00	120.00	117.00
27	B8	602	A	C5-C6-N6	-6.00	118.90	123.70
27	B8	623	C	N3-C4-N4	6.00	122.20	118.00
27	B8	1342	A	C4-C5-C6	6.00	120.00	117.00
27	B8	1795	C	N3-C4-C5	-6.00	119.50	121.90
27	B8	2497	A	C4-C5-C6	6.00	120.00	117.00
1	AA	465	A	C5-C6-N6	-6.00	118.90	123.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	208	C	N3-C4-N4	6.00	122.20	118.00
27	B8	743	A	C4-C5-C6	6.00	120.00	117.00
27	B8	1593	A	C5-C6-N6	-6.00	118.90	123.70
1	AA	673	A	O4'-C1'-N9	5.99	113.00	108.20
3	AV	36	G	O4'-C1'-N9	5.99	113.00	108.20
27	B8	44	A	C4-C5-C6	5.99	120.00	117.00
27	B8	693	A	C5-C6-N6	-5.99	118.91	123.70
27	B8	896	A	O4'-C1'-N9	5.99	113.00	108.20
27	B8	1779	U	O4'-C1'-N1	5.99	113.00	108.20
27	B8	2564	A	C4-C5-C6	5.99	120.00	117.00
27	B8	2853	C	N3-C4-N4	5.99	122.20	118.00
1	AA	327	A	C5-C6-N1	-5.99	114.70	117.70
27	B8	347	A	C4-C5-C6	5.99	120.00	117.00
27	B8	1350	C	N3-C4-N4	5.99	122.19	118.00
27	B8	1932	A	C4-C5-C6	5.99	120.00	117.00
27	B8	2643	G	O4'-C1'-N9	5.99	112.99	108.20
1	AA	328	C	N3-C4-N4	5.99	122.19	118.00
1	AA	356	A	O4'-C1'-N9	5.99	112.99	108.20
1	AA	817	C	N3-C4-N4	5.99	122.19	118.00
2	AX	16	C	N3-C4-N4	5.99	122.19	118.00
27	B8	183	C	N3-C4-N4	5.99	122.19	118.00
27	B8	1193	G	O4'-C1'-N9	5.99	112.99	108.20
27	B8	1361	G	O4'-C1'-N9	5.99	112.99	108.20
27	B8	2381	A	C4-C5-C6	5.99	120.00	117.00
27	B8	2461	A	O4'-C1'-N9	5.99	112.99	108.20
1	AA	374	A	O4'-C1'-N9	5.99	112.99	108.20
1	AA	641	U	O4'-C1'-N1	5.99	112.99	108.20
1	AA	1035	A	C4-C5-C6	5.99	119.99	117.00
1	AA	1369	C	N3-C4-N4	5.99	122.19	118.00
27	B8	643	A	C4-C5-C6	5.99	119.99	117.00
27	B8	912	C	N3-C4-N4	5.99	122.19	118.00
27	B8	1166	G	O4'-C1'-N9	5.99	112.99	108.20
27	B8	1801	A	C4-C5-C6	5.99	120.00	117.00
27	B8	1836	C	N3-C4-N4	5.99	122.19	118.00
27	B8	1890	A	C4-C5-C6	5.99	119.99	117.00
27	B8	2024	G	O4'-C1'-N9	5.99	112.99	108.20
27	B8	2363	G	O4'-C1'-N9	5.99	112.99	108.20
27	B8	2461	A	C5-C6-N6	-5.99	118.91	123.70
27	B8	2616	C	N3-C4-N4	5.99	122.19	118.00
27	B8	2752	C	N3-C4-N4	5.99	122.19	118.00
27	B8	2755	C	N3-C4-N4	5.99	122.19	118.00
26	B7	116	G	O4'-C1'-N9	5.99	112.99	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	292	G	O4'-C1'-N9	5.99	112.99	108.20
1	AA	1147	C	N3-C4-N4	5.99	122.19	118.00
27	B8	1403	A	C4-C5-C6	5.99	119.99	117.00
27	B8	1433	A	C5-C6-N1	-5.99	114.71	117.70
27	B8	1448	G	O4'-C1'-N9	5.99	112.99	108.20
27	B8	2101	A	C4-C5-C6	5.99	119.99	117.00
1	AA	766	A	C4-C5-C6	5.98	119.99	117.00
26	B7	82	U	O4'-C1'-N1	5.98	112.99	108.20
27	B8	439	A	C4-C5-C6	5.98	119.99	117.00
27	B8	1064	C	N3-C4-N4	5.98	122.19	118.00
27	B8	1290	C	N3-C4-N4	5.98	122.19	118.00
27	B8	1844	C	N3-C4-N4	5.98	122.19	118.00
1	AA	1105	A	C5-C6-N6	-5.98	118.91	123.70
27	B8	190	A	C5-C6-N6	-5.98	118.92	123.70
27	B8	1783	A	C4-C5-C6	5.98	119.99	117.00
27	B8	2198	A	C5-C6-N6	-5.98	118.91	123.70
27	B8	2530	A	C1'-O4'-C4'	-5.98	105.11	109.90
45	BQ	23	TYR	CB-CG-CD2	5.98	124.59	121.00
1	AA	120	A	C5-C6-N6	-5.98	118.92	123.70
1	AA	232	G	C5-C6-O6	-5.98	125.01	128.60
1	AA	878	A	C4-C5-C6	5.98	119.99	117.00
1	AA	1287	A	C5-C6-N6	-5.98	118.92	123.70
27	B8	501	A	C4-C5-C6	5.98	119.99	117.00
27	B8	1404	C	N3-C4-N4	5.98	122.19	118.00
27	B8	2027	G	O4'-C1'-N9	5.98	112.98	108.20
27	B8	47	C	N3-C4-N4	5.98	122.19	118.00
27	B8	589	U	O4'-C1'-N1	5.98	112.98	108.20
27	B8	2503	A	C5-C6-N6	-5.98	118.92	123.70
1	AA	182	A	O4'-C1'-N9	5.98	112.98	108.20
1	AA	303	A	C4-C5-C6	5.98	119.99	117.00
1	AA	1032	G	O4'-C1'-N9	5.98	112.98	108.20
1	AA	1103	C	N3-C4-N4	5.98	122.18	118.00
27	B8	538	A	O4'-C1'-N9	5.98	112.98	108.20
27	B8	1152	C	N3-C4-N4	5.98	122.18	118.00
27	B8	1278	C	N3-C4-N4	5.98	122.18	118.00
27	B8	1938	A	C4-C5-C6	5.98	119.99	117.00
1	AA	366	A	C4-C5-C6	5.97	119.99	117.00
1	AA	451	A	C4-C5-C6	5.97	119.99	117.00
1	AA	686	U	O4'-C1'-N1	5.97	112.98	108.20
1	AA	1155	A	O4'-C1'-N9	5.97	112.98	108.20
26	B7	99	A	C5-C6-N1	-5.97	114.71	117.70
1	AA	288	A	C4-C5-C6	5.97	119.99	117.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	609	A	C4-C5-C6	5.97	119.99	117.00
1	AA	743	A	C5-C6-N6	-5.97	118.92	123.70
1	AA	1104	G	O4'-C1'-N9	5.97	112.98	108.20
1	AA	1371	G	C5-C6-O6	-5.97	125.02	128.60
27	B8	481	G	C5-C6-O6	-5.97	125.02	128.60
27	B8	540	C	N3-C4-N4	5.97	122.18	118.00
27	B8	550	C	N3-C4-C5	-5.97	119.51	121.90
27	B8	777	G	O4'-C1'-N9	5.97	112.98	108.20
27	B8	802	A	C5-C6-N1	-5.97	114.71	117.70
27	B8	1091	G	C5-C6-O6	-5.97	125.02	128.60
27	B8	1430	G	O4'-C1'-N9	5.97	112.98	108.20
27	B8	2135	A	C4-C5-C6	5.97	119.99	117.00
27	B8	2221	G	O4'-C1'-N9	5.97	112.98	108.20
27	B8	2758	A	C5-C6-N6	-5.97	118.92	123.70
1	AA	391	G	O4'-C1'-N9	5.97	112.98	108.20
27	B8	1413	A	C4-C5-C6	5.97	119.98	117.00
27	B8	1587	G	C5-C6-O6	-5.97	125.02	128.60
27	B8	2846	G	O4'-C1'-N9	5.97	112.98	108.20
1	AA	716	A	C5-C6-N1	-5.97	114.72	117.70
1	AA	877	G	O4'-C1'-N9	5.97	112.98	108.20
1	AA	1181	G	C5-C6-O6	-5.97	125.02	128.60
1	AA	1428	A	C4-C5-C6	5.97	119.98	117.00
27	B8	241	A	C4-C5-C6	5.97	119.98	117.00
27	B8	1165	A	C5-C6-N1	-5.97	114.72	117.70
27	B8	1854	A	O4'-C1'-N9	5.97	112.98	108.20
27	B8	2099	U	O4'-C1'-N1	5.97	112.97	108.20
27	B8	2172	U	O4'-C1'-N1	5.97	112.97	108.20
27	B8	2211	A	C4-C5-C6	5.97	119.98	117.00
27	B8	2241	A	C4-C5-C6	5.97	119.98	117.00
27	B8	2350	C	N3-C4-N4	5.97	122.18	118.00
27	B8	130	C	N3-C4-N4	5.97	122.18	118.00
27	B8	270	A	C4-C5-C6	5.97	119.98	117.00
27	B8	892	A	O4'-C1'-N9	5.97	112.97	108.20
27	B8	2588	G	O4'-C1'-N9	5.97	112.97	108.20
1	AA	184	G	O4'-C1'-N9	5.97	112.97	108.20
1	AA	1170	A	C5-C6-N6	-5.97	118.93	123.70
1	AA	1196	A	C4-C5-C6	5.97	119.98	117.00
27	B8	1070	A	C4-C5-C6	5.97	119.98	117.00
27	B8	2176	A	O4'-C1'-N9	5.97	112.97	108.20
27	B8	2723	C	N3-C4-N4	5.97	122.18	118.00
1	AA	1059	C	N3-C4-N4	5.96	122.18	118.00
1	AA	1325	C	N3-C4-N4	5.96	122.17	118.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1518	A	C4-C5-C6	5.96	119.98	117.00
27	B8	586	A	C4-C5-C6	5.96	119.98	117.00
27	B8	1367	A	C5-C6-N6	-5.96	118.93	123.70
27	B8	2196	C	N3-C4-N4	5.96	122.18	118.00
27	B8	2382	G	O4'-C1'-N9	5.96	112.97	108.20
27	B8	2888	C	N3-C4-N4	5.96	122.17	118.00
1	AA	1284	C	N3-C4-N4	5.96	122.17	118.00
27	B8	1247	A	C4-C5-C6	5.96	119.98	117.00
1	AA	702	A	C4-C5-C6	5.96	119.98	117.00
1	AA	1081	A	C5-C6-N6	-5.96	118.93	123.70
1	AA	1108	G	O4'-C1'-N9	5.96	112.97	108.20
1	AA	1251	A	C4-C5-C6	5.96	119.98	117.00
27	B8	103	A	O4'-C1'-N9	5.96	112.97	108.20
27	B8	281	C	N3-C4-N4	5.96	122.17	118.00
27	B8	528	A	C4-C5-C6	5.96	119.98	117.00
27	B8	603	A	C4-C5-C6	5.96	119.98	117.00
27	B8	804	A	C4-C5-C6	5.96	119.98	117.00
27	B8	878	A	C5-C6-N6	-5.96	118.93	123.70
27	B8	1919	A	C4-C5-C6	5.96	119.98	117.00
27	B8	2094	A	C5-C6-N6	-5.96	118.93	123.70
46	BR	3	ALA	N-CA-CB	5.96	118.45	110.10
1	AA	793	U	O4'-C1'-N1	5.96	112.97	108.20
27	B8	452	G	O4'-C1'-N9	5.96	112.97	108.20
27	B8	1471	G	O4'-C1'-N9	5.96	112.97	108.20
1	AA	225	C	N3-C4-N4	5.96	122.17	118.00
1	AA	1169	A	C4-C5-C6	5.96	119.98	117.00
1	AA	1239	A	C4-C5-C6	5.96	119.98	117.00
1	AA	1519	A	C4-C5-C6	5.96	119.98	117.00
27	B8	750	A	C5-C6-N6	-5.96	118.93	123.70
27	B8	1118	C	N3-C4-N4	5.96	122.17	118.00
27	B8	1634	A	C5-C6-N1	-5.96	114.72	117.70
27	B8	1650	A	C5-C6-N6	-5.96	118.93	123.70
27	B8	2037	A	C4-C5-C6	5.96	119.98	117.00
27	B8	2143	C	N3-C4-N4	5.96	122.17	118.00
27	B8	2426	A	C4-C5-C6	5.96	119.98	117.00
1	AA	496	A	C4-C5-C6	5.96	119.98	117.00
1	AA	899	C	N3-C4-C5	-5.96	119.52	121.90
1	AA	1082	A	C4-C5-C6	5.96	119.98	117.00
1	AA	1163	A	C4-C5-C6	5.96	119.98	117.00
1	AA	1500	A	C4-C5-C6	5.96	119.98	117.00
27	B8	297	G	O4'-C1'-N9	5.96	112.97	108.20
27	B8	391	A	C5-C6-N6	-5.96	118.94	123.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	936	A	C5-C6-N6	-5.96	118.94	123.70
27	B8	1754	A	C5-C6-N6	-5.96	118.94	123.70
27	B8	1778	U	O4'-C1'-N1	5.96	112.97	108.20
27	B8	1829	A	C4-C5-C6	5.96	119.98	117.00
27	B8	2590	A	C4-C5-C6	5.96	119.98	117.00
27	B8	2796	U	O4'-C1'-N1	5.96	112.97	108.20
1	AA	241	G	O4'-C1'-N9	5.96	112.96	108.20
1	AA	456	A	O4'-C1'-N9	5.96	112.96	108.20
1	AA	469	C	N3-C4-N4	5.96	122.17	118.00
1	AA	1502	A	C5-C6-N1	-5.96	114.72	117.70
27	B8	108	G	O4'-C1'-N9	5.96	112.96	108.20
27	B8	282	A	O4'-C1'-N9	5.96	112.96	108.20
27	B8	346	A	C5-C6-N1	-5.96	114.72	117.70
27	B8	653	U	C2-N1-C1'	5.96	124.85	117.70
27	B8	1286	A	C5-C6-N1	-5.96	114.72	117.70
27	B8	2278	A	C4-C5-C6	5.96	119.98	117.00
1	AA	80	A	C5-C6-N1	-5.95	114.72	117.70
1	AA	681	A	C4-C5-C6	5.95	119.98	117.00
27	B8	89	A	C4-C5-C6	5.95	119.98	117.00
27	B8	361	G	O4'-C1'-N9	5.95	112.96	108.20
27	B8	1826	G	O4'-C1'-N9	5.95	112.96	108.20
1	AA	243	A	C4-C5-C6	5.95	119.98	117.00
27	B8	905	A	C4-C5-C6	5.95	119.98	117.00
27	B8	1866	A	C5-C6-N6	-5.95	118.94	123.70
1	AA	129	A	C4-C5-C6	5.95	119.98	117.00
1	AA	600	A	O4'-C1'-N9	5.95	112.96	108.20
1	AA	767	A	C4-C5-C6	5.95	119.98	117.00
1	AA	1163	A	O4'-C1'-N9	5.95	112.96	108.20
27	B8	147	C	N3-C4-N4	5.95	122.17	118.00
27	B8	156	A	C4-C5-C6	5.95	119.97	117.00
27	B8	179	C	N3-C4-N4	5.95	122.17	118.00
27	B8	456	C	N3-C4-C5	-5.95	119.52	121.90
27	B8	980	A	C4-C5-C6	5.95	119.97	117.00
27	B8	1065	U	O4'-C1'-N1	5.95	112.96	108.20
27	B8	1637	A	C5-C6-N1	-5.95	114.72	117.70
27	B8	2175	C	N3-C4-N4	5.95	122.17	118.00
27	B8	2448	A	C4-C5-C6	5.95	119.97	117.00
1	AA	613	C	N3-C4-N4	5.95	122.17	118.00
1	AA	1520	C	N3-C4-N4	5.95	122.16	118.00
27	B8	102	U	O4'-C1'-N1	5.95	112.96	108.20
27	B8	254	G	O4'-C1'-N9	5.95	112.96	108.20
27	B8	637	A	C5-C6-N6	-5.95	118.94	123.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	806	C	N3-C4-N4	5.95	122.16	118.00
27	B8	2854	G	O4'-C1'-N9	5.95	112.96	108.20
1	AA	28	A	C5-C6-N6	-5.95	118.94	123.70
1	AA	282	A	C4-C5-C6	5.95	119.97	117.00
26	B7	21	G	O4'-C1'-N9	5.95	112.96	108.20
27	B8	611	C	N3-C4-N4	5.95	122.16	118.00
1	AA	156	C	N3-C4-N4	5.95	122.16	118.00
1	AA	363	A	O4'-C1'-N9	5.95	112.96	108.20
1	AA	546	A	C4-C5-C6	5.95	119.97	117.00
27	B8	60	G	O4'-C1'-N9	5.95	112.96	108.20
27	B8	564	C	N3-C4-N4	5.95	122.16	118.00
27	B8	706	A	C4-C5-C6	5.95	119.97	117.00
27	B8	1856	U	O4'-C1'-N1	5.95	112.96	108.20
27	B8	2679	A	C4-C5-C6	5.95	119.97	117.00
1	AA	271	C	N3-C4-N4	5.94	122.16	118.00
1	AA	314	C	N3-C4-N4	5.94	122.16	118.00
1	AA	826	C	N3-C4-C5	-5.94	119.52	121.90
1	AA	912	C	N3-C4-N4	5.94	122.16	118.00
27	B8	1676	A	C4-C5-C6	5.94	119.97	117.00
27	B8	2294	G	O4'-C1'-N9	5.94	112.95	108.20
1	AA	320	A	C4-C5-C6	5.94	119.97	117.00
22	AR	4	PHE	CB-CG-CD1	5.94	124.96	120.80
27	B8	923	G	O4'-C1'-N9	5.94	112.95	108.20
27	B8	1270	C	N3-C4-N4	5.94	122.16	118.00
27	B8	1272	A	C4-C5-C6	5.94	119.97	117.00
27	B8	1845	G	O4'-C1'-N9	5.94	112.95	108.20
27	B8	2374	C	N3-C4-N4	5.94	122.16	118.00
27	B8	2770	G	O4'-C1'-N9	5.94	112.95	108.20
1	AA	73	C	N3-C4-N4	5.94	122.16	118.00
1	AA	874	G	O4'-C1'-N9	5.94	112.95	108.20
26	B7	28	C	N3-C4-N4	5.94	122.16	118.00
27	B8	401	A	C4-C5-C6	5.94	119.97	117.00
27	B8	1042	G	C5-C6-O6	-5.94	125.03	128.60
27	B8	1817	G	C5-C6-O6	-5.94	125.04	128.60
27	B8	2053	G	O4'-C1'-N9	5.94	112.95	108.20
27	B8	2171	A	O4'-C1'-N9	5.94	112.95	108.20
27	B8	841	G	O4'-C1'-N9	5.94	112.95	108.20
27	B8	2129	C	C2-N1-C1'	5.94	125.33	118.80
1	AA	130	A	P-O3'-C3'	5.94	126.83	119.70
1	AA	637	C	N3-C4-N4	5.94	122.16	118.00
1	AA	900	A	C4-C5-C6	5.94	119.97	117.00
1	AA	1340	A	O4'-C1'-N9	5.94	112.95	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	706	A	O4'-C1'-N9	5.94	112.95	108.20
27	B8	1080	A	C4-C5-C6	5.94	119.97	117.00
27	B8	1082	U	O4'-C1'-N1	5.94	112.95	108.20
27	B8	1507	C	N3-C4-N4	5.94	122.16	118.00
27	B8	1730	C	C6-N1-C1'	-5.94	113.67	120.80
27	B8	1810	A	C5-C6-N6	-5.94	118.95	123.70
1	AA	269	C	N3-C4-N4	5.93	122.15	118.00
1	AA	478	A	C5-C6-N6	-5.93	118.95	123.70
1	AA	559	A	C4-C5-C6	5.93	119.97	117.00
1	AA	832	G	C5-C6-O6	-5.93	125.04	128.60
1	AA	893	C	N3-C4-C5	-5.93	119.53	121.90
1	AA	922	G	C5-C6-O6	-5.93	125.04	128.60
1	AA	1230	C	N3-C4-N4	5.93	122.15	118.00
1	AA	1269	A	O4'-C1'-N9	5.93	112.95	108.20
1	AA	1501	C	N3-C4-N4	5.93	122.15	118.00
3	AV	60	A	C4-C5-C6	5.93	119.97	117.00
27	B8	14	A	C4-C5-C6	5.93	119.97	117.00
27	B8	346	A	C4-C5-C6	5.93	119.97	117.00
27	B8	538	A	C4-C5-C6	5.93	119.97	117.00
27	B8	582	A	C4-C5-C6	5.93	119.97	117.00
27	B8	690	G	O4'-C1'-N9	5.93	112.95	108.20
27	B8	1158	C	N3-C4-N4	5.93	122.15	118.00
27	B8	1216	G	O4'-C1'-N9	5.93	112.95	108.20
27	B8	2880	C	N3-C4-N4	5.93	122.15	118.00
1	AA	78	A	O4'-C1'-N9	5.93	112.95	108.20
1	AA	816	A	O4'-C1'-N9	5.93	112.95	108.20
1	AA	1160	G	O4'-C1'-N9	5.93	112.95	108.20
27	B8	89	A	C5-C6-N1	-5.93	114.73	117.70
27	B8	400	G	O4'-C1'-N9	5.93	112.95	108.20
27	B8	1000	A	O4'-C1'-N9	5.93	112.94	108.20
27	B8	1150	C	N3-C4-N4	5.93	122.15	118.00
27	B8	2284	A	O4'-C1'-N9	5.93	112.95	108.20
27	B8	2574	G	O4'-C1'-N9	5.93	112.95	108.20
1	AA	574	A	C5-C6-N6	-5.93	118.95	123.70
1	AA	1272	G	O4'-C1'-N9	5.93	112.94	108.20
1	AA	1333	A	C4-C5-C6	5.93	119.97	117.00
27	B8	104	A	C4-C5-C6	5.93	119.97	117.00
27	B8	287	G	O4'-C1'-N9	5.93	112.94	108.20
27	B8	2281	A	C4-C5-C6	5.93	119.97	117.00
27	B8	2600	A	O4'-C1'-N9	5.93	112.94	108.20
1	AA	596	A	C5-C6-N6	-5.93	118.96	123.70
27	B8	340	A	O4'-C1'-N9	5.93	112.94	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	844	A	C4-C5-C6	5.93	119.96	117.00
27	B8	1392	A	O4'-C1'-N9	5.93	112.94	108.20
27	B8	1572	A	C5-C6-N6	-5.93	118.96	123.70
27	B8	2826	A	O4'-C1'-N9	5.93	112.94	108.20
27	B8	2837	A	C4-C5-C6	5.93	119.97	117.00
1	AA	915	A	C4-C5-C6	5.93	119.96	117.00
1	AA	948	C	N3-C4-N4	5.93	122.15	118.00
27	B8	483	A	C4-C5-C6	5.93	119.96	117.00
27	B8	2397	G	C5-C6-O6	-5.93	125.04	128.60
27	B8	2753	A	C5-C6-N6	-5.93	118.96	123.70
27	B8	2902	C	N3-C4-N4	5.93	122.15	118.00
1	AA	554	A	O4'-C1'-N9	5.93	112.94	108.20
1	AA	735	C	N3-C4-N4	5.93	122.15	118.00
1	AA	768	A	C5-C6-N6	-5.93	118.96	123.70
1	AA	829	G	O4'-C1'-N9	5.93	112.94	108.20
27	B8	84	A	C4-C5-C6	5.93	119.96	117.00
27	B8	862	G	O4'-C1'-N9	5.93	112.94	108.20
27	B8	1127	A	C5-C6-N1	-5.93	114.74	117.70
27	B8	1224	U	O4'-C1'-N1	5.93	112.94	108.20
27	B8	2019	A	C4-C5-C6	5.93	119.96	117.00
1	AA	1110	A	C5-C6-N6	-5.92	118.96	123.70
1	AA	1223	C	N3-C4-N4	5.92	122.15	118.00
1	AA	1234	C	N3-C4-N4	5.92	122.15	118.00
1	AA	1306	A	C5-C6-N6	-5.92	118.96	123.70
3	AV	22	A	C5-C6-N6	-5.92	118.96	123.70
27	B8	83	A	C5-C6-N6	-5.92	118.96	123.70
27	B8	357	C	N3-C4-N4	5.92	122.15	118.00
27	B8	1128	G	O4'-C1'-N9	5.92	112.94	108.20
1	AA	532	A	O4'-C1'-N9	5.92	112.94	108.20
1	AA	1137	C	C2-N1-C1'	5.92	125.32	118.80
27	B8	632	A	C4-C5-C6	5.92	119.96	117.00
27	B8	2031	A	C5-C6-N6	-5.92	118.96	123.70
1	AA	655	A	C4-C5-C6	5.92	119.96	117.00
1	AA	1151	A	C5-C6-N6	-5.92	118.96	123.70
1	AA	1175	G	O4'-C1'-N9	5.92	112.94	108.20
1	AA	1450	U	O4'-C1'-N1	5.92	112.94	108.20
27	B8	152	A	O4'-C1'-N9	5.92	112.94	108.20
27	B8	322	A	C4-C5-C6	5.92	119.96	117.00
27	B8	739	A	C4-C5-C6	5.92	119.96	117.00
27	B8	981	A	C4-C5-C6	5.92	119.96	117.00
27	B8	1200	C	N3-C4-N4	5.92	122.14	118.00
27	B8	1264	A	C4-C5-C6	5.92	119.96	117.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	1265	A	C4-C5-C6	5.92	119.96	117.00
27	B8	1356	G	O4'-C1'-N9	5.92	112.94	108.20
27	B8	1399	C	N3-C4-N4	5.92	122.14	118.00
27	B8	1740	G	O4'-C1'-N9	5.92	112.94	108.20
27	B8	1905	C	N3-C4-N4	5.92	122.14	118.00
27	B8	1927	A	C4-C5-C6	5.92	119.96	117.00
27	B8	1999	C	N3-C4-N4	5.92	122.14	118.00
27	B8	2466	C	N3-C4-N4	5.92	122.14	118.00
1	AA	842	U	C2-N1-C1'	5.92	124.80	117.70
27	B8	274	C	N3-C4-N4	5.92	122.14	118.00
27	B8	323	C	N3-C4-N4	5.92	122.14	118.00
27	B8	902	C	N3-C4-N4	5.92	122.14	118.00
27	B8	2600	A	C5-C6-N6	-5.92	118.96	123.70
27	B8	513	A	O4'-C1'-N9	5.92	112.93	108.20
27	B8	756	A	C4-C5-C6	5.92	119.96	117.00
27	B8	954	G	O4'-C1'-N9	5.92	112.94	108.20
27	B8	1129	A	O4'-C1'-N9	5.92	112.94	108.20
27	B8	1889	A	C4-C5-C6	5.92	119.96	117.00
27	B8	1941	C	N3-C4-N4	5.92	122.14	118.00
27	B8	1953	A	C5-C6-N1	-5.92	114.74	117.70
27	B8	1998	A	O4'-C1'-N9	5.92	112.94	108.20
27	B8	2859	G	C5-C6-O6	-5.92	125.05	128.60
1	AA	59	A	C5-C6-N6	-5.92	118.97	123.70
1	AA	1162	C	N3-C4-N4	5.92	122.14	118.00
1	AA	1432	G	N3-C2-N2	5.92	124.04	119.90
27	B8	84	A	C5-C6-N6	-5.92	118.97	123.70
27	B8	310	A	C5-C6-N1	-5.92	114.74	117.70
27	B8	460	A	C4-C5-C6	5.92	119.96	117.00
27	B8	1010	A	C4-C5-C6	5.92	119.96	117.00
27	B8	1556	C	N3-C4-C5	-5.92	119.53	121.90
27	B8	1805	A	C4-C5-C6	5.92	119.96	117.00
27	B8	2767	C	N3-C4-N4	5.92	122.14	118.00
27	B8	2887	A	C5-C6-N6	-5.92	118.97	123.70
1	AA	796	C	N3-C4-N4	5.92	122.14	118.00
27	B8	19	A	C4-C5-C6	5.92	119.96	117.00
1	AA	344	A	C4-C5-C6	5.91	119.96	117.00
1	AA	581	G	N3-C2-N2	5.91	124.04	119.90
1	AA	896	C	N3-C4-N4	5.91	122.14	118.00
26	B7	119	A	C5-C6-N6	-5.91	118.97	123.70
27	B8	650	C	N3-C4-N4	5.91	122.14	118.00
27	B8	1998	A	C5-C6-N6	-5.91	118.97	123.70
27	B8	2317	A	C5-C6-N6	-5.91	118.97	123.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	2435	A	O4'-C1'-N9	5.91	112.93	108.20
27	B8	2589	A	C5-C6-N1	-5.91	114.74	117.70
27	B8	2725	A	C4-C5-C6	5.91	119.96	117.00
27	B8	2813	A	C4-C5-C6	5.91	119.96	117.00
1	AA	136	C	N3-C4-N4	5.91	122.14	118.00
1	AA	1229	A	C5-C6-N6	-5.91	118.97	123.70
1	AA	1329	A	C4-C5-C6	5.91	119.96	117.00
27	B8	794	A	C4-C5-C6	5.91	119.96	117.00
27	B8	814	C	N3-C4-N4	5.91	122.14	118.00
1	AA	309	A	C4-C5-C6	5.91	119.96	117.00
1	AA	1236	A	C5-C6-N1	-5.91	114.75	117.70
1	AA	1524	C	N3-C4-N4	5.91	122.14	118.00
27	B8	103	A	C4-C5-C6	5.91	119.96	117.00
27	B8	838	C	N3-C4-N4	5.91	122.14	118.00
27	B8	1247	A	C5-C6-N1	-5.91	114.75	117.70
27	B8	1592	C	N3-C4-N4	5.91	122.14	118.00
27	B8	1745	A	C5-C6-N1	-5.91	114.75	117.70
27	B8	1863	G	O4'-C1'-N9	5.91	112.93	108.20
27	B8	1936	A	C5-C6-N6	-5.91	118.97	123.70
27	B8	1960	A	C4-C5-C6	5.91	119.95	117.00
1	AA	539	A	C5-C6-N6	-5.91	118.97	123.70
1	AA	985	C	N3-C4-N4	5.91	122.14	118.00
1	AA	1188	A	C5-C6-N6	-5.91	118.97	123.70
1	AA	1322	C	C6-N1-C1'	-5.91	113.71	120.80
27	B8	5	A	C4-C5-C6	5.91	119.95	117.00
27	B8	97	C	N3-C4-N4	5.91	122.14	118.00
27	B8	422	A	C4-C5-C6	5.91	119.95	117.00
27	B8	627	A	C4-C5-C6	5.91	119.95	117.00
27	B8	2662	A	C5-C6-N1	-5.91	114.75	117.70
27	B8	2829	A	C4-C5-C6	5.91	119.95	117.00
1	AA	131	A	C5-C6-N1	-5.91	114.75	117.70
1	AA	1019	A	O4'-C1'-N9	5.91	112.93	108.20
27	B8	435	C	N3-C4-C5	-5.91	119.54	121.90
27	B8	1450	G	O4'-C1'-N9	5.91	112.93	108.20
27	B8	2545	G	O4'-C1'-N9	5.91	112.93	108.20
1	AA	321	A	C5-C6-N1	-5.91	114.75	117.70
1	AA	1067	A	C4-C5-C6	5.91	119.95	117.00
27	B8	1243	C	N3-C4-N4	5.91	122.13	118.00
27	B8	2009	A	O4'-C1'-N9	5.91	112.92	108.20
27	B8	2147	A	C5-C6-N6	-5.91	118.98	123.70
1	AA	794	A	C4-C5-C6	5.90	119.95	117.00
1	AA	1067	A	C5-C6-N1	-5.90	114.75	117.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1250	A	C5-C6-N6	-5.90	118.98	123.70
27	B8	1109	C	N3-C4-N4	5.90	122.13	118.00
27	B8	1677	A	C4-C5-C6	5.90	119.95	117.00
1	AA	328	C	C2-N1-C1'	5.90	125.29	118.80
27	B8	128	C	N3-C4-N4	5.90	122.13	118.00
27	B8	471	A	C5-C6-N1	-5.90	114.75	117.70
27	B8	599	A	C5-C6-N1	-5.90	114.75	117.70
27	B8	812	C	N3-C4-N4	5.90	122.13	118.00
27	B8	978	G	O4'-C1'-N9	5.90	112.92	108.20
27	B8	1039	A	C5-C6-N6	-5.90	118.98	123.70
27	B8	1155	A	C4-C5-C6	5.90	119.95	117.00
27	B8	1241	A	C4-C5-C6	5.90	119.95	117.00
27	B8	1788	C	N3-C4-N4	5.90	122.13	118.00
1	AA	192	A	C5-C6-N1	-5.90	114.75	117.70
1	AA	396	C	N3-C4-N4	5.90	122.13	118.00
1	AA	462	G	O4'-C1'-N9	5.90	112.92	108.20
1	AA	1171	A	C4-C5-C6	5.90	119.95	117.00
1	AA	1364	U	C2-N1-C1'	5.90	124.78	117.70
1	AA	1480	A	C4-C5-C6	5.90	119.95	117.00
27	B8	211	C	N3-C4-N4	5.90	122.13	118.00
27	B8	749	A	C5-C6-N6	-5.90	118.98	123.70
27	B8	789	A	C5-C6-N6	-5.90	118.98	123.70
27	B8	994	C	N3-C4-N4	5.90	122.13	118.00
27	B8	1114	C	N3-C4-N4	5.90	122.13	118.00
27	B8	1334	G	O4'-C1'-N9	5.90	112.92	108.20
27	B8	1586	A	C5-C6-N6	-5.90	118.98	123.70
27	B8	1615	C	O4'-C1'-N1	5.90	112.92	108.20
27	B8	2191	A	C4-C5-C6	5.90	119.95	117.00
27	B8	2710	C	N3-C4-N4	5.90	122.13	118.00
1	AA	11	G	O4'-C1'-N9	5.90	112.92	108.20
1	AA	1082	A	C5-C6-N1	-5.90	114.75	117.70
27	B8	181	A	O4'-C1'-N9	5.90	112.92	108.20
27	B8	404	A	C4-C5-C6	5.90	119.95	117.00
27	B8	624	C	N3-C4-C5	-5.90	119.54	121.90
1	AA	336	A	C4-C5-C6	5.90	119.95	117.00
27	B8	1194	A	C5-C6-N6	-5.90	118.98	123.70
27	B8	1289	C	N3-C4-N4	5.90	122.13	118.00
27	B8	1760	C	N3-C4-N4	5.90	122.13	118.00
27	B8	2013	A	C5-C6-N6	-5.90	118.98	123.70
27	B8	2133	G	O4'-C1'-N9	5.90	112.92	108.20
27	B8	2170	A	C5-C6-N6	-5.90	118.98	123.70
27	B8	2873	A	O4'-C1'-N9	5.90	112.92	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	800	G	C5-C6-O6	-5.90	125.06	128.60
1	AA	899	C	N3-C4-N4	5.90	122.13	118.00
27	B8	2810	A	C5-C6-N6	-5.90	118.98	123.70
1	AA	323	U	O4'-C1'-N1	5.89	112.92	108.20
1	AA	386	C	N3-C4-N4	5.89	122.13	118.00
1	AA	958	A	C5-C6-N1	-5.89	114.75	117.70
1	AA	1208	C	N3-C4-N4	5.89	122.13	118.00
1	AA	1374	A	C4-C5-C6	5.89	119.95	117.00
1	AA	1446	A	C4-C5-C6	5.89	119.95	117.00
27	B8	38	A	C5-C6-N6	-5.89	118.98	123.70
27	B8	322	A	C5-C6-N6	-5.89	118.98	123.70
27	B8	1208	C	N3-C4-N4	5.89	122.13	118.00
27	B8	1978	A	C5-C6-N6	-5.89	118.98	123.70
27	B8	2308	G	C5-C6-O6	-5.89	125.06	128.60
27	B8	2547	A	C4-C5-C6	5.89	119.95	117.00
1	AA	183	C	C2-N1-C1'	5.89	125.28	118.80
1	AA	938	A	C5-C6-N6	-5.89	118.99	123.70
1	AA	1031	C	N3-C4-C5	-5.89	119.54	121.90
27	B8	295	G	O4'-C1'-N9	5.89	112.91	108.20
27	B8	602	A	C4-C5-C6	5.89	119.95	117.00
27	B8	1191	G	O4'-C1'-N9	5.89	112.91	108.20
27	B8	1230	A	C5-C6-N6	-5.89	118.99	123.70
27	B8	1544	A	O4'-C1'-N9	5.89	112.91	108.20
27	B8	2075	U	O4'-C1'-N1	5.89	112.91	108.20
1	AA	68	G	C5-C6-O6	-5.89	125.06	128.60
1	AA	1214	C	O4'-C1'-N1	5.89	112.91	108.20
1	AA	1410	A	O4'-C1'-N9	5.89	112.91	108.20
27	B8	21	A	O4'-C1'-N9	5.89	112.91	108.20
27	B8	1446	C	N3-C4-N4	5.89	122.12	118.00
27	B8	1553	A	C4-C5-C6	5.89	119.94	117.00
27	B8	2837	A	C5-C6-N6	-5.89	118.99	123.70
1	AA	1049	U	O4'-C1'-N1	5.89	112.91	108.20
1	AA	1427	C	N3-C4-N4	5.89	122.12	118.00
1	AA	1429	A	C4-C5-C6	5.89	119.94	117.00
3	AV	59	A	C4-C5-C6	5.89	119.94	117.00
26	B7	118	C	N3-C4-N4	5.89	122.12	118.00
27	B8	382	A	C4-C5-C6	5.89	119.94	117.00
27	B8	605	G	O4'-C1'-N9	5.89	112.91	108.20
27	B8	855	G	O4'-C1'-N9	5.89	112.91	108.20
27	B8	910	A	C5-C6-N1	-5.89	114.75	117.70
27	B8	989	G	O4'-C1'-N9	5.89	112.91	108.20
27	B8	1090	A	O4'-C1'-N9	5.89	112.91	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	1294	U	O4'-C1'-N1	5.89	112.91	108.20
27	B8	1639	C	O4'-C1'-N1	5.89	112.91	108.20
27	B8	1741	C	N3-C4-N4	5.89	122.12	118.00
27	B8	2317	A	O4'-C1'-N9	5.89	112.91	108.20
1	AA	7	A	C4-C5-C6	5.89	119.94	117.00
27	B8	904	G	O4'-C1'-N9	5.89	112.91	108.20
27	B8	1623	G	O4'-C1'-N9	5.89	112.91	108.20
27	B8	2132	U	C2-N1-C1'	5.89	124.77	117.70
1	AA	414	A	C4-C5-C6	5.89	119.94	117.00
1	AA	1042	A	C4-C5-C6	5.89	119.94	117.00
1	AA	1508	A	C4-C5-C6	5.89	119.94	117.00
26	B7	19	C	N3-C4-N4	5.89	122.12	118.00
27	B8	371	A	C5-C6-N1	-5.89	114.76	117.70
27	B8	1366	A	C5-C6-N6	-5.89	118.99	123.70
27	B8	2115	G	O4'-C1'-N9	5.89	112.91	108.20
27	B8	2200	C	N3-C4-C5	-5.89	119.55	121.90
27	B8	2250	G	C5-C6-O6	-5.89	125.07	128.60
27	B8	2630	G	O4'-C1'-N9	5.89	112.91	108.20
35	BG	108	PHE	CB-CG-CD1	-5.89	116.68	120.80
1	AA	45	G	O4'-C1'-N9	5.88	112.91	108.20
1	AA	694	A	C5-C6-N6	-5.88	118.99	123.70
1	AA	736	C	N3-C4-N4	5.88	122.12	118.00
1	AA	815	A	C4-C5-C6	5.88	119.94	117.00
1	AA	1246	A	C5-C6-N1	-5.88	114.76	117.70
1	AA	1358	U	O4'-C1'-N1	5.88	112.91	108.20
1	AA	1377	A	C5-C6-N6	-5.88	118.99	123.70
27	B8	410	G	N3-C2-N2	5.88	124.02	119.90
27	B8	691	C	N3-C4-N4	5.88	122.12	118.00
27	B8	2162	G	O4'-C1'-N9	5.88	112.91	108.20
27	B8	2198	A	C4-C5-C6	5.88	119.94	117.00
27	B8	2820	A	C4-C5-C6	5.88	119.94	117.00
27	B8	2823	A	C4-C5-C6	5.88	119.94	117.00
1	AA	1176	A	C4-C5-C6	5.88	119.94	117.00
27	B8	847	U	C2-N1-C1'	5.88	124.76	117.70
27	B8	982	C	C6-N1-C1'	-5.88	113.74	120.80
27	B8	1663	G	O4'-C1'-N9	5.88	112.91	108.20
27	B8	2252	G	O4'-C1'-N9	5.88	112.91	108.20
1	AA	301	G	O4'-C1'-N9	5.88	112.90	108.20
1	AA	1155	A	C5-C6-N1	-5.88	114.76	117.70
1	AA	1167	A	C4-C5-C6	5.88	119.94	117.00
1	AA	1339	A	O4'-C1'-N9	5.88	112.91	108.20
1	AA	1492	A	O4'-C1'-N9	5.88	112.91	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	127	A	C4-C5-C6	5.88	119.94	117.00
27	B8	961	C	O4'-C1'-N1	5.88	112.91	108.20
27	B8	2000	C	N3-C4-N4	5.88	122.12	118.00
27	B8	2191	A	C5-C6-N1	-5.88	114.76	117.70
27	B8	2281	A	O4'-C1'-N9	5.88	112.91	108.20
27	B8	2468	A	C4-C5-C6	5.88	119.94	117.00
27	B8	2636	C	N3-C4-N4	5.88	122.12	118.00
27	B8	2706	A	C5-C6-N6	-5.88	118.99	123.70
27	B8	2882	A	C4-C5-C6	5.88	119.94	117.00
1	AA	655	A	C5-C6-N1	-5.88	114.76	117.70
1	AA	949	A	C4-C5-C6	5.88	119.94	117.00
1	AA	1340	A	C4-C5-C6	5.88	119.94	117.00
27	B8	1325	U	O4'-C1'-N1	5.88	112.90	108.20
27	B8	1362	C	N3-C4-N4	5.88	122.12	118.00
27	B8	2169	A	C4-C5-C6	5.88	119.94	117.00
27	B8	455	C	N3-C4-C5	-5.88	119.55	121.90
27	B8	497	A	C5-C6-N1	-5.88	114.76	117.70
27	B8	905	A	O4'-C1'-N9	5.88	112.90	108.20
27	B8	1194	A	C4-C5-C6	5.88	119.94	117.00
27	B8	1768	C	N3-C4-N4	5.88	122.11	118.00
27	B8	2005	A	C4-C5-C6	5.88	119.94	117.00
27	B8	2090	A	C4-C5-C6	5.88	119.94	117.00
27	B8	2722	G	O4'-C1'-N9	5.88	112.90	108.20
1	AA	553	A	C5-C6-N6	-5.88	119.00	123.70
1	AA	974	A	C5-C6-N6	-5.88	119.00	123.70
27	B8	798	G	O4'-C1'-N9	5.88	112.90	108.20
27	B8	1260	A	O4'-C1'-N9	5.88	112.90	108.20
27	B8	1978	A	O4'-C1'-N9	5.88	112.90	108.20
27	B8	2021	C	N3-C4-N4	5.88	122.11	118.00
1	AA	300	A	C4-C5-C6	5.88	119.94	117.00
1	AA	533	A	C5-C6-N1	-5.88	114.76	117.70
1	AA	773	G	O4'-C1'-N9	5.88	112.90	108.20
27	B8	2359	C	N3-C4-N4	5.88	122.11	118.00
1	AA	19	A	C5-C6-N6	-5.87	119.00	123.70
1	AA	629	A	C5-C6-N6	-5.87	119.00	123.70
1	AA	687	A	C4-C5-C6	5.87	119.94	117.00
1	AA	946	A	C5-C6-N1	-5.87	114.76	117.70
27	B8	181	A	C4-C5-C6	5.87	119.94	117.00
27	B8	429	A	C5-C6-N6	-5.87	119.00	123.70
27	B8	544	C	C6-N1-C1'	-5.87	113.75	120.80
27	B8	1757	A	C5-C6-N6	-5.87	119.00	123.70
27	B8	1773	A	O4'-C1'-N9	5.87	112.90	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	2059	A	C4-C5-C6	5.87	119.94	117.00
1	AA	65	A	C4-C5-C6	5.87	119.94	117.00
1	AA	263	A	C5-C6-N6	-5.87	119.00	123.70
1	AA	434	U	O4'-C1'-N1	5.87	112.90	108.20
1	AA	1063	C	O4'-C1'-N1	5.87	112.90	108.20
26	B7	54	G	O4'-C1'-N9	5.87	112.90	108.20
27	B8	746	U	O4'-C1'-N1	5.87	112.90	108.20
1	AA	441	A	C4-C5-C6	5.87	119.94	117.00
1	AA	1058	G	O4'-C1'-N9	5.87	112.90	108.20
27	B8	920	A	C5-C6-N1	-5.87	114.77	117.70
1	AA	223	A	C5-C6-N1	-5.87	114.77	117.70
27	B8	26	G	N3-C2-N2	5.87	124.01	119.90
27	B8	950	G	O4'-C1'-N9	5.87	112.89	108.20
27	B8	1615	C	N3-C4-N4	5.87	122.11	118.00
27	B8	1618	A	C5-C6-N6	-5.87	119.00	123.70
27	B8	1749	A	C5-C6-N1	-5.87	114.77	117.70
27	B8	1881	C	N3-C4-N4	5.87	122.11	118.00
27	B8	1969	A	C5-C6-N1	-5.87	114.77	117.70
27	B8	2108	A	C4-C5-C6	5.87	119.94	117.00
27	B8	2807	U	O4'-C1'-N1	5.87	112.89	108.20
1	AA	3	A	C5-C6-N6	-5.87	119.01	123.70
1	AA	525	C	N3-C4-N4	5.87	122.11	118.00
27	B8	2841	C	N3-C4-N4	5.87	122.11	118.00
1	AA	205	A	O4'-C1'-N9	5.87	112.89	108.20
1	AA	443	C	N3-C4-N4	5.87	122.11	118.00
1	AA	705	G	O4'-C1'-N9	5.87	112.89	108.20
1	AA	1237	C	N3-C4-N4	5.87	122.11	118.00
1	AA	1254	A	C4-C5-C6	5.87	119.93	117.00
1	AA	1513	A	C4-C5-C6	5.87	119.93	117.00
27	B8	395	U	O4'-C1'-N1	5.87	112.89	108.20
27	B8	480	A	O4'-C1'-N9	5.87	112.89	108.20
27	B8	716	A	C5-C6-N6	-5.87	119.01	123.70
27	B8	1126	A	C4-C5-C6	5.87	119.93	117.00
27	B8	2311	A	C5-C6-N1	-5.87	114.77	117.70
27	B8	2362	C	N3-C4-N4	5.87	122.11	118.00
27	B8	2369	A	C4-C5-C6	5.87	119.93	117.00
27	B8	2753	A	O4'-C1'-N9	5.87	112.89	108.20
27	B8	2756	U	P-O3'-C3'	5.87	126.74	119.70
1	AA	182	A	C5-C6-N1	-5.86	114.77	117.70
1	AA	382	A	C4-C5-C6	5.86	119.93	117.00
27	B8	191	A	C5-C6-N1	-5.86	114.77	117.70
27	B8	965	C	N3-C4-C5	-5.86	119.55	121.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	977	G	O4'-C1'-N9	5.86	112.89	108.20
27	B8	1771	C	N3-C4-N4	5.86	122.10	118.00
1	AA	453	G	O4'-C1'-N9	5.86	112.89	108.20
27	B8	1496	A	C4-C5-C6	5.86	119.93	117.00
1	AA	199	A	C5-C6-N1	-5.86	114.77	117.70
1	AA	346	G	O4'-C1'-N9	5.86	112.89	108.20
1	AA	1054	C	N3-C4-N4	5.86	122.10	118.00
27	B8	53	A	C5-C6-N6	-5.86	119.01	123.70
27	B8	2411	A	C5-C6-N6	-5.86	119.01	123.70
27	B8	2829	A	C5-C6-N1	-5.86	114.77	117.70
1	AA	1280	A	C4-C5-C6	5.86	119.93	117.00
27	B8	1050	A	C5-C6-N6	-5.86	119.01	123.70
27	B8	1408	G	O4'-C1'-N9	5.86	112.89	108.20
27	B8	2213	U	O4'-C1'-N1	5.86	112.89	108.20
27	B8	2791	G	O4'-C1'-N9	5.86	112.89	108.20
1	AA	350	G	O4'-C1'-N9	5.86	112.89	108.20
1	AA	441	A	O4'-C1'-N9	5.86	112.89	108.20
1	AA	553	A	C4-C5-C6	5.86	119.93	117.00
1	AA	1021	A	C4-C5-C6	5.86	119.93	117.00
1	AA	1157	A	C4-C5-C6	5.86	119.93	117.00
1	AA	1204	A	C5-C6-N1	-5.86	114.77	117.70
1	AA	1388	C	N3-C4-N4	5.86	122.10	118.00
26	B7	73	A	C5-C6-N1	-5.86	114.77	117.70
27	B8	382	A	C5-C6-N1	-5.86	114.77	117.70
27	B8	421	C	N3-C4-N4	5.86	122.10	118.00
27	B8	1009	A	C5-C6-N6	-5.86	119.01	123.70
27	B8	1090	A	C4-C5-C6	5.86	119.93	117.00
27	B8	1244	A	C4-C5-C6	5.86	119.93	117.00
27	B8	1496	A	O4'-C1'-N9	5.86	112.89	108.20
27	B8	1690	A	O4'-C1'-N9	5.86	112.89	108.20
27	B8	2326	C	N3-C4-N4	5.86	122.10	118.00
27	B8	2518	A	C4-C5-C6	5.86	119.93	117.00
27	B8	2670	A	C5-C6-N6	-5.86	119.01	123.70
27	B8	2814	A	O4'-C1'-N9	5.86	112.89	108.20
1	AA	647	C	N3-C4-N4	5.86	122.10	118.00
1	AA	949	A	C5-C6-N1	-5.86	114.77	117.70
27	B8	945	A	C5-C6-N6	-5.86	119.02	123.70
27	B8	1558	C	N3-C4-C5	-5.86	119.56	121.90
27	B8	1952	A	C5-C6-N6	-5.86	119.02	123.70
27	B8	2206	C	N3-C4-N4	5.86	122.10	118.00
27	B8	2314	A	C5-C6-N1	-5.86	114.77	117.70
27	B8	2449	U	O4'-C1'-N1	5.86	112.89	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	2570	G	O4'-C1'-N9	5.86	112.89	108.20
27	B8	2676	C	N3-C4-N4	5.86	122.10	118.00
26	B7	70	C	N3-C4-N4	5.85	122.10	118.00
27	B8	1014	A	C4-C5-C6	5.85	119.93	117.00
27	B8	2412	A	C5-C6-N6	-5.85	119.02	123.70
1	AA	504	C	N3-C4-C5	-5.85	119.56	121.90
1	AA	771	G	O4'-C1'-N9	5.85	112.88	108.20
1	AA	1377	A	O4'-C1'-N9	5.85	112.88	108.20
1	AA	1413	A	C5-C6-N1	-5.85	114.77	117.70
27	B8	549	G	O4'-C1'-N9	5.85	112.88	108.20
27	B8	715	A	C4-C5-C6	5.85	119.93	117.00
27	B8	1503	A	C5-C6-N1	-5.85	114.77	117.70
1	AA	560	A	C5-C6-N6	-5.85	119.02	123.70
1	AA	737	C	N3-C4-C5	-5.85	119.56	121.90
1	AA	1196	A	C5-C6-N6	-5.85	119.02	123.70
27	B8	429	A	C5-C6-N1	-5.85	114.77	117.70
27	B8	557	C	N3-C4-N4	5.85	122.09	118.00
27	B8	1490	A	C5-C6-N6	-5.85	119.02	123.70
27	B8	1928	A	O4'-C1'-N9	5.85	112.88	108.20
27	B8	2665	A	C5-C6-N6	-5.85	119.02	123.70
1	AA	171	A	O4'-C1'-N9	5.85	112.88	108.20
1	AA	217	C	N3-C4-N4	5.85	122.09	118.00
1	AA	384	G	O4'-C1'-N9	5.85	112.88	108.20
27	B8	1579	A	O4'-C1'-N9	5.85	112.88	108.20
1	AA	236	A	C5-C6-N6	-5.85	119.02	123.70
1	AA	341	C	N3-C4-N4	5.85	122.09	118.00
1	AA	414	A	O4'-C1'-N9	5.85	112.88	108.20
3	AV	63	C	N3-C4-C5	-5.85	119.56	121.90
27	B8	111	A	C5-C6-N6	-5.85	119.02	123.70
27	B8	209	C	N3-C4-N4	5.85	122.09	118.00
27	B8	679	C	N3-C4-N4	5.85	122.09	118.00
27	B8	951	C	N3-C4-N4	5.85	122.09	118.00
27	B8	1502	A	C4-C5-C6	5.85	119.92	117.00
27	B8	2268	A	C5-C6-N1	-5.85	114.78	117.70
27	B8	2781	A	C4-C5-C6	5.85	119.92	117.00
1	AA	1352	C	N3-C4-N4	5.85	122.09	118.00
26	B7	94	A	C5-C6-N6	-5.85	119.02	123.70
27	B8	1167	C	N3-C4-N4	5.85	122.09	118.00
27	B8	2052	A	C4-C5-C6	5.85	119.92	117.00
27	B8	2733	A	O4'-C1'-N9	5.85	112.88	108.20
27	B8	2740	A	C4-C5-C6	5.85	119.92	117.00
27	B8	2781	A	C5-C6-N6	-5.85	119.02	123.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	817	C	N3-C4-N4	5.84	122.09	118.00
27	B8	825	A	C4-C5-C6	5.84	119.92	117.00
27	B8	935	C	N3-C4-N4	5.84	122.09	118.00
27	B8	1609	A	C5-C6-N6	-5.84	119.02	123.70
27	B8	1965	C	N3-C4-N4	5.84	122.09	118.00
27	B8	2093	G	O4'-C1'-N9	5.84	112.88	108.20
27	B8	2386	A	C4-C5-C6	5.84	119.92	117.00
1	AA	959	A	C5-C6-N1	-5.84	114.78	117.70
27	B8	1764	C	N3-C4-N4	5.84	122.09	118.00
27	B8	2376	A	C5-C6-N6	-5.84	119.03	123.70
1	AA	51	A	C5-C6-N1	-5.84	114.78	117.70
1	AA	100	G	O4'-C1'-N9	5.84	112.87	108.20
1	AA	825	A	O4'-C1'-N9	5.84	112.87	108.20
26	B7	47	C	N3-C4-C5	-5.84	119.56	121.90
27	B8	599	A	C4-C5-C6	5.84	119.92	117.00
27	B8	2156	G	C5-C6-O6	-5.84	125.09	128.60
27	B8	2176	A	C4-C5-C6	5.84	119.92	117.00
1	AA	61	G	O4'-C1'-N9	5.84	112.87	108.20
1	AA	257	G	O4'-C1'-N9	5.84	112.87	108.20
1	AA	452	A	O4'-C1'-N9	5.84	112.87	108.20
1	AA	938	A	C4-C5-C6	5.84	119.92	117.00
1	AA	1322	C	N3-C4-C5	-5.84	119.56	121.90
27	B8	394	C	N3-C4-N4	5.84	122.09	118.00
27	B8	917	A	C5-C6-N1	-5.84	114.78	117.70
27	B8	1416	G	O4'-C1'-N9	5.84	112.87	108.20
27	B8	1595	C	N3-C4-N4	5.84	122.09	118.00
1	AA	32	A	C5-C6-N6	-5.84	119.03	123.70
27	B8	1142	A	C5'-C4'-O4'	5.84	116.11	109.10
27	B8	1272	A	O4'-C1'-N9	5.84	112.87	108.20
27	B8	1906	G	O4'-C1'-N9	5.84	112.87	108.20
27	B8	2313	C	N3-C4-N4	5.84	122.09	118.00
27	B8	2691	C	N3-C4-N4	5.84	122.09	118.00
1	AA	243	A	C4'-C3'-C2'	5.84	108.44	102.60
1	AA	1176	A	O4'-C1'-N9	5.84	112.87	108.20
27	B8	203	A	C5-C6-N6	-5.84	119.03	123.70
27	B8	272	A	C4-C5-C6	5.84	119.92	117.00
27	B8	539	G	C5-C6-O6	-5.84	125.10	128.60
27	B8	608	A	C5-C6-N6	-5.84	119.03	123.70
27	B8	764	A	C5-C6-N1	-5.84	114.78	117.70
27	B8	1585	C	N3-C4-N4	5.84	122.09	118.00
27	B8	2060	A	C4-C5-C6	5.84	119.92	117.00
1	AA	435	A	C5-C6-N6	-5.83	119.03	123.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1461	G	O4'-C1'-N9	5.83	112.87	108.20
27	B8	829	A	C4-C5-C6	5.83	119.92	117.00
27	B8	1077	A	O4'-C1'-N9	5.83	112.87	108.20
27	B8	1091	G	O4'-C1'-N9	5.83	112.87	108.20
27	B8	1161	C	N3-C4-N4	5.83	122.08	118.00
27	B8	2183	A	C5-C6-N6	-5.83	119.03	123.70
27	B8	2740	A	C5-C6-N6	-5.83	119.03	123.70
1	AA	246	A	C5-C6-N1	-5.83	114.78	117.70
1	AA	302	G	O4'-C1'-N9	5.83	112.87	108.20
1	AA	497	G	O4'-C1'-N9	5.83	112.87	108.20
1	AA	511	C	N3-C4-N4	5.83	122.08	118.00
1	AA	999	C	N3-C4-N4	5.83	122.08	118.00
1	AA	1155	A	C4-C5-C6	5.83	119.92	117.00
3	AV	52	A	C4-C5-C6	5.83	119.92	117.00
27	B8	146	A	C4-C5-C6	5.83	119.92	117.00
27	B8	203	A	C4-C5-C6	5.83	119.92	117.00
27	B8	949	G	O4'-C1'-N9	5.83	112.87	108.20
27	B8	1079	C	N3-C4-N4	5.83	122.08	118.00
27	B8	1338	G	O4'-C1'-N9	5.83	112.87	108.20
1	AA	819	A	C4-C5-C6	5.83	119.92	117.00
1	AA	1051	C	N3-C4-N4	5.83	122.08	118.00
1	AA	1331	G	N3-C2-N2	5.83	123.98	119.90
3	AV	6	C	N3-C4-N4	5.83	122.08	118.00
26	B7	67	G	C5-C6-O6	-5.83	125.10	128.60
27	B8	300	A	C5-C6-N6	-5.83	119.03	123.70
27	B8	695	G	O4'-C1'-N9	5.83	112.87	108.20
27	B8	1373	A	C5-C6-N1	-5.83	114.78	117.70
27	B8	1654	A	C5-C6-N6	-5.83	119.03	123.70
27	B8	1754	A	O4'-C1'-N9	5.83	112.86	108.20
27	B8	2594	C	N3-C4-N4	5.83	122.08	118.00
27	B8	2734	A	C4-C5-C6	5.83	119.92	117.00
1	AA	634	C	N3-C4-N4	5.83	122.08	118.00
1	AA	1107	C	N3-C4-N4	5.83	122.08	118.00
1	AA	1456	A	O4'-C1'-N9	5.83	112.86	108.20
27	B8	666	A	C4-C5-C6	5.83	119.92	117.00
1	AA	522	C	N3-C4-N4	5.83	122.08	118.00
1	AA	1184	G	O4'-C1'-N9	5.83	112.86	108.20
26	B7	39	A	O4'-C1'-N9	5.83	112.86	108.20
27	B8	320	A	C5-C6-N6	-5.83	119.04	123.70
27	B8	524	G	O4'-C1'-N9	5.83	112.86	108.20
27	B8	733	G	O4'-C1'-N9	5.83	112.86	108.20
27	B8	1129	A	C4-C5-C6	5.83	119.91	117.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	1239	G	O4'-C1'-N9	5.83	112.86	108.20
27	B8	1499	C	N3-C4-N4	5.83	122.08	118.00
27	B8	1609	A	C4-C5-C6	5.83	119.91	117.00
27	B8	345	A	C5-C6-N6	-5.83	119.04	123.70
27	B8	1241	A	C5-C6-N6	-5.83	119.04	123.70
27	B8	1986	C	N3-C4-N4	5.83	122.08	118.00
1	AA	303	A	C5-C6-N1	-5.83	114.79	117.70
1	AA	487	A	C5-C6-N1	-5.83	114.79	117.70
1	AA	780	A	C4-C5-C6	5.83	119.91	117.00
1	AA	781	A	C5-C6-N1	-5.83	114.79	117.70
1	AA	787	A	C5-C6-N6	-5.83	119.04	123.70
3	AV	12	G	O4'-C1'-N9	5.83	112.86	108.20
27	B8	1009	A	C4-C5-C6	5.83	119.91	117.00
27	B8	1040	A	O4'-C1'-N9	5.83	112.86	108.20
27	B8	1359	A	C5-C6-N6	-5.83	119.04	123.70
27	B8	1504	A	C5-C6-N1	-5.83	114.79	117.70
27	B8	2091	C	N3-C4-N4	5.83	122.08	118.00
27	B8	2592	G	O4'-C1'-N9	5.83	112.86	108.20
1	AA	8	A	C5-C6-N6	-5.82	119.04	123.70
27	B8	655	A	C4-C5-C6	5.82	119.91	117.00
27	B8	1012	U	O4'-C1'-N1	5.82	112.86	108.20
27	B8	1257	C	N3-C4-N4	5.82	122.08	118.00
27	B8	2295	C	N3-C4-N4	5.82	122.08	118.00
27	B8	2642	G	O4'-C1'-N9	5.82	112.86	108.20
27	B8	2671	G	O4'-C1'-N9	5.82	112.86	108.20
1	AA	43	C	N3-C4-N4	5.82	122.08	118.00
1	AA	994	A	C5-C6-N6	-5.82	119.04	123.70
26	B7	102	G	O4'-C1'-N9	5.82	112.86	108.20
27	B8	1701	A	O4'-C1'-N9	5.82	112.86	108.20
27	B8	2618	G	O4'-C1'-N9	5.82	112.86	108.20
1	AA	349	A	C4-C5-C6	5.82	119.91	117.00
1	AA	1117	A	C4-C5-C6	5.82	119.91	117.00
26	B7	71	C	N3-C4-N4	5.82	122.07	118.00
27	B8	632	A	C5-C6-N6	-5.82	119.04	123.70
27	B8	717	C	N3-C4-N4	5.82	122.08	118.00
27	B8	1701	A	C4-C5-C6	5.82	119.91	117.00
27	B8	2891	U	O4'-C1'-N1	5.82	112.86	108.20
1	AA	1271	A	O4'-C1'-N9	5.82	112.86	108.20
27	B8	634	C	N3-C4-N4	5.82	122.07	118.00
27	B8	996	A	C5-C6-N6	-5.82	119.05	123.70
27	B8	1456	G	O4'-C1'-N9	5.82	112.86	108.20
1	AA	338	A	C5-C6-N1	-5.82	114.79	117.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	969	A	C4-C5-C6	5.82	119.91	117.00
27	B8	796	C	N3-C4-N4	5.82	122.07	118.00
27	B8	995	C	N3-C4-N4	5.82	122.07	118.00
27	B8	1028	A	C4-C5-C6	5.82	119.91	117.00
27	B8	1548	A	C5-C6-N6	-5.82	119.05	123.70
27	B8	1614	A	C4-C5-C6	5.82	119.91	117.00
27	B8	1711	A	C4-C5-C6	5.82	119.91	117.00
27	B8	1968	G	N3-C2-N2	5.82	123.97	119.90
27	B8	2264	C	N3-C4-N4	5.82	122.07	118.00
27	B8	2340	A	C4-C5-C6	5.82	119.91	117.00
27	B8	2794	C	N3-C4-N4	5.82	122.07	118.00
48	BT	99	ALA	N-CA-CB	5.82	118.24	110.10
1	AA	665	A	C4-C5-C6	5.82	119.91	117.00
1	AA	994	A	O4'-C1'-N9	5.82	112.85	108.20
27	B8	91	A	C5-C6-N1	-5.82	114.79	117.70
27	B8	618	G	O4'-C1'-N9	5.82	112.85	108.20
27	B8	1284	A	C4-C5-C6	5.82	119.91	117.00
27	B8	1480	C	N3-C4-N4	5.82	122.07	118.00
27	B8	1495	A	C5-C6-N6	-5.82	119.05	123.70
27	B8	2406	A	C5-C6-N6	-5.82	119.05	123.70
1	AA	816	A	C5-C6-N6	-5.81	119.05	123.70
27	B8	988	A	C5-C6-N1	-5.81	114.79	117.70
27	B8	1479	G	O4'-C1'-N9	5.81	112.85	108.20
1	AA	149	A	C5-C6-N6	-5.81	119.05	123.70
1	AA	393	A	C5-C6-N1	-5.81	114.79	117.70
1	AA	1140	C	N3-C4-N4	5.81	122.07	118.00
1	AA	1311	A	C4-C5-C6	5.81	119.91	117.00
27	B8	1075	C	N3-C4-N4	5.81	122.07	118.00
27	B8	1399	C	N3-C4-C5	-5.81	119.58	121.90
27	B8	2021	C	N3-C4-C5	-5.81	119.58	121.90
27	B8	2064	C	N3-C4-N4	5.81	122.07	118.00
27	B8	2600	A	C4-C5-C6	5.81	119.91	117.00
27	B8	2651	C	N3-C4-N4	5.81	122.07	118.00
27	B8	2057	G	O4'-C1'-N9	5.81	112.85	108.20
1	AA	124	C	N3-C4-N4	5.81	122.07	118.00
1	AA	411	A	C4-C5-C6	5.81	119.90	117.00
1	AA	1210	C	N3-C4-N4	5.81	122.07	118.00
26	B7	93	C	N3-C4-N4	5.81	122.07	118.00
27	B8	98	G	O4'-C1'-N9	5.81	112.85	108.20
27	B8	1226	A	C5-C6-N1	-5.81	114.80	117.70
27	B8	1276	A	C4-C5-C6	5.81	119.91	117.00
27	B8	1549	A	C4-C5-C6	5.81	119.91	117.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	1591	A	C4-C5-C6	5.81	119.90	117.00
27	B8	2063	C	N3-C4-N4	5.81	122.07	118.00
1	AA	44	A	C5-C6-N1	-5.81	114.80	117.70
1	AA	76	G	P-O5'-C5'	5.81	130.19	120.90
1	AA	1007	U	O4'-C1'-N1	5.81	112.85	108.20
1	AA	1340	A	C5-C6-N1	-5.81	114.80	117.70
27	B8	180	G	O4'-C1'-N9	5.81	112.85	108.20
27	B8	466	A	C5-C6-N1	-5.81	114.80	117.70
27	B8	1679	A	C4-C5-C6	5.81	119.90	117.00
27	B8	2097	A	C4-C5-C6	5.81	119.90	117.00
27	B8	2146	C	N3-C4-C5	-5.81	119.58	121.90
1	AA	1081	A	C4-C5-C6	5.81	119.90	117.00
1	AA	1437	A	C5-C6-N1	-5.81	114.80	117.70
27	B8	608	A	O4'-C1'-N9	5.81	112.84	108.20
27	B8	1260	A	C4-C5-C6	5.81	119.90	117.00
27	B8	2051	A	C4-C5-C6	5.81	119.90	117.00
27	B8	2903	U	C6-N1-C1'	-5.81	113.07	121.20
1	AA	576	C	N3-C4-N4	5.80	122.06	118.00
1	AA	1519	A	C5-C6-N6	-5.80	119.06	123.70
27	B8	146	A	C5-C6-N6	-5.80	119.06	123.70
27	B8	742	A	O4'-C1'-N9	5.80	112.84	108.20
27	B8	1145	C	N3-C4-N4	5.80	122.06	118.00
27	B8	1433	A	C5-C6-N6	-5.80	119.06	123.70
26	B7	115	A	O4'-C1'-N9	5.80	112.84	108.20
27	B8	69	C	N3-C4-C5	-5.80	119.58	121.90
27	B8	299	A	C5-C6-N6	-5.80	119.06	123.70
27	B8	1936	A	C5-C6-N1	-5.80	114.80	117.70
1	AA	353	A	C4-C5-C6	5.80	119.90	117.00
1	AA	1350	A	C4-C5-C6	5.80	119.90	117.00
26	B7	115	A	C4-C5-C6	5.80	119.90	117.00
27	B8	144	A	O4'-C1'-N9	5.80	112.84	108.20
27	B8	1048	A	C5-C6-N1	-5.80	114.80	117.70
27	B8	1293	C	N3-C4-N4	5.80	122.06	118.00
27	B8	1819	A	C5-C6-N6	-5.80	119.06	123.70
27	B8	2158	A	C5-C6-N6	-5.80	119.06	123.70
27	B8	2737	G	O4'-C1'-N9	5.80	112.84	108.20
1	AA	26	A	C5-C6-N6	-5.80	119.06	123.70
1	AA	44	A	C4-C5-C6	5.80	119.90	117.00
1	AA	579	A	C5-C6-N6	-5.80	119.06	123.70
1	AA	749	A	C4-C5-C6	5.80	119.90	117.00
1	AA	784	A	C5-C6-N6	-5.80	119.06	123.70
27	B8	845	A	C5-C6-N6	-5.80	119.06	123.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	1667	G	O4'-C1'-N9	5.80	112.84	108.20
27	B8	1952	A	C4-C5-C6	5.80	119.90	117.00
27	B8	2247	A	C4-C5-C6	5.80	119.90	117.00
1	AA	342	C	N3-C4-N4	5.80	122.06	118.00
26	B7	12	C	N3-C4-N4	5.80	122.06	118.00
27	B8	940	G	O4'-C1'-N9	5.80	112.84	108.20
27	B8	2020	A	C4-C5-C6	5.80	119.90	117.00
27	B8	2070	A	C4-C5-C6	5.80	119.90	117.00
1	AA	648	A	C4-C5-C6	5.80	119.90	117.00
1	AA	649	A	C5-C6-N1	-5.80	114.80	117.70
1	AA	805	C	N3-C4-N4	5.80	122.06	118.00
1	AA	1350	A	C5-C6-N6	-5.80	119.06	123.70
27	B8	466	A	O4'-C1'-N9	5.80	112.84	108.20
27	B8	495	G	O4'-C1'-N9	5.80	112.84	108.20
27	B8	638	G	O4'-C1'-N9	5.80	112.84	108.20
27	B8	1616	A	C4-C5-C6	5.80	119.90	117.00
27	B8	2126	A	C5-C6-N6	-5.80	119.06	123.70
27	B8	2332	C	N3-C4-N4	5.80	122.06	118.00
27	B8	2700	A	C4-C5-C6	5.80	119.90	117.00
1	AA	752	G	O4'-C1'-N9	5.79	112.84	108.20
1	AA	1375	A	C5-C6-N1	-5.79	114.80	117.70
27	B8	226	A	O4'-C1'-N9	5.79	112.84	108.20
27	B8	1949	G	O4'-C1'-N9	5.79	112.84	108.20
27	B8	2328	A	C5-C6-N6	-5.79	119.06	123.70
27	B8	2418	A	C4-C5-C6	5.79	119.90	117.00
27	B8	2806	C	N3-C4-N4	5.79	122.06	118.00
1	AA	215	C	N3-C4-C5	-5.79	119.58	121.90
1	AA	535	A	C4-C5-C6	5.79	119.90	117.00
1	AA	635	A	C4-C5-C6	5.79	119.90	117.00
1	AA	935	A	C5-C6-N6	-5.79	119.06	123.70
27	B8	31	C	N3-C4-N4	5.79	122.06	118.00
27	B8	197	A	C5-C6-N6	-5.79	119.07	123.70
27	B8	238	C	N3-C4-N4	5.79	122.06	118.00
27	B8	256	A	C5-C6-N1	-5.79	114.80	117.70
27	B8	621	A	C4-C5-C6	5.79	119.90	117.00
27	B8	928	A	C4-C5-C6	5.79	119.90	117.00
27	B8	1150	C	N3-C4-C5	-5.79	119.58	121.90
27	B8	1444	G	O4'-C1'-N9	5.79	112.83	108.20
27	B8	1634	A	C5-C6-N6	-5.79	119.06	123.70
27	B8	1772	A	C4-C5-C6	5.79	119.90	117.00
27	B8	1903	G	O4'-C1'-N9	5.79	112.83	108.20
27	B8	2462	C	N3-C4-N4	5.79	122.06	118.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	2626	C	N3-C4-N4	5.79	122.06	118.00
27	B8	2628	C	N3-C4-N4	5.79	122.06	118.00
1	AA	546	A	C5-C6-N6	-5.79	119.07	123.70
1	AA	825	A	C4-C5-C6	5.79	119.90	117.00
1	AA	1229	A	C5-C6-N1	-5.79	114.80	117.70
27	B8	590	A	C4-C5-C6	5.79	119.90	117.00
27	B8	1537	G	P-O3'-C3'	5.79	126.65	119.70
27	B8	1591	A	C5-C6-N1	-5.79	114.80	117.70
27	B8	2142	A	C4-C5-C6	5.79	119.90	117.00
27	B8	2456	C	N3-C4-N4	5.79	122.05	118.00
1	AA	33	A	O4'-C1'-N9	5.79	112.83	108.20
1	AA	802	A	C4-C5-C6	5.79	119.89	117.00
26	B7	98	G	O4'-C1'-N9	5.79	112.83	108.20
27	B8	706	A	C5-C6-N6	-5.79	119.07	123.70
1	AA	564	C	N3-C4-N4	5.79	122.05	118.00
1	AA	578	C	N3-C4-N4	5.79	122.05	118.00
1	AA	747	A	C4-C5-C6	5.79	119.89	117.00
1	AA	1271	A	C4-C5-C6	5.79	119.89	117.00
1	AA	1280	A	C5-C6-N6	-5.79	119.07	123.70
27	B8	473	G	O4'-C1'-N9	5.79	112.83	108.20
27	B8	1172	C	N3-C4-N4	5.79	122.05	118.00
27	B8	1197	G	O4'-C1'-N9	5.79	112.83	108.20
27	B8	1236	G	N3-C2-N2	5.79	123.95	119.90
27	B8	2273	A	O4'-C1'-N9	5.79	112.83	108.20
27	B8	2388	A	C5-C6-N1	-5.79	114.81	117.70
1	AA	1161	C	N3-C4-N4	5.79	122.05	118.00
27	B8	64	A	C4-C5-C6	5.79	119.89	117.00
27	B8	2761	A	C5-C6-N1	-5.79	114.81	117.70
1	AA	569	C	N3-C4-N4	5.79	122.05	118.00
1	AA	1141	C	N3-C4-N4	5.79	122.05	118.00
26	B7	46	A	C4-C5-C6	5.79	119.89	117.00
1	AA	959	A	C4-C5-C6	5.78	119.89	117.00
1	AA	1373	G	O4'-C1'-N9	5.78	112.83	108.20
27	B8	2296	U	O4'-C1'-N1	5.78	112.83	108.20
27	B8	2482	A	C5-C6-N1	-5.78	114.81	117.70
1	AA	1249	C	N3-C4-N4	5.78	122.05	118.00
1	AA	1332	A	C4-C5-C6	5.78	119.89	117.00
27	B8	1276	A	O4'-C1'-N9	5.78	112.83	108.20
27	B8	1367	A	C4-C5-C6	5.78	119.89	117.00
1	AA	600	A	C5-C6-N6	-5.78	119.08	123.70
27	B8	462	C	N3-C4-N4	5.78	122.05	118.00
27	B8	590	A	C5-C6-N6	-5.78	119.08	123.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	869	G	O4'-C1'-N9	5.78	112.82	108.20
27	B8	1111	A	C4-C5-C6	5.78	119.89	117.00
27	B8	1134	A	C5-C6-N6	-5.78	119.08	123.70
27	B8	1169	A	C4-C5-C6	5.78	119.89	117.00
27	B8	1759	A	C4-C5-C6	5.78	119.89	117.00
27	B8	2107	G	O4'-C1'-N9	5.78	112.82	108.20
27	B8	1028	A	O4'-C1'-N9	5.78	112.82	108.20
27	B8	1503	A	C4-C5-C6	5.78	119.89	117.00
1	AA	325	A	O4'-C1'-N9	5.78	112.82	108.20
1	AA	1275	A	O4'-C1'-N9	5.78	112.82	108.20
1	AA	1507	A	C5-C6-N6	-5.78	119.08	123.70
26	B7	90	C	N3-C4-N4	5.78	122.04	118.00
27	B8	689	A	C5-C6-N1	-5.78	114.81	117.70
27	B8	844	A	C5-C6-N1	-5.78	114.81	117.70
27	B8	982	C	N3-C4-N4	5.78	122.04	118.00
27	B8	1728	C	N3-C4-N4	5.78	122.04	118.00
27	B8	1790	C	N3-C4-N4	5.78	122.05	118.00
27	B8	2088	A	C5-C6-N6	-5.78	119.08	123.70
27	B8	2328	A	O4'-C1'-N9	5.78	112.82	108.20
1	AA	50	A	C4-C5-C6	5.78	119.89	117.00
1	AA	407	U	O4'-C1'-N1	5.78	112.82	108.20
1	AA	608	A	C4-C5-C6	5.78	119.89	117.00
1	AA	1106	G	O4'-C1'-N9	5.78	112.82	108.20
1	AA	1128	C	N3-C4-N4	5.78	122.04	118.00
1	AA	1384	C	N3-C4-N4	5.78	122.04	118.00
27	B8	76	C	N3-C4-N4	5.78	122.04	118.00
27	B8	217	A	O4'-C1'-N9	5.78	112.82	108.20
27	B8	783	A	C5-C6-N6	-5.78	119.08	123.70
27	B8	948	C	N3-C4-N4	5.78	122.04	118.00
27	B8	1143	A	C4-C5-C6	5.78	119.89	117.00
27	B8	1230	A	C4-C5-C6	5.78	119.89	117.00
27	B8	1383	A	C5-C6-N6	-5.78	119.08	123.70
27	B8	2058	A	C4-C5-C6	5.78	119.89	117.00
27	B8	2452	C	N3-C4-N4	5.78	122.04	118.00
27	B8	2727	A	C5-C6-N1	-5.78	114.81	117.70
1	AA	1274	A	C5-C6-N6	-5.77	119.08	123.70
27	B8	2119	A	C5-C6-N1	-5.77	114.81	117.70
1	AA	210	C	N3-C4-N4	5.77	122.04	118.00
1	AA	335	C	N3-C4-N4	5.77	122.04	118.00
1	AA	460	A	C4-C5-C6	5.77	119.89	117.00
1	AA	1171	A	C5-C6-N6	-5.77	119.08	123.70
3	AV	5	A	C5-C6-N6	-5.77	119.08	123.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	71	A	C5-C6-N1	-5.77	114.81	117.70
27	B8	532	A	C4-C5-C6	5.77	119.89	117.00
27	B8	1670	C	N3-C4-C5	-5.77	119.59	121.90
27	B8	66	C	N3-C4-C5	-5.77	119.59	121.90
27	B8	352	A	C5-C6-N6	-5.77	119.08	123.70
27	B8	582	A	O4'-C1'-N9	5.77	112.82	108.20
27	B8	783	A	C4-C5-C6	5.77	119.89	117.00
27	B8	1437	C	N3-C4-N4	5.77	122.04	118.00
1	AA	496	A	O4'-C1'-N9	5.77	112.81	108.20
1	AA	573	A	C5-C6-N6	-5.77	119.08	123.70
1	AA	1113	C	N3-C4-N4	5.77	122.04	118.00
1	AA	1277	C	N3-C4-N4	5.77	122.04	118.00
27	B8	269	C	N3-C4-N4	5.77	122.04	118.00
27	B8	721	A	C4-C5-C6	5.77	119.89	117.00
27	B8	1927	A	C5-C6-N6	-5.77	119.08	123.70
27	B8	1933	G	O4'-C1'-N9	5.77	112.81	108.20
27	B8	2325	G	O4'-C1'-N9	5.77	112.81	108.20
27	B8	2422	C	N3-C4-N4	5.77	122.04	118.00
27	B8	2542	A	C4-C5-C6	5.77	119.89	117.00
27	B8	2657	A	C4-C5-C6	5.77	119.89	117.00
1	AA	974	A	C5-C6-N1	-5.77	114.82	117.70
1	AA	1343	G	O4'-C1'-N9	5.77	112.81	108.20
27	B8	75	G	O4'-C1'-N9	5.77	112.81	108.20
27	B8	604	G	O4'-C1'-N9	5.77	112.81	108.20
27	B8	1077	A	C5-C6-N6	-5.77	119.09	123.70
27	B8	1585	C	N3-C4-C5	-5.77	119.59	121.90
27	B8	2365	G	O4'-C1'-N9	5.77	112.81	108.20
27	B8	2521	C	N3-C4-N4	5.77	122.04	118.00
27	B8	2726	A	O4'-C1'-N9	5.77	112.81	108.20
1	AA	228	A	O4'-C1'-N9	5.77	112.81	108.20
26	B7	50	A	C4-C5-C6	5.77	119.88	117.00
27	B8	475	C	N3-C4-N4	5.77	122.04	118.00
27	B8	1040	A	C4-C5-C6	5.77	119.88	117.00
27	B8	1211	C	N3-C4-C5	-5.77	119.59	121.90
27	B8	1246	A	C4-C5-C6	5.77	119.88	117.00
27	B8	2868	A	O4'-C1'-N9	5.77	112.81	108.20
1	AA	728	A	C5-C6-N6	-5.76	119.09	123.70
1	AA	1214	C	N3-C4-N4	5.76	122.03	118.00
1	AA	1507	A	O4'-C1'-N9	5.76	112.81	108.20
27	B8	233	A	O4'-C1'-N9	5.76	112.81	108.20
27	B8	1749	A	C4-C5-C6	5.76	119.88	117.00
27	B8	2179	C	N3-C4-N4	5.76	122.04	118.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	2850	A	C5-C6-N6	-5.76	119.09	123.70
1	AA	1008	U	O4'-C1'-N1	5.76	112.81	108.20
27	B8	155	A	O4'-C1'-N9	5.76	112.81	108.20
27	B8	362	A	O4'-C1'-N9	5.76	112.81	108.20
27	B8	539	G	O4'-C1'-N9	5.76	112.81	108.20
27	B8	749	A	C4-C5-C6	5.76	119.88	117.00
27	B8	1413	A	O4'-C1'-N9	5.76	112.81	108.20
27	B8	1837	C	N3-C4-N4	5.76	122.03	118.00
27	B8	2200	C	N3-C4-N4	5.76	122.03	118.00
27	B8	2556	C	N3-C4-N4	5.76	122.03	118.00
27	B8	2741	A	O4'-C1'-N9	5.76	112.81	108.20
27	B8	2748	A	C5-C6-N1	-5.76	114.82	117.70
1	AA	572	A	C5-C6-N1	-5.76	114.82	117.70
1	AA	699	C	N3-C4-N4	5.76	122.03	118.00
1	AA	792	A	C4-C5-C6	5.76	119.88	117.00
1	AA	1041	G	O4'-C1'-N9	5.76	112.81	108.20
1	AA	1238	A	O4'-C1'-N9	5.76	112.81	108.20
1	AA	1323	G	O4'-C1'-N9	5.76	112.81	108.20
27	B8	223	A	C4-C5-C6	5.76	119.88	117.00
27	B8	553	G	O4'-C1'-N9	5.76	112.81	108.20
27	B8	782	A	C5-C6-N1	-5.76	114.82	117.70
27	B8	2309	A	O4'-C1'-N9	5.76	112.81	108.20
27	B8	2311	A	C5-C6-N6	-5.76	119.09	123.70
1	AA	706	A	O4'-C1'-N9	5.76	112.81	108.20
1	AA	760	G	O4'-C1'-N9	5.76	112.81	108.20
27	B8	227	A	C5-C6-N6	-5.76	119.09	123.70
27	B8	1525	A	C5-C6-N1	-5.76	114.82	117.70
1	AA	431	A	C4-C5-C6	5.76	119.88	117.00
1	AA	508	U	O4'-C1'-N1	5.76	112.81	108.20
1	AA	679	C	N3-C4-N4	5.76	122.03	118.00
1	AA	1201	A	C5-C6-N6	-5.76	119.09	123.70
1	AA	1366	C	N3-C4-N4	5.76	122.03	118.00
27	B8	142	A	C4-C5-C6	5.76	119.88	117.00
27	B8	176	A	C4-C5-C6	5.76	119.88	117.00
27	B8	515	A	C4-C5-C6	5.76	119.88	117.00
27	B8	1162	G	O4'-C1'-N9	5.76	112.81	108.20
27	B8	1353	A	C5-C6-N1	-5.76	114.82	117.70
27	B8	1472	C	N3-C4-N4	5.76	122.03	118.00
27	B8	1678	A	C5-C6-N6	-5.76	119.09	123.70
27	B8	1879	C	N3-C4-N4	5.76	122.03	118.00
27	B8	2116	G	O4'-C1'-N9	5.76	112.81	108.20
27	B8	2317	A	C4-C5-C6	5.76	119.88	117.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	2808	G	O4'-C1'-N9	5.76	112.81	108.20
26	B7	11	C	N3-C4-C5	-5.75	119.60	121.90
27	B8	10	A	C5-C6-N1	-5.75	114.82	117.70
27	B8	944	C	N3-C4-N4	5.75	122.03	118.00
27	B8	1794	A	C5-C6-N6	-5.75	119.10	123.70
27	B8	1913	A	C5-C6-N6	-5.75	119.10	123.70
1	AA	783	C	N3-C4-N4	5.75	122.03	118.00
27	B8	742	A	C4-C5-C6	5.75	119.88	117.00
27	B8	1887	C	N3-C4-N4	5.75	122.03	118.00
27	B8	2451	A	C5-C6-N6	-5.75	119.10	123.70
1	AA	719	C	N3-C4-N4	5.75	122.03	118.00
1	AA	1367	C	N3-C4-N4	5.75	122.03	118.00
27	B8	423	A	O4'-C1'-N9	5.75	112.80	108.20
27	B8	557	C	N3-C4-C5	-5.75	119.60	121.90
27	B8	1445	G	O4'-C1'-N9	5.75	112.80	108.20
27	B8	1637	A	O4'-C1'-N9	5.75	112.80	108.20
27	B8	2682	A	C5-C6-N6	-5.75	119.10	123.70
27	B8	2809	A	C5-C6-N6	-5.75	119.10	123.70
1	AA	513	C	N3-C4-N4	5.75	122.03	118.00
1	AA	1476	A	O4'-C1'-N9	5.75	112.80	108.20
27	B8	601	C	N3-C4-N4	5.75	122.03	118.00
27	B8	2641	G	O4'-C1'-N9	5.75	112.80	108.20
1	AA	274	A	C4-C5-C6	5.75	119.88	117.00
27	B8	223	A	C5-C6-N6	-5.75	119.10	123.70
27	B8	376	G	O4'-C1'-N9	5.75	112.80	108.20
27	B8	693	A	C4-C5-C6	5.75	119.87	117.00
27	B8	1007	C	N3-C4-N4	5.75	122.02	118.00
27	B8	1569	A	C4-C5-C6	5.75	119.88	117.00
27	B8	262	A	C5-C6-N6	-5.75	119.10	123.70
27	B8	294	A	C4-C5-C6	5.75	119.87	117.00
27	B8	965	C	N3-C4-N4	5.75	122.02	118.00
27	B8	1127	A	O4'-C1'-N9	5.75	112.80	108.20
27	B8	1528	A	C5-C6-N1	-5.75	114.83	117.70
27	B8	1590	A	C5-C6-N1	-5.75	114.83	117.70
27	B8	1821	A	C5-C6-N1	-5.75	114.83	117.70
27	B8	2893	A	C5-C6-N1	-5.75	114.83	117.70
28	BA	340	ARG	N-CA-CB	5.75	120.94	110.60
1	AA	919	A	O4'-C1'-N9	5.75	112.80	108.20
27	B8	145	C	N3-C4-N4	5.75	122.02	118.00
27	B8	430	A	C4-C5-C6	5.75	119.87	117.00
1	AA	387	U	O4'-C1'-N1	5.74	112.80	108.20
1	AA	478	A	C4-C5-C6	5.74	119.87	117.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	499	A	C5-C6-N6	-5.74	119.11	123.70
1	AA	902	G	O4'-C1'-N9	5.74	112.79	108.20
1	AA	1181	G	O4'-C1'-N9	5.74	112.80	108.20
1	AA	1293	C	N3-C4-N4	5.74	122.02	118.00
1	AA	1399	C	N3-C4-N4	5.74	122.02	118.00
27	B8	905	A	C5-C6-N6	-5.74	119.10	123.70
27	B8	1211	C	C6-N1-C1'	-5.74	113.91	120.80
27	B8	1600	C	N3-C4-N4	5.74	122.02	118.00
27	B8	1661	G	O4'-C1'-N9	5.74	112.79	108.20
27	B8	1804	C	N3-C4-N4	5.74	122.02	118.00
27	B8	1821	A	C4-C5-C6	5.74	119.87	117.00
27	B8	2184	A	O4'-C1'-N9	5.74	112.80	108.20
27	B8	2417	C	N3-C4-N4	5.74	122.02	118.00
27	B8	2443	C	N3-C4-N4	5.74	122.02	118.00
27	B8	2530	A	C4-C5-C6	5.74	119.87	117.00
27	B8	2733	A	C5-C6-N1	-5.74	114.83	117.70
1	AA	611	C	N3-C4-N4	5.74	122.02	118.00
27	B8	1637	A	C4-C5-C6	5.74	119.87	117.00
27	B8	2792	A	C5-C6-N6	-5.74	119.11	123.70
1	AA	478	A	C5-C6-N1	-5.74	114.83	117.70
1	AA	663	A	C4-C5-C6	5.74	119.87	117.00
1	AA	790	A	C5-C6-N6	-5.74	119.11	123.70
1	AA	807	A	O4'-C1'-N9	5.74	112.79	108.20
1	AA	907	A	C5-C6-N6	-5.74	119.11	123.70
1	AA	1227	A	C5-C6-N6	-5.74	119.11	123.70
1	AA	1433	A	C4-C5-C6	5.74	119.87	117.00
1	AA	1454	G	P-O5'-C5'	5.74	130.09	120.90
27	B8	933	A	C4-C5-C6	5.74	119.87	117.00
27	B8	1054	A	C5-C6-N6	-5.74	119.11	123.70
27	B8	2463	C	N3-C4-C5	-5.74	119.60	121.90
27	B8	2727	A	C5-C6-N6	-5.74	119.11	123.70
28	BA	217	PHE	CB-CG-CD1	5.74	124.82	120.80
1	AA	510	A	C5-C6-N1	-5.74	114.83	117.70
1	AA	583	A	C4-C5-C6	5.74	119.87	117.00
1	AA	669	G	O4'-C1'-N9	5.74	112.79	108.20
1	AA	691	G	N3-C2-N2	5.74	123.92	119.90
1	AA	706	A	C5-C6-N6	-5.74	119.11	123.70
1	AA	815	A	C5-C6-N6	-5.74	119.11	123.70
1	AA	1004	A	C5-C6-N1	-5.74	114.83	117.70
3	AV	67	C	N3-C4-N4	5.74	122.02	118.00
26	B7	50	A	C5-C6-N6	-5.74	119.11	123.70
27	B8	1398	C	N3-C4-N4	5.74	122.02	118.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	1974	C	N3-C4-N4	5.74	122.02	118.00
27	B8	2136	G	O4'-C1'-N9	5.74	112.79	108.20
1	AA	526	C	N3-C4-N4	5.74	122.02	118.00
1	AA	753	A	C5-C6-N1	-5.74	114.83	117.70
1	AA	1152	A	C5-C6-N6	-5.74	119.11	123.70
1	AA	1243	C	N3-C4-C5	-5.74	119.61	121.90
27	B8	79	C	N3-C4-C5	-5.74	119.61	121.90
27	B8	1030	C	N3-C4-N4	5.74	122.02	118.00
27	B8	1806	C	N3-C4-N4	5.74	122.02	118.00
27	B8	2857	G	N3-C2-N2	5.74	123.92	119.90
35	BG	108	PHE	CB-CG-CD2	5.74	124.82	120.80
1	AA	1221	G	O4'-C1'-N9	5.74	112.79	108.20
3	AV	63	C	N3-C4-N4	5.74	122.02	118.00
26	B7	104	A	C4-C5-C6	5.74	119.87	117.00
27	B8	44	A	O4'-C1'-N9	5.74	112.79	108.20
27	B8	282	A	C4-C5-C6	5.74	119.87	117.00
27	B8	1914	C	N3-C4-N4	5.74	122.01	118.00
27	B8	1987	A	C5-C6-N1	-5.74	114.83	117.70
27	B8	2882	A	O4'-C1'-N9	5.74	112.79	108.20
1	AA	635	A	C5-C6-N6	-5.73	119.11	123.70
27	B8	2003	A	C5-C6-N6	-5.73	119.11	123.70
27	B8	2234	G	O4'-C1'-N9	5.73	112.79	108.20
27	B8	2453	A	C5-C6-N1	-5.73	114.83	117.70
27	B8	2453	A	O4'-C1'-N9	5.73	112.79	108.20
1	AA	931	C	N3-C4-N4	5.73	122.01	118.00
1	AA	1071	C	N3-C4-C5	-5.73	119.61	121.90
27	B8	368	A	C5-C6-N6	-5.73	119.11	123.70
27	B8	654	A	C4-C5-C6	5.73	119.87	117.00
27	B8	2603	G	O4'-C1'-N9	5.73	112.79	108.20
1	AA	139	A	C4-C5-C6	5.73	119.86	117.00
1	AA	143	A	C5-C6-N1	-5.73	114.83	117.70
1	AA	415	A	C5-C6-N1	-5.73	114.83	117.70
1	AA	554	A	C4-C5-C6	5.73	119.87	117.00
1	AA	557	G	O4'-C1'-N9	5.73	112.78	108.20
1	AA	1431	A	C5-C6-N6	-5.73	119.11	123.70
1	AA	1446	A	C5-C6-N6	-5.73	119.12	123.70
27	B8	402	A	C5-C6-N1	-5.73	114.83	117.70
27	B8	1420	A	C5-C6-N6	-5.73	119.11	123.70
27	B8	2248	C	N3-C4-N4	5.73	122.01	118.00
27	B8	2619	C	N3-C4-N4	5.73	122.01	118.00
27	B8	2883	A	C4-C5-C6	5.73	119.86	117.00
1	AA	1513	A	O4'-C1'-N9	5.73	112.78	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	1154	G	N3-C2-N2	5.73	123.91	119.90
27	B8	1794	A	C5-C6-N1	-5.73	114.84	117.70
1	AA	523	A	C4-C5-C6	5.73	119.86	117.00
1	AA	1328	C	N3-C4-N4	5.73	122.01	118.00
26	B7	81	G	O4'-C1'-N9	5.73	112.78	108.20
27	B8	53	A	O4'-C1'-N9	5.73	112.78	108.20
27	B8	422	A	C5-C6-N6	-5.73	119.12	123.70
27	B8	727	A	C4-C5-C6	5.73	119.86	117.00
27	B8	1165	A	C4-C5-C6	5.73	119.86	117.00
27	B8	1706	C	N3-C4-N4	5.73	122.01	118.00
27	B8	1772	A	O4'-C1'-N9	5.73	112.78	108.20
27	B8	2688	G	O4'-C1'-N9	5.73	112.78	108.20
1	AA	1011	C	N3-C4-N4	5.73	122.01	118.00
27	B8	14	A	C5-C6-N1	-5.73	114.84	117.70
27	B8	272	A	O4'-C1'-N9	5.73	112.78	108.20
27	B8	587	C	N3-C4-N4	5.73	122.01	118.00
27	B8	1046	A	C5-C6-N6	-5.73	119.12	123.70
27	B8	1339	G	O4'-C1'-N9	5.73	112.78	108.20
27	B8	1477	A	C5-C6-N1	-5.73	114.84	117.70
27	B8	2809	A	C4-C5-C6	5.73	119.86	117.00
1	AA	135	C	N3-C4-N4	5.72	122.01	118.00
1	AA	168	G	O4'-C1'-N9	5.72	112.78	108.20
1	AA	189	A	O4'-C1'-N9	5.72	112.78	108.20
1	AA	243	A	C5-C6-N6	-5.72	119.12	123.70
1	AA	746	A	O4'-C1'-N9	5.72	112.78	108.20
1	AA	807	A	C5-C6-N1	-5.72	114.84	117.70
1	AA	1171	A	C5-C6-N1	-5.72	114.84	117.70
27	B8	155	A	C5-C6-N6	-5.72	119.12	123.70
27	B8	2077	A	C5-C6-N1	-5.72	114.84	117.70
27	B8	2358	A	C5-C6-N6	-5.72	119.12	123.70
27	B8	2412	A	C5-C6-N1	-5.72	114.84	117.70
27	B8	2806	C	N3-C4-C5	-5.72	119.61	121.90
27	B8	2824	C	N3-C4-N4	5.72	122.01	118.00
1	AA	66	A	C5-C6-N1	-5.72	114.84	117.70
1	AA	78	A	C4-C5-C6	5.72	119.86	117.00
1	AA	1324	A	C5-C6-N6	-5.72	119.12	123.70
1	AA	1456	A	C5-C6-N6	-5.72	119.12	123.70
27	B8	622	G	O4'-C1'-N9	5.72	112.78	108.20
27	B8	677	A	C4-C5-C6	5.72	119.86	117.00
27	B8	1354	A	O4'-C1'-N9	5.72	112.78	108.20
27	B8	2005	A	C5-C6-N6	-5.72	119.12	123.70
27	B8	2065	C	N3-C4-C5	-5.72	119.61	121.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	2475	C	O4'-C1'-N1	5.72	112.78	108.20
1	AA	22	G	O4'-C1'-N9	5.72	112.78	108.20
1	AA	602	A	C4-C5-C6	5.72	119.86	117.00
1	AA	1225	A	C5-C6-N1	-5.72	114.84	117.70
3	AV	59	A	C5-C6-N6	-5.72	119.12	123.70
27	B8	497	A	C5-C6-N6	-5.72	119.12	123.70
27	B8	980	A	C5-C6-N6	-5.72	119.12	123.70
1	AA	482	A	C4-C5-C6	5.72	119.86	117.00
1	AA	640	A	C4-C5-C6	5.72	119.86	117.00
1	AA	1346	A	C4-C5-C6	5.72	119.86	117.00
3	AV	37	G	O4'-C1'-N9	5.72	112.78	108.20
27	B8	485	C	N3-C4-N4	5.72	122.00	118.00
27	B8	943	A	C5-C6-N1	-5.72	114.84	117.70
27	B8	1107	G	O4'-C1'-N9	5.72	112.78	108.20
27	B8	1377	G	N3-C2-N2	5.72	123.90	119.90
27	B8	1650	A	C4-C5-C6	5.72	119.86	117.00
27	B8	2761	A	C4-C5-C6	5.72	119.86	117.00
27	B8	2840	C	N3-C4-N4	5.72	122.00	118.00
1	AA	587	G	O4'-C1'-N9	5.72	112.77	108.20
1	AA	1169	A	C5-C6-N6	-5.72	119.13	123.70
27	B8	1102	C	N3-C4-N4	5.72	122.00	118.00
27	B8	2298	A	O4'-C1'-N9	5.72	112.77	108.20
1	AA	926	G	O4'-C1'-N9	5.72	112.77	108.20
1	AA	1105	A	C4-C5-C6	5.72	119.86	117.00
1	AA	1216	A	C5-C6-N1	-5.72	114.84	117.70
27	B8	46	G	O4'-C1'-N9	5.72	112.77	108.20
27	B8	693	A	O4'-C1'-N9	5.72	112.77	108.20
27	B8	1196	C	N3-C4-N4	5.72	122.00	118.00
27	B8	1502	A	C5-C6-N6	-5.72	119.13	123.70
27	B8	2097	A	C5-C6-N6	-5.72	119.13	123.70
1	AA	290	C	N3-C4-N4	5.71	122.00	118.00
1	AA	876	C	N3-C4-N4	5.71	122.00	118.00
27	B8	1069	A	C5-C6-N6	-5.71	119.13	123.70
27	B8	1140	C	N3-C4-N4	5.71	122.00	118.00
27	B8	2205	A	C5-C6-N1	-5.71	114.84	117.70
27	B8	2385	C	N3-C4-C5	-5.71	119.61	121.90
27	B8	2572	A	C5-C6-N6	-5.71	119.13	123.70
1	AA	631	C	N3-C4-N4	5.71	122.00	118.00
1	AA	963	G	O4'-C1'-N9	5.71	112.77	108.20
27	B8	57	C	N3-C4-N4	5.71	122.00	118.00
27	B8	1551	A	C4-C5-C6	5.71	119.86	117.00
27	B8	1694	C	O4'-C1'-N1	5.71	112.77	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	2482	A	C5-C6-N6	-5.71	119.13	123.70
27	B8	2515	C	N3-C4-N4	5.71	122.00	118.00
1	AA	389	A	C5-C6-N6	-5.71	119.13	123.70
1	AA	607	A	O4'-C1'-N9	5.71	112.77	108.20
27	B8	344	A	C4-C5-C6	5.71	119.86	117.00
27	B8	348	A	C4-C5-C6	5.71	119.86	117.00
27	B8	1493	C	N3-C4-N4	5.71	122.00	118.00
27	B8	1656	C	N3-C4-N4	5.71	122.00	118.00
27	B8	2340	A	C5-C6-N6	-5.71	119.13	123.70
27	B8	2377	A	C5-C6-N6	-5.71	119.13	123.70
27	B8	2407	A	C5-C6-N1	-5.71	114.84	117.70
27	B8	2418	A	O4'-C1'-N9	5.71	112.77	108.20
3	AV	49	C	N3-C4-C5	-5.71	119.62	121.90
27	B8	354	A	C4-C5-C6	5.71	119.86	117.00
27	B8	761	A	C4-C5-C6	5.71	119.86	117.00
27	B8	1387	A	C4-C5-C6	5.71	119.86	117.00
1	AA	655	A	C5-C6-N6	-5.71	119.13	123.70
1	AA	712	A	C4-C5-C6	5.71	119.86	117.00
1	AA	754	C	N3-C4-N4	5.71	122.00	118.00
1	AA	839	C	N3-C4-N4	5.71	122.00	118.00
1	AA	1103	C	N3-C4-C5	-5.71	119.62	121.90
27	B8	79	C	N3-C4-N4	5.71	122.00	118.00
27	B8	626	A	C5-C6-N1	-5.71	114.85	117.70
27	B8	851	C	N3-C4-N4	5.71	122.00	118.00
27	B8	1046	A	C4-C5-C6	5.71	119.85	117.00
27	B8	1928	A	C5-C6-N1	-5.71	114.85	117.70
27	B8	2602	A	C5-C6-N6	-5.71	119.13	123.70
1	AA	336	A	C5-C6-N6	-5.71	119.14	123.70
1	AA	759	A	C4-C5-C6	5.71	119.85	117.00
1	AA	1248	A	C5-C6-N6	-5.71	119.13	123.70
1	AA	1446	A	O4'-C1'-N9	5.71	112.76	108.20
27	B8	115	C	N3-C4-N4	5.71	122.00	118.00
27	B8	182	A	C5-C6-N6	-5.71	119.14	123.70
27	B8	878	A	C5-C6-N1	-5.71	114.85	117.70
27	B8	889	C	N3-C4-C5	-5.71	119.62	121.90
27	B8	1363	C	N3-C4-N4	5.71	121.99	118.00
27	B8	1735	A	C5-C6-N1	-5.71	114.85	117.70
27	B8	1908	C	N3-C4-N4	5.71	122.00	118.00
1	AA	60	A	C4-C5-C6	5.71	119.85	117.00
1	AA	983	A	C5-C6-N6	-5.71	119.14	123.70
27	B8	1305	C	N3-C4-N4	5.71	121.99	118.00
1	AA	67	C	N3-C4-C5	-5.70	119.62	121.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	308	C	N3-C4-N4	5.70	121.99	118.00
1	AA	1130	A	C4-C5-C6	5.70	119.85	117.00
27	B8	466	A	C4-C5-C6	5.70	119.85	117.00
27	B8	764	A	C4-C5-C6	5.70	119.85	117.00
27	B8	1426	G	N3-C2-N2	5.70	123.89	119.90
27	B8	2717	C	N3-C4-C5	-5.70	119.62	121.90
27	B8	129	C	N3-C4-N4	5.70	121.99	118.00
27	B8	943	A	C5-C6-N6	-5.70	119.14	123.70
27	B8	1221	C	N3-C4-N4	5.70	121.99	118.00
27	B8	1637	A	C5-C6-N6	-5.70	119.14	123.70
27	B8	2814	A	C5-C6-N6	-5.70	119.14	123.70
1	AA	169	C	N3-C4-C5	-5.70	119.62	121.90
1	AA	882	C	N3-C4-N4	5.70	121.99	118.00
1	AA	1256	A	O4'-C1'-N9	5.70	112.76	108.20
27	B8	163	C	N3-C4-N4	5.70	121.99	118.00
27	B8	245	G	O4'-C1'-N9	5.70	112.76	108.20
27	B8	1328	A	C4-C5-C6	5.70	119.85	117.00
27	B8	1434	A	C4-C5-C6	5.70	119.85	117.00
27	B8	1564	C	N3-C4-C5	-5.70	119.62	121.90
27	B8	1962	C	O4'-C1'-N1	5.70	112.76	108.20
27	B8	1978	A	C4-C5-C6	5.70	119.85	117.00
27	B8	1981	A	C4-C5-C6	5.70	119.85	117.00
27	B8	2624	G	O4'-C1'-N9	5.70	112.76	108.20
1	AA	253	A	C4-C5-C6	5.70	119.85	117.00
1	AA	388	G	O4'-C1'-N9	5.70	112.76	108.20
1	AA	456	A	C4-C5-C6	5.70	119.85	117.00
1	AA	1261	A	C5-C6-N1	-5.70	114.85	117.70
27	B8	981	A	C5-C6-N6	-5.70	119.14	123.70
27	B8	1142	A	C5-C6-N6	-5.70	119.14	123.70
27	B8	1144	A	C5-C6-N1	-5.70	114.85	117.70
27	B8	1225	G	O4'-C1'-N9	5.70	112.76	108.20
27	B8	1719	G	O4'-C1'-N9	5.70	112.76	108.20
27	B8	2156	G	N3-C2-N2	5.70	123.89	119.90
27	B8	2688	G	N3-C2-N2	5.70	123.89	119.90
1	AA	559	A	C5-C6-N6	-5.70	119.14	123.70
1	AA	1513	A	C5-C6-N1	-5.70	114.85	117.70
27	B8	1330	C	N3-C4-N4	5.70	121.99	118.00
27	B8	1901	A	O4'-C1'-N9	5.70	112.76	108.20
27	B8	1971	U	C2-N1-C1'	5.70	124.54	117.70
27	B8	2125	G	C5-C6-O6	-5.70	125.18	128.60
1	AA	222	C	N3-C4-N4	5.70	121.99	118.00
1	AA	901	A	C5-C6-N1	-5.70	114.85	117.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	217	A	C5-C6-N6	-5.70	119.14	123.70
27	B8	592	A	C4-C5-C6	5.70	119.85	117.00
27	B8	1607	C	N3-C4-C5	-5.70	119.62	121.90
27	B8	1784	A	C4-C5-C6	5.70	119.85	117.00
27	B8	2870	C	N3-C4-N4	5.70	121.99	118.00
27	B8	499	U	O4'-C1'-N1	5.69	112.75	108.20
27	B8	627	A	C5-C6-N6	-5.69	119.14	123.70
27	B8	1469	A	C5-C6-N1	-5.69	114.85	117.70
27	B8	1547	C	N3-C4-N4	5.69	121.99	118.00
1	AA	298	A	C4-C5-C6	5.69	119.85	117.00
1	AA	900	A	C5-C6-N6	-5.69	119.15	123.70
27	B8	528	A	C5-C6-N1	-5.69	114.85	117.70
27	B8	1675	C	N3-C4-N4	5.69	121.98	118.00
27	B8	1685	C	N3-C4-N4	5.69	121.98	118.00
27	B8	1772	A	C5-C6-N6	-5.69	119.15	123.70
27	B8	2288	A	C5-C6-N1	-5.69	114.85	117.70
27	B8	2516	A	C4-C5-C6	5.69	119.85	117.00
27	B8	2527	C	N3-C4-N4	5.69	121.98	118.00
1	AA	440	C	N3-C4-C5	-5.69	119.62	121.90
1	AA	1179	A	O4'-C1'-N9	5.69	112.75	108.20
1	AA	1250	A	C4-C5-C6	5.69	119.85	117.00
1	AA	1403	C	N3-C4-C5	-5.69	119.62	121.90
27	B8	131	A	C4-C5-C6	5.69	119.85	117.00
27	B8	466	A	C5-C6-N6	-5.69	119.15	123.70
27	B8	507	A	C4-C5-C6	5.69	119.84	117.00
27	B8	1057	A	C5-C6-N6	-5.69	119.15	123.70
27	B8	1502	A	C5-C6-N1	-5.69	114.86	117.70
27	B8	1916	A	C5-C6-N1	-5.69	114.85	117.70
27	B8	1966	A	O4'-C1'-N9	5.69	112.75	108.20
27	B8	2071	A	C5-C6-N6	-5.69	119.15	123.70
1	AA	649	A	C4-C5-C6	5.69	119.84	117.00
27	B8	1327	A	C5-C6-N6	-5.69	119.15	123.70
27	B8	1705	A	C4-C5-C6	5.69	119.84	117.00
27	B8	1928	A	C5-C6-N6	-5.69	119.15	123.70
1	AA	1055	A	C5-C6-N6	-5.69	119.15	123.70
1	AA	1494	G	O4'-C1'-N9	5.69	112.75	108.20
3	AV	26	C	N3-C4-N4	5.69	121.98	118.00
27	B8	482	A	C5-C6-N6	-5.69	119.15	123.70
27	B8	1032	A	C4-C5-C6	5.69	119.84	117.00
27	B8	1123	C	N3-C4-N4	5.69	121.98	118.00
27	B8	2013	A	C5-C6-N1	-5.69	114.86	117.70
27	B8	2055	C	N3-C4-N4	5.69	121.98	118.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	2309	A	C5-C6-N6	-5.69	119.15	123.70
27	B8	2436	G	O4'-C1'-N9	5.69	112.75	108.20
27	B8	339	U	O4'-C1'-N1	5.69	112.75	108.20
27	B8	2434	A	C5-C6-N1	-5.69	114.86	117.70
27	B8	2663	G	O4'-C1'-N9	5.69	112.75	108.20
1	AA	153	C	N3-C4-N4	5.68	121.98	118.00
1	AA	321	A	C4-C5-C6	5.68	119.84	117.00
1	AA	972	C	N3-C4-C5	-5.68	119.63	121.90
1	AA	1240	U	O4'-C1'-N1	5.68	112.75	108.20
1	AA	1419	G	O4'-C1'-N9	5.68	112.75	108.20
1	AA	1534	A	C5-C6-N1	-5.68	114.86	117.70
3	AV	5	A	C4-C5-C6	5.68	119.84	117.00
3	AV	77	A	C5-C6-N1	-5.68	114.86	117.70
26	B7	109	A	C4-C5-C6	5.68	119.84	117.00
27	B8	619	G	N3-C2-N2	5.68	123.88	119.90
27	B8	920	A	C4-C5-C6	5.68	119.84	117.00
27	B8	1508	A	C5-C6-N6	-5.68	119.15	123.70
27	B8	1558	C	N3-C4-N4	5.68	121.98	118.00
27	B8	2320	U	O4'-C1'-N1	5.68	112.75	108.20
27	B8	2835	A	C5-C6-N6	-5.68	119.15	123.70
1	AA	199	A	C4-C5-C6	5.68	119.84	117.00
1	AA	914	A	C4-C5-C6	5.68	119.84	117.00
1	AA	934	C	O4'-C1'-N1	5.68	112.75	108.20
1	AA	1133	G	O4'-C1'-N9	5.68	112.75	108.20
1	AA	1380	U	O4'-C1'-N1	5.68	112.75	108.20
1	AA	1396	A	C5-C6-N6	-5.68	119.15	123.70
26	B7	38	C	N3-C4-C5	-5.68	119.63	121.90
27	B8	979	A	C5-C6-N6	-5.68	119.15	123.70
27	B8	1088	A	C5-C6-N1	-5.68	114.86	117.70
27	B8	1262	A	C5-C6-N1	-5.68	114.86	117.70
27	B8	1528	A	C5-C6-N6	-5.68	119.16	123.70
27	B8	1570	A	C4-C5-C6	5.68	119.84	117.00
27	B8	1691	C	N3-C4-N4	5.68	121.98	118.00
27	B8	1895	C	N3-C4-C5	-5.68	119.63	121.90
27	B8	2015	A	C4-C5-C6	5.68	119.84	117.00
1	AA	1214	C	C2-N1-C1'	5.68	125.05	118.80
1	AA	1236	A	C4-C5-C6	5.68	119.84	117.00
27	B8	362	A	C5-C6-N6	-5.68	119.16	123.70
27	B8	1711	A	C5-C6-N1	-5.68	114.86	117.70
1	AA	87	C	N3-C4-C5	-5.68	119.63	121.90
1	AA	122	G	O4'-C1'-N9	5.68	112.74	108.20
1	AA	167	A	C4-C5-C6	5.68	119.84	117.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	328	C	N3-C4-C5	-5.68	119.63	121.90
1	AA	549	C	N3-C4-C5	-5.68	119.63	121.90
1	AA	729	A	C4-C5-C6	5.68	119.84	117.00
1	AA	750	C	N3-C4-N4	5.68	121.98	118.00
1	AA	1082	A	O4'-C1'-N9	5.68	112.74	108.20
1	AA	1281	C	N3-C4-N4	5.68	121.97	118.00
3	AV	74	A	C4-C5-C6	5.68	119.84	117.00
27	B8	626	A	C5-C6-N6	-5.68	119.16	123.70
27	B8	1151	A	O4'-C1'-N9	5.68	112.74	108.20
27	B8	1386	C	N3-C4-N4	5.68	121.98	118.00
27	B8	1895	C	N3-C4-N4	5.68	121.98	118.00
27	B8	1909	C	N3-C4-N4	5.68	121.98	118.00
27	B8	2173	A	C5-C6-N1	-5.68	114.86	117.70
27	B8	2434	A	C5-C6-N6	-5.68	119.16	123.70
27	B8	2598	A	C4-C5-C6	5.68	119.84	117.00
1	AA	132	C	N3-C4-N4	5.68	121.97	118.00
1	AA	533	A	O4'-C1'-N9	5.68	112.74	108.20
1	AA	1517	G	O4'-C1'-N9	5.68	112.74	108.20
26	B7	34	A	C4-C5-C6	5.68	119.84	117.00
27	B8	415	A	O4'-C1'-N9	5.68	112.74	108.20
27	B8	478	A	C5-C6-N6	-5.68	119.16	123.70
27	B8	1304	A	C4-C5-C6	5.68	119.84	117.00
27	B8	1319	C	N3-C4-N4	5.68	121.97	118.00
27	B8	1357	C	N3-C4-N4	5.68	121.97	118.00
27	B8	2088	A	C4-C5-C6	5.68	119.84	117.00
1	AA	246	A	C4-C5-C6	5.68	119.84	117.00
1	AA	1021	A	C5-C6-N6	-5.68	119.16	123.70
1	AA	1257	A	C5-C6-N6	-5.68	119.16	123.70
1	AA	1306	A	C5-C6-N1	-5.68	114.86	117.70
26	B7	18	G	O4'-C1'-N9	5.68	112.74	108.20
26	B7	52	A	C5-C6-N6	-5.68	119.16	123.70
27	B8	722	A	C5-C6-N6	-5.68	119.16	123.70
27	B8	1096	A	C5-C6-N1	-5.68	114.86	117.70
28	BA	332	TYR	CB-CG-CD2	5.68	124.41	121.00
1	AA	510	A	C4-C5-C6	5.67	119.84	117.00
1	AA	696	A	C5-C6-N1	-5.67	114.86	117.70
1	AA	1203	C	N3-C4-N4	5.67	121.97	118.00
1	AA	1251	A	C5-C6-N6	-5.67	119.16	123.70
3	AV	2	G	O4'-C1'-N9	5.67	112.74	108.20
3	AV	61	U	O4'-C1'-N1	5.67	112.74	108.20
27	B8	617	G	O4'-C1'-N9	5.67	112.74	108.20
27	B8	946	C	N3-C4-N4	5.67	121.97	118.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	1073	A	C4-C5-C6	5.67	119.84	117.00
27	B8	1762	A	C5-C6-N6	-5.67	119.16	123.70
27	B8	1783	A	C5-C6-N1	-5.67	114.86	117.70
27	B8	2212	A	C5-C6-N1	-5.67	114.86	117.70
27	B8	2258	C	N3-C4-N4	5.67	121.97	118.00
1	AA	648	A	C5-C6-N1	-5.67	114.86	117.70
1	AA	721	G	O4'-C1'-N9	5.67	112.74	108.20
27	B8	160	A	C5-C6-N6	-5.67	119.16	123.70
27	B8	523	C	N3-C4-N4	5.67	121.97	118.00
27	B8	2110	G	P-O3'-C3'	5.67	126.51	119.70
27	B8	2445	G	O4'-C1'-N9	5.67	112.74	108.20
27	B8	2608	G	N3-C2-N2	5.67	123.87	119.90
1	AA	189	A	C5-C6-N6	-5.67	119.16	123.70
1	AA	306	A	O4'-C1'-N9	5.67	112.74	108.20
1	AA	977	A	C5-C6-N6	-5.67	119.16	123.70
1	AA	1081	A	O4'-C1'-N9	5.67	112.74	108.20
27	B8	460	A	O4'-C1'-N9	5.67	112.74	108.20
27	B8	541	A	C5-C6-N1	-5.67	114.86	117.70
27	B8	631	A	C5-C6-N6	-5.67	119.16	123.70
27	B8	1127	A	C4-C5-C6	5.67	119.84	117.00
27	B8	1650	A	O4'-C1'-N9	5.67	112.74	108.20
27	B8	1843	C	N3-C4-N4	5.67	121.97	118.00
27	B8	2009	A	C4-C5-C6	5.67	119.84	117.00
27	B8	2772	C	N3-C4-N4	5.67	121.97	118.00
1	AA	131	A	O4'-C1'-N9	5.67	112.74	108.20
1	AA	408	A	C5-C6-N6	-5.67	119.16	123.70
26	B7	93	C	N3-C4-C5	-5.67	119.63	121.90
27	B8	479	A	P-O3'-C3'	5.67	126.50	119.70
27	B8	1566	A	C5-C6-N6	-5.67	119.16	123.70
27	B8	2080	A	C5-C6-N6	-5.67	119.16	123.70
1	AA	272	C	N3-C4-N4	5.67	121.97	118.00
1	AA	542	G	O4'-C1'-N9	5.67	112.73	108.20
1	AA	609	A	O4'-C1'-N9	5.67	112.73	108.20
1	AA	612	C	N3-C4-C5	-5.67	119.63	121.90
3	AV	28	C	N3-C4-N4	5.67	121.97	118.00
27	B8	143	C	N3-C4-N4	5.67	121.97	118.00
27	B8	366	C	N3-C4-N4	5.67	121.97	118.00
27	B8	922	C	N3-C4-C5	-5.67	119.63	121.90
27	B8	968	C	N3-C4-N4	5.67	121.97	118.00
27	B8	1330	C	N3-C4-C5	-5.67	119.63	121.90
27	B8	1678	A	O4'-C1'-N9	5.67	112.73	108.20
27	B8	1773	A	C4-C5-C6	5.67	119.83	117.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	2205	A	C4-C5-C6	5.67	119.83	117.00
27	B8	2547	A	C5-C6-N1	-5.67	114.87	117.70
1	AA	101	A	C5-C6-N6	-5.67	119.17	123.70
1	AA	261	U	O4'-C1'-N1	5.67	112.73	108.20
1	AA	630	A	C5-C6-N6	-5.67	119.17	123.70
1	AA	978	A	C4-C5-C6	5.67	119.83	117.00
1	AA	1019	A	C5-C6-N6	-5.67	119.17	123.70
27	B8	781	A	C5-C6-N1	-5.67	114.87	117.70
27	B8	833	A	O4'-C1'-N9	5.67	112.73	108.20
27	B8	1307	A	C4-C5-C6	5.67	119.83	117.00
27	B8	1364	G	O4'-C1'-N9	5.67	112.73	108.20
27	B8	2082	A	O4'-C1'-N9	5.67	112.73	108.20
27	B8	2749	A	C4-C5-C6	5.67	119.83	117.00
1	AA	110	C	N3-C4-N4	5.67	121.97	118.00
1	AA	1467	C	N3-C4-N4	5.67	121.97	118.00
27	B8	42	A	C4-C5-C6	5.67	119.83	117.00
27	B8	368	A	C5-C6-N1	-5.67	114.87	117.70
27	B8	1385	A	C4-C5-C6	5.67	119.83	117.00
1	AA	518	C	N3-C4-N4	5.66	121.97	118.00
1	AA	580	C	N3-C4-N4	5.66	121.96	118.00
1	AA	1080	A	C5-C6-N1	-5.66	114.87	117.70
1	AA	1442	G	O4'-C1'-N9	5.66	112.73	108.20
27	B8	155	A	C4-C5-C6	5.66	119.83	117.00
27	B8	793	A	C5-C6-N6	-5.66	119.17	123.70
27	B8	2426	A	C5-C6-N6	-5.66	119.17	123.70
27	B8	44	A	C5-C6-N1	-5.66	114.87	117.70
27	B8	983	A	C5-C6-N6	-5.66	119.17	123.70
27	B8	1384	A	C4-C5-C6	5.66	119.83	117.00
27	B8	1635	A	C5-C6-N6	-5.66	119.17	123.70
27	B8	2703	C	N3-C4-N4	5.66	121.96	118.00
1	AA	394	G	O4'-C1'-N9	5.66	112.73	108.20
1	AA	507	C	N3-C4-N4	5.66	121.96	118.00
26	B7	62	C	N3-C4-C5	-5.66	119.64	121.90
27	B8	203	A	O4'-C1'-N9	5.66	112.73	108.20
27	B8	382	A	C5-C6-N6	-5.66	119.17	123.70
27	B8	483	A	O4'-C1'-N9	5.66	112.73	108.20
27	B8	1246	A	C5-C6-N1	-5.66	114.87	117.70
27	B8	1557	C	N3-C4-C5	-5.66	119.64	121.90
27	B8	1679	A	O4'-C1'-N9	5.66	112.73	108.20
27	B8	1746	A	C4-C5-C6	5.66	119.83	117.00
27	B8	2036	C	N3-C4-N4	5.66	121.96	118.00
27	B8	2177	C	N3-C4-N4	5.66	121.96	118.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	2182	U	O4'-C1'-N1	5.66	112.73	108.20
27	B8	2765	A	C5-C6-N1	-5.66	114.87	117.70
27	B8	2858	C	N3-C4-C5	-5.66	119.64	121.90
1	AA	436	C	N3-C4-N4	5.66	121.96	118.00
1	AA	1243	C	N3-C4-N4	5.66	121.96	118.00
1	AA	1302	C	O4'-C1'-N1	5.66	112.73	108.20
26	B7	50	A	C5-C6-N1	-5.66	114.87	117.70
27	B8	497	A	C4-C5-C6	5.66	119.83	117.00
27	B8	723	C	N3-C4-N4	5.66	121.96	118.00
27	B8	925	A	O4'-C1'-N9	5.66	112.73	108.20
27	B8	952	G	O4'-C1'-N9	5.66	112.73	108.20
27	B8	1138	G	O4'-C1'-N9	5.66	112.73	108.20
27	B8	1274	A	C5-C6-N6	-5.66	119.17	123.70
27	B8	1458	U	O4'-C1'-N1	5.66	112.73	108.20
27	B8	2104	C	N3-C4-C5	-5.66	119.64	121.90
27	B8	2439	A	C5-C6-N1	-5.66	114.87	117.70
27	B8	2614	A	C5-C6-N6	-5.66	119.17	123.70
27	B8	2623	G	O4'-C1'-N9	5.66	112.73	108.20
27	B8	2660	A	C5-C6-N6	-5.66	119.17	123.70
1	AA	23	C	N3-C4-C5	-5.66	119.64	121.90
1	AA	770	C	N3-C4-N4	5.66	121.96	118.00
1	AA	1411	C	N3-C4-N4	5.66	121.96	118.00
27	B8	1912	A	C5-C6-N1	-5.66	114.87	117.70
27	B8	1970	A	C5-C6-N6	-5.66	119.17	123.70
27	B8	2298	A	C4-C5-C6	5.66	119.83	117.00
27	B8	2713	U	O4'-C1'-N1	5.66	112.72	108.20
1	AA	106	C	N3-C4-C5	-5.66	119.64	121.90
1	AA	124	C	N3-C4-C5	-5.66	119.64	121.90
1	AA	174	A	C5-C6-N1	-5.66	114.87	117.70
1	AA	488	C	N3-C4-N4	5.66	121.96	118.00
1	AA	908	A	C5-C6-N1	-5.66	114.87	117.70
1	AA	1163	A	C5-C6-N6	-5.66	119.18	123.70
1	AA	1412	C	N3-C4-N4	5.66	121.96	118.00
26	B7	57	A	C4-C5-C6	5.66	119.83	117.00
27	B8	597	G	O4'-C1'-N9	5.66	112.72	108.20
27	B8	758	C	N3-C4-N4	5.66	121.96	118.00
27	B8	1686	C	N3-C4-N4	5.66	121.96	118.00
27	B8	1721	G	N3-C2-N2	5.66	123.86	119.90
27	B8	1786	A	C4-C5-C6	5.66	119.83	117.00
1	AA	689	C	N3-C4-N4	5.65	121.96	118.00
27	B8	455	C	N3-C4-N4	5.65	121.96	118.00
27	B8	809	G	O4'-C1'-N9	5.65	112.72	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	983	A	O4'-C1'-N9	5.65	112.72	108.20
27	B8	2763	G	O4'-C1'-N9	5.65	112.72	108.20
1	AA	277	C	N3-C4-C5	-5.65	119.64	121.90
1	AA	1500	A	C5-C6-N1	-5.65	114.87	117.70
1	AA	1518	A	C5-C6-N1	-5.65	114.87	117.70
27	B8	270	A	C5-C6-N6	-5.65	119.18	123.70
27	B8	1285	A	O4'-C1'-N9	5.65	112.72	108.20
27	B8	2851	A	O4'-C1'-N9	5.65	112.72	108.20
1	AA	823	C	N3-C4-C5	-5.65	119.64	121.90
1	AA	1248	A	C4-C5-C6	5.65	119.83	117.00
27	B8	101	A	O4'-C1'-N9	5.65	112.72	108.20
27	B8	250	G	C5-C6-O6	-5.65	125.21	128.60
27	B8	2108	A	C5-C6-N1	-5.65	114.87	117.70
27	B8	2224	G	O4'-C1'-N9	5.65	112.72	108.20
27	B8	2290	G	O4'-C1'-N9	5.65	112.72	108.20
27	B8	2439	A	C5-C6-N6	-5.65	119.18	123.70
27	B8	2716	C	N3-C4-N4	5.65	121.95	118.00
27	B8	151	C	N3-C4-N4	5.65	121.95	118.00
27	B8	343	C	N3-C4-N4	5.65	121.95	118.00
27	B8	602	A	O4'-C1'-N9	5.65	112.72	108.20
27	B8	660	C	N3-C4-N4	5.65	121.95	118.00
27	B8	668	A	C5-C6-N1	-5.65	114.88	117.70
27	B8	833	A	C5-C6-N1	-5.65	114.88	117.70
1	AA	503	C	N3-C4-N4	5.65	121.95	118.00
27	B8	239	C	N3-C4-N4	5.65	121.95	118.00
27	B8	247	G	O4'-C1'-N9	5.65	112.72	108.20
27	B8	281	C	N3-C4-C5	-5.65	119.64	121.90
27	B8	526	A	C4-C5-C6	5.65	119.82	117.00
27	B8	714	U	O4'-C1'-N1	5.65	112.72	108.20
27	B8	890	C	N3-C4-N4	5.65	121.95	118.00
27	B8	901	C	P-O5'-C5'	5.65	129.94	120.90
27	B8	1274	A	C5-C6-N1	-5.65	114.88	117.70
27	B8	1304	A	C5-C6-N1	-5.65	114.88	117.70
27	B8	2023	C	N3-C4-N4	5.65	121.95	118.00
27	B8	2164	C	O4'-C1'-N1	5.65	112.72	108.20
27	B8	2275	C	N3-C4-N4	5.65	121.95	118.00
27	B8	2856	A	C4-C5-C6	5.65	119.82	117.00
1	AA	58	C	N3-C4-C5	-5.65	119.64	121.90
1	AA	223	A	C5-C6-N6	-5.65	119.18	123.70
1	AA	885	G	O4'-C1'-N9	5.65	112.72	108.20
3	AV	43	G	O4'-C1'-N9	5.65	112.72	108.20
27	B8	800	A	C5-C6-N1	-5.65	114.88	117.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	866	A	C5-C6-N6	-5.65	119.18	123.70
27	B8	960	A	C5-C6-N6	-5.65	119.18	123.70
27	B8	2821	A	C5-C6-N6	-5.65	119.18	123.70
27	B8	2823	A	C5-C6-N6	-5.65	119.18	123.70
1	AA	130	A	C5-C6-N6	-5.64	119.19	123.70
1	AA	280	C	N3-C4-N4	5.64	121.95	118.00
1	AA	422	C	N3-C4-C5	-5.64	119.64	121.90
1	AA	602	A	C5-C6-N1	-5.64	114.88	117.70
1	AA	1204	A	C4-C5-C6	5.64	119.82	117.00
26	B7	108	A	C4-C5-C6	5.64	119.82	117.00
27	B8	1507	C	N3-C4-C5	-5.64	119.64	121.90
27	B8	2246	G	O4'-C1'-N9	5.64	112.72	108.20
1	AA	345	C	N3-C4-C5	-5.64	119.64	121.90
1	AA	716	A	C5-C6-N6	-5.64	119.19	123.70
1	AA	918	A	C5-C6-N6	-5.64	119.19	123.70
1	AA	1158	C	O4'-C1'-N1	5.64	112.71	108.20
27	B8	101	A	C5-C6-N6	-5.64	119.19	123.70
27	B8	324	A	C5-C6-N6	-5.64	119.19	123.70
27	B8	1938	A	C5-C6-N6	-5.64	119.19	123.70
27	B8	2423	U	O4'-C1'-N1	5.64	112.71	108.20
27	B8	2448	A	C5-C6-N6	-5.64	119.19	123.70
1	AA	315	A	C4-C5-C6	5.64	119.82	117.00
1	AA	676	A	C4-C5-C6	5.64	119.82	117.00
1	AA	1216	A	C4-C5-C6	5.64	119.82	117.00
1	AA	1460	C	N3-C4-N4	5.64	121.95	118.00
27	B8	1164	C	N3-C4-N4	5.64	121.95	118.00
27	B8	1525	A	C5-C6-N6	-5.64	119.19	123.70
27	B8	1677	A	C5-C6-N1	-5.64	114.88	117.70
27	B8	1744	A	C5-C6-N1	-5.64	114.88	117.70
1	AA	348	G	O4'-C1'-N9	5.64	112.71	108.20
1	AA	729	A	C5-C6-N6	-5.64	119.19	123.70
1	AA	928	G	O4'-C1'-N9	5.64	112.71	108.20
27	B8	625	G	O4'-C1'-N9	5.64	112.71	108.20
27	B8	739	A	C5-C6-N6	-5.64	119.19	123.70
27	B8	834	G	O4'-C1'-N9	5.64	112.71	108.20
27	B8	1211	C	P-O3'-C3'	5.64	126.47	119.70
27	B8	2005	A	O4'-C1'-N9	5.64	112.71	108.20
27	B8	2103	C	N3-C4-N4	5.64	121.95	118.00
27	B8	1699	G	O4'-C1'-N9	5.64	112.71	108.20
1	AA	58	C	N3-C4-N4	5.64	121.95	118.00
1	AA	197	A	C4-C5-C6	5.64	119.82	117.00
1	AA	363	A	C5-C6-N6	-5.64	119.19	123.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	946	A	C4-C5-C6	5.64	119.82	117.00
1	AA	968	A	O4'-C1'-N9	5.64	112.71	108.20
1	AA	1322	C	N3-C4-N4	5.64	121.94	118.00
27	B8	272	A	C5-C6-N1	-5.64	114.88	117.70
27	B8	1327	A	C4-C5-C6	5.64	119.82	117.00
27	B8	1672	A	C5-C6-N6	-5.64	119.19	123.70
27	B8	1727	C	N3-C4-N4	5.64	121.95	118.00
27	B8	2428	G	P-O3'-C3'	5.64	126.46	119.70
1	AA	238	A	O4'-C1'-N9	5.63	112.71	108.20
1	AA	620	C	N3-C4-N4	5.63	121.94	118.00
1	AA	747	A	C5-C6-N6	-5.63	119.19	123.70
1	AA	1155	A	C5-C6-N6	-5.63	119.19	123.70
1	AA	1327	C	N3-C4-N4	5.63	121.94	118.00
3	AV	38	G	O4'-C1'-N9	5.63	112.71	108.20
27	B8	88	G	C5-C6-O6	-5.63	125.22	128.60
27	B8	299	A	C5-C6-N1	-5.63	114.88	117.70
27	B8	430	A	C5-C6-N6	-5.63	119.19	123.70
27	B8	1037	G	O4'-C1'-N9	5.63	112.71	108.20
27	B8	1039	A	C5-C6-N1	-5.63	114.88	117.70
27	B8	2058	A	O4'-C1'-N9	5.63	112.71	108.20
27	B8	2705	A	C4-C5-C6	5.63	119.82	117.00
27	B8	2757	A	C4-C5-C6	5.63	119.82	117.00
1	AA	195	A	C4-C5-C6	5.63	119.82	117.00
1	AA	1246	A	C4-C5-C6	5.63	119.82	117.00
3	AV	40	G	O4'-C1'-N9	5.63	112.71	108.20
27	B8	2199	A	C5-C6-N6	-5.63	119.19	123.70
1	AA	395	C	N3-C4-N4	5.63	121.94	118.00
1	AA	600	A	C4-C5-C6	5.63	119.82	117.00
1	AA	1000	A	C4-C5-C6	5.63	119.81	117.00
3	AV	52	A	C5-C6-N1	-5.63	114.88	117.70
3	AV	77	A	C5-C6-N6	-5.63	119.19	123.70
27	B8	172	A	C5-C6-N6	-5.63	119.19	123.70
27	B8	507	A	C5-C6-N6	-5.63	119.19	123.70
27	B8	875	G	P-O3'-C3'	5.63	126.46	119.70
27	B8	1570	A	C5-C6-N6	-5.63	119.19	123.70
27	B8	2635	A	C5-C6-N6	-5.63	119.19	123.70
27	B8	2675	A	C4-C5-C6	5.63	119.81	117.00
1	AA	633	G	C5-C6-O6	-5.63	125.22	128.60
1	AA	913	A	C4-C5-C6	5.63	119.81	117.00
1	AA	959	A	C5-C6-N6	-5.63	119.20	123.70
1	AA	1274	A	C4-C5-C6	5.63	119.81	117.00
1	AA	1430	A	C5-C6-N1	-5.63	114.89	117.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1500	A	O4'-C1'-N9	5.63	112.70	108.20
27	B8	736	C	N3-C4-C5	-5.63	119.65	121.90
27	B8	819	A	C5-C6-N6	-5.63	119.20	123.70
27	B8	1014	A	C5-C6-N6	-5.63	119.20	123.70
27	B8	1353	A	C4-C5-C6	5.63	119.81	117.00
27	B8	1870	C	N3-C4-N4	5.63	121.94	118.00
27	B8	2450	A	C4-C5-C6	5.63	119.81	117.00
1	AA	910	C	N3-C4-N4	5.63	121.94	118.00
1	AA	983	A	C4-C5-C6	5.63	119.81	117.00
1	AA	1117	A	C5-C6-N6	-5.63	119.20	123.70
1	AA	1430	A	C4-C5-C6	5.63	119.81	117.00
27	B8	22	C	N3-C4-N4	5.63	121.94	118.00
27	B8	672	C	N3-C4-N4	5.63	121.94	118.00
27	B8	765	C	N3-C4-N4	5.63	121.94	118.00
1	AA	210	C	N3-C4-C5	-5.63	119.65	121.90
1	AA	978	A	C5-C6-N1	-5.63	114.89	117.70
1	AA	1004	A	C5-C6-N6	-5.63	119.20	123.70
27	B8	1378	A	C5-C6-N1	-5.63	114.89	117.70
27	B8	2104	C	N3-C4-N4	5.63	121.94	118.00
27	B8	2377	A	O4'-C1'-N9	5.63	112.70	108.20
27	B8	2510	C	N3-C4-N4	5.63	121.94	118.00
27	B8	2560	A	O4'-C1'-N9	5.63	112.70	108.20
27	B8	2876	G	O4'-C1'-N9	5.63	112.70	108.20
1	AA	155	A	P-O5'-C5'	5.62	129.90	120.90
1	AA	307	C	N3-C4-N4	5.62	121.94	118.00
1	AA	366	A	C5-C6-N1	-5.62	114.89	117.70
1	AA	1112	C	N3-C4-N4	5.62	121.94	118.00
1	AA	1134	G	O4'-C1'-N9	5.62	112.70	108.20
26	B7	31	C	N3-C4-N4	5.62	121.94	118.00
27	B8	1665	A	C5-C6-N1	-5.62	114.89	117.70
27	B8	1805	A	C5-C6-N1	-5.62	114.89	117.70
27	B8	2059	A	C5-C6-N6	-5.62	119.20	123.70
1	AA	1031	C	N3-C4-N4	5.62	121.94	118.00
1	AA	1203	C	N3-C4-C5	-5.62	119.65	121.90
3	AV	4	C	O4'-C1'-N1	5.62	112.70	108.20
3	AV	26	C	N3-C4-C5	-5.62	119.65	121.90
26	B7	30	C	N3-C4-N4	5.62	121.94	118.00
27	B8	1605	C	N3-C4-C5	-5.62	119.65	121.90
27	B8	1618	A	O4'-C1'-N9	5.62	112.70	108.20
27	B8	2010	G	O4'-C1'-N9	5.62	112.70	108.20
27	B8	2270	A	C5-C6-N1	-5.62	114.89	117.70
27	B8	2306	C	N3-C4-N4	5.62	121.94	118.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	2432	A	C5-C6-N6	-5.62	119.20	123.70
27	B8	2600	A	C5-C6-N1	-5.62	114.89	117.70
1	AA	74	A	C5-C6-N1	-5.62	114.89	117.70
1	AA	248	C	N3-C4-N4	5.62	121.93	118.00
1	AA	276	G	O4'-C1'-N9	5.62	112.70	108.20
1	AA	1430	A	O4'-C1'-N9	5.62	112.70	108.20
1	AA	1510	C	N3-C4-C5	-5.62	119.65	121.90
27	B8	62	U	P-O3'-C3'	5.62	126.45	119.70
27	B8	332	A	C5-C6-N1	-5.62	114.89	117.70
27	B8	391	A	O4'-C1'-N9	5.62	112.70	108.20
27	B8	603	A	C5-C6-N6	-5.62	119.20	123.70
27	B8	890	C	N3-C4-C5	-5.62	119.65	121.90
27	B8	2025	C	N3-C4-N4	5.62	121.94	118.00
27	B8	2483	C	N3-C4-N4	5.62	121.94	118.00
27	B8	2635	A	O4'-C1'-N9	5.62	112.70	108.20
27	B8	2745	C	N3-C4-C5	-5.62	119.65	121.90
1	AA	495	A	O4'-C1'-N9	5.62	112.70	108.20
1	AA	651	C	N3-C4-C5	-5.62	119.65	121.90
1	AA	983	A	C5-C6-N1	-5.62	114.89	117.70
26	B7	11	C	N3-C4-N4	5.62	121.93	118.00
27	B8	226	A	C4-C5-C6	5.62	119.81	117.00
27	B8	1348	C	N3-C4-N4	5.62	121.93	118.00
27	B8	1795	C	N3-C4-N4	5.62	121.93	118.00
27	B8	2178	C	N3-C4-C5	-5.62	119.65	121.90
1	AA	518	C	N3-C4-C5	-5.62	119.65	121.90
1	AA	532	A	C5-C6-N6	-5.62	119.20	123.70
27	B8	131	A	C5-C6-N1	-5.62	114.89	117.70
27	B8	244	A	C4-C5-C6	5.62	119.81	117.00
27	B8	470	A	C5-C6-N1	-5.62	114.89	117.70
27	B8	542	C	N3-C4-N4	5.62	121.93	118.00
27	B8	941	A	C5-C6-N6	-5.62	119.20	123.70
27	B8	1008	A	C5-C6-N6	-5.62	119.20	123.70
27	B8	1912	A	C4-C5-C6	5.62	119.81	117.00
27	B8	2088	A	C5-C6-N1	-5.62	114.89	117.70
27	B8	2101	A	C5-C6-N6	-5.62	119.20	123.70
26	B7	68	C	N3-C4-N4	5.62	121.93	118.00
27	B8	190	A	C5-C6-N1	-5.62	114.89	117.70
27	B8	825	A	C5-C6-N1	-5.62	114.89	117.70
27	B8	1229	C	N3-C4-C5	-5.62	119.65	121.90
27	B8	1395	A	C5-C6-N1	-5.62	114.89	117.70
1	AA	105	G	O4'-C1'-N9	5.62	112.69	108.20
1	AA	712	A	C5-C6-N6	-5.62	119.21	123.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1383	C	N3-C4-N4	5.62	121.93	118.00
27	B8	804	A	O4'-C1'-N9	5.62	112.69	108.20
27	B8	900	A	C4-C5-C6	5.62	119.81	117.00
27	B8	1237	A	C5-C6-N6	-5.62	119.21	123.70
27	B8	1770	G	O4'-C1'-N9	5.62	112.69	108.20
27	B8	1801	A	O4'-C1'-N9	5.62	112.69	108.20
1	AA	456	A	C5-C6-N6	-5.61	119.21	123.70
1	AA	930	C	N3-C4-N4	5.61	121.93	118.00
1	AA	1400	C	C6-N1-C1'	-5.61	114.06	120.80
27	B8	792	A	C5-C6-N6	-5.61	119.21	123.70
27	B8	823	C	N3-C4-N4	5.61	121.93	118.00
27	B8	1284	A	C5-C6-N6	-5.61	119.21	123.70
27	B8	1354	A	C5-C6-N1	-5.61	114.89	117.70
27	B8	1689	A	O4'-C1'-N9	5.61	112.69	108.20
27	B8	1735	A	C5-C6-N6	-5.61	119.21	123.70
27	B8	2384	U	O4'-C1'-N1	5.61	112.69	108.20
27	B8	2607	G	O4'-C1'-N9	5.61	112.69	108.20
1	AA	66	A	C5-C6-N6	-5.61	119.21	123.70
1	AA	325	A	C4-C5-C6	5.61	119.81	117.00
1	AA	897	C	N3-C4-N4	5.61	121.93	118.00
1	AA	1428	A	C5-C6-N6	-5.61	119.21	123.70
27	B8	2164	C	C2-N1-C1'	5.61	124.97	118.80
31	B6	189	ALA	N-CA-CB	5.61	117.96	110.10
1	AA	807	A	C4-C5-C6	5.61	119.81	117.00
1	AA	1349	A	C4-C5-C6	5.61	119.81	117.00
27	B8	853	C	N3-C4-N4	5.61	121.93	118.00
27	B8	1172	C	N3-C4-C5	-5.61	119.66	121.90
27	B8	1428	C	O4'-C1'-N1	5.61	112.69	108.20
27	B8	2247	A	C5-C6-N6	-5.61	119.21	123.70
27	B8	2660	A	C5-C6-N1	-5.61	114.89	117.70
2	AX	21	A	C5-C6-N6	-5.61	119.21	123.70
3	AV	16	C	N3-C4-N4	5.61	121.93	118.00
27	B8	661	A	O4'-C1'-N9	5.61	112.69	108.20
27	B8	2369	A	O4'-C1'-N9	5.61	112.69	108.20
1	AA	187	G	N3-C2-N2	5.61	123.83	119.90
1	AA	461	A	O4'-C1'-N9	5.61	112.69	108.20
1	AA	728	A	C4-C5-C6	5.61	119.80	117.00
1	AA	1360	A	C5-C6-N1	-5.61	114.90	117.70
27	B8	946	C	N3-C4-C5	-5.61	119.66	121.90
27	B8	1597	A	C5-C6-N6	-5.61	119.21	123.70
27	B8	1833	C	N3-C4-C5	-5.61	119.66	121.90
27	B8	2578	G	O4'-C1'-N9	5.61	112.69	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	2583	G	O4'-C1'-N9	5.61	112.69	108.20
27	B8	2590	A	C5-C6-N1	-5.61	114.90	117.70
27	B8	2785	C	N3-C4-N4	5.61	121.93	118.00
1	AA	438	U	O4'-C1'-N1	5.61	112.68	108.20
1	AA	1251	A	C5-C6-N1	-5.61	114.90	117.70
1	AA	1493	A	C5-C6-N6	-5.61	119.22	123.70
27	B8	2154	A	C5-C6-N1	-5.61	114.90	117.70
27	B8	2241	A	C5-C6-N1	-5.61	114.90	117.70
1	AA	1157	A	C5-C6-N1	-5.60	114.90	117.70
1	AA	1311	A	C5-C6-N6	-5.60	119.22	123.70
1	AA	1519	A	O4'-C1'-N9	5.60	112.68	108.20
1	AA	1542	A	C5-C6-N6	-5.60	119.22	123.70
27	B8	814	C	N3-C4-C5	-5.60	119.66	121.90
27	B8	1591	A	C5-C6-N6	-5.60	119.22	123.70
27	B8	1839	G	O4'-C1'-N9	5.60	112.68	108.20
1	AA	635	A	O4'-C1'-N9	5.60	112.68	108.20
27	B8	1987	A	C4-C5-C6	5.60	119.80	117.00
27	B8	2805	C	N3-C4-N4	5.60	121.92	118.00
1	AA	366	A	C5-C6-N6	-5.60	119.22	123.70
1	AA	1151	A	C5-C6-N1	-5.60	114.90	117.70
27	B8	173	A	C4-C5-C6	5.60	119.80	117.00
27	B8	227	A	C5-C6-N1	-5.60	114.90	117.70
27	B8	1322	A	C5-C6-N1	-5.60	114.90	117.70
27	B8	2342	C	N3-C4-N4	5.60	121.92	118.00
1	AA	643	C	N3-C4-N4	5.60	121.92	118.00
1	AA	796	C	N3-C4-C5	-5.60	119.66	121.90
1	AA	1480	A	C5-C6-N1	-5.60	114.90	117.70
26	B7	6	G	O4'-C1'-N9	5.60	112.68	108.20
27	B8	563	A	C5-C6-N1	-5.60	114.90	117.70
27	B8	749	A	C5-C6-N1	-5.60	114.90	117.70
27	B8	1462	C	N3-C4-N4	5.60	121.92	118.00
27	B8	1806	C	N3-C4-C5	-5.60	119.66	121.90
27	B8	1824	G	O4'-C1'-N9	5.60	112.68	108.20
27	B8	2160	C	N3-C4-N4	5.60	121.92	118.00
27	B8	2317	A	C5-C6-N1	-5.60	114.90	117.70
27	B8	2821	A	C5-C6-N1	-5.60	114.90	117.70
1	AA	1	A	C5-C6-N6	-5.60	119.22	123.70
1	AA	1378	C	N3-C4-N4	5.60	121.92	118.00
1	AA	1461	G	C5-C6-O6	-5.60	125.24	128.60
27	B8	63	A	C4-C5-C6	5.60	119.80	117.00
27	B8	128	C	N3-C4-C5	-5.60	119.66	121.90
27	B8	144	A	C5-C6-N1	-5.60	114.90	117.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	782	A	C5-C6-N6	-5.60	119.22	123.70
27	B8	2012	G	O4'-C1'-N9	5.60	112.68	108.20
1	AA	519	C	N3-C4-N4	5.60	121.92	118.00
3	AV	1	C	N3-C4-C5	-5.60	119.66	121.90
27	B8	1001	A	C5-C6-N1	-5.60	114.90	117.70
27	B8	1147	A	C4-C5-C6	5.60	119.80	117.00
27	B8	1615	C	N3-C4-C5	-5.60	119.66	121.90
27	B8	1989	G	O4'-C1'-N9	5.60	112.68	108.20
1	AA	520	A	C5-C6-N1	-5.59	114.90	117.70
1	AA	559	A	C5-C6-N1	-5.59	114.90	117.70
1	AA	648	A	C5-C6-N6	-5.59	119.22	123.70
1	AA	808	C	N3-C4-N4	5.59	121.92	118.00
1	AA	913	A	C5-C6-N1	-5.59	114.90	117.70
1	AA	1413	A	C4-C5-C6	5.59	119.80	117.00
27	B8	83	A	C5-C6-N1	-5.59	114.90	117.70
27	B8	199	A	O4'-C1'-N9	5.59	112.68	108.20
27	B8	240	C	N3-C4-N4	5.59	121.92	118.00
27	B8	332	A	C5-C6-N6	-5.59	119.22	123.70
27	B8	972	A	C5-C6-N6	-5.59	119.22	123.70
27	B8	1095	A	C5-C6-N1	-5.59	114.90	117.70
27	B8	1347	A	C4-C5-C6	5.59	119.80	117.00
27	B8	1349	C	N3-C4-N4	5.59	121.92	118.00
27	B8	1847	A	C5-C6-N6	-5.59	119.22	123.70
27	B8	2112	G	C5-C6-O6	-5.59	125.24	128.60
27	B8	2295	C	N3-C4-C5	-5.59	119.66	121.90
1	AA	1476	A	C4-C5-C6	5.59	119.80	117.00
27	B8	1090	A	C5-C6-N1	-5.59	114.90	117.70
27	B8	1877	A	C5-C6-N6	-5.59	119.23	123.70
27	B8	2178	C	N3-C4-N4	5.59	121.92	118.00
1	AA	372	C	N3-C4-C5	-5.59	119.66	121.90
1	AA	1100	C	N3-C4-N4	5.59	121.92	118.00
27	B8	89	A	C5-C6-N6	-5.59	119.23	123.70
27	B8	514	A	C4-C5-C6	5.59	119.80	117.00
27	B8	564	C	N3-C4-C5	-5.59	119.66	121.90
27	B8	903	C	N3-C4-C5	-5.59	119.66	121.90
27	B8	989	G	N3-C2-N2	5.59	123.81	119.90
27	B8	1583	A	C5-C6-N6	-5.59	119.23	123.70
27	B8	1858	A	C4-C5-C6	5.59	119.80	117.00
27	B8	1960	A	C5-C6-N1	-5.59	114.91	117.70
27	B8	2538	C	N3-C4-N4	5.59	121.91	118.00
27	B8	2758	A	C4-C5-C6	5.59	119.80	117.00
1	AA	206	C	N3-C4-C5	-5.59	119.66	121.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	267	C	N3-C4-C5	-5.59	119.66	121.90
1	AA	704	A	C5-C6-N6	-5.59	119.23	123.70
1	AA	718	A	C5-C6-N1	-5.59	114.91	117.70
1	AA	948	C	N3-C4-C5	-5.59	119.66	121.90
1	AA	1538	C	N3-C4-N4	5.59	121.91	118.00
26	B7	47	C	N3-C4-N4	5.59	121.91	118.00
26	B7	83	G	O4'-C1'-N9	5.59	112.67	108.20
27	B8	278	A	C5-C6-N1	-5.59	114.91	117.70
27	B8	541	A	O4'-C1'-N9	5.59	112.67	108.20
27	B8	753	A	O4'-C1'-N9	5.59	112.67	108.20
27	B8	962	G	N3-C2-N2	5.59	123.81	119.90
27	B8	1959	G	O4'-C1'-N9	5.59	112.67	108.20
27	B8	2055	C	N3-C4-C5	-5.59	119.67	121.90
27	B8	2314	A	C4-C5-C6	5.59	119.80	117.00
27	B8	2478	A	O4'-C1'-N9	5.59	112.67	108.20
1	AA	680	C	N3-C4-N4	5.59	121.91	118.00
1	AA	806	C	N3-C4-N4	5.59	121.91	118.00
27	B8	472	A	C5-C6-N6	-5.59	119.23	123.70
27	B8	592	A	C5-C6-N6	-5.59	119.23	123.70
27	B8	2283	C	P-O5'-C5'	5.59	129.84	120.90
27	B8	2307	G	O4'-C1'-N9	5.59	112.67	108.20
1	AA	510	A	O4'-C1'-N9	5.59	112.67	108.20
1	AA	600	A	C5-C6-N1	-5.59	114.91	117.70
1	AA	658	C	N3-C4-N4	5.59	121.91	118.00
1	AA	767	A	O4'-C1'-N9	5.59	112.67	108.20
1	AA	1005	A	C5-C6-N1	-5.59	114.91	117.70
1	AA	1192	C	N3-C4-N4	5.59	121.91	118.00
27	B8	300	A	C5-C6-N1	-5.59	114.91	117.70
27	B8	341	C	N3-C4-C5	-5.59	119.67	121.90
27	B8	382	A	O4'-C1'-N9	5.59	112.67	108.20
27	B8	693	A	C5-C6-N1	-5.59	114.91	117.70
27	B8	1284	A	O4'-C1'-N9	5.59	112.67	108.20
27	B8	1785	A	O4'-C1'-N9	5.59	112.67	108.20
1	AA	452	A	C4-C5-C6	5.58	119.79	117.00
1	AA	1524	C	N3-C4-C5	-5.58	119.67	121.90
27	B8	430	A	C5-C6-N1	-5.58	114.91	117.70
27	B8	1815	A	C4-C5-C6	5.58	119.79	117.00
27	B8	2254	C	N3-C4-N4	5.58	121.91	118.00
27	B8	2685	G	O4'-C1'-N9	5.58	112.67	108.20
27	B8	2813	A	C5-C6-N6	-5.58	119.23	123.70
1	AA	172	A	C4-C5-C6	5.58	119.79	117.00
1	AA	243	A	C2'-C3'-O3'	5.58	122.64	113.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	309	A	C5-C6-N6	-5.58	119.23	123.70
27	B8	559	G	O4'-C1'-N9	5.58	112.67	108.20
27	B8	1013	C	N3-C4-N4	5.58	121.91	118.00
27	B8	1913	A	C5-C6-N1	-5.58	114.91	117.70
27	B8	2498	C	N3-C4-N4	5.58	121.91	118.00
27	B8	2539	C	N3-C4-C5	-5.58	119.67	121.90
27	B8	2665	A	O4'-C1'-N9	5.58	112.67	108.20
1	AA	233	C	N3-C4-N4	5.58	121.91	118.00
1	AA	549	C	N3-C4-N4	5.58	121.91	118.00
27	B8	165	A	C5-C6-N1	-5.58	114.91	117.70
27	B8	309	A	O4'-C1'-N9	5.58	112.67	108.20
27	B8	745	G	N3-C2-N2	5.58	123.81	119.90
27	B8	901	C	N3-C4-N4	5.58	121.91	118.00
27	B8	1106	G	O4'-C1'-N9	5.58	112.67	108.20
27	B8	1392	A	C5-C6-N6	-5.58	119.23	123.70
27	B8	1418	G	N3-C2-N2	5.58	123.81	119.90
27	B8	1447	C	N3-C4-C5	-5.58	119.67	121.90
27	B8	2196	C	N3-C4-C5	-5.58	119.67	121.90
27	B8	2255	G	O4'-C1'-N9	5.58	112.66	108.20
27	B8	2310	C	N3-C4-C5	-5.58	119.67	121.90
27	B8	2540	C	N3-C4-N4	5.58	121.91	118.00
1	AA	87	C	N3-C4-N4	5.58	121.91	118.00
1	AA	263	A	C5-C6-N1	-5.58	114.91	117.70
1	AA	607	A	C5-C6-N6	-5.58	119.24	123.70
1	AA	1320	C	N3-C4-C5	-5.58	119.67	121.90
3	AV	24	C	N3-C4-C5	-5.58	119.67	121.90
27	B8	1033	U	O4'-C1'-N1	5.58	112.66	108.20
27	B8	1043	C	N3-C4-N4	5.58	121.91	118.00
27	B8	1548	A	C4-C5-C6	5.58	119.79	117.00
27	B8	1966	A	C5-C6-N6	-5.58	119.24	123.70
27	B8	2346	A	C5-C6-N6	-5.58	119.24	123.70
1	AA	80	A	C5-C6-N6	-5.58	119.24	123.70
1	AA	1147	C	N3-C4-C5	-5.58	119.67	121.90
1	AA	1462	C	N3-C4-N4	5.58	121.91	118.00
3	AV	18	U	O4'-C1'-N1	5.58	112.66	108.20
3	AV	49	C	N3-C4-N4	5.58	121.91	118.00
26	B7	97	C	N3-C4-N4	5.58	121.91	118.00
27	B8	173	A	C5-C6-N6	-5.58	119.24	123.70
27	B8	585	G	O4'-C1'-N9	5.58	112.66	108.20
27	B8	804	A	C5-C6-N6	-5.58	119.24	123.70
27	B8	1454	C	C2-N1-C1'	5.58	124.94	118.80
27	B8	1551	A	C5-C6-N6	-5.58	119.24	123.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	1552	A	O4'-C1'-N9	5.58	112.66	108.20
27	B8	1967	C	N3-C4-N4	5.58	121.90	118.00
27	B8	2577	A	C5-C6-N1	-5.58	114.91	117.70
27	B8	2638	G	O4'-C1'-N9	5.58	112.66	108.20
27	B8	2747	G	O4'-C1'-N9	5.58	112.66	108.20
1	AA	1050	G	O4'-C1'-N9	5.58	112.66	108.20
26	B7	57	A	O4'-C1'-N9	5.58	112.66	108.20
27	B8	264	C	N3-C4-N4	5.58	121.90	118.00
27	B8	2335	A	C5-C6-N1	-5.58	114.91	117.70
1	AA	7	A	O4'-C1'-N9	5.58	112.66	108.20
1	AA	344	A	C5-C6-N6	-5.58	119.24	123.70
1	AA	351	G	O4'-C1'-N9	5.58	112.66	108.20
1	AA	754	C	N3-C4-C5	-5.58	119.67	121.90
3	AV	14	A	C5-C6-N1	-5.58	114.91	117.70
27	B8	719	C	N3-C4-N4	5.58	121.90	118.00
27	B8	1378	A	O4'-C1'-N9	5.58	112.66	108.20
1	AA	1110	A	C5-C6-N1	-5.57	114.91	117.70
1	AA	1198	G	O4'-C1'-N9	5.57	112.66	108.20
27	B8	7	G	O4'-C1'-N9	5.57	112.66	108.20
27	B8	504	A	C5-C6-N6	-5.57	119.24	123.70
27	B8	634	C	N3-C4-C5	-5.57	119.67	121.90
27	B8	1403	A	C5-C6-N1	-5.57	114.91	117.70
27	B8	1494	A	C4-C5-C6	5.57	119.79	117.00
27	B8	1494	A	C5-C6-N1	-5.57	114.91	117.70
27	B8	1518	C	N3-C4-N4	5.57	121.90	118.00
27	B8	1552	A	P-O5'-C5'	5.57	129.82	120.90
27	B8	1877	A	C5-C6-N1	-5.57	114.91	117.70
27	B8	2433	A	C5-C6-N6	-5.57	119.24	123.70
27	B8	795	C	N3-C4-C5	-5.57	119.67	121.90
27	B8	865	C	N3-C4-N4	5.57	121.90	118.00
27	B8	2417	C	N3-C4-C5	-5.57	119.67	121.90
29	BB	104	MET	CG-SD-CE	-5.57	91.28	100.20
1	AA	1382	C	N3-C4-N4	5.57	121.90	118.00
27	B8	163	C	N3-C4-C5	-5.57	119.67	121.90
27	B8	272	A	C5-C6-N6	-5.57	119.24	123.70
27	B8	351	C	N3-C4-N4	5.57	121.90	118.00
27	B8	1006	C	N3-C4-N4	5.57	121.90	118.00
27	B8	1052	C	N3-C4-C5	-5.57	119.67	121.90
27	B8	1218	G	O4'-C1'-N9	5.57	112.66	108.20
27	B8	1308	A	C4-C5-C6	5.57	119.78	117.00
27	B8	1786	A	C5-C6-N6	-5.57	119.24	123.70
27	B8	1794	A	C4-C5-C6	5.57	119.79	117.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	2061	G	O4'-C1'-N9	5.57	112.66	108.20
27	B8	2314	A	O4'-C1'-N9	5.57	112.66	108.20
27	B8	2776	A	C5-C6-N6	-5.57	119.24	123.70
27	B8	41	C	N3-C4-N4	5.57	121.90	118.00
27	B8	262	A	O4'-C1'-N9	5.57	112.66	108.20
27	B8	344	A	C5-C6-N6	-5.57	119.25	123.70
27	B8	433	C	N3-C4-N4	5.57	121.90	118.00
27	B8	1414	C	N3-C4-N4	5.57	121.90	118.00
27	B8	2023	C	N3-C4-C5	-5.57	119.67	121.90
27	B8	2164	C	N3-C4-N4	5.57	121.90	118.00
1	AA	996	A	O4'-C1'-N9	5.57	112.66	108.20
3	AV	51	G	O4'-C1'-N9	5.57	112.66	108.20
27	B8	450	G	O4'-C1'-N9	5.57	112.65	108.20
27	B8	637	A	C5-C6-N1	-5.57	114.92	117.70
27	B8	1532	A	C5-C6-N1	-5.57	114.92	117.70
27	B8	2193	G	O4'-C1'-N9	5.57	112.65	108.20
1	AA	143	A	C5-C6-N6	-5.57	119.25	123.70
26	B7	101	A	C4-C5-C6	5.57	119.78	117.00
27	B8	833	A	C5-C6-N6	-5.57	119.25	123.70
27	B8	1020	A	C5-C6-N6	-5.57	119.25	123.70
27	B8	1169	A	C5-C6-N1	-5.57	114.92	117.70
27	B8	1214	A	C4-C5-C6	5.57	119.78	117.00
27	B8	1429	G	O4'-C1'-N9	5.57	112.65	108.20
27	B8	1937	A	C4-C5-C6	5.57	119.78	117.00
27	B8	1969	A	C5-C6-N6	-5.57	119.25	123.70
27	B8	2058	A	C5-C6-N6	-5.57	119.25	123.70
1	AA	1026	G	O4'-C1'-N9	5.56	112.65	108.20
1	AA	1191	A	C5-C6-N1	-5.56	114.92	117.70
27	B8	2114	A	C5-C6-N1	-5.56	114.92	117.70
27	B8	2699	C	N3-C4-N4	5.56	121.89	118.00
1	AA	104	G	O4'-C1'-N9	5.56	112.65	108.20
1	AA	503	C	N3-C4-C5	-5.56	119.67	121.90
1	AA	980	C	N3-C4-N4	5.56	121.89	118.00
1	AA	1302	C	N3-C4-C5	-5.56	119.67	121.90
26	B7	37	C	N3-C4-C5	-5.56	119.67	121.90
27	B8	739	A	O4'-C1'-N9	5.56	112.65	108.20
27	B8	908	C	N3-C4-C5	-5.56	119.67	121.90
27	B8	1027	A	C5-C6-N1	-5.56	114.92	117.70
27	B8	1211	C	O4'-C1'-N1	5.56	112.65	108.20
27	B8	1281	G	O4'-C1'-N9	5.56	112.65	108.20
27	B8	1654	A	C5-C6-N1	-5.56	114.92	117.70
27	B8	2047	C	N3-C4-C5	-5.56	119.67	121.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	2712	C	N3-C4-N4	5.56	121.89	118.00
27	B8	1632	A	C5-C6-N6	-5.56	119.25	123.70
27	B8	2525	G	O4'-C1'-N9	5.56	112.65	108.20
27	B8	2799	A	C5-C6-N6	-5.56	119.25	123.70
1	AA	234	C	N3-C4-N4	5.56	121.89	118.00
1	AA	432	A	O4'-C1'-N9	5.56	112.65	108.20
1	AA	642	A	C5-C6-N1	-5.56	114.92	117.70
1	AA	924	C	N3-C4-C5	-5.56	119.68	121.90
1	AA	1408	A	C4-C5-C6	5.56	119.78	117.00
26	B7	30	C	N3-C4-C5	-5.56	119.68	121.90
27	B8	209	C	N3-C4-C5	-5.56	119.68	121.90
27	B8	334	C	N3-C4-N4	5.56	121.89	118.00
27	B8	643	A	C5-C6-N6	-5.56	119.25	123.70
27	B8	1291	C	N3-C4-N4	5.56	121.89	118.00
27	B8	1295	C	N3-C4-N4	5.56	121.89	118.00
27	B8	1403	A	C5-C6-N6	-5.56	119.25	123.70
27	B8	1431	A	O4'-C1'-N9	5.56	112.65	108.20
27	B8	1625	C	N3-C4-N4	5.56	121.89	118.00
1	AA	178	C	N3-C4-N4	5.56	121.89	118.00
1	AA	306	A	C5-C6-N6	-5.56	119.25	123.70
1	AA	573	A	C5-C6-N1	-5.56	114.92	117.70
27	B8	480	A	C5-C6-N6	-5.56	119.25	123.70
27	B8	882	G	O4'-C1'-N9	5.56	112.65	108.20
27	B8	1313	U	O4'-C1'-N1	5.56	112.65	108.20
27	B8	1323	C	N3-C4-N4	5.56	121.89	118.00
27	B8	1761	C	N3-C4-N4	5.56	121.89	118.00
27	B8	1890	A	O4'-C1'-N9	5.56	112.64	108.20
1	AA	749	A	C5-C6-N1	-5.56	114.92	117.70
1	AA	1516	G	O4'-C1'-N9	5.56	112.64	108.20
3	AV	14	A	C5-C6-N6	-5.56	119.25	123.70
27	B8	156	A	C5-C6-N6	-5.56	119.25	123.70
27	B8	610	C	N3-C4-N4	5.56	121.89	118.00
1	AA	392	C	N3-C4-N4	5.55	121.89	118.00
1	AA	767	A	C5-C6-N6	-5.55	119.26	123.70
1	AA	1389	C	N3-C4-N4	5.55	121.89	118.00
27	B8	788	A	C5-C6-N6	-5.55	119.26	123.70
27	B8	1349	C	N3-C4-C5	-5.55	119.68	121.90
27	B8	2029	G	N3-C2-N2	5.55	123.79	119.90
27	B8	2705	A	C5-C6-N6	-5.55	119.26	123.70
27	B8	2764	A	C5-C6-N1	-5.55	114.92	117.70
1	AA	78	A	C5-C6-N1	-5.55	114.92	117.70
27	B8	348	A	C5-C6-N1	-5.55	114.92	117.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	621	A	C5-C6-N6	-5.55	119.26	123.70
1	AA	965	U	O4'-C1'-N1	5.55	112.64	108.20
1	AA	1394	A	C5-C6-N1	-5.55	114.92	117.70
1	AA	1402	C	N3-C4-C5	-5.55	119.68	121.90
3	AV	10	G	O4'-C1'-N9	5.55	112.64	108.20
27	B8	218	A	C5-C6-N6	-5.55	119.26	123.70
27	B8	731	C	N3-C4-C5	-5.55	119.68	121.90
27	B8	889	C	N3-C4-N4	5.55	121.89	118.00
27	B8	899	A	C4-C5-C6	5.55	119.78	117.00
27	B8	1000	A	C5-C6-N1	-5.55	114.92	117.70
27	B8	1005	C	N3-C4-N4	5.55	121.89	118.00
27	B8	1226	A	C5-C6-N6	-5.55	119.26	123.70
27	B8	1569	A	O4'-C1'-N9	5.55	112.64	108.20
27	B8	1804	C	N3-C4-C5	-5.55	119.68	121.90
27	B8	1985	C	N3-C4-N4	5.55	121.89	118.00
27	B8	2171	A	C5-C6-N1	-5.55	114.92	117.70
1	AA	1092	A	C5-C6-N1	-5.55	114.92	117.70
1	AA	1479	C	N3-C4-N4	5.55	121.89	118.00
27	B8	959	A	C4-C5-C6	5.55	119.77	117.00
27	B8	1871	A	C5-C6-N6	-5.55	119.26	123.70
27	B8	2134	A	C5-C6-N1	-5.55	114.92	117.70
27	B8	2425	A	C5-C6-N1	-5.55	114.92	117.70
27	B8	2480	C	N3-C4-N4	5.55	121.89	118.00
27	B8	2666	C	N3-C4-C5	-5.55	119.68	121.90
1	AA	744	C	N3-C4-N4	5.55	121.88	118.00
27	B8	727	A	C5-C6-N6	-5.55	119.26	123.70
27	B8	1089	A	C5-C6-N1	-5.55	114.93	117.70
27	B8	1090	A	C5-C6-N6	-5.55	119.26	123.70
27	B8	1153	C	N3-C4-C5	-5.55	119.68	121.90
27	B8	1730	C	N3-C4-N4	5.55	121.88	118.00
27	B8	2019	A	C5-C6-N1	-5.55	114.93	117.70
27	B8	2418	A	C5-C6-N1	-5.55	114.93	117.70
1	AA	466	A	C5-C6-N6	-5.55	119.26	123.70
1	AA	622	A	C5-C6-N6	-5.55	119.26	123.70
1	AA	1421	G	O4'-C1'-N9	5.55	112.64	108.20
1	AA	1499	A	C5-C6-N6	-5.55	119.26	123.70
1	AA	1515	G	O4'-C1'-N9	5.55	112.64	108.20
27	B8	140	C	N3-C4-C5	-5.55	119.68	121.90
27	B8	157	C	N3-C4-N4	5.55	121.88	118.00
27	B8	195	A	O4'-C1'-N9	5.55	112.64	108.20
27	B8	650	C	N3-C4-C5	-5.55	119.68	121.90
27	B8	995	C	N3-C4-C5	-5.55	119.68	121.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	1370	C	N3-C4-N4	5.55	121.88	118.00
27	B8	2152	G	C5'-C4'-O4'	5.55	115.76	109.10
27	B8	2886	A	C5-C6-N6	-5.55	119.26	123.70
1	AA	1186	G	O4'-C1'-N9	5.54	112.64	108.20
27	B8	318	C	N3-C4-C5	-5.54	119.68	121.90
27	B8	800	A	C4-C5-C6	5.54	119.77	117.00
27	B8	2241	A	C5-C6-N6	-5.54	119.26	123.70
27	B8	2475	C	N3-C4-N4	5.54	121.88	118.00
1	AA	280	C	C2-N1-C1'	5.54	124.90	118.80
1	AA	526	C	N3-C4-C5	-5.54	119.68	121.90
1	AA	646	G	O4'-C1'-N9	5.54	112.63	108.20
1	AA	869	G	N3-C2-N2	5.54	123.78	119.90
1	AA	1045	C	N3-C4-N4	5.54	121.88	118.00
1	AA	1136	C	N3-C4-N4	5.54	121.88	118.00
1	AA	1349	A	O4'-C1'-N9	5.54	112.63	108.20
27	B8	821	A	C4-C5-C6	5.54	119.77	117.00
27	B8	1439	A	O4'-C1'-N9	5.54	112.64	108.20
27	B8	2573	C	N3-C4-C5	-5.54	119.68	121.90
27	B8	2691	C	N3-C4-C5	-5.54	119.68	121.90
1	AA	702	A	C5-C6-N1	-5.54	114.93	117.70
26	B7	53	A	C5-C6-N1	-5.54	114.93	117.70
27	B8	772	C	N3-C4-C5	-5.54	119.68	121.90
27	B8	941	A	C4-C5-C6	5.54	119.77	117.00
27	B8	1205	A	C5-C6-N1	-5.54	114.93	117.70
27	B8	2322	A	C5-C6-N1	-5.54	114.93	117.70
1	AA	166	U	O4'-C1'-N1	5.54	112.63	108.20
1	AA	459	A	C5-C6-N6	-5.54	119.27	123.70
1	AA	1180	A	C5-C6-N6	-5.54	119.27	123.70
1	AA	1483	A	O4'-C1'-N9	5.54	112.63	108.20
27	B8	480	A	C5-C6-N1	-5.54	114.93	117.70
27	B8	896	A	C5-C6-N6	-5.54	119.27	123.70
27	B8	1129	A	C5-C6-N6	-5.54	119.27	123.70
27	B8	1151	A	C5-C6-N6	-5.54	119.27	123.70
27	B8	2174	C	N3-C4-C5	-5.54	119.68	121.90
27	B8	2364	C	N3-C4-N4	5.54	121.88	118.00
27	B8	2889	C	N3-C4-N4	5.54	121.88	118.00
1	AA	1092	A	C5-C6-N6	-5.54	119.27	123.70
1	AA	1271	A	C5-C6-N1	-5.54	114.93	117.70
1	AA	1395	C	N3-C4-N4	5.54	121.88	118.00
27	B8	380	G	O4'-C1'-N9	5.54	112.63	108.20
27	B8	432	A	O4'-C1'-N9	5.54	112.63	108.20
27	B8	440	C	N3-C4-N4	5.54	121.88	118.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	849	A	C4-C5-C6	5.54	119.77	117.00
27	B8	861	A	C4-C5-C6	5.54	119.77	117.00
27	B8	2333	A	C4-C5-C6	5.54	119.77	117.00
27	B8	2670	A	C5-C6-N1	-5.54	114.93	117.70
1	AA	1046	A	C4-C5-C6	5.54	119.77	117.00
27	B8	311	A	C5-C6-N6	-5.54	119.27	123.70
27	B8	1919	A	C5-C6-N6	-5.54	119.27	123.70
1	AA	213	G	O4'-C1'-N9	5.54	112.63	108.20
1	AA	668	G	O4'-C1'-N9	5.54	112.63	108.20
1	AA	936	C	N3-C4-N4	5.54	121.88	118.00
1	AA	1368	A	C4-C5-C6	5.54	119.77	117.00
27	B8	752	A	C5-C6-N1	-5.54	114.93	117.70
27	B8	1167	C	N3-C4-C5	-5.54	119.69	121.90
27	B8	1302	A	C4-C5-C6	5.54	119.77	117.00
27	B8	1805	A	C5-C6-N6	-5.54	119.27	123.70
27	B8	1848	A	C5-C6-N1	-5.54	114.93	117.70
27	B8	2215	C	N3-C4-C5	-5.54	119.69	121.90
27	B8	2352	A	C5-C6-N6	-5.54	119.27	123.70
27	B8	2858	C	N3-C4-N4	5.54	121.88	118.00
27	B8	2883	A	C5-C6-N6	-5.54	119.27	123.70
27	B8	2893	A	C5-C6-N6	-5.54	119.27	123.70
1	AA	36	C	N3-C4-C5	-5.53	119.69	121.90
1	AA	198	G	O4'-C1'-N9	5.53	112.63	108.20
1	AA	306	A	C5-C6-N1	-5.53	114.93	117.70
1	AA	811	C	N3-C4-C5	-5.53	119.69	121.90
26	B7	114	C	N3-C4-N4	5.53	121.87	118.00
27	B8	194	G	O4'-C1'-N9	5.53	112.63	108.20
27	B8	1028	A	C5-C6-N6	-5.53	119.27	123.70
27	B8	1816	C	N3-C4-N4	5.53	121.87	118.00
27	B8	1997	C	N3-C4-N4	5.53	121.87	118.00
27	B8	2082	A	C5-C6-N6	-5.53	119.27	123.70
27	B8	2163	A	O4'-C1'-N9	5.53	112.63	108.20
1	AA	298	A	C5-C6-N6	-5.53	119.27	123.70
1	AA	629	A	C5-C6-N1	-5.53	114.93	117.70
1	AA	1161	C	C6-N1-C2	-5.53	118.09	120.30
27	B8	992	C	N3-C4-N4	5.53	121.87	118.00
27	B8	1461	C	N3-C4-C5	-5.53	119.69	121.90
27	B8	2589	A	C5-C6-N6	-5.53	119.28	123.70
1	AA	74	A	C4-C5-C6	5.53	119.77	117.00
1	AA	490	C	N3-C4-N4	5.53	121.87	118.00
1	AA	909	A	C5-C6-N6	-5.53	119.28	123.70
1	AA	1094	G	O4'-C1'-N9	5.53	112.62	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	B7	52	A	C4-C5-C6	5.53	119.77	117.00
27	B8	231	A	O4'-C1'-N9	5.53	112.62	108.20
27	B8	417	C	N3-C4-C5	-5.53	119.69	121.90
27	B8	590	A	O4'-C1'-N9	5.53	112.62	108.20
27	B8	1156	A	C5-C6-N6	-5.53	119.28	123.70
27	B8	1535	A	C5-C6-N6	-5.53	119.28	123.70
27	B8	1676	A	O4'-C1'-N9	5.53	112.62	108.20
27	B8	1817	G	O4'-C1'-N9	5.53	112.62	108.20
1	AA	161	A	C5-C6-N6	-5.53	119.28	123.70
1	AA	826	C	N3-C4-N4	5.53	121.87	118.00
27	B8	1869	G	N3-C2-N2	5.53	123.77	119.90
27	B8	2851	A	C4-C5-C6	5.53	119.76	117.00
1	AA	706	A	C5-C6-N1	-5.53	114.94	117.70
1	AA	747	A	O4'-C1'-N9	5.53	112.62	108.20
1	AA	1437	A	O4'-C1'-N9	5.53	112.62	108.20
1	AA	1523	G	O4'-C1'-N9	5.53	112.62	108.20
27	B8	14	A	C5-C6-N6	-5.53	119.28	123.70
27	B8	1051	G	O4'-C1'-N9	5.53	112.62	108.20
27	B8	1652	A	C4-C5-C6	5.53	119.76	117.00
27	B8	1732	C	N3-C4-C5	-5.53	119.69	121.90
27	B8	1990	C	N3-C4-C5	-5.53	119.69	121.90
27	B8	2425	A	C5-C6-N6	-5.53	119.28	123.70
27	B8	2634	A	C5-C6-N1	-5.53	114.94	117.70
1	AA	131	A	C5-C6-N6	-5.53	119.28	123.70
1	AA	182	A	C5-C6-N6	-5.53	119.28	123.70
1	AA	951	G	O4'-C1'-N9	5.53	112.62	108.20
1	AA	1371	G	O4'-C1'-N9	5.53	112.62	108.20
27	B8	49	A	C5-C6-N6	-5.53	119.28	123.70
27	B8	118	A	C4-C5-C6	5.53	119.76	117.00
27	B8	1343	G	O4'-C1'-N9	5.53	112.62	108.20
27	B8	1604	C	N3-C4-C5	-5.53	119.69	121.90
27	B8	1748	C	N3-C4-N4	5.53	121.87	118.00
27	B8	2129	C	N3-C4-N4	5.53	121.87	118.00
27	B8	2340	A	C5-C6-N1	-5.53	114.94	117.70
27	B8	2367	G	O4'-C1'-N9	5.53	112.62	108.20
27	B8	2459	A	C5-C6-N1	-5.53	114.94	117.70
1	AA	286	C	N3-C4-C5	-5.52	119.69	121.90
1	AA	711	G	O4'-C1'-N9	5.52	112.62	108.20
1	AA	1011	C	N3-C4-C5	-5.52	119.69	121.90
3	AV	9	A	C5-C6-N1	-5.52	114.94	117.70
26	B7	15	A	C5-C6-N1	-5.52	114.94	117.70
27	B8	792	A	C5-C6-N1	-5.52	114.94	117.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	906	A	C4-C5-C6	5.52	119.76	117.00
1	AA	1176	A	C5-C6-N1	-5.52	114.94	117.70
26	B7	109	A	O4'-C1'-N9	5.52	112.62	108.20
27	B8	432	A	C5-C6-N6	-5.52	119.28	123.70
27	B8	804	A	C5-C6-N1	-5.52	114.94	117.70
27	B8	1265	A	C5-C6-N1	-5.52	114.94	117.70
27	B8	1328	A	C5-C6-N6	-5.52	119.28	123.70
27	B8	1376	C	N3-C4-C5	-5.52	119.69	121.90
27	B8	1759	A	C5-C6-N6	-5.52	119.28	123.70
27	B8	1816	C	N3-C4-C5	-5.52	119.69	121.90
27	B8	2469	A	C4-C5-C6	5.52	119.76	117.00
27	B8	2565	A	C5-C6-N1	-5.52	114.94	117.70
27	B8	2646	C	N3-C4-C5	-5.52	119.69	121.90
2	AX	13	C	N3-C4-C5	-5.52	119.69	121.90
27	B8	125	A	C5-C6-N6	-5.52	119.28	123.70
27	B8	547	A	C5-C6-N6	-5.52	119.28	123.70
27	B8	1274	A	C4-C5-C6	5.52	119.76	117.00
27	B8	2009	A	C5-C6-N1	-5.52	114.94	117.70
27	B8	2559	C	N3-C4-N4	5.52	121.86	118.00
1	AA	403	C	N3-C4-C5	-5.52	119.69	121.90
1	AA	612	C	N3-C4-N4	5.52	121.86	118.00
26	B7	42	C	N3-C4-C5	-5.52	119.69	121.90
27	B8	393	C	N3-C4-C5	-5.52	119.69	121.90
27	B8	502	A	C5-C6-N1	-5.52	114.94	117.70
27	B8	990	A	C4-C5-C6	5.52	119.76	117.00
27	B8	1013	C	N3-C4-C5	-5.52	119.69	121.90
27	B8	1077	A	C5-C6-N1	-5.52	114.94	117.70
27	B8	1899	A	C4-C5-C6	5.52	119.76	117.00
27	B8	2534	A	C5-C6-N1	-5.52	114.94	117.70
27	B8	2812	G	O4'-C1'-N9	5.52	112.62	108.20
1	AA	719	C	N3-C4-C5	-5.52	119.69	121.90
1	AA	1069	C	N3-C4-N4	5.52	121.86	118.00
1	AA	1213	A	C5-C6-N1	-5.52	114.94	117.70
2	AX	16	C	N3-C4-C5	-5.52	119.69	121.90
27	B8	449	A	C5-C6-N1	-5.52	114.94	117.70
27	B8	601	C	N3-C4-C5	-5.52	119.69	121.90
27	B8	984	A	C5-C6-N6	-5.52	119.29	123.70
27	B8	1789	A	C5-C6-N6	-5.52	119.29	123.70
27	B8	2101	A	C5-C6-N1	-5.52	114.94	117.70
1	AA	117	G	O4'-C1'-N9	5.52	112.61	108.20
1	AA	777	A	C5-C6-N1	-5.52	114.94	117.70
1	AA	1180	A	C5-C6-N1	-5.52	114.94	117.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	201	C	N3-C4-C5	-5.52	119.69	121.90
27	B8	2019	A	C5-C6-N6	-5.52	119.29	123.70
27	B8	2146	C	N3-C4-N4	5.52	121.86	118.00
27	B8	2609	U	O4'-C1'-N1	5.52	112.61	108.20
1	AA	162	A	C5-C6-N6	-5.51	119.29	123.70
1	AA	171	A	C5-C6-N1	-5.51	114.94	117.70
1	AA	715	A	C5-C6-N6	-5.51	119.29	123.70
1	AA	1368	A	C5-C6-N1	-5.51	114.94	117.70
26	B7	46	A	O4'-C1'-N9	5.51	112.61	108.20
27	B8	91	A	C5-C6-N6	-5.51	119.29	123.70
27	B8	152	A	C5-C6-N1	-5.51	114.94	117.70
27	B8	543	G	O4'-C1'-N9	5.51	112.61	108.20
27	B8	1987	A	C5-C6-N6	-5.51	119.29	123.70
27	B8	2033	A	C5-C6-N1	-5.51	114.94	117.70
1	AA	1169	A	C5-C6-N1	-5.51	114.94	117.70
1	AA	1318	A	C5-C6-N6	-5.51	119.29	123.70
2	AX	15	C	N3-C4-N4	5.51	121.86	118.00
27	B8	1096	A	C5-C6-N6	-5.51	119.29	123.70
1	AA	217	C	N3-C4-C5	-5.51	119.69	121.90
1	AA	620	C	N3-C4-C5	-5.51	119.69	121.90
7	AC	36	PHE	CB-CG-CD2	5.51	124.66	120.80
27	B8	635	C	N3-C4-C5	-5.51	119.69	121.90
27	B8	661	A	C5-C6-N6	-5.51	119.29	123.70
27	B8	673	C	N3-C4-N4	5.51	121.86	118.00
27	B8	1610	A	C4-C5-C6	5.51	119.75	117.00
27	B8	2001	C	N3-C4-C5	-5.51	119.70	121.90
27	B8	2094	A	O4'-C1'-N9	5.51	112.61	108.20
27	B8	2287	A	C5-C6-N1	-5.51	114.94	117.70
27	B8	2342	C	N3-C4-C5	-5.51	119.70	121.90
27	B8	2711	A	C4-C5-C6	5.51	119.75	117.00
1	AA	655	A	O4'-C1'-N9	5.51	112.61	108.20
1	AA	907	A	C5-C6-N1	-5.51	114.94	117.70
1	AA	1093	A	O4'-C1'-N9	5.51	112.61	108.20
1	AA	1137	C	N3-C4-C5	-5.51	119.70	121.90
1	AA	1158	C	N3-C4-C5	-5.51	119.70	121.90
1	AA	1466	C	N3-C4-N4	5.51	121.86	118.00
27	B8	311	A	C5-C6-N1	-5.51	114.94	117.70
27	B8	477	A	O4'-C1'-N9	5.51	112.61	108.20
27	B8	645	C	N3-C4-C5	-5.51	119.70	121.90
27	B8	668	A	C4-C5-C6	5.51	119.75	117.00
27	B8	1006	C	N3-C4-C5	-5.51	119.70	121.90
27	B8	1942	C	N3-C4-C5	-5.51	119.70	121.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	2332	C	N3-C4-C5	-5.51	119.70	121.90
27	B8	2681	C	N3-C4-N4	5.51	121.86	118.00
26	B7	42	C	N3-C4-N4	5.51	121.86	118.00
27	B8	24	G	O4'-C1'-N9	5.51	112.61	108.20
27	B8	1160	G	O4'-C1'-N9	5.51	112.61	108.20
27	B8	1550	C	N3-C4-C5	-5.51	119.70	121.90
27	B8	1610	A	O4'-C1'-N9	5.51	112.61	108.20
27	B8	1758	U	O4'-C1'-N1	5.51	112.61	108.20
27	B8	2870	C	N3-C4-C5	-5.51	119.70	121.90
1	AA	915	A	O4'-C1'-N9	5.51	112.61	108.20
1	AA	1303	C	N3-C4-N4	5.51	121.85	118.00
26	B7	36	C	N3-C4-N4	5.51	121.85	118.00
27	B8	301	G	O4'-C1'-N9	5.51	112.61	108.20
27	B8	520	G	O4'-C1'-N9	5.51	112.61	108.20
27	B8	815	C	N3-C4-C5	-5.51	119.70	121.90
27	B8	951	C	N3-C4-C5	-5.51	119.70	121.90
27	B8	1320	C	N3-C4-C5	-5.51	119.70	121.90
27	B8	1854	A	C4-C5-C6	5.51	119.75	117.00
27	B8	2275	C	N3-C4-C5	-5.51	119.70	121.90
27	B8	2327	A	C5-C6-N1	-5.51	114.95	117.70
27	B8	2839	G	O4'-C1'-N9	5.51	112.61	108.20
1	AA	165	G	O4'-C1'-N9	5.50	112.60	108.20
26	B7	17	C	N3-C4-N4	5.50	121.85	118.00
27	B8	12	U	P-O3'-C3'	5.50	126.31	119.70
1	AA	823	C	N3-C4-N4	5.50	121.85	118.00
1	AA	912	C	N3-C4-C5	-5.50	119.70	121.90
1	AA	1093	A	C5-C6-N6	-5.50	119.30	123.70
27	B8	318	C	N3-C4-N4	5.50	121.85	118.00
27	B8	453	A	O4'-C1'-N9	5.50	112.60	108.20
27	B8	819	A	C5-C6-N1	-5.50	114.95	117.70
27	B8	889	C	C6-N1-C1'	-5.50	114.20	120.80
27	B8	1158	C	N3-C4-C5	-5.50	119.70	121.90
27	B8	1169	A	C5-C6-N6	-5.50	119.30	123.70
27	B8	1351	C	N3-C4-N4	5.50	121.85	118.00
27	B8	1552	A	C5-C6-N1	-5.50	114.95	117.70
27	B8	1748	C	N3-C4-C5	-5.50	119.70	121.90
27	B8	2020	A	C5-C6-N1	-5.50	114.95	117.70
1	AA	2	A	C5-C6-N6	-5.50	119.30	123.70
1	AA	10	A	C5-C6-N1	-5.50	114.95	117.70
1	AA	280	C	N3-C4-C5	-5.50	119.70	121.90
1	AA	1145	A	C4-C5-C6	5.50	119.75	117.00
1	AA	1195	C	N3-C4-C5	-5.50	119.70	121.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	17	G	O4'-C1'-N9	5.50	112.60	108.20
27	B8	454	A	C5-C6-N1	-5.50	114.95	117.70
27	B8	1020	A	C5-C6-N1	-5.50	114.95	117.70
27	B8	1901	A	C5-C6-N1	-5.50	114.95	117.70
27	B8	2454	G	O4'-C1'-N9	5.50	112.60	108.20
27	B8	2820	A	C5-C6-N6	-5.50	119.30	123.70
1	AA	556	C	N3-C4-C5	-5.50	119.70	121.90
1	AA	1396	A	C5-C6-N1	-5.50	114.95	117.70
26	B7	94	A	C5-C6-N1	-5.50	114.95	117.70
27	B8	384	A	C5-C6-N1	-5.50	114.95	117.70
27	B8	563	A	C5-C6-N6	-5.50	119.30	123.70
27	B8	1230	A	O4'-C1'-N9	5.50	112.60	108.20
1	AA	83	C	N3-C4-N4	5.50	121.85	118.00
1	AA	260	G	O4'-C1'-N9	5.50	112.60	108.20
27	B8	716	A	O4'-C1'-N9	5.50	112.60	108.20
27	B8	772	C	N3-C4-N4	5.50	121.85	118.00
27	B8	1439	A	C5-C6-N1	-5.50	114.95	117.70
27	B8	1548	A	C5-C6-N1	-5.50	114.95	117.70
27	B8	2073	C	N3-C4-C5	-5.50	119.70	121.90
27	B8	2432	A	C5-C6-N1	-5.50	114.95	117.70
27	B8	2781	A	C5-C6-N1	-5.50	114.95	117.70
1	AA	196	A	C4-C5-C6	5.50	119.75	117.00
1	AA	430	A	O4'-C1'-N9	5.50	112.60	108.20
1	AA	448	A	C4-C5-C6	5.50	119.75	117.00
1	AA	994	A	C5-C6-N1	-5.50	114.95	117.70
1	AA	1336	C	N3-C4-N4	5.50	121.85	118.00
27	B8	482	A	C5-C6-N1	-5.50	114.95	117.70
27	B8	1630	A	C4-C5-C6	5.50	119.75	117.00
27	B8	2801	G	O4'-C1'-N9	5.50	112.60	108.20
1	AA	336	A	O4'-C1'-N9	5.50	112.60	108.20
1	AA	630	A	C5-C6-N1	-5.50	114.95	117.70
1	AA	995	C	N3-C4-C5	-5.50	119.70	121.90
1	AA	1410	A	C5-C6-N1	-5.50	114.95	117.70
26	B7	88	C	N3-C4-C5	-5.50	119.70	121.90
27	B8	56	A	O4'-C1'-N9	5.50	112.60	108.20
1	AA	57	G	O4'-C1'-N9	5.49	112.59	108.20
1	AA	109	A	O4'-C1'-N9	5.49	112.59	108.20
1	AA	264	C	N3-C4-N4	5.49	121.84	118.00
1	AA	610	U	C6-N1-C1'	-5.49	113.51	121.20
1	AA	1013	G	N3-C2-N2	5.49	123.75	119.90
3	AV	58	A	C5-C6-N6	-5.49	119.31	123.70
27	B8	486	C	N3-C4-N4	5.49	121.85	118.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	908	C	N3-C4-N4	5.49	121.85	118.00
27	B8	1050	A	C4-C5-C6	5.49	119.75	117.00
27	B8	1496	A	P-O3'-C3'	5.49	126.29	119.70
27	B8	1833	C	N3-C4-N4	5.49	121.84	118.00
33	BE	85	PHE	CB-CG-CD1	5.49	124.64	120.80
27	B8	666	A	O4'-C1'-N9	5.49	112.59	108.20
27	B8	1626	A	C5-C6-N1	-5.49	114.95	117.70
1	AA	197	A	C5-C6-N1	-5.49	114.95	117.70
1	AA	925	G	O4'-C1'-N9	5.49	112.59	108.20
1	AA	1120	C	N3-C4-N4	5.49	121.84	118.00
1	AA	1456	A	C5-C6-N1	-5.49	114.95	117.70
3	AV	52	A	O4'-C1'-N9	5.49	112.59	108.20
27	B8	491	G	O4'-C1'-N9	5.49	112.59	108.20
27	B8	526	A	C5-C6-N6	-5.49	119.31	123.70
27	B8	888	C	N3-C4-N4	5.49	121.84	118.00
27	B8	1556	C	N3-C4-N4	5.49	121.84	118.00
27	B8	2003	A	O4'-C1'-N9	5.49	112.59	108.20
1	AA	322	C	N3-C4-N4	5.49	121.84	118.00
1	AA	510	A	C5-C6-N6	-5.49	119.31	123.70
1	AA	611	C	N3-C4-C5	-5.49	119.70	121.90
1	AA	784	A	C5-C6-N1	-5.49	114.96	117.70
27	B8	659	G	O4'-C1'-N9	5.49	112.59	108.20
27	B8	806	C	N3-C4-C5	-5.49	119.70	121.90
27	B8	837	C	N3-C4-N4	5.49	121.84	118.00
27	B8	1072	C	N3-C4-C5	-5.49	119.70	121.90
27	B8	1080	A	C5-C6-N1	-5.49	114.96	117.70
27	B8	1370	C	N3-C4-C5	-5.49	119.70	121.90
27	B8	1449	G	O4'-C1'-N9	5.49	112.59	108.20
27	B8	2407	A	C5-C6-N6	-5.49	119.31	123.70
27	B8	685	A	C4-C5-C6	5.49	119.74	117.00
1	AA	449	G	O4'-C1'-N9	5.49	112.59	108.20
1	AA	622	A	C4-C5-C6	5.49	119.74	117.00
1	AA	715	A	C5-C6-N1	-5.49	114.96	117.70
1	AA	1250	A	O4'-C1'-N9	5.49	112.59	108.20
26	B7	63	C	N3-C4-N4	5.49	121.84	118.00
27	B8	13	A	C5-C6-N1	-5.49	114.96	117.70
27	B8	218	A	C5-C6-N1	-5.49	114.96	117.70
27	B8	385	C	N3-C4-C5	-5.49	119.71	121.90
27	B8	715	A	C5-C6-N6	-5.49	119.31	123.70
27	B8	1286	A	C5-C6-N6	-5.49	119.31	123.70
27	B8	1994	C	N3-C4-C5	-5.49	119.71	121.90
27	B8	2067	G	P-O3'-C3'	5.49	126.28	119.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	2281	A	C5-C6-N1	-5.49	114.96	117.70
27	B8	2346	A	C5-C6-N1	-5.49	114.96	117.70
1	AA	716	A	C4-C5-C6	5.48	119.74	117.00
1	AA	1271	A	C5-C6-N6	-5.48	119.31	123.70
27	B8	205	G	O4'-C1'-N9	5.48	112.59	108.20
27	B8	1509	A	C5-C6-N6	-5.48	119.31	123.70
27	B8	1990	C	N3-C4-N4	5.48	121.84	118.00
27	B8	2539	C	N3-C4-N4	5.48	121.84	118.00
1	AA	50	A	C5-C6-N6	-5.48	119.31	123.70
1	AA	1204	A	O4'-C1'-N9	5.48	112.59	108.20
27	B8	348	A	C5-C6-N6	-5.48	119.31	123.70
27	B8	420	C	N3-C4-C5	-5.48	119.71	121.90
27	B8	848	C	N3-C4-N4	5.48	121.84	118.00
27	B8	1153	C	N3-C4-N4	5.48	121.84	118.00
27	B8	1647	U	O4'-C1'-N1	5.48	112.59	108.20
27	B8	2153	C	N3-C4-N4	5.48	121.84	118.00
27	B8	2232	C	N3-C4-N4	5.48	121.84	118.00
1	AA	623	C	N3-C4-C5	-5.48	119.71	121.90
1	AA	923	A	O4'-C1'-N9	5.48	112.58	108.20
1	AA	1146	A	O4'-C1'-N9	5.48	112.58	108.20
3	AV	16	C	N3-C4-C5	-5.48	119.71	121.90
26	B7	94	A	C4-C5-C6	5.48	119.74	117.00
26	B7	106	G	O4'-C1'-N9	5.48	112.58	108.20
27	B8	316	C	N3-C4-N4	5.48	121.84	118.00
27	B8	752	A	C5-C6-N6	-5.48	119.31	123.70
27	B8	1809	A	C4-C5-C6	5.48	119.74	117.00
27	B8	1925	C	N3-C4-N4	5.48	121.84	118.00
1	AA	411	A	C5-C6-N6	-5.48	119.32	123.70
1	AA	441	A	C5-C6-N6	-5.48	119.32	123.70
1	AA	1492	A	C4-C5-C6	5.48	119.74	117.00
27	B8	2497	A	C5-C6-N1	-5.48	114.96	117.70
27	B8	2823	A	C5-C6-N1	-5.48	114.96	117.70
1	AA	77	A	O4'-C1'-N9	5.48	112.58	108.20
1	AA	621	A	C5-C6-N1	-5.48	114.96	117.70
1	AA	1081	A	C5-C6-N1	-5.48	114.96	117.70
1	AA	1280	A	C5-C6-N1	-5.48	114.96	117.70
1	AA	1400	C	N3-C4-C5	-5.48	119.71	121.90
27	B8	196	A	C5-C6-N6	-5.48	119.32	123.70
27	B8	302	C	N3-C4-C5	-5.48	119.71	121.90
27	B8	351	C	N3-C4-C5	-5.48	119.71	121.90
27	B8	369	U	O4'-C1'-N1	5.48	112.58	108.20
27	B8	423	A	C4-C5-C6	5.48	119.74	117.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	730	A	O4'-C1'-N9	5.48	112.58	108.20
27	B8	996	A	O4'-C1'-N9	5.48	112.58	108.20
27	B8	1169	A	O4'-C1'-N9	5.48	112.58	108.20
27	B8	1332	G	O4'-C1'-N9	5.48	112.58	108.20
27	B8	1360	G	C5-C6-O6	-5.48	125.31	128.60
27	B8	1800	C	N3-C4-C5	-5.48	119.71	121.90
27	B8	2278	A	C5-C6-N1	-5.48	114.96	117.70
27	B8	2360	G	O4'-C1'-N9	5.48	112.58	108.20
27	B8	2572	A	O4'-C1'-N9	5.48	112.58	108.20
1	AA	975	A	C5-C6-N6	-5.48	119.32	123.70
1	AA	1170	A	O4'-C1'-N9	5.48	112.58	108.20
27	B8	631	A	O4'-C1'-N9	5.48	112.58	108.20
27	B8	1549	A	C5-C6-N6	-5.48	119.32	123.70
27	B8	1658	C	N3-C4-C5	-5.48	119.71	121.90
27	B8	2063	C	N3-C4-C5	-5.48	119.71	121.90
27	B8	2386	A	O4'-C1'-N9	5.48	112.58	108.20
1	AA	303	A	C5-C6-N6	-5.47	119.32	123.70
1	AA	547	A	C5-C6-N1	-5.47	114.96	117.70
1	AA	1412	C	N3-C4-C5	-5.47	119.71	121.90
27	B8	393	C	N3-C4-N4	5.47	121.83	118.00
27	B8	445	C	N3-C4-N4	5.47	121.83	118.00
27	B8	508	A	C5-C6-N6	-5.47	119.32	123.70
27	B8	886	A	C5-C6-N1	-5.47	114.96	117.70
27	B8	1590	A	C4-C5-C6	5.47	119.74	117.00
27	B8	1774	C	N3-C4-C5	-5.47	119.71	121.90
27	B8	1810	A	C5-C6-N1	-5.47	114.96	117.70
27	B8	2165	C	N3-C4-N4	5.47	121.83	118.00
27	B8	2314	A	C5-C6-N6	-5.47	119.32	123.70
27	B8	2830	C	N3-C4-C5	-5.47	119.71	121.90
1	AA	307	C	N3-C4-C5	-5.47	119.71	121.90
1	AA	1431	A	C4-C5-C6	5.47	119.74	117.00
27	B8	475	C	N3-C4-C5	-5.47	119.71	121.90
27	B8	502	A	C4-C5-C6	5.47	119.74	117.00
27	B8	943	A	O4'-C1'-N9	5.47	112.58	108.20
27	B8	1266	G	O4'-C1'-N9	5.47	112.58	108.20
27	B8	2526	G	O4'-C1'-N9	5.47	112.58	108.20
1	AA	839	C	N3-C4-C5	-5.47	119.71	121.90
1	AA	1042	A	O4'-C1'-N9	5.47	112.58	108.20
1	AA	1152	A	C5-C6-N1	-5.47	114.97	117.70
27	B8	115	C	N3-C4-C5	-5.47	119.71	121.90
27	B8	529	A	C5-C6-N1	-5.47	114.97	117.70
27	B8	1694	C	N3-C4-C5	-5.47	119.71	121.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	1802	A	O4'-C1'-N9	5.47	112.58	108.20
1	AA	535	A	O4'-C1'-N9	5.47	112.58	108.20
1	AA	845	A	C5-C6-N6	-5.47	119.32	123.70
1	AA	1109	C	N3-C4-N4	5.47	121.83	118.00
1	AA	1166	G	N3-C2-N2	5.47	123.73	119.90
3	AV	13	C	N3-C4-C5	-5.47	119.71	121.90
27	B8	680	C	N3-C4-C5	-5.47	119.71	121.90
27	B8	927	A	C5-C6-N6	-5.47	119.33	123.70
27	B8	985	C	N3-C4-C5	-5.47	119.71	121.90
27	B8	1093	G	O4'-C1'-N9	5.47	112.58	108.20
27	B8	1981	A	C5-C6-N1	-5.47	114.97	117.70
27	B8	2078	C	N3-C4-N4	5.47	121.83	118.00
27	B8	2565	A	C5-C6-N6	-5.47	119.32	123.70
27	B8	2718	G	O4'-C1'-N9	5.47	112.58	108.20
27	B8	2874	C	N3-C4-C5	-5.47	119.71	121.90
32	BD	127	PHE	CB-CG-CD2	5.47	124.63	120.80
1	AA	935	A	O4'-C1'-N9	5.47	112.58	108.20
1	AA	1093	A	C5-C6-N1	-5.47	114.97	117.70
27	B8	111	A	C5-C6-N1	-5.47	114.97	117.70
27	B8	961	C	N3-C4-N4	5.47	121.83	118.00
27	B8	1871	A	C5-C6-N1	-5.47	114.97	117.70
27	B8	2369	A	C5-C6-N1	-5.47	114.97	117.70
27	B8	2422	C	N3-C4-C5	-5.47	119.71	121.90
1	AA	163	C	N3-C4-N4	5.47	121.83	118.00
1	AA	640	A	C5-C6-N1	-5.47	114.97	117.70
1	AA	654	G	O4'-C1'-N9	5.47	112.57	108.20
26	B7	59	A	O4'-C1'-N9	5.47	112.57	108.20
27	B8	345	A	C4-C5-C6	5.47	119.73	117.00
27	B8	624	C	N3-C4-N4	5.47	121.83	118.00
27	B8	863	A	O4'-C1'-N9	5.47	112.57	108.20
27	B8	981	A	C5-C6-N1	-5.47	114.97	117.70
27	B8	1348	C	N3-C4-C5	-5.47	119.71	121.90
27	B8	1622	G	O4'-C1'-N9	5.47	112.57	108.20
27	B8	2038	G	O4'-C1'-N9	5.47	112.57	108.20
1	AA	95	C	C6-N1-C2	-5.46	118.11	120.30
1	AA	968	A	C5-C6-N6	-5.46	119.33	123.70
1	AA	1191	A	O4'-C1'-N9	5.46	112.57	108.20
27	B8	9	G	O4'-C1'-N9	5.46	112.57	108.20
27	B8	1010	A	C5-C6-N1	-5.46	114.97	117.70
27	B8	1544	A	C5-C6-N6	-5.46	119.33	123.70
27	B8	1665	A	C5-C6-N6	-5.46	119.33	123.70
34	BF	7	TYR	CB-CG-CD1	-5.46	117.72	121.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	364	A	C5-C6-N6	-5.46	119.33	123.70
27	B8	142	A	C5-C6-N1	-5.46	114.97	117.70
1	AA	233	C	N3-C4-C5	-5.46	119.72	121.90
1	AA	397	A	C5-C6-N6	-5.46	119.33	123.70
1	AA	1311	A	C5-C6-N1	-5.46	114.97	117.70
2	AX	18	C	N3-C4-C5	-5.46	119.72	121.90
27	B8	964	C	N3-C4-C5	-5.46	119.72	121.90
27	B8	1981	A	C5-C6-N6	-5.46	119.33	123.70
27	B8	2358	A	C5-C6-N1	-5.46	114.97	117.70
27	B8	2749	A	O4'-C1'-N9	5.46	112.57	108.20
1	AA	821	G	O4'-C1'-N9	5.46	112.57	108.20
2	AX	22	A	C5-C6-N1	-5.46	114.97	117.70
27	B8	443	A	C5-C6-N1	-5.46	114.97	117.70
27	B8	1111	A	C5-C6-N1	-5.46	114.97	117.70
27	B8	1808	A	C5-C6-N6	-5.46	119.33	123.70
1	AA	269	C	N3-C4-C5	-5.46	119.72	121.90
1	AA	694	A	C5-C6-N1	-5.46	114.97	117.70
1	AA	1257	A	O4'-C1'-N9	5.46	112.57	108.20
1	AA	1395	C	N3-C4-C5	-5.46	119.72	121.90
3	AV	76	C	N3-C4-C5	-5.46	119.72	121.90
27	B8	1135	C	N3-C4-N4	5.46	121.82	118.00
27	B8	1918	A	C5-C6-N1	-5.46	114.97	117.70
27	B8	2368	C	N3-C4-N4	5.46	121.82	118.00
27	B8	2873	A	C5-C6-N1	-5.46	114.97	117.70
1	AA	452	A	C5-C6-N6	-5.46	119.33	123.70
1	AA	461	A	C5-C6-N6	-5.46	119.33	123.70
1	AA	490	C	N3-C4-C5	-5.46	119.72	121.90
1	AA	935	A	C5-C6-N1	-5.46	114.97	117.70
1	AA	1213	A	C5-C6-N6	-5.46	119.33	123.70
1	AA	1317	C	N3-C4-N4	5.46	121.82	118.00
1	AA	1357	A	O4'-C1'-N9	5.46	112.56	108.20
1	AA	1499	A	O4'-C1'-N9	5.46	112.57	108.20
26	B7	12	C	N3-C4-C5	-5.46	119.72	121.90
27	B8	255	A	C5-C6-N1	-5.46	114.97	117.70
27	B8	314	C	N3-C4-N4	5.46	121.82	118.00
27	B8	668	A	C5-C6-N6	-5.46	119.33	123.70
27	B8	1175	A	C5-C6-N1	-5.46	114.97	117.70
27	B8	1365	A	C5-C6-N6	-5.46	119.33	123.70
27	B8	1759	A	C5-C6-N1	-5.46	114.97	117.70
27	B8	1801	A	C5-C6-N1	-5.46	114.97	117.70
27	B8	1878	G	O4'-C1'-N9	5.46	112.56	108.20
27	B8	2798	U	C2-N1-C1'	5.46	124.25	117.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	BA	158	PHE	CB-CG-CD1	5.46	124.62	120.80
3	AV	52	A	C5-C6-N6	-5.46	119.34	123.70
27	B8	492	A	C5-C6-N1	-5.46	114.97	117.70
27	B8	1000	A	C5-C6-N6	-5.46	119.34	123.70
27	B8	1419	A	C5-C6-N1	-5.46	114.97	117.70
27	B8	1570	A	C5-C6-N1	-5.46	114.97	117.70
27	B8	1837	C	N3-C4-C5	-5.46	119.72	121.90
1	AA	330	C	N3-C4-C5	-5.45	119.72	121.90
1	AA	1218	C	N3-C4-N4	5.45	121.82	118.00
27	B8	176	A	C5-C6-N1	-5.45	114.97	117.70
27	B8	1505	A	C5-C6-N6	-5.45	119.34	123.70
27	B8	2062	A	C5-C6-N6	-5.45	119.34	123.70
27	B8	2872	A	C5-C6-N6	-5.45	119.34	123.70
1	AA	279	A	C4-C5-C6	5.45	119.73	117.00
1	AA	325	A	C5-C6-N6	-5.45	119.34	123.70
1	AA	1027	C	N3-C4-C5	-5.45	119.72	121.90
1	AA	1452	C	N3-C4-C5	-5.45	119.72	121.90
27	B8	1024	G	O4'-C1'-N9	5.45	112.56	108.20
27	B8	1251	C	N3-C4-C5	-5.45	119.72	121.90
1	AA	66	A	O4'-C1'-N9	5.45	112.56	108.20
1	AA	67	C	N3-C4-N4	5.45	121.81	118.00
1	AA	73	C	N3-C4-C5	-5.45	119.72	121.90
1	AA	708	C	N3-C4-N4	5.45	121.82	118.00
1	AA	1267	C	N3-C4-C5	-5.45	119.72	121.90
1	AA	1503	A	C5-C6-N1	-5.45	114.97	117.70
27	B8	544	C	N3-C4-N4	5.45	121.81	118.00
27	B8	1125	G	O4'-C1'-N9	5.45	112.56	108.20
27	B8	1301	A	C5-C6-N6	-5.45	119.34	123.70
27	B8	1614	A	C5-C6-N6	-5.45	119.34	123.70
27	B8	2736	A	C5-C6-N6	-5.45	119.34	123.70
1	AA	722	G	O4'-C1'-N9	5.45	112.56	108.20
1	AA	1179	A	C5-C6-N6	-5.45	119.34	123.70
1	AA	1480	A	C5-C6-N6	-5.45	119.34	123.70
3	AV	74	A	C5-C6-N6	-5.45	119.34	123.70
27	B8	472	A	C5-C6-N1	-5.45	114.98	117.70
27	B8	632	A	O4'-C1'-N9	5.45	112.56	108.20
27	B8	805	G	O4'-C1'-N9	5.45	112.56	108.20
27	B8	857	G	O4'-C1'-N9	5.45	112.56	108.20
27	B8	1951	U	O4'-C1'-N1	5.45	112.56	108.20
27	B8	2411	A	C5-C6-N1	-5.45	114.98	117.70
27	B8	2442	C	N3-C4-C5	-5.45	119.72	121.90
1	AA	470	C	N3-C4-C5	-5.45	119.72	121.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	AV	42	C	N3-C4-C5	-5.45	119.72	121.90
27	B8	1549	A	C5-C6-N1	-5.45	114.98	117.70
27	B8	1626	A	C5-C6-N6	-5.45	119.34	123.70
27	B8	2001	C	N3-C4-N4	5.45	121.81	118.00
27	B8	2322	A	C5-C6-N6	-5.45	119.34	123.70
1	AA	113	G	O4'-C1'-N9	5.45	112.56	108.20
1	AA	774	G	O4'-C1'-N9	5.45	112.56	108.20
26	B7	35	C	N3-C4-N4	5.45	121.81	118.00
27	B8	161	A	C4-C5-C6	5.45	119.72	117.00
27	B8	217	A	C5-C6-N1	-5.45	114.98	117.70
27	B8	1670	C	N3-C4-N4	5.45	121.81	118.00
27	B8	1808	A	C5-C6-N1	-5.45	114.98	117.70
27	B8	2159	G	O4'-C1'-N9	5.45	112.56	108.20
27	B8	2516	A	C5-C6-N1	-5.45	114.98	117.70
28	BA	314	GLN	CA-C-N	5.45	132.35	117.10
1	AA	8	A	C5-C6-N1	-5.44	114.98	117.70
1	AA	1042	A	C5-C6-N6	-5.44	119.34	123.70
1	AA	1362	A	C4-C5-C6	5.44	119.72	117.00
27	B8	1762	A	C5-C6-N1	-5.44	114.98	117.70
27	B8	2260	C	N3-C4-C5	-5.44	119.72	121.90
27	B8	2776	A	C5-C6-N1	-5.44	114.98	117.70
33	BE	85	PHE	CB-CG-CD2	-5.44	116.99	120.80
1	AA	385	C	N3-C4-C5	-5.44	119.72	121.90
1	AA	775	G	O4'-C1'-N9	5.44	112.55	108.20
1	AA	1024	G	N3-C2-N2	5.44	123.71	119.90
1	AA	1363	A	C5-C6-N1	-5.44	114.98	117.70
1	AA	1394	A	C5-C6-N6	-5.44	119.35	123.70
2	AX	13	C	N3-C4-N4	5.44	121.81	118.00
27	B8	61	C	N3-C4-N4	5.44	121.81	118.00
27	B8	836	G	O4'-C1'-N9	5.44	112.55	108.20
27	B8	1536	C	N3-C4-C5	-5.44	119.72	121.90
1	AA	197	A	C5-C6-N6	-5.44	119.35	123.70
1	AA	265	G	C5-C6-O6	-5.44	125.33	128.60
1	AA	443	C	N3-C4-C5	-5.44	119.72	121.90
1	AA	778	G	O4'-C1'-N9	5.44	112.55	108.20
1	AA	845	A	P-O3'-C3'	5.44	126.23	119.70
1	AA	1137	C	C6-N1-C1'	-5.44	114.27	120.80
1	AA	1256	A	C5-C6-N6	-5.44	119.35	123.70
1	AA	1483	A	C5-C6-N6	-5.44	119.35	123.70
1	AA	1539	C	N3-C4-C5	-5.44	119.72	121.90
2	AX	22	A	C5-C6-N6	-5.44	119.35	123.70
27	B8	716	A	C5-C6-N1	-5.44	114.98	117.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	749	A	O4'-C1'-N9	5.44	112.55	108.20
27	B8	1246	A	C5-C6-N6	-5.44	119.35	123.70
27	B8	1253	A	C5-C6-N6	-5.44	119.35	123.70
27	B8	1366	A	C5-C6-N1	-5.44	114.98	117.70
27	B8	1893	C	N3-C4-N4	5.44	121.81	118.00
27	B8	2235	G	O4'-C1'-N9	5.44	112.55	108.20
27	B8	2654	A	C4-C5-C6	5.44	119.72	117.00
27	B8	2829	A	O4'-C1'-N9	5.44	112.55	108.20
1	AA	967	C	N3-C4-C5	-5.44	119.72	121.90
27	B8	330	A	C5-C6-N1	-5.44	114.98	117.70
27	B8	444	C	N3-C4-N4	5.44	121.81	118.00
27	B8	1612	C	N3-C4-N4	5.44	121.81	118.00
27	B8	2158	A	C5-C6-N1	-5.44	114.98	117.70
1	AA	7	A	C5-C6-N6	-5.44	119.35	123.70
1	AA	665	A	C5-C6-N6	-5.44	119.35	123.70
1	AA	1163	A	C5-C6-N1	-5.44	114.98	117.70
27	B8	1254	A	C5-C6-N1	-5.44	114.98	117.70
27	B8	1321	A	O4'-C1'-N9	5.44	112.55	108.20
27	B8	1597	A	O4'-C1'-N9	5.44	112.55	108.20
27	B8	1914	C	N3-C4-C5	-5.44	119.72	121.90
27	B8	1920	C	N3-C4-C5	-5.44	119.72	121.90
27	B8	1940	U	O4'-C1'-N1	5.44	112.55	108.20
27	B8	2579	C	N3-C4-C5	-5.44	119.72	121.90
27	B8	2675	A	O4'-C1'-N9	5.44	112.55	108.20
27	B8	2753	A	C5-C6-N1	-5.44	114.98	117.70
27	B8	2894	G	O4'-C1'-N9	5.44	112.55	108.20
1	AA	430	A	C4-C5-C6	5.44	119.72	117.00
1	AA	1416	G	O4'-C1'-N9	5.44	112.55	108.20
27	B8	1935	G	O4'-C1'-N9	5.44	112.55	108.20
27	B8	2665	A	C5-C6-N1	-5.44	114.98	117.70
27	B8	2841	C	N3-C4-C5	-5.44	119.73	121.90
1	AA	44	A	C5-C6-N6	-5.43	119.35	123.70
1	AA	640	A	O4'-C1'-N9	5.43	112.55	108.20
1	AA	900	A	C5-C6-N1	-5.43	114.98	117.70
1	AA	1491	G	O4'-C1'-N9	5.43	112.55	108.20
27	B8	531	C	N3-C4-N4	5.43	121.81	118.00
27	B8	574	A	C5-C6-N6	-5.43	119.35	123.70
27	B8	1071	G	O4'-C1'-N9	5.43	112.55	108.20
27	B8	1173	U	O4'-C1'-N1	5.43	112.55	108.20
27	B8	1447	C	N3-C4-N4	5.43	121.81	118.00
27	B8	2070	A	C5-C6-N6	-5.43	119.35	123.70
27	B8	2147	A	C5-C6-N1	-5.43	114.98	117.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	2170	A	O4'-C1'-N9	5.43	112.55	108.20
27	B8	2288	A	C5-C6-N6	-5.43	119.35	123.70
27	B8	2601	C	O4'-C1'-N1	5.43	112.55	108.20
27	B8	2644	G	O4'-C1'-N9	5.43	112.55	108.20
1	AA	90	C	N3-C4-C5	-5.43	119.73	121.90
1	AA	749	A	C5-C6-N6	-5.43	119.35	123.70
1	AA	840	C	N3-C4-N4	5.43	121.80	118.00
1	AA	1132	C	N3-C4-C5	-5.43	119.73	121.90
1	AA	1136	C	N3-C4-C5	-5.43	119.73	121.90
1	AA	1137	C	N3-C4-N4	5.43	121.80	118.00
1	AA	1346	A	C5-C6-N1	-5.43	114.98	117.70
27	B8	69	C	N3-C4-N4	5.43	121.80	118.00
27	B8	140	C	N3-C4-N4	5.43	121.80	118.00
27	B8	1102	C	N3-C4-C5	-5.43	119.73	121.90
27	B8	1109	C	N3-C4-C5	-5.43	119.73	121.90
27	B8	1290	C	N3-C4-C5	-5.43	119.73	121.90
27	B8	1489	C	O4'-C1'-N1	5.43	112.55	108.20
27	B8	2451	A	C4-C5-C6	5.43	119.72	117.00
27	B8	2634	A	C5-C6-N6	-5.43	119.35	123.70
1	AA	167	A	C5-C6-N6	-5.43	119.36	123.70
1	AA	339	C	N3-C4-N4	5.43	121.80	118.00
1	AA	392	C	N3-C4-C5	-5.43	119.73	121.90
1	AA	468	A	C5-C6-N6	-5.43	119.36	123.70
1	AA	810	C	N3-C4-N4	5.43	121.80	118.00
27	B8	478	A	C4-C5-C6	5.43	119.72	117.00
27	B8	1658	C	N3-C4-N4	5.43	121.80	118.00
27	B8	2266	A	C5-C6-N6	-5.43	119.36	123.70
1	AA	183	C	N3-C4-N4	5.43	121.80	118.00
1	AA	1217	C	N3-C4-N4	5.43	121.80	118.00
27	B8	10	A	C5-C6-N6	-5.43	119.36	123.70
27	B8	384	A	C5-C6-N6	-5.43	119.36	123.70
27	B8	733	G	N3-C2-N2	5.43	123.70	119.90
27	B8	903	C	N3-C4-N4	5.43	121.80	118.00
27	B8	1175	A	C5-C6-N6	-5.43	119.36	123.70
27	B8	1490	A	C5-C6-N1	-5.43	114.98	117.70
27	B8	1690	A	C5-C6-N1	-5.43	114.99	117.70
27	B8	2459	A	C5-C6-N6	-5.43	119.36	123.70
27	B8	2830	C	N3-C4-N4	5.43	121.80	118.00
1	AA	72	A	C5-C6-N1	-5.43	114.99	117.70
1	AA	277	C	N3-C4-N4	5.43	121.80	118.00
27	B8	160	A	C5-C6-N1	-5.43	114.99	117.70
27	B8	222	A	C5-C6-N6	-5.43	119.36	123.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	1114	C	N3-C4-C5	-5.43	119.73	121.90
27	B8	2250	G	N3-C2-N2	5.43	123.70	119.90
27	B8	2381	A	C5-C6-N1	-5.43	114.99	117.70
1	AA	546	A	O4'-C1'-N9	5.43	112.54	108.20
1	AA	602	A	C5-C6-N6	-5.43	119.36	123.70
1	AA	970	C	N3-C4-N4	5.43	121.80	118.00
1	AA	1228	C	N3-C4-N4	5.43	121.80	118.00
1	AA	1483	A	C5-C6-N1	-5.43	114.99	117.70
3	AV	33	A	C5-C6-N6	-5.43	119.36	123.70
22	AR	4	PHE	CB-CG-CD2	-5.43	117.00	120.80
27	B8	671	C	C5'-C4'-C3'	-5.43	107.32	116.00
27	B8	1358	G	N3-C2-N2	5.43	123.70	119.90
27	B8	1746	A	C5-C6-N6	-5.43	119.36	123.70
27	B8	2005	A	C5-C6-N1	-5.43	114.99	117.70
27	B8	2042	A	C5-C6-N1	-5.43	114.99	117.70
27	B8	2184	A	C5-C6-N1	-5.43	114.99	117.70
27	B8	2201	G	O4'-C1'-N9	5.43	112.54	108.20
27	B8	2573	C	N3-C4-N4	5.43	121.80	118.00
1	AA	110	C	N3-C4-C5	-5.42	119.73	121.90
1	AA	616	G	O4'-C1'-N9	5.42	112.54	108.20
1	AA	1285	A	C5'-C4'-C3'	-5.42	107.32	116.00
1	AA	1484	C	N3-C4-N4	5.42	121.80	118.00
3	AV	24	C	N3-C4-N4	5.42	121.80	118.00
27	B8	979	A	O4'-C1'-N9	5.42	112.54	108.20
27	B8	1708	C	N3-C4-C5	-5.42	119.73	121.90
1	AA	984	C	N3-C4-C5	-5.42	119.73	121.90
1	AA	1003	G	O4'-C1'-N9	5.42	112.54	108.20
1	AA	1037	C	N3-C4-N4	5.42	121.80	118.00
27	B8	873	C	N3-C4-N4	5.42	121.80	118.00
27	B8	1008	A	C5-C6-N1	-5.42	114.99	117.70
27	B8	1801	A	C5-C6-N6	-5.42	119.36	123.70
1	AA	236	A	C5-C6-N1	-5.42	114.99	117.70
1	AA	330	C	N3-C4-N4	5.42	121.79	118.00
3	AV	5	A	C5-C6-N1	-5.42	114.99	117.70
27	B8	845	A	C5-C6-N1	-5.42	114.99	117.70
27	B8	1262	A	C5-C6-N6	-5.42	119.36	123.70
27	B8	1592	C	N3-C4-C5	-5.42	119.73	121.90
27	B8	1819	A	C5-C6-N1	-5.42	114.99	117.70
27	B8	2734	A	O4'-C1'-N9	5.42	112.54	108.20
1	AA	492	C	N3-C4-N4	5.42	121.79	118.00
1	AA	1045	C	N3-C4-C5	-5.42	119.73	121.90
1	AA	1226	C	N3-C4-N4	5.42	121.79	118.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1484	C	N3-C4-C5	-5.42	119.73	121.90
1	AA	1503	A	C5-C6-N6	-5.42	119.36	123.70
27	B8	73	A	C5-C6-N1	-5.42	114.99	117.70
27	B8	412	A	C5-C6-N1	-5.42	114.99	117.70
27	B8	1505	A	C5-C6-N1	-5.42	114.99	117.70
27	B8	1708	C	N3-C4-N4	5.42	121.79	118.00
1	AA	640	A	C5-C6-N6	-5.42	119.36	123.70
1	AA	688	G	O4'-C1'-N9	5.42	112.53	108.20
1	AA	1118	U	O4'-C1'-N1	5.42	112.54	108.20
27	B8	517	C	N3-C4-N4	5.42	121.79	118.00
27	B8	865	C	N3-C4-C5	-5.42	119.73	121.90
27	B8	1049	C	N3-C4-N4	5.42	121.79	118.00
27	B8	1136	G	O4'-C1'-N9	5.42	112.53	108.20
27	B8	1194	A	C5-C6-N1	-5.42	114.99	117.70
27	B8	1780	A	C5-C6-N1	-5.42	114.99	117.70
27	B8	1889	A	C5-C6-N6	-5.42	119.36	123.70
27	B8	2117	A	C5-C6-N6	-5.42	119.36	123.70
27	B8	2467	C	N3-C4-C5	-5.42	119.73	121.90
1	AA	32	A	C5-C6-N1	-5.42	114.99	117.70
1	AA	225	C	N3-C4-C5	-5.42	119.73	121.90
1	AA	250	A	C5-C6-N1	-5.42	114.99	117.70
1	AA	660	C	N3-C4-N4	5.42	121.79	118.00
1	AA	1408	A	C5-C6-N6	-5.42	119.37	123.70
27	B8	42	A	C5-C6-N1	-5.42	114.99	117.70
27	B8	125	A	C5-C6-N1	-5.42	114.99	117.70
27	B8	233	A	C5-C6-N1	-5.42	114.99	117.70
27	B8	342	A	C5-C6-N1	-5.42	114.99	117.70
27	B8	363	G	P-O5'-C5'	5.42	129.56	120.90
27	B8	735	A	C4-C5-C6	5.42	119.71	117.00
27	B8	1313	U	C6-N1-C1'	-5.42	113.62	121.20
27	B8	1353	A	C5-C6-N6	-5.42	119.37	123.70
27	B8	2530	A	C5-C6-N6	-5.42	119.37	123.70
27	B8	2710	C	N3-C4-C5	-5.42	119.73	121.90
27	B8	1953	A	C5-C6-N6	-5.42	119.37	123.70
1	AA	129	A	C5-C6-N1	-5.41	114.99	117.70
1	AA	1410	A	C4-C5-C6	5.41	119.71	117.00
1	AA	1467	C	N3-C4-C5	-5.41	119.73	121.90
1	AA	1538	C	N3-C4-C5	-5.41	119.73	121.90
27	B8	692	C	N3-C4-C5	-5.41	119.73	121.90
27	B8	1269	A	O4'-C1'-N9	5.41	112.53	108.20
27	B8	1665	A	O4'-C1'-N9	5.41	112.53	108.20
27	B8	1739	A	C4-C5-C6	5.41	119.71	117.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	2805	C	N3-C4-C5	-5.41	119.73	121.90
1	AA	811	C	N3-C4-N4	5.41	121.79	118.00
27	B8	542	C	N3-C4-C5	-5.41	119.73	121.90
27	B8	1161	C	N3-C4-C5	-5.41	119.73	121.90
27	B8	1588	G	O4'-C1'-N9	5.41	112.53	108.20
27	B8	2037	A	C5-C6-N1	-5.41	114.99	117.70
27	B8	2300	C	N3-C4-C5	-5.41	119.73	121.90
3	AV	29	C	N3-C4-C5	-5.41	119.74	121.90
27	B8	1569	A	C5-C6-N6	-5.41	119.37	123.70
27	B8	817	C	N3-C4-C5	-5.41	119.74	121.90
27	B8	984	A	C5-C6-N1	-5.41	115.00	117.70
27	B8	1014	A	C5-C6-N1	-5.41	115.00	117.70
27	B8	1079	C	N3-C4-C5	-5.41	119.74	121.90
27	B8	1493	C	N3-C4-C5	-5.41	119.74	121.90
27	B8	2208	C	N3-C4-N4	5.41	121.79	118.00
27	B8	2542	A	C5-C6-N6	-5.41	119.37	123.70
27	B8	2721	A	C5-C6-N6	-5.41	119.37	123.70
27	B8	509	C	N3-C4-N4	5.41	121.78	118.00
27	B8	1889	A	C5-C6-N1	-5.41	115.00	117.70
27	B8	2328	A	C5-C6-N1	-5.41	115.00	117.70
1	AA	250	A	C5-C6-N6	-5.41	119.38	123.70
1	AA	264	C	N3-C4-C5	-5.41	119.74	121.90
1	AA	777	A	C5-C6-N6	-5.41	119.38	123.70
1	AA	1362	A	C5-C6-N6	-5.41	119.38	123.70
1	AA	1536	C	N3-C4-N4	5.41	121.78	118.00
2	AX	15	C	N3-C4-C5	-5.41	119.74	121.90
3	AV	29	C	N3-C4-N4	5.41	121.78	118.00
27	B8	63	A	O4'-C1'-N9	5.41	112.53	108.20
27	B8	207	A	C4-C5-C6	5.41	119.70	117.00
27	B8	323	C	N3-C4-C5	-5.41	119.74	121.90
27	B8	456	C	N3-C4-N4	5.41	121.78	118.00
27	B8	888	C	N3-C4-C5	-5.41	119.74	121.90
27	B8	1655	A	C4-C5-C6	5.41	119.70	117.00
27	B8	1938	A	C5-C6-N1	-5.41	115.00	117.70
27	B8	2064	C	N3-C4-C5	-5.41	119.74	121.90
27	B8	2145	C	O4'-C1'-N1	5.41	112.52	108.20
27	B8	2177	C	N3-C4-C5	-5.41	119.74	121.90
27	B8	2183	A	C5-C6-N1	-5.41	115.00	117.70
27	B8	2226	C	N3-C4-N4	5.41	121.78	118.00
27	B8	2468	A	C5-C6-N6	-5.41	119.38	123.70
27	B8	2824	C	N3-C4-C5	-5.41	119.74	121.90
1	AA	378	G	O4'-C1'-N9	5.40	112.52	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	878	A	C5-C6-N6	-5.40	119.38	123.70
1	AA	1149	C	N3-C4-C5	-5.40	119.74	121.90
1	AA	1333	A	C5-C6-N6	-5.40	119.38	123.70
1	AA	1441	A	C5-C6-N1	-5.40	115.00	117.70
27	B8	307	G	O4'-C1'-N9	5.40	112.52	108.20
27	B8	645	C	N3-C4-N4	5.40	121.78	118.00
27	B8	2285	C	N3-C4-C5	-5.40	119.74	121.90
27	B8	2347	C	N3-C4-N4	5.40	121.78	118.00
27	B8	2731	G	O4'-C1'-N9	5.40	112.52	108.20
1	AA	305	G	O4'-C1'-N9	5.40	112.52	108.20
1	AA	582	C	N3-C4-N4	5.40	121.78	118.00
27	B8	236	C	N3-C4-C5	-5.40	119.74	121.90
27	B8	632	A	C5-C6-N1	-5.40	115.00	117.70
27	B8	1596	A	C5-C6-N1	-5.40	115.00	117.70
27	B8	1685	C	N3-C4-C5	-5.40	119.74	121.90
27	B8	1733	G	O4'-C1'-N9	5.40	112.52	108.20
27	B8	2073	C	N3-C4-N4	5.40	121.78	118.00
27	B8	2388	A	C5-C6-N6	-5.40	119.38	123.70
1	AA	339	C	N3-C4-C5	-5.40	119.74	121.90
1	AA	505	G	O4'-C1'-N9	5.40	112.52	108.20
1	AA	509	A	C5-C6-N1	-5.40	115.00	117.70
1	AA	548	G	O4'-C1'-N9	5.40	112.52	108.20
1	AA	1141	C	N3-C4-C5	-5.40	119.74	121.90
1	AA	1174	G	O4'-C1'-N9	5.40	112.52	108.20
1	AA	1214	C	N3-C4-C5	-5.40	119.74	121.90
26	B7	43	C	N3-C4-N4	5.40	121.78	118.00
27	B8	753	A	C5-C6-N1	-5.40	115.00	117.70
27	B8	1566	A	C5-C6-N1	-5.40	115.00	117.70
27	B8	1597	A	C5-C6-N1	-5.40	115.00	117.70
27	B8	2705	A	O4'-C1'-N9	5.40	112.52	108.20
27	B8	2736	A	C5-C6-N1	-5.40	115.00	117.70
27	B8	2835	A	C4-C5-C6	5.40	119.70	117.00
1	AA	1430	A	C5-C6-N6	-5.40	119.38	123.70
27	B8	84	A	C5-C6-N1	-5.40	115.00	117.70
27	B8	2762	C	N3-C4-N4	5.40	121.78	118.00
27	B8	2889	C	N3-C4-C5	-5.40	119.74	121.90
1	AA	381	C	N3-C4-C5	-5.40	119.74	121.90
1	AA	1114	C	N3-C4-C5	-5.40	119.74	121.90
1	AA	1509	C	N3-C4-N4	5.40	121.78	118.00
1	AA	1531	A	C5-C6-N1	-5.40	115.00	117.70
26	B7	31	C	N3-C4-C5	-5.40	119.74	121.90
26	B7	58	A	C5-C6-N1	-5.40	115.00	117.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	675	A	C5-C6-N1	-5.40	115.00	117.70
27	B8	1453	A	C5-C6-N6	-5.40	119.38	123.70
27	B8	1586	A	C5-C6-N1	-5.40	115.00	117.70
27	B8	2176	A	C5-C6-N6	-5.40	119.38	123.70
1	AA	661	G	O4'-C1'-N9	5.40	112.52	108.20
27	B8	21	A	C5-C6-N6	-5.40	119.38	123.70
27	B8	893	C	N3-C4-C5	-5.40	119.74	121.90
27	B8	2266	A	C5-C6-N1	-5.40	115.00	117.70
1	AA	183	C	N3-C4-C5	-5.39	119.74	121.90
1	AA	618	C	N3-C4-C5	-5.39	119.74	121.90
1	AA	1179	A	C5-C6-N1	-5.39	115.00	117.70
1	AA	1542	A	C5-C6-N1	-5.39	115.00	117.70
26	B7	59	A	C5-C6-N6	-5.39	119.39	123.70
27	B8	255	A	O4'-C1'-N9	5.39	112.52	108.20
27	B8	334	C	N3-C4-C5	-5.39	119.74	121.90
27	B8	575	A	C5-C6-N6	-5.39	119.38	123.70
27	B8	1274	A	O4'-C1'-N9	5.39	112.52	108.20
27	B8	1418	G	O4'-C1'-N9	5.39	112.52	108.20
27	B8	2209	G	O4'-C1'-N9	5.39	112.52	108.20
27	B8	2251	G	O4'-C1'-N9	5.39	112.52	108.20
1	AA	163	C	N3-C4-C5	-5.39	119.74	121.90
1	AA	992	U	O4'-C1'-N1	5.39	112.51	108.20
3	AV	1	C	N3-C4-N4	5.39	121.78	118.00
3	AV	22	A	O4'-C1'-N9	5.39	112.51	108.20
27	B8	196	A	C5-C6-N1	-5.39	115.00	117.70
27	B8	627	A	C5-C6-N1	-5.39	115.00	117.70
27	B8	1133	A	C5-C6-N1	-5.39	115.00	117.70
27	B8	1420	A	C5-C6-N1	-5.39	115.00	117.70
27	B8	1565	C	N3-C4-N4	5.39	121.78	118.00
27	B8	1925	C	N3-C4-C5	-5.39	119.74	121.90
27	B8	2031	A	C5-C6-N1	-5.39	115.00	117.70
27	B8	2496	C	N3-C4-N4	5.39	121.78	118.00
28	BA	158	PHE	CB-CG-CD2	-5.39	117.03	120.80
1	AA	107	G	O4'-C1'-N9	5.39	112.51	108.20
1	AA	1097	C	N3-C4-C5	-5.39	119.74	121.90
27	B8	404	A	C5-C6-N6	-5.39	119.39	123.70
27	B8	761	A	C5-C6-N1	-5.39	115.00	117.70
27	B8	2009	A	C5-C6-N6	-5.39	119.39	123.70
27	B8	2129	C	C6-N1-C1'	-5.39	114.33	120.80
27	B8	2191	A	C5-C6-N6	-5.39	119.39	123.70
27	B8	2792	A	C5-C6-N1	-5.39	115.00	117.70
1	AA	26	A	C4-C5-C6	5.39	119.69	117.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	379	C	N3-C4-N4	5.39	121.77	118.00
1	AA	412	A	C5-C6-N6	-5.39	119.39	123.70
1	AA	460	A	C5-C6-N6	-5.39	119.39	123.70
1	AA	532	A	C5-C6-N1	-5.39	115.01	117.70
3	AV	65	C	N3-C4-N4	5.39	121.77	118.00
27	B8	22	C	N3-C4-C5	-5.39	119.74	121.90
27	B8	226	A	C5-C6-N1	-5.39	115.00	117.70
27	B8	947	A	O4'-C1'-N9	5.39	112.51	108.20
27	B8	1129	A	C5-C6-N1	-5.39	115.00	117.70
27	B8	1877	A	O4'-C1'-N9	5.39	112.51	108.20
27	B8	2476	A	C5-C6-N1	-5.39	115.01	117.70
27	B8	2541	A	C5-C6-N1	-5.39	115.01	117.70
27	B8	537	G	O4'-C1'-N9	5.39	112.51	108.20
27	B8	550	C	N3-C4-N4	5.39	121.77	118.00
27	B8	1044	C	N3-C4-N4	5.39	121.77	118.00
27	B8	2339	C	N3-C4-N4	5.39	121.77	118.00
1	AA	356	A	C4-C5-C6	5.39	119.69	117.00
1	AA	412	A	C5-C6-N1	-5.39	115.01	117.70
1	AA	535	A	C5-C6-N1	-5.39	115.01	117.70
1	AA	566	G	C5-C6-O6	-5.39	125.37	128.60
1	AA	1080	A	C4-C5-C6	5.39	119.69	117.00
1	AA	1226	C	N3-C4-C5	-5.39	119.75	121.90
27	B8	453	A	C5-C6-N6	-5.39	119.39	123.70
27	B8	915	C	N3-C4-C5	-5.39	119.75	121.90
27	B8	1583	A	C4-C5-C6	5.39	119.69	117.00
27	B8	2092	U	C2-N1-C1'	5.39	124.16	117.70
1	AA	568	G	O4'-C1'-N9	5.38	112.51	108.20
1	AA	705	G	N1-C6-O6	5.38	123.13	119.90
1	AA	996	A	C5-C6-N1	-5.38	115.01	117.70
27	B8	483	A	C5-C6-N1	-5.38	115.01	117.70
27	B8	1503	A	C5-C6-N6	-5.38	119.39	123.70
27	B8	1521	G	N3-C2-N2	5.38	123.67	119.90
27	B8	2030	A	C5-C6-N6	-5.38	119.39	123.70
27	B8	2058	A	C5-C6-N1	-5.38	115.01	117.70
27	B8	2448	A	C5-C6-N1	-5.38	115.01	117.70
27	B8	2572	A	C5-C6-N1	-5.38	115.01	117.70
27	B8	2712	C	N3-C4-C5	-5.38	119.75	121.90
1	AA	1509	C	N3-C4-C5	-5.38	119.75	121.90
27	B8	914	G	O4'-C1'-N9	5.38	112.51	108.20
27	B8	944	C	N3-C4-C5	-5.38	119.75	121.90
27	B8	1595	C	N3-C4-C5	-5.38	119.75	121.90
27	B8	1745	A	O4'-C1'-N9	5.38	112.51	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	2052	A	O4'-C1'-N9	5.38	112.51	108.20
27	B8	2364	C	N3-C4-C5	-5.38	119.75	121.90
1	AA	1192	C	N3-C4-C5	-5.38	119.75	121.90
27	B8	972	A	C4-C5-C6	5.38	119.69	117.00
27	B8	979	A	C5-C6-N1	-5.38	115.01	117.70
27	B8	1463	C	N3-C4-N4	5.38	121.77	118.00
27	B8	1847	A	C5-C6-N1	-5.38	115.01	117.70
27	B8	2002	G	O4'-C1'-N9	5.38	112.50	108.20
27	B8	2751	G	O4'-C1'-N9	5.38	112.51	108.20
1	AA	2	A	C5-C6-N1	-5.38	115.01	117.70
1	AA	212	G	O4'-C1'-N9	5.38	112.50	108.20
1	AA	381	C	N3-C4-N4	5.38	121.77	118.00
1	AA	880	C	N3-C4-C5	-5.38	119.75	121.90
3	AV	46	G	O4'-C1'-N9	5.38	112.50	108.20
27	B8	1287	A	C5-C6-N1	-5.38	115.01	117.70
27	B8	1488	C	N3-C4-N4	5.38	121.77	118.00
27	B8	1947	C	N3-C4-N4	5.38	121.77	118.00
1	AA	207	C	N3-C4-N4	5.38	121.77	118.00
1	AA	335	C	N3-C4-C5	-5.38	119.75	121.90
1	AA	584	G	O4'-C1'-N9	5.38	112.50	108.20
1	AA	969	A	C5-C6-N6	-5.38	119.40	123.70
26	B7	66	A	C4-C5-C6	5.38	119.69	117.00
27	B8	302	C	N3-C4-N4	5.38	121.77	118.00
27	B8	442	G	O4'-C1'-N9	5.38	112.50	108.20
27	B8	484	C	N3-C4-C5	-5.38	119.75	121.90
27	B8	565	C	N3-C4-C5	-5.38	119.75	121.90
27	B8	1048	A	C5-C6-N6	-5.38	119.40	123.70
27	B8	1419	A	C5-C6-N6	-5.38	119.40	123.70
27	B8	1545	A	C4-C5-C6	5.38	119.69	117.00
27	B8	1763	G	O4'-C1'-N9	5.38	112.50	108.20
27	B8	1966	A	C5-C6-N1	-5.38	115.01	117.70
27	B8	1970	A	C5-C6-N1	-5.38	115.01	117.70
27	B8	2205	A	C5-C6-N6	-5.38	119.40	123.70
27	B8	2815	C	N3-C4-N4	5.38	121.77	118.00
27	B8	2868	A	C5-C6-N1	-5.38	115.01	117.70
1	AA	383	A	C5-C6-N6	-5.38	119.40	123.70
1	AA	447	G	O4'-C1'-N9	5.38	112.50	108.20
1	AA	566	G	O4'-C1'-N9	5.38	112.50	108.20
1	AA	807	A	C5-C6-N6	-5.38	119.40	123.70
1	AA	1324	A	C5-C6-N1	-5.38	115.01	117.70
1	AA	1408	A	C5-C6-N1	-5.38	115.01	117.70
27	B8	176	A	C5-C6-N6	-5.38	119.40	123.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	854	C	N3-C4-N4	5.38	121.76	118.00
27	B8	1307	A	C5-C6-N6	-5.38	119.40	123.70
27	B8	1598	A	O4'-C1'-N9	5.38	112.50	108.20
27	B8	1645	G	O4'-C1'-N9	5.38	112.50	108.20
27	B8	1757	A	C5-C6-N1	-5.38	115.01	117.70
27	B8	2276	G	O4'-C1'-N9	5.38	112.50	108.20
27	B8	2501	C	O4'-C1'-N1	5.38	112.50	108.20
1	AA	363	A	C5-C6-N1	-5.38	115.01	117.70
1	AA	663	A	O4'-C1'-N9	5.38	112.50	108.20
1	AA	764	C	N3-C4-C5	-5.38	119.75	121.90
1	AA	1539	C	N3-C4-N4	5.38	121.76	118.00
27	B8	49	A	C5-C6-N1	-5.38	115.01	117.70
27	B8	1272	A	C5-C6-N1	-5.38	115.01	117.70
27	B8	1451	C	N3-C4-N4	5.38	121.76	118.00
27	B8	2799	A	C5-C6-N1	-5.38	115.01	117.70
1	AA	160	A	C5-C6-N1	-5.37	115.01	117.70
1	AA	482	A	O4'-C1'-N9	5.37	112.50	108.20
1	AA	1265	C	N3-C4-N4	5.37	121.76	118.00
27	B8	44	A	C5-C6-N6	-5.37	119.40	123.70
27	B8	320	A	O4'-C1'-N9	5.37	112.50	108.20
27	B8	1005	C	N3-C4-C5	-5.37	119.75	121.90
27	B8	1134	A	C5-C6-N1	-5.37	115.01	117.70
27	B8	1276	A	C5-C6-N6	-5.37	119.40	123.70
27	B8	1985	C	N3-C4-C5	-5.37	119.75	121.90
1	AA	1493	A	C5-C6-N1	-5.37	115.01	117.70
1	AA	1499	A	C5-C6-N1	-5.37	115.01	117.70
27	B8	537	G	N3-C2-N2	5.37	123.66	119.90
27	B8	928	A	O4'-C1'-N9	5.37	112.50	108.20
27	B8	1511	G	O4'-C1'-N9	5.37	112.50	108.20
27	B8	1596	A	C4-C5-C6	5.37	119.69	117.00
27	B8	1944	U	O4'-C1'-N1	5.37	112.50	108.20
27	B8	2126	A	C5-C6-N1	-5.37	115.01	117.70
27	B8	2307	G	C5-C6-O6	-5.37	125.38	128.60
27	B8	2336	A	C5-C6-N6	-5.37	119.40	123.70
27	B8	2476	A	C5-C6-N6	-5.37	119.40	123.70
1	AA	488	C	N3-C4-C5	-5.37	119.75	121.90
1	AA	635	A	C5-C6-N1	-5.37	115.02	117.70
1	AA	794	A	C5-C6-N6	-5.37	119.40	123.70
3	AV	42	C	N3-C4-N4	5.37	121.76	118.00
27	B8	1126	A	C5-C6-N6	-5.37	119.40	123.70
1	AA	1319	A	C5-C6-N1	-5.37	115.02	117.70
1	AA	1366	C	N3-C4-C5	-5.37	119.75	121.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1448	C	N3-C4-C5	-5.37	119.75	121.90
26	B7	100	G	O4'-C1'-N9	5.37	112.50	108.20
27	B8	73	A	C5-C6-N6	-5.37	119.41	123.70
27	B8	470	A	C5-C6-N6	-5.37	119.40	123.70
27	B8	692	C	N3-C4-N4	5.37	121.76	118.00
27	B8	909	A	C4-C5-C6	5.37	119.68	117.00
27	B8	1010	A	C5-C6-N6	-5.37	119.41	123.70
27	B8	1522	A	C5-C6-N6	-5.37	119.41	123.70
27	B8	2462	C	N3-C4-C5	-5.37	119.75	121.90
27	B8	2874	C	N3-C4-N4	5.37	121.76	118.00
1	AA	397	A	C5-C6-N1	-5.37	115.02	117.70
27	B8	848	C	N3-C4-C5	-5.37	119.75	121.90
27	B8	1080	A	C5-C6-N6	-5.37	119.41	123.70
27	B8	1538	G	O4'-C1'-N9	5.37	112.49	108.20
27	B8	1787	A	C5-C6-N1	-5.37	115.02	117.70
1	AA	298	A	O4'-C1'-N9	5.37	112.49	108.20
1	AA	374	A	C5-C6-N1	-5.37	115.02	117.70
1	AA	720	C	N3-C4-N4	5.37	121.76	118.00
1	AA	819	A	C5-C6-N6	-5.37	119.41	123.70
1	AA	1536	C	N3-C4-C5	-5.37	119.75	121.90
27	B8	1889	A	O4'-C1'-N9	5.37	112.49	108.20
27	B8	2327	A	O4'-C1'-N9	5.37	112.49	108.20
27	B8	2759	G	O4'-C1'-N9	5.37	112.49	108.20
1	AA	186	C	N3-C4-C5	-5.36	119.75	121.90
1	AA	189	A	C5-C6-N1	-5.36	115.02	117.70
1	AA	1036	A	C5-C6-N1	-5.36	115.02	117.70
27	B8	147	C	N3-C4-C5	-5.36	119.75	121.90
27	B8	404	A	C5-C6-N1	-5.36	115.02	117.70
27	B8	516	C	N3-C4-N4	5.36	121.75	118.00
27	B8	603	A	C5-C6-N1	-5.36	115.02	117.70
27	B8	1040	A	C5-C6-N1	-5.36	115.02	117.70
27	B8	1057	A	O4'-C1'-N9	5.36	112.49	108.20
27	B8	1672	A	C5-C6-N1	-5.36	115.02	117.70
27	B8	2117	A	C5-C6-N1	-5.36	115.02	117.70
27	B8	2468	A	C5-C6-N1	-5.36	115.02	117.70
1	AA	374	A	C5-C6-N6	-5.36	119.41	123.70
1	AA	907	A	O4'-C1'-N9	5.36	112.49	108.20
1	AA	1347	G	O4'-C1'-N9	5.36	112.49	108.20
27	B8	840	C	N3-C4-C5	-5.36	119.75	121.90
27	B8	1170	C	N3-C4-C5	-5.36	119.75	121.90
27	B8	2327	A	C5-C6-N6	-5.36	119.41	123.70
1	AA	153	C	N3-C4-C5	-5.36	119.76	121.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	161	A	C5-C6-N1	-5.36	115.02	117.70
1	AA	489	C	N3-C4-N4	5.36	121.75	118.00
1	AA	528	C	N3-C4-C5	-5.36	119.75	121.90
1	AA	841	C	N3-C4-N4	5.36	121.75	118.00
1	AA	972	C	N3-C4-N4	5.36	121.75	118.00
1	AA	1227	A	C4-C5-C6	5.36	119.68	117.00
1	AA	1363	A	C5-C6-N6	-5.36	119.41	123.70
3	AV	57	C	N3-C4-N4	5.36	121.75	118.00
27	B8	762	U	O4'-C1'-N1	5.36	112.49	108.20
27	B8	922	C	N3-C4-N4	5.36	121.75	118.00
27	B8	1335	C	N3-C4-N4	5.36	121.75	118.00
27	B8	1392	A	C5-C6-N1	-5.36	115.02	117.70
27	B8	2094	A	C5-C6-N1	-5.36	115.02	117.70
27	B8	2788	C	N3-C4-C5	-5.36	119.76	121.90
1	AA	815	A	C5-C6-N1	-5.36	115.02	117.70
1	AA	967	C	N3-C4-N4	5.36	121.75	118.00
1	AA	1012	A	C5-C6-N1	-5.36	115.02	117.70
27	B8	1151	A	C5-C6-N1	-5.36	115.02	117.70
1	AA	567	G	O4'-C1'-N9	5.36	112.49	108.20
26	B7	76	G	O4'-C1'-N9	5.36	112.49	108.20
27	B8	729	G	O4'-C1'-N9	5.36	112.49	108.20
27	B8	753	A	C5-C6-N6	-5.36	119.41	123.70
27	B8	820	A	C5-C6-N1	-5.36	115.02	117.70
27	B8	1086	A	C4-C5-C6	5.36	119.68	117.00
27	B8	1140	C	N3-C4-C5	-5.36	119.76	121.90
27	B8	1451	C	N3-C4-C5	-5.36	119.76	121.90
27	B8	1761	C	N3-C4-C5	-5.36	119.76	121.90
27	B8	1876	A	C4-C5-C6	5.36	119.68	117.00
27	B8	2066	C	N3-C4-C5	-5.36	119.76	121.90
27	B8	2066	C	N3-C4-N4	5.36	121.75	118.00
27	B8	2347	C	N3-C4-C5	-5.36	119.76	121.90
1	AA	172	A	C5-C6-N1	-5.36	115.02	117.70
1	AA	889	A	C4-C5-C6	5.36	119.68	117.00
1	AA	1110	A	O4'-C1'-N9	5.36	112.48	108.20
27	B8	742	A	C5-C6-N1	-5.36	115.02	117.70
27	B8	788	A	C5-C6-N1	-5.36	115.02	117.70
27	B8	1537	G	O4'-C1'-N9	5.36	112.48	108.20
27	B8	1952	A	C5-C6-N1	-5.36	115.02	117.70
27	B8	2170	A	C5-C6-N1	-5.36	115.02	117.70
27	B8	2730	C	N3-C4-C5	-5.36	119.76	121.90
1	AA	779	C	N3-C4-C5	-5.35	119.76	121.90
27	B8	764	A	C5-C6-N6	-5.35	119.42	123.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	1605	C	N3-C4-N4	5.35	121.75	118.00
27	B8	1958	C	N3-C4-C5	-5.35	119.76	121.90
27	B8	2522	U	O4'-C1'-N1	5.35	112.48	108.20
1	AA	167	A	O4'-C1'-N9	5.35	112.48	108.20
1	AA	401	C	N3-C4-N4	5.35	121.75	118.00
1	AA	783	C	N3-C4-C5	-5.35	119.76	121.90
1	AA	919	A	C5-C6-N6	-5.35	119.42	123.70
1	AA	968	A	C5-C6-N1	-5.35	115.02	117.70
1	AA	1089	G	O4'-C1'-N9	5.35	112.48	108.20
1	AA	1111	A	C5-C6-N1	-5.35	115.02	117.70
1	AA	1201	A	C5-C6-N1	-5.35	115.02	117.70
1	AA	1296	C	N3-C4-N4	5.35	121.75	118.00
1	AA	1389	C	N3-C4-C5	-5.35	119.76	121.90
1	AA	1535	C	N3-C4-N4	5.35	121.75	118.00
3	AV	67	C	N3-C4-C5	-5.35	119.76	121.90
27	B8	118	A	O4'-C1'-N9	5.35	112.48	108.20
27	B8	446	G	N3-C2-N2	5.35	123.65	119.90
27	B8	636	G	O4'-C1'-N9	5.35	112.48	108.20
27	B8	802	A	C5-C6-N6	-5.35	119.42	123.70
27	B8	996	A	C5-C6-N1	-5.35	115.02	117.70
27	B8	2284	A	C5-C6-N1	-5.35	115.02	117.70
1	AA	188	C	N3-C4-N4	5.35	121.75	118.00
27	B8	1746	A	C5-C6-N1	-5.35	115.03	117.70
27	B8	2331	G	O4'-C1'-N9	5.35	112.48	108.20
1	AA	1377	A	C5-C6-N1	-5.35	115.03	117.70
3	AV	17	C	N3-C4-C5	-5.35	119.76	121.90
27	B8	173	A	C5-C6-N1	-5.35	115.03	117.70
27	B8	249	C	N3-C4-C5	-5.35	119.76	121.90
27	B8	446	G	O4'-C1'-N9	5.35	112.48	108.20
27	B8	477	A	C5-C6-N1	-5.35	115.03	117.70
27	B8	614	A	C5-C6-N6	-5.35	119.42	123.70
27	B8	666	A	C5-C6-N1	-5.35	115.03	117.70
27	B8	1495	A	C5-C6-N1	-5.35	115.03	117.70
27	B8	1522	A	O4'-C1'-N9	5.35	112.48	108.20
1	AA	244	U	O4'-C1'-N1	5.35	112.48	108.20
3	AV	65	C	N3-C4-C5	-5.35	119.76	121.90
3	AV	75	C	N3-C4-N4	5.35	121.74	118.00
5	A0	192	TYR	CB-CG-CD1	-5.35	117.79	121.00
26	B7	66	A	C5-C6-N1	-5.35	115.03	117.70
27	B8	348	A	O4'-C1'-N9	5.35	112.48	108.20
27	B8	761	A	O4'-C1'-N9	5.35	112.48	108.20
27	B8	1235	G	N3-C2-N2	5.35	123.64	119.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	1554	U	O4'-C1'-N1	5.35	112.48	108.20
27	B8	1580	A	O4'-C1'-N9	5.35	112.48	108.20
27	B8	1631	G	O4'-C1'-N9	5.35	112.48	108.20
27	B8	1707	G	O4'-C1'-N9	5.35	112.48	108.20
27	B8	2070	A	C5-C6-N1	-5.35	115.03	117.70
27	B8	2377	A	C5-C6-N1	-5.35	115.03	117.70
27	B8	2855	C	N3-C4-C5	-5.35	119.76	121.90
1	AA	901	A	O4'-C1'-N9	5.35	112.48	108.20
1	AA	792	A	C5-C6-N6	-5.34	119.42	123.70
1	AA	1054	C	C2-N1-C1'	5.34	124.68	118.80
26	B7	101	A	C5-C6-N1	-5.34	115.03	117.70
27	B8	608	A	C5-C6-N1	-5.34	115.03	117.70
27	B8	937	C	N3-C4-C5	-5.34	119.76	121.90
27	B8	2096	C	N3-C4-N4	5.34	121.74	118.00
27	B8	2108	A	O4'-C1'-N9	5.34	112.48	108.20
27	B8	2771	C	N3-C4-C5	-5.34	119.76	121.90
27	B8	19	A	C5-C6-N1	-5.34	115.03	117.70
27	B8	1076	C	N3-C4-N4	5.34	121.74	118.00
27	B8	1357	C	N3-C4-C5	-5.34	119.76	121.90
27	B8	1436	G	O4'-C1'-N9	5.34	112.47	108.20
27	B8	1785	A	C4-C5-C6	5.34	119.67	117.00
27	B8	2261	C	N3-C4-C5	-5.34	119.76	121.90
1	AA	240	G	O4'-C1'-N9	5.34	112.47	108.20
1	AA	465	A	C4-C5-C6	5.34	119.67	117.00
1	AA	523	A	C5-C6-N6	-5.34	119.43	123.70
1	AA	720	C	N3-C4-C5	-5.34	119.76	121.90
1	AA	1195	C	P-O3'-C3'	5.34	126.11	119.70
27	B8	38	A	C5-C6-N1	-5.34	115.03	117.70
27	B8	1275	A	C5-C6-N1	-5.34	115.03	117.70
27	B8	1321	A	C5-C6-N1	-5.34	115.03	117.70
27	B8	2247	A	C5-C6-N1	-5.34	115.03	117.70
27	B8	2394	C	N3-C4-C5	-5.34	119.76	121.90
27	B8	2727	A	O4'-C1'-N9	5.34	112.47	108.20
1	AA	768	A	C5-C6-N1	-5.34	115.03	117.70
1	AA	1054	C	N3-C4-C5	-5.34	119.77	121.90
1	AA	1508	A	C5-C6-N6	-5.34	119.43	123.70
27	B8	1053	C	N3-C4-C5	-5.34	119.76	121.90
27	B8	1327	A	C5-C6-N1	-5.34	115.03	117.70
27	B8	2080	A	C5-C6-N1	-5.34	115.03	117.70
27	B8	2472	G	O4'-C1'-N9	5.34	112.47	108.20
27	B8	2875	C	N3-C4-N4	5.34	121.74	118.00
1	AA	806	C	N3-C4-C5	-5.34	119.77	121.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	1211	C	N3-C4-N4	5.34	121.74	118.00
27	B8	1809	A	O4'-C1'-N9	5.34	112.47	108.20
27	B8	2403	C	N3-C4-C5	-5.34	119.77	121.90
1	AA	28	A	C5-C6-N1	-5.34	115.03	117.70
1	AA	609	A	C5-C6-N6	-5.34	119.43	123.70
1	AA	853	C	N3-C4-N4	5.34	121.74	118.00
1	AA	892	A	C5-C6-N1	-5.34	115.03	117.70
1	AA	985	C	N3-C4-C5	-5.34	119.77	121.90
1	AA	1342	C	N3-C4-N4	5.34	121.73	118.00
1	AA	1369	C	N3-C4-C5	-5.34	119.77	121.90
27	B8	161	A	C5-C6-N1	-5.34	115.03	117.70
27	B8	942	G	O4'-C1'-N9	5.34	112.47	108.20
27	B8	1232	G	O4'-C1'-N9	5.34	112.47	108.20
27	B8	1789	A	C5-C6-N1	-5.34	115.03	117.70
27	B8	1870	C	N3-C4-C5	-5.34	119.77	121.90
27	B8	2095	A	C5-C6-N1	-5.34	115.03	117.70
27	B8	2497	A	C5-C6-N6	-5.34	119.43	123.70
27	B8	2507	C	N3-C4-C5	-5.34	119.77	121.90
27	B8	2610	C	N3-C4-C5	-5.34	119.77	121.90
27	B8	2699	C	N3-C4-C5	-5.34	119.77	121.90
1	AA	167	A	C5-C6-N1	-5.33	115.03	117.70
1	AA	1329	A	C5-C6-N1	-5.33	115.03	117.70
27	B8	340	A	C5-C6-N6	-5.33	119.43	123.70
27	B8	2406	A	C5-C6-N1	-5.33	115.03	117.70
27	B8	2814	A	C5-C6-N1	-5.33	115.03	117.70
1	AA	1396	A	C4-C5-C6	5.33	119.67	117.00
1	AA	1510	C	N3-C4-N4	5.33	121.73	118.00
27	B8	717	C	N3-C4-C5	-5.33	119.77	121.90
27	B8	948	C	N3-C4-C5	-5.33	119.77	121.90
27	B8	1204	A	C5-C6-N1	-5.33	115.03	117.70
27	B8	2124	G	O4'-C1'-N9	5.33	112.47	108.20
27	B8	2469	A	C5-C6-N6	-5.33	119.43	123.70
27	B8	2534	A	C5-C6-N6	-5.33	119.43	123.70
1	AA	18	C	N3-C4-C5	-5.33	119.77	121.90
1	AA	309	A	C5-C6-N1	-5.33	115.03	117.70
1	AA	321	A	C5-C6-N6	-5.33	119.44	123.70
1	AA	344	A	C5-C6-N1	-5.33	115.03	117.70
1	AA	595	A	C5-C6-N1	-5.33	115.03	117.70
1	AA	781	A	C5-C6-N6	-5.33	119.44	123.70
27	B8	490	C	N3-C4-C5	-5.33	119.77	121.90
27	B8	778	G	O4'-C1'-N9	5.33	112.47	108.20
27	B8	1273	U	O4'-C1'-N1	5.33	112.47	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	1314	C	N3-C4-C5	-5.33	119.77	121.90
27	B8	1518	C	N3-C4-C5	-5.33	119.77	121.90
27	B8	2394	C	N3-C4-N4	5.33	121.73	118.00
27	B8	2602	A	C5-C6-N1	-5.33	115.03	117.70
3	AV	11	C	N3-C4-C5	-5.33	119.77	121.90
27	B8	968	C	N3-C4-C5	-5.33	119.77	121.90
27	B8	1040	A	C5-C6-N6	-5.33	119.44	123.70
27	B8	1616	A	C5-C6-N1	-5.33	115.03	117.70
27	B8	2161	C	N3-C4-N4	5.33	121.73	118.00
1	AA	214	C	N3-C4-C5	-5.33	119.77	121.90
1	AA	958	A	C5-C6-N6	-5.33	119.44	123.70
27	B8	203	A	C5-C6-N1	-5.33	115.04	117.70
27	B8	251	A	C5-C6-N6	-5.33	119.44	123.70
27	B8	487	C	N3-C4-C5	-5.33	119.77	121.90
27	B8	501	A	C5-C6-N1	-5.33	115.04	117.70
27	B8	1103	A	C5-C6-N1	-5.33	115.04	117.70
27	B8	1322	A	C5-C6-N6	-5.33	119.44	123.70
27	B8	1570	A	O4'-C1'-N9	5.33	112.46	108.20
27	B8	1611	C	N3-C4-N4	5.33	121.73	118.00
27	B8	1679	A	C5-C6-N1	-5.33	115.03	117.70
1	AA	787	A	C5-C6-N1	-5.33	115.04	117.70
1	AA	1021	A	C5-C6-N1	-5.33	115.04	117.70
1	AA	1384	C	N3-C4-C5	-5.33	119.77	121.90
27	B8	213	A	O4'-C1'-N9	5.33	112.46	108.20
27	B8	536	G	O4'-C1'-N9	5.33	112.46	108.20
27	B8	1069	A	C5-C6-N1	-5.33	115.04	117.70
27	B8	1342	A	C5-C6-N1	-5.33	115.04	117.70
27	B8	2478	A	C5-C6-N1	-5.33	115.04	117.70
1	AA	228	A	C5-C6-N1	-5.33	115.04	117.70
1	AA	1507	A	C5-C6-N1	-5.33	115.04	117.70
1	AA	1519	A	C5-C6-N1	-5.33	115.04	117.70
3	AV	57	C	N3-C4-C5	-5.33	119.77	121.90
27	B8	278	A	O4'-C1'-N9	5.33	112.46	108.20
27	B8	354	A	C5-C6-N6	-5.33	119.44	123.70
27	B8	1941	C	N3-C4-C5	-5.33	119.77	121.90
27	B8	2513	A	O4'-C1'-N9	5.33	112.46	108.20
27	B8	2547	A	C5-C6-N6	-5.33	119.44	123.70
1	AA	382	A	C5-C6-N1	-5.32	115.04	117.70
1	AA	624	C	N3-C4-C5	-5.32	119.77	121.90
1	AA	627	G	O4'-C1'-N9	5.32	112.46	108.20
1	AA	934	C	N3-C4-N4	5.32	121.73	118.00
1	AA	975	A	C5-C6-N1	-5.32	115.04	117.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1260	G	N3-C2-N2	5.32	123.63	119.90
27	B8	63	A	C5-C6-N6	-5.32	119.44	123.70
27	B8	213	A	C5-C6-N1	-5.32	115.04	117.70
27	B8	685	A	C5-C6-N1	-5.32	115.04	117.70
27	B8	751	A	O4'-C1'-N9	5.32	112.46	108.20
27	B8	1147	A	C5-C6-N6	-5.32	119.44	123.70
27	B8	1553	A	O4'-C1'-N9	5.32	112.46	108.20
27	B8	1629	U	O4'-C1'-N1	5.32	112.46	108.20
27	B8	1998	A	C5-C6-N1	-5.32	115.04	117.70
27	B8	2553	G	O4'-C1'-N9	5.32	112.46	108.20
27	B8	1461	C	N3-C4-N4	5.32	121.72	118.00
1	AA	889	A	C5-C6-N1	-5.32	115.04	117.70
1	AA	1293	C	N3-C4-C5	-5.32	119.77	121.90
27	B8	126	A	C5-C6-N6	-5.32	119.44	123.70
27	B8	527	C	C2-N1-C1'	5.32	124.65	118.80
27	B8	1328	A	C5-C6-N1	-5.32	115.04	117.70
27	B8	1727	C	N3-C4-C5	-5.32	119.77	121.90
27	B8	891	G	C5'-C4'-O4'	5.32	115.48	109.10
1	AA	34	C	N3-C4-C5	-5.32	119.77	121.90
1	AA	499	A	C5-C6-N1	-5.32	115.04	117.70
1	AA	546	A	C5-C6-N1	-5.32	115.04	117.70
1	AA	1327	C	N3-C4-C5	-5.32	119.77	121.90
27	B8	28	A	C5-C6-N1	-5.32	115.04	117.70
27	B8	616	A	O4'-C1'-N9	5.32	112.45	108.20
27	B8	1204	A	O4'-C1'-N9	5.32	112.45	108.20
27	B8	1853	A	C5-C6-N6	-5.32	119.45	123.70
27	B8	1947	C	N3-C4-C5	-5.32	119.77	121.90
27	B8	2309	A	C5-C6-N1	-5.32	115.04	117.70
27	B8	2520	C	N3-C4-N4	5.32	121.72	118.00
1	AA	585	G	O4'-C1'-N9	5.32	112.45	108.20
1	AA	815	A	O4'-C1'-N9	5.32	112.45	108.20
27	B8	11	C	N3-C4-N4	5.32	121.72	118.00
27	B8	104	A	C5-C6-N1	-5.32	115.04	117.70
27	B8	613	A	C5-C6-N6	-5.32	119.45	123.70
27	B8	1509	A	C5-C6-N1	-5.32	115.04	117.70
27	B8	2662	A	O4'-C1'-N9	5.32	112.45	108.20
27	B8	2682	A	C5-C6-N1	-5.32	115.04	117.70
1	AA	1274	A	C5-C6-N1	-5.31	115.04	117.70
1	AA	1518	A	C5-C6-N6	-5.31	119.45	123.70
27	B8	1067	A	C5-C6-N1	-5.31	115.04	117.70
27	B8	1514	G	O4'-C1'-N9	5.31	112.45	108.20
27	B8	1853	A	C4-C5-C6	5.31	119.66	117.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	338	A	C5-C6-N6	-5.31	119.45	123.70
1	AA	702	A	O4'-C1'-N9	5.31	112.45	108.20
1	AA	1288	A	C5-C6-N1	-5.31	115.04	117.70
1	AA	1399	C	N3-C4-C5	-5.31	119.78	121.90
27	B8	2270	A	C5-C6-N6	-5.31	119.45	123.70
27	B8	2651	C	N3-C4-C5	-5.31	119.78	121.90
1	AA	54	C	N3-C4-N4	5.31	121.72	118.00
1	AA	1069	C	N3-C4-C5	-5.31	119.78	121.90
2	AX	20	G	O4'-C1'-N9	5.31	112.45	108.20
27	B8	252	G	O4'-C1'-N9	5.31	112.45	108.20
27	B8	1156	A	C5-C6-N1	-5.31	115.05	117.70
27	B8	1606	C	N3-C4-C5	-5.31	119.78	121.90
27	B8	2380	C	N3-C4-C5	-5.31	119.78	121.90
27	B8	2427	C	N3-C4-N4	5.31	121.72	118.00
1	AA	395	C	N3-C4-C5	-5.31	119.78	121.90
1	AA	844	G	C5'-C4'-O4'	5.31	115.47	109.10
1	AA	1117	A	C5-C6-N1	-5.31	115.05	117.70
1	AA	1332	A	C5-C6-N6	-5.31	119.45	123.70
27	B8	106	C	N3-C4-N4	5.31	121.72	118.00
27	B8	322	A	O4'-C1'-N9	5.31	112.45	108.20
27	B8	1125	G	N3-C2-N2	5.31	123.62	119.90
27	B8	1428	C	N3-C4-N4	5.31	121.72	118.00
27	B8	1792	G	O4'-C1'-N9	5.31	112.45	108.20
1	AA	1238	A	C4-C5-C6	5.31	119.65	117.00
27	B8	74	A	C5-C6-N6	-5.31	119.45	123.70
27	B8	238	C	N3-C4-C5	-5.31	119.78	121.90
27	B8	1009	A	C5-C6-N1	-5.31	115.05	117.70
27	B8	1270	C	N3-C4-C5	-5.31	119.78	121.90
27	B8	2239	G	O4'-C1'-N9	5.31	112.45	108.20
27	B8	2273	A	C5-C6-N1	-5.31	115.05	117.70
1	AA	135	C	N3-C4-C5	-5.31	119.78	121.90
1	AA	1427	C	N3-C4-C5	-5.31	119.78	121.90
27	B8	74	A	C5-C6-N1	-5.31	115.05	117.70
27	B8	512	G	O4'-C1'-N9	5.31	112.44	108.20
27	B8	713	G	N3-C2-N2	5.31	123.61	119.90
27	B8	715	A	C5-C6-N1	-5.31	115.05	117.70
27	B8	748	G	O4'-C1'-N9	5.31	112.44	108.20
27	B8	960	A	C5-C6-N1	-5.31	115.05	117.70
27	B8	1822	C	N3-C4-C5	-5.31	119.78	121.90
27	B8	2376	A	C5-C6-N1	-5.31	115.05	117.70
27	B8	2577	A	C5-C6-N6	-5.31	119.45	123.70
1	AA	78	A	C5-C6-N6	-5.30	119.46	123.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	99	C	N3-C4-N4	5.30	121.71	118.00
1	AA	637	C	N3-C4-C5	-5.30	119.78	121.90
1	AA	701	U	O4'-C1'-N1	5.30	112.44	108.20
1	AA	1429	A	C5-C6-N1	-5.30	115.05	117.70
26	B7	88	C	N3-C4-N4	5.30	121.71	118.00
27	B8	361	G	N3-C2-N2	5.30	123.61	119.90
27	B8	445	C	N3-C4-C5	-5.30	119.78	121.90
27	B8	829	A	C5-C6-N1	-5.30	115.05	117.70
27	B8	961	C	N3-C4-C5	-5.30	119.78	121.90
27	B8	1365	A	C5-C6-N1	-5.30	115.05	117.70
27	B8	1800	C	O4'-C1'-N1	5.30	112.44	108.20
27	B8	2501	C	N3-C4-N4	5.30	121.71	118.00
27	B8	2763	G	N3-C2-N2	5.30	123.61	119.90
28	BA	217	PHE	CB-CG-CD2	-5.30	117.09	120.80
1	AA	422	C	N3-C4-N4	5.30	121.71	118.00
1	AA	845	A	C5-C6-N1	-5.30	115.05	117.70
1	AA	55	A	C5-C6-N1	-5.30	115.05	117.70
1	AA	136	C	N3-C4-C5	-5.30	119.78	121.90
1	AA	242	G	O4'-C1'-N9	5.30	112.44	108.20
3	AV	72	C	N3-C4-N4	5.30	121.71	118.00
27	B8	52	A	O4'-C1'-N9	5.30	112.44	108.20
27	B8	94	A	C5-C6-N1	-5.30	115.05	117.70
27	B8	208	C	N3-C4-C5	-5.30	119.78	121.90
27	B8	2084	C	N3-C4-C5	-5.30	119.78	121.90
27	B8	2129	C	N3-C4-C5	-5.30	119.78	121.90
27	B8	2282	G	C2'-C3'-O3'	5.30	122.18	113.70
27	B8	2726	A	C5-C6-N1	-5.30	115.05	117.70
1	AA	3	A	C5-C6-N1	-5.30	115.05	117.70
1	AA	65	A	C5-C6-N1	-5.30	115.05	117.70
1	AA	432	A	C5-C6-N6	-5.30	119.46	123.70
1	AA	1404	C	N3-C4-C5	-5.30	119.78	121.90
3	AV	58	A	O4'-C1'-N9	5.30	112.44	108.20
26	B7	4	C	N3-C4-N4	5.30	121.71	118.00
27	B8	127	A	C5'-C4'-C3'	-5.30	107.52	116.00
27	B8	191	A	C5-C6-N6	-5.30	119.46	123.70
27	B8	398	C	N3-C4-N4	5.30	121.71	118.00
27	B8	614	A	C5-C6-N1	-5.30	115.05	117.70
27	B8	1243	C	N3-C4-C5	-5.30	119.78	121.90
27	B8	1376	C	N3-C4-N4	5.30	121.71	118.00
27	B8	1744	A	C5-C6-N6	-5.30	119.46	123.70
27	B8	1960	A	C5-C6-N6	-5.30	119.46	123.70
27	B8	2420	C	N3-C4-C5	-5.30	119.78	121.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	856	C	N3-C4-N4	5.30	121.71	118.00
1	AA	1152	A	O4'-C1'-N9	5.30	112.44	108.20
27	B8	264	C	N3-C4-C5	-5.30	119.78	121.90
27	B8	368	A	O4'-C1'-N9	5.30	112.44	108.20
27	B8	527	C	N3-C4-N4	5.30	121.71	118.00
27	B8	1575	C	N3-C4-N4	5.30	121.71	118.00
27	B8	172	A	C5-C6-N1	-5.30	115.05	117.70
27	B8	555	G	N3-C2-N2	5.30	123.61	119.90
27	B8	846	U	C2-N1-C1'	5.30	124.06	117.70
27	B8	1133	A	C5-C6-N6	-5.30	119.46	123.70
27	B8	1254	A	C5-C6-N6	-5.30	119.46	123.70
27	B8	1698	A	C5-C6-N1	-5.30	115.05	117.70
27	B8	2095	A	C5-C6-N6	-5.30	119.46	123.70
27	B8	2338	C	N3-C4-N4	5.30	121.71	118.00
27	B8	2840	C	N3-C4-C5	-5.30	119.78	121.90
1	AA	1102	A	O4'-C1'-N9	5.29	112.44	108.20
1	AA	1188	A	C5-C6-N1	-5.29	115.05	117.70
27	B8	11	C	N3-C4-C5	-5.29	119.78	121.90
1	AA	40	C	N3-C4-C5	-5.29	119.78	121.90
1	AA	160	A	C5-C6-N6	-5.29	119.47	123.70
1	AA	685	G	O4'-C1'-N9	5.29	112.44	108.20
3	AV	3	G	O4'-C1'-N9	5.29	112.43	108.20
26	B7	44	G	O4'-C1'-N9	5.29	112.44	108.20
27	B8	546	U	O4'-C1'-N1	5.29	112.44	108.20
27	B8	697	G	O4'-C1'-N9	5.29	112.44	108.20
27	B8	1616	A	C5-C6-N6	-5.29	119.47	123.70
27	B8	1760	C	N3-C4-C5	-5.29	119.78	121.90
27	B8	1965	C	N3-C4-C5	-5.29	119.78	121.90
27	B8	2395	C	N3-C4-C5	-5.29	119.78	121.90
27	B8	2440	C	N3-C4-N4	5.29	121.71	118.00
1	AA	72	A	C5-C6-N6	-5.29	119.47	123.70
1	AA	101	A	C5-C6-N1	-5.29	115.05	117.70
1	AA	158	G	O4'-C1'-N9	5.29	112.43	108.20
1	AA	572	A	C5-C6-N6	-5.29	119.47	123.70
1	AA	607	A	C5-C6-N1	-5.29	115.05	117.70
1	AA	675	A	C5-C6-N1	-5.29	115.05	117.70
1	AA	1167	A	C5-C6-N1	-5.29	115.06	117.70
1	AA	1410	A	C5-C6-N6	-5.29	119.47	123.70
1	AA	1535	C	N3-C4-C5	-5.29	119.78	121.90
27	B8	308	G	O4'-C1'-N9	5.29	112.43	108.20
27	B8	352	A	C5-C6-N1	-5.29	115.05	117.70
27	B8	1939	U	O4'-C1'-N1	5.29	112.43	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	2078	C	N3-C4-C5	-5.29	119.78	121.90
27	B8	2821	A	O4'-C1'-N9	5.29	112.43	108.20
27	B8	2853	C	N3-C4-C5	-5.29	119.78	121.90
1	AA	1109	C	N3-C4-C5	-5.29	119.78	121.90
1	AA	1531	A	C5-C6-N6	-5.29	119.47	123.70
27	B8	137	U	P-O5'-C5'	5.29	129.36	120.90
27	B8	1701	A	C5-C6-N6	-5.29	119.47	123.70
1	AA	576	C	N3-C4-C5	-5.29	119.78	121.90
1	AA	1270	G	O4'-C1'-N9	5.29	112.43	108.20
1	AA	1342	C	N3-C4-C5	-5.29	119.78	121.90
27	B8	342	A	O4'-C1'-N9	5.29	112.43	108.20
27	B8	1057	A	C5-C6-N1	-5.29	115.06	117.70
27	B8	1146	C	N3-C4-N4	5.29	121.70	118.00
27	B8	1176	U	O4'-C1'-N1	5.29	112.43	108.20
27	B8	1213	A	C5-C6-N6	-5.29	119.47	123.70
27	B8	1489	C	N3-C4-N4	5.29	121.70	118.00
27	B8	2425	A	O4'-C1'-N9	5.29	112.43	108.20
27	B8	2426	A	C5-C6-N1	-5.29	115.06	117.70
1	AA	676	A	C5-C6-N6	-5.29	119.47	123.70
1	AA	1360	A	O4'-C1'-N9	5.29	112.43	108.20
27	B8	897	C	N3-C4-C5	-5.29	119.78	121.90
27	B8	1395	A	O4'-C1'-N9	5.29	112.43	108.20
27	B8	1710	G	O4'-C1'-N9	5.29	112.43	108.20
27	B8	2287	A	C5-C6-N6	-5.29	119.47	123.70
1	AA	415	A	C5-C6-N6	-5.29	119.47	123.70
3	AV	58	A	C5-C6-N1	-5.29	115.06	117.70
27	B8	32	C	N3-C4-C5	-5.29	119.79	121.90
27	B8	1303	G	O4'-C1'-N9	5.29	112.43	108.20
27	B8	1504	A	C5-C6-N6	-5.29	119.47	123.70
27	B8	1942	C	N3-C4-N4	5.29	121.70	118.00
27	B8	2267	A	C5-C6-N1	-5.29	115.06	117.70
27	B8	2628	C	N3-C4-C5	-5.29	119.79	121.90
1	AA	523	A	C5-C6-N1	-5.28	115.06	117.70
27	B8	751	A	C5-C6-N6	-5.28	119.47	123.70
27	B8	1067	A	C5-C6-N6	-5.28	119.47	123.70
27	B8	1322	A	C4-C5-C6	5.28	119.64	117.00
27	B8	1803	A	O4'-C1'-N9	5.28	112.43	108.20
27	B8	2090	A	C5-C6-N1	-5.28	115.06	117.70
1	AA	461	A	C5-C6-N1	-5.28	115.06	117.70
27	B8	579	G	O4'-C1'-N9	5.28	112.43	108.20
1	AA	238	A	C5-C6-N1	-5.28	115.06	117.70
1	AA	466	A	C5-C6-N1	-5.28	115.06	117.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	946	A	C5-C6-N6	-5.28	119.47	123.70
27	B8	118	A	C5-C6-N6	-5.28	119.48	123.70
27	B8	309	A	C5-C6-N1	-5.28	115.06	117.70
27	B8	354	A	O4'-C1'-N9	5.28	112.42	108.20
27	B8	750	A	O4'-C1'-N9	5.28	112.42	108.20
27	B8	1271	G	O4'-C1'-N9	5.28	112.42	108.20
27	B8	1381	G	O4'-C1'-N9	5.28	112.42	108.20
27	B8	2468	A	O4'-C1'-N9	5.28	112.42	108.20
27	B8	2619	C	N3-C4-C5	-5.28	119.79	121.90
27	B8	2652	C	N3-C4-N4	5.28	121.70	118.00
27	B8	2823	A	O4'-C1'-N9	5.28	112.42	108.20
1	AA	609	A	C5-C6-N1	-5.28	115.06	117.70
1	AA	1012	A	C4-C5-C6	5.28	119.64	117.00
1	AA	51	A	C5-C6-N6	-5.28	119.48	123.70
1	AA	235	C	N3-C4-C5	-5.28	119.79	121.90
1	AA	1216	A	C5-C6-N6	-5.28	119.48	123.70
1	AA	1402	C	N3-C4-N4	5.28	121.69	118.00
26	B7	57	A	C5-C6-N6	-5.28	119.48	123.70
27	B8	504	A	C5-C6-N1	-5.28	115.06	117.70
27	B8	1212	G	N3-C2-N2	5.28	123.59	119.90
27	B8	1602	U	O4'-C1'-N1	5.28	112.42	108.20
27	B8	1730	C	N3-C4-C5	-5.28	119.79	121.90
27	B8	2019	A	O4'-C1'-N9	5.28	112.42	108.20
27	B8	2164	C	N3-C4-C5	-5.28	119.79	121.90
27	B8	2890	G	O4'-C1'-N9	5.28	112.42	108.20
1	AA	704	A	O4'-C1'-N9	5.28	112.42	108.20
1	AA	1359	C	N3-C4-C5	-5.28	119.79	121.90
2	AX	21	A	C5-C6-N1	-5.28	115.06	117.70
27	B8	660	C	N3-C4-C5	-5.28	119.79	121.90
1	AA	162	A	C8-N9-C4	-5.27	103.69	105.80
1	AA	410	G	C5-C6-O6	-5.27	125.44	128.60
27	B8	357	C	N3-C4-C5	-5.27	119.79	121.90
27	B8	1790	C	N3-C4-C5	-5.27	119.79	121.90
27	B8	2849	U	O4'-C1'-N1	5.27	112.42	108.20
1	AA	74	A	C5-C6-N6	-5.27	119.48	123.70
1	AA	149	A	C5-C6-N1	-5.27	115.06	117.70
1	AA	382	A	C5-C6-N6	-5.27	119.48	123.70
1	AA	736	C	N3-C4-C5	-5.27	119.79	121.90
1	AA	825	A	C5-C6-N1	-5.27	115.06	117.70
1	AA	1101	A	C4-C5-C6	5.27	119.64	117.00
27	B8	383	C	N3-C4-C5	-5.27	119.79	121.90
27	B8	436	C	N3-C4-C5	-5.27	119.79	121.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	508	A	C5-C6-N1	-5.27	115.06	117.70
27	B8	921	C	N3-C4-C5	-5.27	119.79	121.90
27	B8	1272	A	C5-C6-N6	-5.27	119.48	123.70
27	B8	1500	G	O4'-C1'-N9	5.27	112.42	108.20
27	B8	1983	G	O4'-C1'-N9	5.27	112.42	108.20
27	B8	2051	A	C5-C6-N1	-5.27	115.06	117.70
1	AA	580	C	N3-C4-C5	-5.27	119.79	121.90
27	B8	1924	C	N3-C4-C5	-5.27	119.79	121.90
1	AA	352	C	N3-C4-C5	-5.27	119.79	121.90
1	AA	949	A	O4'-C1'-N9	5.27	112.42	108.20
1	AA	1428	A	O4'-C1'-N9	5.27	112.42	108.20
3	AV	4	C	N3-C4-C5	-5.27	119.79	121.90
27	B8	27	G	N3-C2-N2	5.27	123.59	119.90
27	B8	41	C	N3-C4-C5	-5.27	119.79	121.90
27	B8	182	A	O4'-C1'-N9	5.27	112.42	108.20
27	B8	793	A	O4'-C1'-N9	5.27	112.42	108.20
27	B8	1103	A	C5-C6-N6	-5.27	119.48	123.70
27	B8	1968	G	O4'-C1'-N9	5.27	112.42	108.20
27	B8	2161	C	N3-C4-C5	-5.27	119.79	121.90
1	AA	373	A	C5-C6-N6	-5.27	119.49	123.70
1	AA	380	G	O4'-C1'-N9	5.27	112.41	108.20
1	AA	861	G	O4'-C1'-N9	5.27	112.41	108.20
26	B7	53	A	C5-C6-N6	-5.27	119.49	123.70
27	B8	739	A	C5-C6-N1	-5.27	115.07	117.70
27	B8	925	A	C5-C6-N6	-5.27	119.49	123.70
27	B8	959	A	O4'-C1'-N9	5.27	112.42	108.20
27	B8	1089	A	C5-C6-N6	-5.27	119.49	123.70
27	B8	1254	A	O4'-C1'-N9	5.27	112.41	108.20
27	B8	1498	C	N3-C4-C5	-5.27	119.79	121.90
27	B8	1780	A	C4-C5-C6	5.27	119.63	117.00
27	B8	2405	G	O4'-C1'-N9	5.27	112.41	108.20
27	B8	2450	A	O4'-C1'-N9	5.27	112.41	108.20
27	B8	2564	A	C5-C6-N6	-5.27	119.49	123.70
17	AM	105	ALA	N-CA-CB	5.27	117.47	110.10
27	B8	279	A	C5-C6-N1	-5.27	115.07	117.70
27	B8	2681	C	N3-C4-C5	-5.27	119.79	121.90
27	B8	2887	A	C5-C6-N1	-5.27	115.07	117.70
1	AA	47	C	N3-C4-C5	-5.26	119.80	121.90
1	AA	90	C	N3-C4-N4	5.26	121.69	118.00
1	AA	511	C	P-O3'-C3'	5.26	126.02	119.70
27	B8	270	A	O4'-C1'-N9	5.26	112.41	108.20
27	B8	514	A	C5-C6-N6	-5.26	119.49	123.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	1689	A	C5-C6-N1	-5.26	115.07	117.70
1	AA	119	A	C5-C6-N6	-5.26	119.49	123.70
1	AA	691	G	O4'-C1'-N9	5.26	112.41	108.20
1	AA	1059	C	N3-C4-C5	-5.26	119.80	121.90
27	B8	943	A	C4-C5-C6	5.26	119.63	117.00
27	B8	1032	A	C5-C6-N1	-5.26	115.07	117.70
27	B8	1810	A	O4'-C1'-N9	5.26	112.41	108.20
1	AA	1004	A	O4'-C1'-N9	5.26	112.41	108.20
1	AA	1311	A	O4'-C1'-N9	5.26	112.41	108.20
27	B8	225	C	N3-C4-N4	5.26	121.68	118.00
27	B8	241	A	C5-C6-N1	-5.26	115.07	117.70
1	AA	545	C	N3-C4-C5	-5.26	119.80	121.90
1	AA	560	A	C5-C6-N1	-5.26	115.07	117.70
1	AA	1383	C	N3-C4-C5	-5.26	119.80	121.90
1	AA	1411	C	N3-C4-C5	-5.26	119.80	121.90
26	B7	29	A	C5-C6-N1	-5.26	115.07	117.70
27	B8	386	G	O4'-C1'-N9	5.26	112.41	108.20
27	B8	631	A	C5-C6-N1	-5.26	115.07	117.70
27	B8	785	G	O4'-C1'-N9	5.26	112.41	108.20
27	B8	885	C	N3-C4-C5	-5.26	119.80	121.90
27	B8	2050	C	N3-C4-N4	5.26	121.68	118.00
27	B8	2866	U	O4'-C1'-N1	5.26	112.41	108.20
1	AA	71	A	C4-C5-C6	5.26	119.63	117.00
1	AA	1533	C	N3-C4-N4	5.26	121.68	118.00
27	B8	57	C	N3-C4-C5	-5.26	119.80	121.90
27	B8	621	A	C5-C6-N6	-5.26	119.49	123.70
27	B8	1531	C	N3-C4-C5	-5.26	119.80	121.90
27	B8	1894	C	N3-C4-C5	-5.26	119.80	121.90
27	B8	2067	G	O4'-C1'-N9	5.26	112.41	108.20
27	B8	2254	C	N3-C4-C5	-5.26	119.80	121.90
27	B8	2714	G	N3-C2-N2	5.26	123.58	119.90
1	AA	143	A	O4'-C1'-N9	5.26	112.41	108.20
1	AA	162	A	O4'-C1'-N9	5.26	112.41	108.20
1	AA	178	C	N3-C4-C5	-5.26	119.80	121.90
1	AA	274	A	C5-C6-N6	-5.26	119.50	123.70
1	AA	1196	A	C5-C6-N1	-5.26	115.07	117.70
1	AA	1429	A	C5-C6-N6	-5.26	119.49	123.70
26	B7	68	C	N3-C4-C5	-5.26	119.80	121.90
27	B8	1025	G	O4'-C1'-N9	5.26	112.41	108.20
27	B8	1276	A	C5-C6-N1	-5.26	115.07	117.70
27	B8	1669	A	C5-C6-N6	-5.26	119.50	123.70
27	B8	1678	A	C5-C6-N1	-5.26	115.07	117.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	126	A	C5-C6-N1	-5.25	115.07	117.70
27	B8	335	C	N3-C4-N4	5.25	121.68	118.00
1	AA	95	C	N3-C4-C5	-5.25	119.80	121.90
1	AA	1229	A	O4'-C1'-N9	5.25	112.40	108.20
1	AA	1250	A	C5-C6-N1	-5.25	115.07	117.70
26	B7	35	C	N3-C4-C5	-5.25	119.80	121.90
27	B8	159	G	N3-C2-N2	5.25	123.58	119.90
27	B8	1525	A	O4'-C1'-N9	5.25	112.40	108.20
27	B8	1598	A	C5-C6-N1	-5.25	115.07	117.70
27	B8	2097	A	C5-C6-N1	-5.25	115.07	117.70
27	B8	2611	C	N3-C4-C5	-5.25	119.80	121.90
27	B8	2726	A	C5-C6-N6	-5.25	119.50	123.70
27	B8	2813	A	C5-C6-N1	-5.25	115.07	117.70
27	B8	2850	A	C5-C6-N1	-5.25	115.07	117.70
1	AA	864	A	C5-C6-N6	-5.25	119.50	123.70
1	AA	1054	C	C6-N1-C1'	-5.25	114.50	120.80
1	AA	1067	A	C5-C6-N6	-5.25	119.50	123.70
1	AA	1392	G	O4'-C1'-N9	5.25	112.40	108.20
27	B8	146	A	C5-C6-N1	-5.25	115.07	117.70
27	B8	479	A	C5-C6-N6	-5.25	119.50	123.70
27	B8	687	C	N3-C4-C5	-5.25	119.80	121.90
27	B8	844	A	C5-C6-N6	-5.25	119.50	123.70
27	B8	983	A	C5-C6-N1	-5.25	115.08	117.70
27	B8	1321	A	C5-C6-N6	-5.25	119.50	123.70
27	B8	2176	A	C5-C6-N1	-5.25	115.07	117.70
27	B8	2471	A	C4-C5-C6	5.25	119.62	117.00
27	B8	2660	A	O4'-C1'-N9	5.25	112.40	108.20
27	B8	2820	A	C5-C6-N1	-5.25	115.07	117.70
1	AA	1	A	C5-C6-N1	-5.25	115.08	117.70
26	B7	45	A	C4-C5-C6	5.25	119.62	117.00
27	B8	1752	C	N3-C4-N4	5.25	121.67	118.00
1	AA	196	A	C5-C6-N1	-5.25	115.08	117.70
1	AA	345	C	O4'-C1'-N1	5.25	112.40	108.20
1	AA	554	A	C5-C6-N1	-5.25	115.08	117.70
1	AA	808	C	N3-C4-C5	-5.25	119.80	121.90
1	AA	1353	G	O4'-C1'-N9	5.25	112.40	108.20
3	AV	38	G	C5-C6-O6	-5.25	125.45	128.60
3	AV	60	A	C5-C6-N1	-5.25	115.08	117.70
27	B8	86	G	O4'-C1'-N9	5.25	112.40	108.20
27	B8	673	C	N3-C4-C5	-5.25	119.80	121.90
27	B8	793	A	C5-C6-N1	-5.25	115.08	117.70
27	B8	851	C	N3-C4-C5	-5.25	119.80	121.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	895	U	O4'-C1'-N1	5.25	112.40	108.20
27	B8	994	C	N3-C4-C5	-5.25	119.80	121.90
27	B8	1265	A	C5-C6-N6	-5.25	119.50	123.70
27	B8	1323	C	N3-C4-C5	-5.25	119.80	121.90
27	B8	1477	A	C5-C6-N6	-5.25	119.50	123.70
27	B8	1700	A	C5-C6-N1	-5.25	115.08	117.70
27	B8	1910	G	O4'-C1'-N9	5.25	112.40	108.20
27	B8	2103	C	N3-C4-C5	-5.25	119.80	121.90
27	B8	2248	C	N3-C4-C5	-5.25	119.80	121.90
27	B8	2345	G	O4'-C1'-N9	5.25	112.40	108.20
27	B8	2416	C	N3-C4-C5	-5.25	119.80	121.90
27	B8	2556	C	N3-C4-C5	-5.25	119.80	121.90
1	AA	1284	C	O4'-C1'-N1	5.25	112.40	108.20
1	AA	1331	G	O4'-C1'-N9	5.25	112.40	108.20
1	AA	1533	C	N3-C4-C5	-5.25	119.80	121.90
27	B8	99	U	C6-N1-C1'	-5.25	113.86	121.20
27	B8	704	G	N3-C2-N2	5.25	123.57	119.90
27	B8	1324	G	C5'-C4'-C3'	-5.25	107.61	116.00
27	B8	1630	A	C5-C6-N1	-5.25	115.08	117.70
27	B8	1632	A	C5-C6-N1	-5.25	115.08	117.70
27	B8	2590	A	O4'-C1'-N9	5.25	112.40	108.20
27	B8	2721	A	C5-C6-N1	-5.25	115.08	117.70
1	AA	53	A	C5-C6-N1	-5.25	115.08	117.70
1	AA	328	C	C6-N1-C1'	-5.25	114.51	120.80
1	AA	1267	C	N3-C4-N4	5.25	121.67	118.00
27	B8	1555	G	O4'-C1'-N9	5.25	112.40	108.20
27	B8	1580	A	C5-C6-N1	-5.25	115.08	117.70
27	B8	2515	C	N3-C4-C5	-5.25	119.80	121.90
27	B8	2587	A	C5-C6-N1	-5.25	115.08	117.70
1	AA	195	A	C5-C6-N6	-5.24	119.50	123.70
1	AA	708	C	N3-C4-C5	-5.24	119.80	121.90
1	AA	767	A	C5-C6-N1	-5.24	115.08	117.70
1	AA	918	A	O4'-C1'-N9	5.24	112.39	108.20
2	AX	14	G	O4'-C1'-N9	5.24	112.39	108.20
27	B8	418	C	N3-C4-C5	-5.24	119.80	121.90
27	B8	609	A	C5-C6-N1	-5.24	115.08	117.70
27	B8	610	C	N3-C4-C5	-5.24	119.80	121.90
27	B8	1821	A	C5-C6-N6	-5.24	119.51	123.70
1	AA	322	C	N3-C4-C5	-5.24	119.80	121.90
1	AA	574	A	C5-C6-N1	-5.24	115.08	117.70
27	B8	472	A	O4'-C1'-N9	5.24	112.39	108.20
27	B8	743	A	C5-C6-N1	-5.24	115.08	117.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	1327	A	O4'-C1'-N9	5.24	112.39	108.20
27	B8	2175	C	N3-C4-C5	-5.24	119.80	121.90
27	B8	2321	U	O4'-C1'-N1	5.24	112.39	108.20
1	AA	852	G	O4'-C1'-N9	5.24	112.39	108.20
1	AA	1320	C	N3-C4-N4	5.24	121.67	118.00
27	B8	47	C	N3-C4-C5	-5.24	119.80	121.90
27	B8	149	A	C5-C6-N1	-5.24	115.08	117.70
27	B8	444	C	N3-C4-C5	-5.24	119.80	121.90
27	B8	1256	G	O4'-C1'-N9	5.24	112.39	108.20
27	B8	1384	A	C5-C6-N1	-5.24	115.08	117.70
27	B8	1908	C	N3-C4-C5	-5.24	119.80	121.90
27	B8	2674	G	O4'-C1'-N9	5.24	112.39	108.20
27	B8	2837	A	C5-C6-N1	-5.24	115.08	117.70
1	AA	535	A	C5-C6-N6	-5.24	119.51	123.70
1	AA	680	C	N3-C4-C5	-5.24	119.81	121.90
1	AA	770	C	N3-C4-C5	-5.24	119.81	121.90
1	AA	1019	A	C5-C6-N1	-5.24	115.08	117.70
1	AA	1033	G	O4'-C1'-N9	5.24	112.39	108.20
1	AA	1105	A	C5-C6-N1	-5.24	115.08	117.70
1	AA	1257	A	C5-C6-N1	-5.24	115.08	117.70
2	AX	17	C	N3-C4-N4	5.24	121.67	118.00
27	B8	31	C	N3-C4-C5	-5.24	119.80	121.90
27	B8	1029	A	C5-C6-N6	-5.24	119.51	123.70
27	B8	1068	G	O4'-C1'-N9	5.24	112.39	108.20
27	B8	1189	A	C5-C6-N1	-5.24	115.08	117.70
27	B8	2020	A	O4'-C1'-N9	5.24	112.39	108.20
27	B8	2060	A	C5-C6-N1	-5.24	115.08	117.70
27	B8	2333	A	C5-C6-N1	-5.24	115.08	117.70
27	B8	165	A	O4'-C1'-N9	5.24	112.39	108.20
27	B8	1547	C	N3-C4-C5	-5.24	119.81	121.90
27	B8	2616	C	N3-C4-C5	-5.24	119.81	121.90
27	B8	2693	G	O4'-C1'-N9	5.24	112.39	108.20
1	AA	587	G	P-O3'-C3'	5.24	125.98	119.70
1	AA	873	A	C5-C6-N6	-5.24	119.51	123.70
1	AA	1118	U	C2-N1-C1'	5.24	123.98	117.70
27	B8	640	C	N3-C4-C5	-5.24	119.81	121.90
27	B8	1337	G	O4'-C1'-N9	5.24	112.39	108.20
27	B8	1535	A	C5-C6-N1	-5.24	115.08	117.70
27	B8	1609	A	O4'-C1'-N9	5.24	112.39	108.20
27	B8	1618	A	C5-C6-N1	-5.24	115.08	117.70
27	B8	2062	A	C5-C6-N1	-5.24	115.08	117.70
27	B8	2397	G	O4'-C1'-N9	5.24	112.39	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	60	A	C5-C6-N6	-5.23	119.51	123.70
1	AA	1172	C	N3-C4-C5	-5.23	119.81	121.90
27	B8	274	C	N3-C4-C5	-5.23	119.81	121.90
27	B8	1499	C	N3-C4-C5	-5.23	119.81	121.90
27	B8	1646	C	N3-C4-N4	5.23	121.66	118.00
28	BA	435	LYS	N-CA-CB	5.23	120.02	110.60
1	AA	415	A	O4'-C1'-N9	5.23	112.39	108.20
1	AA	622	A	C5-C6-N1	-5.23	115.08	117.70
1	AA	667	G	O4'-C1'-N9	5.23	112.39	108.20
1	AA	909	A	C5-C6-N1	-5.23	115.08	117.70
27	B8	1614	A	C5-C6-N1	-5.23	115.08	117.70
27	B8	1626	A	O4'-C1'-N9	5.23	112.39	108.20
27	B8	2114	A	C5-C6-N6	-5.23	119.51	123.70
27	B8	2153	C	N3-C4-C5	-5.23	119.81	121.90
27	B8	2211	A	C5-C6-N1	-5.23	115.08	117.70
27	B8	2391	G	O4'-C1'-N9	5.23	112.39	108.20
1	AA	964	A	C5-C6-N1	-5.23	115.08	117.70
1	AA	1217	C	N3-C4-C5	-5.23	119.81	121.90
27	B8	751	A	C5-C6-N1	-5.23	115.08	117.70
27	B8	1567	G	O4'-C1'-N9	5.23	112.38	108.20
27	B8	2418	A	C5-C6-N6	-5.23	119.52	123.70
1	AA	98	A	C5-C6-N1	-5.23	115.09	117.70
1	AA	1443	C	N3-C4-C5	-5.23	119.81	121.90
27	B8	129	C	N3-C4-C5	-5.23	119.81	121.90
27	B8	143	C	N3-C4-C5	-5.23	119.81	121.90
27	B8	145	C	N3-C4-C5	-5.23	119.81	121.90
27	B8	422	A	O4'-C1'-N9	5.23	112.38	108.20
27	B8	1152	C	N3-C4-C5	-5.23	119.81	121.90
27	B8	1536	C	N3-C4-N4	5.23	121.66	118.00
27	B8	2738	A	C5-C6-N6	-5.23	119.52	123.70
27	B8	53	A	C5-C6-N1	-5.23	115.09	117.70
27	B8	199	A	C4-C5-C6	5.23	119.61	117.00
27	B8	1428	C	N3-C4-C5	-5.23	119.81	121.90
27	B8	2563	U	O4'-C1'-N1	5.23	112.38	108.20
27	B8	2639	A	C5-C6-N6	-5.23	119.52	123.70
1	AA	800	G	O4'-C1'-N9	5.22	112.38	108.20
1	AA	1254	A	C5-C6-N6	-5.22	119.52	123.70
3	AV	22	A	C5-C6-N1	-5.22	115.09	117.70
3	AV	28	C	N3-C4-C5	-5.22	119.81	121.90
3	AV	60	A	C5-C6-N6	-5.22	119.52	123.70
27	B8	655	A	C5-C6-N1	-5.22	115.09	117.70
27	B8	896	A	C5-C6-N1	-5.22	115.09	117.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	1021	A	C5-C6-N6	-5.22	119.52	123.70
27	B8	1463	C	N3-C4-C5	-5.22	119.81	121.90
27	B8	1788	C	N3-C4-C5	-5.22	119.81	121.90
1	AA	414	A	C5-C6-N1	-5.22	115.09	117.70
1	AA	918	A	C5-C6-N1	-5.22	115.09	117.70
1	AA	1082	A	C5-C6-N6	-5.22	119.52	123.70
1	AA	1150	A	C5-C6-N1	-5.22	115.09	117.70
27	B8	241	A	O4'-C1'-N9	5.22	112.38	108.20
27	B8	518	G	O4'-C1'-N9	5.22	112.38	108.20
27	B8	2160	C	N3-C4-C5	-5.22	119.81	121.90
1	AA	7	A	C5-C6-N1	-5.22	115.09	117.70
1	AA	223	A	O4'-C1'-N9	5.22	112.38	108.20
1	AA	1012	A	C5-C6-N6	-5.22	119.52	123.70
1	AA	1154	G	O4'-C1'-N9	5.22	112.38	108.20
27	B8	706	A	C5-C6-N1	-5.22	115.09	117.70
27	B8	1118	C	N3-C4-C5	-5.22	119.81	121.90
27	B8	1285	A	C5-C6-N1	-5.22	115.09	117.70
1	AA	132	C	N3-C4-C5	-5.22	119.81	121.90
1	AA	308	C	N3-C4-C5	-5.22	119.81	121.90
26	B7	90	C	N3-C4-C5	-5.22	119.81	121.90
27	B8	144	A	C5-C6-N6	-5.22	119.52	123.70
27	B8	344	A	C5-C6-N1	-5.22	115.09	117.70
27	B8	1257	C	N3-C4-C5	-5.22	119.81	121.90
27	B8	1315	C	N3-C4-C5	-5.22	119.81	121.90
27	B8	1512	C	N3-C4-C5	-5.22	119.81	121.90
27	B8	2590	A	C5-C6-N6	-5.22	119.53	123.70
27	B8	2675	A	C5-C6-N6	-5.22	119.53	123.70
1	AA	1447	A	C5-C6-N6	-5.22	119.53	123.70
27	B8	320	A	C5-C6-N1	-5.22	115.09	117.70
27	B8	1049	C	N3-C4-C5	-5.22	119.81	121.90
1	AA	349	A	C5-C6-N6	-5.22	119.53	123.70
1	AA	825	A	C5-C6-N6	-5.22	119.53	123.70
1	AA	1269	A	C5-C6-N1	-5.22	115.09	117.70
27	B8	219	A	C5-C6-N1	-5.22	115.09	117.70
27	B8	270	A	C5-C6-N1	-5.22	115.09	117.70
27	B8	278	A	C5-C6-N6	-5.22	119.53	123.70
27	B8	609	A	O4'-C1'-N9	5.22	112.37	108.20
27	B8	613	A	O4'-C1'-N9	5.22	112.37	108.20
27	B8	1460	U	C2-N1-C1'	5.22	123.96	117.70
27	B8	2060	A	C5-C6-N6	-5.22	119.53	123.70
1	AA	936	C	N3-C4-C5	-5.21	119.81	121.90
27	B8	156	A	C5-C6-N1	-5.21	115.09	117.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	590	A	C5-C6-N1	-5.21	115.09	117.70
27	B8	721	A	C5-C6-N6	-5.21	119.53	123.70
27	B8	854	C	N3-C4-C5	-5.21	119.81	121.90
27	B8	1401	G	O4'-C1'-N9	5.21	112.37	108.20
27	B8	1717	A	C5-C6-N6	-5.21	119.53	123.70
27	B8	1726	C	N3-C4-C5	-5.21	119.81	121.90
32	BD	156	PHE	CB-CG-CD1	5.21	124.45	120.80
1	AA	1409	C	N3-C4-N4	5.21	121.65	118.00
1	AA	215	C	N3-C4-N4	5.21	121.65	118.00
1	AA	498	A	C5-C6-N1	-5.21	115.09	117.70
1	AA	569	C	N3-C4-C5	-5.21	119.81	121.90
1	AA	702	A	C5-C6-N6	-5.21	119.53	123.70
1	AA	1132	C	N3-C4-N4	5.21	121.65	118.00
1	AA	1286	U	O4'-C1'-N1	5.21	112.37	108.20
1	AA	1350	A	O4'-C1'-N9	5.21	112.37	108.20
27	B8	275	C	N3-C4-N4	5.21	121.65	118.00
27	B8	547	A	C5-C6-N1	-5.21	115.09	117.70
27	B8	990	A	C5-C6-N6	-5.21	119.53	123.70
27	B8	1085	A	O4'-C1'-N9	5.21	112.37	108.20
27	B8	1544	A	C5-C6-N1	-5.21	115.09	117.70
27	B8	1609	A	C5-C6-N1	-5.21	115.09	117.70
27	B8	2198	A	C5-C6-N1	-5.21	115.09	117.70
1	AA	1344	C	N3-C4-C5	-5.21	119.82	121.90
26	B7	78	A	C4-C5-C6	5.21	119.61	117.00
27	B8	223	A	C5-C6-N1	-5.21	115.09	117.70
27	B8	497	A	O4'-C1'-N9	5.21	112.37	108.20
27	B8	917	A	C5-C6-N6	-5.21	119.53	123.70
1	AA	288	A	O4'-C1'-N9	5.21	112.37	108.20
1	AA	631	C	N3-C4-C5	-5.21	119.82	121.90
1	AA	998	C	N3-C4-N4	5.21	121.64	118.00
1	AA	1336	C	N3-C4-C5	-5.21	119.82	121.90
27	B8	1070	A	C5-C6-N1	-5.21	115.09	117.70
27	B8	1145	C	N3-C4-C5	-5.21	119.82	121.90
27	B8	1960	A	O4'-C1'-N9	5.21	112.37	108.20
1	AA	48	C	N3-C4-C5	-5.21	119.82	121.90
1	AA	1042	A	C5-C6-N1	-5.21	115.10	117.70
1	AA	1462	C	N3-C4-C5	-5.21	119.82	121.90
27	B8	879	G	O4'-C1'-N9	5.21	112.37	108.20
27	B8	913	U	O4'-C1'-N1	5.21	112.37	108.20
27	B8	945	A	C5-C6-N1	-5.21	115.10	117.70
27	B8	957	C	N3-C4-C5	-5.21	119.82	121.90
27	B8	1293	C	N3-C4-C5	-5.21	119.82	121.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	1650	A	C5-C6-N1	-5.21	115.10	117.70
27	B8	2608	G	O4'-C1'-N9	5.21	112.36	108.20
27	B8	2892	G	O4'-C1'-N9	5.21	112.36	108.20
1	AA	858	G	O4'-C1'-N9	5.21	112.36	108.20
1	AA	1482	G	N3-C2-N2	5.21	123.54	119.90
27	B8	1912	A	C5-C6-N6	-5.21	119.54	123.70
27	B8	2503	A	O4'-C1'-N9	5.21	112.36	108.20
1	AA	33	A	C5-C6-N1	-5.20	115.10	117.70
1	AA	787	A	C4-C5-C6	5.20	119.60	117.00
1	AA	792	A	C5-C6-N1	-5.20	115.10	117.70
1	AA	1099	G	O4'-C1'-N9	5.20	112.36	108.20
1	AA	1253	G	O4'-C1'-N9	5.20	112.36	108.20
27	B8	440	C	N3-C4-C5	-5.20	119.82	121.90
27	B8	730	A	C5-C6-N1	-5.20	115.10	117.70
27	B8	1729	U	O4'-C1'-N1	5.20	112.36	108.20
1	AA	728	A	C5-C6-N1	-5.20	115.10	117.70
1	AA	878	A	O4'-C1'-N9	5.20	112.36	108.20
3	AV	72	C	N3-C4-C5	-5.20	119.82	121.90
26	B7	43	C	N3-C4-C5	-5.20	119.82	121.90
27	B8	165	A	C5-C6-N6	-5.20	119.54	123.70
27	B8	332	A	P-O3'-C3'	5.20	125.94	119.70
27	B8	347	A	C5-C6-N1	-5.20	115.10	117.70
27	B8	976	G	O4'-C1'-N9	5.20	112.36	108.20
27	B8	1189	A	C5-C6-N6	-5.20	119.54	123.70
27	B8	1850	G	O4'-C1'-N9	5.20	112.36	108.20
27	B8	2532	G	O4'-C1'-N9	5.20	112.36	108.20
27	B8	2856	A	C5-C6-N1	-5.20	115.10	117.70
1	AA	553	A	O4'-C1'-N9	5.20	112.36	108.20
1	AA	864	A	C5-C6-N1	-5.20	115.10	117.70
1	AA	1158	C	N3-C4-N4	5.20	121.64	118.00
1	AA	1338	G	C4-N9-C1'	5.20	133.26	126.50
27	B8	1362	C	N3-C4-C5	-5.20	119.82	121.90
27	B8	1569	A	C5-C6-N1	-5.20	115.10	117.70
27	B8	2480	C	N3-C4-C5	-5.20	119.82	121.90
1	AA	1314	C	N3-C4-C5	-5.20	119.82	121.90
26	B7	23	G	O4'-C1'-N9	5.20	112.36	108.20
27	B8	331	C	N3-C4-C5	-5.20	119.82	121.90
27	B8	600	G	O4'-C1'-N9	5.20	112.36	108.20
27	B8	1244	A	C5-C6-N1	-5.20	115.10	117.70
27	B8	2163	A	C5-C6-N1	-5.20	115.10	117.70
1	AA	320	A	C5-C6-N1	-5.20	115.10	117.70
1	AA	643	C	N3-C4-C5	-5.20	119.82	121.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	860	A	C5-C6-N1	-5.20	115.10	117.70
27	B8	1652	A	O4'-C1'-N9	5.20	112.36	108.20
27	B8	1854	A	C5-C6-N1	-5.20	115.10	117.70
1	AA	520	A	O4'-C1'-N9	5.20	112.36	108.20
1	AA	521	G	O4'-C1'-N9	5.20	112.36	108.20
1	AA	1375	A	C5-C6-N6	-5.20	119.54	123.70
3	AV	32	C	N3-C4-N4	5.20	121.64	118.00
27	B8	131	A	C5-C6-N6	-5.20	119.54	123.70
27	B8	531	C	N3-C4-C5	-5.20	119.82	121.90
27	B8	705	A	C5-C6-N1	-5.20	115.10	117.70
27	B8	2414	G	O4'-C1'-N9	5.20	112.36	108.20
27	B8	2639	A	C4-C5-C6	5.20	119.60	117.00
27	B8	2755	C	N3-C4-C5	-5.20	119.82	121.90
32	BD	156	PHE	CB-CG-CD2	-5.20	117.16	120.80
27	B8	401	A	C5-C6-N1	-5.19	115.10	117.70
27	B8	1034	G	O4'-C1'-N9	5.19	112.36	108.20
1	AA	687	A	P-O3'-C3'	5.19	125.93	119.70
1	AA	819	A	C5-C6-N1	-5.19	115.10	117.70
1	AA	1378	C	N3-C4-C5	-5.19	119.82	121.90
3	AV	76	C	P-O5'-C5'	5.19	129.21	120.90
27	B8	457	A	C5-C6-N1	-5.19	115.10	117.70
27	B8	661	A	C5-C6-N1	-5.19	115.10	117.70
27	B8	1147	A	C5-C6-N1	-5.19	115.10	117.70
27	B8	2350	C	N3-C4-C5	-5.19	119.82	121.90
27	B8	2815	C	N3-C4-C5	-5.19	119.82	121.90
1	AA	272	C	N3-C4-C5	-5.19	119.82	121.90
1	AA	608	A	C5-C6-N6	-5.19	119.55	123.70
1	AA	884	U	O4'-C1'-N1	5.19	112.35	108.20
27	B8	32	C	N3-C4-N4	5.19	121.63	118.00
27	B8	527	C	N3-C4-C5	-5.19	119.82	121.90
27	B8	980	A	C5-C6-N1	-5.19	115.10	117.70
27	B8	1749	A	O4'-C1'-N9	5.19	112.35	108.20
27	B8	1865	U	P-O3'-C3'	5.19	125.93	119.70
27	B8	2071	A	C5-C6-N1	-5.19	115.11	117.70
27	B8	2456	C	N3-C4-C5	-5.19	119.82	121.90
27	B8	2510	C	N3-C4-C5	-5.19	119.82	121.90
1	AA	990	C	N3-C4-C5	-5.19	119.82	121.90
27	B8	613	A	C5-C6-N1	-5.19	115.11	117.70
27	B8	1070	A	C5-C6-N6	-5.19	119.55	123.70
27	B8	1732	C	O4'-C1'-N1	5.19	112.35	108.20
27	B8	338	G	N3-C2-N2	5.19	123.53	119.90
27	B8	432	A	C5-C6-N1	-5.19	115.11	117.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	595	C	N3-C4-C5	-5.19	119.83	121.90
27	B8	640	C	N3-C4-N4	5.19	121.63	118.00
27	B8	935	C	N3-C4-C5	-5.19	119.83	121.90
27	B8	1295	C	N3-C4-C5	-5.19	119.83	121.90
27	B8	1385	A	C5-C6-N6	-5.19	119.55	123.70
27	B8	2498	C	N3-C4-C5	-5.19	119.83	121.90
27	B8	2856	A	C5-C6-N6	-5.19	119.55	123.70
1	AA	84	U	C2-N1-C1'	5.19	123.92	117.70
1	AA	1100	C	N3-C4-C5	-5.19	119.83	121.90
1	AA	1193	G	O4'-C1'-N9	5.19	112.35	108.20
27	B8	1718	G	O4'-C1'-N9	5.19	112.35	108.20
27	B8	1892	C	N3-C4-C5	-5.19	119.83	121.90
27	B8	2750	A	C5-C6-N6	-5.19	119.55	123.70
1	AA	253	A	C5-C6-N1	-5.18	115.11	117.70
27	B8	20	C	N3-C4-C5	-5.18	119.83	121.90
27	B8	1155	A	C5-C6-N1	-5.18	115.11	117.70
27	B8	2030	A	C5-C6-N1	-5.18	115.11	117.70
27	B8	2179	C	N3-C4-C5	-5.18	119.83	121.90
27	B8	2558	C	N3-C4-C5	-5.18	119.83	121.90
1	AA	315	A	C5-C6-N6	-5.18	119.56	123.70
1	AA	431	A	C5-C6-N6	-5.18	119.55	123.70
1	AA	913	A	C5-C6-N6	-5.18	119.56	123.70
1	AA	1016	A	C5-C6-N6	-5.18	119.55	123.70
1	AA	1346	A	C5-C6-N6	-5.18	119.55	123.70
1	AA	1486	G	O4'-C1'-N9	5.18	112.35	108.20
1	AA	1508	A	C5-C6-N1	-5.18	115.11	117.70
27	B8	453	A	C5-C6-N1	-5.18	115.11	117.70
27	B8	775	G	P-O3'-C3'	5.18	125.92	119.70
27	B8	796	C	N3-C4-C5	-5.18	119.83	121.90
27	B8	972	A	C5-C6-N1	-5.18	115.11	117.70
27	B8	1580	A	C5-C6-N6	-5.18	119.56	123.70
27	B8	1962	C	N3-C4-C5	-5.18	119.83	121.90
27	B8	2044	C	N3-C4-C5	-5.18	119.83	121.90
1	AA	1394	A	O4'-C1'-N9	5.18	112.34	108.20
27	B8	821	A	C5-C6-N1	-5.18	115.11	117.70
27	B8	1393	A	C5-C6-N1	-5.18	115.11	117.70
27	B8	1803	A	C5-C6-N1	-5.18	115.11	117.70
27	B8	2301	C	N3-C4-C5	-5.18	119.83	121.90
27	B8	162	U	O4'-C1'-N1	5.18	112.34	108.20
27	B8	1489	C	N3-C4-C5	-5.18	119.83	121.90
27	B8	1768	C	N3-C4-C5	-5.18	119.83	121.90
27	B8	1891	G	O4'-C1'-N9	5.18	112.34	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	1916	A	C5-C6-N6	-5.18	119.56	123.70
27	B8	2326	C	N3-C4-C5	-5.18	119.83	121.90
1	AA	759	A	N1-C6-N6	5.18	121.71	118.60
1	AA	1534	A	C5-C6-N6	-5.18	119.56	123.70
27	B8	366	C	N3-C4-C5	-5.18	119.83	121.90
27	B8	2359	C	N3-C4-C5	-5.18	119.83	121.90
3	AV	45	G	O4'-C1'-N9	5.18	112.34	108.20
27	B8	37	C	N3-C4-C5	-5.18	119.83	121.90
27	B8	276	U	C6-N1-C1'	-5.18	113.95	121.20
27	B8	990	A	O4'-C1'-N9	5.18	112.34	108.20
27	B8	1164	C	N3-C4-C5	-5.18	119.83	121.90
27	B8	1195	G	O4'-C1'-N9	5.18	112.34	108.20
27	B8	1297	C	N3-C4-C5	-5.18	119.83	121.90
27	B8	1858	A	O4'-C1'-N9	5.18	112.34	108.20
27	B8	2083	G	O4'-C1'-N9	5.18	112.34	108.20
1	AA	188	C	N3-C4-C5	-5.17	119.83	121.90
1	AA	406	G	O4'-C1'-N9	5.17	112.34	108.20
1	AA	1279	G	C4-N9-C1'	5.17	133.23	126.50
26	B7	119	A	C5-C6-N1	-5.17	115.11	117.70
27	B8	181	A	C5-C6-N1	-5.17	115.11	117.70
27	B8	239	C	N3-C4-C5	-5.17	119.83	121.90
27	B8	897	C	N3-C4-N4	5.17	121.62	118.00
27	B8	995	C	C6-N1-C1'	-5.17	114.59	120.80
27	B8	1488	C	N3-C4-C5	-5.17	119.83	121.90
27	B8	2135	A	C5-C6-N6	-5.17	119.56	123.70
27	B8	2227	A	C5-C6-N1	-5.17	115.11	117.70
27	B8	2433	A	C5-C6-N1	-5.17	115.11	117.70
27	B8	2443	C	N3-C4-C5	-5.17	119.83	121.90
1	AA	298	A	C5-C6-N1	-5.17	115.11	117.70
1	AA	1521	C	N3-C4-C5	-5.17	119.83	121.90
27	B8	1289	C	N3-C4-C5	-5.17	119.83	121.90
27	B8	2512	C	N3-C4-C5	-5.17	119.83	121.90
27	B8	2636	C	N3-C4-C5	-5.17	119.83	121.90
1	AA	1101	A	C5-C6-N6	-5.17	119.56	123.70
27	B8	61	C	N3-C4-C5	-5.17	119.83	121.90
27	B8	648	G	O4'-C1'-N9	5.17	112.34	108.20
27	B8	910	A	O4'-C1'-N9	5.17	112.34	108.20
27	B8	1345	C	N3-C4-C5	-5.17	119.83	121.90
27	B8	1527	G	O4'-C1'-N9	5.17	112.34	108.20
27	B8	1652	A	C5-C6-N1	-5.17	115.11	117.70
27	B8	2141	G	O4'-C1'-N9	5.17	112.34	108.20
27	B8	2310	C	N3-C4-N4	5.17	121.62	118.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1234	C	N3-C4-C5	-5.17	119.83	121.90
26	B7	60	C	N3-C4-C5	-5.17	119.83	121.90
27	B8	42	A	C5-C6-N6	-5.17	119.56	123.70
27	B8	66	C	N3-C4-N4	5.17	121.62	118.00
27	B8	106	C	N3-C4-C5	-5.17	119.83	121.90
27	B8	2809	A	C5-C6-N1	-5.17	115.11	117.70
1	AA	201	G	O4'-C1'-N9	5.17	112.33	108.20
1	AA	203	G	N3-C2-N2	5.17	123.52	119.90
1	AA	450	G	O4'-C1'-N9	5.17	112.33	108.20
1	AA	715	A	O4'-C1'-N9	5.17	112.33	108.20
1	AA	805	C	N3-C4-C5	-5.17	119.83	121.90
27	B8	691	C	N3-C4-C5	-5.17	119.83	121.90
27	B8	1596	A	C5-C6-N6	-5.17	119.56	123.70
27	B8	1617	C	N3-C4-C5	-5.17	119.83	121.90
27	B8	2355	G	O4'-C1'-N9	5.17	112.33	108.20
1	AA	55	A	O4'-C1'-N9	5.17	112.33	108.20
1	AA	372	C	N3-C4-N4	5.17	121.62	118.00
1	AA	547	A	C5-C6-N6	-5.17	119.57	123.70
1	AA	606	G	O4'-C1'-N9	5.17	112.33	108.20
1	AA	614	C	N3-C4-C5	-5.17	119.83	121.90
1	AA	676	A	O4'-C1'-N9	5.17	112.33	108.20
1	AA	831	A	C5-C6-N1	-5.17	115.12	117.70
1	AA	836	G	O4'-C1'-N9	5.17	112.33	108.20
1	AA	1225	A	O4'-C1'-N9	5.17	112.33	108.20
1	AA	1405	G	O4'-C1'-N9	5.17	112.33	108.20
27	B8	715	A	O4'-C1'-N9	5.17	112.33	108.20
27	B8	765	C	N3-C4-C5	-5.17	119.83	121.90
27	B8	898	C	N3-C4-N4	5.17	121.62	118.00
27	B8	973	A	C5-C6-N1	-5.17	115.12	117.70
27	B8	1046	A	C5-C6-N1	-5.17	115.12	117.70
27	B8	1366	A	O4'-C1'-N9	5.17	112.33	108.20
27	B8	2150	C	N3-C4-C5	-5.17	119.83	121.90
27	B8	2774	C	N3-C4-C5	-5.17	119.83	121.90
1	AA	933	G	O4'-C1'-N9	5.17	112.33	108.20
1	AA	1005	A	O4'-C1'-N9	5.17	112.33	108.20
1	AA	1035	A	C5-C6-N1	-5.17	115.12	117.70
1	AA	1449	C	N3-C4-C5	-5.17	119.83	121.90
26	B7	14	U	O4'-C1'-N1	5.17	112.33	108.20
27	B8	101	A	C5-C6-N1	-5.17	115.12	117.70
27	B8	340	A	C5-C6-N1	-5.17	115.12	117.70
27	B8	856	G	O4'-C1'-N9	5.17	112.33	108.20
27	B8	1881	C	N3-C4-C5	-5.17	119.83	121.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	2015	A	C5-C6-N6	-5.17	119.57	123.70
1	AA	79	G	O4'-C1'-N9	5.16	112.33	108.20
1	AA	998	C	N3-C4-C5	-5.16	119.83	121.90
1	AA	1400	C	N3-C4-N4	5.16	121.61	118.00
27	B8	21	A	C5-C6-N1	-5.16	115.12	117.70
27	B8	701	G	O4'-C1'-N9	5.16	112.33	108.20
27	B8	1974	C	N3-C4-C5	-5.16	119.83	121.90
1	AA	50	A	C5-C6-N1	-5.16	115.12	117.70
1	AA	199	A	O4'-C1'-N9	5.16	112.33	108.20
1	AA	888	G	N3-C2-N2	5.16	123.51	119.90
3	AV	27	A	C5-C6-N1	-5.16	115.12	117.70
27	B8	555	G	O4'-C1'-N9	5.16	112.33	108.20
27	B8	611	C	N3-C4-C5	-5.16	119.83	121.90
27	B8	1304	A	C5-C6-N6	-5.16	119.57	123.70
37	BI	87	SER	N-CA-CB	5.16	118.24	110.50
1	AA	364	A	O4'-C1'-N9	5.16	112.33	108.20
27	B8	479	A	C5-C6-N1	-5.16	115.12	117.70
27	B8	507	A	C5-C6-N1	-5.16	115.12	117.70
27	B8	900	A	C5-C6-N6	-5.16	119.57	123.70
27	B8	1085	A	C4-C5-C6	5.16	119.58	117.00
27	B8	1644	C	N3-C4-C5	-5.16	119.84	121.90
27	B8	1836	C	N3-C4-C5	-5.16	119.84	121.90
27	B8	2336	A	C5-C6-N1	-5.16	115.12	117.70
27	B8	2649	C	N3-C4-C5	-5.16	119.83	121.90
1	AA	1150	A	C5-C6-N6	-5.16	119.57	123.70
3	AV	17	C	N3-C4-N4	5.16	121.61	118.00
26	B7	70	C	N3-C4-C5	-5.16	119.84	121.90
27	B8	305	C	N3-C4-C5	-5.16	119.84	121.90
27	B8	1527	G	N3-C2-N2	5.16	123.51	119.90
27	B8	1600	C	N3-C4-C5	-5.16	119.84	121.90
27	B8	1638	C	N3-C4-C5	-5.16	119.84	121.90
26	B7	61	G	O4'-C1'-N9	5.16	112.33	108.20
27	B8	643	A	C5-C6-N1	-5.16	115.12	117.70
27	B8	1078	U	C2-N1-C1'	5.16	123.89	117.70
27	B8	1296	G	O4'-C1'-N9	5.16	112.33	108.20
1	AA	160	A	O4'-C1'-N9	5.16	112.32	108.20
1	AA	383	A	O4'-C1'-N9	5.16	112.33	108.20
27	B8	85	G	O4'-C1'-N9	5.16	112.32	108.20
27	B8	1872	A	C5-C6-N6	-5.16	119.58	123.70
1	AA	177	G	C5-C6-O6	-5.15	125.51	128.60
1	AA	1431	A	C5-C6-N1	-5.15	115.12	117.70
1	AA	695	A	C5-C6-N1	-5.15	115.12	117.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1287	A	C5-C6-N1	-5.15	115.12	117.70
27	B8	127	A	C5-C6-N1	-5.15	115.12	117.70
27	B8	670	A	C5-C6-N1	-5.15	115.12	117.70
27	B8	911	A	O4'-C1'-N9	5.15	112.32	108.20
27	B8	2012	G	N3-C2-N2	5.15	123.51	119.90
27	B8	2145	C	C2-N1-C1'	5.15	124.47	118.80
1	AA	369	G	O4'-C1'-N9	5.15	112.32	108.20
1	AA	558	G	O4'-C1'-N9	5.15	112.32	108.20
1	AA	613	C	N3-C4-C5	-5.15	119.84	121.90
1	AA	969	A	C5-C6-N1	-5.15	115.12	117.70
1	AA	1285	A	C5-C6-N1	-5.15	115.12	117.70
1	AA	1318	A	C5-C6-N1	-5.15	115.12	117.70
1	AA	1332	A	C5-C6-N1	-5.15	115.12	117.70
1	AA	1352	C	N3-C4-C5	-5.15	119.84	121.90
27	B8	6	A	O4'-C1'-N9	5.15	112.32	108.20
27	B8	1496	A	C5-C6-N1	-5.15	115.12	117.70
27	B8	2082	A	C5-C6-N1	-5.15	115.12	117.70
27	B8	2430	A	C5-C6-N1	-5.15	115.12	117.70
27	B8	2598	A	C5-C6-N1	-5.15	115.12	117.70
27	B8	121	G	O4'-C1'-N9	5.15	112.32	108.20
27	B8	1495	A	O4'-C1'-N9	5.15	112.32	108.20
27	B8	1628	G	O4'-C1'-N9	5.15	112.32	108.20
27	B8	2673	G	O4'-C1'-N9	5.15	112.32	108.20
27	B8	2682	A	O4'-C1'-N9	5.15	112.32	108.20
1	AA	59	A	C5-C6-N1	-5.15	115.13	117.70
1	AA	630	A	O4'-C1'-N9	5.15	112.32	108.20
1	AA	833	G	O4'-C1'-N9	5.15	112.32	108.20
27	B8	314	C	N3-C4-C5	-5.15	119.84	121.90
27	B8	477	A	C5-C6-N6	-5.15	119.58	123.70
27	B8	570	G	O4'-C1'-N9	5.15	112.32	108.20
27	B8	789	A	C5-C6-N1	-5.15	115.13	117.70
27	B8	1741	C	N3-C4-C5	-5.15	119.84	121.90
27	B8	1893	C	N3-C4-C5	-5.15	119.84	121.90
27	B8	2664	G	O4'-C1'-N9	5.15	112.32	108.20
27	B8	2765	A	C5-C6-N6	-5.15	119.58	123.70
1	AA	1142	G	O4'-C1'-N9	5.15	112.32	108.20
2	AX	17	C	N3-C4-C5	-5.15	119.84	121.90
3	AV	44	G	O4'-C1'-N9	5.15	112.32	108.20
27	B8	2595	G	O4'-C1'-N9	5.15	112.32	108.20
1	AA	489	C	N3-C4-C5	-5.14	119.84	121.90
1	AA	999	C	N3-C4-C5	-5.14	119.84	121.90
1	AA	1022	A	C5-C6-N6	-5.14	119.58	123.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1107	C	N3-C4-C5	-5.14	119.84	121.90
1	AA	1111	A	O4'-C1'-N9	5.14	112.32	108.20
27	B8	844	A	O4'-C1'-N9	5.14	112.32	108.20
27	B8	2530	A	C5-C6-N1	-5.14	115.13	117.70
1	AA	331	G	O4'-C1'-N9	5.14	112.31	108.20
1	AA	750	C	N3-C4-C5	-5.14	119.84	121.90
1	AA	857	C	N3-C4-N4	5.14	121.60	118.00
1	AA	1044	A	O4'-C1'-N9	5.14	112.31	108.20
1	AA	1492	A	C5-C6-N1	-5.14	115.13	117.70
27	B8	505	A	C5-C6-N1	-5.14	115.13	117.70
27	B8	1587	G	O4'-C1'-N9	5.14	112.31	108.20
27	B8	1753	G	O4'-C1'-N9	5.14	112.31	108.20
27	B8	2750	A	C5-C6-N1	-5.14	115.13	117.70
41	BM	122	ALA	N-CA-CB	5.14	117.30	110.10
1	AA	1214	C	C6-N1-C1'	-5.14	114.63	120.80
1	AA	1281	C	N3-C4-C5	-5.14	119.84	121.90
3	AV	27	A	O4'-C1'-N9	5.14	112.31	108.20
27	B8	616	A	C5-C6-N1	-5.14	115.13	117.70
27	B8	873	C	N3-C4-C5	-5.14	119.84	121.90
1	AA	236	A	O4'-C1'-N9	5.14	112.31	108.20
1	AA	914	A	O4'-C1'-N9	5.14	112.31	108.20
1	AA	1418	A	C5-C6-N1	-5.14	115.13	117.70
27	B8	1048	A	O4'-C1'-N9	5.14	112.31	108.20
27	B8	1722	A	C5-C6-N6	-5.14	119.59	123.70
27	B8	2762	C	N3-C4-C5	-5.14	119.84	121.90
1	AA	435	A	C5-C6-N1	-5.14	115.13	117.70
1	AA	608	A	C5-C6-N1	-5.14	115.13	117.70
1	AA	880	C	N3-C4-N4	5.14	121.60	118.00
27	B8	216	A	C5-C6-N6	-5.14	119.59	123.70
27	B8	719	C	N3-C4-C5	-5.14	119.84	121.90
27	B8	2455	G	O4'-C1'-N9	5.14	112.31	108.20
27	B8	2503	A	C5-C6-N1	-5.14	115.13	117.70
1	AA	980	C	N3-C4-C5	-5.14	119.84	121.90
1	AA	1368	A	C5-C6-N6	-5.14	119.59	123.70
1	AA	1468	A	C5-C6-N6	-5.14	119.59	123.70
26	B7	34	A	C5-C6-N6	-5.14	119.59	123.70
27	B8	94	A	C5-C6-N6	-5.14	119.59	123.70
27	B8	644	A	C5-C6-N1	-5.14	115.13	117.70
27	B8	905	A	C5-C6-N1	-5.14	115.13	117.70
27	B8	2208	C	N3-C4-C5	-5.14	119.85	121.90
1	AA	116	A	C5-C6-N6	-5.13	119.59	123.70
1	AA	1120	C	N3-C4-C5	-5.13	119.85	121.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	316	C	N3-C4-C5	-5.13	119.85	121.90
27	B8	516	C	N3-C4-C5	-5.13	119.85	121.90
27	B8	1454	C	N3-C4-N4	5.13	121.59	118.00
27	B8	2620	C	N3-C4-C5	-5.13	119.85	121.90
27	B8	2875	C	N3-C4-C5	-5.13	119.85	121.90
27	B8	1879	C	N3-C4-C5	-5.13	119.85	121.90
1	AA	727	G	N3-C2-N2	5.13	123.49	119.90
1	AA	1285	A	C5-C6-N6	-5.13	119.59	123.70
1	AA	1447	A	C4-C5-C6	5.13	119.56	117.00
27	B8	142	A	C5-C6-N6	-5.13	119.59	123.70
27	B8	385	C	N3-C4-N4	5.13	121.59	118.00
27	B8	1075	C	N3-C4-C5	-5.13	119.85	121.90
27	B8	1302	A	C5-C6-N6	-5.13	119.59	123.70
27	B8	1909	C	N3-C4-C5	-5.13	119.85	121.90
1	AA	60	A	C5-C6-N1	-5.13	115.14	117.70
1	AA	452	A	C5-C6-N1	-5.13	115.14	117.70
1	AA	959	A	O4'-C1'-N9	5.13	112.30	108.20
27	B8	1383	A	C5-C6-N1	-5.13	115.14	117.70
27	B8	2509	G	O4'-C1'-N9	5.13	112.30	108.20
27	B8	2832	U	O4'-C1'-N1	5.13	112.30	108.20
1	AA	712	A	C5-C6-N1	-5.13	115.14	117.70
26	B7	17	C	N3-C4-C5	-5.13	119.85	121.90
27	B8	195	A	C5-C6-N1	-5.13	115.14	117.70
27	B8	457	A	C4-C5-C6	5.13	119.56	117.00
27	B8	1298	C	N3-C4-C5	-5.13	119.85	121.90
27	B8	2134	A	C5-C6-N6	-5.13	119.60	123.70
27	B8	2427	C	N3-C4-C5	-5.13	119.85	121.90
27	B8	2833	U	O4'-C1'-N1	5.13	112.30	108.20
27	B8	2883	A	C5-C6-N1	-5.13	115.14	117.70
1	AA	1027	C	C5-C4-N4	-5.13	116.61	120.20
1	AA	1188	A	O4'-C1'-N9	5.13	112.30	108.20
27	B8	251	A	O4'-C1'-N9	5.13	112.30	108.20
27	B8	849	A	C5-C6-N1	-5.13	115.14	117.70
27	B8	2499	C	N3-C4-C5	-5.13	119.85	121.90
1	AA	648	A	O4'-C1'-N9	5.12	112.30	108.20
1	AA	139	A	C5-C6-N1	-5.12	115.14	117.70
1	AA	507	C	N3-C4-C5	-5.12	119.85	121.90
1	AA	1269	A	C4-C5-C6	5.12	119.56	117.00
1	AA	1350	A	C5-C6-N1	-5.12	115.14	117.70
26	B7	26	C	N3-C4-N4	5.12	121.59	118.00
27	B8	34	U	C2-N1-C1'	5.12	123.85	117.70
27	B8	56	A	C5-C6-N1	-5.12	115.14	117.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	513	A	C5-C6-N1	-5.12	115.14	117.70
27	B8	599	A	O4'-C1'-N9	5.12	112.30	108.20
27	B8	1264	A	C5-C6-N1	-5.12	115.14	117.70
27	B8	1529	G	O4'-C1'-N9	5.12	112.30	108.20
27	B8	1572	A	O4'-C1'-N9	5.12	112.30	108.20
27	B8	1668	A	C5-C6-N1	-5.12	115.14	117.70
27	B8	2761	A	O4'-C1'-N9	5.12	112.30	108.20
1	AA	54	C	N3-C4-C5	-5.12	119.85	121.90
26	B7	107	G	N3-C2-N2	5.12	123.49	119.90
27	B8	737	C	N3-C4-C5	-5.12	119.85	121.90
27	B8	878	A	O4'-C1'-N9	5.12	112.30	108.20
27	B8	1996	C	O4'-C1'-N1	5.12	112.30	108.20
27	B8	2706	A	C5-C6-N1	-5.12	115.14	117.70
1	AA	177	G	O4'-C1'-N9	5.12	112.30	108.20
27	B8	1	G	O4'-C1'-N9	5.12	112.30	108.20
27	B8	218	A	O4'-C1'-N9	5.12	112.30	108.20
27	B8	250	G	O4'-C1'-N9	5.12	112.30	108.20
27	B8	387	U	O4'-C1'-N1	5.12	112.30	108.20
27	B8	899	A	C5-C6-N1	-5.12	115.14	117.70
1	AA	699	C	N3-C4-C5	-5.12	119.85	121.90
1	AA	888	G	O4'-C1'-N9	5.12	112.30	108.20
27	B8	38	A	O4'-C1'-N9	5.12	112.30	108.20
27	B8	231	A	C5-C6-N6	-5.12	119.60	123.70
27	B8	1117	C	N3-C4-C5	-5.12	119.85	121.90
27	B8	1367	A	C5-C6-N1	-5.12	115.14	117.70
27	B8	2274	A	O4'-C1'-N9	5.12	112.30	108.20
1	AA	560	A	O4'-C1'-N9	5.12	112.29	108.20
1	AA	1014	A	C5-C6-N1	-5.12	115.14	117.70
27	B8	120	U	O4'-C1'-N1	5.12	112.29	108.20
27	B8	621	A	C5-C6-N1	-5.12	115.14	117.70
27	B8	2020	A	C5-C6-N6	-5.12	119.61	123.70
27	B8	2467	C	N3-C4-N4	5.12	121.58	118.00
27	B8	2666	C	N3-C4-N4	5.12	121.58	118.00
1	AA	342	C	N3-C4-C5	-5.12	119.85	121.90
1	AA	579	A	C5-C6-N1	-5.12	115.14	117.70
1	AA	938	A	C5-C6-N1	-5.12	115.14	117.70
1	AA	1266	G	O4'-C1'-N9	5.12	112.29	108.20
1	AA	1340	A	C5-C6-N6	-5.12	119.61	123.70
1	AA	1434	A	C5-C6-N1	-5.12	115.14	117.70
27	B8	70	G	O4'-C1'-N9	5.12	112.29	108.20
27	B8	1074	G	O4'-C1'-N9	5.12	112.29	108.20
27	B8	2365	G	N3-C2-N2	5.12	123.48	119.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	2440	C	N3-C4-C5	-5.12	119.85	121.90
1	AA	190	A	C5-C6-N6	-5.11	119.61	123.70
1	AA	1047	G	O4'-C1'-N9	5.11	112.29	108.20
1	AA	1096	C	N3-C4-C5	-5.11	119.86	121.90
6	AB	212	TYR	CB-CG-CD2	-5.11	117.93	121.00
27	B8	330	A	O4'-C1'-N9	5.11	112.29	108.20
27	B8	398	C	N3-C4-C5	-5.11	119.86	121.90
27	B8	1308	A	O4'-C1'-N9	5.11	112.29	108.20
27	B8	1428	C	P-O3'-C3'	5.11	125.84	119.70
27	B8	1674	G	O4'-C1'-N9	5.11	112.29	108.20
27	B8	1978	A	C5-C6-N1	-5.11	115.14	117.70
27	B8	2164	C	C6-N1-C1'	-5.11	114.67	120.80
28	BA	200	PRO	CA-C-N	5.11	131.42	117.10
1	AA	1245	C	N3-C4-C5	-5.11	119.86	121.90
27	B8	91	A	O4'-C1'-N9	5.11	112.29	108.20
47	BS	89	ALA	N-CA-CB	5.11	117.26	110.10
1	AA	530	G	O4'-C1'-N9	5.11	112.29	108.20
1	AA	1113	C	P-O5'-C5'	5.11	129.08	120.90
1	AA	1252	A	C5-C6-N1	-5.11	115.14	117.70
27	B8	52	A	C5-C6-N6	-5.11	119.61	123.70
27	B8	2258	C	N3-C4-C5	-5.11	119.86	121.90
27	B8	2531	A	C5-C6-N6	-5.11	119.61	123.70
27	B8	2711	A	C5-C6-N1	-5.11	115.14	117.70
1	AA	810	C	N3-C4-C5	-5.11	119.86	121.90
27	B8	1208	C	N3-C4-C5	-5.11	119.86	121.90
27	B8	1711	A	C5-C6-N6	-5.11	119.61	123.70
27	B8	910	A	C5-C6-N6	-5.11	119.61	123.70
1	AA	285	C	N3-C4-C5	-5.11	119.86	121.90
1	AA	475	C	N3-C4-C5	-5.11	119.86	121.90
1	AA	639	G	O4'-C1'-N9	5.11	112.28	108.20
27	B8	124	G	O4'-C1'-N9	5.11	112.28	108.20
27	B8	1454	C	N3-C4-C5	-5.11	119.86	121.90
27	B8	1494	A	O4'-C1'-N9	5.11	112.28	108.20
27	B8	1553	A	C5-C6-N1	-5.11	115.15	117.70
27	B8	2321	U	C2-N1-C1'	5.11	123.83	117.70
27	B8	2704	C	N3-C4-C5	-5.11	119.86	121.90
27	B8	2787	C	N3-C4-C5	-5.11	119.86	121.90
1	AA	1469	C	N3-C4-C5	-5.10	119.86	121.90
27	B8	2810	A	C5-C6-N1	-5.10	115.15	117.70
42	BN	21	PHE	CB-CG-CD2	5.10	124.37	120.80
1	AA	528	C	N3-C4-N4	5.10	121.57	118.00
1	AA	966	G	O4'-C1'-N9	5.10	112.28	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1502	A	C5-C6-N6	-5.10	119.62	123.70
3	AV	54	G	O4'-C1'-N9	5.10	112.28	108.20
27	B8	529	A	C5-C6-N6	-5.10	119.62	123.70
27	B8	633	A	C5-C6-N6	-5.10	119.62	123.70
27	B8	2214	C	N3-C4-C5	-5.10	119.86	121.90
1	AA	134	G	O4'-C1'-N9	5.10	112.28	108.20
27	B8	867	C	N3-C4-N4	5.10	121.57	118.00
27	B8	1414	C	N3-C4-C5	-5.10	119.86	121.90
27	B8	1789	A	O4'-C1'-N9	5.10	112.28	108.20
1	AA	326	G	O4'-C1'-N9	5.10	112.28	108.20
27	B8	343	C	N3-C4-C5	-5.10	119.86	121.90
27	B8	1403	A	O4'-C1'-N9	5.10	112.28	108.20
27	B8	1866	A	C5-C6-N1	-5.10	115.15	117.70
27	B8	2035	G	O4'-C1'-N9	5.10	112.28	108.20
27	B8	2678	C	N3-C4-C5	-5.10	119.86	121.90
27	B8	2785	C	N3-C4-C5	-5.10	119.86	121.90
1	AA	364	A	C5-C6-N1	-5.10	115.15	117.70
1	AA	865	A	C5-C6-N1	-5.10	115.15	117.70
27	B8	63	A	C5-C6-N1	-5.10	115.15	117.70
27	B8	167	A	C5-C6-N1	-5.10	115.15	117.70
27	B8	1695	G	O4'-C1'-N9	5.10	112.28	108.20
1	AA	1325	C	N3-C4-C5	-5.10	119.86	121.90
27	B8	5	A	O4'-C1'-N9	5.10	112.28	108.20
1	AA	282	A	C5-C6-N1	-5.09	115.15	117.70
1	AA	647	C	N3-C4-C5	-5.09	119.86	121.90
1	AA	743	A	O4'-C1'-N9	5.09	112.28	108.20
1	AA	1113	C	N3-C4-C5	-5.09	119.86	121.90
1	AA	1397	C	N3-C4-C5	-5.09	119.86	121.90
26	B7	37	C	N3-C4-N4	5.09	121.57	118.00
27	B8	109	C	N3-C4-C5	-5.09	119.86	121.90
27	B8	469	G	N3-C2-N2	5.09	123.47	119.90
27	B8	668	A	O4'-C1'-N9	5.09	112.28	108.20
27	B8	874	G	O4'-C1'-N9	5.09	112.28	108.20
27	B8	1387	A	C5-C6-N1	-5.09	115.15	117.70
27	B8	1630	A	C5-C6-N6	-5.09	119.62	123.70
27	B8	2368	C	N3-C4-C5	-5.09	119.86	121.90
27	B8	2620	C	N3-C4-N4	5.09	121.57	118.00
27	B8	2793	C	N3-C4-C5	-5.09	119.86	121.90
27	B8	2857	G	O4'-C1'-N9	5.09	112.28	108.20
27	B8	2879	A	C5-C6-N1	-5.09	115.15	117.70
1	AA	910	C	N3-C4-C5	-5.09	119.86	121.90
27	B8	626	A	O4'-C1'-N9	5.09	112.28	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	973	A	C5'-C4'-O4'	5.09	115.21	109.10
27	B8	1640	A	C5-C6-N1	-5.09	115.15	117.70
1	AA	52	C	N3-C4-C5	-5.09	119.86	121.90
1	AA	411	A	C5-C6-N1	-5.09	115.15	117.70
1	AA	1446	A	C5-C6-N1	-5.09	115.16	117.70
27	B8	39	G	O4'-C1'-N9	5.09	112.27	108.20
27	B8	1287	A	C5-C6-N6	-5.09	119.63	123.70
27	B8	1533	C	N3-C4-C5	-5.09	119.86	121.90
27	B8	1902	C	N3-C4-N4	5.09	121.56	118.00
27	B8	2077	A	C5-C6-N6	-5.09	119.63	123.70
27	B8	2306	C	N3-C4-C5	-5.09	119.86	121.90
1	AA	71	A	C5-C6-N1	-5.09	115.16	117.70
1	AA	280	C	O4'-C1'-N1	5.09	112.27	108.20
1	AA	876	C	N3-C4-C5	-5.09	119.86	121.90
3	AV	11	C	N3-C4-N4	5.09	121.56	118.00
27	B8	1111	A	C5-C6-N6	-5.09	119.63	123.70
27	B8	2386	A	C5-C6-N1	-5.09	115.16	117.70
27	B8	2520	C	N3-C4-C5	-5.09	119.86	121.90
27	B8	2654	A	C5-C6-N1	-5.09	115.16	117.70
1	AA	539	A	C5-C6-N1	-5.09	115.16	117.70
27	B8	1050	A	C5-C6-N1	-5.09	115.16	117.70
27	B8	1522	A	C4-C5-C6	5.09	119.54	117.00
27	B8	1679	A	C5-C6-N6	-5.09	119.63	123.70
1	AA	109	A	C5-C6-N6	-5.09	119.63	123.70
1	AA	234	C	N3-C4-C5	-5.09	119.87	121.90
1	AA	896	C	N3-C4-C5	-5.09	119.87	121.90
27	B8	1233	C	N3-C4-C5	-5.09	119.87	121.90
27	B8	2091	C	N3-C4-C5	-5.09	119.87	121.90
27	B8	2679	A	C5-C6-N1	-5.09	115.16	117.70
1	AA	1261	A	O4'-C1'-N9	5.08	112.27	108.20
27	B8	794	A	O4'-C1'-N9	5.08	112.27	108.20
27	B8	2486	C	N3-C4-C5	-5.08	119.87	121.90
1	AA	1236	A	O4'-C1'-N9	5.08	112.27	108.20
2	AX	19	U	O4'-C1'-N1	5.08	112.27	108.20
27	B8	1565	C	P-O3'-C3'	5.08	125.80	119.70
27	B8	1854	A	C5-C6-N6	-5.08	119.63	123.70
27	B8	1961	C	N3-C4-C5	-5.08	119.87	121.90
27	B8	2366	A	O4'-C1'-N9	5.08	112.27	108.20
27	B8	2487	G	O4'-C1'-N9	5.08	112.27	108.20
1	AA	432	A	C5-C6-N1	-5.08	115.16	117.70
1	AA	766	A	C5-C6-N1	-5.08	115.16	117.70
1	AA	1265	C	N3-C4-C5	-5.08	119.87	121.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	104	A	O4'-C1'-N9	5.08	112.27	108.20
27	B8	586	A	O4'-C1'-N9	5.08	112.27	108.20
27	B8	1044	C	N3-C4-C5	-5.08	119.87	121.90
27	B8	2542	A	C5-C6-N1	-5.08	115.16	117.70
1	AA	393	A	C5-C6-N6	-5.08	119.64	123.70
1	AA	1178	G	N3-C2-N2	5.08	123.46	119.90
27	B8	74	A	O4'-C1'-N9	5.08	112.26	108.20
1	AA	115	G	N3-C2-N2	5.08	123.46	119.90
1	AA	954	G	O4'-C1'-N9	5.08	112.26	108.20
27	B8	71	A	C5-C6-N6	-5.08	119.64	123.70
27	B8	1607	C	N3-C4-N4	5.08	121.55	118.00
27	B8	1977	A	O4'-C1'-N9	5.08	112.26	108.20
27	B8	2626	C	N3-C4-C5	-5.08	119.87	121.90
1	AA	729	A	C5-C6-N1	-5.08	115.16	117.70
1	AA	790	A	O4'-C1'-N9	5.08	112.26	108.20
1	AA	1417	G	N3-C2-N2	5.08	123.45	119.90
27	B8	792	A	O4'-C1'-N9	5.08	112.26	108.20
27	B8	1574	C	N3-C4-C5	-5.08	119.87	121.90
1	AA	660	C	N3-C4-C5	-5.08	119.87	121.90
1	AA	1208	C	N3-C4-C5	-5.08	119.87	121.90
1	AA	1275	A	C5-C6-N6	-5.08	119.64	123.70
3	AV	59	A	C5-C6-N1	-5.08	115.16	117.70
27	B8	242	G	P-O3'-C3'	5.08	125.79	119.70
27	B8	958	U	O4'-C1'-N1	5.08	112.26	108.20
27	B8	2366	A	C5-C6-N6	-5.08	119.64	123.70
27	B8	2822	G	O4'-C1'-N9	5.08	112.26	108.20
1	AA	744	C	N3-C4-C5	-5.07	119.87	121.90
1	AA	802	A	C5-C6-N1	-5.07	115.16	117.70
1	AA	878	A	C5-C6-N1	-5.07	115.16	117.70
1	AA	1218	C	N3-C4-C5	-5.07	119.87	121.90
27	B8	581	C	N3-C4-C5	-5.07	119.87	121.90
27	B8	1395	A	C5-C6-N6	-5.07	119.64	123.70
27	B8	2795	C	N3-C4-C5	-5.07	119.87	121.90
1	AA	704	A	C5-C6-N1	-5.07	115.16	117.70
1	AA	864	A	O4'-C1'-N9	5.07	112.26	108.20
1	AA	1112	C	N3-C4-C5	-5.07	119.87	121.90
27	B8	1515	A	C4-C5-C6	5.07	119.54	117.00
27	B8	2003	A	C5-C6-N1	-5.07	115.16	117.70
27	B8	2015	A	C5-C6-N1	-5.07	115.16	117.70
27	B8	2705	A	C5-C6-N1	-5.07	115.16	117.70
1	AA	389	A	C5-C6-N1	-5.07	115.17	117.70
1	AA	685	G	N3-C2-N2	5.07	123.45	119.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	799	G	O4'-C1'-N9	5.07	112.26	108.20
26	B7	24	G	N3-C2-N2	5.07	123.45	119.90
27	B8	675	A	C5-C6-N6	-5.07	119.64	123.70
27	B8	676	A	C5-C6-N1	-5.07	115.17	117.70
27	B8	1749	A	C5-C6-N6	-5.07	119.64	123.70
27	B8	1791	A	C5-C6-N1	-5.07	115.17	117.70
27	B8	2392	A	C5-C6-N1	-5.07	115.17	117.70
1	AA	181	A	C5-C6-N1	-5.07	115.17	117.70
27	B8	2115	G	N3-C2-N2	5.07	123.45	119.90
1	AA	353	A	C5-C6-N1	-5.07	115.17	117.70
1	AA	890	G	O4'-C1'-N9	5.07	112.25	108.20
1	AA	1476	A	C5-C6-N6	-5.07	119.65	123.70
27	B8	204	A	C4-C5-C6	5.07	119.53	117.00
27	B8	916	G	O4'-C1'-N9	5.07	112.25	108.20
27	B8	2080	A	O4'-C1'-N9	5.07	112.25	108.20
1	AA	746	A	C5-C6-N1	-5.07	115.17	117.70
26	B7	28	C	N3-C4-C5	-5.07	119.87	121.90
27	B8	353	C	N3-C4-C5	-5.07	119.87	121.90
27	B8	374	A	C5-C6-N6	-5.07	119.65	123.70
27	B8	893	C	N3-C4-N4	5.07	121.55	118.00
27	B8	1545	A	O4'-C1'-N9	5.07	112.25	108.20
27	B8	2090	A	O4'-C1'-N9	5.07	112.25	108.20
27	B8	2224	G	N3-C2-N2	5.07	123.45	119.90
1	AA	523	A	O4'-C1'-N9	5.06	112.25	108.20
1	AA	595	A	O4'-C1'-N9	5.06	112.25	108.20
3	AV	25	G	O4'-C1'-N9	5.06	112.25	108.20
27	B8	721	A	O4'-C1'-N9	5.06	112.25	108.20
27	B8	735	A	O4'-C1'-N9	5.06	112.25	108.20
1	AA	187	G	O4'-C1'-N9	5.06	112.25	108.20
1	AA	561	U	P-O3'-C3'	5.06	125.78	119.70
1	AA	1037	C	N3-C4-C5	-5.06	119.88	121.90
27	B8	267	C	N3-C4-C5	-5.06	119.88	121.90
27	B8	310	A	C5-C6-N6	-5.06	119.65	123.70
27	B8	745	G	O4'-C1'-N9	5.06	112.25	108.20
27	B8	1502	A	O4'-C1'-N9	5.06	112.25	108.20
27	B8	1635	A	C5-C6-N1	-5.06	115.17	117.70
27	B8	2004	G	O4'-C1'-N9	5.06	112.25	108.20
27	B8	2733	A	C5-C6-N6	-5.06	119.65	123.70
1	AA	553	A	C5-C6-N1	-5.06	115.17	117.70
1	AA	1388	C	N3-C4-C5	-5.06	119.88	121.90
27	B8	644	A	O4'-C1'-N9	5.06	112.25	108.20
27	B8	679	C	N3-C4-C5	-5.06	119.88	121.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	1241	A	C5-C6-N1	-5.06	115.17	117.70
27	B8	1462	C	N3-C4-C5	-5.06	119.88	121.90
27	B8	2354	C	N3-C4-C5	-5.06	119.88	121.90
27	B8	2446	G	O4'-C1'-N9	5.06	112.25	108.20
1	AA	334	C	N3-C4-C5	-5.06	119.88	121.90
1	AA	525	C	N3-C4-C5	-5.06	119.88	121.90
1	AA	1268	G	N3-C2-N2	5.06	123.44	119.90
27	B8	117	G	N3-C2-N2	5.06	123.44	119.90
27	B8	687	C	N3-C4-N4	5.06	121.54	118.00
27	B8	723	C	N3-C4-C5	-5.06	119.88	121.90
27	B8	880	G	O4'-C1'-N9	5.06	112.25	108.20
27	B8	1196	C	N3-C4-C5	-5.06	119.88	121.90
27	B8	2169	A	C5-C6-N1	-5.06	115.17	117.70
27	B8	2729	G	C5'-C4'-O4'	5.06	115.17	109.10
1	AA	698	G	O4'-C1'-N9	5.06	112.25	108.20
1	AA	841	C	N3-C4-C5	-5.06	119.88	121.90
26	B7	109	A	C5-C6-N1	-5.06	115.17	117.70
27	B8	517	C	N3-C4-C5	-5.06	119.88	121.90
27	B8	1336	A	C5'-C4'-O4'	5.06	115.17	109.10
1	AA	1304	G	N3-C2-N2	5.06	123.44	119.90
27	B8	139	U	O4'-C1'-N1	5.06	112.25	108.20
27	B8	439	A	C5-C6-N6	-5.06	119.66	123.70
27	B8	478	A	C5-C6-N1	-5.06	115.17	117.70
27	B8	1668	A	C5-C6-N6	-5.06	119.66	123.70
1	AA	207	C	N3-C4-C5	-5.05	119.88	121.90
1	AA	300	A	C5-C6-N1	-5.05	115.17	117.70
1	AA	617	G	O4'-C1'-N9	5.05	112.24	108.20
1	AA	795	C	N3-C4-N4	5.05	121.54	118.00
1	AA	816	A	C5-C6-N1	-5.05	115.17	117.70
1	AA	1102	A	C5-C6-N6	-5.05	119.66	123.70
1	AA	1124	G	N3-C2-N2	5.05	123.44	119.90
1	AA	1300	G	O4'-C1'-N9	5.05	112.24	108.20
27	B8	791	C	N3-C4-N4	5.05	121.54	118.00
27	B8	1047	G	N3-C2-N2	5.05	123.44	119.90
27	B8	2880	C	N3-C4-C5	-5.05	119.88	121.90
27	B8	556	A	C5-C6-N1	-5.05	115.17	117.70
27	B8	892	A	C5-C6-N1	-5.05	115.17	117.70
27	B8	1814	G	N3-C2-N2	5.05	123.44	119.90
27	B8	2452	C	N3-C4-C5	-5.05	119.88	121.90
27	B8	1021	A	C5-C6-N1	-5.05	115.17	117.70
27	B8	1508	A	C5-C6-N1	-5.05	115.17	117.70
27	B8	1848	A	C5-C6-N6	-5.05	119.66	123.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	2379	G	O4'-C1'-N9	5.05	112.24	108.20
1	AA	329	A	C5-C6-N6	-5.05	119.66	123.70
1	AA	1447	A	O4'-C1'-N9	5.05	112.24	108.20
27	B8	1030	C	N3-C4-C5	-5.05	119.88	121.90
27	B8	2197	U	P-O3'-C3'	5.05	125.76	119.70
27	B8	2676	C	N3-C4-C5	-5.05	119.88	121.90
1	AA	120	A	C5-C6-N1	-5.05	115.18	117.70
27	B8	654	A	C5-C6-N1	-5.05	115.18	117.70
27	B8	1266	G	P-O3'-C3'	5.05	125.76	119.70
27	B8	1575	C	N3-C4-C5	-5.05	119.88	121.90
27	B8	1654	A	O4'-C1'-N9	5.05	112.24	108.20
27	B8	2154	A	O4'-C1'-N9	5.05	112.24	108.20
27	B8	2559	C	N3-C4-C5	-5.05	119.88	121.90
1	AA	26	A	O4'-C1'-N9	5.05	112.24	108.20
1	AA	43	C	N3-C4-C5	-5.05	119.88	121.90
1	AA	169	C	N3-C4-N4	5.05	121.53	118.00
1	AA	345	C	N3-C4-N4	5.05	121.53	118.00
1	AA	554	A	C5-C6-N6	-5.05	119.66	123.70
1	AA	738	C	N3-C4-C5	-5.05	119.88	121.90
1	AA	1125	U	O4'-C1'-N1	5.05	112.24	108.20
27	B8	127	A	O4'-C1'-N9	5.05	112.24	108.20
27	B8	345	A	C5-C6-N1	-5.05	115.18	117.70
27	B8	1612	C	N3-C4-C5	-5.05	119.88	121.90
27	B8	2567	G	O4'-C1'-N9	5.05	112.24	108.20
27	B8	2589	A	O4'-C1'-N9	5.05	112.24	108.20
27	B8	1282	U	P-O3'-C3'	5.04	125.75	119.70
27	B8	1919	A	O4'-C1'-N9	5.04	112.24	108.20
27	B8	2199	A	O4'-C1'-N9	5.04	112.24	108.20
1	AA	1012	A	O4'-C1'-N9	5.04	112.23	108.20
1	AA	1289	A	C5-C6-N1	-5.04	115.18	117.70
27	B8	933	A	C5-C6-N6	-5.04	119.67	123.70
1	AA	1263	C	N3-C4-C5	-5.04	119.88	121.90
27	B8	103	A	C5-C6-N6	-5.04	119.67	123.70
27	B8	927	A	C5-C6-N1	-5.04	115.18	117.70
27	B8	1393	A	C5-C6-N6	-5.04	119.67	123.70
27	B8	1494	A	C5-C6-N6	-5.04	119.67	123.70
27	B8	1656	C	N3-C4-C5	-5.04	119.88	121.90
27	B8	1919	A	C5-C6-N1	-5.04	115.18	117.70
27	B8	2054	A	C5-C6-N6	-5.04	119.67	123.70
27	B8	2283	C	N3-C4-C5	-5.04	119.88	121.90
27	B8	2433	A	O4'-C1'-N9	5.04	112.23	108.20
27	B8	2886	A	C5-C6-N1	-5.04	115.18	117.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	251	G	O4'-C1'-N9	5.04	112.23	108.20
1	AA	1124	G	O4'-C1'-N9	5.04	112.23	108.20
1	AA	1166	G	O4'-C1'-N9	5.04	112.23	108.20
27	B8	1177	G	O4'-C1'-N9	5.04	112.23	108.20
27	B8	2366	A	C5-C6-N1	-5.04	115.18	117.70
1	AA	129	A	C5-C6-N6	-5.04	119.67	123.70
1	AA	690	G	N3-C2-N2	5.04	123.43	119.90
1	AA	1357	A	C5-C6-N1	-5.04	115.18	117.70
27	B8	181	A	C5-C6-N6	-5.04	119.67	123.70
27	B8	787	C	N3-C4-C5	-5.04	119.89	121.90
27	B8	1691	C	N3-C4-C5	-5.04	119.89	121.90
27	B8	2006	C	N3-C4-C5	-5.04	119.89	121.90
27	B8	2014	A	C5-C6-N6	-5.04	119.67	123.70
27	B8	2767	C	N3-C4-C5	-5.04	119.89	121.90
27	B8	2879	A	O4'-C1'-N9	5.04	112.23	108.20
40	BL	113	ALA	N-CA-CB	5.04	117.15	110.10
1	AA	687	A	C5-C6-N1	-5.04	115.18	117.70
1	AA	766	A	C5-C6-N6	-5.04	119.67	123.70
1	AA	1256	A	C5-C6-N1	-5.04	115.18	117.70
27	B8	972	A	O4'-C1'-N9	5.04	112.23	108.20
27	B8	1652	A	C5-C6-N6	-5.04	119.67	123.70
1	AA	183	C	C6-N1-C1'	-5.04	114.76	120.80
1	AA	784	A	O4'-C1'-N9	5.04	112.23	108.20
26	B7	71	C	N3-C4-C5	-5.04	119.89	121.90
27	B8	279	A	C5-C6-N6	-5.04	119.67	123.70
27	B8	975	A	C5-C6-N6	-5.04	119.67	123.70
27	B8	2052	A	C5-C6-N6	-5.04	119.67	123.70
1	AA	77	A	C5-C6-N1	-5.03	115.18	117.70
1	AA	130	A	C5-C6-N1	-5.03	115.18	117.70
1	AA	281	G	N3-C2-N2	5.03	123.42	119.90
1	AA	483	C	O4'-C1'-N1	5.03	112.23	108.20
1	AA	883	C	N3-C4-C5	-5.03	119.89	121.90
27	B8	886	A	C5-C6-N6	-5.03	119.67	123.70
1	AA	1292	G	O4'-C1'-N9	5.03	112.22	108.20
27	B8	791	C	N3-C4-C5	-5.03	119.89	121.90
1	AA	194	C	N3-C4-C5	-5.03	119.89	121.90
1	AA	370	C	N3-C4-N4	5.03	121.52	118.00
1	AA	400	C	N3-C4-C5	-5.03	119.89	121.90
1	AA	511	C	N3-C4-C5	-5.03	119.89	121.90
1	AA	914	A	C5-C6-N1	-5.03	115.19	117.70
1	AA	1219	A	C5-C6-N1	-5.03	115.18	117.70
26	B7	59	A	C5-C6-N1	-5.03	115.19	117.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	394	C	N3-C4-C5	-5.03	119.89	121.90
27	B8	1492	G	O4'-C1'-N9	5.03	112.22	108.20
27	B8	1785	A	C5-C6-N1	-5.03	115.19	117.70
1	AA	495	A	P-O3'-C3'	5.03	125.73	119.70
1	AA	860	A	C5-C6-N6	-5.03	119.68	123.70
1	AA	914	A	C5-C6-N6	-5.03	119.68	123.70
27	B8	478	A	O4'-C1'-N9	5.03	112.22	108.20
27	B8	2250	G	O4'-C1'-N9	5.03	112.22	108.20
1	AA	618	C	N3-C4-N4	5.03	121.52	118.00
26	B7	26	C	N3-C4-C5	-5.03	119.89	121.90
26	B7	72	G	O4'-C1'-N9	5.03	112.22	108.20
27	B8	5	A	C5-C6-N1	-5.03	115.19	117.70
27	B8	1093	G	N3-C2-N2	5.03	123.42	119.90
27	B8	1728	C	N3-C4-C5	-5.03	119.89	121.90
27	B8	1771	C	N3-C4-C5	-5.03	119.89	121.90
27	B8	1802	A	C5-C6-N6	-5.03	119.68	123.70
27	B8	2304	G	O4'-C1'-N9	5.03	112.22	108.20
26	B7	107	G	C5'-C4'-O4'	5.03	115.13	109.10
27	B8	422	A	C5-C6-N1	-5.03	115.19	117.70
27	B8	858	G	N3-C2-N2	5.03	123.42	119.90
27	B8	1032	A	C5-C6-N6	-5.03	119.68	123.70
27	B8	2140	G	O4'-C1'-N9	5.03	112.22	108.20
27	B8	2700	A	C5-C6-N1	-5.03	115.19	117.70
1	AA	370	C	N3-C4-C5	-5.02	119.89	121.90
27	B8	486	C	N3-C4-C5	-5.02	119.89	121.90
27	B8	911	A	C5-C6-N1	-5.02	115.19	117.70
27	B8	1230	A	C5-C6-N1	-5.02	115.19	117.70
27	B8	2108	A	C5-C6-N6	-5.02	119.68	123.70
1	AA	65	A	O4'-C1'-N9	5.02	112.22	108.20
1	AA	393	A	O4'-C1'-N9	5.02	112.22	108.20
1	AA	1225	A	C5-C6-N6	-5.02	119.68	123.70
27	B8	335	C	N3-C4-C5	-5.02	119.89	121.90
27	B8	602	A	C5-C6-N1	-5.02	115.19	117.70
27	B8	1830	C	N3-C4-C5	-5.02	119.89	121.90
27	B8	2278	A	O4'-C1'-N9	5.02	112.22	108.20
27	B8	2538	C	N3-C4-C5	-5.02	119.89	121.90
1	AA	274	A	C5-C6-N1	-5.02	115.19	117.70
1	AA	1246	A	C5-C6-N6	-5.02	119.68	123.70
27	B8	157	C	N3-C4-C5	-5.02	119.89	121.90
27	B8	247	G	N3-C2-N2	5.02	123.42	119.90
27	B8	2032	G	O4'-C1'-N9	5.02	112.22	108.20
3	AV	23	G	O4'-C1'-N9	5.02	112.22	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	AV	33	A	C5-C6-N1	-5.02	115.19	117.70
26	B7	97	C	N3-C4-C5	-5.02	119.89	121.90
27	B8	244	A	C5-C6-N6	-5.02	119.68	123.70
27	B8	435	C	N3-C4-N4	5.02	121.51	118.00
27	B8	781	A	C5-C6-N6	-5.02	119.69	123.70
27	B8	816	C	N3-C4-C5	-5.02	119.89	121.90
27	B8	1284	A	C5-C6-N1	-5.02	115.19	117.70
27	B8	1635	A	O4'-C1'-N9	5.02	112.22	108.20
27	B8	2645	G	O4'-C1'-N9	5.02	112.22	108.20
27	B8	228	C	N3-C4-C5	-5.02	119.89	121.90
1	AA	586	C	N3-C4-C5	-5.02	119.89	121.90
27	B8	654	A	C5-C6-N6	-5.02	119.69	123.70
27	B8	1565	C	N3-C4-C5	-5.02	119.89	121.90
27	B8	2349	G	C5-C6-O6	-5.02	125.59	128.60
1	AA	221	C	N3-C4-C5	-5.01	119.89	121.90
1	AA	316	C	N3-C4-C5	-5.01	119.89	121.90
1	AA	583	A	C5-C6-N1	-5.01	115.19	117.70
1	AA	1170	A	C5-C6-N1	-5.01	115.19	117.70
27	B8	301	G	P-O3'-C3'	5.01	125.72	119.70
27	B8	548	G	O4'-C1'-N9	5.01	112.21	108.20
27	B8	800	A	C5-C6-N6	-5.01	119.69	123.70
27	B8	936	A	O4'-C1'-N9	5.01	112.21	108.20
27	B8	1029	A	O4'-C1'-N9	5.01	112.21	108.20
27	B8	1335	C	N3-C4-C5	-5.01	119.89	121.90
27	B8	2050	C	N3-C4-C5	-5.01	119.89	121.90
1	AA	939	G	O4'-C1'-N9	5.01	112.21	108.20
27	B8	2501	C	N3-C4-C5	-5.01	119.89	121.90
1	AA	83	C	N3-C4-C5	-5.01	119.89	121.90
1	AA	152	A	O4'-C1'-N9	5.01	112.21	108.20
1	AA	1329	A	C5-C6-N6	-5.01	119.69	123.70
27	B8	1526	C	N3-C4-C5	-5.01	119.89	121.90
27	B8	1972	G	O4'-C1'-N9	5.01	112.21	108.20
27	B8	240	C	N3-C4-C5	-5.01	119.90	121.90
27	B8	722	A	C5-C6-N1	-5.01	115.19	117.70
27	B8	1329	U	O4'-C1'-N1	5.01	112.21	108.20
27	B8	2657	A	O4'-C1'-N9	5.01	112.21	108.20
1	AA	232	G	N3-C2-N2	5.01	123.41	119.90
27	B8	1027	A	O4'-C1'-N9	5.01	112.21	108.20
27	B8	1469	A	C5-C6-N6	-5.01	119.69	123.70
27	B8	1828	G	O4'-C1'-N9	5.01	112.21	108.20
27	B8	2740	A	C5-C6-N1	-5.01	115.20	117.70
27	B8	116	C	N3-C4-N4	5.01	121.50	118.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	249	C	N3-C4-N4	5.01	121.50	118.00
27	B8	582	A	C5-C6-N1	-5.01	115.20	117.70
27	B8	883	G	O4'-C1'-N9	5.01	112.20	108.20
27	B8	912	C	N3-C4-C5	-5.01	119.90	121.90
27	B8	1997	C	N3-C4-C5	-5.01	119.90	121.90
27	B8	2232	C	N3-C4-C5	-5.01	119.90	121.90
27	B8	2782	G	O4'-C1'-N9	5.01	112.21	108.20
27	B8	2860	A	O4'-C1'-N9	5.01	112.20	108.20
1	AA	349	A	O4'-C1'-N9	5.00	112.20	108.20
1	AA	1249	C	N3-C4-C5	-5.00	119.90	121.90
27	B8	532	A	C5-C6-N1	-5.00	115.20	117.70
27	B8	2338	C	N3-C4-C5	-5.00	119.90	121.90
27	B8	2614	A	C5-C6-N1	-5.00	115.20	117.70
27	B8	2750	A	O4'-C1'-N9	5.00	112.20	108.20
1	AA	782	A	C5-C6-N1	-5.00	115.20	117.70
27	B8	299	A	O4'-C1'-N9	5.00	112.20	108.20
27	B8	1155	A	O4'-C1'-N9	5.00	112.20	108.20
27	B8	1743	G	O4'-C1'-N9	5.00	112.20	108.20
27	B8	2474	U	C2-N1-C1'	5.00	123.70	117.70
27	B8	2901	C	N3-C4-C5	-5.00	119.90	121.90
1	AA	386	C	N3-C4-C5	-5.00	119.90	121.90
1	AA	578	C	N3-C4-C5	-5.00	119.90	121.90
1	AA	1142	G	N1-C6-O6	5.00	122.90	119.90
27	B8	423	A	C5-C6-N1	-5.00	115.20	117.70
27	B8	758	C	N3-C4-C5	-5.00	119.90	121.90
27	B8	2263	C	N3-C4-C5	-5.00	119.90	121.90
27	B8	2298	A	C5-C6-N6	-5.00	119.70	123.70
27	B8	2319	G	O4'-C1'-N9	5.00	112.20	108.20

There are no chirality outliers.

All (189) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	A1	237	THR	Peptide
1	AA	102	G	Sidechain
1	AA	1024	G	Sidechain
1	AA	1027	C	Sidechain
1	AA	1044	A	Sidechain
1	AA	1094	G	Sidechain
1	AA	1095	U	Sidechain
1	AA	1101	A	Sidechain
1	AA	1125	U	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	AA	1129	C	Sidechain
1	AA	1131	G	Sidechain
1	AA	1139	G	Sidechain
1	AA	1144	G	Sidechain
1	AA	115	G	Sidechain
1	AA	1179	A	Sidechain
1	AA	1226	C	Sidechain
1	AA	1268	G	Sidechain
1	AA	1269	A	Sidechain
1	AA	1289	A	Sidechain
1	AA	1299	A	Sidechain
1	AA	13	U	Sidechain
1	AA	130	A	Sidechain
1	AA	1323	G	Sidechain
1	AA	1346	A	Sidechain
1	AA	1347	G	Sidechain
1	AA	1417	G	Sidechain
1	AA	1418	A	Sidechain
1	AA	1465	A	Sidechain
1	AA	1502	A	Sidechain
1	AA	1516	G	Sidechain
1	AA	152	A	Sidechain
1	AA	1526	G	Sidechain
1	AA	1529	G	Sidechain
1	AA	173	U	Sidechain
1	AA	180	U	Sidechain
1	AA	181	A	Sidechain
1	AA	184	G	Sidechain
1	AA	185	U	Sidechain
1	AA	202	G	Sidechain
1	AA	204	G	Sidechain
1	AA	244	U	Sidechain
1	AA	262	A	Sidechain
1	AA	265	G	Sidechain
1	AA	298	A	Sidechain
1	AA	315	A	Sidechain
1	AA	353	A	Sidechain
1	AA	378	G	Sidechain
1	AA	380	G	Sidechain
1	AA	439	U	Sidechain
1	AA	450	G	Sidechain
1	AA	454	G	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	AA	496	A	Sidechain
1	AA	527	G	Sidechain
1	AA	557	G	Sidechain
1	AA	565	U	Sidechain
1	AA	566	G	Sidechain
1	AA	581	G	Sidechain
1	AA	587	G	Sidechain
1	AA	588	G	Sidechain
1	AA	620	C	Sidechain
1	AA	622	A	Sidechain
1	AA	69	G	Sidechain
1	AA	718	A	Sidechain
1	AA	728	A	Sidechain
1	AA	752	G	Sidechain
1	AA	874	G	Sidechain
1	AA	883	C	Sidechain
1	AA	884	U	Sidechain
1	AA	927	G	Sidechain
1	AA	95	C	Sidechain
1	AA	960	U	Sidechain
1	AA	974	A	Sidechain
1	AA	978	A	Sidechain
7	AC	218	LYS	Peptide
12	AH	14	ARG	Sidechain
13	AI	6	TYR	Sidechain
3	AV	53	G	Sidechain
3	AV	7	G	Sidechain
57	B2	12	ARG	Sidechain
26	B7	111	U	Sidechain
26	B7	5	U	Sidechain
27	B8	1025	G	Sidechain
27	B8	1027	A	Sidechain
27	B8	1070	A	Sidechain
27	B8	1084	A	Sidechain
27	B8	1095	A	Sidechain
27	B8	1099	G	Sidechain
27	B8	1130	U	Sidechain
27	B8	1138	G	Sidechain
27	B8	120	U	Sidechain
27	B8	1204	A	Sidechain
27	B8	1224	U	Sidechain
27	B8	1235	G	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
27	B8	1236	G	Sidechain
27	B8	1296	G	Sidechain
27	B8	1327	A	Sidechain
27	B8	1334	G	Sidechain
27	B8	1360	G	Sidechain
27	B8	1383	A	Sidechain
27	B8	1394	U	Sidechain
27	B8	1427	A	Sidechain
27	B8	1515	A	Sidechain
27	B8	1517	G	Sidechain
27	B8	1530	G	Sidechain
27	B8	1573	G	Sidechain
27	B8	161	A	Sidechain
27	B8	1672	A	Sidechain
27	B8	1680	U	Sidechain
27	B8	1682	G	Sidechain
27	B8	1699	G	Sidechain
27	B8	1738	G	Sidechain
27	B8	1743	G	Sidechain
27	B8	1784	A	Sidechain
27	B8	1813	G	Sidechain
27	B8	1846	G	Sidechain
27	B8	1904	G	Sidechain
27	B8	1920	C	Sidechain
27	B8	1927	A	Sidechain
27	B8	1952	A	Sidechain
27	B8	1954	G	Sidechain
27	B8	2005	A	Sidechain
27	B8	205	G	Sidechain
27	B8	2125	G	Sidechain
27	B8	2143	C	Sidechain
27	B8	2148	G	Sidechain
27	B8	2155	U	Sidechain
27	B8	2272	U	Sidechain
27	B8	2345	G	Sidechain
27	B8	2365	G	Sidechain
27	B8	2382	G	Sidechain
27	B8	2460	U	Sidechain
27	B8	2471	A	Sidechain
27	B8	250	G	Sidechain
27	B8	2517	C	Sidechain
27	B8	2580	U	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
27	B8	2596	U	Sidechain
27	B8	261	G	Sidechain
27	B8	2637	U	Sidechain
27	B8	265	A	Sidechain
27	B8	2689	U	Sidechain
27	B8	27	G	Sidechain
27	B8	2746	U	Sidechain
27	B8	2756	U	Sidechain
27	B8	2857	G	Sidechain
27	B8	2858	C	Sidechain
27	B8	2866	U	Sidechain
27	B8	2903	U	Sidechain
27	B8	303	G	Sidechain
27	B8	346	A	Sidechain
27	B8	362	A	Sidechain
27	B8	370	G	Sidechain
27	B8	395	U	Sidechain
27	B8	428	A	Sidechain
27	B8	445	C	Sidechain
27	B8	446	G	Sidechain
27	B8	457	A	Sidechain
27	B8	467	G	Sidechain
27	B8	480	A	Sidechain
27	B8	505	A	Sidechain
27	B8	507	A	Sidechain
27	B8	532	A	Sidechain
27	B8	569	U	Sidechain
27	B8	60	G	Sidechain
27	B8	630	G	Sidechain
27	B8	642	U	Sidechain
27	B8	674	G	Sidechain
27	B8	675	A	Sidechain
27	B8	676	A	Sidechain
27	B8	684	G	Sidechain
27	B8	705	A	Sidechain
27	B8	712	G	Sidechain
27	B8	72	U	Sidechain
27	B8	728	G	Sidechain
27	B8	738	G	Sidechain
27	B8	773	U	Sidechain
27	B8	821	A	Sidechain
27	B8	849	A	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
27	B8	858	G	Sidechain
27	B8	877	A	Sidechain
27	B8	899	A	Sidechain
27	B8	959	A	Sidechain
28	BA	181	ARG	Peptide
28	BA	198	GLY	Peptide
28	BA	293	TRP	Peptide
28	BA	314	GLN	Peptide
28	BA	72	LEU	Peptide
34	BF	137	PHE	Peptide
36	BH	31	VAL	Peptide
49	BU	48	VAL	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	33080	0	16649	21	0
2	AX	231	0	120	0	0
3	AV	1649	0	834	1	0
4	AZ	779	0	798	4	0
5	A0	1640	0	1641	0	0
5	A1	1640	0	1641	0	0
6	AB	1872	0	1885	3	0
7	AC	1822	0	1913	2	0
8	AD	1643	0	1710	1	0
9	AE	1225	0	1273	1	0
10	AF	1101	0	1050	1	0
11	AG	1400	0	1449	0	0
12	AH	979	0	1034	1	0
13	AI	1036	0	1084	0	0
14	AJ	825	0	865	2	0
15	AK	965	0	997	0	0
16	AL	955	0	1019	2	0
17	AM	910	0	981	0	0
18	AN	805	0	847	1	0
19	AO	716	0	742	0	0
20	AP	649	0	666	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	AQ	672	0	716	1	0
22	AR	626	0	651	0	0
23	AS	727	0	769	0	0
24	AT	670	0	722	2	0
25	AU	590	0	631	1	0
26	B7	2570	0	1301	0	0
27	B8	62341	0	31354	41	0
28	BA	3362	0	3511	38	0
29	BB	889	0	982	1	0
30	B5	1733	0	1824	1	0
31	B6	2092	0	2170	2	0
32	BD	1565	0	1616	1	0
33	BE	1552	0	1619	1	0
34	BF	1420	0	1460	1	0
35	BG	1323	0	1374	0	0
36	BH	1111	0	1148	2	0
37	BI	1032	0	1088	0	0
38	BJ	1129	0	1162	0	0
39	BK	947	0	1023	0	0
40	BL	1053	0	1129	1	0
41	BM	1074	0	1157	1	0
42	BN	1008	0	1045	1	0
43	BO	900	0	935	0	0
44	BP	917	0	965	0	0
45	BQ	947	0	1022	0	0
46	BR	816	0	839	1	0
47	BS	857	0	922	0	0
48	BT	787	0	846	0	0
49	BU	789	0	847	0	0
50	BV	753	0	780	0	0
51	BW	634	0	656	0	0
52	BX	625	0	655	0	0
53	BY	509	0	543	0	0
54	BZ	449	0	491	0	0
55	B0	444	0	461	0	0
56	B1	441	0	485	2	0
57	B2	377	0	418	1	0
58	B3	504	0	574	1	0
59	B4	302	0	343	0	0
60	A0	1078	0	1694	1	0
60	A1	1225	0	1925	4	0
60	AZ	245	0	385	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
60	B8	294	0	462	2	0
60	BA	1568	0	2464	34	0
60	BB	539	0	847	0	0
61	A0	510	0	760	0	0
61	A1	204	0	304	2	0
61	AZ	102	0	152	0	0
61	B8	51	0	76	0	0
61	BA	408	0	608	1	0
61	BB	357	0	532	0	0
All	All	163040	0	119641	141	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 0.

All (141) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:BA:416:PHE:CD1	28:BA:416:PHE:CE1	1.92	1.58
28:BA:416:PHE:CD2	28:BA:416:PHE:CE2	1.95	1.54
28:BA:416:PHE:CE2	28:BA:416:PHE:CZ	1.95	1.53
28:BA:416:PHE:CE1	28:BA:416:PHE:CZ	1.95	1.51
28:BA:416:PHE:CD1	28:BA:416:PHE:CG	1.98	1.49
28:BA:416:PHE:CD2	28:BA:416:PHE:CG	2.01	1.46
28:BA:416:PHE:CG	60:BA:533:PEV:H401	1.82	1.13
28:BA:416:PHE:CD2	60:BA:533:PEV:C39	2.32	1.12
28:BA:416:PHE:CE2	60:BA:533:PEV:C39	2.33	1.12
28:BA:416:PHE:CD1	60:BA:533:PEV:C39	2.33	1.12
28:BA:416:PHE:CD2	60:BA:533:PEV:H392	1.84	1.12
28:BA:416:PHE:CE2	60:BA:533:PEV:C40	2.33	1.12
28:BA:416:PHE:CG	60:BA:533:PEV:C40	2.33	1.12
28:BA:416:PHE:CD1	60:BA:533:PEV:C40	2.33	1.11
28:BA:416:PHE:CD2	60:BA:533:PEV:H402	1.85	1.11
28:BA:416:PHE:CE1	60:BA:533:PEV:C39	2.33	1.11
28:BA:416:PHE:CD2	60:BA:533:PEV:C40	2.32	1.11
28:BA:416:PHE:CZ	60:BA:533:PEV:C40	2.33	1.11
28:BA:416:PHE:CE1	60:BA:533:PEV:C40	2.34	1.11
28:BA:416:PHE:CZ	60:BA:533:PEV:C39	2.33	1.11
28:BA:416:PHE:CG	60:BA:533:PEV:C39	2.33	1.10
28:BA:416:PHE:CG	60:BA:533:PEV:H391	1.86	1.10
28:BA:416:PHE:CE2	60:BA:533:PEV:H402	1.91	1.04
28:BA:416:PHE:CD1	60:BA:533:PEV:H391	1.94	1.03

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:BA:416:PHE:CE2	60:BA:533:PEV:H392	1.96	1.01
28:BA:416:PHE:CD1	60:BA:533:PEV:H401	1.97	0.99
60:BA:533:PEV:C39	60:BA:533:PEV:C40	2.52	0.87
4:AZ:81:LEU:HD13	4:AZ:82:GLY:H	1.53	0.72
28:BA:324:ALA:HB2	60:BA:531:PEV:H402	1.73	0.70
28:BA:416:PHE:CZ	60:BA:533:PEV:C38	2.77	0.68
28:BA:416:PHE:CE1	60:BA:533:PEV:C38	2.79	0.65
28:BA:416:PHE:CZ	60:BA:533:PEV:H381	2.33	0.63
28:BA:416:PHE:CE1	60:BA:533:PEV:C41	2.82	0.62
28:BA:416:PHE:CZ	60:BA:533:PEV:C41	2.85	0.59
28:BA:416:PHE:CE1	60:BA:533:PEV:H381	2.39	0.57
27:B8:2091:C:H3'	27:B8:2092:U:H5''	1.87	0.56
27:B8:1021:A:H61	27:B8:1142:A:H61	1.53	0.56
3:AV:27:A:H61	3:AV:45:G:H1	1.52	0.55
27:B8:1024:G:H3'	27:B8:1025:G:H5''	1.88	0.55
1:AA:664:G:H22	1:AA:741:G:H1	1.54	0.55
27:B8:500:G:H21	27:B8:505:A:H62	1.55	0.55
27:B8:2792:A:H3'	27:B8:2793:C:H5''	1.90	0.53
27:B8:871:U:H3	27:B8:906:U:H3	1.56	0.53
27:B8:962:G:H21	27:B8:2250:G:H1	1.57	0.53
27:B8:870:U:H2'	27:B8:871:U:H5''	1.90	0.53
61:BA:512:PGV:H72	60:BA:513:PEV:H401	1.91	0.53
27:B8:1083:U:HO2'	27:B8:1084:A:H8	1.58	0.51
14:AJ:15:HIS:CD2	14:AJ:16:ARG:HE	2.29	0.51
1:AA:507:C:H3'	1:AA:508:U:H5''	1.92	0.50
4:AZ:39:LEU:HD13	28:BA:286:PHE:HB3	1.93	0.50
60:B8:3001:PEV:H401	60:B8:3002:PEV:H401	1.92	0.50
21:AQ:18:LYS:H	21:AQ:50:ASN:HD21	1.59	0.50
1:AA:1239:A:H62	1:AA:1299:A:H62	1.60	0.50
25:AU:33:ARG:HE	25:AU:34:ARG:H	1.59	0.50
1:AA:1305:G:H21	1:AA:1332:A:H8	1.59	0.49
27:B8:1065:U:H3	27:B8:1069:A:H2'	1.76	0.49
36:BH:126:GLY:H	36:BH:128:HIS:CE1	2.30	0.49
1:AA:82:G:H3'	1:AA:83:C:H4'	1.95	0.49
27:B8:713:G:H21	27:B8:718:A:H2	1.60	0.49
1:AA:632:U:H3'	1:AA:633:G:H5'	1.95	0.49
28:BA:416:PHE:CZ	60:BA:533:PEV:H411	2.48	0.49
27:B8:870:U:C2'	27:B8:871:U:H5''	2.43	0.48
1:AA:243:A:H4'	1:AA:244:U:H5'	1.94	0.48
27:B8:1551:A:H3'	27:B8:1552:A:H5''	1.95	0.48
9:AE:89:THR:HG22	9:AE:90:GLY:H	1.77	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:AP:54:LEU:H	20:AP:54:LEU:HD12	1.78	0.48
60:BA:503:PEV:H442	60:BA:503:PEV:H401	1.95	0.48
1:AA:1122:U:H5''	7:AC:222:GLN:H	1.78	0.48
28:BA:416:PHE:CE1	60:BA:533:PEV:H411	2.48	0.48
12:AH:60:LEU:H	12:AH:60:LEU:HD23	1.79	0.48
20:AP:78:VAL:HG23	20:AP:81:ALA:H	1.79	0.48
60:A1:301:PEV:H392	61:A1:303:PGV:H02	1.96	0.47
24:AT:67:HIS:CD2	24:AT:69:ASN:H	2.32	0.47
27:B8:82:U:H3	27:B8:104:A:H61	1.63	0.47
30:B5:165:ASN:HD21	30:B5:169:GLY:H	1.63	0.47
1:AA:1223:C:H3'	1:AA:1224:U:C5'	2.45	0.47
58:B3:36:ALA:H	58:B3:39:ARG:HE	1.62	0.47
60:A0:315:PEV:H391	60:A1:302:PEV:H401	1.96	0.47
27:B8:957:C:H42	27:B8:2494:G:H21	1.61	0.47
27:B8:2091:C:H3'	27:B8:2092:U:C5'	2.46	0.46
36:BH:101:ASP:H	36:BH:111:ALA:HB3	1.80	0.46
4:AZ:25:LEU:CB	28:BA:333:THR:HG23	2.46	0.46
27:B8:2371:G:H21	56:B1:45:HIS:HE1	1.63	0.46
27:B8:63:A:H2'	27:B8:64:A:C8	2.51	0.46
60:A1:323:PEV:H142	60:A1:323:PEV:H392	1.97	0.46
27:B8:2171:A:H1'	27:B8:2172:U:C6	2.50	0.45
27:B8:480:A:H3'	27:B8:481:G:H5''	1.98	0.45
1:AA:262:A:H4'	24:AT:67:HIS:CD2	2.52	0.44
60:A1:319:PEV:H361	60:A1:319:PEV:H392	1.91	0.44
27:B8:2371:G:H21	56:B1:45:HIS:CE1	2.35	0.44
1:AA:973:G:H3'	1:AA:974:A:H5''	1.99	0.44
6:AB:14:HIS:CE1	6:AB:200:PRO:HB3	2.53	0.44
27:B8:890:C:H3'	27:B8:891:G:H4'	2.00	0.44
27:B8:1203:U:H3'	27:B8:1204:A:H5''	1.99	0.44
10:AF:94:HIS:CG	10:AF:95:ALA:H	2.37	0.43
1:AA:404:G:H1	1:AA:499:A:H62	1.65	0.43
8:AD:96:ARG:HB2	8:AD:99:ASN:HD22	1.82	0.43
32:BD:33:ARG:HH11	32:BD:93:GLY:H	1.67	0.43
27:B8:1273:U:H3	27:B8:2002:G:H21	1.67	0.43
27:B8:2874:C:H4'	42:BN:4:ARG:HH21	1.84	0.43
27:B8:532:A:H4'	27:B8:533:G:C8	2.54	0.43
57:B2:24:THR:HG23	57:B2:27:GLY:H	1.84	0.43
27:B8:572:A:H5''	46:BR:80:ARG:HH21	1.84	0.43
27:B8:1567:G:H5'	31:B6:57:HIS:CD2	2.54	0.43
6:AB:103:TRP:HE1	6:AB:107:ARG:HH21	1.66	0.42
27:B8:2682:A:C2	27:B8:2683:C:C5	3.06	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:B8:1205:A:C5	33:BE:165:HIS:HB3	2.54	0.42
27:B8:880:G:H2'	27:B8:881:G:C8	2.55	0.42
27:B8:877:A:C2	27:B8:901:C:C2	3.08	0.42
27:B8:1391:U:H2'	27:B8:1393:A:C2	2.53	0.42
29:BB:123:THR:HA	29:BB:126:ARG:HH12	1.84	0.42
31:B6:264:LYS:H	31:B6:264:LYS:HD2	1.85	0.42
34:BF:106:ALA:HA	34:BF:111:ARG:HH11	1.85	0.42
1:AA:413:G:H4'	1:AA:414:A:H5''	2.02	0.42
6:AB:169:HIS:H	6:AB:169:HIS:CD2	2.37	0.42
27:B8:962:G:N2	27:B8:2250:G:H1	2.17	0.42
27:B8:2233:U:H2'	27:B8:2234:G:C8	2.55	0.42
1:AA:995:C:H2'	1:AA:996:A:H5''	2.02	0.42
1:AA:537:G:H5''	16:AL:109:ARG:HH12	1.85	0.41
1:AA:1130:A:H61	1:AA:1144:G:H1'	1.86	0.41
1:AA:1144:G:N2	1:AA:1146:A:H62	2.19	0.41
16:AL:41:PRO:HG2	16:AL:45:ASN:H	1.85	0.41
27:B8:900:A:H2'	27:B8:901:C:H5'	2.02	0.41
27:B8:1082:U:N3	27:B8:1086:A:C2	2.88	0.41
1:AA:412:A:H3'	1:AA:413:G:C5'	2.51	0.41
60:BA:514:PEV:H362	60:BA:514:PEV:H391	1.94	0.41
27:B8:1283:G:H22	27:B8:1286:A:H5'	1.85	0.41
27:B8:251:A:H4'	40:BL:49:GLY:HA2	2.02	0.41
27:B8:2351:G:H2'	27:B8:2365:G:H22	1.84	0.41
4:AZ:25:LEU:HB3	28:BA:333:THR:HG23	2.03	0.41
61:A1:315:PGV:H132	61:A1:315:PGV:H102	1.98	0.41
1:AA:781:A:H2'	1:AA:782:A:H5'	2.02	0.41
27:B8:2645:G:H3'	27:B8:2646:C:H5'	2.02	0.41
60:B8:3002:PEV:H362	60:B8:3002:PEV:H392	1.94	0.41
1:AA:1118:U:H1'	1:AA:1179:A:C4	2.55	0.41
7:AC:10:ARG:HH21	7:AC:175:HIS:HA	1.85	0.40
14:AJ:15:HIS:HA	14:AJ:18:ILE:HG22	2.01	0.40
60:BA:520:PEV:H402	60:BA:526:PEV:H441	2.04	0.40
1:AA:483:C:H2'	1:AA:484:G:C8	2.57	0.40
18:AN:60:ARG:HA	18:AN:60:ARG:HE	1.86	0.40
41:BM:78:LEU:H	41:BM:78:LEU:HD23	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	
4	AZ	96/98 (98%)	74 (77%)	13 (14%)	9 (9%)	0	10
5	A0	198/200 (99%)	174 (88%)	20 (10%)	4 (2%)	7	38
5	A1	198/200 (99%)	169 (85%)	23 (12%)	6 (3%)	4	28
6	AB	238/240 (99%)	190 (80%)	42 (18%)	6 (2%)	5	32
7	AC	230/232 (99%)	184 (80%)	31 (14%)	15 (6%)	1	16
8	AD	203/205 (99%)	163 (80%)	28 (14%)	12 (6%)	1	17
9	AE	164/166 (99%)	137 (84%)	21 (13%)	6 (4%)	3	24
10	AF	133/135 (98%)	109 (82%)	22 (16%)	2 (2%)	10	46
11	AG	176/178 (99%)	142 (81%)	29 (16%)	5 (3%)	5	30
12	AH	127/129 (98%)	102 (80%)	23 (18%)	2 (2%)	9	44
13	AI	127/129 (98%)	108 (85%)	11 (9%)	8 (6%)	1	17
14	AJ	101/103 (98%)	85 (84%)	9 (9%)	7 (7%)	1	15
15	AK	126/128 (98%)	106 (84%)	15 (12%)	5 (4%)	3	23
16	AL	121/123 (98%)	108 (89%)	12 (10%)	1 (1%)	19	60
17	AM	115/117 (98%)	96 (84%)	13 (11%)	6 (5%)	2	19
18	AN	98/100 (98%)	81 (83%)	9 (9%)	8 (8%)	1	12
19	AO	86/88 (98%)	79 (92%)	5 (6%)	2 (2%)	6	34
20	AP	80/82 (98%)	73 (91%)	5 (6%)	2 (2%)	5	32
21	AQ	81/83 (98%)	67 (83%)	8 (10%)	6 (7%)	1	13
22	AR	72/74 (97%)	59 (82%)	9 (12%)	4 (6%)	2	18
23	AS	89/91 (98%)	73 (82%)	12 (14%)	4 (4%)	2	22
24	AT	84/86 (98%)	76 (90%)	7 (8%)	1 (1%)	13	50
25	AU	68/70 (97%)	64 (94%)	4 (6%)	0	100	100
28	BA	433/435 (100%)	313 (72%)	66 (15%)	54 (12%)	0	5
29	BB	114/116 (98%)	96 (84%)	12 (10%)	6 (5%)	2	19

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
30	B5	232/234 (99%)	211 (91%)	15 (6%)	6 (3%)	5	31
31	B6	270/272 (99%)	227 (84%)	31 (12%)	12 (4%)	2	22
32	BD	207/209 (99%)	172 (83%)	24 (12%)	11 (5%)	2	19
33	BE	199/201 (99%)	169 (85%)	20 (10%)	10 (5%)	2	20
34	BF	176/178 (99%)	137 (78%)	27 (15%)	12 (7%)	1	15
35	BG	174/176 (99%)	137 (79%)	28 (16%)	9 (5%)	2	19
36	BH	147/149 (99%)	108 (74%)	31 (21%)	8 (5%)	2	19
37	BI	139/141 (99%)	125 (90%)	11 (8%)	3 (2%)	6	35
38	BJ	140/142 (99%)	117 (84%)	19 (14%)	4 (3%)	4	29
39	BK	121/123 (98%)	99 (82%)	16 (13%)	6 (5%)	2	20
40	BL	142/144 (99%)	129 (91%)	10 (7%)	3 (2%)	7	36
41	BM	134/136 (98%)	107 (80%)	17 (13%)	10 (8%)	1	13
42	BN	125/127 (98%)	104 (83%)	12 (10%)	9 (7%)	1	14
43	BO	115/117 (98%)	97 (84%)	15 (13%)	3 (3%)	5	31
44	BP	112/114 (98%)	94 (84%)	11 (10%)	7 (6%)	1	17
45	BQ	115/117 (98%)	94 (82%)	15 (13%)	6 (5%)	2	19
46	BR	101/103 (98%)	83 (82%)	13 (13%)	5 (5%)	2	20
47	BS	108/110 (98%)	81 (75%)	18 (17%)	9 (8%)	1	12
48	BT	98/100 (98%)	71 (72%)	20 (20%)	7 (7%)	1	14
49	BU	101/103 (98%)	84 (83%)	14 (14%)	3 (3%)	4	28
50	BV	92/94 (98%)	82 (89%)	9 (10%)	1 (1%)	14	52
51	BW	82/84 (98%)	59 (72%)	19 (23%)	4 (5%)	2	20
52	BX	75/77 (97%)	57 (76%)	12 (16%)	6 (8%)	1	12
53	BY	61/63 (97%)	48 (79%)	11 (18%)	2 (3%)	4	26
54	BZ	56/58 (97%)	49 (88%)	4 (7%)	3 (5%)	2	19
55	B0	54/56 (96%)	47 (87%)	6 (11%)	1 (2%)	8	38
56	B1	52/54 (96%)	46 (88%)	5 (10%)	1 (2%)	8	38
57	B2	44/46 (96%)	31 (70%)	10 (23%)	3 (7%)	1	15
58	B3	62/64 (97%)	52 (84%)	9 (14%)	1 (2%)	9	44
59	B4	36/38 (95%)	32 (89%)	3 (8%)	1 (3%)	5	30
All	All	7128/7238 (98%)	5877 (82%)	904 (13%)	347 (5%)	4	20

All (347) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	AZ	48	TRP
4	AZ	61	VAL
4	AZ	81	LEU
5	A1	177	ARG
7	AC	206	ILE
7	AC	219	PRO
9	AE	17	VAL
13	AI	127	SER
14	AJ	57	VAL
14	AJ	67	ILE
17	AM	3	ILE
18	AN	80	ARG
28	BA	48	VAL
28	BA	56	GLN
28	BA	68	SER
28	BA	72	LEU
28	BA	79	ALA
28	BA	148	LEU
28	BA	200	PRO
28	BA	237	VAL
28	BA	249	ALA
28	BA	275	ILE
28	BA	314	GLN
28	BA	319	LEU
28	BA	332	TYR
28	BA	353	VAL
28	BA	358	PRO
28	BA	373	LEU
29	BB	67	ALA
31	B6	132	ARG
31	B6	197	ALA
31	B6	231	HIS
31	B6	261	ARG
33	BE	4	VAL
34	BF	82	TYR
34	BF	136	ILE
35	BG	2	ARG
35	BG	94	ARG
36	BH	32	PRO
36	BH	115	VAL
38	BJ	40	HIS
39	BK	71	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
41	BM	43	ALA
41	BM	56	ALA
41	BM	122	ALA
44	BP	25	VAL
45	BQ	71	ASN
46	BR	3	ALA
46	BR	48	LYS
46	BR	101	ILE
47	BS	76	VAL
48	BT	35	ALA
48	BT	36	LYS
48	BT	99	ALA
49	BU	49	PRO
4	AZ	49	MET
6	AB	95	TRP
6	AB	224	ARG
7	AC	190	THR
8	AD	7	LYS
10	AF	85	ILE
11	AG	77	ARG
12	AH	73	SER
14	AJ	85	ASP
15	AK	11	VAL
16	AL	54	VAL
17	AM	29	SER
17	AM	87	GLY
18	AN	21	ALA
21	AQ	12	VAL
21	AQ	13	SER
21	AQ	81	ALA
22	AR	24	ASP
23	AS	28	LYS
28	BA	235	VAL
28	BA	256	ARG
28	BA	267	LEU
28	BA	308	LEU
28	BA	320	LEU
28	BA	333	THR
28	BA	340	ARG
28	BA	351	ALA
28	BA	362	THR
28	BA	363	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
28	BA	369	VAL
28	BA	371	THR
28	BA	401	PHE
28	BA	431	SER
29	BB	19	TRP
29	BB	71	PHE
31	B6	142	ASN
32	BD	31	ALA
32	BD	46	ARG
32	BD	107	VAL
33	BE	12	LEU
33	BE	30	GLN
34	BF	74	ALA
34	BF	84	ILE
34	BF	103	ILE
34	BF	138	PRO
37	BI	87	SER
40	BL	113	ALA
41	BM	55	ARG
41	BM	72	PRO
41	BM	73	ILE
41	BM	135	VAL
42	BN	63	ARG
44	BP	106	ALA
45	BQ	101	ASP
46	BR	65	ALA
47	BS	12	SER
47	BS	53	SER
47	BS	89	ALA
48	BT	72	GLN
53	BY	2	LYS
53	BY	37	LEU
4	AZ	109	ASP
5	A0	170	LEU
5	A1	228	SER
7	AC	53	ARG
7	AC	106	ARG
7	AC	116	ALA
8	AD	6	PRO
8	AD	21	LYS
8	AD	146	GLU
8	AD	176	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	AE	120	HIS
11	AG	80	GLY
11	AG	138	GLU
12	AH	116	ARG
13	AI	35	GLU
13	AI	59	LYS
14	AJ	17	LEU
17	AM	105	ALA
19	AO	87	ARG
20	AP	54	LEU
23	AS	86	LYS
28	BA	57	ARG
28	BA	71	ALA
28	BA	78	PHE
28	BA	145	MET
28	BA	236	PHE
28	BA	254	GLY
28	BA	260	ALA
28	BA	278	ILE
28	BA	356	ILE
28	BA	391	MET
28	BA	432	ALA
29	BB	45	ALA
29	BB	69	VAL
30	B5	87	ALA
30	B5	159	GLY
31	B6	112	GLY
31	B6	152	GLN
31	B6	189	ALA
31	B6	205	GLY
32	BD	65	ALA
32	BD	140	HIS
32	BD	175	LEU
33	BE	16	GLU
33	BE	130	LYS
33	BE	154	ASP
34	BF	42	ALA
34	BF	77	LYS
34	BF	123	GLY
34	BF	124	ARG
35	BG	21	GLN
36	BH	14	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
36	BH	75	LEU
36	BH	84	ALA
38	BJ	111	LYS
39	BK	36	GLY
40	BL	53	GLY
42	BN	13	ASN
42	BN	122	ALA
43	BO	89	ASP
43	BO	113	ALA
44	BP	54	LEU
44	BP	113	LEU
48	BT	97	GLY
50	BV	44	HIS
51	BW	27	GLY
51	BW	41	GLY
51	BW	52	CYS
52	BX	27	ARG
52	BX	32	LEU
54	BZ	8	GLN
54	BZ	10	ARG
57	B2	23	ALA
57	B2	35	ARG
4	AZ	55	LEU
4	AZ	101	GLN
5	A0	154	ALA
5	A1	71	PHE
5	A1	164	ALA
6	AB	74	ALA
7	AC	82	ASP
8	AD	20	LEU
8	AD	28	ASP
8	AD	35	GLN
8	AD	36	ALA
8	AD	174	ALA
9	AE	9	GLU
10	AF	114	ASP
13	AI	121	ARG
14	AJ	78	GLU
15	AK	2	LYS
17	AM	16	ILE
18	AN	38	GLU
18	AN	68	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
21	AQ	15	LYS
21	AQ	51	GLU
22	AR	2	ARG
22	AR	26	ALA
23	AS	55	GLN
23	AS	87	LYS
28	BA	39	ILE
28	BA	42	PRO
28	BA	151	ASN
28	BA	214	ASP
28	BA	346	LEU
28	BA	352	PHE
28	BA	435	LYS
30	B5	52	ALA
30	B5	82	ALA
30	B5	89	ALA
30	B5	147	PRO
31	B6	214	GLY
31	B6	240	GLY
32	BD	122	VAL
32	BD	203	VAL
33	BE	106	LYS
35	BG	31	GLU
35	BG	47	ASN
37	BI	97	VAL
38	BJ	68	LYS
39	BK	113	MET
40	BL	66	PHE
41	BM	134	THR
42	BN	10	LEU
42	BN	32	GLU
42	BN	80	PHE
42	BN	121	LYS
43	BO	16	ARG
44	BP	35	SER
44	BP	81	ASP
45	BQ	9	ALA
46	BR	27	ILE
47	BS	31	GLN
47	BS	64	ALA
49	BU	12	VAL
49	BU	75	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
52	BX	15	ASN
54	BZ	29	ARG
57	B2	8	SER
4	AZ	72	ASP
4	AZ	94	ILE
5	A1	157	ASP
6	AB	28	PRO
6	AB	33	ALA
7	AC	9	ILE
7	AC	47	ALA
7	AC	61	LYS
7	AC	128	MET
7	AC	218	LYS
8	AD	47	LEU
8	AD	147	LYS
9	AE	44	ARG
11	AG	2	ARG
11	AG	4	ARG
14	AJ	59	LYS
15	AK	101	ALA
17	AM	116	LYS
18	AN	28	ALA
18	AN	43	ALA
18	AN	66	THR
19	AO	73	ASP
24	AT	47	GLN
28	BA	61	ILE
28	BA	330	PHE
29	BB	65	GLY
32	BD	9	VAL
32	BD	109	VAL
33	BE	2	GLU
33	BE	83	VAL
33	BE	96	VAL
34	BF	148	VAL
35	BG	100	ASN
35	BG	136	ASP
35	BG	155	PRO
36	BH	55	GLU
36	BH	87	GLU
39	BK	92	GLU
39	BK	122	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
41	BM	67	VAL
42	BN	72	ASP
44	BP	76	HIS
45	BQ	27	ARG
45	BQ	81	GLY
47	BS	32	ALA
47	BS	40	ASN
48	BT	10	VAL
52	BX	41	SER
56	B1	33	LEU
5	A0	47	LEU
5	A0	156	VAL
6	AB	132	GLU
7	AC	111	ASP
7	AC	205	GLU
7	AC	213	VAL
13	AI	58	GLU
13	AI	109	GLN
13	AI	110	VAL
14	AJ	48	ARG
15	AK	12	ARG
22	AR	14	ALA
28	BA	337	PHE
31	B6	59	GLN
34	BF	111	ARG
35	BG	156	TYR
36	BH	41	LYS
37	BI	30	GLN
41	BM	70	ASP
42	BN	100	CYS
48	BT	29	THR
52	BX	3	VAL
52	BX	6	VAL
55	B0	44	ALA
58	B3	53	ASP
5	A1	227	VAL
13	AI	57	VAL
18	AN	33	VAL
59	B4	16	ILE
9	AE	15	ILE
20	AP	36	VAL
39	BK	35	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
45	BQ	33	VAL
9	AE	105	ILE
15	AK	88	PRO
21	AQ	11	VAL
28	BA	306	ILE
28	BA	403	GLY
32	BD	152	PRO
38	BJ	96	ARG
28	BA	318	VAL
51	BW	73	PRO
47	BS	45	VAL

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	
4	AZ	85/85 (100%)	72 (85%)	13 (15%)	2	14
5	A0	176/176 (100%)	174 (99%)	2 (1%)	73	84
5	A1	176/176 (100%)	173 (98%)	3 (2%)	60	78
6	AB	198/198 (100%)	194 (98%)	4 (2%)	55	74
7	AC	189/189 (100%)	183 (97%)	6 (3%)	39	61
8	AD	172/172 (100%)	166 (96%)	6 (4%)	36	59
9	AE	125/125 (100%)	122 (98%)	3 (2%)	49	69
10	AF	116/116 (100%)	111 (96%)	5 (4%)	29	53
11	AG	146/146 (100%)	146 (100%)	0	100	100
12	AH	104/104 (100%)	101 (97%)	3 (3%)	42	64
13	AI	106/106 (100%)	101 (95%)	5 (5%)	26	51
14	AJ	90/90 (100%)	88 (98%)	2 (2%)	52	71
15	AK	98/98 (100%)	95 (97%)	3 (3%)	40	62
16	AL	103/103 (100%)	102 (99%)	1 (1%)	76	86
17	AM	95/95 (100%)	92 (97%)	3 (3%)	39	61

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	AN	83/83 (100%)	81 (98%)	2 (2%)	49	69
19	AO	76/76 (100%)	74 (97%)	2 (3%)	46	66
20	AP	65/65 (100%)	65 (100%)	0	100	100
21	AQ	77/77 (100%)	74 (96%)	3 (4%)	32	56
22	AR	64/64 (100%)	63 (98%)	1 (2%)	62	79
23	AS	78/78 (100%)	78 (100%)	0	100	100
24	AT	65/65 (100%)	65 (100%)	0	100	100
25	AU	60/60 (100%)	58 (97%)	2 (3%)	38	61
28	BA	353/353 (100%)	326 (92%)	27 (8%)	13	37
29	BB	92/92 (100%)	88 (96%)	4 (4%)	29	53
30	B5	181/181 (100%)	178 (98%)	3 (2%)	60	78
31	B6	217/217 (100%)	212 (98%)	5 (2%)	50	70
32	BD	164/164 (100%)	158 (96%)	6 (4%)	34	58
33	BE	165/165 (100%)	164 (99%)	1 (1%)	86	92
34	BF	149/149 (100%)	145 (97%)	4 (3%)	44	65
35	BG	137/137 (100%)	134 (98%)	3 (2%)	52	71
36	BH	114/114 (100%)	108 (95%)	6 (5%)	22	47
37	BI	109/109 (100%)	106 (97%)	3 (3%)	43	65
38	BJ	116/116 (100%)	113 (97%)	3 (3%)	46	66
39	BK	104/104 (100%)	99 (95%)	5 (5%)	25	50
40	BL	103/103 (100%)	102 (99%)	1 (1%)	76	86
41	BM	109/109 (100%)	109 (100%)	0	100	100
42	BN	103/103 (100%)	100 (97%)	3 (3%)	42	64
43	BO	87/87 (100%)	87 (100%)	0	100	100
44	BP	99/99 (100%)	96 (97%)	3 (3%)	41	63
45	BQ	89/89 (100%)	89 (100%)	0	100	100
46	BR	84/84 (100%)	84 (100%)	0	100	100
47	BS	93/93 (100%)	93 (100%)	0	100	100
48	BT	84/84 (100%)	79 (94%)	5 (6%)	19	44
49	BU	84/84 (100%)	82 (98%)	2 (2%)	49	69
50	BV	78/78 (100%)	77 (99%)	1 (1%)	69	81

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
51	BW	62/62 (100%)	61 (98%)	1 (2%)	62	79
52	BX	67/67 (100%)	66 (98%)	1 (2%)	65	80
53	BY	55/55 (100%)	54 (98%)	1 (2%)	59	77
54	BZ	48/48 (100%)	47 (98%)	1 (2%)	53	72
55	B0	47/47 (100%)	46 (98%)	1 (2%)	53	72
56	B1	48/48 (100%)	47 (98%)	1 (2%)	53	72
57	B2	38/38 (100%)	37 (97%)	1 (3%)	46	66
58	B3	51/51 (100%)	50 (98%)	1 (2%)	55	74
59	B4	34/34 (100%)	34 (100%)	0	100	100
All	All	5911/5911 (100%)	5749 (97%)	162 (3%)	48	65

All (162) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	AZ	28	ILE
4	AZ	54	ARG
4	AZ	60	LEU
4	AZ	71	ASN
4	AZ	75	ARG
4	AZ	78	ILE
4	AZ	79	LEU
4	AZ	81	LEU
4	AZ	95	ILE
4	AZ	97	THR
4	AZ	99	ILE
4	AZ	107	ARG
4	AZ	115	HIS
5	A0	132	GLN
5	A0	133	LYS
5	A1	112	MET
5	A1	132	GLN
5	A1	237	THR
6	AB	103	TRP
6	AB	164	ASP
6	AB	169	HIS
6	AB	174	GLU
7	AC	106	ARG
7	AC	114	LEU
7	AC	131	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	AC	214	GLU
7	AC	219	PRO
7	AC	225	LYS
8	AD	13	ARG
8	AD	20	LEU
8	AD	43	ARG
8	AD	110	ARG
8	AD	170	LEU
8	AD	182	LYS
9	AE	75	LEU
9	AE	89	THR
9	AE	150	GLU
10	AF	16	GLU
10	AF	44	ARG
10	AF	47	LEU
10	AF	104	LYS
10	AF	107	ASP
12	AH	2	MET
12	AH	26	MET
12	AH	123	GLU
13	AI	17	ARG
13	AI	40	ARG
13	AI	44	ARG
13	AI	58	GLU
13	AI	129	ARG
14	AJ	31	ARG
14	AJ	81	GLU
15	AK	10	ARG
15	AK	75	GLU
15	AK	79	LYS
16	AL	50	LYS
17	AM	69	ARG
17	AM	91	ARG
17	AM	113	LYS
18	AN	53	ASP
18	AN	64	ARG
19	AO	16	ARG
19	AO	87	ARG
21	AQ	5	ARG
21	AQ	17	GLU
21	AQ	26	ARG
22	AR	11	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
25	AU	18	PHE
25	AU	69	LEU
28	BA	53	LEU
28	BA	55	GLN
28	BA	85	TYR
28	BA	130	PHE
28	BA	180	GLU
28	BA	189	ILE
28	BA	192	PHE
28	BA	195	ILE
28	BA	212	GLN
28	BA	228	PHE
28	BA	237	VAL
28	BA	252	GLN
28	BA	256	ARG
28	BA	290	ILE
28	BA	309	TYR
28	BA	317	TYR
28	BA	336	VAL
28	BA	340	ARG
28	BA	347	LYS
28	BA	352	PHE
28	BA	356	ILE
28	BA	357	ARG
28	BA	361	GLN
28	BA	372	ARG
28	BA	373	LEU
28	BA	374	THR
28	BA	441	TYR
29	BB	44	ARG
29	BB	76	ARG
29	BB	77	THR
29	BB	104	MET
30	B5	7	ARG
30	B5	9	ARG
30	B5	166	ASP
31	B6	129	LEU
31	B6	212	TRP
31	B6	227	VAL
31	B6	264	LYS
31	B6	269	ARG
32	BD	74	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	BD	84	LEU
32	BD	86	GLU
32	BD	124	ARG
32	BD	128	ARG
32	BD	201	LEU
33	BE	60	TRP
34	BF	80	GLN
34	BF	119	LYS
34	BF	129	MET
34	BF	136	ILE
35	BG	34	ARG
35	BG	61	TRP
35	BG	94	ARG
36	BH	8	LYS
36	BH	21	VAL
36	BH	32	PRO
36	BH	70	GLU
36	BH	109	GLU
36	BH	144	VAL
37	BI	10	LEU
37	BI	35	MET
37	BI	95	ASP
38	BJ	23	LYS
38	BJ	35	ARG
38	BJ	129	GLU
39	BK	41	ILE
39	BK	70	ARG
39	BK	89	ASN
39	BK	114	LYS
39	BK	121	GLU
40	BL	126	ARG
42	BN	8	ARG
42	BN	49	GLU
42	BN	64	ARG
44	BP	43	GLU
44	BP	50	ARG
44	BP	87	ARG
48	BT	36	LYS
48	BT	61	LEU
48	BT	66	LYS
48	BT	69	ARG
48	BT	96	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
49	BU	49	PRO
49	BU	91	LYS
50	BV	46	LYS
51	BW	23	LYS
52	BX	26	ARG
53	BY	27	ASN
54	BZ	55	LYS
55	B0	31	LYS
56	B1	27	ARG
57	B2	12	ARG
58	B3	6	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
6	AB	14	HIS
6	AB	169	HIS
6	AB	189	ASN
7	AC	175	HIS
7	AC	215	GLN
8	AD	40	HIS
8	AD	99	ASN
14	AJ	15	HIS
15	AK	108	ASN
16	AL	71	HIS
18	AN	48	GLN
20	AP	9	HIS
20	AP	18	GLN
21	AQ	50	ASN
22	AR	53	GLN
23	AS	13	HIS
24	AT	60	GLN
24	AT	67	HIS
28	BA	55	GLN
28	BA	212	GLN
31	B6	52	HIS
31	B6	57	HIS
31	B6	229	HIS
31	B6	238	ASN
33	BE	92	HIS
35	BG	100	ASN
35	BG	115	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
36	BH	2	GLN
36	BH	20	ASN
36	BH	128	HIS
36	BH	133	GLN
38	BJ	80	HIS
38	BJ	132	HIS
39	BK	5	GLN
39	BK	89	ASN
42	BN	16	HIS
43	BO	34	HIS
45	BQ	13	HIS
46	BR	82	HIS
46	BR	87	GLN
50	BV	88	HIS
52	BX	35	HIS
55	B0	18	HIS
58	B3	42	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1541/1542 (99%)	273 (17%)	23 (1%)
2	AX	10/11 (90%)	5 (50%)	0
26	B7	119/120 (99%)	19 (15%)	2 (1%)
27	B8	2903/2904 (99%)	442 (15%)	47 (1%)
3	AV	76/77 (98%)	14 (18%)	1 (1%)
All	All	4649/4654 (99%)	753 (16%)	73 (1%)

All (753) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	2	A
1	AA	5	U
1	AA	7	A
1	AA	9	G
1	AA	15	G
1	AA	31	G
1	AA	32	A
1	AA	39	G
1	AA	47	C
1	AA	48	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	AA	51	A
1	AA	52	C
1	AA	55	A
1	AA	61	G
1	AA	66	A
1	AA	67	C
1	AA	70	U
1	AA	71	A
1	AA	75	G
1	AA	79	G
1	AA	80	A
1	AA	83	C
1	AA	84	U
1	AA	85	U
1	AA	86	G
1	AA	88	U
1	AA	91	U
1	AA	101	A
1	AA	121	U
1	AA	144	G
1	AA	149	A
1	AA	155	A
1	AA	182	A
1	AA	196	A
1	AA	197	A
1	AA	204	G
1	AA	205	A
1	AA	209	U
1	AA	210	C
1	AA	211	G
1	AA	239	U
1	AA	240	G
1	AA	243	A
1	AA	244	U
1	AA	245	U
1	AA	247	G
1	AA	252	U
1	AA	253	A
1	AA	257	G
1	AA	258	G
1	AA	266	G
1	AA	267	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	AA	280	C
1	AA	289	G
1	AA	306	A
1	AA	308	C
1	AA	316	C
1	AA	328	C
1	AA	329	A
1	AA	332	G
1	AA	345	C
1	AA	352	C
1	AA	354	G
1	AA	367	U
1	AA	373	A
1	AA	374	A
1	AA	381	C
1	AA	382	A
1	AA	397	A
1	AA	398	U
1	AA	406	G
1	AA	408	A
1	AA	409	U
1	AA	411	A
1	AA	412	A
1	AA	413	G
1	AA	414	A
1	AA	416	G
1	AA	421	U
1	AA	424	G
1	AA	429	U
1	AA	430	A
1	AA	435	A
1	AA	451	A
1	AA	456	A
1	AA	459	A
1	AA	460	A
1	AA	461	A
1	AA	462	G
1	AA	463	U
1	AA	465	A
1	AA	466	A
1	AA	468	A
1	AA	482	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	AA	484	G
1	AA	485	U
1	AA	486	U
1	AA	493	A
1	AA	494	G
1	AA	499	A
1	AA	508	U
1	AA	511	C
1	AA	512	U
1	AA	518	C
1	AA	524	G
1	AA	527	G
1	AA	532	A
1	AA	533	A
1	AA	535	A
1	AA	547	A
1	AA	561	U
1	AA	563	A
1	AA	564	C
1	AA	572	A
1	AA	573	A
1	AA	576	C
1	AA	577	G
1	AA	596	A
1	AA	611	C
1	AA	633	G
1	AA	653	U
1	AA	654	G
1	AA	665	A
1	AA	666	G
1	AA	721	G
1	AA	724	G
1	AA	731	G
1	AA	747	A
1	AA	748	G
1	AA	752	G
1	AA	755	G
1	AA	781	A
1	AA	782	A
1	AA	793	U
1	AA	794	A
1	AA	812	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	AA	815	A
1	AA	817	C
1	AA	818	G
1	AA	821	G
1	AA	828	U
1	AA	841	C
1	AA	842	U
1	AA	843	U
1	AA	844	G
1	AA	845	A
1	AA	846	G
1	AA	847	G
1	AA	849	G
1	AA	873	A
1	AA	914	A
1	AA	926	G
1	AA	927	G
1	AA	934	C
1	AA	935	A
1	AA	945	G
1	AA	960	U
1	AA	961	U
1	AA	966	G
1	AA	968	A
1	AA	969	A
1	AA	971	G
1	AA	974	A
1	AA	975	A
1	AA	976	G
1	AA	977	A
1	AA	981	U
1	AA	993	G
1	AA	994	A
1	AA	996	A
1	AA	1004	A
1	AA	1014	A
1	AA	1015	G
1	AA	1018	G
1	AA	1020	G
1	AA	1028	C
1	AA	1030	U
1	AA	1032	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	AA	1034	G
1	AA	1036	A
1	AA	1043	G
1	AA	1050	G
1	AA	1053	G
1	AA	1065	U
1	AA	1066	C
1	AA	1070	U
1	AA	1085	U
1	AA	1086	U
1	AA	1094	G
1	AA	1095	U
1	AA	1101	A
1	AA	1112	C
1	AA	1118	U
1	AA	1119	C
1	AA	1124	G
1	AA	1125	U
1	AA	1130	A
1	AA	1133	G
1	AA	1135	U
1	AA	1136	C
1	AA	1139	G
1	AA	1140	C
1	AA	1141	C
1	AA	1143	G
1	AA	1145	A
1	AA	1146	A
1	AA	1152	A
1	AA	1154	G
1	AA	1159	U
1	AA	1160	G
1	AA	1167	A
1	AA	1181	G
1	AA	1184	G
1	AA	1191	A
1	AA	1196	A
1	AA	1197	A
1	AA	1202	U
1	AA	1212	U
1	AA	1213	A
1	AA	1215	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	AA	1225	A
1	AA	1226	C
1	AA	1227	A
1	AA	1238	A
1	AA	1249	C
1	AA	1250	A
1	AA	1258	G
1	AA	1261	A
1	AA	1270	G
1	AA	1279	G
1	AA	1280	A
1	AA	1285	A
1	AA	1286	U
1	AA	1287	A
1	AA	1297	G
1	AA	1300	G
1	AA	1301	U
1	AA	1303	C
1	AA	1305	G
1	AA	1316	G
1	AA	1320	C
1	AA	1323	G
1	AA	1331	G
1	AA	1346	A
1	AA	1353	G
1	AA	1363	A
1	AA	1364	U
1	AA	1380	U
1	AA	1399	C
1	AA	1419	G
1	AA	1432	G
1	AA	1446	A
1	AA	1448	C
1	AA	1452	C
1	AA	1454	G
1	AA	1493	A
1	AA	1494	G
1	AA	1497	G
1	AA	1499	A
1	AA	1503	A
1	AA	1506	U
1	AA	1507	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	AA	1517	G
1	AA	1520	C
1	AA	1526	G
1	AA	1528	U
1	AA	1529	G
1	AA	1530	G
1	AA	1535	C
1	AA	1539	C
1	AA	1540	U
1	AA	1541	U
1	AA	1542	A
2	AX	13	C
2	AX	14	G
2	AX	18	C
2	AX	19	U
2	AX	22	A
3	AV	4	C
3	AV	5	A
3	AV	6	C
3	AV	8	U
3	AV	20	G
3	AV	22	A
3	AV	32	C
3	AV	44	G
3	AV	49	C
3	AV	50	G
3	AV	54	G
3	AV	68	G
3	AV	72	C
3	AV	77	A
26	B7	9	G
26	B7	13	G
26	B7	14	U
26	B7	15	A
26	B7	16	G
26	B7	26	C
26	B7	29	A
26	B7	30	C
26	B7	42	C
26	B7	45	A
26	B7	52	A
26	B7	53	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
26	B7	66	A
26	B7	67	G
26	B7	90	C
26	B7	91	C
26	B7	99	A
26	B7	109	A
26	B7	120	U
27	B8	13	A
27	B8	34	U
27	B8	35	G
27	B8	46	G
27	B8	63	A
27	B8	64	A
27	B8	71	A
27	B8	74	A
27	B8	75	G
27	B8	84	A
27	B8	90	U
27	B8	91	A
27	B8	92	U
27	B8	93	G
27	B8	95	A
27	B8	100	U
27	B8	103	A
27	B8	118	A
27	B8	120	U
27	B8	136	G
27	B8	137	U
27	B8	139	U
27	B8	141	G
27	B8	143	C
27	B8	144	A
27	B8	160	A
27	B8	181	A
27	B8	196	A
27	B8	199	A
27	B8	216	A
27	B8	221	A
27	B8	222	A
27	B8	228	C
27	B8	233	A
27	B8	241	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
27	B8	248	G
27	B8	252	G
27	B8	255	A
27	B8	265	A
27	B8	266	G
27	B8	268	C
27	B8	271	G
27	B8	273	G
27	B8	277	G
27	B8	278	A
27	B8	281	C
27	B8	283	G
27	B8	285	G
27	B8	286	U
27	B8	294	A
27	B8	311	A
27	B8	321	U
27	B8	329	G
27	B8	330	A
27	B8	333	G
27	B8	346	A
27	B8	352	A
27	B8	353	C
27	B8	362	A
27	B8	363	G
27	B8	364	C
27	B8	371	A
27	B8	372	G
27	B8	386	G
27	B8	387	U
27	B8	405	U
27	B8	406	G
27	B8	411	G
27	B8	412	A
27	B8	424	G
27	B8	455	C
27	B8	457	A
27	B8	479	A
27	B8	481	G
27	B8	491	G
27	B8	505	A
27	B8	508	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
27	B8	509	C
27	B8	510	C
27	B8	512	G
27	B8	528	A
27	B8	531	C
27	B8	533	G
27	B8	544	C
27	B8	545	U
27	B8	546	U
27	B8	547	A
27	B8	548	G
27	B8	549	G
27	B8	555	G
27	B8	563	A
27	B8	573	U
27	B8	575	A
27	B8	586	A
27	B8	588	U
27	B8	603	A
27	B8	613	A
27	B8	637	A
27	B8	646	U
27	B8	647	G
27	B8	654	A
27	B8	655	A
27	B8	671	C
27	B8	686	U
27	B8	730	A
27	B8	747	U
27	B8	757	G
27	B8	764	A
27	B8	775	G
27	B8	776	G
27	B8	782	A
27	B8	784	G
27	B8	785	G
27	B8	788	A
27	B8	789	A
27	B8	793	A
27	B8	802	A
27	B8	805	G
27	B8	812	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
27	B8	819	A
27	B8	827	U
27	B8	828	U
27	B8	830	G
27	B8	846	U
27	B8	847	U
27	B8	859	G
27	B8	869	G
27	B8	871	U
27	B8	875	G
27	B8	876	C
27	B8	881	G
27	B8	887	U
27	B8	891	G
27	B8	896	A
27	B8	897	C
27	B8	900	A
27	B8	901	C
27	B8	910	A
27	B8	912	C
27	B8	919	U
27	B8	931	U
27	B8	932	U
27	B8	941	A
27	B8	945	A
27	B8	946	C
27	B8	961	C
27	B8	973	A
27	B8	974	G
27	B8	980	A
27	B8	982	C
27	B8	983	A
27	B8	985	C
27	B8	991	C
27	B8	995	C
27	B8	996	A
27	B8	1005	C
27	B8	1012	U
27	B8	1013	C
27	B8	1022	G
27	B8	1025	G
27	B8	1033	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
27	B8	1054	A
27	B8	1056	G
27	B8	1061	U
27	B8	1062	G
27	B8	1070	A
27	B8	1071	G
27	B8	1078	U
27	B8	1088	A
27	B8	1090	A
27	B8	1095	A
27	B8	1096	A
27	B8	1104	C
27	B8	1112	G
27	B8	1116	G
27	B8	1130	U
27	B8	1132	U
27	B8	1133	A
27	B8	1134	A
27	B8	1135	C
27	B8	1136	G
27	B8	1139	G
27	B8	1142	A
27	B8	1176	U
27	B8	1206	G
27	B8	1237	A
27	B8	1238	G
27	B8	1241	A
27	B8	1242	U
27	B8	1248	G
27	B8	1250	G
27	B8	1253	A
27	B8	1256	G
27	B8	1266	G
27	B8	1271	G
27	B8	1272	A
27	B8	1273	U
27	B8	1275	A
27	B8	1276	A
27	B8	1300	G
27	B8	1301	A
27	B8	1312	U
27	B8	1313	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
27	B8	1316	U
27	B8	1325	U
27	B8	1326	U
27	B8	1334	G
27	B8	1336	A
27	B8	1337	G
27	B8	1352	U
27	B8	1365	A
27	B8	1374	G
27	B8	1379	U
27	B8	1386	C
27	B8	1394	U
27	B8	1396	U
27	B8	1416	G
27	B8	1419	A
27	B8	1420	A
27	B8	1421	G
27	B8	1427	A
27	B8	1428	C
27	B8	1451	C
27	B8	1454	C
27	B8	1459	G
27	B8	1460	U
27	B8	1461	C
27	B8	1469	A
27	B8	1476	U
27	B8	1477	A
27	B8	1478	G
27	B8	1482	G
27	B8	1490	A
27	B8	1497	U
27	B8	1504	A
27	B8	1505	A
27	B8	1507	C
27	B8	1508	A
27	B8	1509	A
27	B8	1523	U
27	B8	1524	G
27	B8	1532	A
27	B8	1535	A
27	B8	1538	G
27	B8	1552	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
27	B8	1560	G
27	B8	1569	A
27	B8	1578	U
27	B8	1583	A
27	B8	1585	C
27	B8	1608	A
27	B8	1609	A
27	B8	1610	A
27	B8	1618	A
27	B8	1634	A
27	B8	1635	A
27	B8	1640	A
27	B8	1647	U
27	B8	1648	U
27	B8	1654	A
27	B8	1674	G
27	B8	1677	A
27	B8	1700	A
27	B8	1714	U
27	B8	1715	G
27	B8	1729	U
27	B8	1730	C
27	B8	1731	G
27	B8	1733	G
27	B8	1738	G
27	B8	1756	G
27	B8	1758	U
27	B8	1761	C
27	B8	1764	C
27	B8	1773	A
27	B8	1776	G
27	B8	1781	U
27	B8	1782	U
27	B8	1784	A
27	B8	1800	C
27	B8	1801	A
27	B8	1808	A
27	B8	1809	A
27	B8	1816	C
27	B8	1819	A
27	B8	1829	A
27	B8	1870	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
27	B8	1896	G
27	B8	1906	G
27	B8	1913	A
27	B8	1914	C
27	B8	1929	G
27	B8	1930	G
27	B8	1940	U
27	B8	1955	U
27	B8	1965	C
27	B8	1966	A
27	B8	1967	C
27	B8	1970	A
27	B8	1971	U
27	B8	1972	G
27	B8	1991	U
27	B8	1993	U
27	B8	1997	C
27	B8	2020	A
27	B8	2022	U
27	B8	2023	C
27	B8	2031	A
27	B8	2033	A
27	B8	2043	C
27	B8	2055	C
27	B8	2056	G
27	B8	2059	A
27	B8	2061	G
27	B8	2062	A
27	B8	2065	C
27	B8	2069	G
27	B8	2077	A
27	B8	2102	G
27	B8	2104	C
27	B8	2111	U
27	B8	2116	G
27	B8	2117	A
27	B8	2118	U
27	B8	2119	A
27	B8	2120	G
27	B8	2128	G
27	B8	2133	G
27	B8	2135	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
27	B8	2136	G
27	B8	2137	U
27	B8	2138	G
27	B8	2145	C
27	B8	2146	C
27	B8	2147	A
27	B8	2148	G
27	B8	2149	U
27	B8	2153	C
27	B8	2155	U
27	B8	2158	A
27	B8	2164	C
27	B8	2165	C
27	B8	2166	U
27	B8	2167	U
27	B8	2176	A
27	B8	2179	C
27	B8	2181	U
27	B8	2192	U
27	B8	2198	A
27	B8	2199	A
27	B8	2204	G
27	B8	2212	A
27	B8	2213	U
27	B8	2214	C
27	B8	2225	A
27	B8	2238	G
27	B8	2239	G
27	B8	2250	G
27	B8	2251	G
27	B8	2266	A
27	B8	2271	G
27	B8	2278	A
27	B8	2279	G
27	B8	2283	C
27	B8	2286	G
27	B8	2287	A
27	B8	2297	A
27	B8	2305	U
27	B8	2307	G
27	B8	2308	G
27	B8	2311	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
27	B8	2322	A
27	B8	2324	U
27	B8	2325	G
27	B8	2333	A
27	B8	2335	A
27	B8	2336	A
27	B8	2337	G
27	B8	2347	C
27	B8	2357	G
27	B8	2383	G
27	B8	2385	C
27	B8	2396	G
27	B8	2407	A
27	B8	2426	A
27	B8	2429	G
27	B8	2430	A
27	B8	2434	A
27	B8	2441	U
27	B8	2448	A
27	B8	2458	G
27	B8	2472	G
27	B8	2473	U
27	B8	2476	A
27	B8	2478	A
27	B8	2491	U
27	B8	2498	C
27	B8	2505	G
27	B8	2506	U
27	B8	2518	A
27	B8	2529	G
27	B8	2530	A
27	B8	2534	A
27	B8	2535	G
27	B8	2554	U
27	B8	2566	A
27	B8	2567	G
27	B8	2573	C
27	B8	2585	U
27	B8	2586	U
27	B8	2602	A
27	B8	2609	U
27	B8	2613	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
27	B8	2629	U
27	B8	2630	G
27	B8	2689	U
27	B8	2690	U
27	B8	2714	G
27	B8	2726	A
27	B8	2729	G
27	B8	2744	G
27	B8	2748	A
27	B8	2757	A
27	B8	2765	A
27	B8	2778	A
27	B8	2791	G
27	B8	2793	C
27	B8	2799	A
27	B8	2800	A
27	B8	2808	G
27	B8	2809	A
27	B8	2820	A
27	B8	2821	A
27	B8	2832	U
27	B8	2836	U
27	B8	2849	U
27	B8	2850	A
27	B8	2867	G
27	B8	2872	A
27	B8	2873	A
27	B8	2883	A
27	B8	2904	U

All (73) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	AA	51	A
1	AA	60	A
1	AA	85	U
1	AA	243	A
1	AA	279	A
1	AA	328	C
1	AA	366	A
1	AA	372	C
1	AA	428	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	AA	429	U
1	AA	484	G
1	AA	653	U
1	AA	700	G
1	AA	960	U
1	AA	1049	U
1	AA	1065	U
1	AA	1159	U
1	AA	1201	A
1	AA	1226	C
1	AA	1300	G
1	AA	1301	U
1	AA	1319	A
1	AA	1541	U
3	AV	16	C
26	B7	14	U
26	B7	66	A
27	B8	91	A
27	B8	241	A
27	B8	320	A
27	B8	329	G
27	B8	507	A
27	B8	670	A
27	B8	792	A
27	B8	827	U
27	B8	858	G
27	B8	876	C
27	B8	880	G
27	B8	890	C
27	B8	891	G
27	B8	973	A
27	B8	984	A
27	B8	1061	U
27	B8	1133	A
27	B8	1205	A
27	B8	1272	A
27	B8	1312	U
27	B8	1608	A
27	B8	1699	G
27	B8	1730	C
27	B8	1786	A
27	B8	1808	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
27	B8	2076	U
27	B8	2116	G
27	B8	2118	U
27	B8	2144	G
27	B8	2145	C
27	B8	2152	G
27	B8	2159	G
27	B8	2164	C
27	B8	2172	U
27	B8	2282	G
27	B8	2286	G
27	B8	2324	U
27	B8	2336	A
27	B8	2402	U
27	B8	2425	A
27	B8	2430	A
27	B8	2491	U
27	B8	2601	C
27	B8	2713	U
27	B8	2756	U
27	B8	2797	U
27	B8	2903	U

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

133 ligands 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	$\# Z > 2$
60	PEV	A0	316	-	48,48,48	0.80	1 (2%)	51,53,53	0.84	2 (3%)
60	PEV	A0	322	-	48,48,48	0.79	1 (2%)	51,53,53	0.74	2 (3%)
60	PEV	AZ	201	-	48,48,48	0.75	1 (2%)	51,53,53	0.70	2 (3%)
60	PEV	A0	329	-	48,48,48	0.78	1 (2%)	51,53,53	0.72	2 (3%)
61	PGV	BA	515	-	50,50,50	1.05	2 (4%)	53,56,56	0.73	2 (3%)
61	PGV	A0	331	-	50,50,50	1.04	2 (4%)	53,56,56	0.77	2 (3%)
60	PEV	A1	304	-	48,48,48	0.77	1 (2%)	51,53,53	0.63	2 (3%)
60	PEV	BA	530	-	48,48,48	0.77	1 (2%)	51,53,53	0.67	2 (3%)
60	PEV	A1	321	-	48,48,48	0.78	1 (2%)	51,53,53	0.67	2 (3%)
60	PEV	A0	311	-	48,48,48	0.78	1 (2%)	51,53,53	0.67	2 (3%)
61	PGV	A0	305	-	50,50,50	1.04	2 (4%)	53,56,56	0.73	2 (3%)
60	PEV	BB	211	-	48,48,48	0.77	1 (2%)	51,53,53	0.73	2 (3%)
60	PEV	BA	520	-	48,48,48	0.78	1 (2%)	51,53,53	0.64	2 (3%)
60	PEV	BB	214	-	48,48,48	0.78	1 (2%)	51,53,53	0.71	2 (3%)
60	PEV	BB	210	-	48,48,48	0.77	1 (2%)	51,53,53	0.72	2 (3%)
60	PEV	A0	309	-	48,48,48	0.79	1 (2%)	51,53,53	0.70	2 (3%)
60	PEV	BA	506	-	48,48,48	0.75	1 (2%)	51,53,53	0.70	2 (3%)
60	PEV	A1	323	-	48,48,48	0.76	1 (2%)	51,53,53	0.66	2 (3%)
61	PGV	BB	207	-	50,50,50	1.06	2 (4%)	53,56,56	0.77	2 (3%)
60	PEV	A1	302	-	48,48,48	0.79	1 (2%)	51,53,53	0.71	2 (3%)
60	PEV	A1	301	-	48,48,48	0.78	2 (4%)	51,53,53	0.71	2 (3%)
60	PEV	A1	328	-	48,48,48	0.76	1 (2%)	51,53,53	0.68	2 (3%)
60	PEV	A1	319	-	48,48,48	0.77	1 (2%)	51,53,53	0.65	1 (1%)
60	PEV	B8	3004	-	48,48,48	0.78	1 (2%)	51,53,53	0.70	2 (3%)
60	PEV	BB	218	-	48,48,48	0.77	1 (2%)	51,53,53	0.70	2 (3%)
60	PEV	B8	3006	-	48,48,48	0.78	1 (2%)	51,53,53	0.67	2 (3%)
60	PEV	A0	313	-	48,48,48	0.80	1 (2%)	51,53,53	0.74	2 (3%)
60	PEV	BB	215	-	48,48,48	0.76	1 (2%)	51,53,53	0.69	2 (3%)
60	PEV	A1	313	-	48,48,48	0.77	1 (2%)	51,53,53	0.73	2 (3%)
60	PEV	BA	526	-	48,48,48	0.77	1 (2%)	51,53,53	0.69	2 (3%)
61	PGV	A0	328	-	50,50,50	1.05	2 (4%)	53,56,56	0.76	2 (3%)
60	PEV	BA	539	-	48,48,48	0.78	1 (2%)	51,53,53	0.79	2 (3%)
60	PEV	A0	330	-	48,48,48	0.78	1 (2%)	51,53,53	0.65	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
60	PEV	AZ	203	-	48,48,48	0.77	1 (2%)	51,53,53	0.63	2 (3%)
60	PEV	BB	216	-	48,48,48	0.78	1 (2%)	51,53,53	0.77	2 (3%)
60	PEV	BB	201	-	48,48,48	0.79	1 (2%)	51,53,53	0.70	2 (3%)
60	PEV	BA	529	-	48,48,48	0.80	1 (2%)	51,53,53	0.70	2 (3%)
61	PGV	A1	311	-	50,50,50	1.06	2 (4%)	53,56,56	0.80	2 (3%)
60	PEV	B8	3003	-	48,48,48	0.79	1 (2%)	51,53,53	0.71	2 (3%)
60	PEV	BA	504	-	48,48,48	0.79	1 (2%)	51,53,53	0.80	2 (3%)
61	PGV	BA	501	-	50,50,50	1.05	2 (4%)	53,56,56	0.81	2 (3%)
61	PGV	BA	512	-	50,50,50	1.04	2 (4%)	53,56,56	0.75	2 (3%)
61	PGV	A0	332	-	50,50,50	1.06	2 (4%)	53,56,56	0.76	2 (3%)
61	PGV	BA	505	-	50,50,50	1.05	2 (4%)	53,56,56	0.77	2 (3%)
60	PEV	BB	202	-	48,48,48	0.78	1 (2%)	51,53,53	0.71	2 (3%)
60	PEV	A1	308	-	48,48,48	0.79	1 (2%)	51,53,53	0.65	2 (3%)
60	PEV	A1	314	-	48,48,48	0.78	1 (2%)	51,53,53	0.69	2 (3%)
60	PEV	A1	309	-	48,48,48	0.78	1 (2%)	51,53,53	0.74	2 (3%)
60	PEV	A1	329	-	48,48,48	0.78	1 (2%)	51,53,53	0.72	2 (3%)
60	PEV	AZ	202	-	48,48,48	0.77	1 (2%)	51,53,53	0.72	2 (3%)
60	PEV	BA	535	-	48,48,48	0.78	1 (2%)	51,53,53	0.67	2 (3%)
60	PEV	B8	3007	-	48,48,48	0.77	1 (2%)	51,53,53	0.64	2 (3%)
60	PEV	A1	310	-	48,48,48	0.77	1 (2%)	51,53,53	0.72	2 (3%)
60	PEV	A1	316	-	48,48,48	0.78	1 (2%)	51,53,53	0.74	2 (3%)
60	PEV	A0	321	-	48,48,48	0.79	1 (2%)	51,53,53	0.81	3 (5%)
60	PEV	A0	315	-	48,48,48	0.76	1 (2%)	51,53,53	0.64	2 (3%)
61	PGV	BB	205	-	50,50,50	1.05	2 (4%)	53,56,56	0.80	2 (3%)
60	PEV	B8	3001	-	48,48,48	0.79	1 (2%)	51,53,53	0.71	2 (3%)
60	PEV	A1	320	-	48,48,48	0.79	1 (2%)	51,53,53	0.71	2 (3%)
61	PGV	A0	306	-	50,50,50	1.05	2 (4%)	53,56,56	0.75	2 (3%)
61	PGV	A0	304	-	50,50,50	1.06	2 (4%)	53,56,56	0.81	2 (3%)
60	PEV	BA	502	-	48,48,48	0.77	1 (2%)	51,53,53	0.70	2 (3%)
60	PEV	BA	537	-	48,48,48	0.80	2 (4%)	51,53,53	0.74	2 (3%)
60	PEV	BB	206	-	48,48,48	0.78	1 (2%)	51,53,53	0.70	2 (3%)
61	PGV	A1	303	-	50,50,50	1.05	2 (4%)	53,56,56	0.75	2 (3%)
60	PEV	A1	327	-	48,48,48	0.76	1 (2%)	51,53,53	0.69	2 (3%)
60	PEV	AZ	204	-	48,48,48	0.78	1 (2%)	51,53,53	0.67	2 (3%)
60	PEV	A1	322	-	48,48,48	0.76	1 (2%)	51,53,53	0.69	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
60	PEV	BA	528	-	48,48,48	0.78	1 (2%)	51,53,53	0.73	2 (3%)
61	PGV	BA	536	-	50,50,50	1.05	2 (4%)	53,56,56	0.73	2 (3%)
61	PGV	BB	213	-	50,50,50	1.06	2 (4%)	53,56,56	0.81	2 (3%)
60	PEV	BA	532	-	48,48,48	0.76	1 (2%)	51,53,53	0.74	2 (3%)
60	PEV	A1	317	-	48,48,48	0.79	2 (4%)	51,53,53	0.69	2 (3%)
61	PGV	BB	203	-	50,50,50	1.06	2 (4%)	53,56,56	0.76	2 (3%)
60	PEV	BA	525	-	48,48,48	0.79	1 (2%)	51,53,53	0.74	2 (3%)
61	PGV	BB	208	-	50,50,50	1.06	2 (4%)	53,56,56	0.74	2 (3%)
60	PEV	A1	324	-	48,48,48	0.78	1 (2%)	51,53,53	0.64	2 (3%)
60	PEV	BA	521	-	48,48,48	0.78	1 (2%)	51,53,53	0.67	2 (3%)
61	PGV	A0	327	-	50,50,50	1.06	2 (4%)	53,56,56	0.71	2 (3%)
60	PEV	BA	524	-	48,48,48	0.80	1 (2%)	51,53,53	0.70	2 (3%)
60	PEV	A1	325	-	48,48,48	0.78	1 (2%)	51,53,53	0.66	2 (3%)
60	PEV	BA	531	-	48,48,48	0.77	1 (2%)	51,53,53	0.66	2 (3%)
60	PEV	BA	507	-	48,48,48	0.78	1 (2%)	51,53,53	0.69	2 (3%)
61	PGV	BA	516	-	50,50,50	1.06	2 (4%)	53,56,56	0.70	2 (3%)
61	PGV	BA	522	-	50,50,50	1.06	2 (4%)	53,56,56	0.71	2 (3%)
61	PGV	AZ	207	-	50,50,50	1.05	2 (4%)	53,56,56	0.76	2 (3%)
61	PGV	B8	3005	-	50,50,50	1.05	2 (4%)	53,56,56	0.72	2 (3%)
60	PEV	A0	320	-	48,48,48	0.80	1 (2%)	51,53,53	0.65	2 (3%)
61	PGV	A0	325	-	50,50,50	1.05	2 (4%)	53,56,56	0.86	2 (3%)
60	PEV	BA	533	-	48,48,48	2.69	1 (2%)	51,53,53	1.32	2 (3%)
61	PGV	BA	540	-	50,50,50	1.04	2 (4%)	53,56,56	0.77	2 (3%)
61	PGV	A0	318	-	50,50,50	1.06	2 (4%)	53,56,56	0.74	2 (3%)
60	PEV	BA	514	-	48,48,48	0.80	1 (2%)	51,53,53	0.75	2 (3%)
60	PEV	A0	307	-	48,48,48	0.77	1 (2%)	51,53,53	0.65	2 (3%)
60	PEV	B8	3002	-	48,48,48	0.77	1 (2%)	51,53,53	0.66	2 (3%)
60	PEV	BA	503	-	48,48,48	0.79	1 (2%)	51,53,53	0.74	2 (3%)
61	PGV	A1	315	-	50,50,50	1.07	2 (4%)	53,56,56	0.79	2 (3%)
60	PEV	BA	518	-	48,48,48	0.77	1 (2%)	51,53,53	0.67	2 (3%)
60	PEV	A0	310	-	48,48,48	0.79	1 (2%)	51,53,53	0.82	2 (3%)
60	PEV	BA	519	-	48,48,48	0.78	1 (2%)	51,53,53	0.74	2 (3%)
61	PGV	BB	204	-	50,50,50	1.06	2 (4%)	53,56,56	0.81	2 (3%)
60	PEV	A0	303	-	48,48,48	0.80	1 (2%)	51,53,53	0.69	2 (3%)
60	PEV	A0	319	-	48,48,48	0.79	1 (2%)	51,53,53	0.75	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
60	PEV	BA	538	-	48,48,48	0.75	1 (2%)	51,53,53	0.65	2 (3%)
60	PEV	BA	517	-	48,48,48	0.78	1 (2%)	51,53,53	0.69	2 (3%)
60	PEV	BB	212	-	48,48,48	0.78	1 (2%)	51,53,53	0.66	2 (3%)
60	PEV	A0	314	-	48,48,48	0.80	1 (2%)	51,53,53	0.69	2 (3%)
60	PEV	A0	326	-	48,48,48	0.76	1 (2%)	51,53,53	0.71	2 (3%)
60	PEV	BA	509	-	48,48,48	0.79	1 (2%)	51,53,53	0.75	2 (3%)
60	PEV	AZ	206	-	48,48,48	0.78	1 (2%)	51,53,53	0.61	2 (3%)
60	PEV	A0	324	-	48,48,48	0.79	1 (2%)	51,53,53	0.71	2 (3%)
60	PEV	A0	302	-	48,48,48	0.77	1 (2%)	51,53,53	0.71	2 (3%)
60	PEV	BA	513	-	48,48,48	0.77	1 (2%)	51,53,53	0.68	2 (3%)
60	PEV	BA	510	-	48,48,48	0.77	1 (2%)	51,53,53	0.69	2 (3%)
60	PEV	BA	534	-	48,48,48	0.82	1 (2%)	51,53,53	0.75	2 (3%)
60	PEV	BA	527	-	48,48,48	0.79	1 (2%)	51,53,53	0.76	2 (3%)
60	PEV	A0	323	-	48,48,48	0.77	1 (2%)	51,53,53	0.71	2 (3%)
60	PEV	A1	306	-	48,48,48	0.79	1 (2%)	51,53,53	0.63	2 (3%)
60	PEV	A0	301	-	48,48,48	0.78	1 (2%)	51,53,53	0.68	2 (3%)
60	PEV	A1	305	-	48,48,48	0.78	1 (2%)	51,53,53	0.68	2 (3%)
60	PEV	A0	308	-	48,48,48	0.78	1 (2%)	51,53,53	0.75	2 (3%)
61	PGV	BB	217	-	50,50,50	1.05	2 (4%)	53,56,56	0.76	2 (3%)
60	PEV	A1	326	-	48,48,48	0.76	1 (2%)	51,53,53	0.68	2 (3%)
60	PEV	A0	312	-	48,48,48	0.79	1 (2%)	51,53,53	0.61	2 (3%)
60	PEV	BA	508	-	48,48,48	0.78	1 (2%)	51,53,53	0.68	2 (3%)
60	PEV	BB	209	-	48,48,48	0.76	1 (2%)	51,53,53	0.69	2 (3%)
60	PEV	BA	511	-	48,48,48	0.75	1 (2%)	51,53,53	0.70	2 (3%)
61	PGV	A0	317	-	50,50,50	1.05	2 (4%)	53,56,56	0.84	2 (3%)
61	PGV	A1	318	-	50,50,50	1.06	2 (4%)	53,56,56	0.79	2 (3%)
60	PEV	BA	523	-	48,48,48	0.78	1 (2%)	51,53,53	0.74	2 (3%)
60	PEV	A1	312	-	48,48,48	0.78	1 (2%)	51,53,53	0.68	2 (3%)
61	PGV	AZ	205	-	50,50,50	1.05	2 (4%)	53,56,56	0.76	2 (3%)
60	PEV	A1	307	-	48,48,48	0.78	1 (2%)	51,53,53	0.70	2 (3%)

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
60	PEV	A0	316	-	-	10/52/52/52	-
60	PEV	A0	322	-	-	6/52/52/52	-
60	PEV	AZ	201	-	-	5/52/52/52	-
61	PGV	BA	515	-	2/2/5/7	6/55/55/55	-
60	PEV	A0	329	-	-	4/52/52/52	-
61	PGV	A0	331	-	2/2/5/7	4/55/55/55	-
60	PEV	A1	304	-	-	5/52/52/52	-
60	PEV	BA	530	-	1/1/4/4	11/52/52/52	-
60	PEV	A1	321	-	-	7/52/52/52	-
60	PEV	A0	311	-	-	7/52/52/52	-
61	PGV	A0	305	-	1/1/5/7	10/55/55/55	-
60	PEV	BB	211	-	-	8/52/52/52	-
60	PEV	BA	520	-	-	5/52/52/52	-
60	PEV	BB	214	-	-	8/52/52/52	-
60	PEV	BB	210	-	-	13/52/52/52	-
60	PEV	A0	309	-	-	6/52/52/52	-
60	PEV	BA	506	-	-	5/52/52/52	-
60	PEV	A1	323	-	-	4/52/52/52	-
61	PGV	BB	207	-	2/2/5/7	4/55/55/55	-
60	PEV	A1	302	-	-	10/52/52/52	-
60	PEV	A1	301	-	1/1/4/4	13/52/52/52	-
60	PEV	A1	328	-	-	12/52/52/52	-
60	PEV	A1	319	-	-	4/52/52/52	-
60	PEV	B8	3004	-	-	9/52/52/52	-
60	PEV	BB	218	-	-	9/52/52/52	-
60	PEV	B8	3006	-	-	7/52/52/52	-
60	PEV	A0	313	-	-	5/52/52/52	-
60	PEV	BB	215	-	-	6/52/52/52	-
60	PEV	A1	313	-	1/1/4/4	8/52/52/52	-
60	PEV	BA	526	-	1/1/4/4	5/52/52/52	-
61	PGV	A0	328	-	2/2/5/7	10/55/55/55	-
60	PEV	BA	539	-	-	4/52/52/52	-
60	PEV	A0	330	-	-	10/52/52/52	-
60	PEV	AZ	203	-	-	8/52/52/52	-
60	PEV	BB	216	-	-	5/52/52/52	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
60	PEV	BB	201	-	-	11/52/52/52	-
60	PEV	BA	529	-	-	4/52/52/52	-
61	PGV	A1	311	-	2/2/5/7	8/55/55/55	-
60	PEV	B8	3003	-	-	15/52/52/52	-
60	PEV	BA	504	-	-	5/52/52/52	-
61	PGV	BA	501	-	1/1/5/7	7/55/55/55	-
61	PGV	BA	512	-	1/1/5/7	10/55/55/55	-
61	PGV	A0	332	-	2/2/5/7	7/55/55/55	-
61	PGV	BA	505	-	2/2/5/7	7/55/55/55	-
60	PEV	BB	202	-	1/1/4/4	3/52/52/52	-
60	PEV	A1	308	-	-	12/52/52/52	-
60	PEV	A1	314	-	-	6/52/52/52	-
60	PEV	A1	309	-	-	6/52/52/52	-
60	PEV	A1	329	-	-	5/52/52/52	-
60	PEV	AZ	202	-	-	8/52/52/52	-
60	PEV	BA	535	-	1/1/4/4	7/52/52/52	-
60	PEV	B8	3007	-	-	3/52/52/52	-
60	PEV	A1	310	-	-	8/52/52/52	-
60	PEV	A1	316	-	-	3/52/52/52	-
60	PEV	A0	321	-	-	11/52/52/52	-
60	PEV	A0	315	-	-	9/52/52/52	-
61	PGV	BB	205	-	2/2/5/7	6/55/55/55	-
60	PEV	B8	3001	-	1/1/4/4	3/52/52/52	-
60	PEV	A1	320	-	-	9/52/52/52	-
61	PGV	A0	306	-	2/2/5/7	7/55/55/55	-
61	PGV	A0	304	-	2/2/5/7	5/55/55/55	-
60	PEV	BA	502	-	1/1/4/4	8/52/52/52	-
60	PEV	BA	537	-	1/1/4/4	9/52/52/52	-
60	PEV	BB	206	-	1/1/4/4	9/52/52/52	-
61	PGV	A1	303	-	2/2/5/7	5/55/55/55	-
60	PEV	A1	327	-	-	7/52/52/52	-
60	PEV	AZ	204	-	1/1/4/4	8/52/52/52	-
61	PGV	BA	536	-	2/2/5/7	7/55/55/55	-
61	PGV	BB	213	-	1/1/5/7	9/55/55/55	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
60	PEV	A1	322	-	-	4/52/52/52	-
60	PEV	BA	528	-	-	9/52/52/52	-
60	PEV	BA	532	-	-	12/52/52/52	-
60	PEV	A1	317	-	1/1/4/4	9/52/52/52	-
61	PGV	BB	203	-	2/2/5/7	8/55/55/55	-
60	PEV	BA	525	-	-	11/52/52/52	-
61	PGV	BB	208	-	2/2/5/7	8/55/55/55	-
60	PEV	A1	324	-	-	5/52/52/52	-
61	PGV	A0	327	-	2/2/5/7	6/55/55/55	-
60	PEV	BA	521	-	-	8/52/52/52	-
60	PEV	BA	524	-	-	12/52/52/52	-
60	PEV	A1	325	-	-	12/52/52/52	-
60	PEV	BA	531	-	-	3/52/52/52	-
61	PGV	BA	516	-	2/2/5/7	7/55/55/55	-
60	PEV	BA	507	-	-	4/52/52/52	-
61	PGV	BA	522	-	2/2/5/7	2/55/55/55	-
61	PGV	AZ	207	-	2/2/5/7	8/55/55/55	-
61	PGV	B8	3005	-	2/2/5/7	8/55/55/55	-
60	PEV	A0	320	-	-	5/52/52/52	-
61	PGV	A0	325	-	2/2/5/7	8/55/55/55	-
61	PGV	BA	540	-	2/2/5/7	6/55/55/55	-
60	PEV	BA	533	-	-	10/52/52/52	-
61	PGV	A0	318	-	2/2/5/7	9/55/55/55	-
60	PEV	BA	514	-	-	8/52/52/52	-
60	PEV	A0	307	-	-	9/52/52/52	-
60	PEV	B8	3002	-	-	4/52/52/52	-
61	PGV	A1	315	-	2/2/5/7	13/55/55/55	-
60	PEV	BA	503	-	-	11/52/52/52	-
60	PEV	BA	518	-	-	9/52/52/52	-
60	PEV	A0	310	-	-	5/52/52/52	-
60	PEV	BA	519	-	-	11/52/52/52	-
61	PGV	BB	204	-	2/2/5/7	10/55/55/55	-
60	PEV	A0	303	-	-	7/52/52/52	-
60	PEV	BA	538	-	1/1/4/4	9/52/52/52	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
60	PEV	A0	319	-	-	8/52/52/52	-
60	PEV	BA	517	-	-	5/52/52/52	-
60	PEV	BB	212	-	-	6/52/52/52	-
60	PEV	A0	314	-	1/1/4/4	8/52/52/52	-
60	PEV	A0	326	-	-	9/52/52/52	-
60	PEV	BA	509	-	-	13/52/52/52	-
60	PEV	AZ	206	-	-	4/52/52/52	-
60	PEV	A0	324	-	-	7/52/52/52	-
60	PEV	A0	302	-	-	8/52/52/52	-
60	PEV	BA	513	-	-	7/52/52/52	-
60	PEV	BA	510	-	-	8/52/52/52	-
60	PEV	BA	534	-	-	5/52/52/52	-
60	PEV	BA	527	-	-	8/52/52/52	-
60	PEV	A0	323	-	1/1/4/4	7/52/52/52	-
60	PEV	A1	306	-	-	6/52/52/52	-
60	PEV	A0	301	-	-	11/52/52/52	-
60	PEV	A1	305	-	1/1/4/4	6/52/52/52	-
60	PEV	A0	308	-	1/1/4/4	5/52/52/52	-
61	PGV	BB	217	-	2/2/5/7	7/55/55/55	-
60	PEV	A1	326	-	-	4/52/52/52	-
60	PEV	A0	312	-	-	7/52/52/52	-
60	PEV	BA	508	-	1/1/4/4	5/52/52/52	-
61	PGV	A0	317	-	2/2/5/7	8/55/55/55	-
60	PEV	BA	511	-	-	5/52/52/52	-
60	PEV	BB	209	-	-	8/52/52/52	-
61	PGV	A1	318	-	2/2/5/7	11/55/55/55	-
60	PEV	BA	523	-	-	7/52/52/52	-
60	PEV	A1	312	-	-	5/52/52/52	-
61	PGV	AZ	205	-	2/2/5/7	15/55/55/55	-
60	PEV	A1	307	-	-	4/52/52/52	-

All (168) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
60	BA	533	PEV	C39-C40	17.92	2.52	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
61	BA	516	PGV	C9-C10	-4.44	1.34	1.52
61	BB	213	PGV	C9-C10	-4.42	1.34	1.52
61	BA	522	PGV	C9-C10	-4.38	1.34	1.52
61	A1	315	PGV	C9-C10	-4.38	1.34	1.52
61	BB	204	PGV	C9-C10	-4.38	1.34	1.52
61	BA	501	PGV	C9-C10	-4.37	1.34	1.52
61	BB	205	PGV	C9-C10	-4.37	1.34	1.52
61	AZ	207	PGV	C9-C10	-4.36	1.34	1.52
61	BA	515	PGV	C9-C10	-4.36	1.34	1.52
61	A0	327	PGV	C9-C10	-4.35	1.34	1.52
61	A0	331	PGV	C9-C10	-4.35	1.35	1.52
61	A0	318	PGV	C9-C10	-4.35	1.35	1.52
61	BB	208	PGV	C9-C10	-4.34	1.35	1.52
61	BA	540	PGV	C9-C10	-4.34	1.35	1.52
61	A0	305	PGV	C9-C10	-4.34	1.35	1.52
61	AZ	205	PGV	C9-C10	-4.33	1.35	1.52
61	BB	207	PGV	C9-C10	-4.33	1.35	1.52
61	A1	303	PGV	C9-C10	-4.32	1.35	1.52
61	A1	311	PGV	C9-C10	-4.32	1.35	1.52
61	A0	317	PGV	C9-C10	-4.32	1.35	1.52
61	BB	217	PGV	C9-C10	-4.31	1.35	1.52
61	BA	512	PGV	C9-C10	-4.30	1.35	1.52
61	A0	328	PGV	C9-C10	-4.30	1.35	1.52
61	BA	536	PGV	C9-C10	-4.30	1.35	1.52
61	A0	306	PGV	C9-C10	-4.30	1.35	1.52
61	A0	304	PGV	C9-C10	-4.29	1.35	1.52
61	B8	3005	PGV	C9-C10	-4.29	1.35	1.52
61	A1	318	PGV	C9-C10	-4.29	1.35	1.52
61	BA	505	PGV	C9-C10	-4.28	1.35	1.52
61	BB	203	PGV	C9-C10	-4.28	1.35	1.52
61	A0	332	PGV	C9-C10	-4.27	1.35	1.52
61	A0	325	PGV	C9-C10	-4.26	1.35	1.52
61	A0	325	PGV	C12-C11	4.01	1.55	1.31
61	BA	522	PGV	C12-C11	4.00	1.54	1.31
61	BB	203	PGV	C12-C11	4.00	1.54	1.31
61	BA	505	PGV	C12-C11	3.99	1.54	1.31
61	BA	516	PGV	C12-C11	3.99	1.54	1.31
61	BB	213	PGV	C12-C11	3.99	1.54	1.31
61	A1	303	PGV	C12-C11	3.98	1.54	1.31
61	A1	315	PGV	C12-C11	3.97	1.54	1.31
61	A0	327	PGV	C12-C11	3.97	1.54	1.31
61	A0	306	PGV	C12-C11	3.96	1.54	1.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
61	BB	204	PGV	C12-C11	3.96	1.54	1.31
61	A1	311	PGV	C12-C11	3.95	1.54	1.31
61	A0	332	PGV	C12-C11	3.95	1.54	1.31
61	A0	304	PGV	C12-C11	3.95	1.54	1.31
61	A0	318	PGV	C12-C11	3.95	1.54	1.31
61	BA	536	PGV	C12-C11	3.94	1.54	1.31
61	BB	217	PGV	C12-C11	3.94	1.54	1.31
61	BA	540	PGV	C12-C11	3.94	1.54	1.31
61	A1	318	PGV	C12-C11	3.94	1.54	1.31
61	A0	328	PGV	C12-C11	3.93	1.54	1.31
61	BB	208	PGV	C12-C11	3.93	1.54	1.31
61	A0	317	PGV	C12-C11	3.92	1.54	1.31
61	AZ	205	PGV	C12-C11	3.92	1.54	1.31
61	AZ	207	PGV	C12-C11	3.92	1.54	1.31
61	A0	331	PGV	C12-C11	3.92	1.54	1.31
61	BB	207	PGV	C12-C11	3.92	1.54	1.31
61	BA	501	PGV	C12-C11	3.91	1.54	1.31
61	A0	305	PGV	C12-C11	3.91	1.54	1.31
61	BA	512	PGV	C12-C11	3.90	1.54	1.31
61	B8	3005	PGV	C12-C11	3.89	1.54	1.31
61	BA	515	PGV	C12-C11	3.88	1.54	1.31
61	BB	205	PGV	C12-C11	3.88	1.54	1.31
60	A1	319	PEV	C39-C40	-3.00	1.34	1.51
60	B8	3004	PEV	C39-C40	-3.00	1.34	1.51
60	A0	309	PEV	C39-C40	-2.99	1.34	1.51
60	B8	3002	PEV	C39-C40	-2.98	1.34	1.51
60	BA	519	PEV	C39-C40	-2.98	1.34	1.51
60	BA	531	PEV	C39-C40	-2.98	1.34	1.51
60	A1	308	PEV	C39-C40	-2.98	1.34	1.51
60	A1	326	PEV	C39-C40	-2.97	1.34	1.51
60	AZ	204	PEV	C39-C40	-2.97	1.34	1.51
60	A0	314	PEV	C39-C40	-2.97	1.34	1.51
60	A1	301	PEV	C39-C40	-2.97	1.34	1.51
60	A0	308	PEV	C39-C40	-2.97	1.34	1.51
60	B8	3007	PEV	C39-C40	-2.97	1.34	1.51
60	BA	518	PEV	C39-C40	-2.97	1.34	1.51
60	BA	528	PEV	C39-C40	-2.96	1.34	1.51
60	BA	532	PEV	C39-C40	-2.96	1.34	1.51
60	BA	514	PEV	C39-C40	-2.96	1.34	1.51
60	BA	507	PEV	C39-C40	-2.96	1.34	1.51
60	A0	330	PEV	C39-C40	-2.96	1.34	1.51
60	AZ	206	PEV	C39-C40	-2.96	1.35	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
60	BA	530	PEV	C39-C40	-2.96	1.35	1.51
60	AZ	202	PEV	C39-C40	-2.96	1.35	1.51
60	A1	323	PEV	C39-C40	-2.96	1.35	1.51
60	BA	534	PEV	C39-C40	-2.96	1.35	1.51
60	A1	310	PEV	C39-C40	-2.96	1.35	1.51
60	A1	305	PEV	C39-C40	-2.96	1.35	1.51
60	A1	322	PEV	C39-C40	-2.96	1.35	1.51
60	BA	521	PEV	C39-C40	-2.96	1.35	1.51
60	A0	310	PEV	C39-C40	-2.96	1.35	1.51
60	BA	539	PEV	C39-C40	-2.96	1.35	1.51
60	BB	211	PEV	C39-C40	-2.96	1.35	1.51
60	A0	322	PEV	C39-C40	-2.95	1.35	1.51
60	A1	324	PEV	C39-C40	-2.95	1.35	1.51
60	A0	315	PEV	C39-C40	-2.95	1.35	1.51
60	A1	304	PEV	C39-C40	-2.95	1.35	1.51
60	A1	306	PEV	C39-C40	-2.95	1.35	1.51
60	A1	329	PEV	C39-C40	-2.95	1.35	1.51
60	BB	201	PEV	C39-C40	-2.95	1.35	1.51
60	A0	319	PEV	C39-C40	-2.95	1.35	1.51
60	A0	326	PEV	C39-C40	-2.95	1.35	1.51
60	B8	3006	PEV	C39-C40	-2.95	1.35	1.51
60	A1	328	PEV	C39-C40	-2.95	1.35	1.51
60	BA	517	PEV	C39-C40	-2.95	1.35	1.51
60	BA	504	PEV	C39-C40	-2.95	1.35	1.51
60	BA	535	PEV	C39-C40	-2.95	1.35	1.51
60	A0	313	PEV	C39-C40	-2.95	1.35	1.51
60	A0	329	PEV	C39-C40	-2.94	1.35	1.51
60	AZ	201	PEV	C39-C40	-2.94	1.35	1.51
60	A1	327	PEV	C39-C40	-2.94	1.35	1.51
60	BB	212	PEV	C39-C40	-2.94	1.35	1.51
60	BB	218	PEV	C39-C40	-2.94	1.35	1.51
60	A0	302	PEV	C39-C40	-2.94	1.35	1.51
60	BB	216	PEV	C39-C40	-2.94	1.35	1.51
60	AZ	203	PEV	C39-C40	-2.94	1.35	1.51
60	A0	324	PEV	C39-C40	-2.94	1.35	1.51
60	BA	538	PEV	C39-C40	-2.94	1.35	1.51
60	A0	312	PEV	C39-C40	-2.94	1.35	1.51
60	BA	527	PEV	C39-C40	-2.94	1.35	1.51
60	BB	202	PEV	C39-C40	-2.94	1.35	1.51
60	BA	508	PEV	C39-C40	-2.94	1.35	1.51
60	BB	210	PEV	C39-C40	-2.94	1.35	1.51
60	A1	302	PEV	C39-C40	-2.94	1.35	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
60	A1	314	PEV	C39-C40	-2.94	1.35	1.51
60	BA	537	PEV	C39-C40	-2.94	1.35	1.51
60	A0	303	PEV	C39-C40	-2.94	1.35	1.51
60	BA	509	PEV	C39-C40	-2.94	1.35	1.51
60	BB	214	PEV	C39-C40	-2.93	1.35	1.51
60	BA	526	PEV	C39-C40	-2.93	1.35	1.51
60	BA	520	PEV	C39-C40	-2.93	1.35	1.51
60	BA	506	PEV	C39-C40	-2.93	1.35	1.51
60	B8	3003	PEV	C39-C40	-2.93	1.35	1.51
60	A0	301	PEV	C39-C40	-2.93	1.35	1.51
60	BA	513	PEV	C39-C40	-2.93	1.35	1.51
60	A1	321	PEV	C39-C40	-2.93	1.35	1.51
60	BA	503	PEV	C39-C40	-2.93	1.35	1.51
60	BA	529	PEV	C39-C40	-2.93	1.35	1.51
60	BA	502	PEV	C39-C40	-2.93	1.35	1.51
60	A0	311	PEV	C39-C40	-2.93	1.35	1.51
60	A0	320	PEV	C39-C40	-2.92	1.35	1.51
60	BA	510	PEV	C39-C40	-2.92	1.35	1.51
60	BA	523	PEV	C39-C40	-2.92	1.35	1.51
60	A1	317	PEV	C39-C40	-2.92	1.35	1.51
60	A1	309	PEV	C39-C40	-2.92	1.35	1.51
60	A1	316	PEV	C39-C40	-2.92	1.35	1.51
60	A0	321	PEV	C39-C40	-2.92	1.35	1.51
60	B8	3001	PEV	C39-C40	-2.92	1.35	1.51
60	A1	320	PEV	C39-C40	-2.92	1.35	1.51
60	A1	307	PEV	C39-C40	-2.92	1.35	1.51
60	BB	209	PEV	C39-C40	-2.92	1.35	1.51
60	A1	312	PEV	C39-C40	-2.92	1.35	1.51
60	BA	525	PEV	C39-C40	-2.91	1.35	1.51
60	A0	307	PEV	C39-C40	-2.91	1.35	1.51
60	A0	323	PEV	C39-C40	-2.91	1.35	1.51
60	A1	313	PEV	C39-C40	-2.91	1.35	1.51
60	BA	524	PEV	C39-C40	-2.91	1.35	1.51
60	BB	206	PEV	C39-C40	-2.90	1.35	1.51
60	A1	325	PEV	C39-C40	-2.90	1.35	1.51
60	BB	215	PEV	C39-C40	-2.90	1.35	1.51
60	BA	511	PEV	C39-C40	-2.88	1.35	1.51
60	A0	316	PEV	C39-C40	-2.87	1.35	1.51
60	A1	317	PEV	C3-C2	2.06	1.57	1.50
60	BA	537	PEV	C3-C2	2.06	1.57	1.50
60	A1	301	PEV	C3-C2	2.04	1.57	1.50

All (266) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
60	BA	533	PEV	C39-C40-C41	6.06	145.17	114.42
60	BA	533	PEV	C38-C39-C40	5.54	142.55	114.42
60	A0	316	PEV	C38-C39-C40	3.57	132.56	114.42
61	A0	325	PGV	C8-C9-C10	3.34	128.33	113.79
61	BB	205	PGV	C8-C9-C10	3.26	127.98	113.79
61	A0	332	PGV	C8-C9-C10	3.22	127.84	113.79
61	A1	311	PGV	C8-C9-C10	3.22	127.80	113.79
61	A0	328	PGV	C8-C9-C10	3.21	127.78	113.79
61	BB	213	PGV	C8-C9-C10	3.20	127.73	113.79
60	A0	316	PEV	C39-C40-C41	3.19	130.63	114.42
61	BA	505	PGV	C8-C9-C10	3.15	127.53	113.79
61	BA	512	PGV	C8-C9-C10	3.09	127.27	113.79
61	BB	203	PGV	C8-C9-C10	3.09	127.24	113.79
61	A0	304	PGV	C8-C9-C10	3.08	127.21	113.79
61	BA	501	PGV	C8-C9-C10	3.07	127.16	113.79
61	BB	208	PGV	C8-C9-C10	3.06	127.10	113.79
61	A1	315	PGV	C8-C9-C10	3.05	127.08	113.79
61	A0	318	PGV	C8-C9-C10	3.04	127.03	113.79
60	A0	321	PEV	C2-O2-C31	3.04	125.27	117.79
61	A0	317	PGV	C8-C9-C10	3.02	126.94	113.79
61	A0	306	PGV	C8-C9-C10	3.01	126.90	113.79
61	A1	318	PGV	C8-C9-C10	3.00	126.88	113.79
61	AZ	205	PGV	C8-C9-C10	2.98	126.77	113.79
61	BA	540	PGV	C8-C9-C10	2.97	126.73	113.79
61	BB	217	PGV	C8-C9-C10	2.96	126.69	113.79
61	BB	207	PGV	C8-C9-C10	2.95	126.65	113.79
61	A0	331	PGV	C8-C9-C10	2.95	126.63	113.79
61	AZ	207	PGV	C8-C9-C10	2.93	126.57	113.79
61	A1	303	PGV	C8-C9-C10	2.93	126.54	113.79
61	BA	536	PGV	C8-C9-C10	2.88	126.34	113.79
61	BB	204	PGV	C8-C9-C10	2.87	126.31	113.79
61	B8	3005	PGV	C8-C9-C10	2.87	126.31	113.79
61	BA	515	PGV	C8-C9-C10	2.86	126.25	113.79
60	A0	308	PEV	C38-C39-C40	2.81	128.67	114.42
60	BB	211	PEV	C38-C39-C40	2.81	128.67	114.42
60	BA	532	PEV	C38-C39-C40	2.80	128.64	114.42
61	BB	205	PGV	C9-C10-C11	2.79	128.44	112.43
60	BA	503	PEV	C38-C39-C40	2.77	128.49	114.42
60	A1	329	PEV	C38-C39-C40	2.77	128.47	114.42
60	A1	307	PEV	C38-C39-C40	2.76	128.44	114.42
61	A0	327	PGV	C8-C9-C10	2.76	125.81	113.79
60	BA	534	PEV	C39-C40-C41	2.75	128.41	114.42
61	BB	207	PGV	C9-C10-C11	2.75	128.21	112.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
60	BA	517	PEV	C38-C39-C40	2.75	128.40	114.42
60	A0	323	PEV	C38-C39-C40	2.75	128.37	114.42
61	A0	325	PGV	C9-C10-C11	2.75	128.18	112.43
60	BB	210	PEV	C39-C40-C41	2.75	128.37	114.42
60	BB	211	PEV	C39-C40-C41	2.73	128.28	114.42
60	A0	323	PEV	C39-C40-C41	2.73	128.28	114.42
60	BA	503	PEV	C39-C40-C41	2.72	128.25	114.42
60	BA	527	PEV	C38-C39-C40	2.72	128.23	114.42
61	A0	332	PGV	C9-C10-C11	2.71	127.98	112.43
60	A1	307	PEV	C39-C40-C41	2.71	128.19	114.42
60	A0	319	PEV	C38-C39-C40	2.71	128.16	114.42
60	BB	210	PEV	C38-C39-C40	2.71	128.16	114.42
60	B8	3004	PEV	C39-C40-C41	2.70	128.11	114.42
60	BA	532	PEV	C39-C40-C41	2.69	128.10	114.42
60	BA	506	PEV	C39-C40-C41	2.69	128.08	114.42
60	AZ	202	PEV	C39-C40-C41	2.69	128.07	114.42
60	BA	534	PEV	C38-C39-C40	2.69	128.06	114.42
60	BB	206	PEV	C38-C39-C40	2.69	128.06	114.42
60	AZ	202	PEV	C38-C39-C40	2.68	128.05	114.42
60	BA	528	PEV	C39-C40-C41	2.68	128.05	114.42
60	A0	329	PEV	C39-C40-C41	2.67	128.00	114.42
60	A0	301	PEV	C39-C40-C41	2.67	128.00	114.42
60	BB	218	PEV	C38-C39-C40	2.67	128.00	114.42
60	B8	3004	PEV	C38-C39-C40	2.67	127.99	114.42
60	BA	526	PEV	C39-C40-C41	2.67	127.98	114.42
60	A0	329	PEV	C38-C39-C40	2.67	127.98	114.42
60	BA	506	PEV	C38-C39-C40	2.66	127.95	114.42
61	A0	305	PGV	C8-C9-C10	2.66	125.37	113.79
61	A1	311	PGV	C9-C10-C11	2.65	127.65	112.43
61	BB	213	PGV	C9-C10-C11	2.65	127.62	112.43
60	A1	323	PEV	C38-C39-C40	2.65	127.87	114.42
60	AZ	201	PEV	C38-C39-C40	2.65	127.87	114.42
60	A0	319	PEV	C39-C40-C41	2.64	127.85	114.42
60	BA	525	PEV	C38-C39-C40	2.64	127.85	114.42
60	BA	535	PEV	C39-C40-C41	2.64	127.84	114.42
60	BA	525	PEV	C39-C40-C41	2.64	127.83	114.42
60	A1	314	PEV	C39-C40-C41	2.64	127.82	114.42
60	A0	308	PEV	C39-C40-C41	2.64	127.81	114.42
60	BA	528	PEV	C38-C39-C40	2.64	127.81	114.42
60	AZ	201	PEV	C39-C40-C41	2.63	127.79	114.42
61	BA	516	PGV	C8-C9-C10	2.63	125.25	113.79
61	BB	203	PGV	C9-C10-C11	2.63	127.49	112.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
60	BB	214	PEV	C39-C40-C41	2.63	127.75	114.42
61	A0	331	PGV	C9-C10-C11	2.62	127.46	112.43
60	BA	517	PEV	C39-C40-C41	2.62	127.73	114.42
60	A1	322	PEV	C39-C40-C41	2.62	127.73	114.42
60	A1	305	PEV	C38-C39-C40	2.62	127.73	114.42
60	BA	507	PEV	C39-C40-C41	2.62	127.73	114.42
60	A0	311	PEV	C39-C40-C41	2.62	127.72	114.42
60	BA	527	PEV	C39-C40-C41	2.62	127.72	114.42
60	BA	539	PEV	C38-C39-C40	2.61	127.69	114.42
60	BA	511	PEV	C39-C40-C41	2.61	127.69	114.42
60	A0	326	PEV	C39-C40-C41	2.61	127.69	114.42
60	BA	524	PEV	C39-C40-C41	2.61	127.69	114.42
60	BA	504	PEV	C39-C40-C41	2.61	127.69	114.42
60	BA	514	PEV	C38-C39-C40	2.61	127.68	114.42
60	BA	535	PEV	C38-C39-C40	2.61	127.68	114.42
60	BB	216	PEV	C38-C39-C40	2.61	127.67	114.42
60	BA	526	PEV	C38-C39-C40	2.60	127.64	114.42
60	A1	309	PEV	C39-C40-C41	2.60	127.63	114.42
60	BA	510	PEV	C39-C40-C41	2.60	127.63	114.42
61	BB	208	PGV	C9-C10-C11	2.60	127.34	112.43
60	B8	3001	PEV	C39-C40-C41	2.60	127.62	114.42
60	BB	206	PEV	C39-C40-C41	2.60	127.62	114.42
60	A0	326	PEV	C38-C39-C40	2.60	127.62	114.42
60	BB	214	PEV	C38-C39-C40	2.60	127.61	114.42
60	BA	510	PEV	C38-C39-C40	2.60	127.60	114.42
60	A0	320	PEV	C39-C40-C41	2.60	127.60	114.42
60	B8	3003	PEV	C39-C40-C41	2.59	127.58	114.42
60	A1	314	PEV	C38-C39-C40	2.59	127.58	114.42
60	BA	523	PEV	C39-C40-C41	2.59	127.57	114.42
60	A1	309	PEV	C38-C39-C40	2.59	127.56	114.42
60	BA	507	PEV	C38-C39-C40	2.59	127.55	114.42
60	BA	508	PEV	C38-C39-C40	2.59	127.55	114.42
60	BB	212	PEV	C38-C39-C40	2.59	127.55	114.42
61	BA	522	PGV	C9-C10-C11	2.58	127.24	112.43
61	BA	505	PGV	C9-C10-C11	2.58	127.24	112.43
61	BA	512	PGV	C9-C10-C11	2.58	127.22	112.43
60	BA	502	PEV	C39-C40-C41	2.58	127.52	114.42
61	A0	328	PGV	C9-C10-C11	2.58	127.19	112.43
60	A1	313	PEV	C39-C40-C41	2.57	127.50	114.42
60	BA	509	PEV	C38-C39-C40	2.57	127.49	114.42
60	A1	325	PEV	C39-C40-C41	2.57	127.49	114.42
60	A1	301	PEV	C38-C39-C40	2.57	127.47	114.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
60	A0	301	PEV	C38-C39-C40	2.57	127.47	114.42
60	A0	320	PEV	C38-C39-C40	2.57	127.47	114.42
60	BA	509	PEV	C39-C40-C41	2.56	127.45	114.42
60	A1	322	PEV	C38-C39-C40	2.56	127.44	114.42
60	A1	328	PEV	C39-C40-C41	2.56	127.43	114.42
60	BA	508	PEV	C39-C40-C41	2.56	127.43	114.42
60	B8	3002	PEV	C39-C40-C41	2.56	127.42	114.42
61	BA	540	PGV	C9-C10-C11	2.56	127.09	112.43
61	BA	501	PGV	C9-C10-C11	2.56	127.09	112.43
60	BA	539	PEV	C39-C40-C41	2.56	127.40	114.42
60	A0	311	PEV	C38-C39-C40	2.55	127.39	114.42
60	A0	307	PEV	C39-C40-C41	2.55	127.39	114.42
60	A1	328	PEV	C38-C39-C40	2.55	127.39	114.42
60	BA	521	PEV	C38-C39-C40	2.55	127.38	114.42
60	BA	502	PEV	C38-C39-C40	2.55	127.38	114.42
60	A0	322	PEV	C39-C40-C41	2.55	127.37	114.42
60	B8	3006	PEV	C39-C40-C41	2.55	127.35	114.42
60	A1	313	PEV	C38-C39-C40	2.55	127.35	114.42
60	A1	324	PEV	C38-C39-C40	2.55	127.35	114.42
60	A1	327	PEV	C39-C40-C41	2.55	127.35	114.42
60	BA	524	PEV	C38-C39-C40	2.55	127.35	114.42
60	BA	530	PEV	C38-C39-C40	2.55	127.35	114.42
61	AZ	207	PGV	C9-C10-C11	2.54	127.02	112.43
60	A1	329	PEV	C39-C40-C41	2.54	127.33	114.42
61	A0	317	PGV	C9-C10-C11	2.54	127.00	112.43
61	A1	303	PGV	C9-C10-C11	2.54	126.99	112.43
60	A0	310	PEV	C38-C39-C40	2.54	127.31	114.42
60	BB	216	PEV	C39-C40-C41	2.53	127.29	114.42
60	A1	325	PEV	C38-C39-C40	2.53	127.29	114.42
60	BB	212	PEV	C39-C40-C41	2.53	127.27	114.42
60	BA	538	PEV	C39-C40-C41	2.53	127.25	114.42
60	BB	202	PEV	C39-C40-C41	2.53	127.25	114.42
60	A1	321	PEV	C39-C40-C41	2.53	127.24	114.42
60	A1	301	PEV	C39-C40-C41	2.52	127.24	114.42
60	A0	307	PEV	C38-C39-C40	2.52	127.23	114.42
60	BB	202	PEV	C38-C39-C40	2.52	127.20	114.42
60	B8	3006	PEV	C38-C39-C40	2.52	127.19	114.42
60	BA	504	PEV	C38-C39-C40	2.51	127.19	114.42
61	BA	536	PGV	C9-C10-C11	2.51	126.84	112.43
61	A1	315	PGV	C9-C10-C11	2.51	126.83	112.43
60	BA	521	PEV	C39-C40-C41	2.51	127.18	114.42
60	BA	514	PEV	C39-C40-C41	2.51	127.17	114.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
61	A0	304	PGV	C9-C10-C11	2.51	126.80	112.43
60	B8	3003	PEV	C38-C39-C40	2.51	127.14	114.42
60	A1	321	PEV	C38-C39-C40	2.50	127.14	114.42
60	BA	520	PEV	C38-C39-C40	2.50	127.13	114.42
60	A1	316	PEV	C39-C40-C41	2.50	127.12	114.42
61	A1	318	PGV	C9-C10-C11	2.50	126.76	112.43
60	B8	3001	PEV	C38-C39-C40	2.50	127.09	114.42
60	A0	324	PEV	C39-C40-C41	2.49	127.08	114.42
60	A0	322	PEV	C38-C39-C40	2.49	127.07	114.42
60	BA	519	PEV	C39-C40-C41	2.49	127.06	114.42
61	A0	306	PGV	C9-C10-C11	2.49	126.70	112.43
60	A0	309	PEV	C39-C40-C41	2.49	127.05	114.42
60	BA	511	PEV	C38-C39-C40	2.49	127.05	114.42
60	A1	310	PEV	C38-C39-C40	2.49	127.04	114.42
60	A0	313	PEV	C38-C39-C40	2.49	127.04	114.42
60	A1	323	PEV	C39-C40-C41	2.49	127.04	114.42
60	A0	321	PEV	C39-C40-C41	2.48	127.03	114.42
60	A1	316	PEV	C38-C39-C40	2.48	127.03	114.42
60	BA	523	PEV	C38-C39-C40	2.48	127.01	114.42
60	A0	313	PEV	C39-C40-C41	2.48	127.00	114.42
60	A1	302	PEV	C39-C40-C41	2.48	127.00	114.42
60	BA	513	PEV	C39-C40-C41	2.47	126.99	114.42
60	A1	317	PEV	C39-C40-C41	2.47	126.97	114.42
60	BA	538	PEV	C38-C39-C40	2.47	126.97	114.42
60	A0	315	PEV	C39-C40-C41	2.47	126.96	114.42
60	BB	209	PEV	C39-C40-C41	2.47	126.95	114.42
60	BB	201	PEV	C39-C40-C41	2.47	126.95	114.42
60	A1	317	PEV	C38-C39-C40	2.46	126.92	114.42
60	A0	321	PEV	C38-C39-C40	2.46	126.92	114.42
61	A0	327	PGV	C9-C10-C11	2.46	126.54	112.43
60	BA	530	PEV	C39-C40-C41	2.46	126.90	114.42
61	BB	204	PGV	C9-C10-C11	2.46	126.52	112.43
60	A0	309	PEV	C38-C39-C40	2.45	126.89	114.42
60	A1	326	PEV	C39-C40-C41	2.45	126.88	114.42
60	A0	303	PEV	C38-C39-C40	2.45	126.88	114.42
60	A1	306	PEV	C38-C39-C40	2.45	126.88	114.42
60	A0	324	PEV	C38-C39-C40	2.45	126.87	114.42
61	BB	217	PGV	C9-C10-C11	2.45	126.48	112.43
60	B8	3002	PEV	C38-C39-C40	2.45	126.85	114.42
60	BB	209	PEV	C38-C39-C40	2.45	126.85	114.42
60	BA	531	PEV	C39-C40-C41	2.44	126.84	114.42
61	AZ	205	PGV	C9-C10-C11	2.44	126.44	112.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
60	AZ	204	PEV	C39-C40-C41	2.44	126.82	114.42
60	A1	324	PEV	C39-C40-C41	2.44	126.81	114.42
60	A1	327	PEV	C38-C39-C40	2.44	126.80	114.42
60	A1	306	PEV	C39-C40-C41	2.44	126.79	114.42
60	BB	215	PEV	C39-C40-C41	2.43	126.77	114.42
60	A1	326	PEV	C38-C39-C40	2.43	126.75	114.42
60	BA	520	PEV	C39-C40-C41	2.43	126.75	114.42
60	A1	305	PEV	C39-C40-C41	2.43	126.75	114.42
60	A1	320	PEV	C38-C39-C40	2.42	126.71	114.42
60	A1	320	PEV	C39-C40-C41	2.42	126.69	114.42
60	A1	310	PEV	C39-C40-C41	2.42	126.69	114.42
60	BA	531	PEV	C38-C39-C40	2.41	126.67	114.42
61	A0	318	PGV	C9-C10-C11	2.41	126.26	112.43
60	A1	302	PEV	C38-C39-C40	2.41	126.65	114.42
60	B8	3007	PEV	C39-C40-C41	2.40	126.63	114.42
60	A0	314	PEV	C38-C39-C40	2.40	126.63	114.42
61	BA	515	PGV	C9-C10-C11	2.40	126.20	112.43
60	A0	315	PEV	C38-C39-C40	2.40	126.61	114.42
60	A1	312	PEV	C39-C40-C41	2.40	126.61	114.42
61	BA	522	PGV	C8-C9-C10	2.39	124.19	113.79
60	A1	308	PEV	C38-C39-C40	2.38	126.53	114.42
60	A0	303	PEV	C39-C40-C41	2.38	126.49	114.42
60	BB	215	PEV	C38-C39-C40	2.38	126.48	114.42
60	BB	201	PEV	C38-C39-C40	2.37	126.47	114.42
60	BA	537	PEV	C38-C39-C40	2.37	126.47	114.42
60	A1	319	PEV	C38-C39-C40	2.37	126.44	114.42
60	A0	314	PEV	C39-C40-C41	2.36	126.41	114.42
60	BA	529	PEV	C39-C40-C41	2.36	126.40	114.42
60	A1	308	PEV	C39-C40-C41	2.36	126.38	114.42
60	BA	518	PEV	C38-C39-C40	2.36	126.38	114.42
60	BA	519	PEV	C38-C39-C40	2.35	126.38	114.42
60	A1	312	PEV	C38-C39-C40	2.35	126.37	114.42
61	A0	305	PGV	C9-C10-C11	2.35	125.90	112.43
60	BB	218	PEV	C39-C40-C41	2.35	126.35	114.42
60	B8	3007	PEV	C38-C39-C40	2.35	126.35	114.42
60	A0	302	PEV	C39-C40-C41	2.35	126.35	114.42
60	BA	513	PEV	C38-C39-C40	2.34	126.32	114.42
61	B8	3005	PGV	C9-C10-C11	2.34	125.86	112.43
60	AZ	206	PEV	C39-C40-C41	2.33	126.27	114.42
60	AZ	204	PEV	C38-C39-C40	2.33	126.24	114.42
60	A0	312	PEV	C38-C39-C40	2.33	126.24	114.42
60	A0	302	PEV	C38-C39-C40	2.32	126.22	114.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
60	A0	310	PEV	C39-C40-C41	2.32	126.21	114.42
60	BA	537	PEV	C39-C40-C41	2.30	126.11	114.42
61	BA	516	PGV	C9-C10-C11	2.30	125.61	112.43
60	BA	518	PEV	C39-C40-C41	2.30	126.08	114.42
60	BA	529	PEV	C38-C39-C40	2.28	126.02	114.42
60	A1	304	PEV	C38-C39-C40	2.28	125.99	114.42
60	A0	330	PEV	C39-C40-C41	2.26	125.88	114.42
60	AZ	206	PEV	C38-C39-C40	2.20	125.57	114.42
60	AZ	203	PEV	C39-C40-C41	2.19	125.55	114.42
60	A0	312	PEV	C39-C40-C41	2.16	125.38	114.42
60	A0	330	PEV	C38-C39-C40	2.15	125.34	114.42
60	AZ	203	PEV	C38-C39-C40	2.13	125.25	114.42
60	A1	304	PEV	C39-C40-C41	2.13	125.24	114.42

All (78) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
60	AZ	204	PEV	C2
60	A0	308	PEV	C2
60	A0	314	PEV	C2
60	A0	323	PEV	C2
60	A1	301	PEV	C2
60	A1	305	PEV	C2
60	A1	313	PEV	C2
60	A1	317	PEV	C2
60	B8	3001	PEV	C2
60	BA	502	PEV	C2
60	BA	508	PEV	C2
60	BA	526	PEV	C2
60	BA	530	PEV	C2
60	BA	535	PEV	C2
60	BA	537	PEV	C2
60	BA	538	PEV	C2
60	BB	202	PEV	C2
60	BB	206	PEV	C2
61	AZ	205	PGV	C05
61	AZ	205	PGV	C02
61	AZ	207	PGV	C05
61	AZ	207	PGV	C02
61	A0	304	PGV	C05
61	A0	304	PGV	C02
61	A0	305	PGV	C05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
61	A0	306	PGV	C05
61	A0	306	PGV	C02
61	A0	317	PGV	C05
61	A0	317	PGV	C02
61	A0	318	PGV	C05
61	A0	318	PGV	C02
61	A0	325	PGV	C05
61	A0	325	PGV	C02
61	A0	327	PGV	C05
61	A0	327	PGV	C02
61	A0	328	PGV	C05
61	A0	328	PGV	C02
61	A0	331	PGV	C05
61	A0	331	PGV	C02
61	A0	332	PGV	C05
61	A0	332	PGV	C02
61	A1	303	PGV	C05
61	A1	303	PGV	C02
61	A1	311	PGV	C05
61	A1	311	PGV	C02
61	A1	315	PGV	C05
61	A1	315	PGV	C02
61	A1	318	PGV	C05
61	A1	318	PGV	C02
61	B8	3005	PGV	C05
61	B8	3005	PGV	C02
61	BA	501	PGV	C05
61	BA	505	PGV	C05
61	BA	505	PGV	C02
61	BA	512	PGV	C05
61	BA	515	PGV	C05
61	BA	515	PGV	C02
61	BA	516	PGV	C05
61	BA	516	PGV	C02
61	BA	522	PGV	C05
61	BA	522	PGV	C02
61	BA	536	PGV	C05
61	BA	536	PGV	C02
61	BA	540	PGV	C05
61	BA	540	PGV	C02
61	BB	203	PGV	C05
61	BB	203	PGV	C02

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
61	BB	204	PGV	C05
61	BB	204	PGV	C02
61	BB	205	PGV	C05
61	BB	205	PGV	C02
61	BB	207	PGV	C05
61	BB	207	PGV	C02
61	BB	208	PGV	C05
61	BB	208	PGV	C02
61	BB	213	PGV	C05
61	BB	217	PGV	C05
61	BB	217	PGV	C02

All (987) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
60	AZ	203	PEV	C4-O4P-P-O2P
60	A0	301	PEV	C4-O4P-P-O2P
60	A0	301	PEV	O11-C11-O3-C3
60	A0	301	PEV	C12-C11-O3-C3
60	A0	303	PEV	C1-O3P-P-O1P
60	A0	303	PEV	C1-O3P-P-O2P
60	A0	308	PEV	C1-O3P-P-O4P
60	A0	316	PEV	O11-C11-O3-C3
60	A0	316	PEV	C12-C11-O3-C3
60	A0	319	PEV	C1-O3P-P-O1P
60	A0	319	PEV	C1-O3P-P-O4P
60	A0	321	PEV	C32-C31-O2-C2
60	A0	321	PEV	O31-C31-O2-C2
60	A0	321	PEV	C1-O3P-P-O1P
60	A0	322	PEV	C1-O3P-P-O1P
60	A0	326	PEV	C1-O3P-P-O1P
60	A0	326	PEV	C1-O3P-P-O2P
60	A0	330	PEV	C4-O4P-P-O1P
60	A1	301	PEV	C4-O4P-P-O2P
60	A1	308	PEV	C4-O4P-P-O1P
60	A1	308	PEV	C4-O4P-P-O2P
60	A1	310	PEV	C4-O4P-P-O1P
60	A1	312	PEV	C4-O4P-P-O3P
60	A1	312	PEV	C4-O4P-P-O1P
60	A1	313	PEV	C4-O4P-P-O1P
60	A1	314	PEV	C4-O4P-P-O3P
60	A1	314	PEV	C4-O4P-P-O1P

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
60	A1	314	PEV	C4-O4P-P-O2P
60	A1	317	PEV	C1-O3P-P-O1P
60	A1	320	PEV	C4-O4P-P-O1P
60	A1	321	PEV	C4-O4P-P-O1P
60	A1	325	PEV	O11-C11-O3-C3
60	A1	325	PEV	C12-C11-O3-C3
60	A1	327	PEV	C4-O4P-P-O3P
60	A1	328	PEV	C1-O3P-P-O1P
60	A1	328	PEV	C4-O4P-P-O1P
60	B8	3003	PEV	C1-O3P-P-O2P
60	B8	3004	PEV	C1-O3P-P-O1P
60	B8	3004	PEV	C4-O4P-P-O2P
60	B8	3006	PEV	C4-O4P-P-O2P
60	BA	502	PEV	C1-O3P-P-O2P
60	BA	503	PEV	C1-O3P-P-O1P
60	BA	503	PEV	C1-O3P-P-O2P
60	BA	509	PEV	C1-O3P-P-O1P
60	BA	509	PEV	C1-O3P-P-O4P
60	BA	510	PEV	C1-O3P-P-O1P
60	BA	510	PEV	C1-O3P-P-O2P
60	BA	521	PEV	C4-O4P-P-O3P
60	BA	521	PEV	C4-O4P-P-O1P
60	BA	521	PEV	C4-O4P-P-O2P
60	BA	524	PEV	C1-O3P-P-O2P
60	BA	525	PEV	C1-O3P-P-O1P
60	BA	525	PEV	C1-O3P-P-O2P
60	BA	525	PEV	C4-O4P-P-O2P
60	BA	527	PEV	C4-O4P-P-O1P
60	BA	530	PEV	C4-O4P-P-O2P
60	BA	532	PEV	C4-O4P-P-O1P
60	BA	532	PEV	C4-O4P-P-O2P
60	BA	538	PEV	C1-O3P-P-O1P
60	BB	201	PEV	C4-O4P-P-O3P
60	BB	201	PEV	C4-O4P-P-O1P
60	BB	209	PEV	C1-O3P-P-O2P
60	BB	210	PEV	C1-O3P-P-O1P
60	BB	210	PEV	C1-O3P-P-O2P
60	BB	210	PEV	C1-O3P-P-O4P
60	BB	210	PEV	C4-O4P-P-O1P
60	BB	211	PEV	C4-O4P-P-O1P
60	BB	214	PEV	C4-O4P-P-O3P
60	BB	214	PEV	C4-O4P-P-O1P

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
60	BB	214	PEV	C4-O4P-P-O2P
60	BB	215	PEV	C1-O3P-P-O1P
60	BB	218	PEV	C1-O3P-P-O1P
60	BB	218	PEV	C4-O4P-P-O2P
61	AZ	205	PGV	C03-O11-P-O13
61	AZ	205	PGV	C04-O12-P-O13
61	AZ	205	PGV	C11-C10-C9-C8
61	AZ	207	PGV	C11-C10-C9-C8
61	A0	304	PGV	C11-C10-C9-C8
61	A0	305	PGV	C11-C10-C9-C8
61	A0	306	PGV	C11-C10-C9-C8
61	A0	317	PGV	C03-O11-P-O13
61	A0	317	PGV	C11-C10-C9-C8
61	A0	318	PGV	C03-O11-P-O14
61	A0	318	PGV	C11-C10-C9-C8
61	A0	325	PGV	C11-C10-C9-C8
61	A0	327	PGV	C11-C10-C9-C8
61	A0	328	PGV	C03-O11-P-O13
61	A0	328	PGV	C11-C10-C9-C8
61	A0	331	PGV	C11-C10-C9-C8
61	A0	332	PGV	C03-O11-P-O12
61	A0	332	PGV	C03-O11-P-O13
61	A0	332	PGV	C11-C10-C9-C8
61	A1	303	PGV	C11-C10-C9-C8
61	A1	311	PGV	C03-O11-P-O12
61	A1	311	PGV	C11-C10-C9-C8
61	A1	315	PGV	C03-O11-P-O12
61	A1	315	PGV	C03-O11-P-O13
61	A1	315	PGV	C03-O11-P-O14
61	A1	315	PGV	C11-C10-C9-C8
61	A1	318	PGV	C11-C10-C9-C8
61	B8	3005	PGV	C03-O11-P-O12
61	B8	3005	PGV	C11-C10-C9-C8
61	BA	501	PGV	C11-C10-C9-C8
61	BA	505	PGV	C11-C10-C9-C8
61	BA	512	PGV	C04-O12-P-O14
61	BA	512	PGV	C11-C10-C9-C8
61	BA	515	PGV	C11-C10-C9-C8
61	BA	536	PGV	C11-C10-C9-C8
61	BA	540	PGV	C11-C10-C9-C8
61	BB	203	PGV	C03-O11-P-O12
61	BB	203	PGV	O04-C19-O03-C01

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
61	BB	203	PGV	C20-C19-O03-C01
61	BB	203	PGV	C11-C10-C9-C8
61	BB	204	PGV	C11-C10-C9-C8
61	BB	205	PGV	C03-O11-P-O12
61	BB	205	PGV	C11-C10-C9-C8
61	BB	207	PGV	C11-C10-C9-C8
61	BB	208	PGV	C11-C10-C9-C8
61	BB	213	PGV	C04-O12-P-O14
61	BB	213	PGV	C11-C10-C9-C8
61	BB	217	PGV	C03-O11-P-O12
61	BB	217	PGV	C03-O11-P-O13
61	BB	217	PGV	C03-O11-P-O14
61	BB	217	PGV	C11-C10-C9-C8
60	AZ	201	PEV	C38-C39-C40-C41
60	AZ	202	PEV	C38-C39-C40-C41
60	AZ	204	PEV	C38-C39-C40-C41
60	A0	303	PEV	C38-C39-C40-C41
60	A0	308	PEV	C38-C39-C40-C41
60	A0	312	PEV	C37-C38-C39-C40
60	A0	316	PEV	C37-C38-C39-C40
60	A0	319	PEV	C38-C39-C40-C41
60	A0	321	PEV	C38-C39-C40-C41
60	A0	323	PEV	C38-C39-C40-C41
60	A0	329	PEV	C38-C39-C40-C41
60	A1	305	PEV	C38-C39-C40-C41
60	A1	314	PEV	C38-C39-C40-C41
60	A1	316	PEV	C38-C39-C40-C41
60	A1	320	PEV	C38-C39-C40-C41
60	A1	323	PEV	C38-C39-C40-C41
60	A1	324	PEV	C38-C39-C40-C41
60	A1	325	PEV	C38-C39-C40-C41
60	A1	326	PEV	C38-C39-C40-C41
60	B8	3001	PEV	C38-C39-C40-C41
60	B8	3004	PEV	C38-C39-C40-C41
60	BA	504	PEV	C38-C39-C40-C41
60	BA	506	PEV	C38-C39-C40-C41
60	BA	507	PEV	C38-C39-C40-C41
60	BA	509	PEV	C38-C39-C40-C41
60	BA	510	PEV	C38-C39-C40-C41
60	BA	511	PEV	C38-C39-C40-C41
60	BA	514	PEV	C38-C39-C40-C41
60	BA	520	PEV	C38-C39-C40-C41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
60	BA	524	PEV	C38-C39-C40-C41
60	BA	525	PEV	C38-C39-C40-C41
60	BA	527	PEV	C38-C39-C40-C41
60	BA	538	PEV	C38-C39-C40-C41
60	BA	539	PEV	C38-C39-C40-C41
60	BB	206	PEV	C38-C39-C40-C41
60	BB	210	PEV	C38-C39-C40-C41
60	BB	214	PEV	C38-C39-C40-C41
60	BB	216	PEV	C38-C39-C40-C41
60	BB	218	PEV	C38-C39-C40-C41
61	A1	303	PGV	C10-C11-C12-C13
61	A1	318	PGV	C10-C11-C12-C13
61	BA	505	PGV	C10-C11-C12-C13
61	BB	204	PGV	C10-C11-C12-C13
61	BB	208	PGV	C10-C11-C12-C13
60	AZ	206	PEV	C38-C39-C40-C41
60	A0	301	PEV	C38-C39-C40-C41
60	A0	302	PEV	C38-C39-C40-C41
60	A0	307	PEV	C38-C39-C40-C41
60	A0	310	PEV	C38-C39-C40-C41
60	A0	311	PEV	C38-C39-C40-C41
60	A0	315	PEV	C38-C39-C40-C41
60	A0	320	PEV	C38-C39-C40-C41
60	A1	301	PEV	C38-C39-C40-C41
60	A1	306	PEV	C38-C39-C40-C41
60	A1	309	PEV	C38-C39-C40-C41
60	A1	312	PEV	C38-C39-C40-C41
60	A1	313	PEV	C38-C39-C40-C41
60	A1	321	PEV	C38-C39-C40-C41
60	A1	328	PEV	C38-C39-C40-C41
60	B8	3002	PEV	C38-C39-C40-C41
60	B8	3007	PEV	C38-C39-C40-C41
60	BA	503	PEV	C38-C39-C40-C41
60	BA	508	PEV	C38-C39-C40-C41
60	BA	513	PEV	C38-C39-C40-C41
60	BA	517	PEV	C38-C39-C40-C41
60	BA	521	PEV	C38-C39-C40-C41
60	BA	528	PEV	C38-C39-C40-C41
60	BA	530	PEV	C38-C39-C40-C41
60	BA	535	PEV	C38-C39-C40-C41
60	BB	201	PEV	C38-C39-C40-C41
60	BB	212	PEV	C38-C39-C40-C41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
60	BB	215	PEV	C38-C39-C40-C41
60	A0	322	PEV	C38-C39-C40-C41
60	A0	326	PEV	C38-C39-C40-C41
60	A1	307	PEV	C38-C39-C40-C41
60	A1	308	PEV	C38-C39-C40-C41
60	A1	329	PEV	C38-C39-C40-C41
60	B8	3003	PEV	C38-C39-C40-C41
60	BA	502	PEV	C38-C39-C40-C41
60	BA	519	PEV	C38-C39-C40-C41
60	BA	526	PEV	C38-C39-C40-C41
60	BA	531	PEV	C38-C39-C40-C41
60	BA	534	PEV	C38-C39-C40-C41
60	BB	202	PEV	C38-C39-C40-C41
60	BB	211	PEV	C38-C39-C40-C41
60	A0	309	PEV	C38-C39-C40-C41
60	A0	313	PEV	C38-C39-C40-C41
60	A0	316	PEV	C38-C39-C40-C41
60	A0	324	PEV	C38-C39-C40-C41
60	A1	302	PEV	C38-C39-C40-C41
60	A1	310	PEV	C38-C39-C40-C41
60	A1	317	PEV	C38-C39-C40-C41
60	A1	322	PEV	C38-C39-C40-C41
60	A1	327	PEV	C38-C39-C40-C41
60	BA	518	PEV	C38-C39-C40-C41
60	BA	529	PEV	C38-C39-C40-C41
60	BA	532	PEV	C38-C39-C40-C41
60	BA	537	PEV	C38-C39-C40-C41
60	BB	209	PEV	C38-C39-C40-C41
60	A0	330	PEV	C38-C39-C40-C41
60	B8	3006	PEV	C38-C39-C40-C41
60	BA	533	PEV	C38-C39-C40-C41
60	AZ	203	PEV	C38-C39-C40-C41
60	A0	314	PEV	C38-C39-C40-C41
60	A1	304	PEV	C38-C39-C40-C41
60	BA	523	PEV	C38-C39-C40-C41
60	BA	509	PEV	C2-C1-O3P-P
61	A0	325	PGV	C10-C11-C12-C13
61	BA	536	PGV	C10-C11-C12-C13
61	BB	203	PGV	C10-C11-C12-C13
61	A0	332	PGV	C05-C04-O12-P
61	BA	516	PGV	C10-C11-C12-C13
60	AZ	203	PEV	C4-O4P-P-O3P

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
60	A0	303	PEV	C1-O3P-P-O4P
60	A0	315	PEV	C1-O3P-P-O4P
60	A0	316	PEV	C4-O4P-P-O3P
60	A0	321	PEV	C1-O3P-P-O4P
60	A0	326	PEV	C1-O3P-P-O4P
60	A1	301	PEV	C1-O3P-P-O4P
60	A1	305	PEV	C1-O3P-P-O4P
60	A1	308	PEV	C1-O3P-P-O4P
60	A1	308	PEV	C4-O4P-P-O3P
60	A1	310	PEV	C4-O4P-P-O3P
60	A1	313	PEV	C4-O4P-P-O3P
60	A1	320	PEV	C4-O4P-P-O3P
60	A1	321	PEV	C4-O4P-P-O3P
60	A1	328	PEV	C4-O4P-P-O3P
60	B8	3004	PEV	C4-O4P-P-O3P
60	BA	502	PEV	C1-O3P-P-O4P
60	BA	503	PEV	C1-O3P-P-O4P
60	BA	510	PEV	C1-O3P-P-O4P
60	BA	514	PEV	C4-O4P-P-O3P
60	BA	525	PEV	C1-O3P-P-O4P
60	BA	525	PEV	C4-O4P-P-O3P
60	BA	527	PEV	C1-O3P-P-O4P
60	BA	527	PEV	C4-O4P-P-O3P
60	BA	528	PEV	C1-O3P-P-O4P
60	BA	530	PEV	C4-O4P-P-O3P
60	BA	532	PEV	C4-O4P-P-O3P
60	BA	533	PEV	C1-O3P-P-O4P
60	BA	538	PEV	C4-O4P-P-O3P
60	BB	209	PEV	C1-O3P-P-O4P
60	BB	210	PEV	C4-O4P-P-O3P
61	A0	305	PGV	C04-O12-P-O11
61	A0	306	PGV	C03-O11-P-O12
61	A0	318	PGV	C03-O11-P-O12
61	BA	512	PGV	C04-O12-P-O11
61	BA	540	PGV	C04-O12-P-O11
61	BB	213	PGV	C04-O12-P-O11
60	A0	308	PEV	C39-C40-C41-C42
60	A1	302	PEV	C39-C40-C41-C42
60	A1	314	PEV	C39-C40-C41-C42
60	B8	3001	PEV	C37-C38-C39-C40
60	BA	513	PEV	C39-C40-C41-C42
60	BA	537	PEV	C37-C38-C39-C40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
61	BA	505	PGV	C7-C8-C9-C10
60	A0	301	PEV	C39-C40-C41-C42
60	A0	309	PEV	C16-C17-C18-C19
60	A0	310	PEV	C39-C40-C41-C42
60	A0	311	PEV	C39-C40-C41-C42
60	A0	312	PEV	C39-C40-C41-C42
60	A0	315	PEV	C39-C40-C41-C42
60	A0	319	PEV	C39-C40-C41-C42
60	A0	320	PEV	C39-C40-C41-C42
60	A1	308	PEV	C39-C40-C41-C42
60	A1	309	PEV	C39-C40-C41-C42
60	A1	312	PEV	C39-C40-C41-C42
60	A1	325	PEV	C44-C45-C46-C47
60	A1	327	PEV	C39-C40-C41-C42
60	A1	328	PEV	C39-C40-C41-C42
60	BA	503	PEV	C37-C38-C39-C40
60	BA	504	PEV	C39-C40-C41-C42
60	BA	504	PEV	C37-C38-C39-C40
60	BA	524	PEV	C39-C40-C41-C42
60	BA	525	PEV	C37-C38-C39-C40
60	BA	532	PEV	C37-C38-C39-C40
60	BA	535	PEV	C39-C40-C41-C42
60	BA	538	PEV	C39-C40-C41-C42
60	BB	212	PEV	C37-C38-C39-C40
60	BB	214	PEV	C37-C38-C39-C40
60	BB	216	PEV	C37-C38-C39-C40
61	BA	501	PGV	C7-C8-C9-C10
61	BA	522	PGV	C7-C8-C9-C10
61	BA	536	PGV	C7-C8-C9-C10
60	AZ	201	PEV	C39-C40-C41-C42
60	A0	302	PEV	C37-C38-C39-C40
60	A0	308	PEV	C37-C38-C39-C40
60	A0	322	PEV	C37-C38-C39-C40
60	A0	329	PEV	C37-C38-C39-C40
60	A1	306	PEV	C37-C38-C39-C40
60	B8	3002	PEV	C39-C40-C41-C42
60	B8	3007	PEV	C39-C40-C41-C42
60	BA	506	PEV	C37-C38-C39-C40
60	BA	507	PEV	C39-C40-C41-C42
60	BA	507	PEV	C37-C38-C39-C40
60	BA	508	PEV	C39-C40-C41-C42
60	BA	511	PEV	C37-C38-C39-C40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
60	BA	521	PEV	C39-C40-C41-C42
60	BA	523	PEV	C37-C38-C39-C40
60	BA	530	PEV	C37-C38-C39-C40
60	BB	201	PEV	C37-C38-C39-C40
60	BB	210	PEV	C37-C38-C39-C40
60	BB	218	PEV	C37-C38-C39-C40
61	A0	304	PGV	C7-C8-C9-C10
61	A0	318	PGV	C7-C8-C9-C10
60	A1	309	PEV	C37-C38-C39-C40
60	A1	313	PEV	C37-C38-C39-C40
60	A1	327	PEV	C37-C38-C39-C40
60	BA	539	PEV	C37-C38-C39-C40
60	BB	211	PEV	C39-C40-C41-C42
60	BB	218	PEV	C39-C40-C41-C42
60	A1	321	PEV	C2-C1-O3P-P
61	BA	516	PGV	C05-C04-O12-P
61	A0	318	PGV	C10-C11-C12-C13
61	BB	213	PGV	C10-C11-C12-C13
60	A0	309	PEV	C39-C40-C41-C42
60	A0	326	PEV	C37-C38-C39-C40
60	A1	317	PEV	C37-C38-C39-C40
60	A1	321	PEV	C37-C38-C39-C40
60	A1	325	PEV	C39-C40-C41-C42
60	BA	527	PEV	C37-C38-C39-C40
60	BB	216	PEV	C39-C40-C41-C42
61	AZ	205	PGV	C7-C8-C9-C10
61	BA	512	PGV	C7-C8-C9-C10
60	A0	303	PEV	C37-C38-C39-C40
60	A0	315	PEV	C37-C38-C39-C40
60	A0	321	PEV	C37-C38-C39-C40
60	A1	310	PEV	C37-C38-C39-C40
60	B8	3003	PEV	C37-C38-C39-C40
60	BA	527	PEV	C39-C40-C41-C42
60	BA	529	PEV	C39-C40-C41-C42
60	AZ	202	PEV	C39-C40-C41-C42
60	A0	311	PEV	C37-C38-C39-C40
60	A1	324	PEV	C39-C40-C41-C42
60	A1	325	PEV	C37-C38-C39-C40
60	BA	506	PEV	C39-C40-C41-C42
60	BA	521	PEV	C37-C38-C39-C40
60	BA	528	PEV	C37-C38-C39-C40
60	BA	538	PEV	C37-C38-C39-C40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
60	BB	202	PEV	C39-C40-C41-C42
60	BB	209	PEV	C39-C40-C41-C42
60	A1	326	PEV	C39-C40-C41-C42
60	A1	328	PEV	C37-C38-C39-C40
60	A1	329	PEV	C39-C40-C41-C42
60	B8	3001	PEV	C39-C40-C41-C42
60	BA	518	PEV	C37-C38-C39-C40
60	BA	519	PEV	C39-C40-C41-C42
60	BA	531	PEV	C37-C38-C39-C40
60	BB	214	PEV	C39-C40-C41-C42
61	B8	3005	PGV	C19-C20-C21-C22
60	A0	319	PEV	C37-C38-C39-C40
60	A0	324	PEV	C39-C40-C41-C42
60	A1	314	PEV	C37-C38-C39-C40
60	BA	514	PEV	C39-C40-C41-C42
60	BA	526	PEV	C39-C40-C41-C42
60	BB	202	PEV	C37-C38-C39-C40
60	BB	206	PEV	C39-C40-C41-C42
61	A1	303	PGV	C7-C8-C9-C10
61	BB	217	PGV	C7-C8-C9-C10
60	AZ	202	PEV	C37-C38-C39-C40
60	A0	307	PEV	C39-C40-C41-C42
60	A0	310	PEV	C37-C38-C39-C40
60	A0	321	PEV	C39-C40-C41-C42
60	A1	301	PEV	C37-C38-C39-C40
60	A1	302	PEV	C37-C38-C39-C40
60	BA	503	PEV	C39-C40-C41-C42
60	BA	525	PEV	C39-C40-C41-C42
60	BB	210	PEV	C39-C40-C41-C42
61	A1	311	PGV	C7-C8-C9-C10
61	B8	3005	PGV	C7-C8-C9-C10
60	A0	320	PEV	C37-C38-C39-C40
60	A1	307	PEV	C39-C40-C41-C42
60	B8	3006	PEV	C37-C38-C39-C40
61	A0	325	PGV	C7-C8-C9-C10
61	A1	315	PGV	C7-C8-C9-C10
60	A1	307	PEV	C11-C12-C13-C14
60	AZ	201	PEV	C37-C38-C39-C40
60	A1	305	PEV	C37-C38-C39-C40
60	A1	307	PEV	C37-C38-C39-C40
60	A1	321	PEV	C39-C40-C41-C42
60	A1	322	PEV	C37-C38-C39-C40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
60	BA	533	PEV	C37-C38-C39-C40
60	BB	212	PEV	C39-C40-C41-C42
61	A1	318	PGV	C7-C8-C9-C10
61	BA	540	PGV	C7-C8-C9-C10
60	A0	301	PEV	C37-C38-C39-C40
60	A0	307	PEV	C37-C38-C39-C40
60	A0	313	PEV	C37-C38-C39-C40
60	A0	323	PEV	C37-C38-C39-C40
60	A0	326	PEV	C39-C40-C41-C42
60	A1	319	PEV	C39-C40-C41-C42
60	A1	319	PEV	C37-C38-C39-C40
60	BA	511	PEV	C39-C40-C41-C42
60	BA	528	PEV	C39-C40-C41-C42
60	BA	534	PEV	C37-C38-C39-C40
60	BB	206	PEV	C37-C38-C39-C40
61	A0	332	PGV	C7-C8-C9-C10
60	A0	314	PEV	C37-C38-C39-C40
60	A1	329	PEV	C37-C38-C39-C40
60	BA	502	PEV	C39-C40-C41-C42
60	BA	514	PEV	C37-C38-C39-C40
60	BA	517	PEV	C37-C38-C39-C40
60	BA	526	PEV	C37-C38-C39-C40
60	BA	533	PEV	C39-C40-C41-C42
60	BA	535	PEV	C37-C38-C39-C40
60	BB	201	PEV	C39-C40-C41-C42
60	BB	209	PEV	C37-C38-C39-C40
61	A0	327	PGV	C1-C2-C3-C4
60	AZ	203	PEV	C39-C40-C41-C42
60	BA	517	PEV	C39-C40-C41-C42
60	BB	211	PEV	C37-C38-C39-C40
60	BB	215	PEV	C37-C38-C39-C40
60	AZ	206	PEV	C39-C40-C41-C42
60	A1	313	PEV	C39-C40-C41-C42
60	A1	316	PEV	C37-C38-C39-C40
61	BA	516	PGV	C7-C8-C9-C10
60	A0	323	PEV	C39-C40-C41-C42
60	A1	301	PEV	C39-C40-C41-C42
60	BA	530	PEV	C39-C40-C41-C42
61	BA	515	PGV	C7-C8-C9-C10
61	BB	205	PGV	C7-C8-C9-C10
60	A1	323	PEV	C39-C40-C41-C42
61	A0	327	PGV	C10-C11-C12-C13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
60	A1	304	PEV	C37-C38-C39-C40
60	B8	3004	PEV	C39-C40-C41-C42
61	AZ	207	PGV	C23-C24-C25-C26
61	A0	317	PGV	C7-C8-C9-C10
60	BA	523	PEV	C39-C40-C41-C42
60	BA	523	PEV	C12-C13-C14-C15
60	A1	324	PEV	C37-C38-C39-C40
60	BA	508	PEV	C37-C38-C39-C40
61	A0	325	PGV	C20-C21-C22-C23
61	A0	328	PGV	C7-C8-C9-C10
61	BB	207	PGV	C24-C25-C26-C27
60	A0	330	PEV	C39-C40-C41-C42
60	A1	323	PEV	C37-C38-C39-C40
60	A1	317	PEV	C39-C40-C41-C42
61	AZ	207	PGV	C7-C8-C9-C10
60	A1	304	PEV	C39-C40-C41-C42
60	BA	506	PEV	C35-C36-C37-C38
61	A0	331	PGV	C7-C8-C9-C10
60	BA	509	PEV	C39-C40-C41-C42
60	BA	510	PEV	C37-C38-C39-C40
60	BB	215	PEV	C39-C40-C41-C42
60	BA	520	PEV	C39-C40-C41-C42
60	BA	537	PEV	C39-C40-C41-C42
61	A1	315	PGV	C10-C11-C12-C13
60	B8	3003	PEV	C39-C40-C41-C42
60	A1	322	PEV	C39-C40-C41-C42
61	B8	3005	PGV	C5-C6-C7-C8
60	A0	310	PEV	C20-C21-C22-C23
60	A1	302	PEV	C12-C13-C14-C15
60	A0	324	PEV	C37-C38-C39-C40
60	BA	537	PEV	C18-C19-C20-C21
60	A0	303	PEV	C39-C40-C41-C42
60	A0	313	PEV	C39-C40-C41-C42
60	A1	308	PEV	C37-C38-C39-C40
60	BA	532	PEV	C39-C40-C41-C42
60	A1	312	PEV	C37-C38-C39-C40
60	A0	309	PEV	C37-C38-C39-C40
61	A0	305	PGV	C7-C8-C9-C10
60	BA	510	PEV	C39-C40-C41-C42
60	BB	212	PEV	C44-C45-C46-C47
60	BA	520	PEV	C21-C22-C23-C24
60	B8	3004	PEV	C37-C38-C39-C40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
60	AZ	204	PEV	C39-C40-C41-C42
60	A0	329	PEV	C39-C40-C41-C42
60	A0	301	PEV	C4-O4P-P-O3P
60	A0	302	PEV	C1-O3P-P-O4P
60	A0	315	PEV	C4-O4P-P-O3P
60	A1	313	PEV	C1-O3P-P-O4P
60	BA	524	PEV	C1-O3P-P-O4P
60	BA	528	PEV	C4-O4P-P-O3P
60	BB	215	PEV	C1-O3P-P-O4P
60	BB	218	PEV	C1-O3P-P-O4P
61	AZ	207	PGV	C02-C03-O11-P
61	A1	311	PGV	C02-C03-O11-P
60	BA	503	PEV	C41-C42-C43-C44
60	A1	316	PEV	C39-C40-C41-C42
61	A0	306	PGV	C7-C8-C9-C10
60	A0	322	PEV	C39-C40-C41-C42
61	A0	305	PGV	C12-C13-C14-C15
60	BA	520	PEV	C37-C38-C39-C40
60	AZ	203	PEV	C37-C38-C39-C40
60	BA	524	PEV	C37-C38-C39-C40
60	B8	3007	PEV	C37-C38-C39-C40
60	A1	319	PEV	C34-C35-C36-C37
61	BB	204	PGV	C7-C8-C9-C10
60	BA	509	PEV	C37-C38-C39-C40
60	A0	316	PEV	C39-C40-C41-C42
60	BA	534	PEV	C39-C40-C41-C42
60	BA	539	PEV	C39-C40-C41-C42
61	BB	208	PGV	C7-C8-C9-C10
60	A1	306	PEV	C39-C40-C41-C42
60	A1	329	PEV	C42-C43-C44-C45
61	A1	311	PGV	C13-C14-C15-C16
60	BA	513	PEV	C37-C38-C39-C40
61	BB	207	PGV	C7-C8-C9-C10
60	B8	3002	PEV	C37-C38-C39-C40
60	A1	320	PEV	C39-C40-C41-C42
60	A1	320	PEV	C37-C38-C39-C40
60	BA	531	PEV	C39-C40-C41-C42
60	BA	532	PEV	C31-C32-C33-C34
60	A0	324	PEV	C14-C15-C16-C17
61	AZ	205	PGV	C23-C24-C25-C26
61	BB	203	PGV	C7-C8-C9-C10
60	A0	314	PEV	C39-C40-C41-C42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
60	A0	326	PEV	C2-C1-O3P-P
61	AZ	205	PGV	C05-C04-O12-P
61	A0	318	PGV	C02-C03-O11-P
61	A1	315	PGV	C02-C03-O11-P
61	A0	305	PGV	C11-C12-C13-C14
60	BA	514	PEV	C32-C33-C34-C35
60	BA	533	PEV	C40-C41-C42-C43
60	A1	326	PEV	C45-C46-C47-C48
60	BA	513	PEV	C1-C2-C3-O3
60	BA	504	PEV	C21-C22-C23-C24
60	AZ	204	PEV	C1-O3P-P-O4P
60	A0	330	PEV	C1-O3P-P-O4P
60	A1	301	PEV	C4-O4P-P-O3P
60	A1	328	PEV	C1-O3P-P-O4P
60	BA	523	PEV	C1-O3P-P-O4P
61	AZ	205	PGV	C03-O11-P-O12
61	A0	328	PGV	C03-O11-P-O12
60	A1	313	PEV	C43-C44-C45-C46
60	A1	327	PEV	C35-C36-C37-C38
60	A0	330	PEV	C37-C38-C39-C40
61	BB	204	PGV	C22-C23-C24-C25
60	A1	328	PEV	C43-C44-C45-C46
60	A1	302	PEV	C2-C1-O3P-P
60	BA	502	PEV	C2-C1-O3P-P
60	BA	519	PEV	C2-C1-O3P-P
61	A0	318	PGV	C12-C13-C14-C15
60	A1	310	PEV	C39-C40-C41-C42
60	BA	524	PEV	C15-C16-C17-C18
60	BA	532	PEV	C32-C33-C34-C35
61	A0	327	PGV	C11-C12-C13-C14
61	A0	332	PGV	C23-C24-C25-C26
60	BA	532	PEV	C42-C43-C44-C45
60	BA	533	PEV	C36-C37-C38-C39
61	A0	327	PGV	C7-C8-C9-C10
61	BA	540	PGV	C11-C12-C13-C14
60	BA	524	PEV	C16-C17-C18-C19
60	A0	316	PEV	C2-C1-O3P-P
60	A0	323	PEV	C2-C1-O3P-P
60	BB	210	PEV	C2-C1-O3P-P
61	A1	318	PGV	C05-C04-O12-P
61	BA	501	PGV	C02-C03-O11-P
61	A1	315	PGV	O01-C02-C03-O11

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
60	BA	502	PEV	C37-C38-C39-C40
61	BB	213	PGV	C7-C8-C9-C10
60	A1	322	PEV	C17-C18-C19-C20
60	B8	3006	PEV	C39-C40-C41-C42
60	B8	3003	PEV	C13-C14-C15-C16
61	A1	318	PGV	C4-C5-C6-C7
60	A1	308	PEV	C12-C13-C14-C15
60	BA	518	PEV	C39-C40-C41-C42
60	A0	313	PEV	C1-O3P-P-O4P
60	A1	304	PEV	C4-O4P-P-O3P
60	B8	3006	PEV	C4-O4P-P-O3P
60	BB	209	PEV	C4-O4P-P-O3P
60	BB	211	PEV	C4-O4P-P-O3P
60	BB	218	PEV	C4-O4P-P-O3P
61	A0	325	PGV	C03-O11-P-O12
61	A0	331	PGV	C03-O11-P-O12
61	BB	204	PGV	C04-O12-P-O11
60	AZ	206	PEV	C2-C1-O3P-P
60	A0	307	PEV	C2-C1-O3P-P
60	A0	324	PEV	C2-C1-O3P-P
60	BA	537	PEV	C2-C1-O3P-P
61	B8	3005	PGV	C05-C04-O12-P
61	BA	512	PGV	C05-C04-O12-P
61	BB	217	PGV	C05-C04-O12-P
60	A0	301	PEV	C4-O4P-P-O1P
60	A0	308	PEV	C1-O3P-P-O2P
60	A0	315	PEV	C1-O3P-P-O1P
60	A0	315	PEV	C4-O4P-P-O1P
60	A0	315	PEV	C4-O4P-P-O2P
60	A0	316	PEV	C4-O4P-P-O1P
60	A0	321	PEV	C1-O3P-P-O2P
60	A1	301	PEV	C1-O3P-P-O1P
60	A1	301	PEV	C1-O3P-P-O2P
60	A1	301	PEV	C4-O4P-P-O1P
60	A1	305	PEV	C1-O3P-P-O1P
60	A1	308	PEV	C1-O3P-P-O1P
60	A1	308	PEV	C1-O3P-P-O2P
60	A1	310	PEV	C4-O4P-P-O2P
60	A1	313	PEV	C4-O4P-P-O2P
60	A1	320	PEV	C4-O4P-P-O2P
60	A1	321	PEV	C4-O4P-P-O2P
60	A1	327	PEV	C4-O4P-P-O2P

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
60	A1	328	PEV	C4-O4P-P-O2P
60	B8	3006	PEV	C4-O4P-P-O1P
60	BA	514	PEV	C4-O4P-P-O1P
60	BA	524	PEV	C1-O3P-P-O1P
60	BA	525	PEV	C4-O4P-P-O1P
60	BA	527	PEV	C1-O3P-P-O1P
60	BA	527	PEV	C4-O4P-P-O2P
60	BA	528	PEV	C1-O3P-P-O2P
60	BA	530	PEV	C4-O4P-P-O1P
60	BA	538	PEV	C4-O4P-P-O1P
60	BB	218	PEV	C4-O4P-P-O1P
61	A0	305	PGV	C04-O12-P-O13
61	A0	306	PGV	C03-O11-P-O14
61	A0	328	PGV	C03-O11-P-O14
61	A1	311	PGV	C03-O11-P-O14
61	B8	3005	PGV	C03-O11-P-O14
61	BA	540	PGV	C04-O12-P-O13
61	BB	203	PGV	C03-O11-P-O14
61	BB	205	PGV	C03-O11-P-O14
61	BB	213	PGV	C04-O12-P-O13
60	BB	206	PEV	C18-C19-C20-C21
61	A1	315	PGV	C01-C02-C03-O11
60	A0	301	PEV	C5-C4-O4P-P
60	A0	321	PEV	C5-C4-O4P-P
60	A0	326	PEV	C5-C4-O4P-P
60	B8	3004	PEV	C5-C4-O4P-P
60	BA	509	PEV	C5-C4-O4P-P
60	BA	510	PEV	C5-C4-O4P-P
60	BA	511	PEV	C5-C4-O4P-P
60	BA	514	PEV	C5-C4-O4P-P
60	BA	519	PEV	C5-C4-O4P-P
60	BA	525	PEV	C5-C4-O4P-P
60	BA	530	PEV	C5-C4-O4P-P
60	BB	206	PEV	C5-C4-O4P-P
60	BB	218	PEV	C5-C4-O4P-P
61	BB	208	PGV	C22-C23-C24-C25
60	A1	328	PEV	C12-C13-C14-C15
61	A0	306	PGV	C11-C12-C13-C14
60	AZ	204	PEV	C32-C33-C34-C35
60	BB	216	PEV	C31-C32-C33-C34
61	A0	328	PGV	C11-C12-C13-C14
61	BA	522	PGV	C11-C12-C13-C14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
61	BB	204	PGV	C11-C12-C13-C14
61	BA	512	PGV	C02-C03-O11-P
61	A1	318	PGV	C11-C12-C13-C14
61	BA	540	PGV	C12-C13-C14-C15
60	BA	502	PEV	C18-C19-C20-C21
61	BB	205	PGV	C11-C12-C13-C14
60	A0	319	PEV	C12-C13-C14-C15
60	BB	214	PEV	C20-C21-C22-C23
60	BA	503	PEV	C31-C32-C33-C34
60	BA	529	PEV	C37-C38-C39-C40
61	B8	3005	PGV	C11-C12-C13-C14
61	BB	203	PGV	C11-C12-C13-C14
60	A1	305	PEV	C39-C40-C41-C42
60	AZ	203	PEV	C1-O3P-P-O4P
60	A0	312	PEV	C1-O3P-P-O4P
60	A0	314	PEV	C4-O4P-P-O3P
60	A0	322	PEV	C1-O3P-P-O4P
60	A0	323	PEV	C1-O3P-P-O4P
60	A0	324	PEV	C1-O3P-P-O4P
60	A0	330	PEV	C4-O4P-P-O3P
60	A1	325	PEV	C1-O3P-P-O4P
60	A1	327	PEV	C1-O3P-P-O4P
60	A1	329	PEV	C1-O3P-P-O4P
60	B8	3003	PEV	C4-O4P-P-O3P
60	BA	519	PEV	C1-O3P-P-O4P
60	BA	526	PEV	C1-O3P-P-O4P
60	BA	537	PEV	C4-O4P-P-O3P
60	BA	538	PEV	C1-O3P-P-O4P
60	BB	206	PEV	C1-O3P-P-O4P
60	BB	211	PEV	C1-O3P-P-O4P
60	BB	215	PEV	C4-O4P-P-O3P
61	AZ	207	PGV	C04-O12-P-O11
61	A0	317	PGV	C03-O11-P-O12
61	A0	328	PGV	C04-O12-P-O11
61	A1	311	PGV	C04-O12-P-O11
61	A1	318	PGV	C03-O11-P-O12
61	BA	501	PGV	C04-O12-P-O11
61	BA	536	PGV	C04-O12-P-O11
61	BB	213	PGV	C03-O11-P-O12
60	BA	513	PEV	C34-C35-C36-C37
60	B8	3003	PEV	C1-C2-C3-O3
61	BA	536	PGV	C11-C12-C13-C14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
61	BB	213	PGV	C11-C12-C13-C14
61	BB	208	PGV	C13-C14-C15-C16
60	A0	330	PEV	C33-C34-C35-C36
60	A0	311	PEV	C19-C20-C21-C22
60	BA	518	PEV	C12-C13-C14-C15
60	B8	3003	PEV	C2-C1-O3P-P
61	A0	325	PGV	C11-C12-C13-C14
61	BA	501	PGV	C11-C12-C13-C14
61	BA	512	PGV	C11-C12-C13-C14
61	A0	304	PGV	C11-C12-C13-C14
61	A0	332	PGV	C11-C12-C13-C14
60	A1	308	PEV	C32-C33-C34-C35
60	A1	319	PEV	C43-C44-C45-C46
60	BA	518	PEV	C13-C14-C15-C16
61	BB	207	PGV	C11-C12-C13-C14
60	BA	533	PEV	C41-C42-C43-C44
60	B8	3003	PEV	C32-C33-C34-C35
61	A0	305	PGV	C2-C3-C4-C5
61	BB	204	PGV	C4-C5-C6-C7
60	BA	508	PEV	C2-C1-O3P-P
61	A0	304	PGV	C05-C04-O12-P
61	A0	305	PGV	C05-C04-O12-P
61	A0	318	PGV	C11-C12-C13-C14
60	A0	314	PEV	C36-C37-C38-C39
60	A0	307	PEV	C35-C36-C37-C38
60	A0	315	PEV	C19-C20-C21-C22
60	B8	3003	PEV	C34-C35-C36-C37
60	A0	310	PEV	C1-C2-O2-C31
60	A0	322	PEV	C1-C2-O2-C31
60	BA	504	PEV	C1-C2-O2-C31
60	BA	514	PEV	C1-C2-O2-C31
60	BA	533	PEV	C3-C2-O2-C31
60	BA	537	PEV	C3-C2-O2-C31
60	BA	539	PEV	C1-C2-O2-C31
60	BB	201	PEV	C1-C2-O2-C31
61	BA	516	PGV	C11-C12-C13-C14
60	BB	209	PEV	C14-C15-C16-C17
61	BA	536	PGV	C2-C3-C4-C5
60	B8	3003	PEV	C1-O3P-P-O4P
60	A1	325	PEV	C32-C33-C34-C35
60	A0	312	PEV	C2-C1-O3P-P
60	BB	209	PEV	C2-C1-O3P-P

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
60	BA	511	PEV	C34-C35-C36-C37
60	BA	519	PEV	C37-C38-C39-C40
61	BA	515	PGV	C11-C12-C13-C14
60	A0	302	PEV	C39-C40-C41-C42
60	BB	211	PEV	C41-C42-C43-C44
60	AZ	202	PEV	C33-C34-C35-C36
61	A0	327	PGV	C5-C6-C7-C8
60	A1	325	PEV	C31-C32-C33-C34
60	A1	317	PEV	C32-C33-C34-C35
60	A1	310	PEV	C42-C43-C44-C45
60	AZ	206	PEV	C17-C18-C19-C20
61	BB	204	PGV	C27-C28-C29-C30
60	BA	517	PEV	C32-C33-C34-C35
61	AZ	205	PGV	C11-C12-C13-C14
61	A0	317	PGV	C11-C12-C13-C14
60	BA	509	PEV	C12-C13-C14-C15
60	BA	513	PEV	C17-C18-C19-C20
60	BA	537	PEV	C16-C17-C18-C19
60	BA	524	PEV	C17-C18-C19-C20
60	A0	320	PEV	C35-C36-C37-C38
60	A1	309	PEV	C17-C18-C19-C20
60	AZ	204	PEV	C14-C15-C16-C17
61	A1	315	PGV	C11-C12-C13-C14
60	A1	324	PEV	C21-C22-C23-C24
60	BA	532	PEV	C36-C37-C38-C39
60	A0	311	PEV	O3-C11-C12-C13
60	B8	3003	PEV	O3-C11-C12-C13
60	A1	302	PEV	O2-C31-C32-C33
60	BB	201	PEV	O2-C31-C32-C33
60	B8	3004	PEV	C1-O3P-P-O4P
61	BB	208	PGV	C04-O12-P-O11
60	BB	201	PEV	O3-C11-C12-C13
60	A1	306	PEV	O3-C11-C12-C13
60	BA	519	PEV	O2-C31-C32-C33
61	AZ	205	PGV	O03-C19-C20-C21
61	A0	331	PGV	C11-C12-C13-C14
61	A1	303	PGV	C11-C12-C13-C14
60	A0	313	PEV	C3-C2-O2-C31
60	A1	309	PEV	C3-C2-O2-C31
60	BA	509	PEV	C3-C2-O2-C31
60	BA	519	PEV	C3-C2-O2-C31
60	BA	523	PEV	C3-C2-O2-C31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
61	A0	304	PGV	C01-C02-O01-C1
61	A0	317	PGV	C01-C02-O01-C1
60	AZ	202	PEV	O3-C11-C12-C13
60	A1	317	PEV	O2-C31-C32-C33
60	A1	328	PEV	O3-C11-C12-C13
60	A0	307	PEV	O2-C31-C32-C33
60	A0	307	PEV	O3-C11-C12-C13
60	BA	509	PEV	O2-C31-C32-C33
60	BA	535	PEV	O3-C11-C12-C13
61	BA	512	PGV	O01-C1-C2-C3
61	A1	311	PGV	C11-C12-C13-C14
61	BA	505	PGV	C11-C12-C13-C14
60	BA	533	PEV	C15-C16-C17-C18
60	AZ	201	PEV	O3-C11-C12-C13
60	A1	301	PEV	O3-C11-C12-C13
60	BA	530	PEV	O2-C31-C32-C33
60	BA	532	PEV	O3-C11-C12-C13
60	BA	538	PEV	O3-C11-C12-C13
60	BB	210	PEV	O2-C31-C32-C33
61	A0	305	PGV	O03-C19-C20-C21
60	BA	502	PEV	C19-C20-C21-C22
60	BB	212	PEV	C16-C17-C18-C19
60	BA	526	PEV	C32-C33-C34-C35
61	BA	512	PGV	C4-C5-C6-C7
60	BA	519	PEV	O3-C11-C12-C13
60	BA	528	PEV	O3-C11-C12-C13
61	A0	328	PGV	O01-C1-C2-C3
60	BA	537	PEV	O2-C2-C3-O3
61	BA	515	PGV	C28-C29-C30-C31
61	A0	317	PGV	O01-C1-C2-C3
60	A0	301	PEV	C12-C13-C14-C15
60	A1	320	PEV	O2-C31-C32-C33
60	BA	521	PEV	O3-C11-C12-C13
60	A0	316	PEV	C17-C18-C19-C20
60	A1	324	PEV	C31-C32-C33-C34
61	BB	217	PGV	C11-C12-C13-C14
61	AZ	205	PGV	O01-C1-C2-C3
60	A0	314	PEV	C44-C45-C46-C47
60	BA	509	PEV	C16-C17-C18-C19
60	A1	328	PEV	O11-C11-C12-C13
61	A1	315	PGV	C2-C3-C4-C5
60	A0	323	PEV	C13-C14-C15-C16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
60	A0	330	PEV	C32-C33-C34-C35
60	A0	312	PEV	O2-C31-C32-C33
60	BA	524	PEV	O2-C31-C32-C33
61	BB	204	PGV	C6-C7-C8-C9
60	BA	530	PEV	O31-C31-C32-C33
61	A0	305	PGV	O04-C19-C20-C21
60	A1	325	PEV	C18-C19-C20-C21
60	BA	520	PEV	C35-C36-C37-C38
60	BA	530	PEV	C15-C16-C17-C18
60	BA	508	PEV	C44-C45-C46-C47
61	BB	208	PGV	C11-C12-C13-C14
60	AZ	201	PEV	O11-C11-C12-C13
60	A0	307	PEV	O31-C31-C32-C33
60	A1	310	PEV	C17-C18-C19-C20
60	B8	3002	PEV	C36-C37-C38-C39
60	BB	206	PEV	O3-C11-C12-C13
60	BB	201	PEV	O11-C11-C12-C13
60	BA	518	PEV	C34-C35-C36-C37
60	A0	302	PEV	C20-C21-C22-C23
60	A1	301	PEV	O11-C11-C12-C13
60	BA	519	PEV	O31-C31-C32-C33
60	BA	535	PEV	O11-C11-C12-C13
60	BB	201	PEV	O31-C31-C32-C33
60	BB	210	PEV	O31-C31-C32-C33
61	BA	512	PGV	O02-C1-C2-C3
60	A0	321	PEV	C32-C33-C34-C35
61	A0	306	PGV	C21-C22-C23-C24
61	AZ	207	PGV	C11-C12-C13-C14
60	A0	307	PEV	O11-C11-C12-C13
60	A1	302	PEV	O31-C31-C32-C33
60	BA	538	PEV	O11-C11-C12-C13
61	AZ	205	PGV	O04-C19-C20-C21
61	BA	536	PGV	C3-C4-C5-C6
60	A0	311	PEV	O11-C11-C12-C13
60	BA	532	PEV	O11-C11-C12-C13
60	A1	306	PEV	O2-C31-C32-C33
61	BB	208	PGV	C05-C04-O12-P
60	BA	503	PEV	C32-C33-C34-C35
60	B8	3003	PEV	O11-C11-C12-C13
60	BA	519	PEV	O11-C11-C12-C13
60	AZ	202	PEV	C1-O3P-P-O1P
60	AZ	203	PEV	C1-O3P-P-O1P

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
60	AZ	204	PEV	C1-O3P-P-O1P
60	A0	301	PEV	C1-O3P-P-O1P
60	A0	302	PEV	C1-O3P-P-O2P
60	A0	312	PEV	C4-O4P-P-O1P
60	A0	314	PEV	C1-O3P-P-O1P
60	A0	314	PEV	C4-O4P-P-O1P
60	A0	321	PEV	C4-O4P-P-O1P
60	A0	323	PEV	C1-O3P-P-O1P
60	A0	326	PEV	C4-O4P-P-O1P
60	A0	329	PEV	C1-O3P-P-O1P
60	A0	330	PEV	C1-O3P-P-O1P
60	A1	317	PEV	C1-O3P-P-O2P
60	B8	3003	PEV	C1-O3P-P-O1P
60	B8	3003	PEV	C4-O4P-P-O1P
60	BA	506	PEV	C4-O4P-P-O1P
60	BA	509	PEV	C4-O4P-P-O1P
60	BA	518	PEV	C4-O4P-P-O1P
60	BA	524	PEV	C4-O4P-P-O1P
60	BA	528	PEV	C4-O4P-P-O1P
60	BA	533	PEV	C1-O3P-P-O1P
60	BA	535	PEV	C1-O3P-P-O1P
60	BB	210	PEV	C4-O4P-P-O2P
60	BB	211	PEV	C1-O3P-P-O1P
61	AZ	205	PGV	C04-O12-P-O14
61	AZ	207	PGV	C03-O11-P-O13
61	AZ	207	PGV	C04-O12-P-O13
61	A0	306	PGV	C04-O12-P-O13
61	A0	328	PGV	C04-O12-P-O13
61	A1	303	PGV	C03-O11-P-O13
61	A1	315	PGV	C04-O12-P-O13
61	A1	318	PGV	C03-O11-P-O13
61	BA	501	PGV	C03-O11-P-O13
61	BA	501	PGV	C04-O12-P-O13
61	BA	515	PGV	C04-O12-P-O13
61	BA	516	PGV	C04-O12-P-O13
61	BB	205	PGV	C04-O12-P-O13
61	BB	213	PGV	C03-O11-P-O13
60	A1	306	PEV	O11-C11-C12-C13
60	A1	317	PEV	O31-C31-C32-C33
60	BA	509	PEV	O31-C31-C32-C33
60	BA	528	PEV	O11-C11-C12-C13
61	AZ	205	PGV	C22-C23-C24-C25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
60	A0	311	PEV	C32-C33-C34-C35
60	AZ	202	PEV	O11-C11-C12-C13
61	A0	317	PGV	O02-C1-C2-C3
60	A1	325	PEV	C15-C16-C17-C18
60	A1	302	PEV	O3-C11-C12-C13
60	A1	309	PEV	O2-C31-C32-C33
60	BB	206	PEV	C32-C33-C34-C35
61	BB	204	PGV	C3-C4-C5-C6
60	A0	302	PEV	C3-C2-O2-C31
60	A0	303	PEV	C3-C2-O2-C31
60	A0	309	PEV	C3-C2-O2-C31
60	A0	319	PEV	C3-C2-O2-C31
60	A0	319	PEV	C5-C4-O4P-P
60	A0	324	PEV	C1-C2-O2-C31
60	A0	330	PEV	C5-C4-O4P-P
60	A1	302	PEV	C3-C2-O2-C31
60	A1	302	PEV	C5-C4-O4P-P
60	A1	308	PEV	C5-C4-O4P-P
60	A1	320	PEV	C3-C2-O2-C31
60	A1	323	PEV	C5-C4-O4P-P
60	B8	3006	PEV	C5-C4-O4P-P
60	BA	503	PEV	C3-C2-O2-C31
60	BA	517	PEV	C5-C4-O4P-P
60	BA	518	PEV	C5-C4-O4P-P
60	BA	525	PEV	C1-C2-O2-C31
60	BB	214	PEV	C5-C4-O4P-P
60	BB	216	PEV	C5-C4-O4P-P
61	A0	325	PGV	C03-C02-O01-C1
61	A1	315	PGV	C03-C02-O01-C1
61	A1	318	PGV	C01-C02-O01-C1
61	A1	318	PGV	C03-C02-O01-C1
60	A1	304	PEV	C42-C43-C44-C45
60	A1	325	PEV	C42-C43-C44-C45
60	B8	3004	PEV	C14-C15-C16-C17
60	A0	309	PEV	O2-C31-C32-C33
60	A1	301	PEV	O2-C31-C32-C33
61	BA	505	PGV	O01-C1-C2-C3
60	BA	535	PEV	C14-C15-C16-C17
60	BA	529	PEV	O3-C11-C12-C13
61	BA	515	PGV	C24-C25-C26-C27
60	A1	326	PEV	C40-C41-C42-C43
60	A0	312	PEV	O31-C31-C32-C33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
60	AZ	204	PEV	C37-C38-C39-C40
60	BA	513	PEV	C32-C33-C34-C35
60	BA	503	PEV	O3-C11-C12-C13
61	A0	325	PGV	O03-C19-C20-C21
61	AZ	205	PGV	C21-C22-C23-C24
60	A0	302	PEV	C31-C32-C33-C34
60	BA	534	PEV	O11-C11-C12-C13
61	A0	328	PGV	O02-C1-C2-C3
60	A0	320	PEV	C2-C1-O3P-P
60	BA	530	PEV	C2-C1-O3P-P
60	A0	316	PEV	C16-C17-C18-C19
60	BA	510	PEV	C20-C21-C22-C23
60	AZ	202	PEV	C31-C32-C33-C34
60	BA	518	PEV	C31-C32-C33-C34
60	A1	301	PEV	O31-C31-C32-C33
60	A1	305	PEV	O2-C31-C32-C33
60	BA	507	PEV	O2-C31-C32-C33
60	BA	534	PEV	O3-C11-C12-C13
60	BB	212	PEV	O2-C31-C32-C33
61	A1	318	PGV	O01-C1-C2-C3
61	BA	505	PGV	O03-C19-C20-C21
60	AZ	203	PEV	C40-C41-C42-C43
60	BA	521	PEV	O11-C11-C12-C13
61	BA	505	PGV	O02-C1-C2-C3
60	BA	523	PEV	C42-C43-C44-C45
61	BA	516	PGV	O03-C19-C20-C21
60	BB	201	PEV	C16-C17-C18-C19
60	A1	320	PEV	O31-C31-C32-C33
60	BA	524	PEV	O31-C31-C32-C33
61	BA	516	PGV	O04-C19-C20-C21
60	BB	210	PEV	C12-C13-C14-C15
61	AZ	205	PGV	O02-C1-C2-C3
60	A1	317	PEV	C43-C44-C45-C46
60	BB	206	PEV	O11-C11-C12-C13
61	A0	318	PGV	C30-C31-C32-C33
60	AZ	204	PEV	O2-C31-C32-C33

There are no ring outliers.

17 monomers are involved in 41 short contacts:

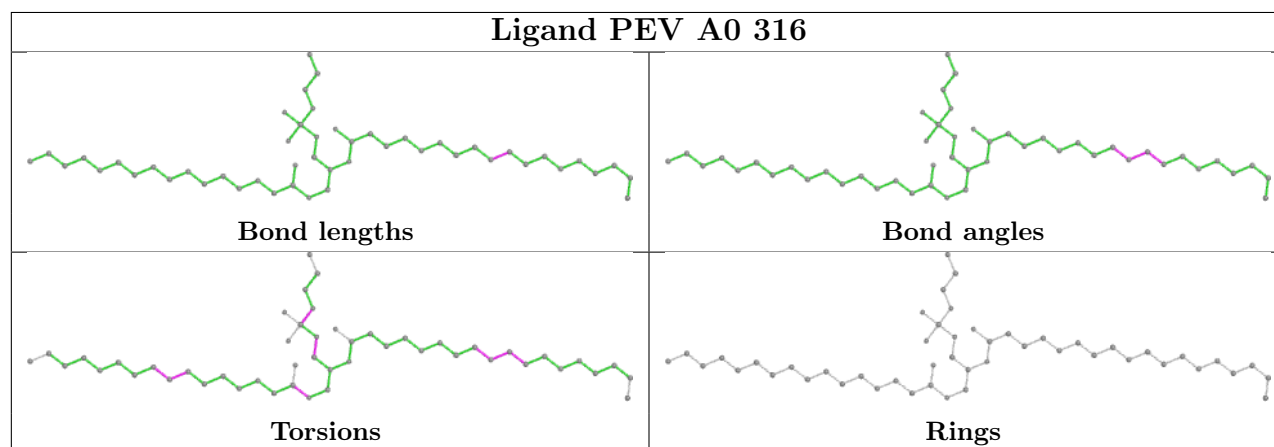
Mol	Chain	Res	Type	Clashes	Symm-Clashes
60	BA	520	PEV	1	0

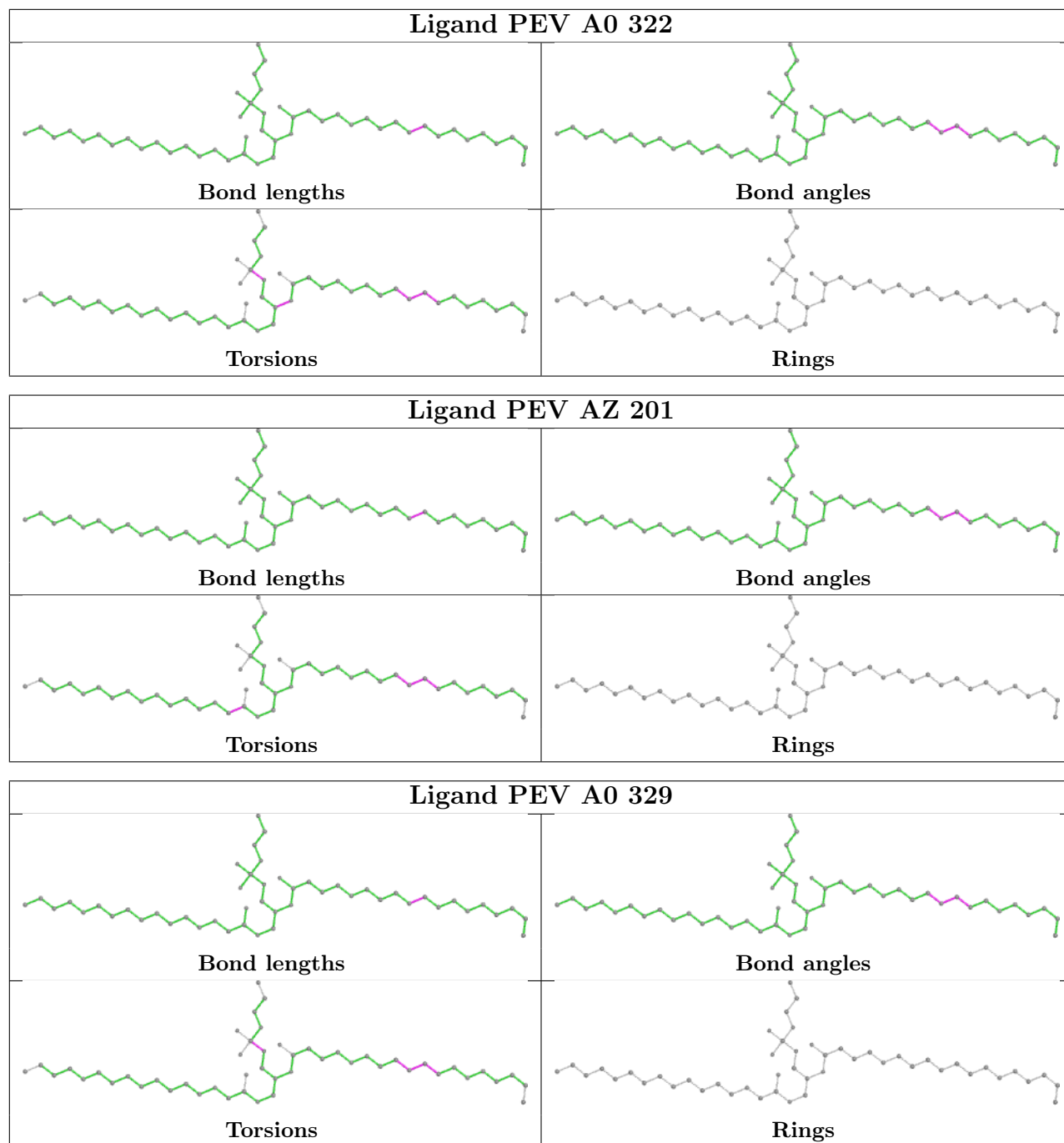
Continued on next page...

Continued from previous page...

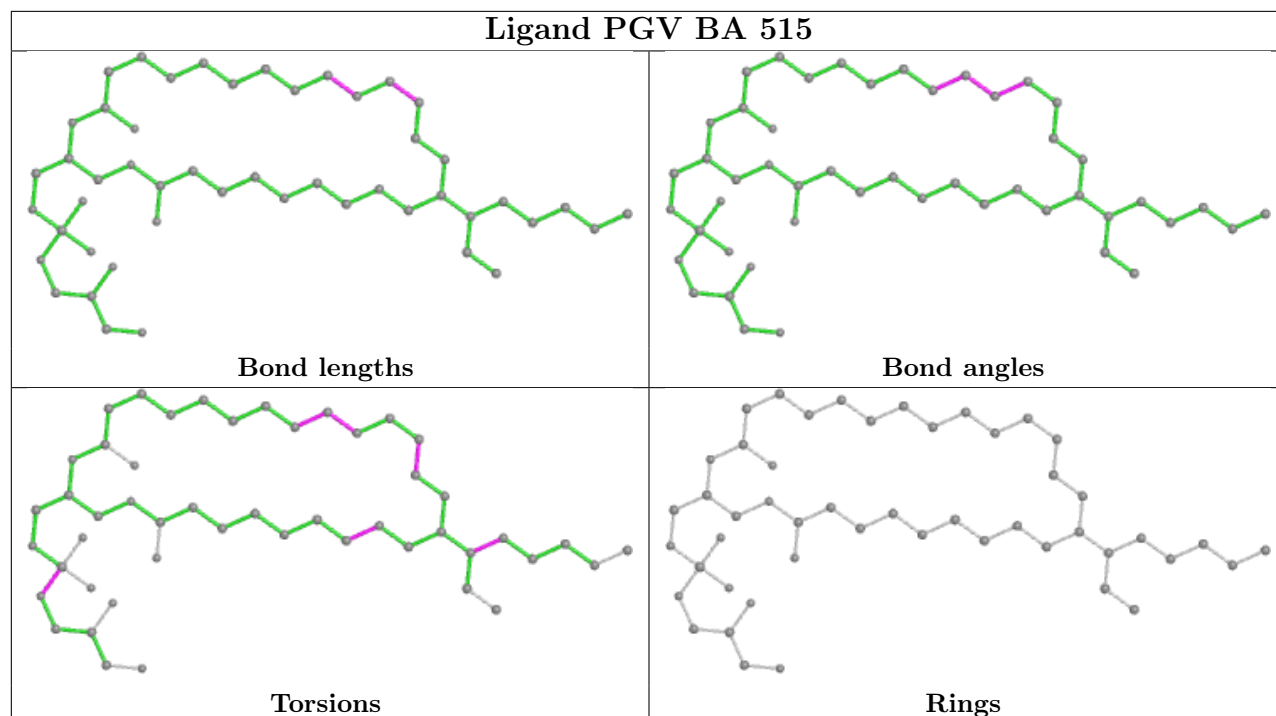
Mol	Chain	Res	Type	Clashes	Symm-Clashes
60	A1	323	PEV	1	0
60	A1	302	PEV	1	0
60	A1	301	PEV	1	0
60	A1	319	PEV	1	0
60	BA	526	PEV	1	0
61	BA	512	PGV	1	0
60	A0	315	PEV	1	0
60	B8	3001	PEV	1	0
61	A1	303	PGV	1	0
60	BA	531	PEV	1	0
60	BA	533	PEV	29	0
60	BA	514	PEV	1	0
60	B8	3002	PEV	2	0
60	BA	503	PEV	1	0
61	A1	315	PGV	1	0
60	BA	513	PEV	1	0

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.

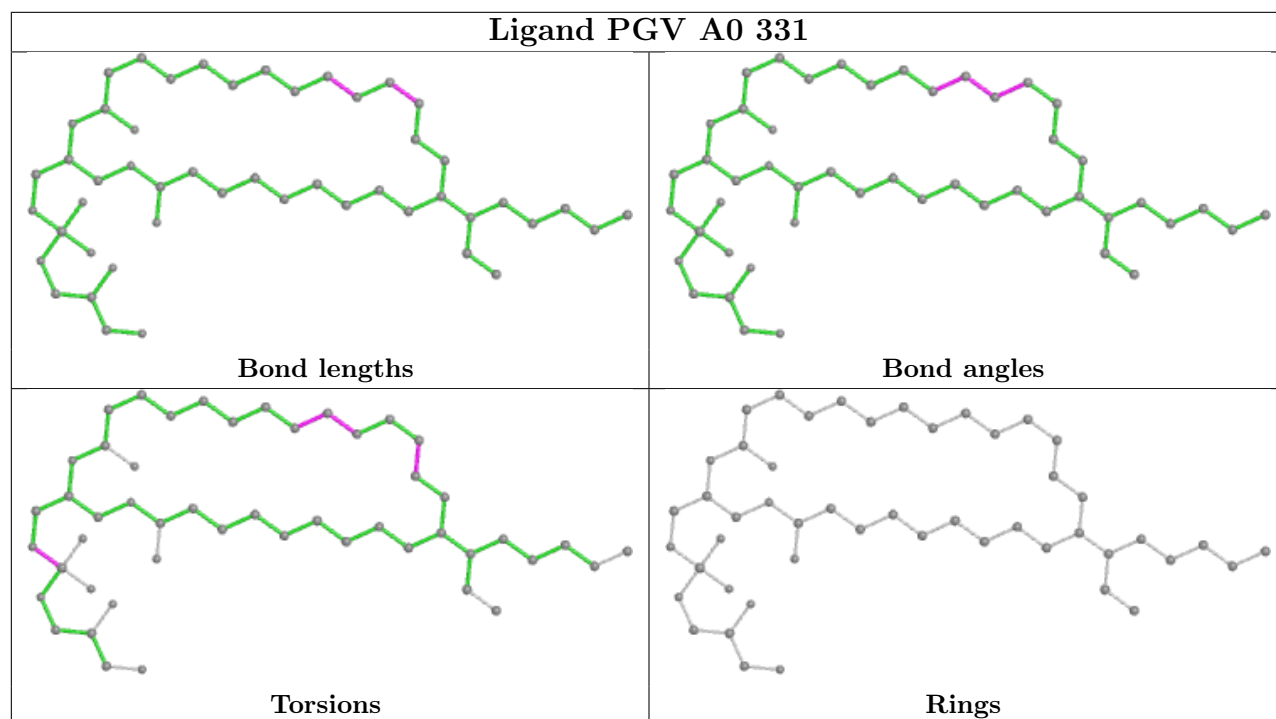


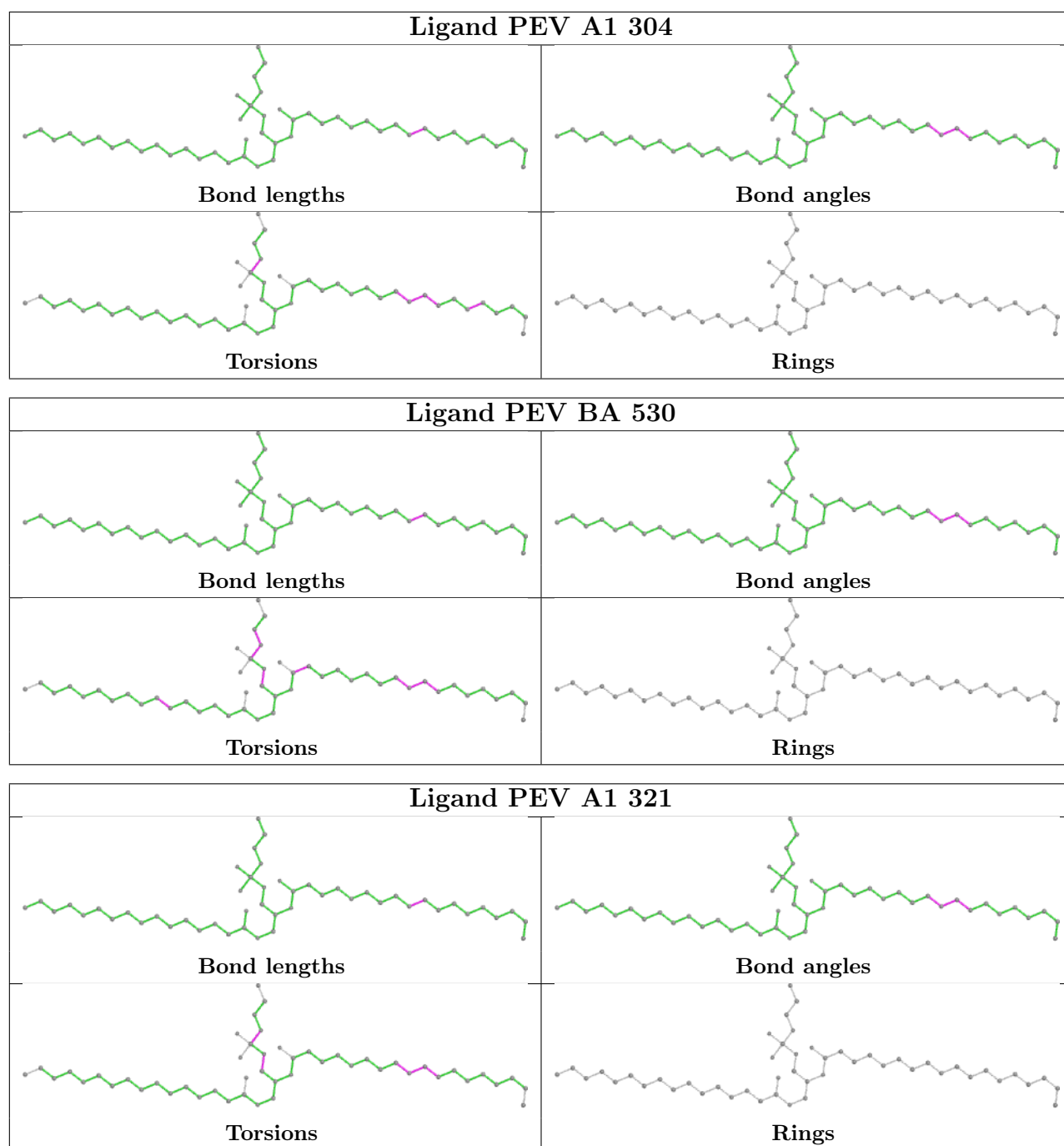


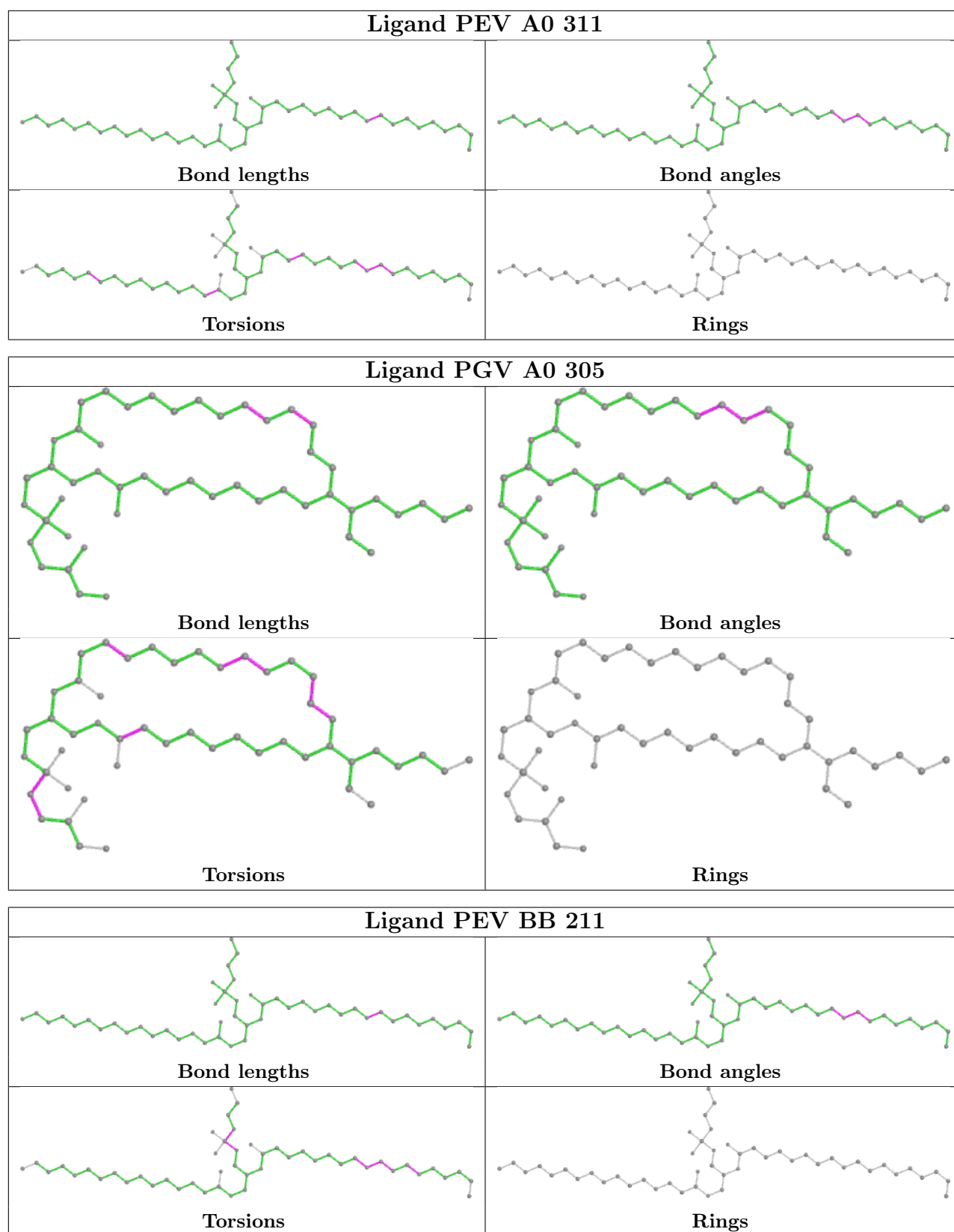
Ligand PGV BA 515

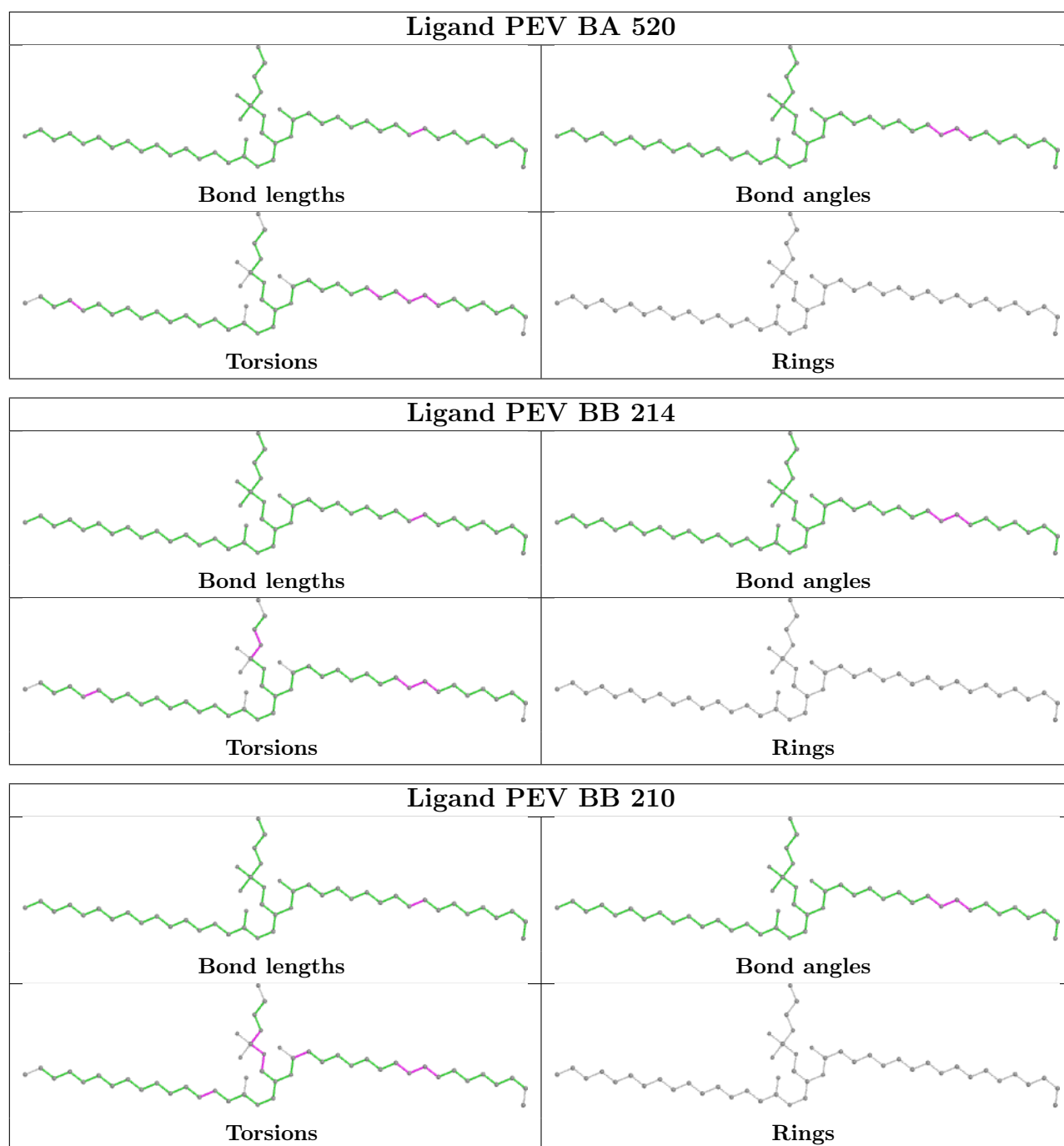


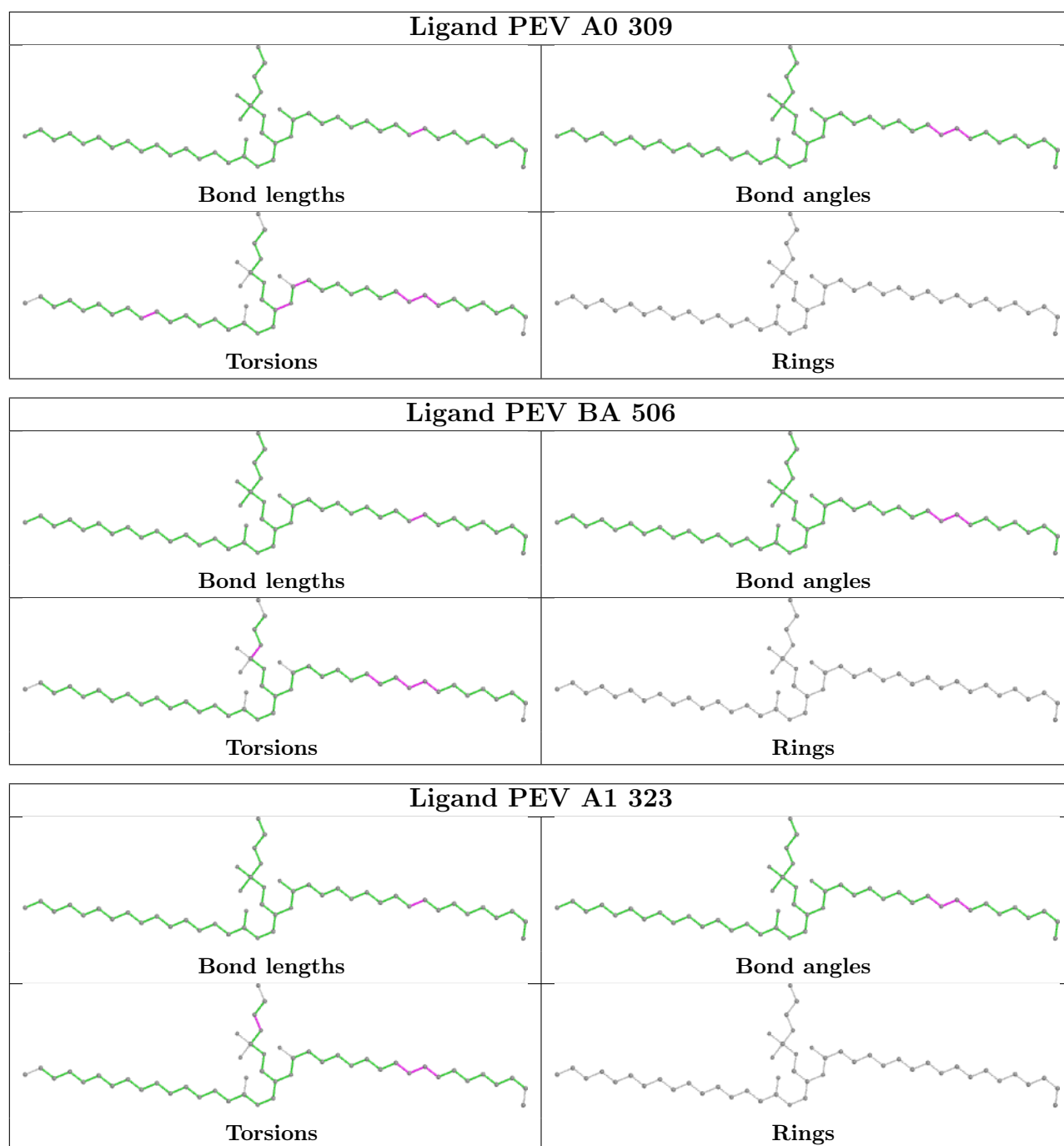
Ligand PGV A0 331

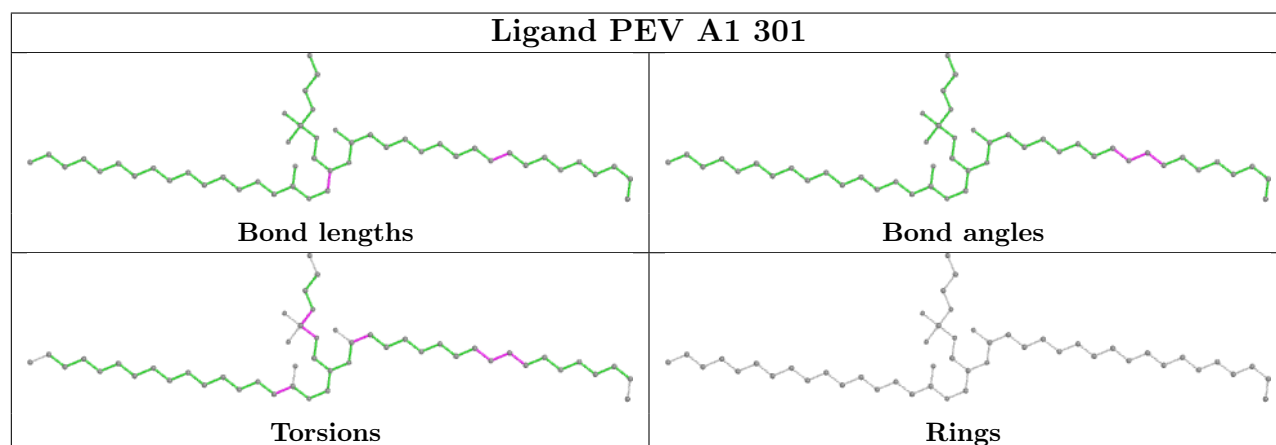
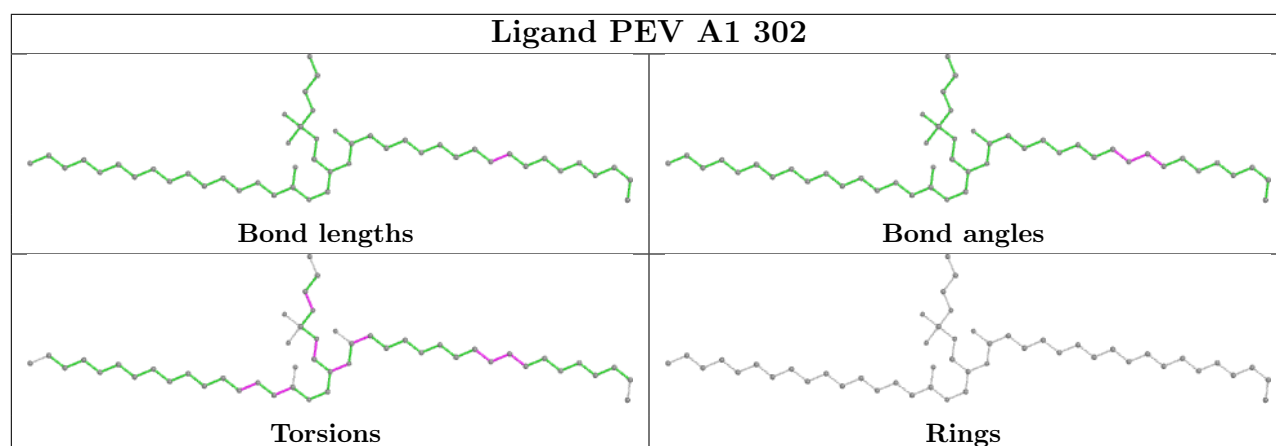
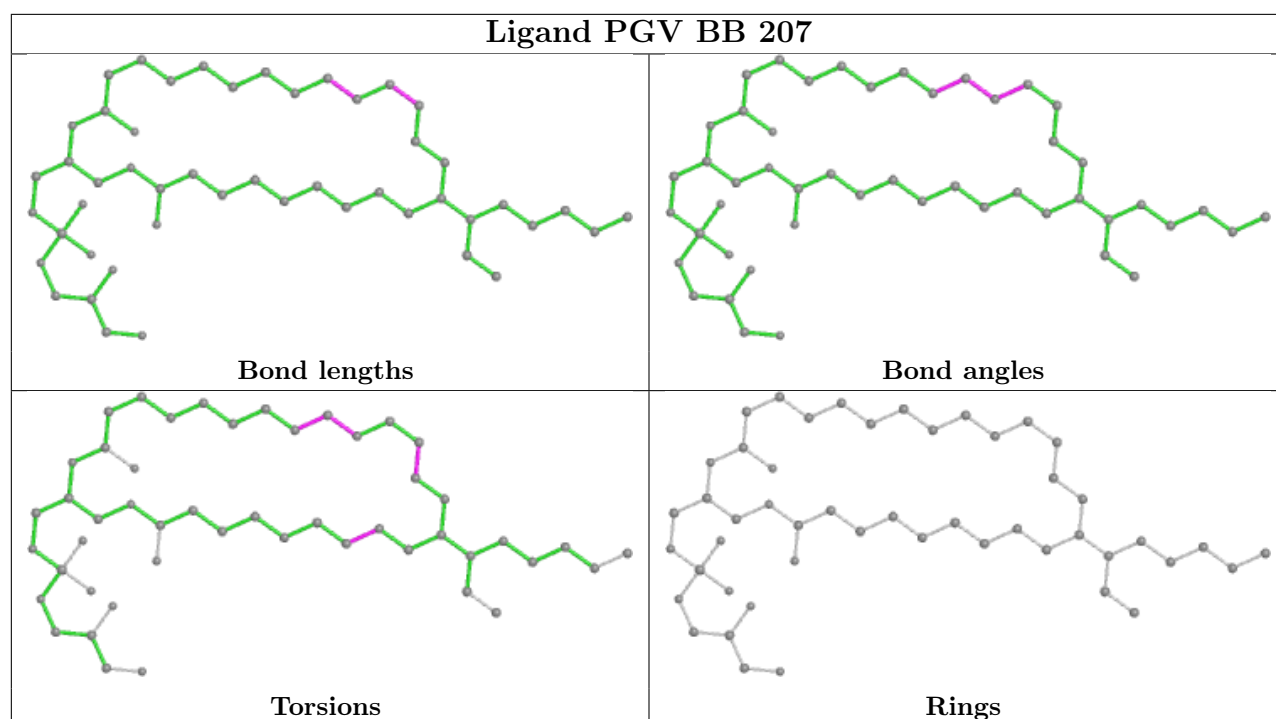


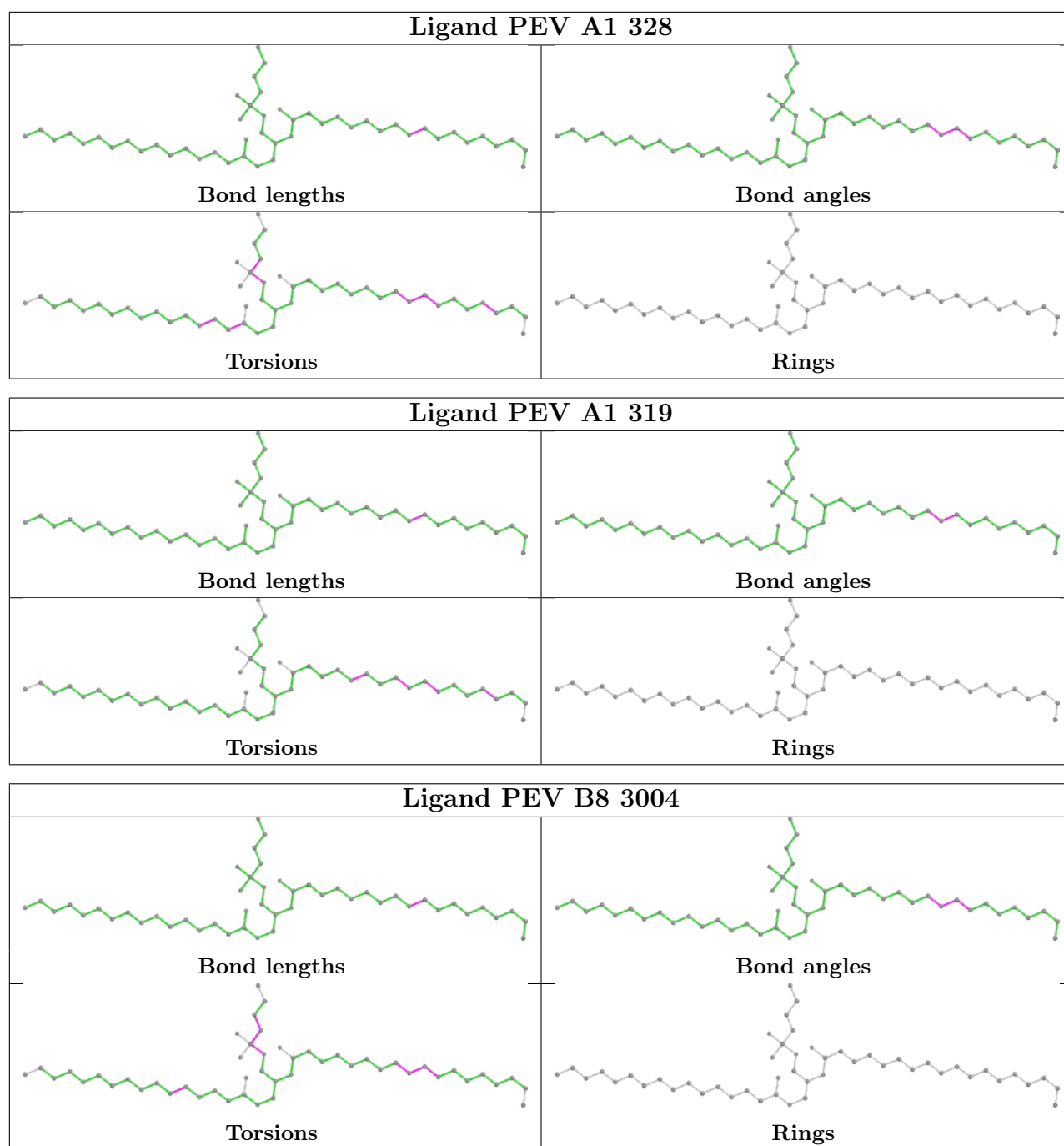


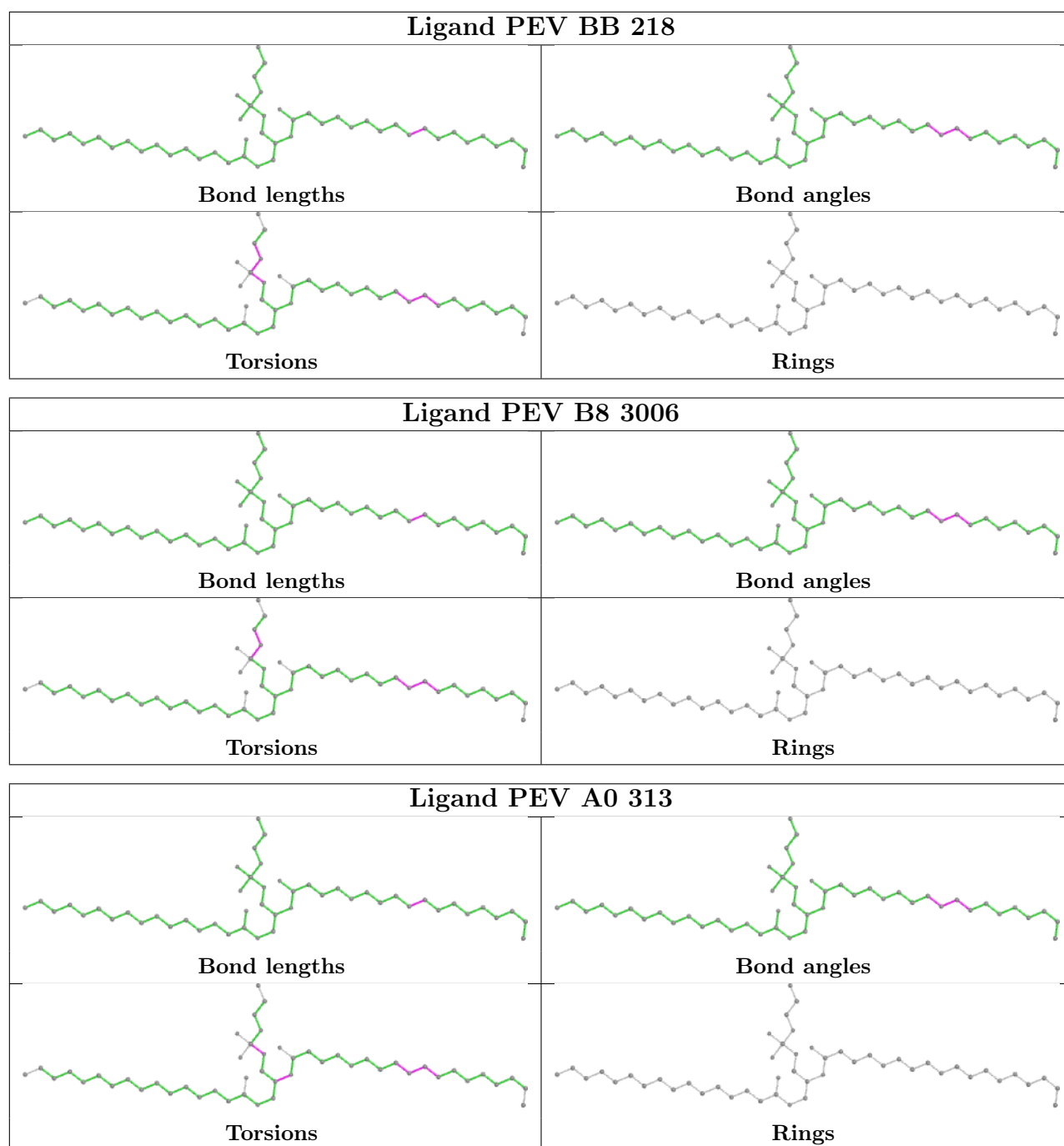


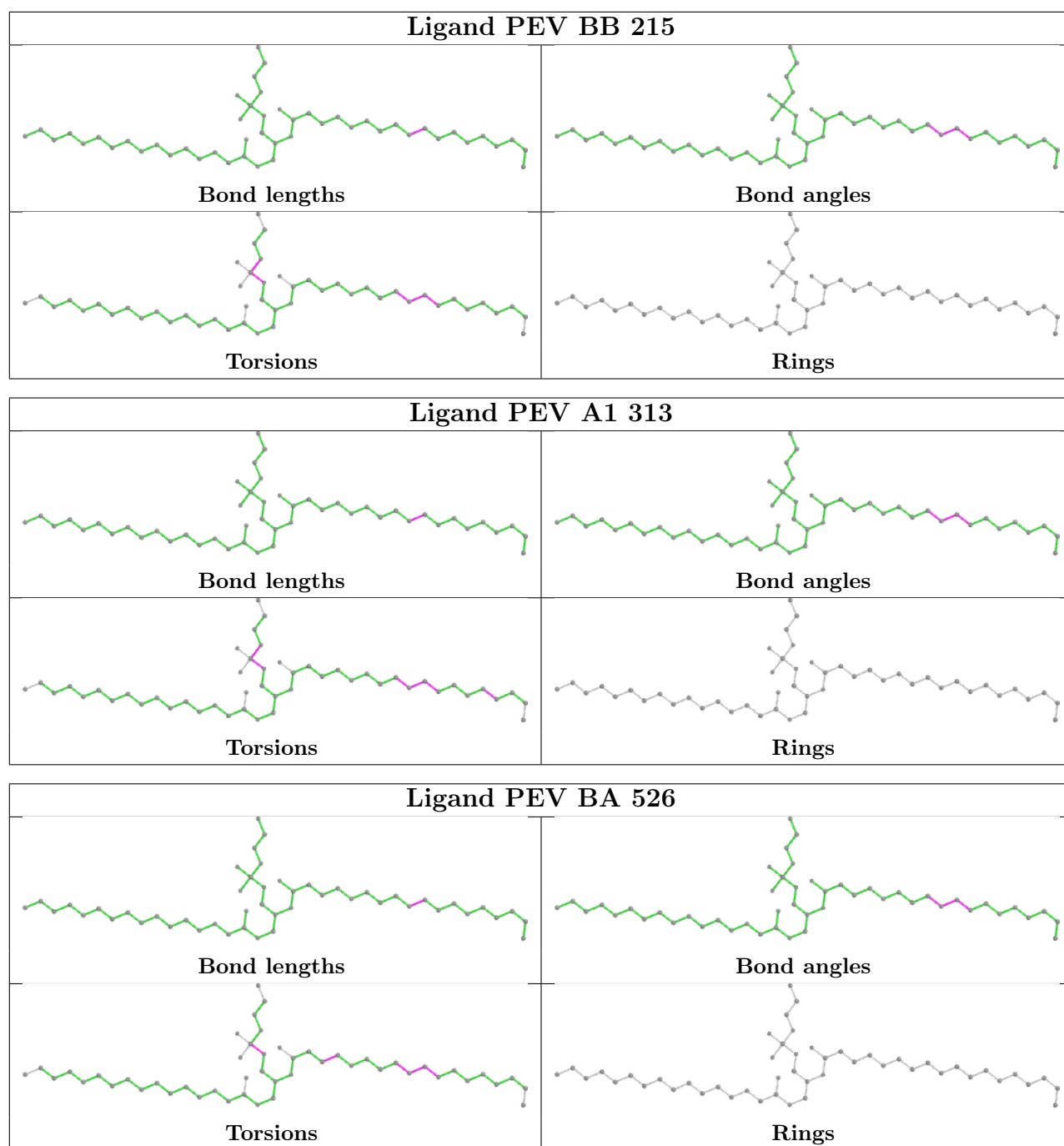


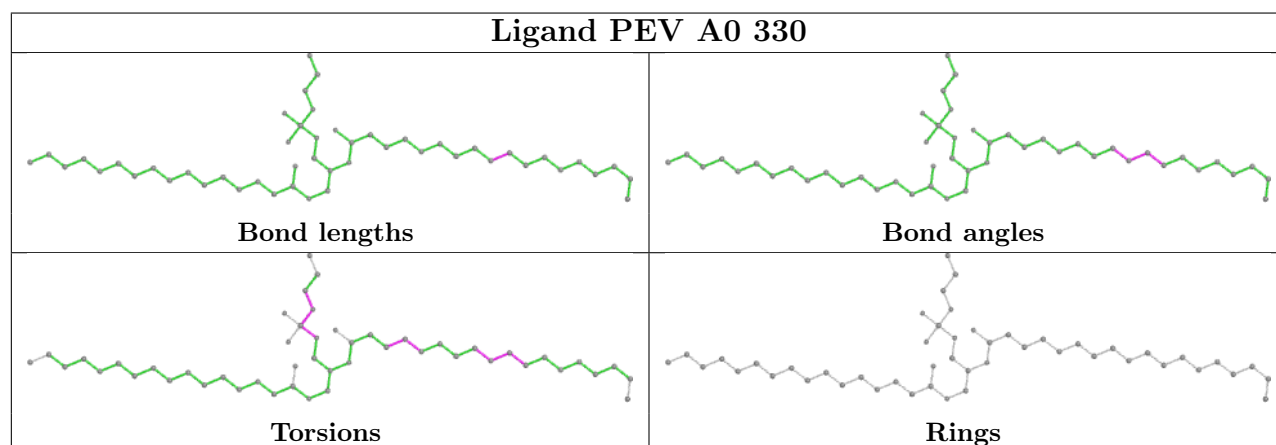
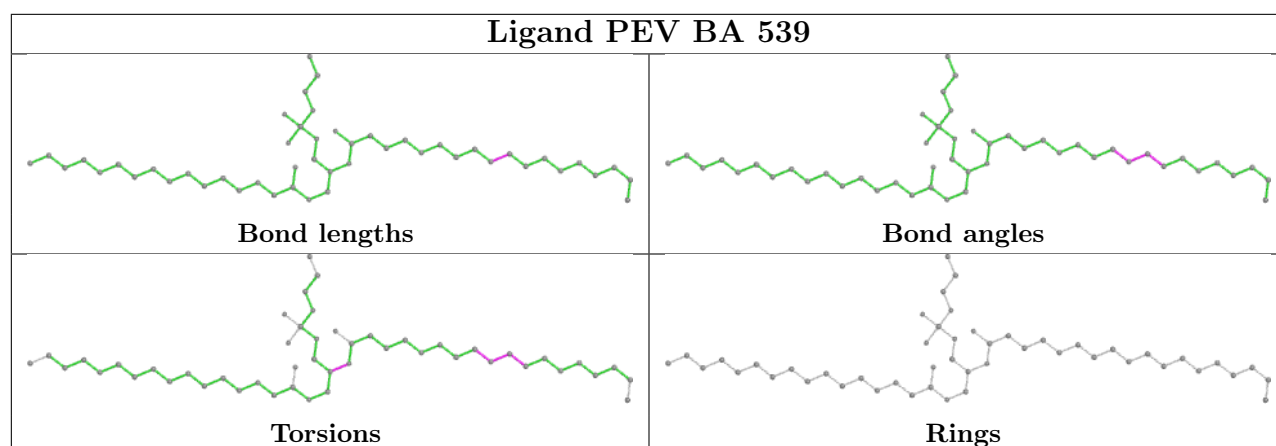
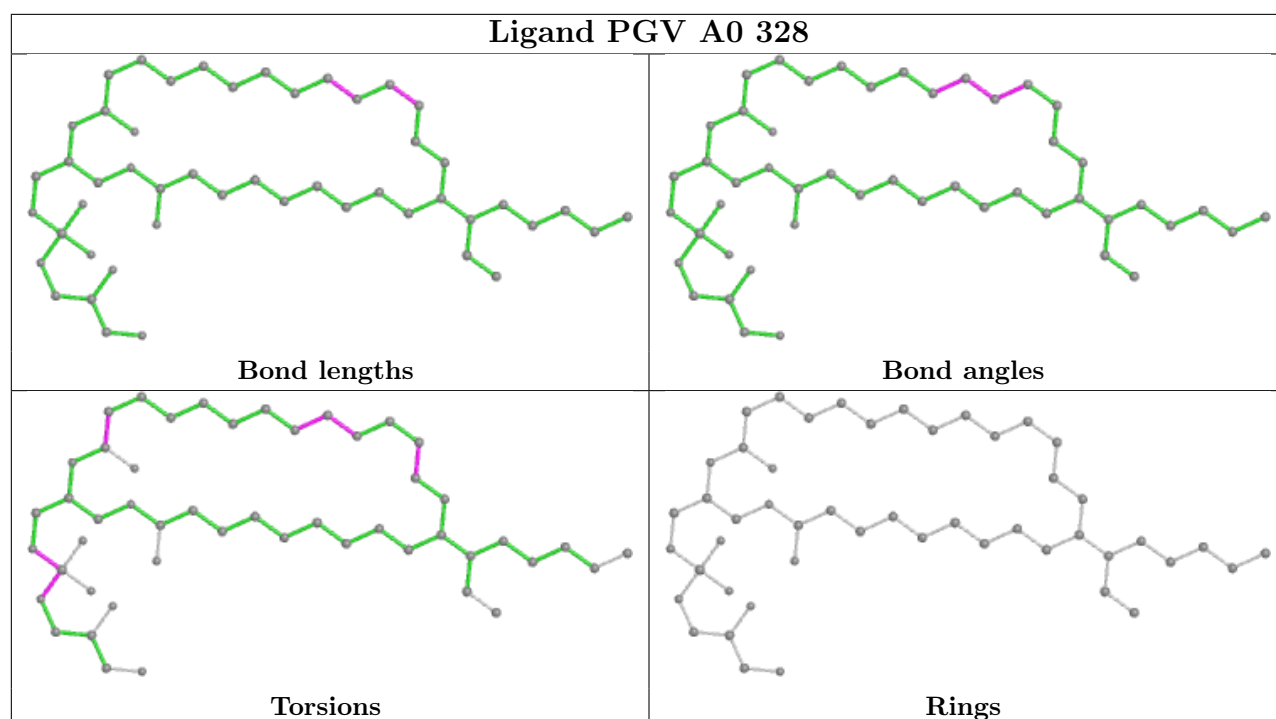


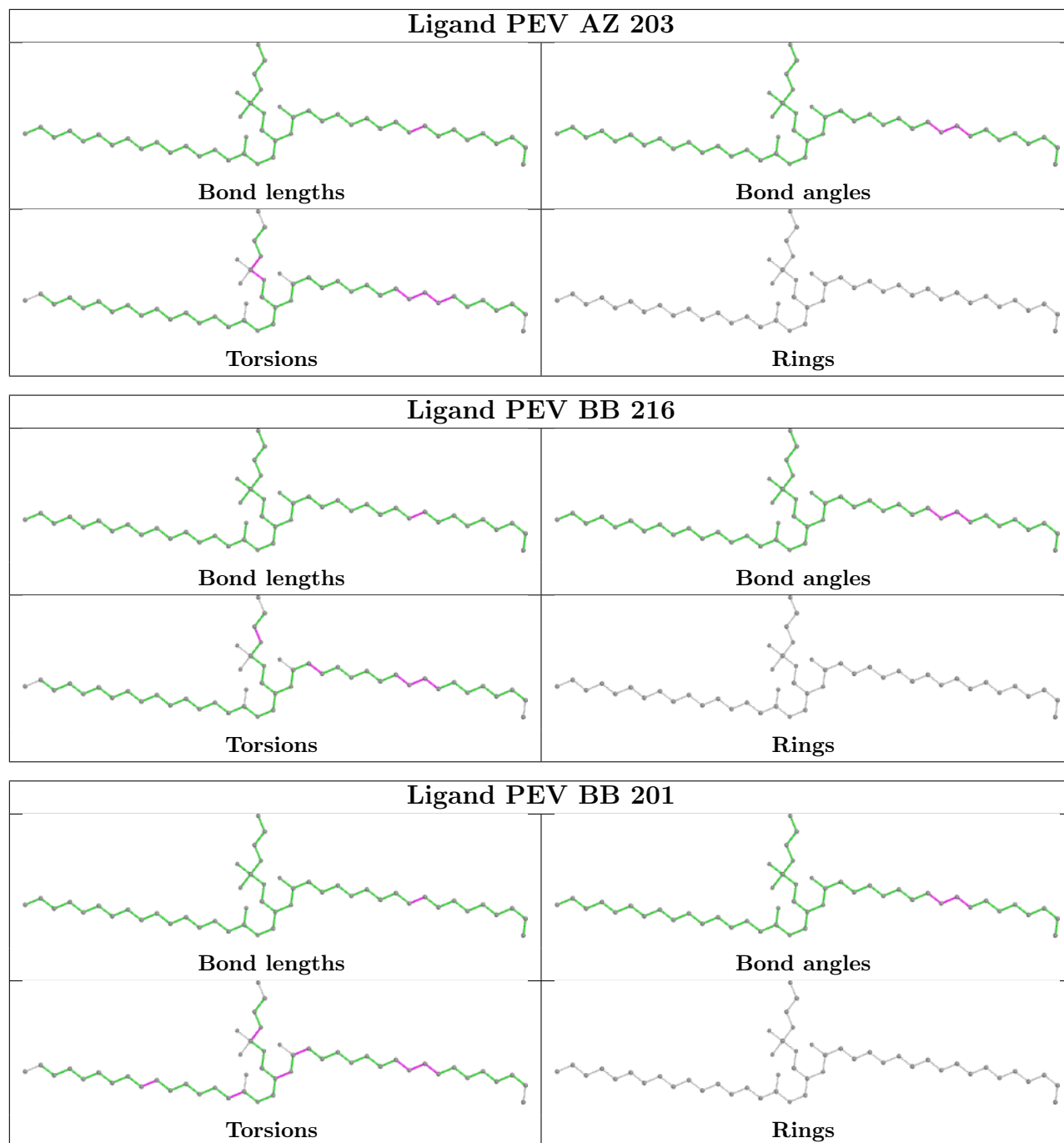


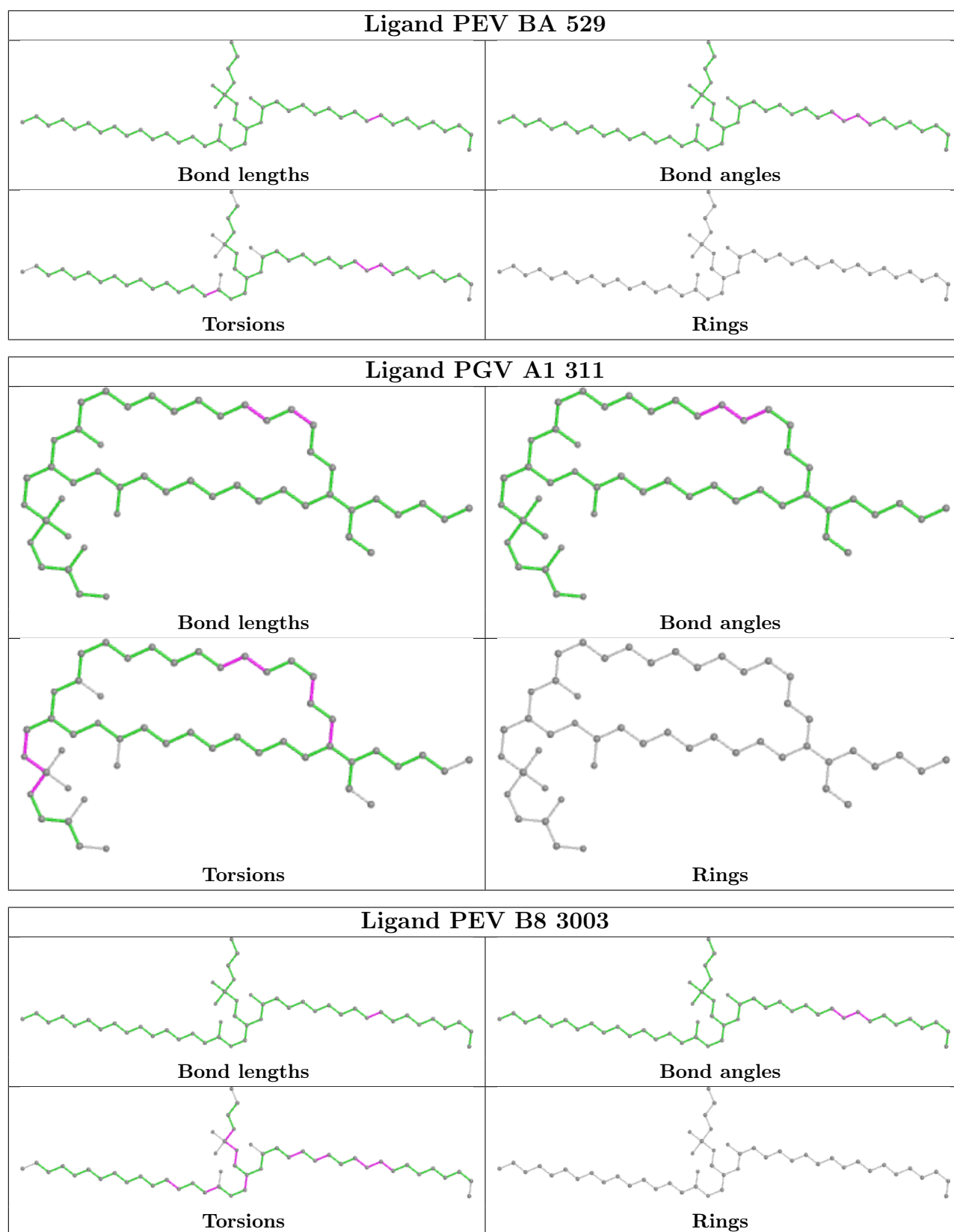


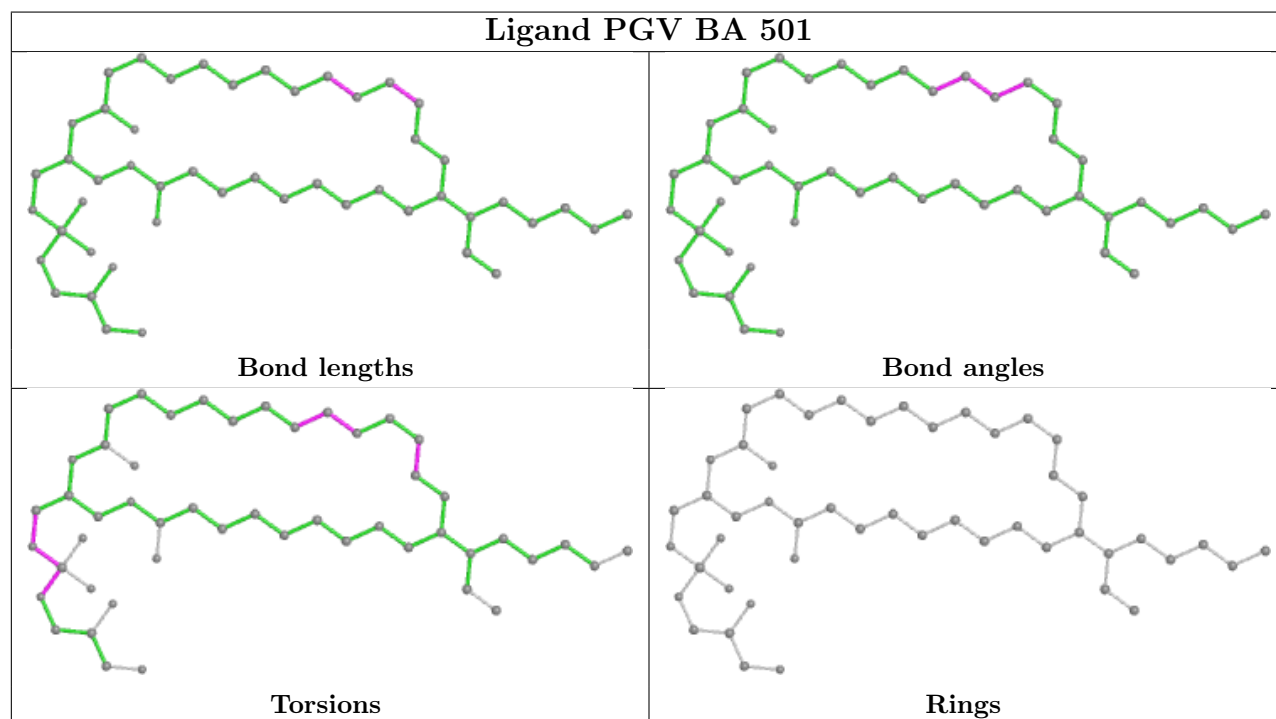
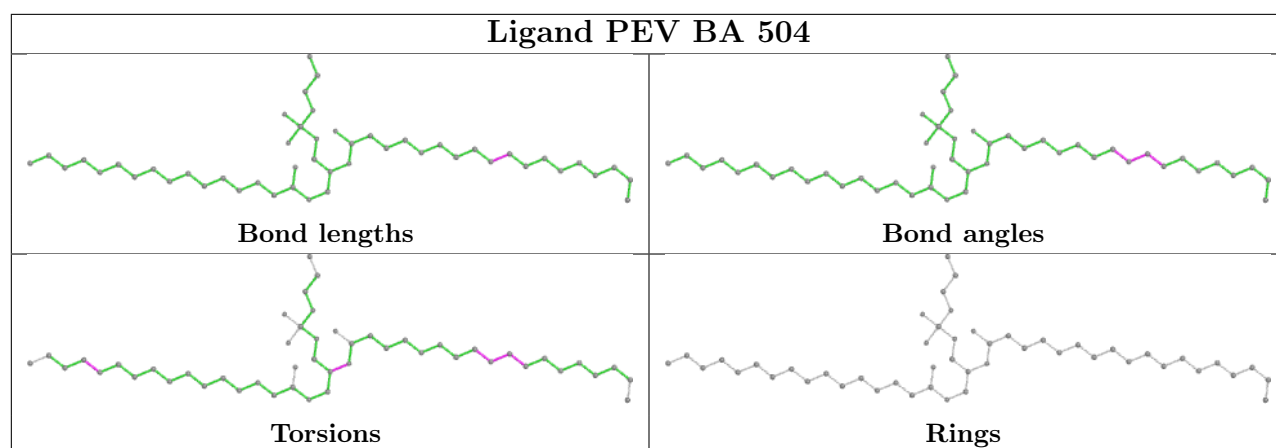




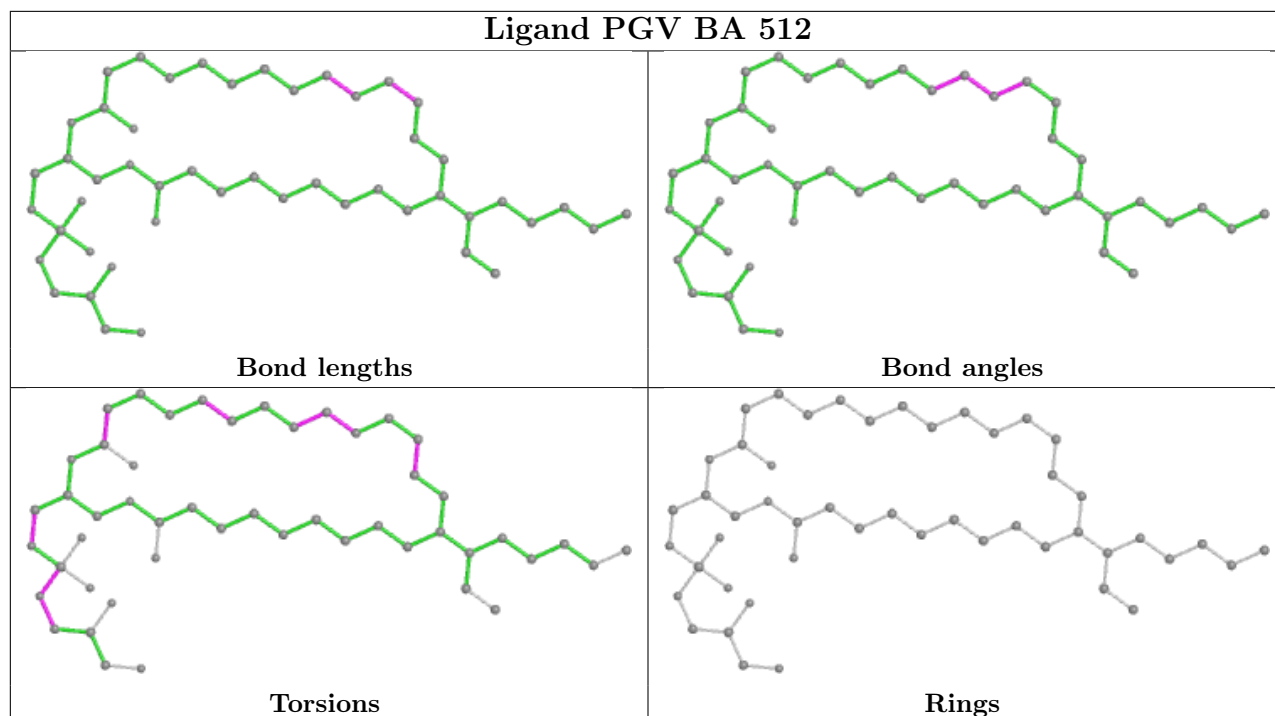




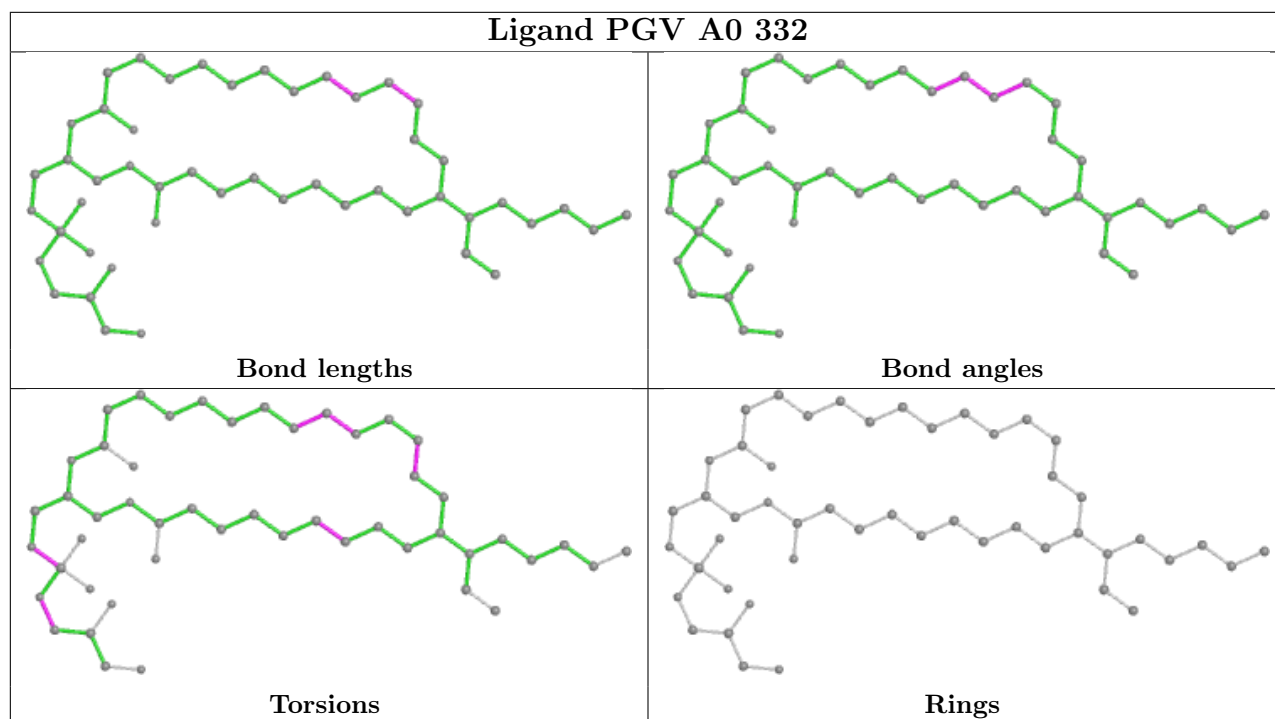


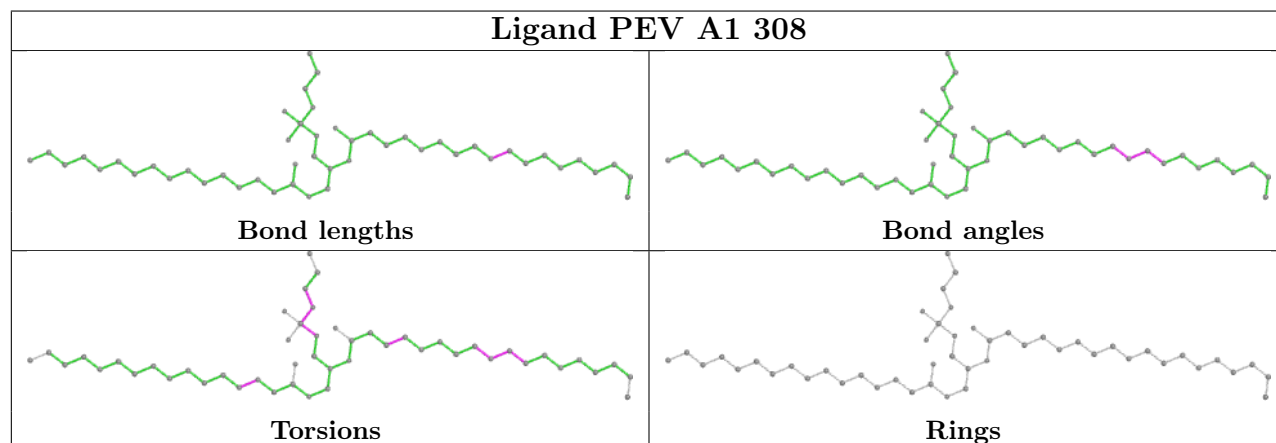
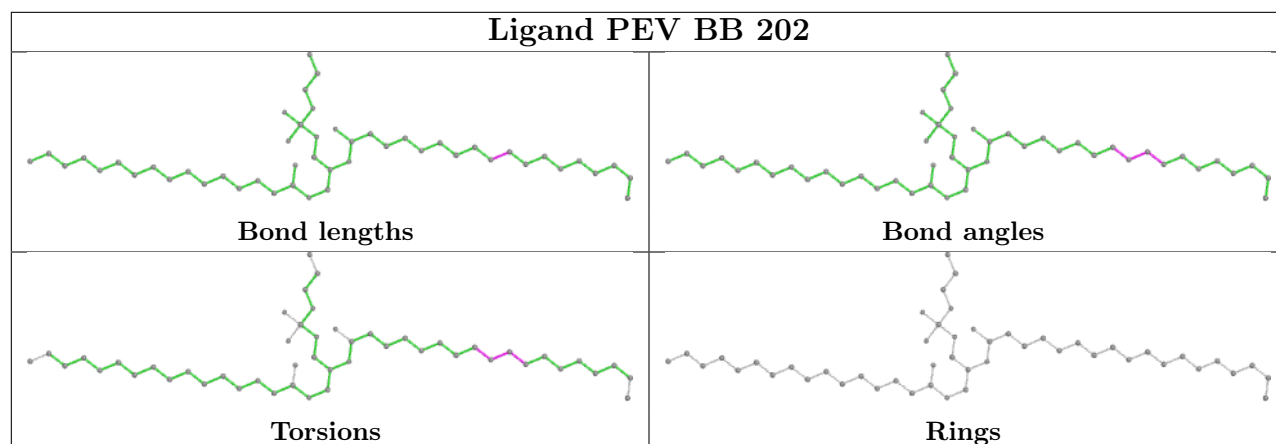
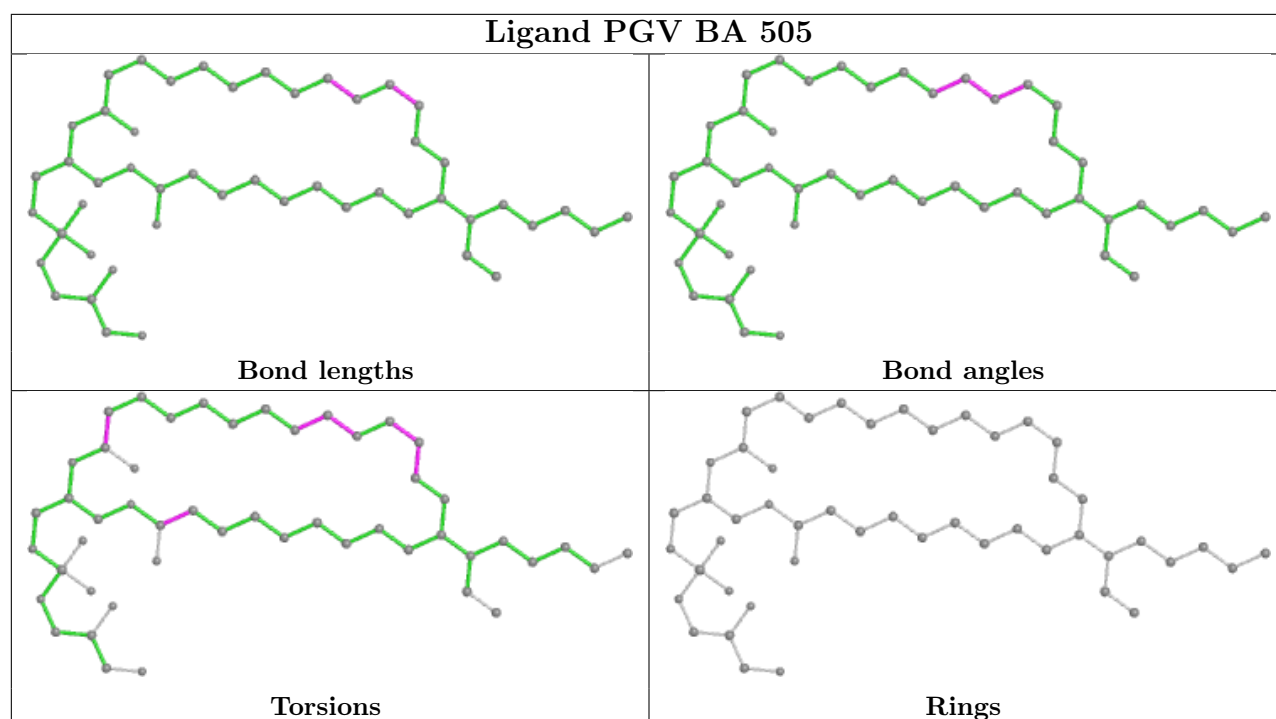


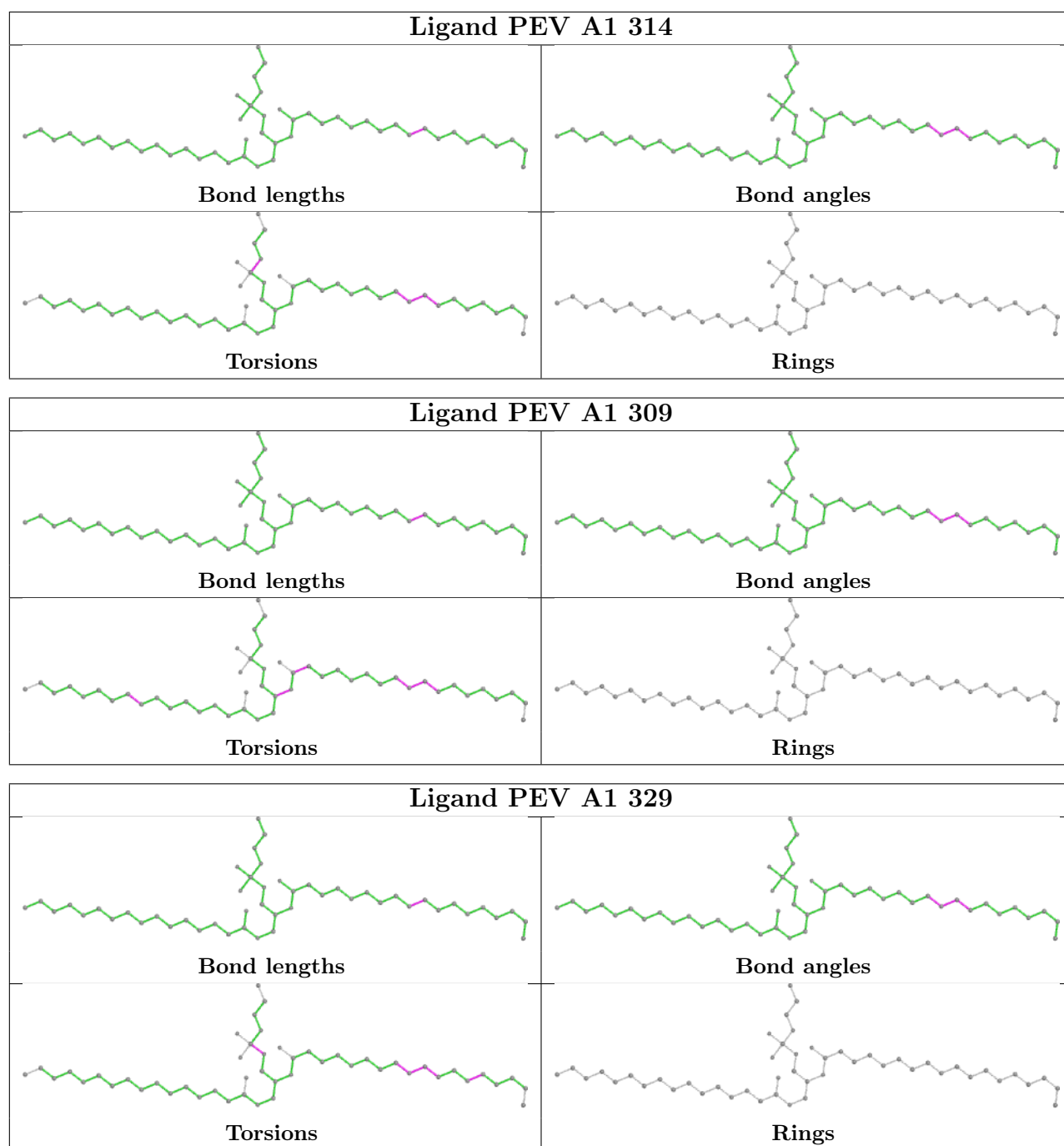
Ligand PGV BA 512

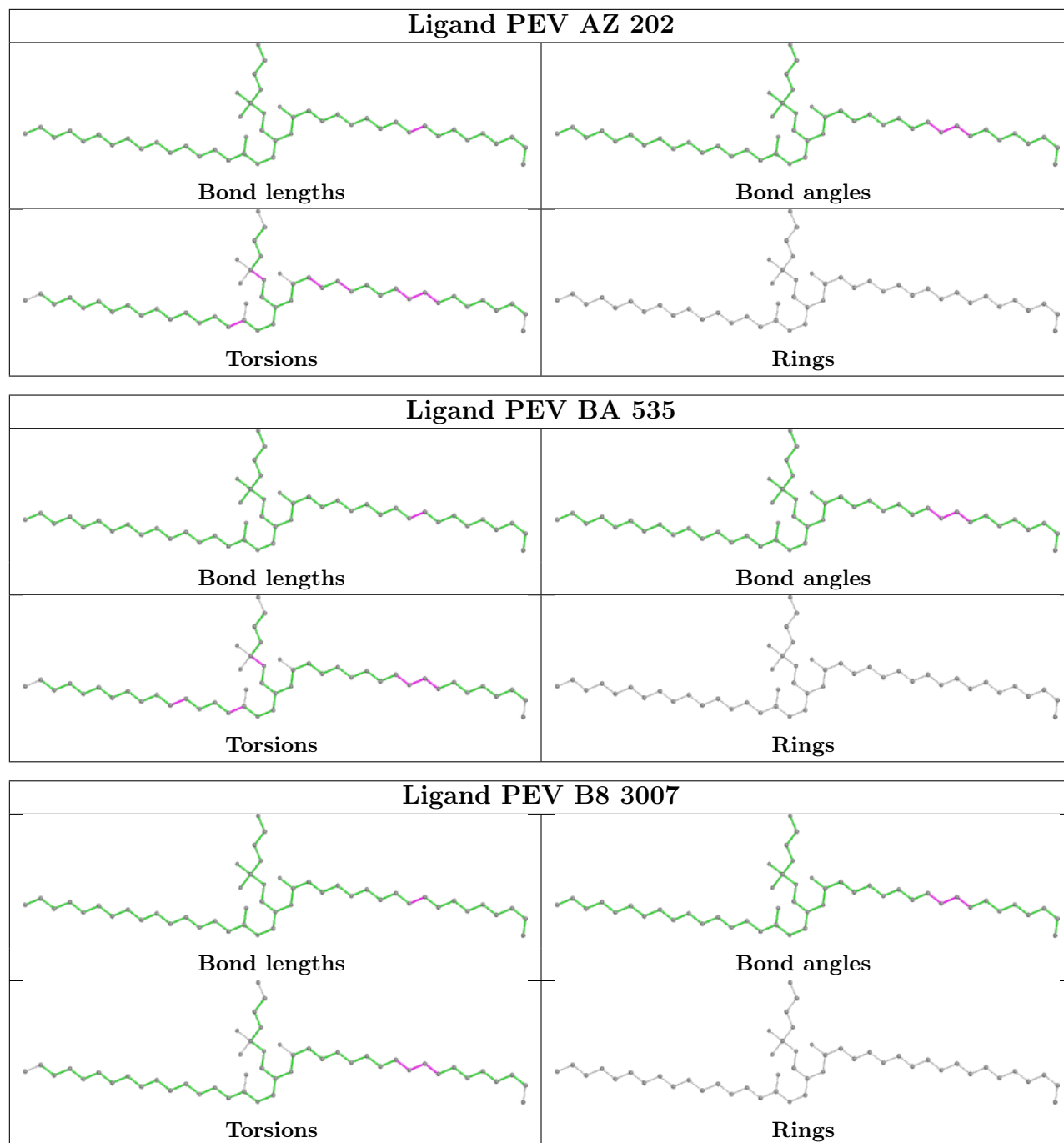


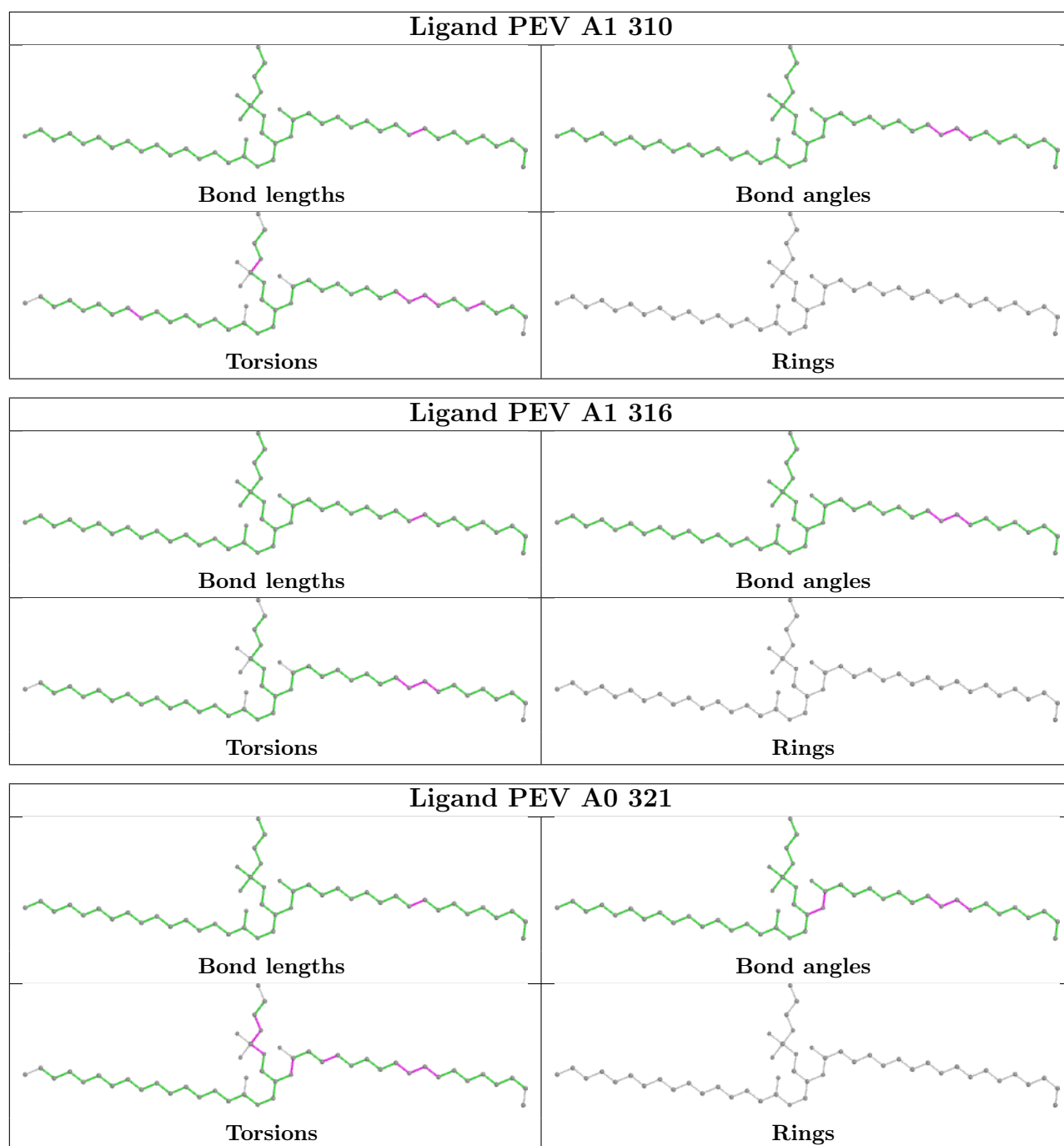
Ligand PGV A0 332

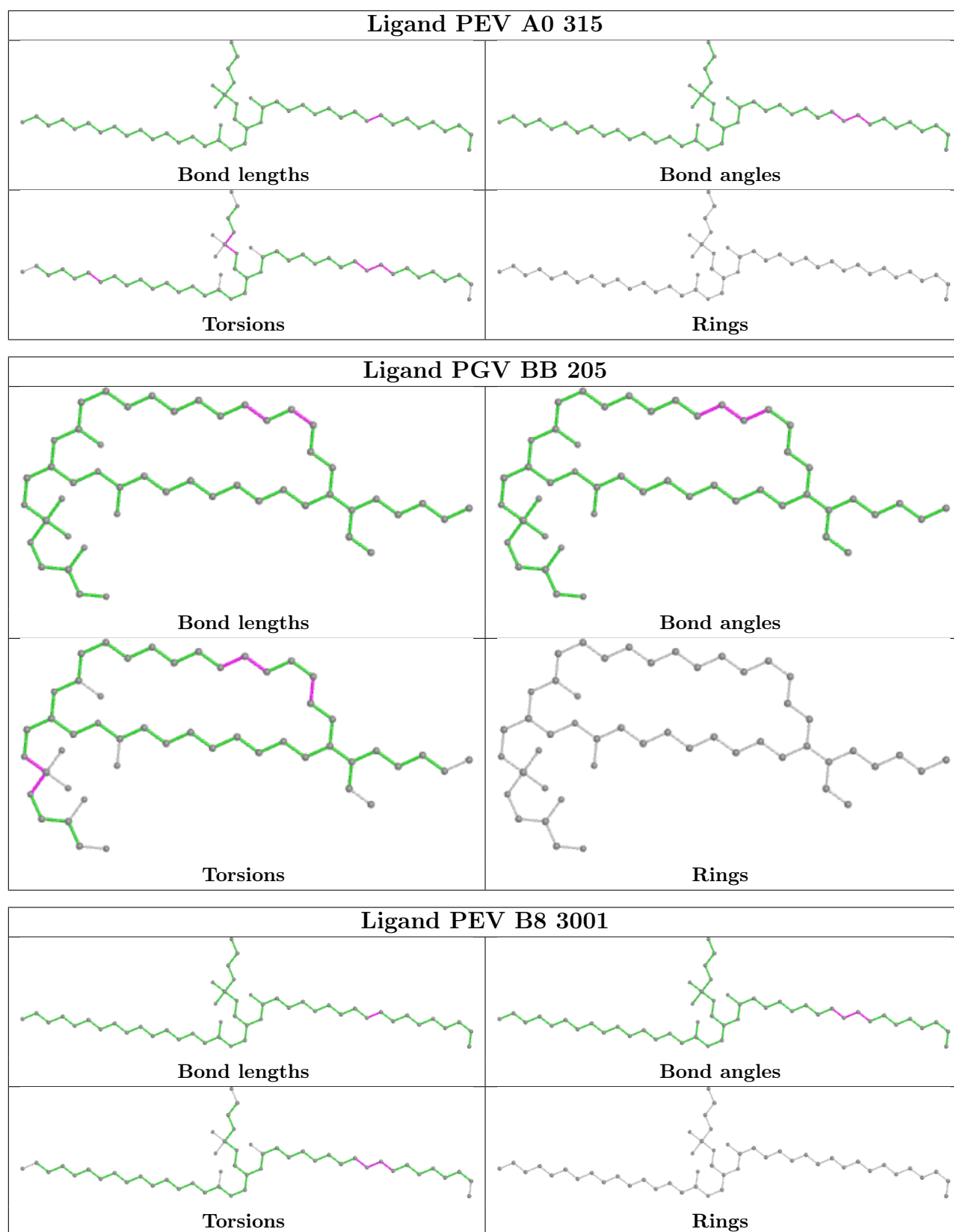


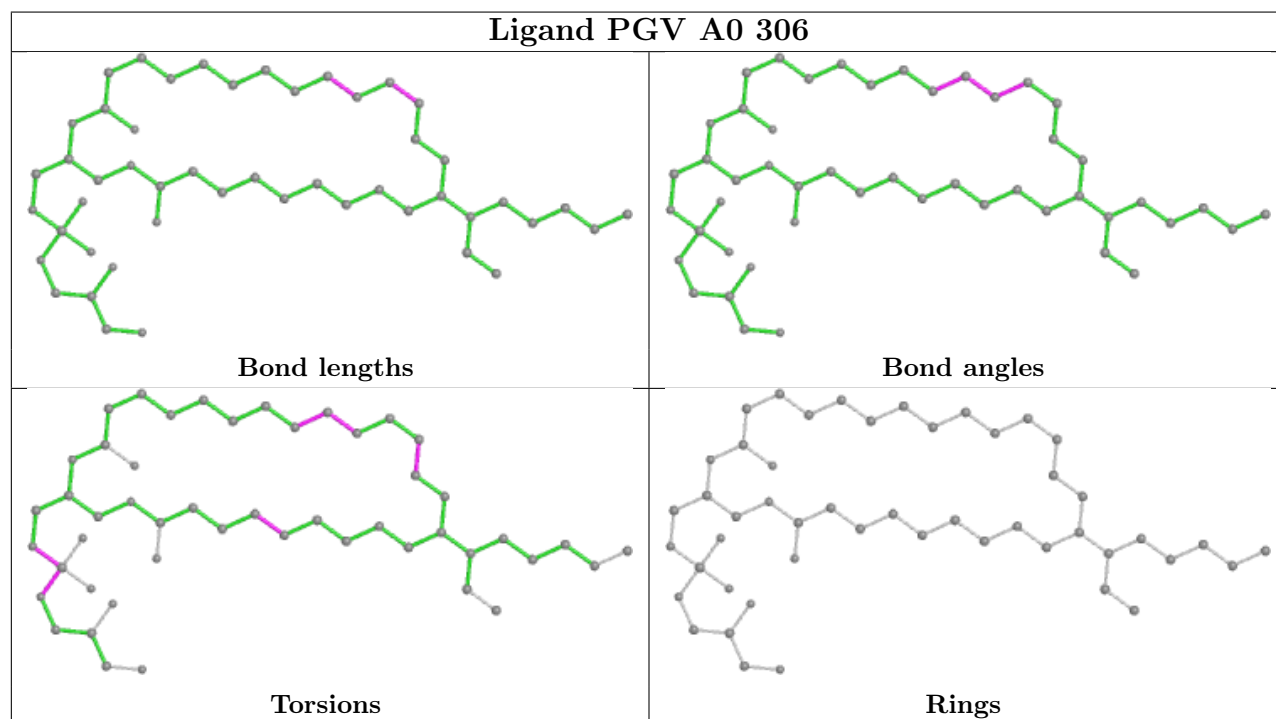
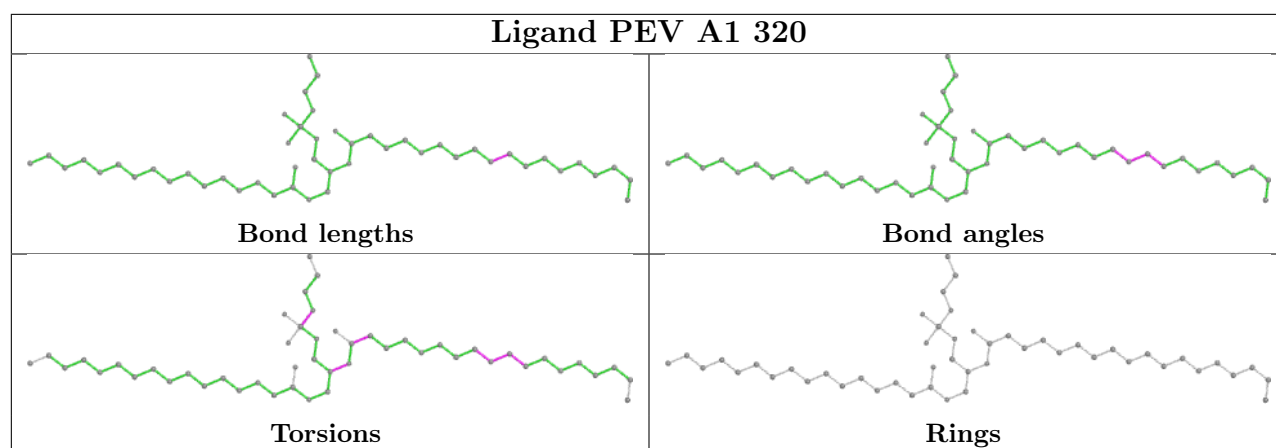


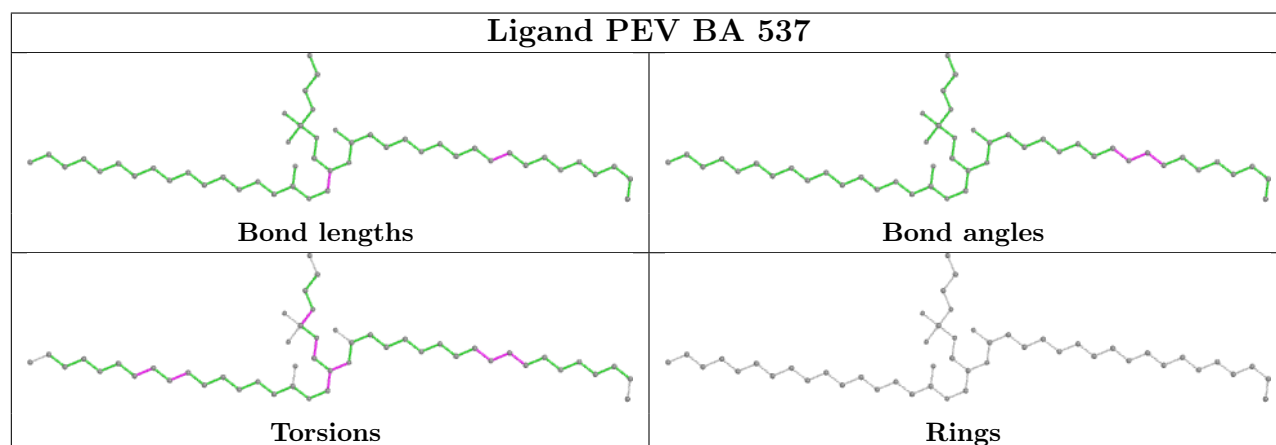
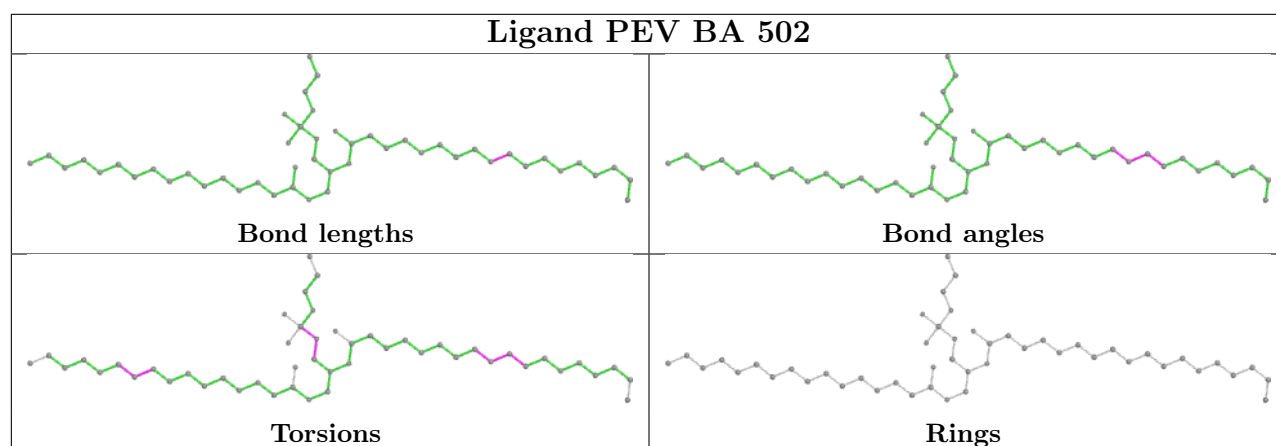
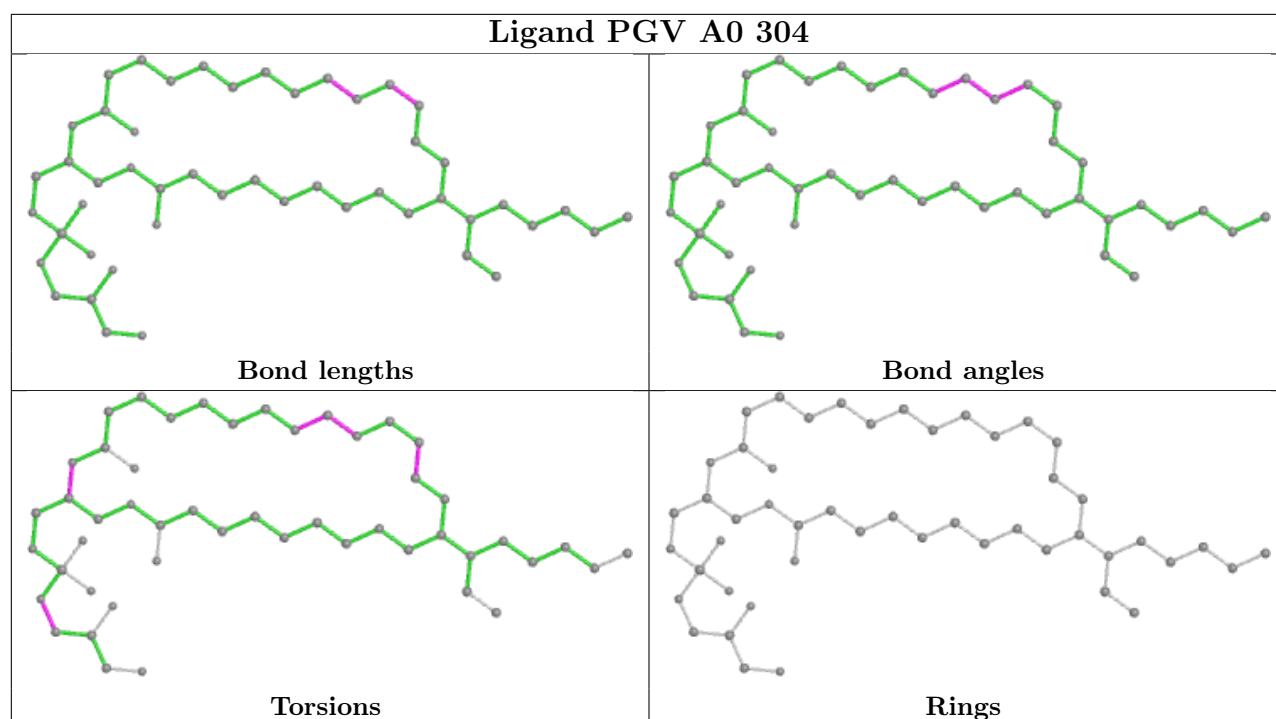


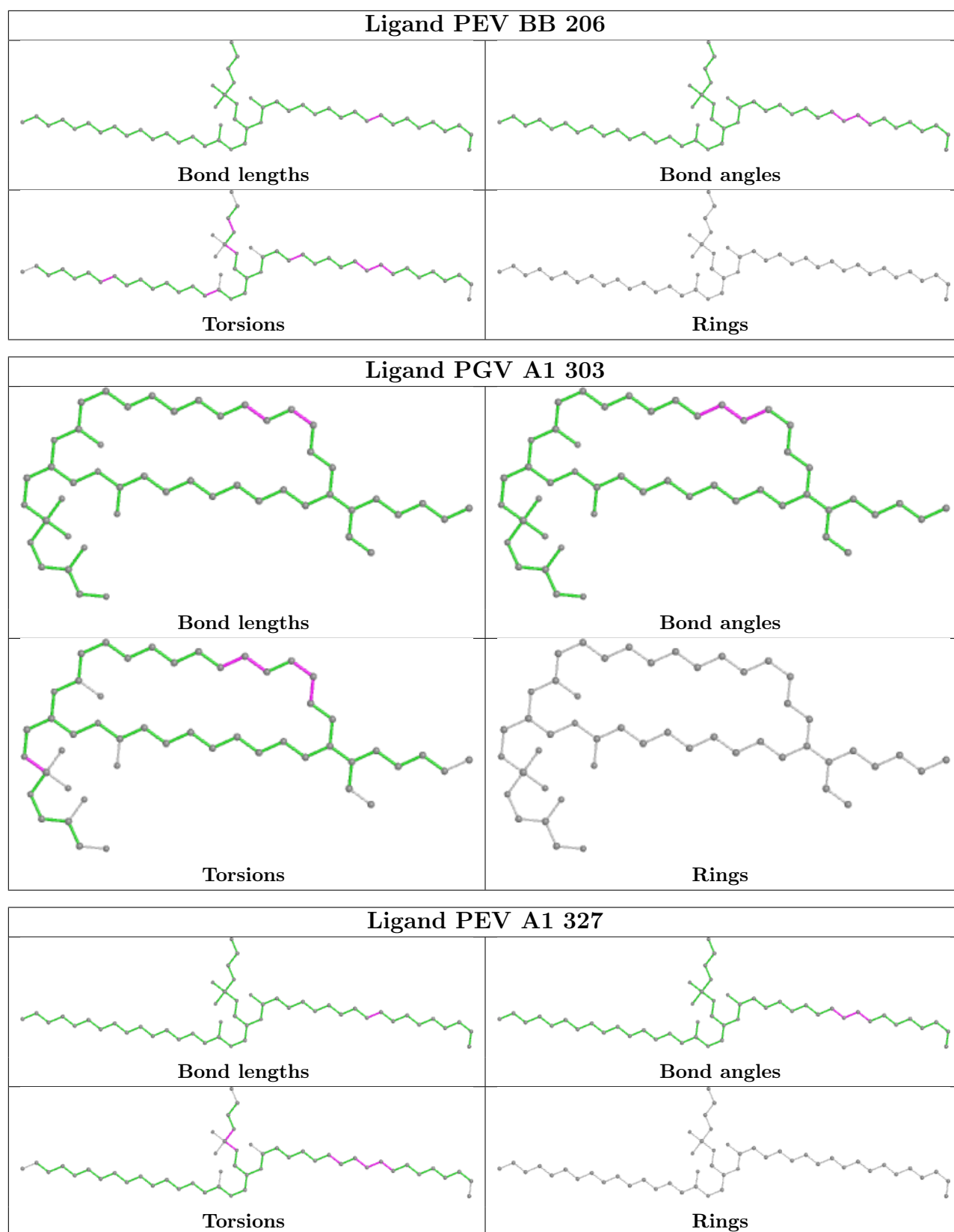


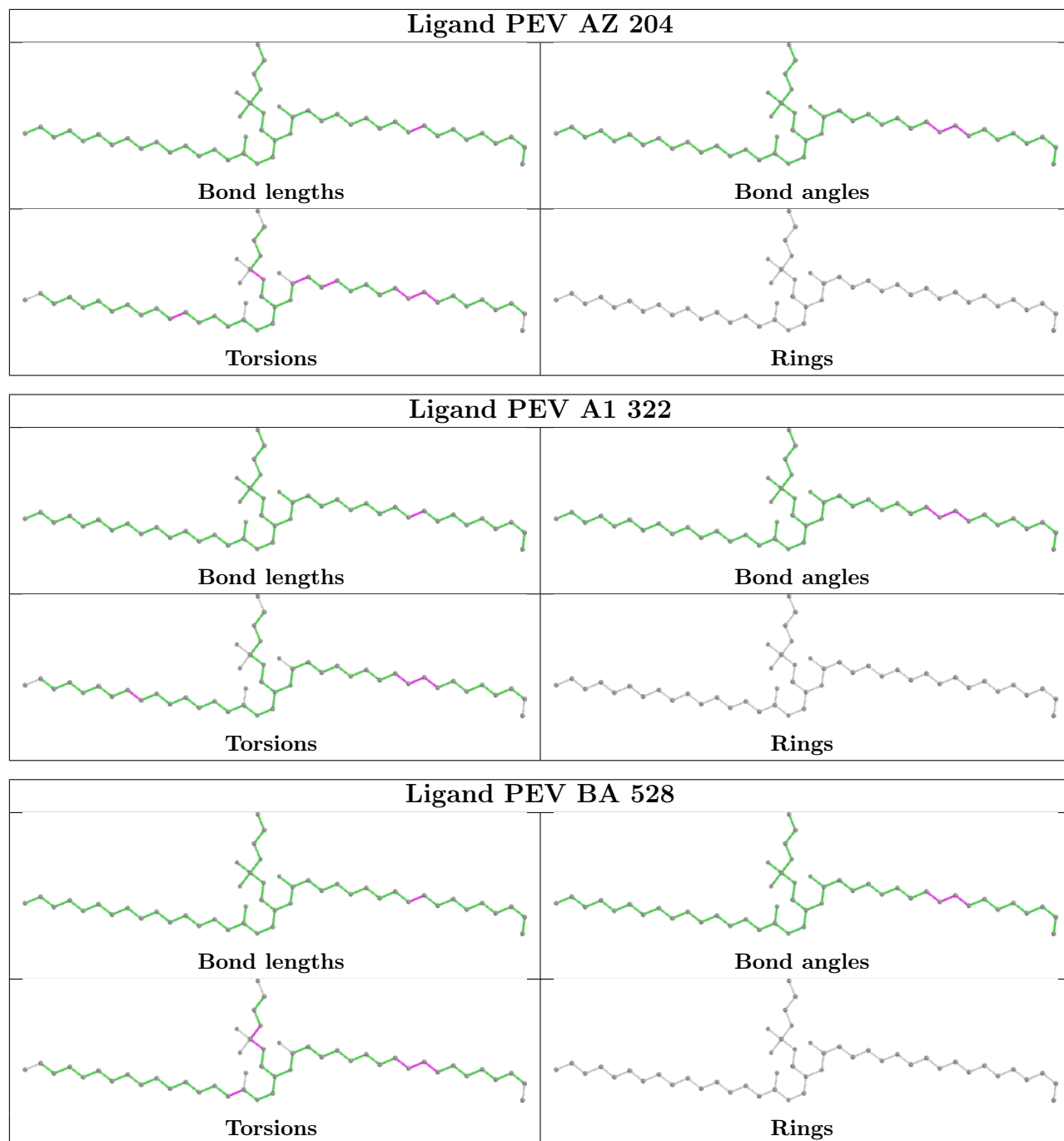




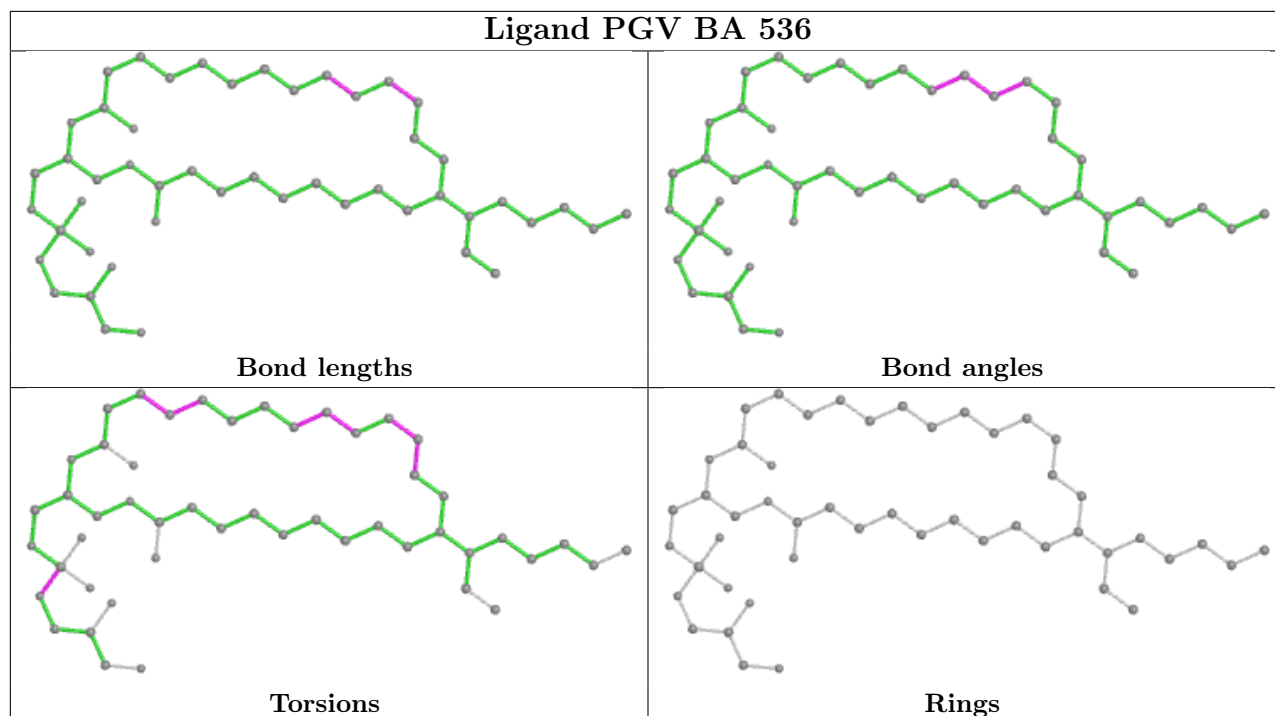




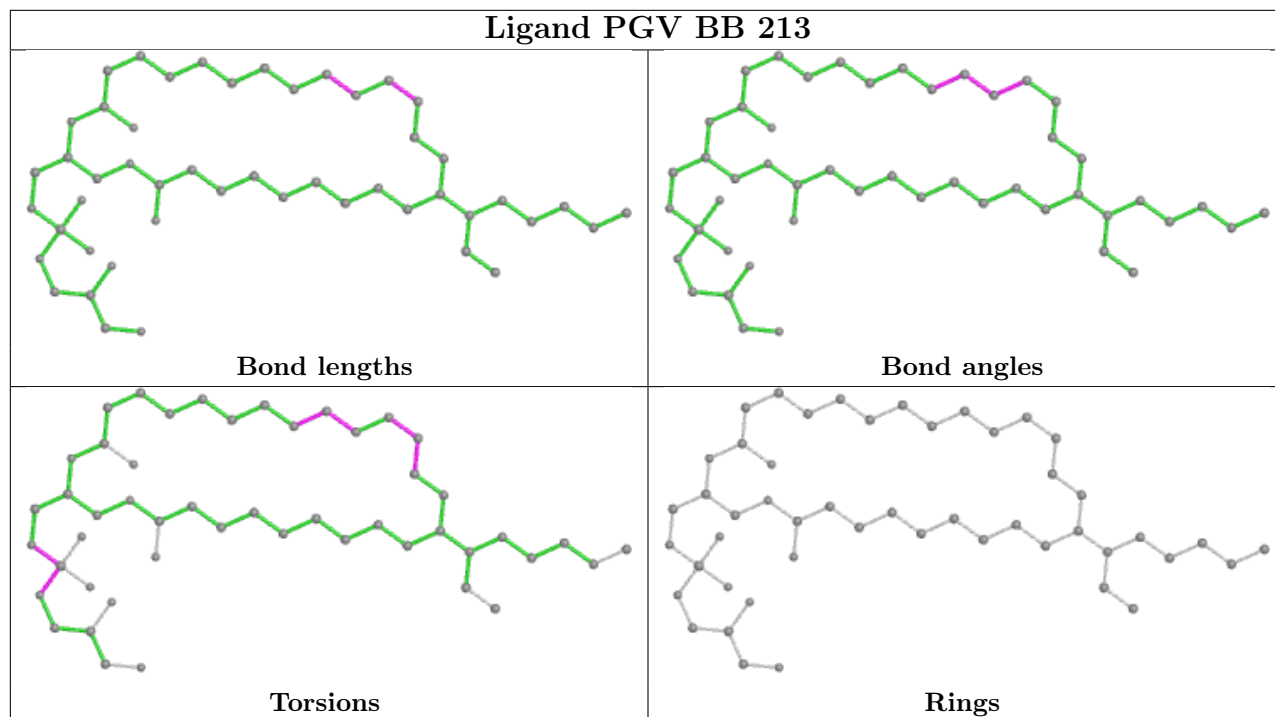


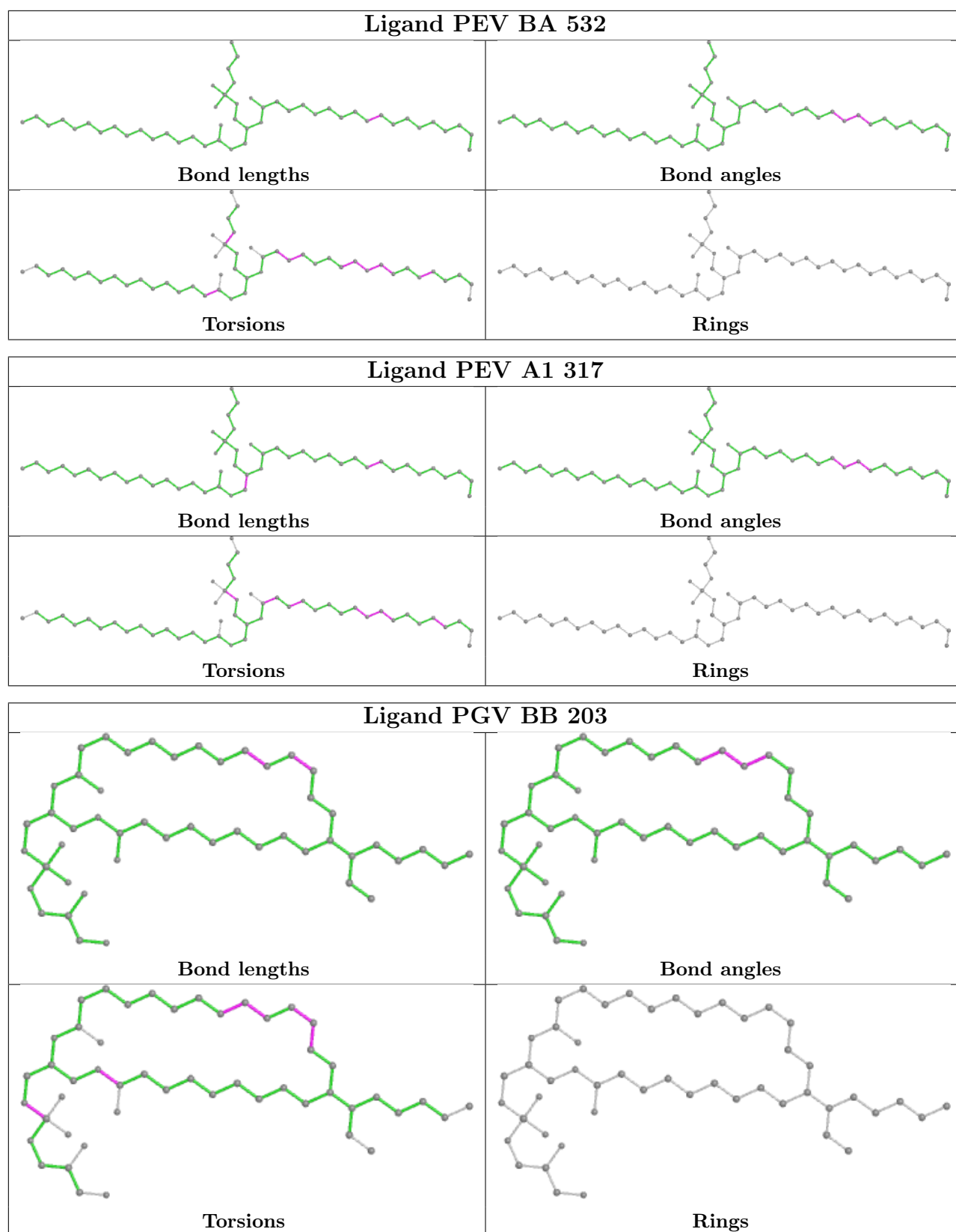


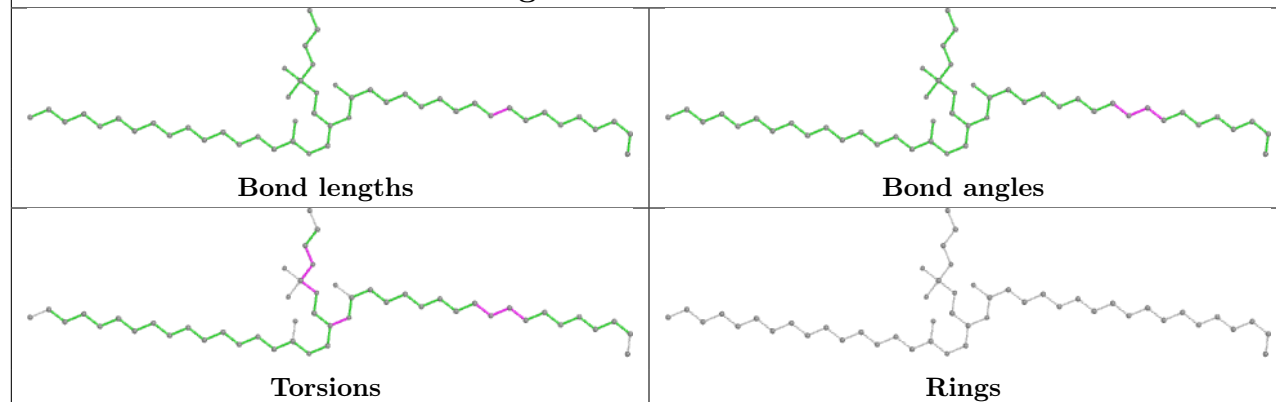
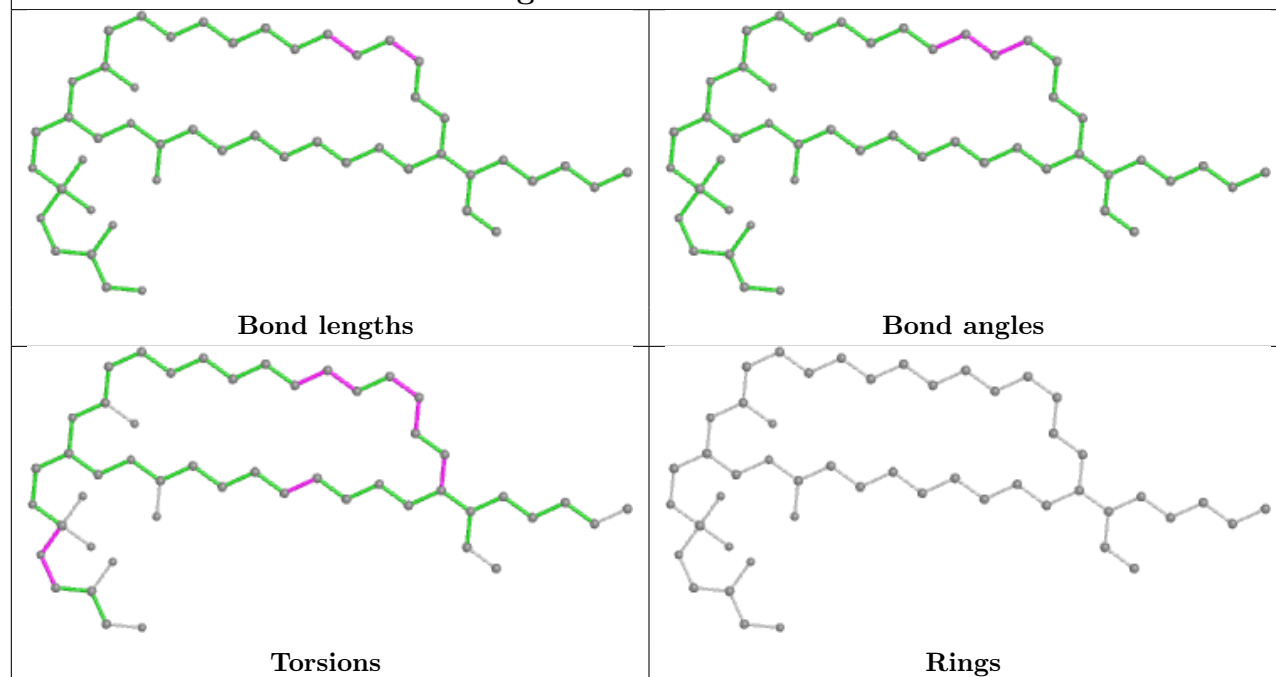
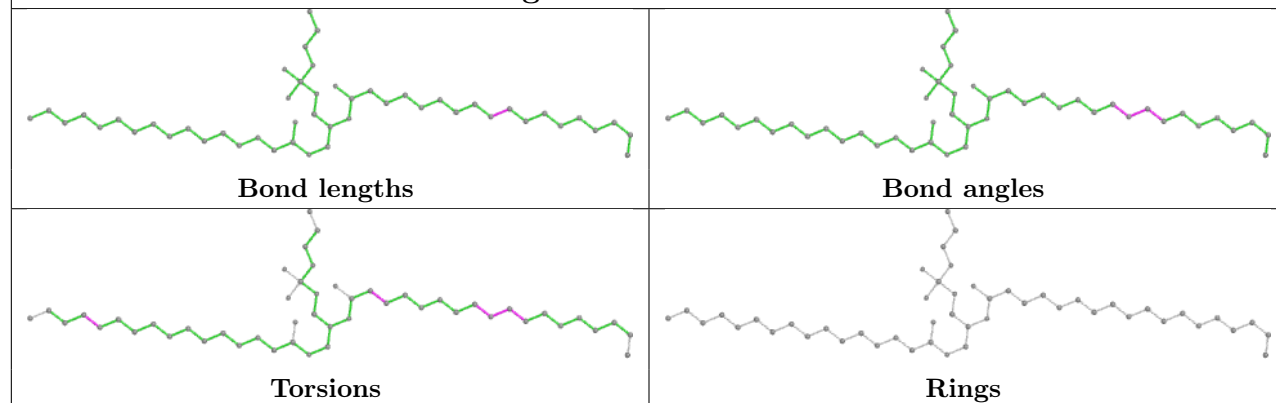
Ligand PGV BA 536

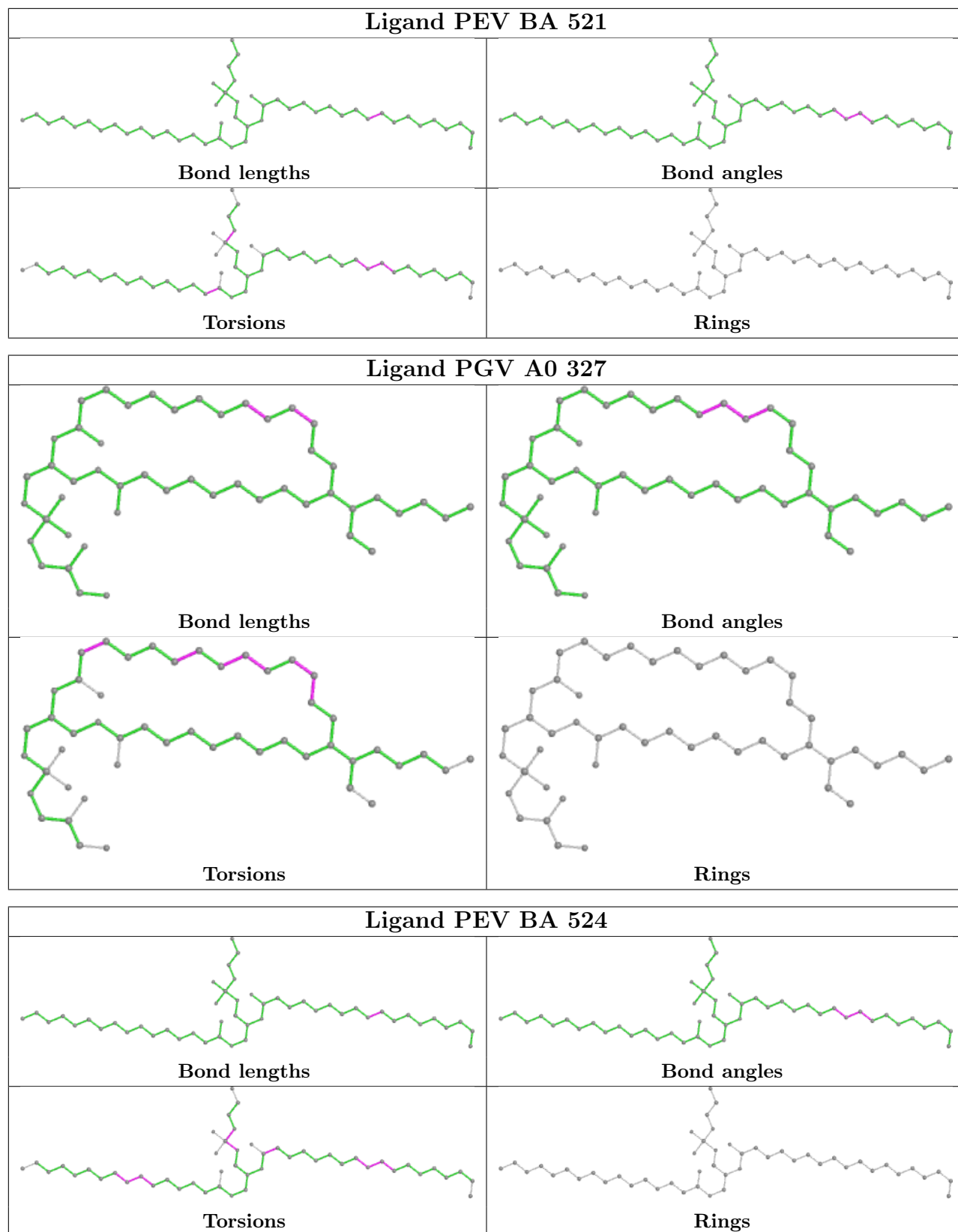


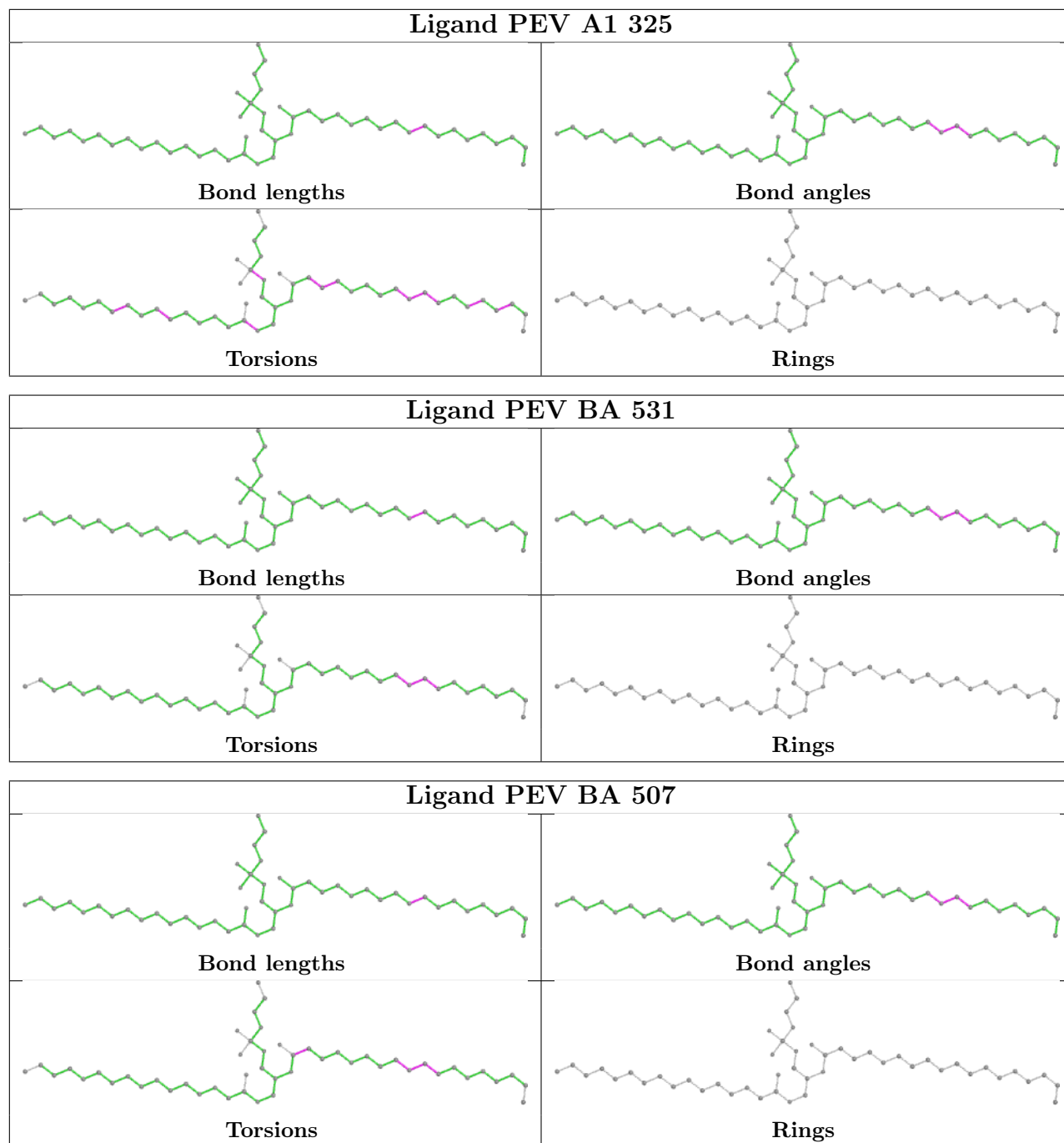
Ligand PGV BB 213

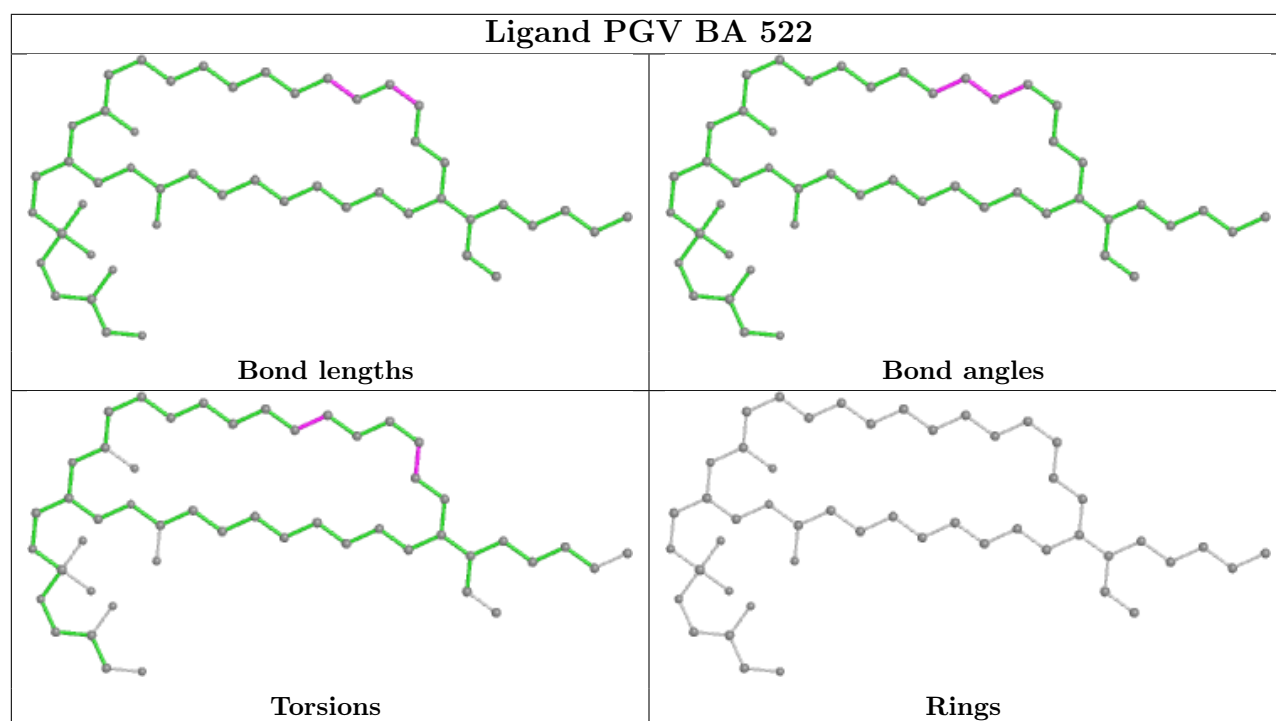
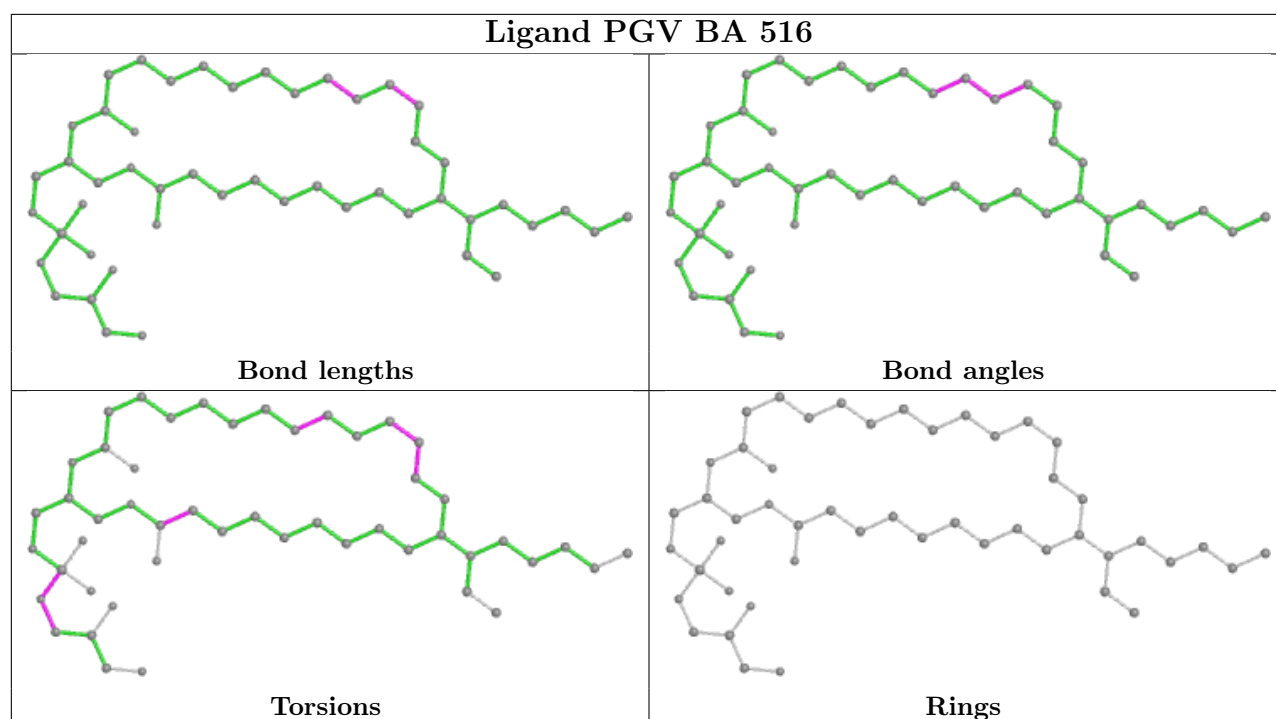




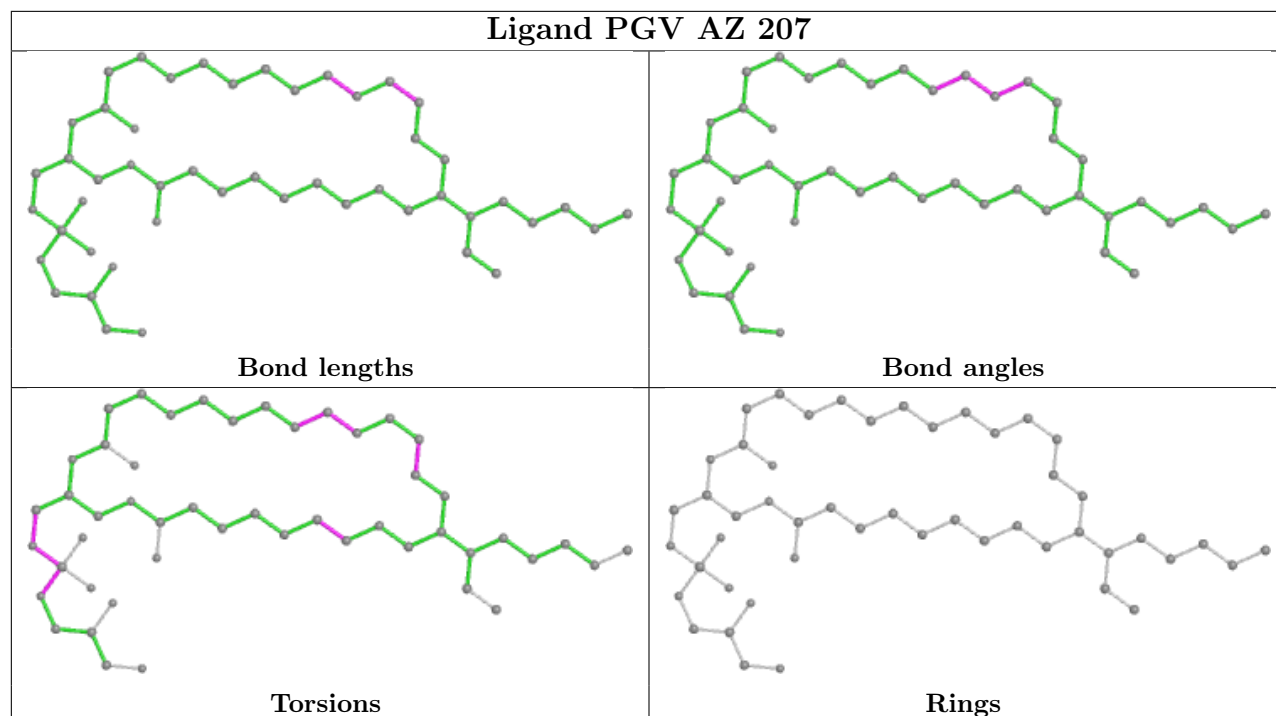
Ligand PEV BA 525**Ligand PGV BB 208****Ligand PEV A1 324**



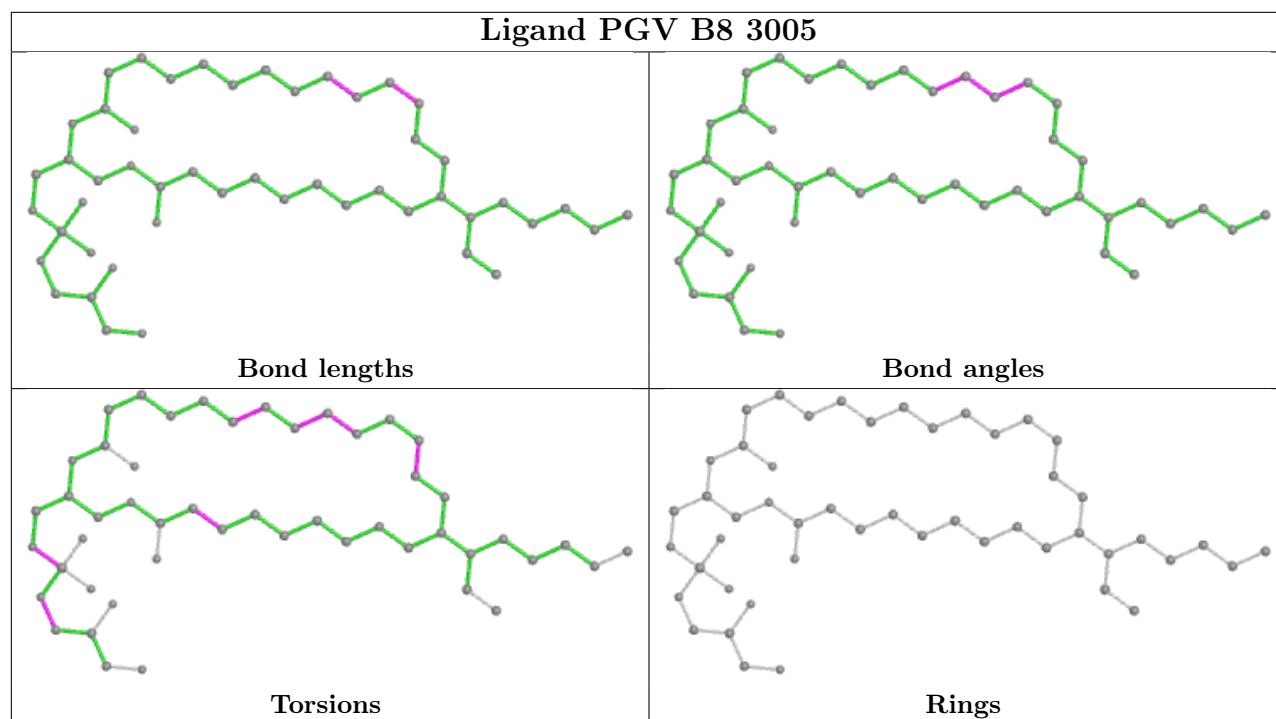


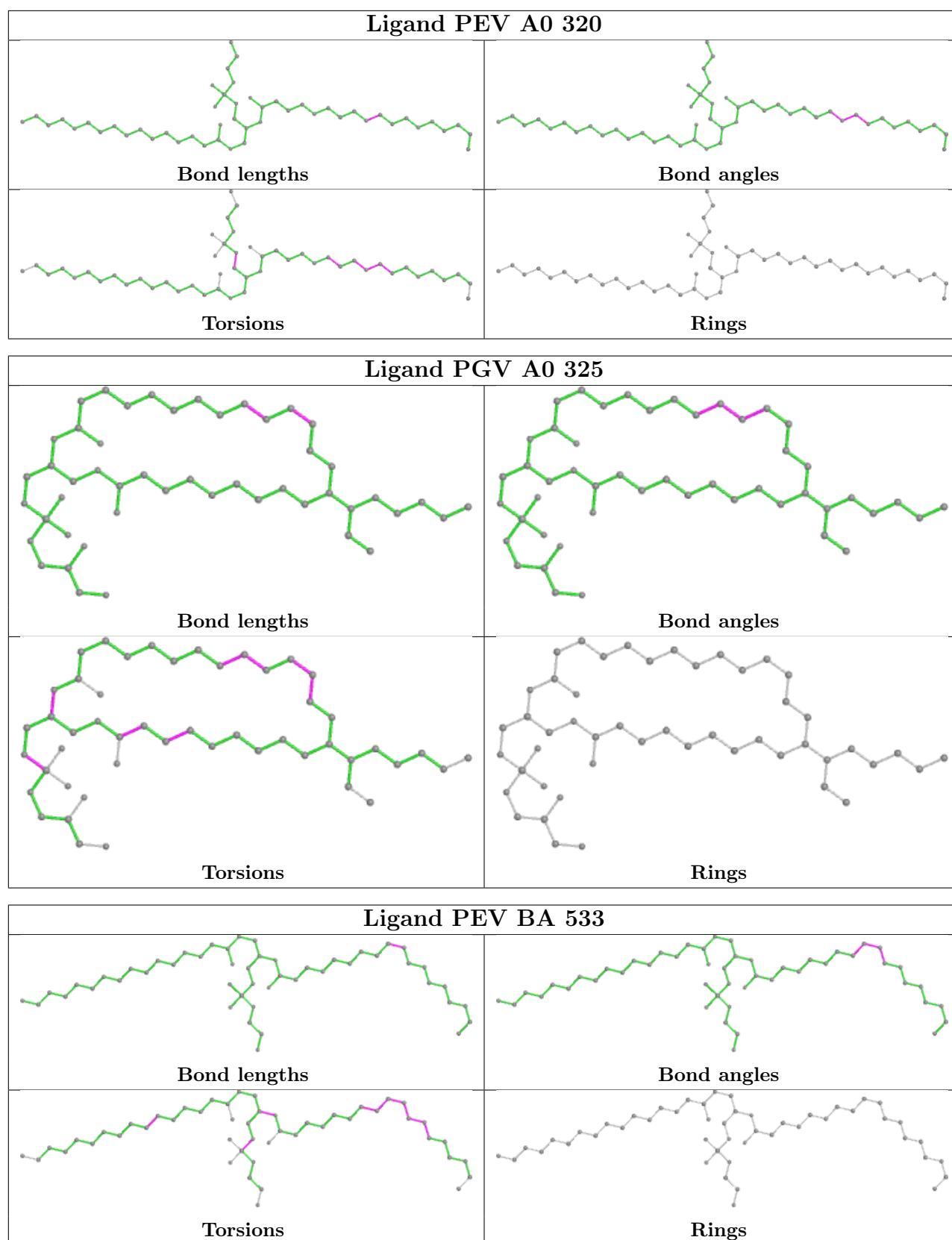


Ligand PGV AZ 207

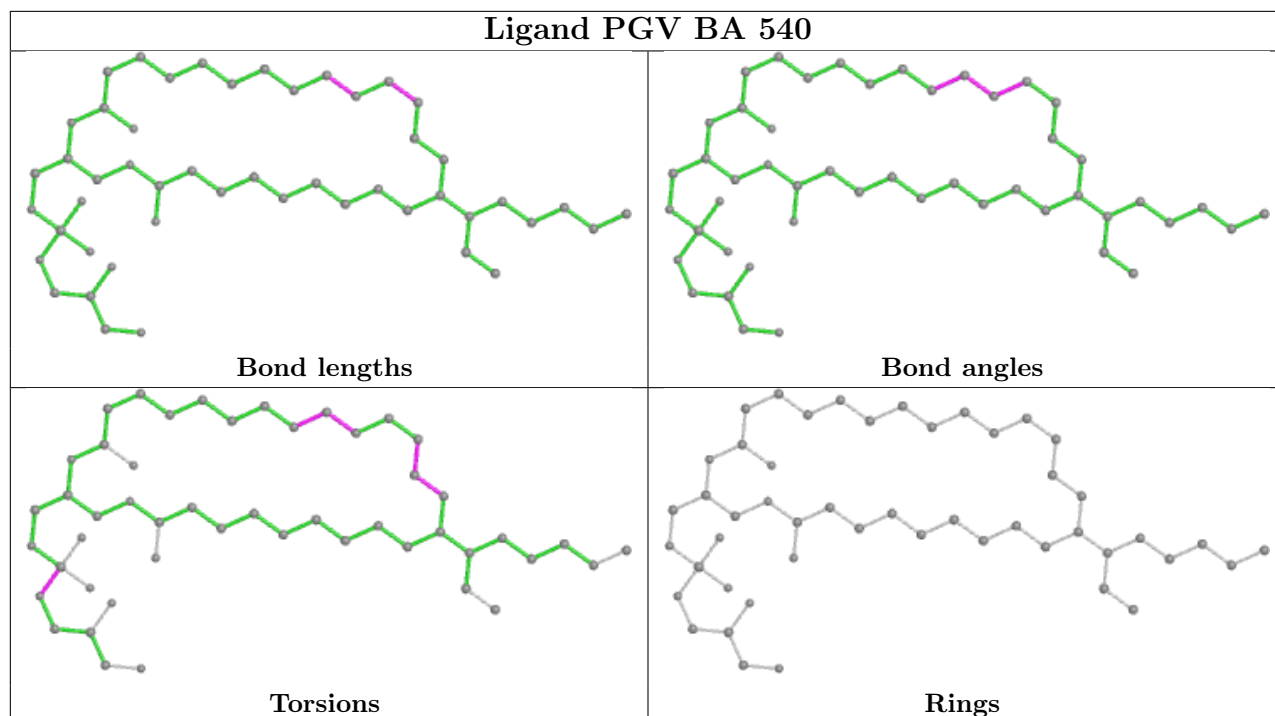


Ligand PGV B8 3005

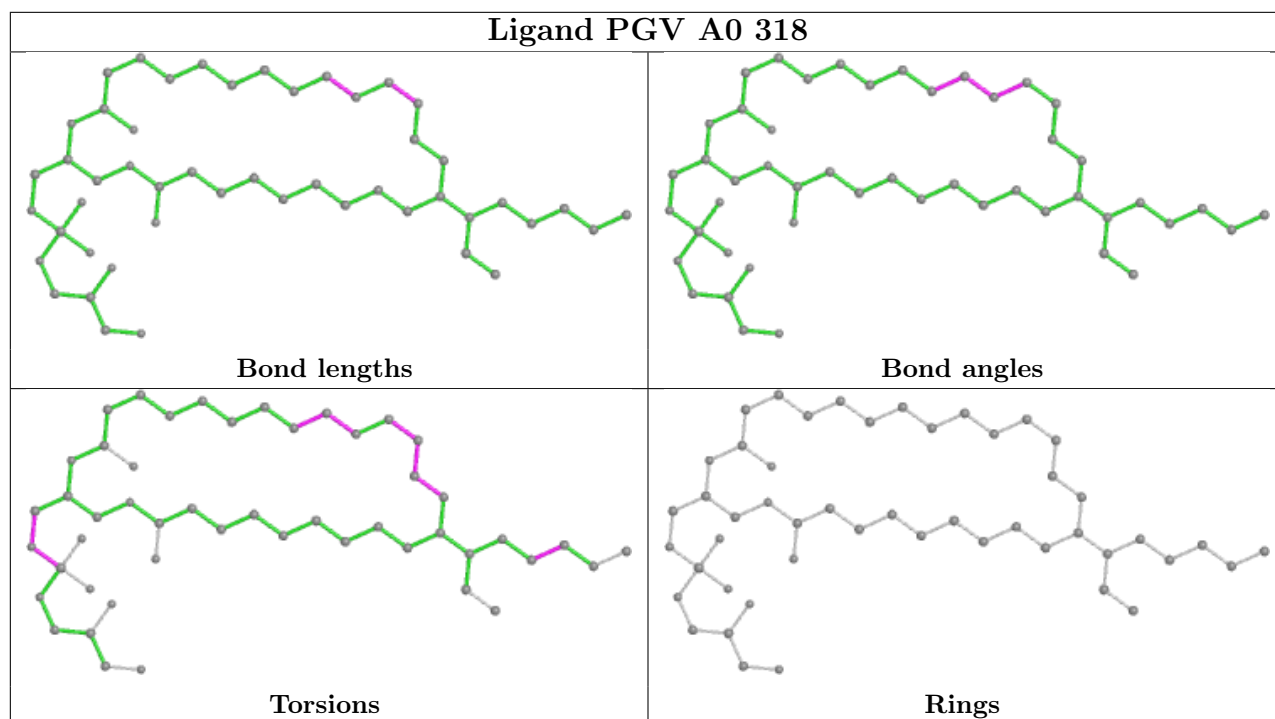


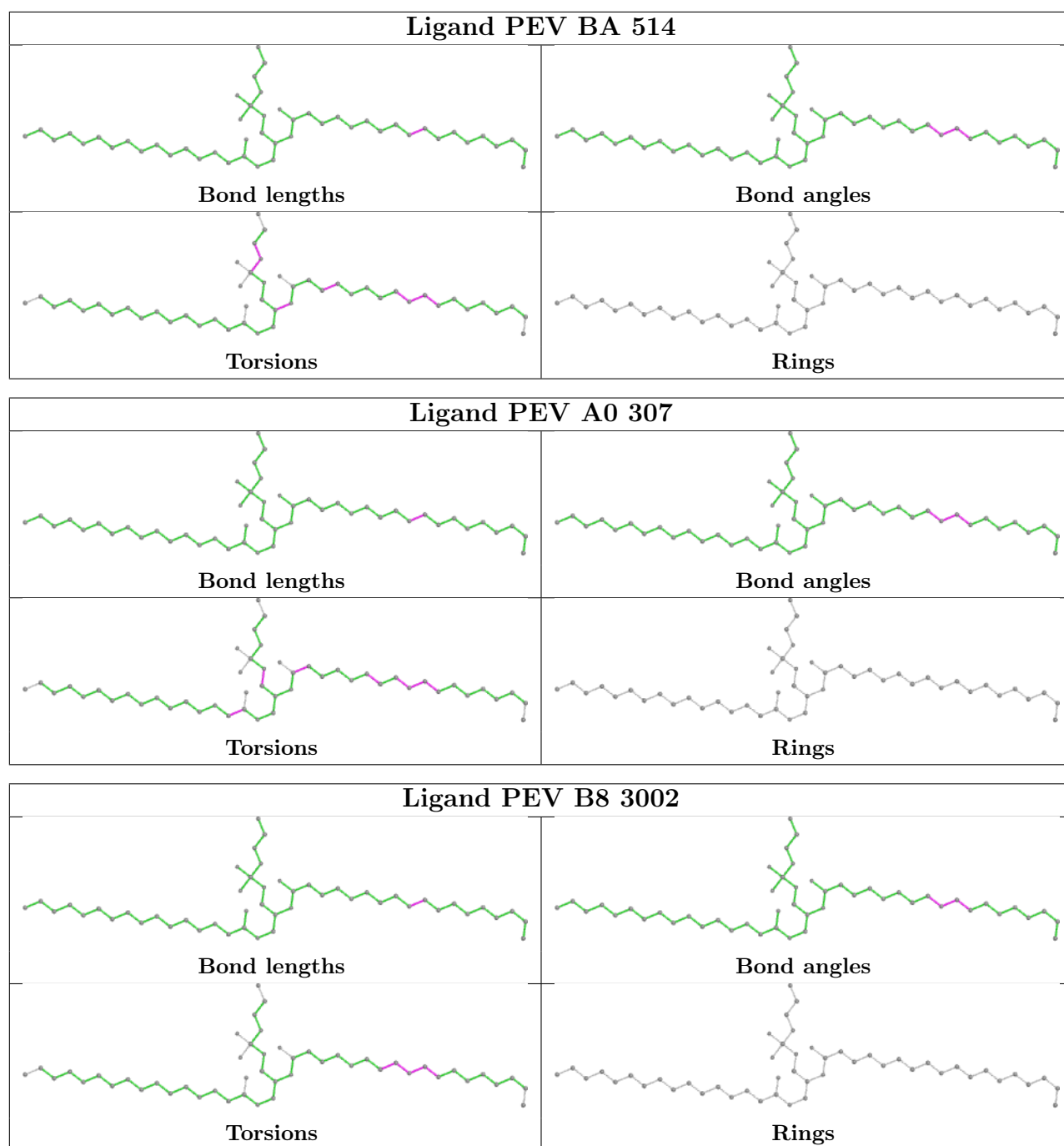


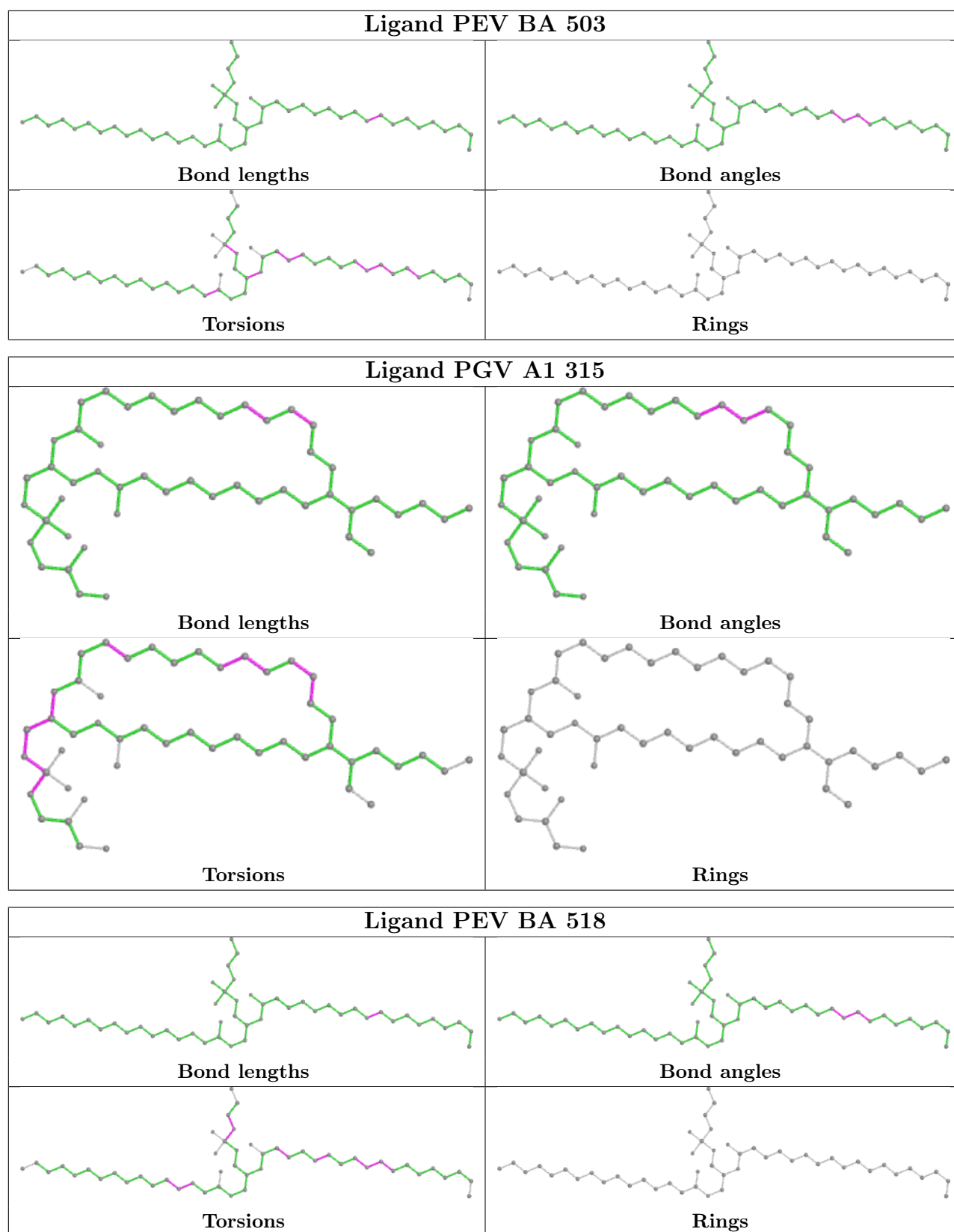
Ligand PGV BA 540

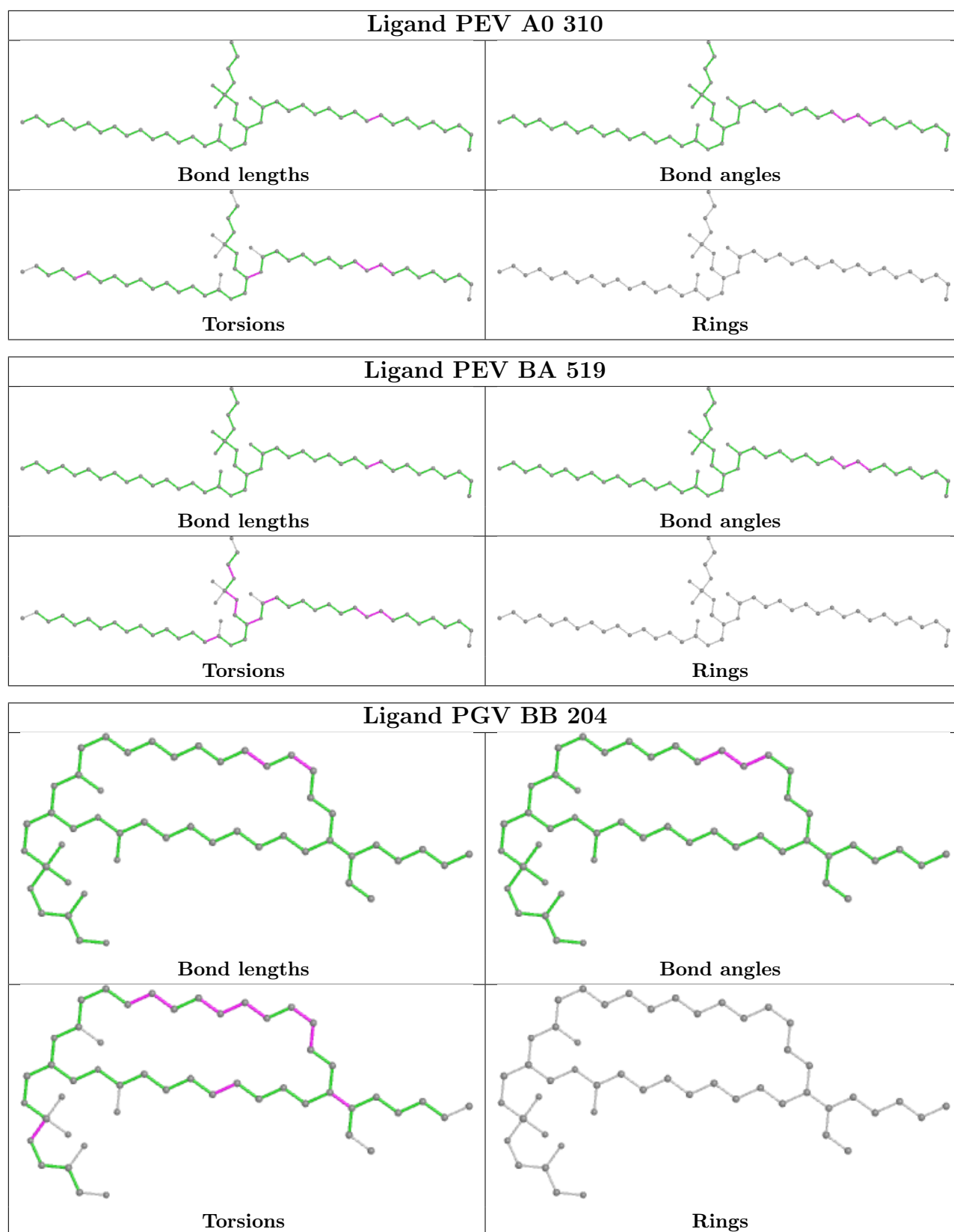


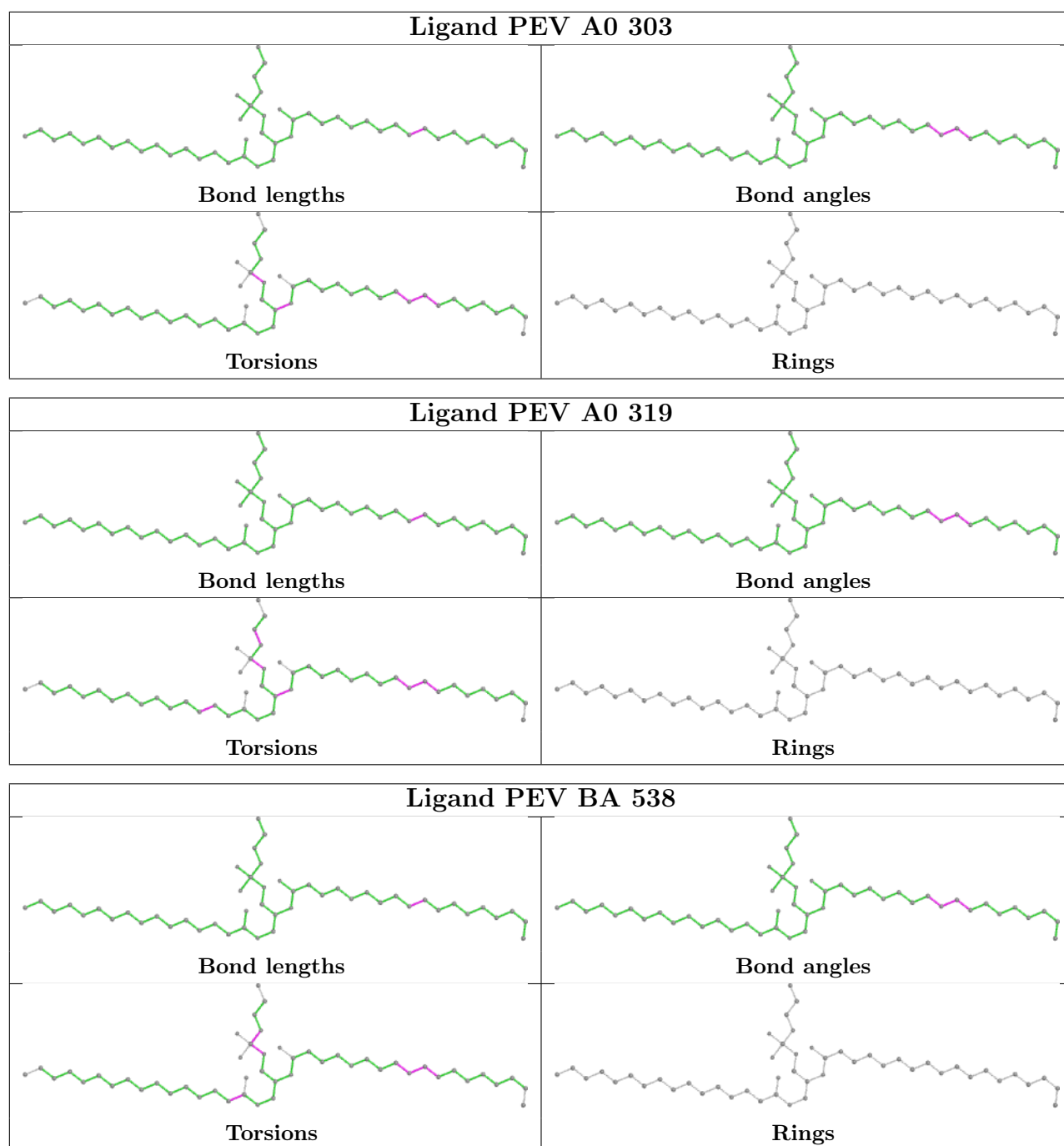
Ligand PGV A0 318

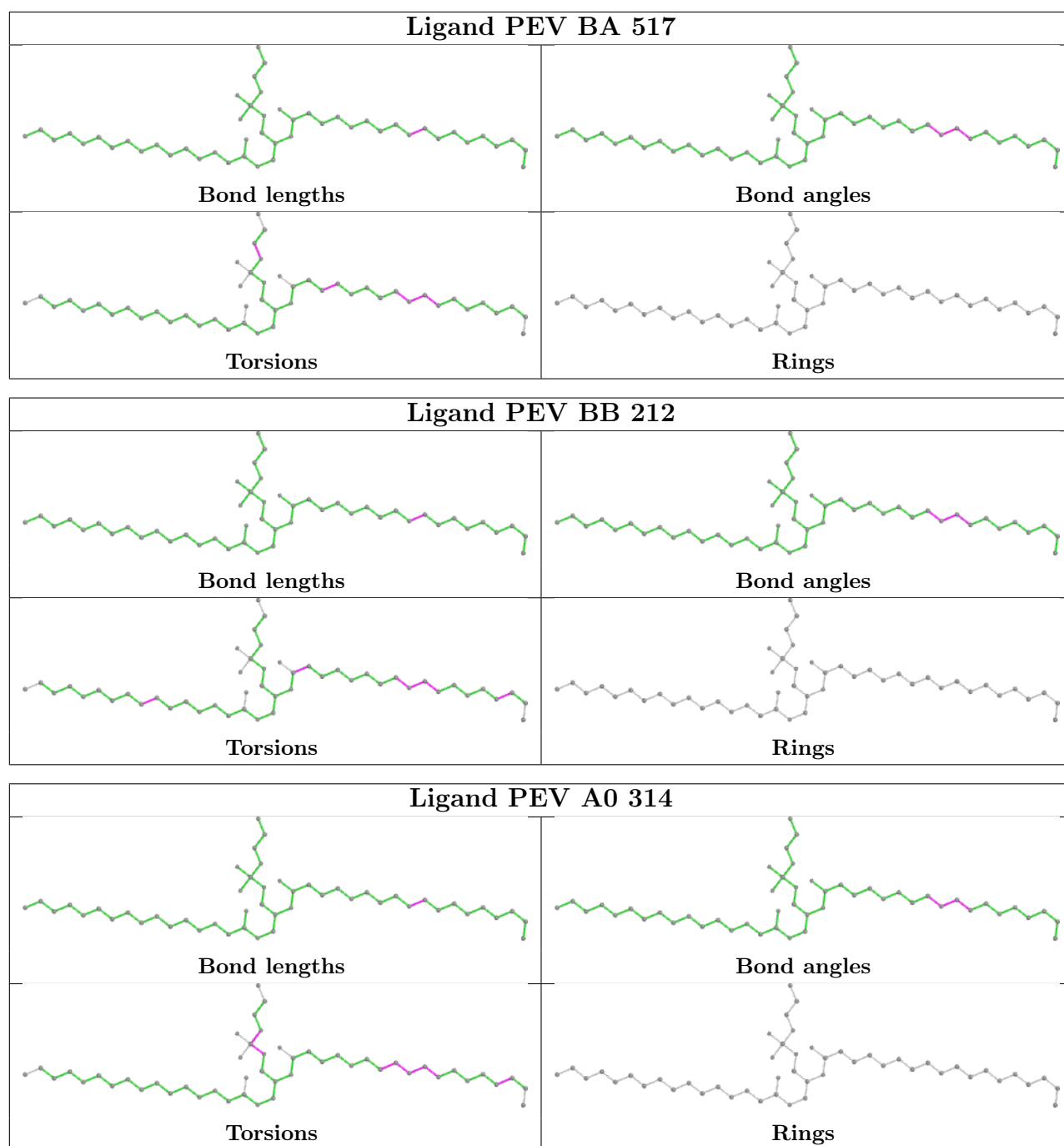


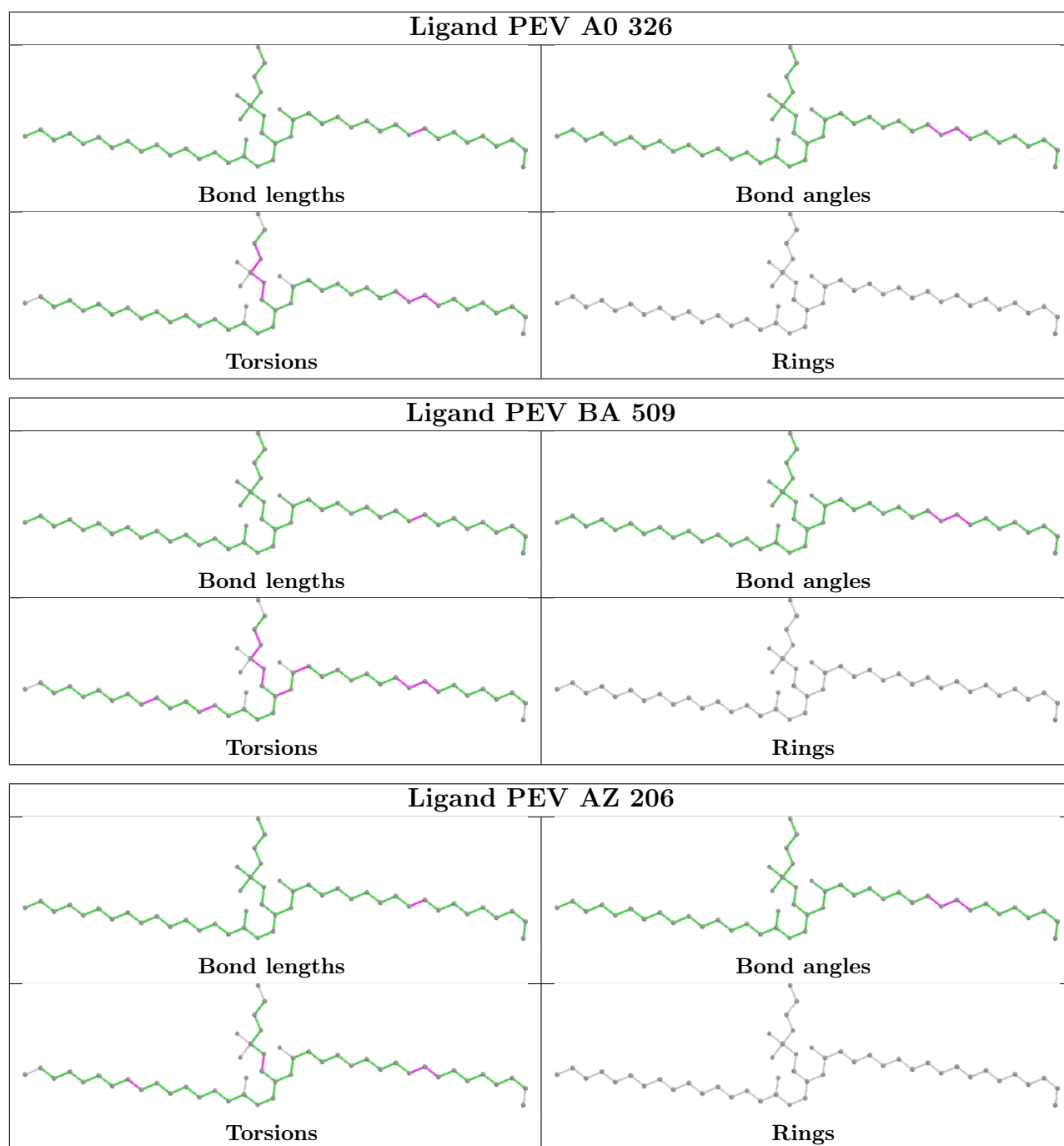


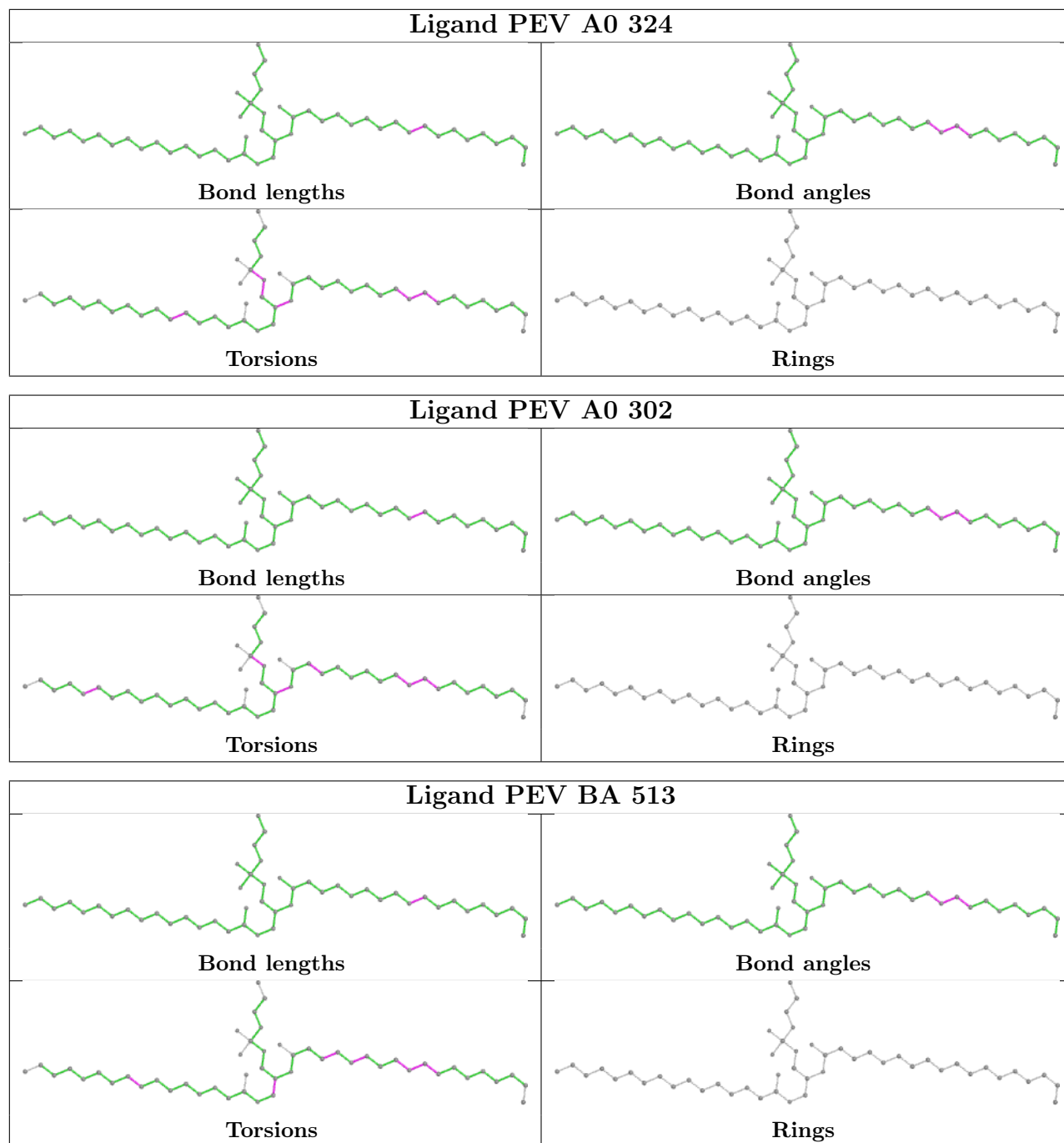


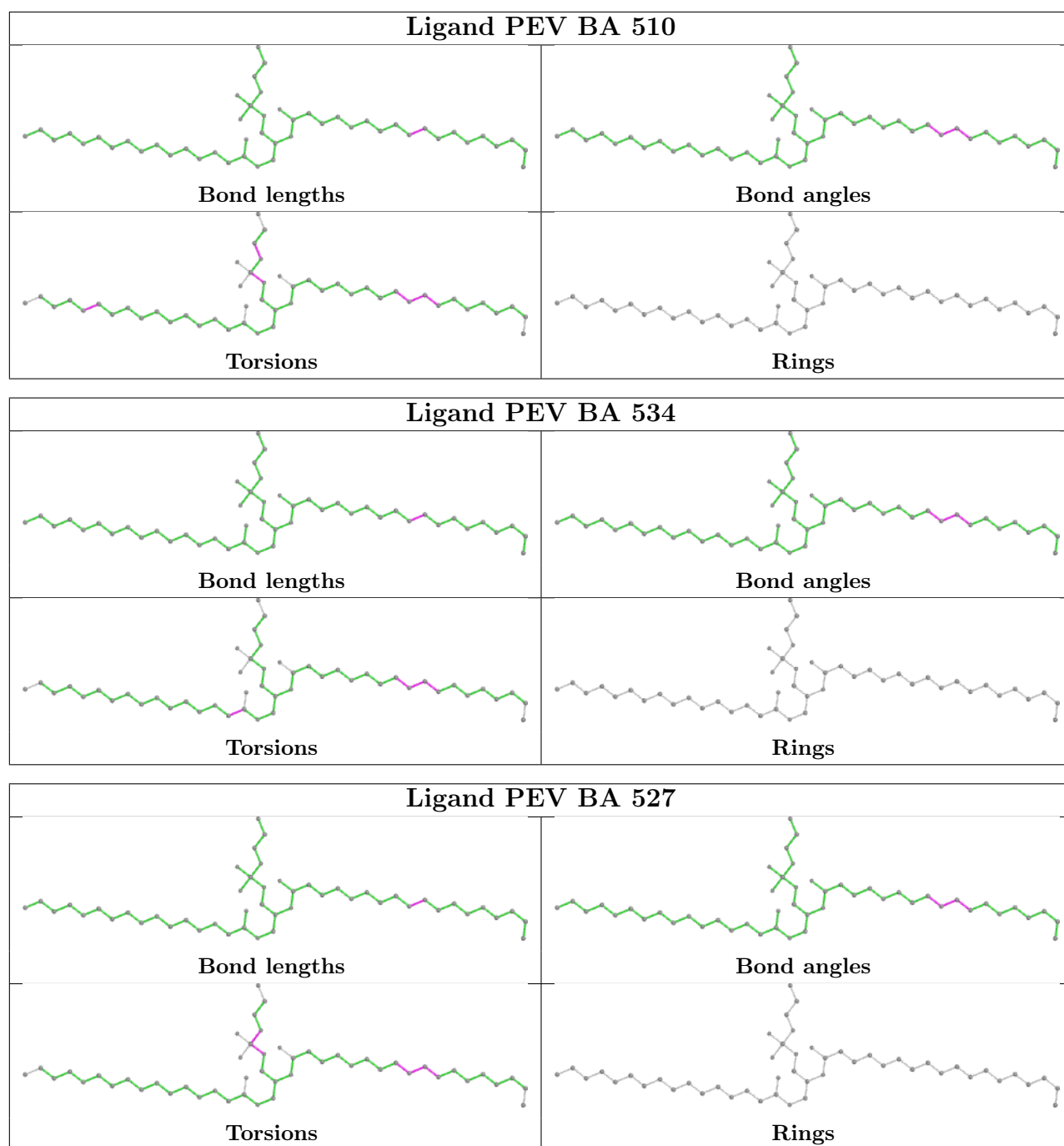


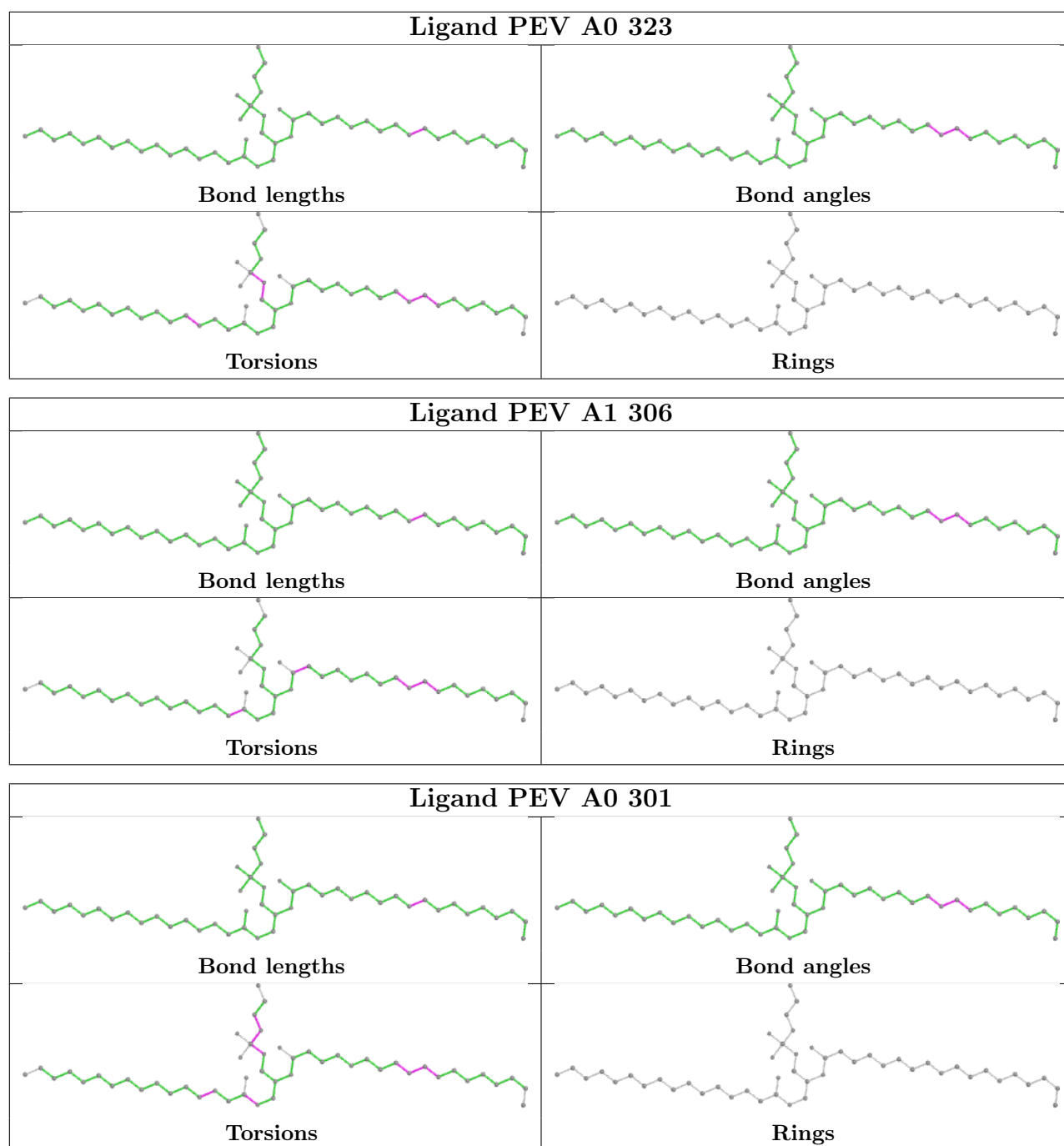


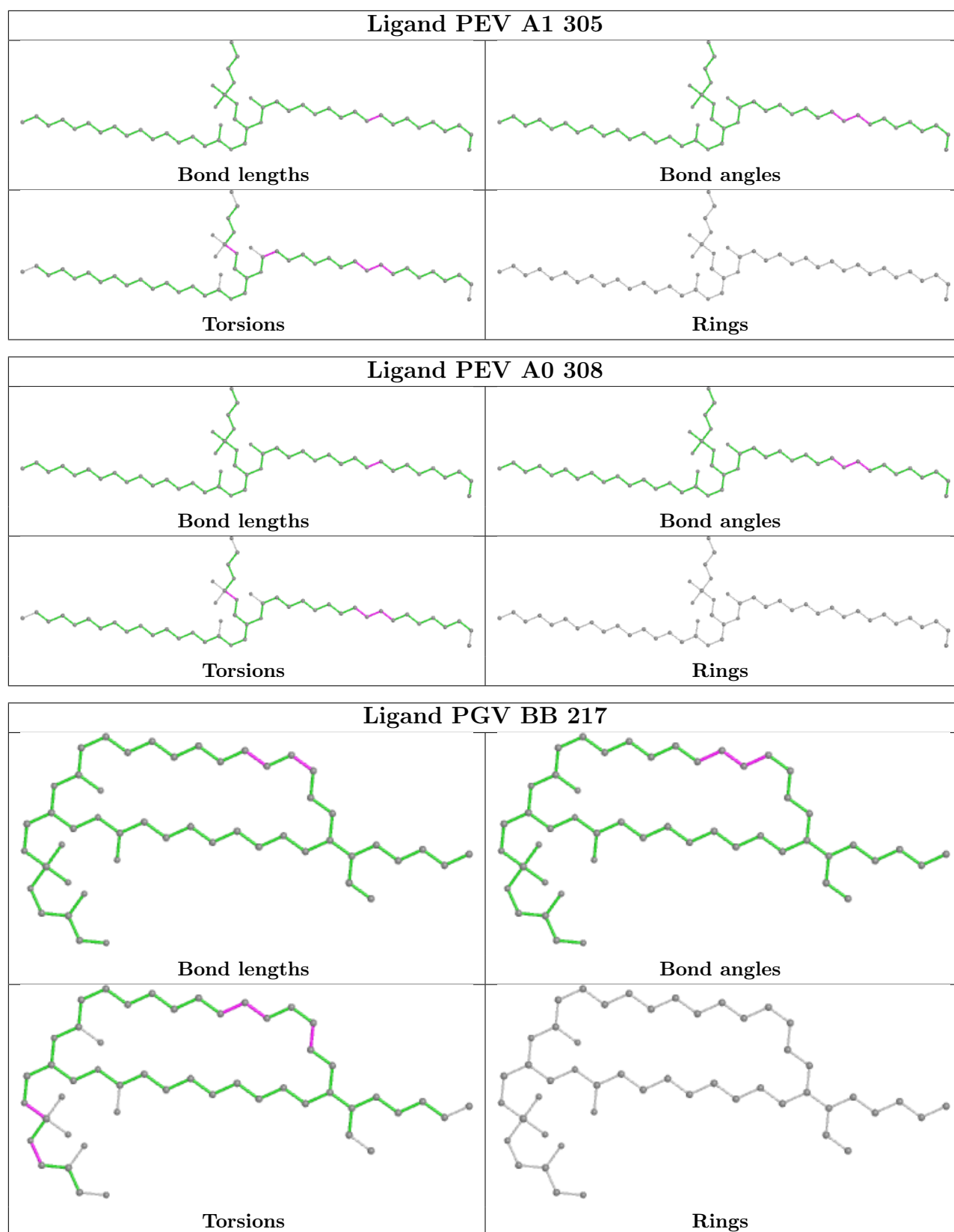


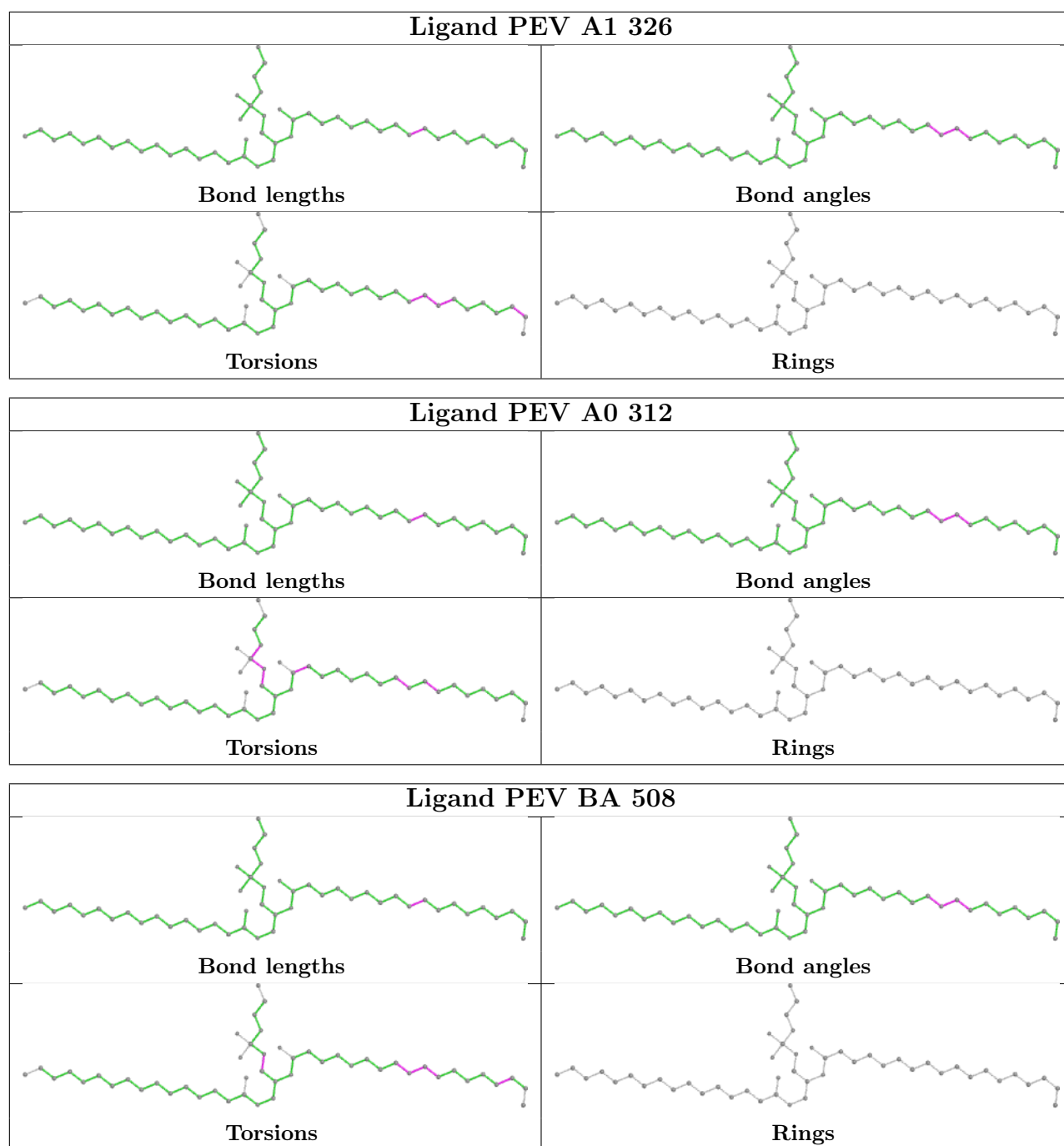


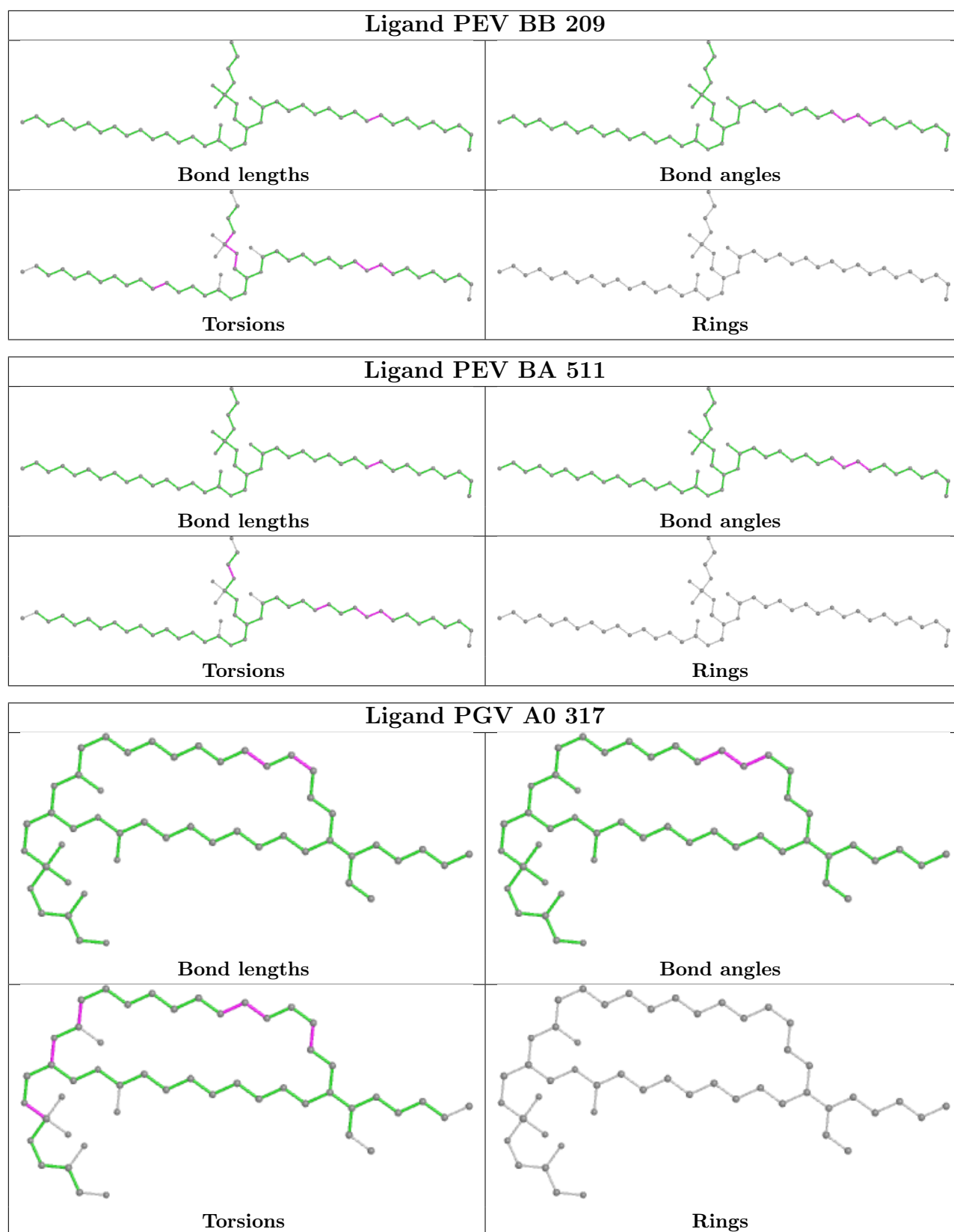


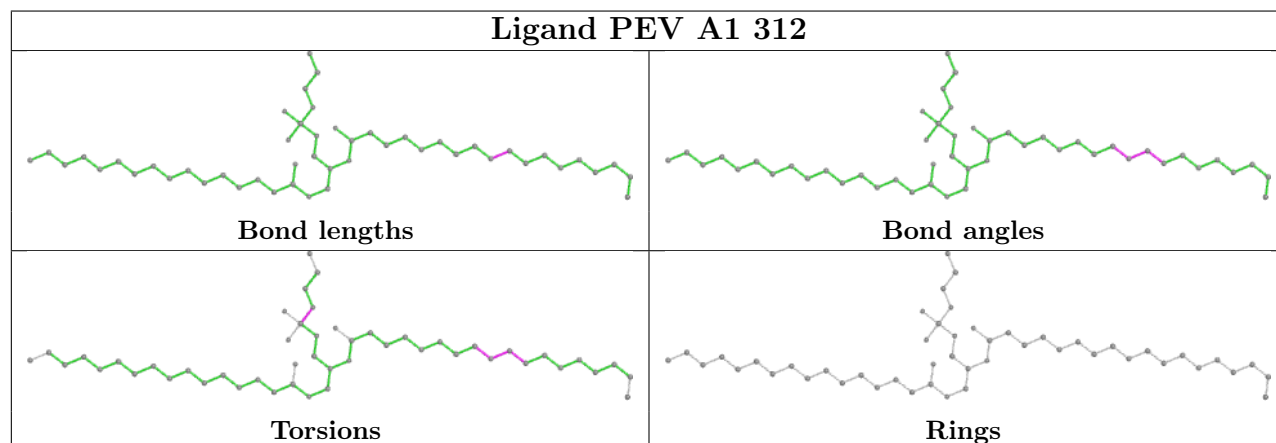
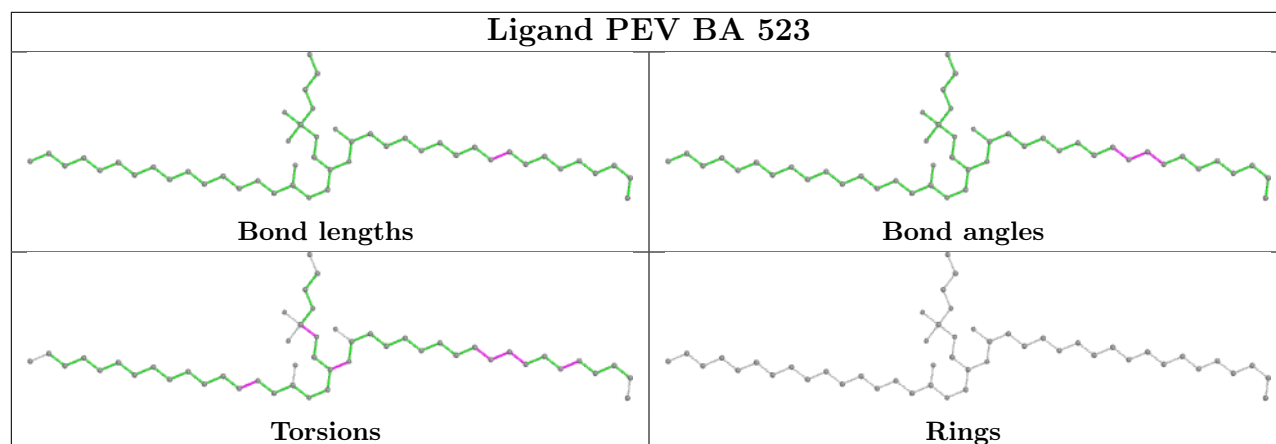
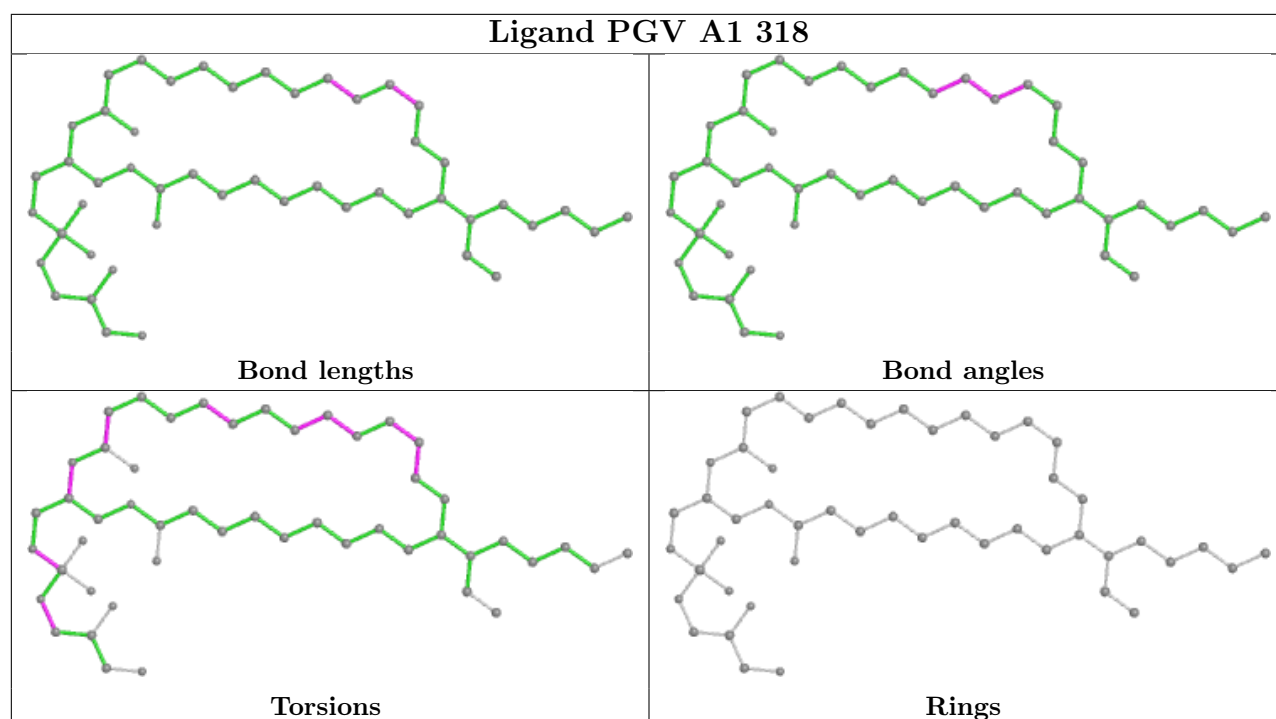


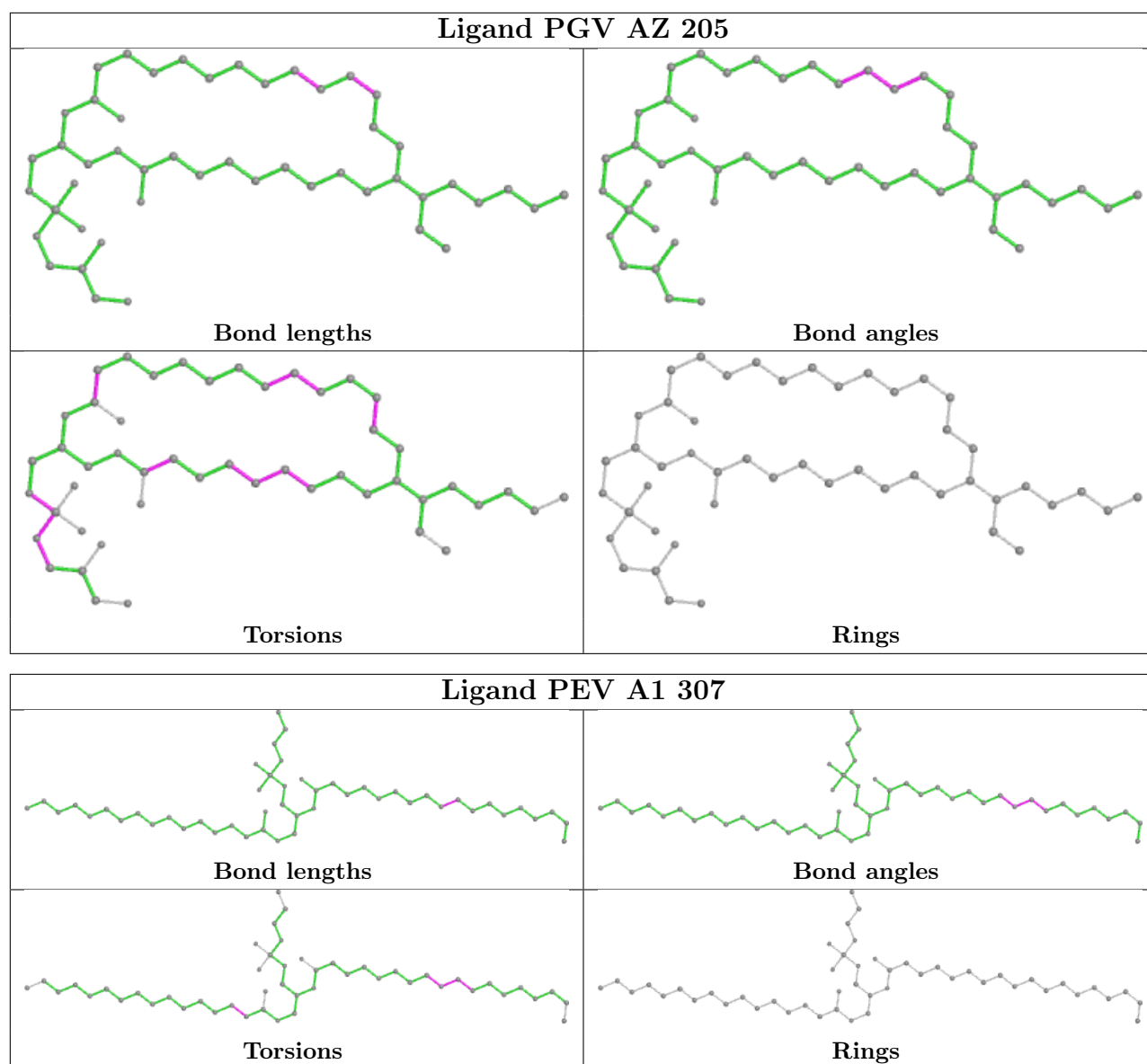












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

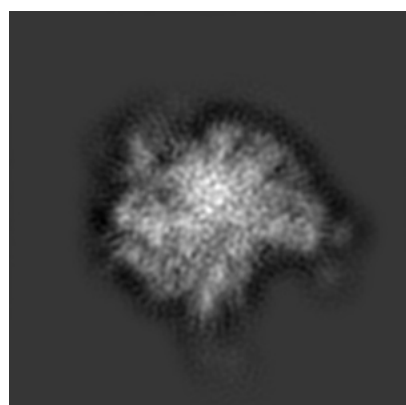
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-1858. These allow visual inspection of the internal detail of the map and identification of artifacts.

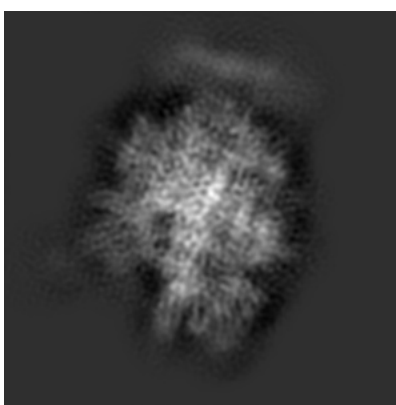
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

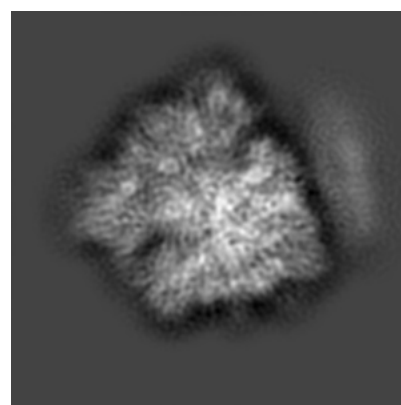
6.1.1 Primary map



X



Y

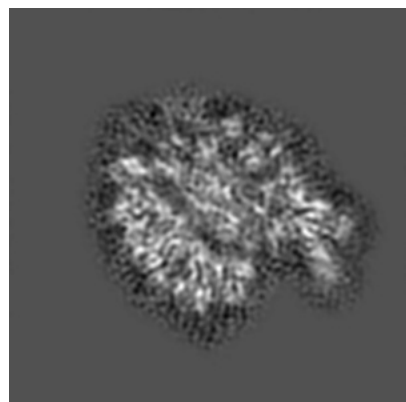


Z

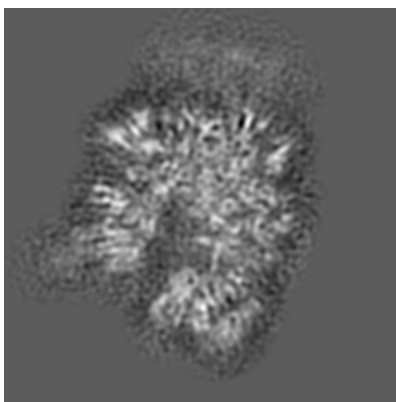
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

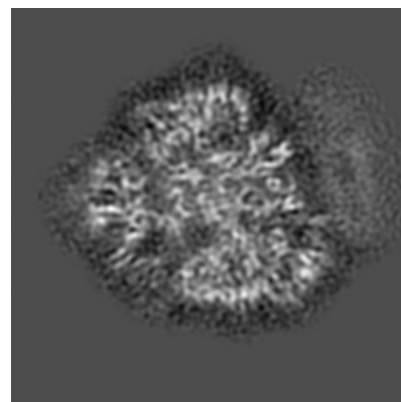
6.2.1 Primary map



X Index: 160



Y Index: 160

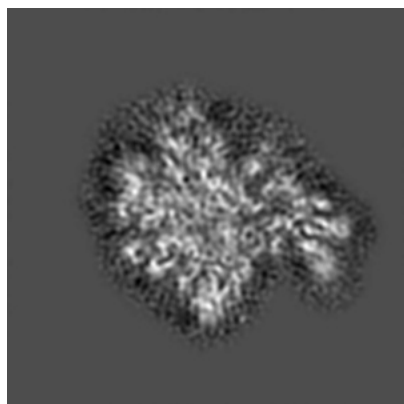


Z Index: 160

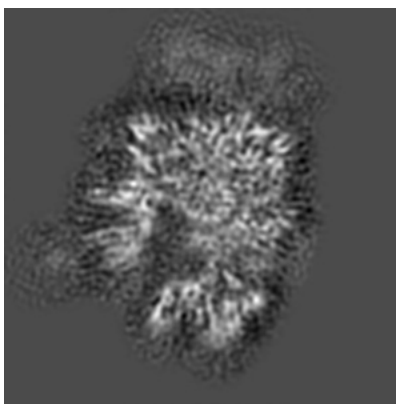
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

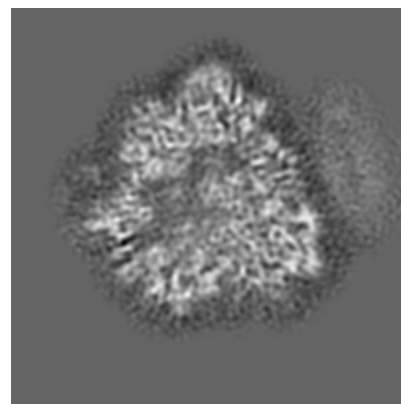
6.3.1 Primary map



X Index: 166



Y Index: 167

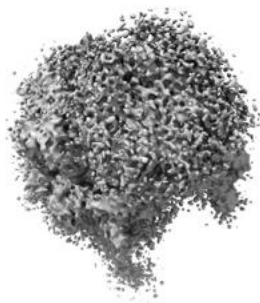


Z Index: 146

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

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

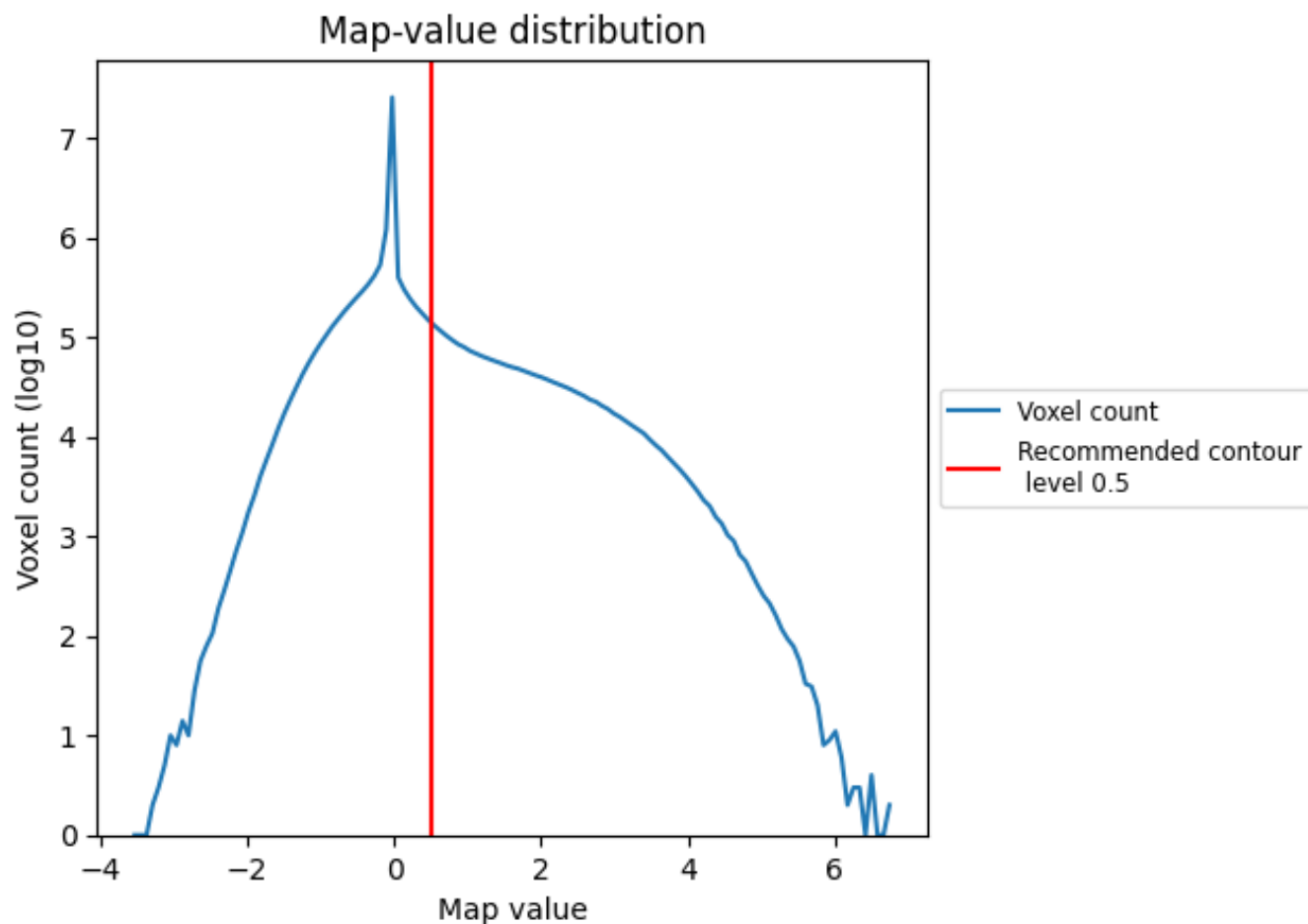
6.5 Mask visualisation

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

7 Map analysis [i](#)

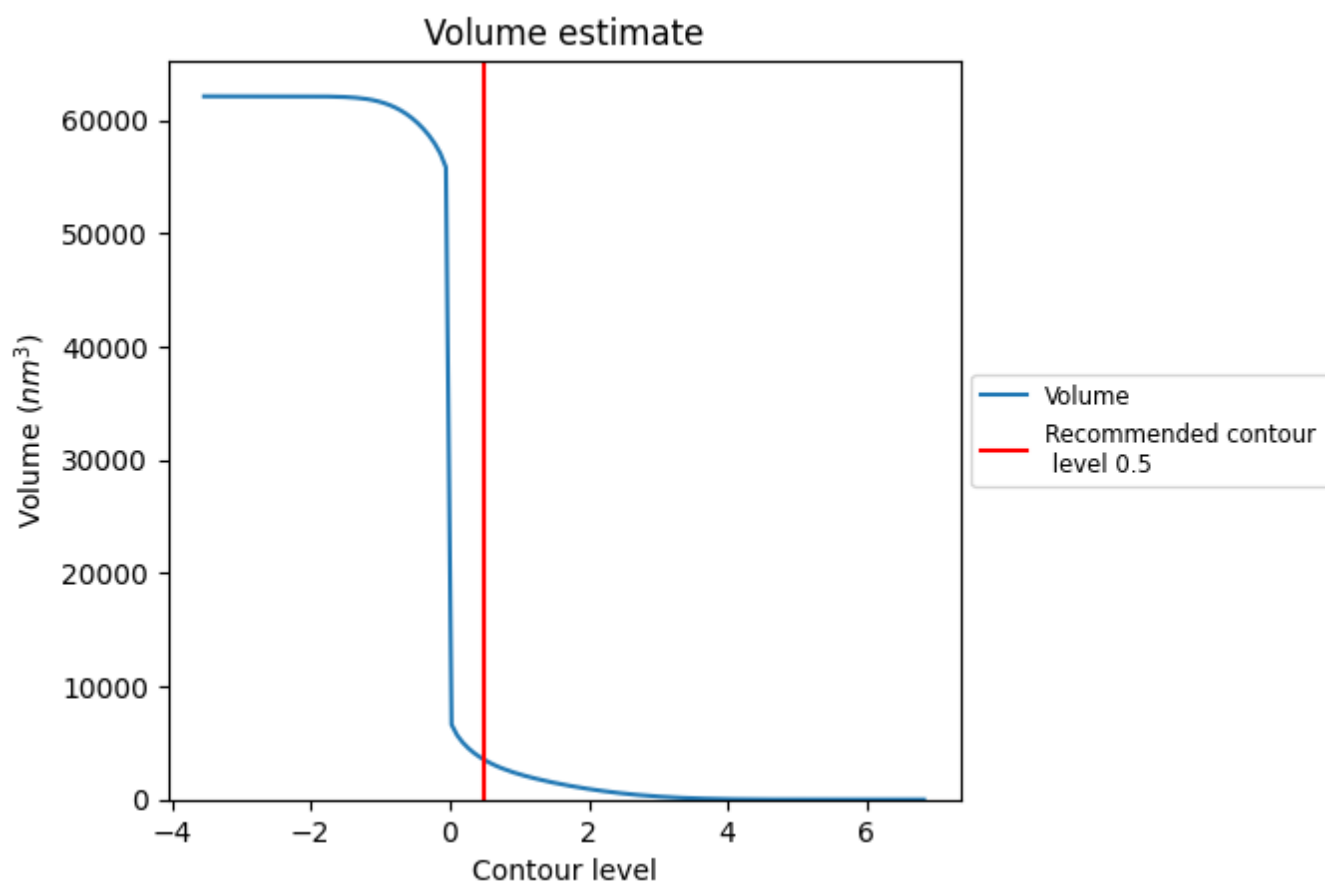
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

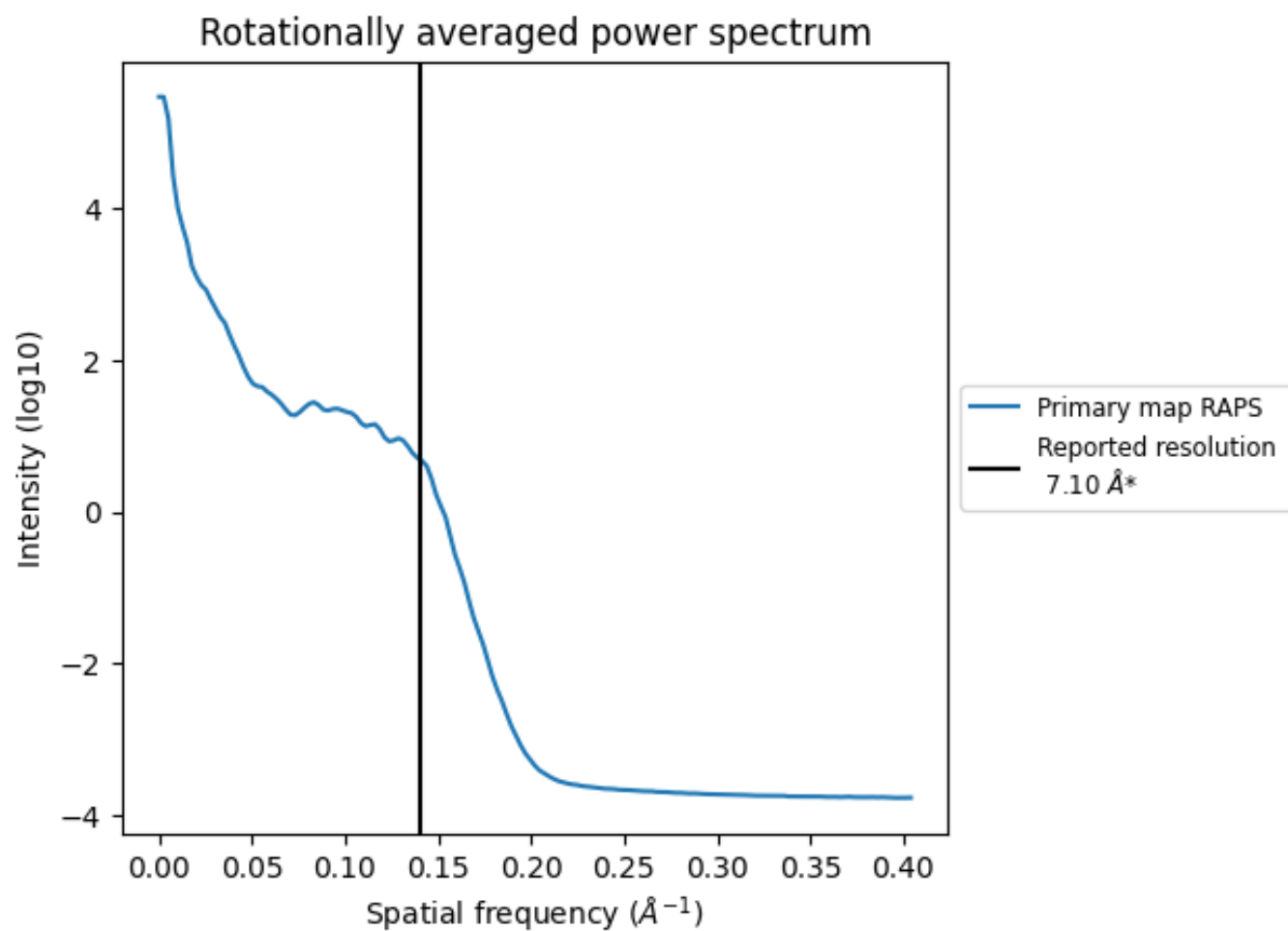
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 3504 nm³; this corresponds to an approximate mass of 3166 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.141 Å⁻¹

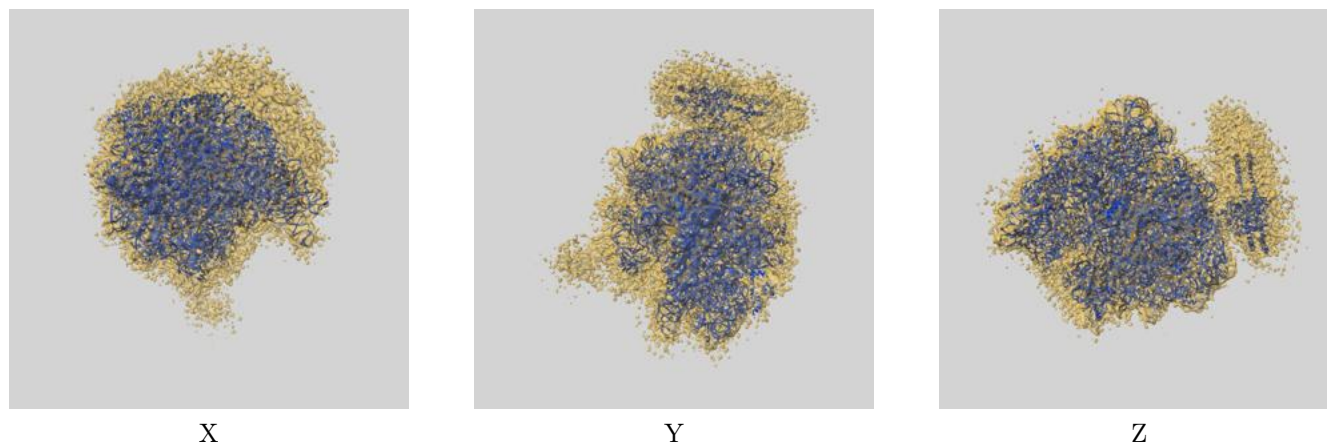
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

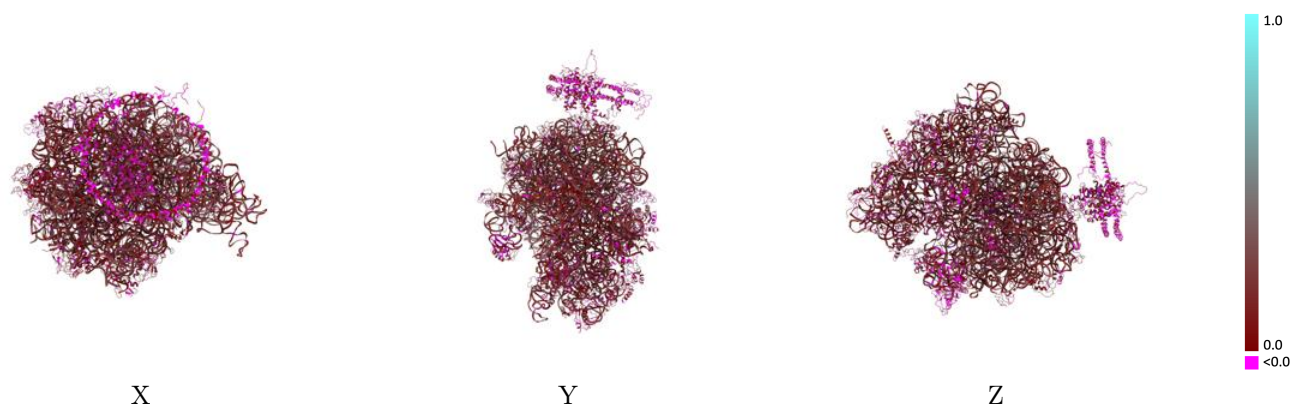
This section contains information regarding the fit between EMDB map EMD-1858 and PDB model 4V6M. Per-residue inclusion information can be found in section [3](#) on page [24](#).

9.1 Map-model overlay [i](#)



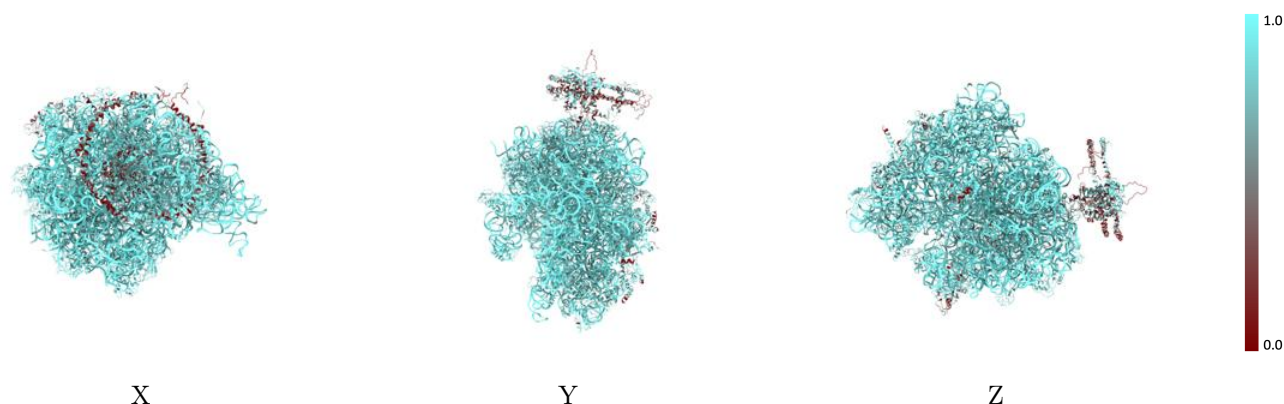
The images above show the 3D surface view of the map at the recommended contour level 0.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



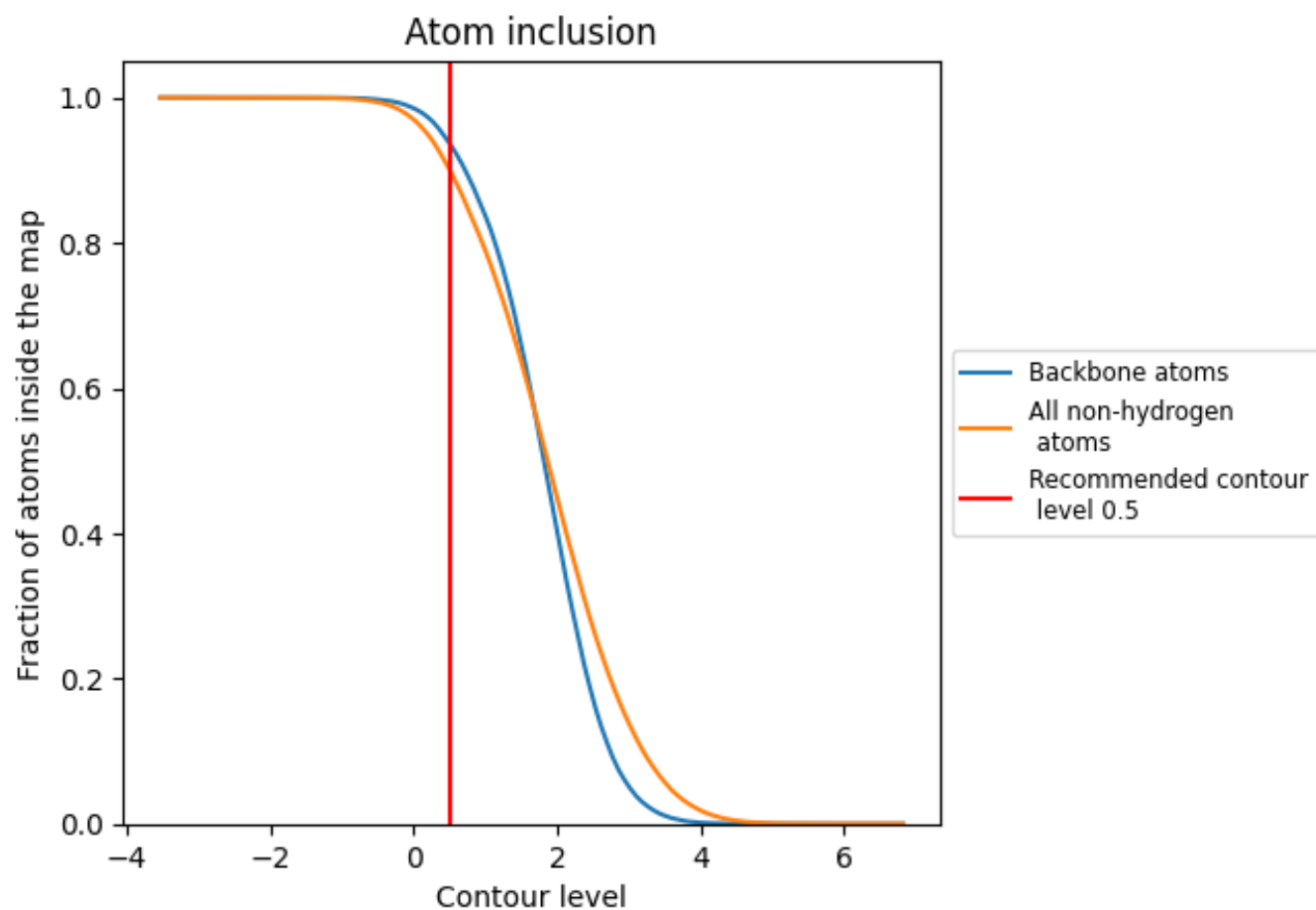
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.5).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 90% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ





















































The table lists the average atom inclusion at the recommended contour level (0.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9008	 0.1450
A0	 0.3258	 0.0170
A1	 0.5625	 0.0090
AA	 0.9846	 0.1740
AB	 0.7507	 0.1210
AC	 0.8279	 0.1200
AD	 0.8390	 0.1240
AE	 0.7781	 0.1190
AF	 0.7183	 0.1060
AG	 0.9093	 0.1350
AH	 0.8542	 0.1350
AI	 0.8731	 0.0980
AJ	 0.8950	 0.0950
AK	 0.8481	 0.1140
AL	 0.9251	 0.1180
AM	 0.8861	 0.1220
AN	 0.8669	 0.1230
AO	 0.9174	 0.1390
AP	 0.8852	 0.1220
AQ	 0.8994	 0.1230
AR	 0.8003	 0.1240
AS	 0.8903	 0.1060
AT	 0.8290	 0.1370
AU	 0.8357	 0.1220
AV	 0.9588	 0.1410
AX	 0.7922	 0.1000
AZ	 0.5154	 0.0640
B0	 0.8551	 0.1190
B1	 0.9423	 0.1170
B2	 0.9268	 0.0860
B3	 0.8961	 0.1220
B4	 0.9144	 0.1000
B5	 0.6780	 0.0570
B6	 0.9294	 0.1300
B7	 0.9883	 0.1840



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
B8	 0.9841	 0.1750
BA	 0.4615	 0.0370
BB	 0.4381	 0.0650
BD	 0.8973	 0.1180
BE	 0.8829	 0.1230
BF	 0.8966	 0.1180
BG	 0.9329	 0.1550
BH	 0.7436	 0.1150
BI	 0.9706	 0.0670
BJ	 0.8964	 0.1410
BK	 0.8970	 0.1400
BL	 0.9102	 0.1230
BM	 0.9463	 0.1330
BN	 0.8443	 0.1070
BO	 0.8990	 0.1260
BP	 0.8682	 0.1360
BQ	 0.8392	 0.1050
BR	 0.8821	 0.1390
BS	 0.8110	 0.1050
BT	 0.7847	 0.1180
BU	 0.8803	 0.1290
BV	 0.9350	 0.1430
BW	 0.9013	 0.0760
BX	 0.8486	 0.1040
BY	 0.8551	 0.1100
BZ	 0.8787	 0.1540